wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 07:22 AM EST

PDB ID	:	6DHP
Title	:	RT XFEL structure of the three-flash state of Photosystem II (3F, S0-rich) at 2.04 Angstrom resolution
Authors	:	Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2018-05-20
Resolution	:	2.04 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 (1)) were used in the production of this report:

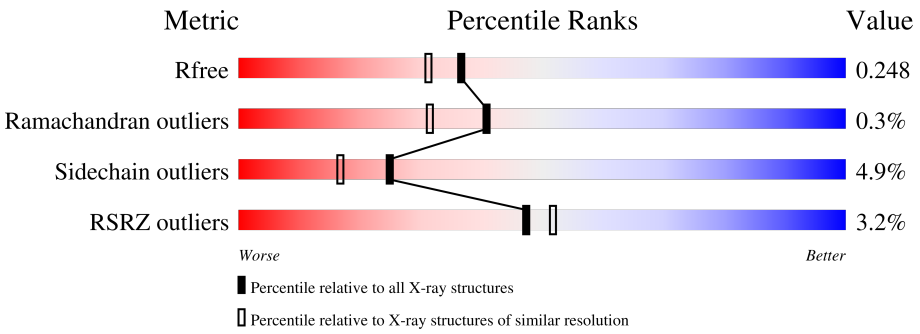
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

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 2.04 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	1692 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	334	% 97% •
1	a	334	% 96% •

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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)	:	2.36

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Mol	Chain	Length	Quality of chain
2	B	505	%, 96%
2	b	505	3%, 97%
3	C	451	%, 96%
3	c	451	%, 95%, 5%
4	D	341	99%
4	d	341	%, 98%
5	E	82	5%, 89%, 10%
5	e	82	5%, 90%, 10%
6	F	34	3%, 100%
6	f	34	3%, 88%, 12%
7	H	65	3%, 95%, 5%
7	h	65	2%, 89%, 8%
8	I	36	3%, 86%, 14%
8	i	36	3%, 94%, 6%
9	J	36	11%, 97%
9	j	36	14%, 94%, 6%
10	K	37	92%, 8%
10	k	37	3%, 89%, 11%
11	L	37	100%
11	l	37	89%, 8%
12	M	33	3%, 94%, 6%
12	m	33	94%
13	O	244	5%, 94%, 6%
13	o	244	5%, 94%, 5%
14	R	34	35%, 82%, 18%

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Mol	Chain	Length	Quality of chain
14	r	34	53% 74% 18% 9%
15	T	30	7% 83% 13%
15	t	30	7% 97%
16	U	97	3% 97%
16	u	97	% 99%
17	V	137	96%
17	v	137	% 97%
18	X	38	8% 97%
18	x	38	8% 95% 5%
19	Y	30	30% 77% 10% 10%
19	y	30	17% 87% 13%
20	Z	62	24% 82% 16%
20	z	62	19% 85% 15%

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
23	CLA	A	603	X	-	-	-
23	CLA	A	607	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	603	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	612	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 105751 atoms, of which 52470 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 II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	334	6018	2010	2937	507	545	19	0	59	0
1	a	334	6006	2007	2928	507	545	19	0	59	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	505	7849	2631	3845	666	694	13	0	5	0
2	b	505	7789	2610	3811	665	690	13	0	0	0

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	442	6868	2282	3392	579	601	14	0	7	0
3	c	451	7017	2324	3464	596	619	14	0	8	0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	341	5350	1806	2624	445	463	12	0	1	0
4	d	341	5362	1810	2630	445	465	12	0	2	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	81	1309	434	647	106	122	0	1	0
5	e	82	1311	434	647	108	122	0	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	34	556	187	281	45	42	1	0	0	0
6	f	34	556	187	281	45	42	1	0	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
7	H	65	1030	338	523	82	85	2	0	0	0
7	h	63	1016	333	518	80	83	2	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
8	I	36	607	200	311	46	49	1	0	0	0
8	i	36	607	200	311	46	49	1	0	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
9	J	36	525	174	268	40	42	1	0	0	0
9	j	36	516	172	261	40	42	1	0	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
10	K	37	620	209	318	46	47	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
10	k	37	598	204	305	43	46	0	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
11	L	37	620	202	316	48	53	1	0	0	0
			Total	C	H	N	O				
11	l	36	600	197	304	47	52		0	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
12	M	33	525	171	269	37	47	1	0	0	0
			Total	C	H	N	O	S			
12	m	32	518	168	267	36	46	1	0	0	0

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
13	O	244	3730	1174	1850	317	385	4	0	1	0
			Total	C	H	N	O	S			
13	o	244	3718	1170	1844	317	383	4	0	0	0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
14	R	34	569	184	298	47	40	0	0	0
			Total	C	H	N	O			
14	r	31	461	154	234	40	33	0	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
15	T	30	519	181	261	36	39	2	0	0	0
			Total	C	H	N	O	S			
15	t	30	512	180	256	36	38	2	0	0	0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
16	U	97	1546	491	772	129	154	0	0	0
16	u	97	1546	491	772	129	154	0	0	0

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
17	V	137	2134	675	1070	177	208	4	0	0	0
17	v	137	2134	675	1070	177	208	4	0	0	0

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
18	X	38	593	188	312	45	48	0	0	0
18	x	38	593	188	312	45	48	0	0	0

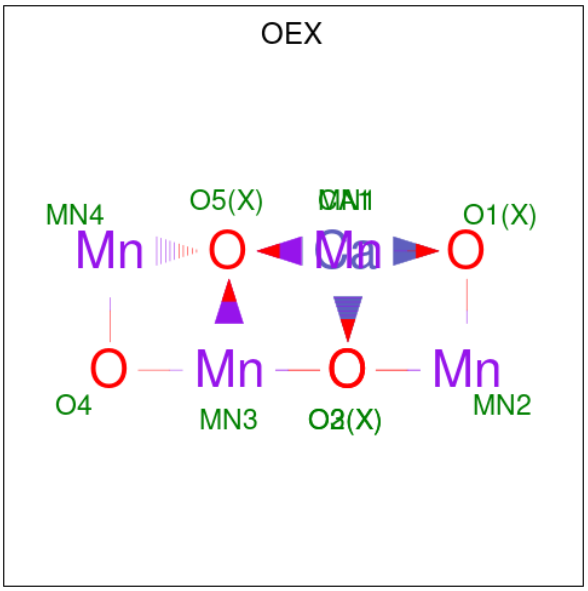
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
19	Y	27	404	128	208	35	30	3	0	0	0
19	y	30	459	144	241	35	36	3	0	0	0

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
20	Z	62	988	328	509	72	77	2	0	0	0
20	z	62	986	326	509	72	77	2	0	0	0

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



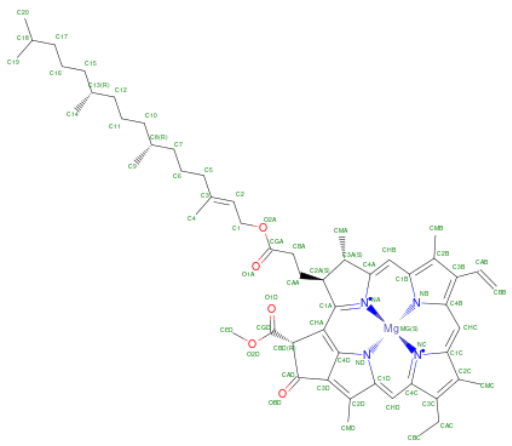
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
21	A	1	10	1	4	5	0	1
21	a	1	10	1	4	5	0	1

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
22	A	1	1	1	0	0
22	a	1	1	1	0	0

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).

CLA



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
23	A	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	A	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	A	1	102	44	48	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	A	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	B	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	117	49	58	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	D	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
23	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	b	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0

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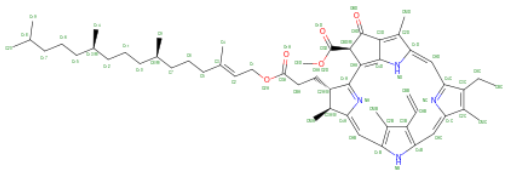
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	132	54	68	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	d	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	d	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
23	h	1	137	55	72	1	4	5	0	0

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

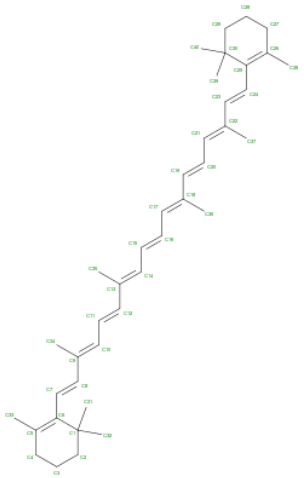
PHO



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
24	A	1	138	55	74	4	5	0	0
			Total	C	H	N	O		
24	A	1	138	55	74	4	5	0	0
			Total	C	H	N	O		
24	a	1	138	55	74	4	5	0	0
			Total	C	H	N	O		
24	d	1	138	55	74	4	5	0	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR

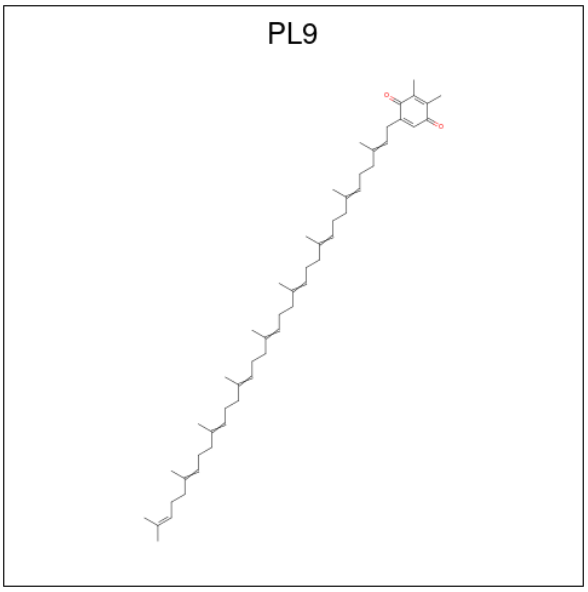


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
25	A	1	96	40	56	0	0
25	B	1	96	40	56	0	0
25	B	1	96	40	56	0	0
25	B	1	96	40	56	0	0
25	C	1	96	40	56	0	0
25	C	1	96	40	56	0	0
25	C	1	96	40	56	0	0
25	D	1	96	40	56	0	0
25	H	1	96	40	56	0	0
25	T	1	96	40	56	0	0
25	Y	1	96	40	56	0	0
25	a	1	96	40	56	0	0
25	b	1	96	40	56	0	0
25	b	1	96	40	56	0	0
25	b	1	96	40	56	0	0
25	c	1	96	40	56	0	0
25	c	1	96	40	56	0	0
25	d	1	96	40	56	0	0
25	h	1	96	40	56	0	0
25	k	1	96	40	56	0	0
25	k	1	96	40	56	0	0
25	t	1	96	40	56	0	0

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

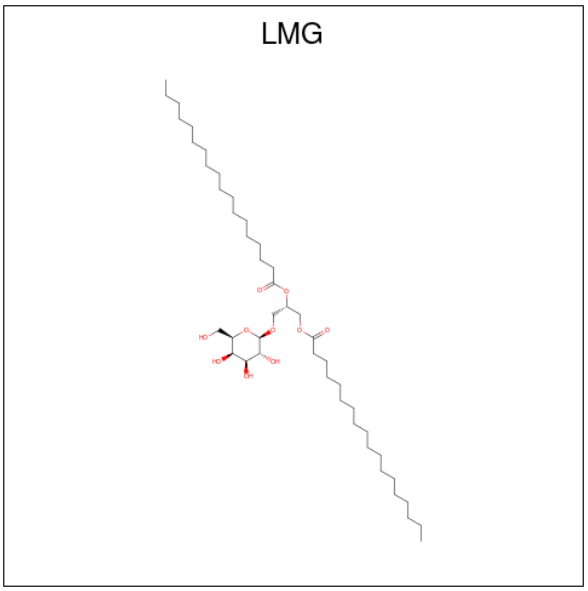
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
26	A	2	2	2	0	0
			Total	Cl		
26	a	2	2	2	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	A	1	135	53	80	2	0	0
			Total	C	H	O		
27	D	1	135	53	80	2	0	0
			Total	C	H	O		
27	a	1	135	53	80	2	0	0
			Total	C	H	O		
27	d	1	135	53	80	2	0	0

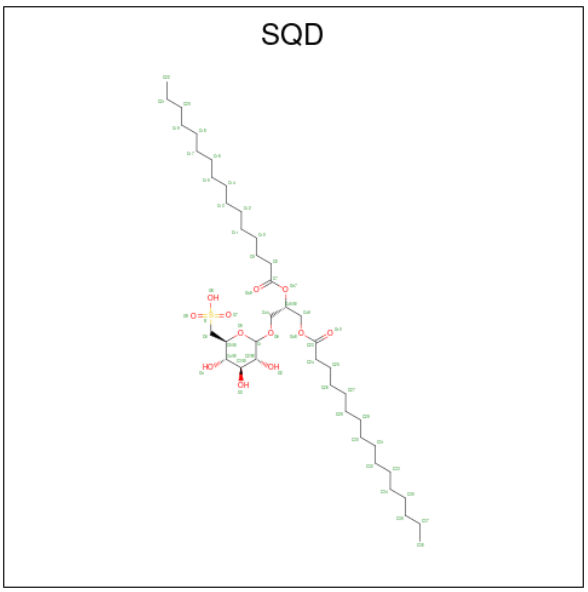
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
28	A	1	114	38	66	10	0	0
			Total	C	H	O		
28	B	1	123	41	72	10	0	0
			Total	C	H	O		
28	B	1	68	24	40	4	0	0
			Total	C	H	O		
28	C	1	114	38	66	10	0	0
			Total	C	H	O		
28	D	1	123	41	72	10	0	0
			Total	C	H	O		
28	D	1	78	27	45	6	0	0
			Total	C	H	O		
28	b	1	141	45	86	10	0	0
			Total	C	H	O		
28	c	1	81	27	44	10	0	0
			Total	C	H	O		
28	c	1	117	38	69	10	0	0
			Total	C	H	O		
28	c	1	117	39	68	10	0	0
			Total	C	H	O		
28	d	1	102	34	58	10	0	0
			Total	C	H	O		
28	d	1	57	21	34	2	0	0
			Total	C	H	O		
28	m	1	123	41	72	10	0	0

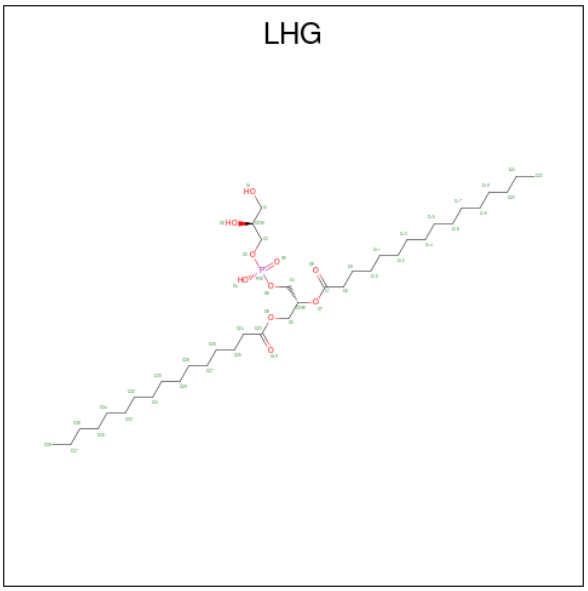
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 122 39 70 12 1	0	0
29	A	1	Total C H O 104 35 65 4	0	0
29	B	1	Total C H O S 132 41 78 12 1	0	0
29	F	1	Total C H O S 81 25 45 10 1	0	0
29	a	1	Total C H O S 132 41 78 12 1	0	0
29	a	1	Total C H O 92 31 56 5	0	0
29	b	1	Total C H O S 114 36 65 12 1	0	0
29	f	1	Total C H O S 90 28 49 12 1	0	0

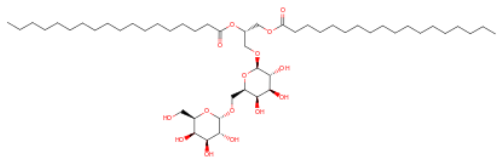
- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
30	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

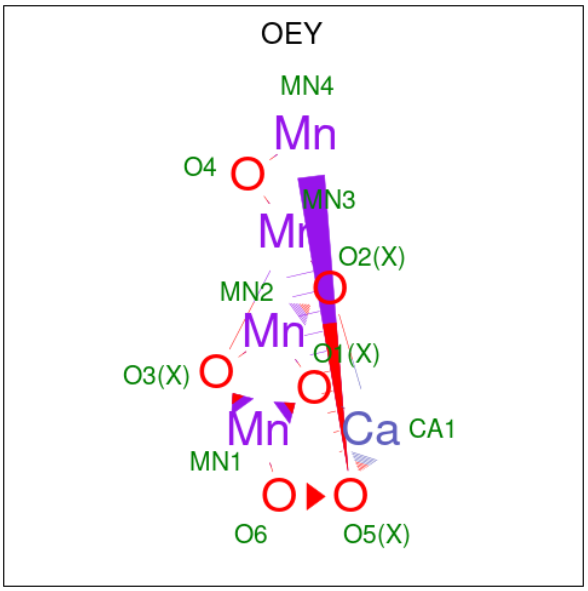
- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
31	A	1	162	51	96	15	0	0
31	C	1	144	47	82	15	0	0
31	C	1	144	47	82	15	0	0
31	C	1	144	47	82	15	0	0
31	H	1	144	47	82	15	0	0
31	a	1	119	39	75	5	0	0
31	c	1	144	47	82	15	0	0
31	c	1	144	47	82	15	0	0
31	c	1	144	47	82	15	0	0
31	h	1	144	47	82	15	0	0

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Ca Mn O 11 1 4 6	0	1
32	a	1	Total Ca Mn O 11 1 4 6	0	1

- Molecule 33 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	5	Total C H O 192 67 117 8	0	0
33	C	3	Total C H O 103 36 63 4	0	0
33	E	1	Total C H O 28 10 16 2	0	0
33	H	1	Total C H 53 18 35	0	0
33	I	1	Total C H 41 15 26	0	0
33	J	1	Total C H O 28 10 16 2	0	0
33	M	2	Total C H O 63 23 38 2	0	0
33	T	2	Total C H 91 31 60	0	0
33	X	1	Total C H O 55 18 35 2	0	0
33	a	1	Total C H O 28 10 16 2	0	0

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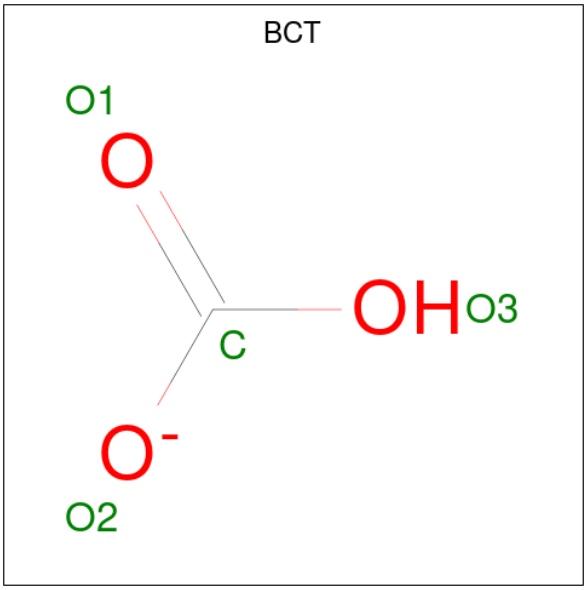
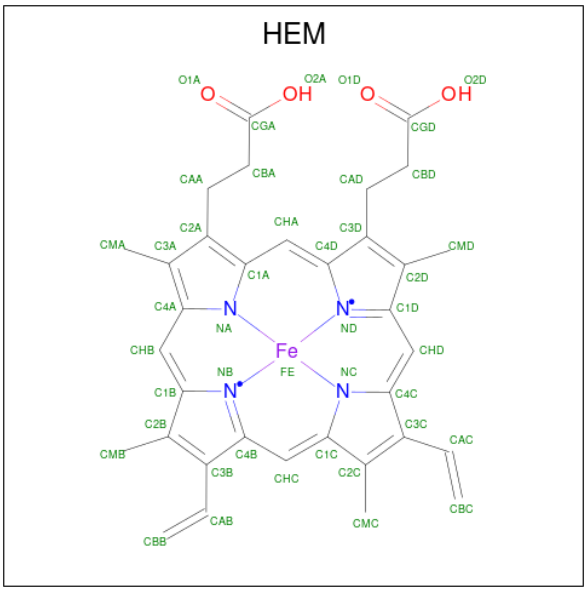
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	b	4	Total C H O 176 60 110 6	0	0
33	c	2	Total C H O 83 28 51 4	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	j	1	Total C H O 28 10 16 2	0	0
33	l	1	Total C H 53 18 35	0	0
33	m	1	Total C H O 28 10 16 2	0	0
33	t	2	Total C H O 60 22 36 2	0	0
33	x	1	Total C H O 55 18 35 2	0	0

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



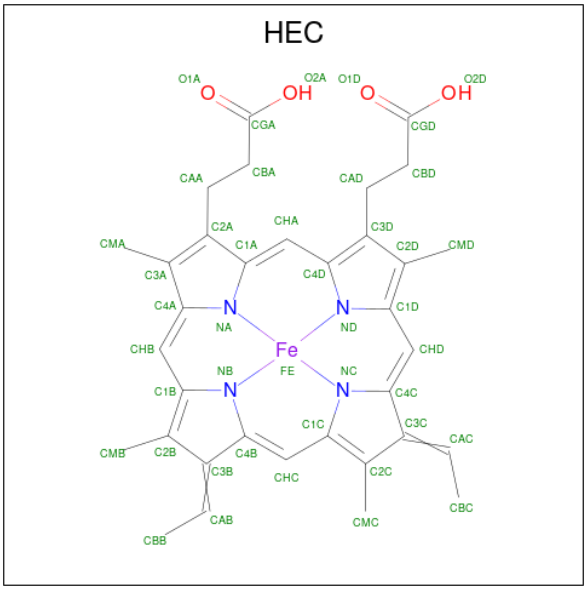
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	D	1	Total C H O 5 1 1 3	0	0
34	a	1	Total C H O 5 1 1 3	0	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
35	F	1	73	34	1	30	4	4	0	0
35	f	1	73	34	1	30	4	4	0	0

- Molecule 36 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
36	V	1	73	34	1	30	4	4	0	0
36	v	1	73	34	1	30	4	4	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	147	Total O 147 147	0	8
37	B	218	Total O 218 218	0	0
37	C	190	Total O 190 190	0	0
37	D	129	Total O 129 129	0	0
37	E	30	Total O 30 30	0	0
37	F	13	Total O 13 13	0	0
37	H	28	Total O 28 28	0	0
37	I	12	Total O 12 12	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	9	Total O 9 9	0	0
37	M	6	Total O 6 6	0	0
37	O	129	Total O 129 129	0	0
37	R	4	Total O 4 4	0	0
37	T	13	Total O 13 13	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	8	Total O 8 8	0	0
37	Y	5	Total O 5 5	0	0
37	Z	5	Total O 5 5	0	0
37	a	132	Total O 132 132	0	8

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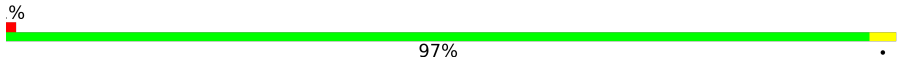
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	b	188	Total O 188 188	0	0
37	c	155	Total O 155 155	0	0
37	d	118	Total O 118 118	0	0
37	e	19	Total O 19 19	0	0
37	f	8	Total O 8 8	0	0
37	h	19	Total O 19 19	0	0
37	i	10	Total O 10 10	0	0
37	j	10	Total O 10 10	0	0
37	k	6	Total O 6 6	0	0
37	l	13	Total O 13 13	0	0
37	m	7	Total O 7 7	0	0
37	o	109	Total O 109 109	0	0
37	r	5	Total O 5 5	0	0
37	t	14	Total O 14 14	0	0
37	u	54	Total O 54 54	0	0
37	v	59	Total O 59 59	0	0
37	x	10	Total O 10 10	0	0
37	y	4	Total O 4 4	0	0
37	z	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

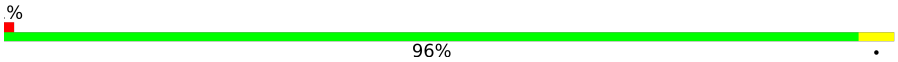
• Molecule 1: Photosystem II protein D1 1

Chain A:



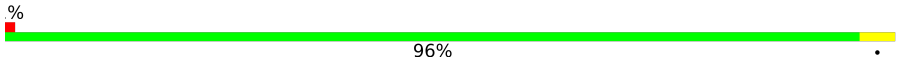
• Molecule 1: Photosystem II protein D1 1

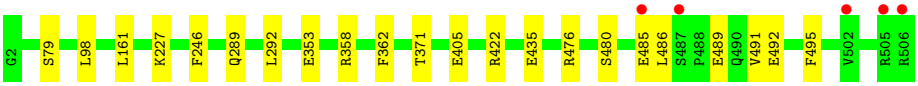
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

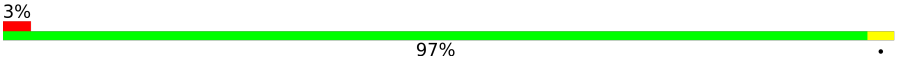
Chain B:





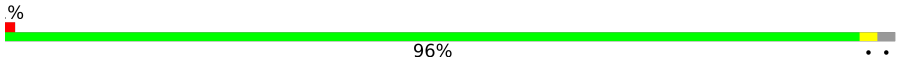
• Molecule 2: Photosystem II CP47 reaction center protein

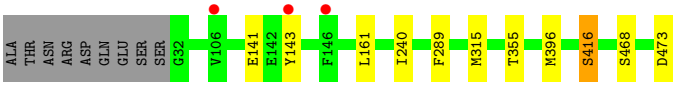
Chain b:



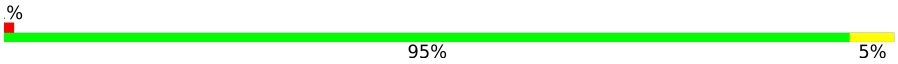
• Molecule 3: Photosystem II CP43 reaction center protein

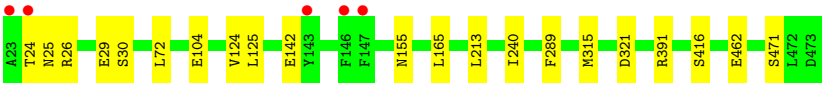
Chain C:



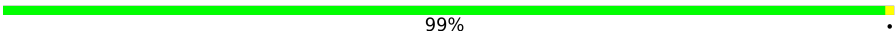


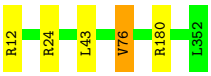
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 

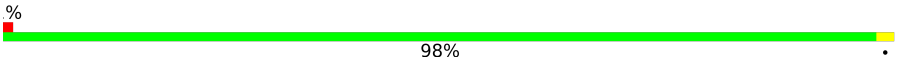


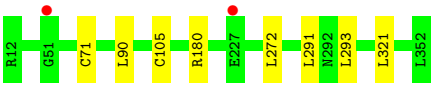
• Molecule 4: Photosystem II D2 protein

Chain D: 



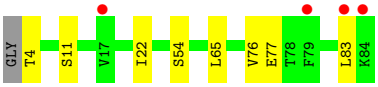
• Molecule 4: Photosystem II D2 protein

Chain d: 

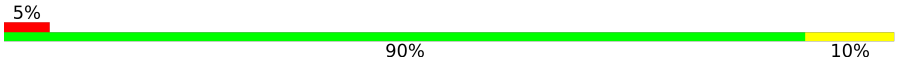


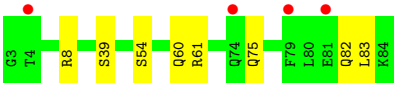
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

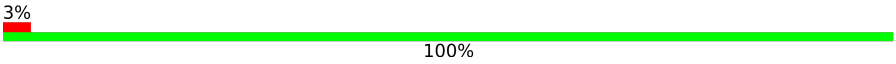


• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 

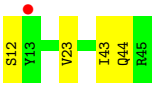


• Molecule 6: Cytochrome b559 subunit beta

Chain F: 

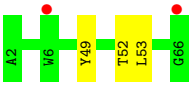
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



• Molecule 7: Photosystem II reaction center protein H

Chain H: 3% 95% 5%

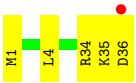


• Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 89% 8%

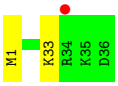
• Molecule 8: Photosystem II reaction center protein I

Chain I: 3% 86% 14%



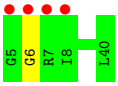
• Molecule 8: Photosystem II reaction center protein I

Chain i: 3% 94% 6%



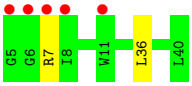
• Molecule 9: Photosystem II reaction center protein J

Chain J: 11% 97%



• Molecule 9: Photosystem II reaction center protein J

Chain j: 14% 94% 6%

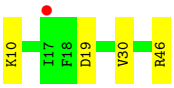


• Molecule 10: Photosystem II reaction center protein K

Chain K: 92% 8%

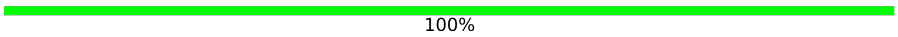
• Molecule 10: Photosystem II reaction center protein K

Chain k:



• Molecule 11: Photosystem II reaction center protein L

Chain L:



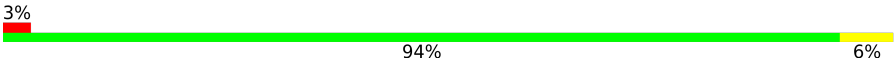
There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem II reaction center protein L

Chain l:

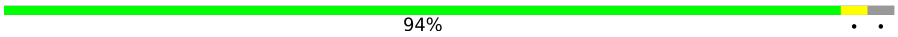
• Molecule 12: Photosystem II reaction center protein M

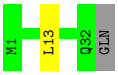
Chain M:



• Molecule 12: Photosystem II reaction center protein M

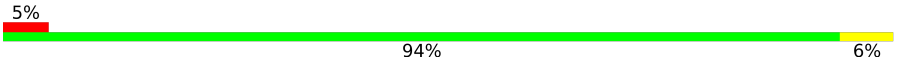
Chain m:





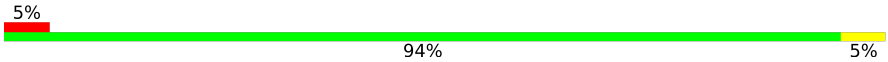
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

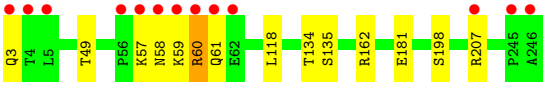
Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

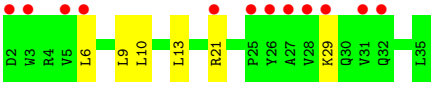
Chain o:





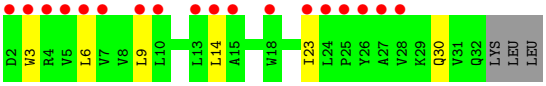
• Molecule 14: Photosystem II protein Y

Chain R:



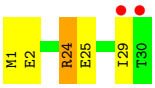
• Molecule 14: Photosystem II protein Y

Chain r:



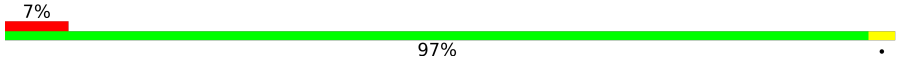
• Molecule 15: Photosystem II reaction center protein T

Chain T:



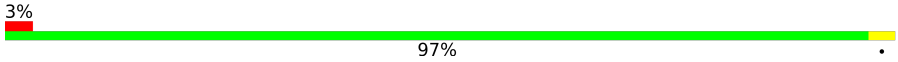
• Molecule 15: Photosystem II reaction center protein T

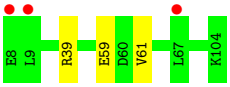
Chain t:



• Molecule 16: Photosystem II 12 kDa extrinsic protein

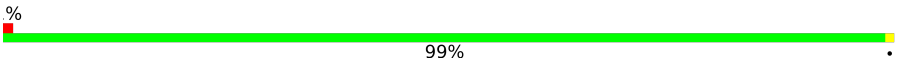
Chain U:

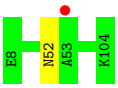




• Molecule 16: Photosystem II 12 kDa extrinsic protein

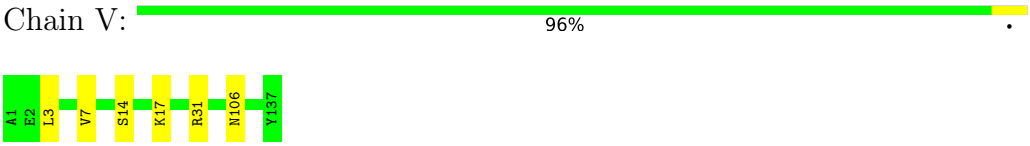
Chain u:





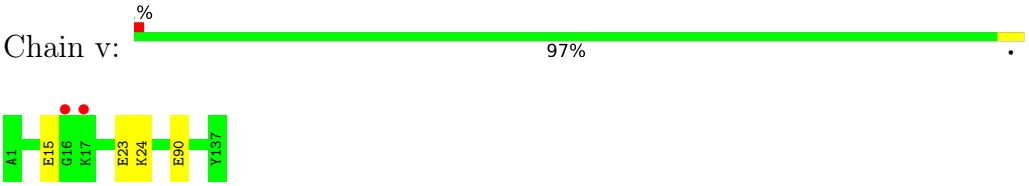
• Molecule 17: Cytochrome c-550

Chain V:



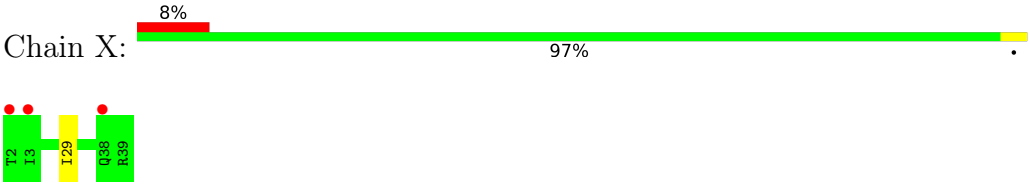
• Molecule 17: Cytochrome c-550

Chain v:



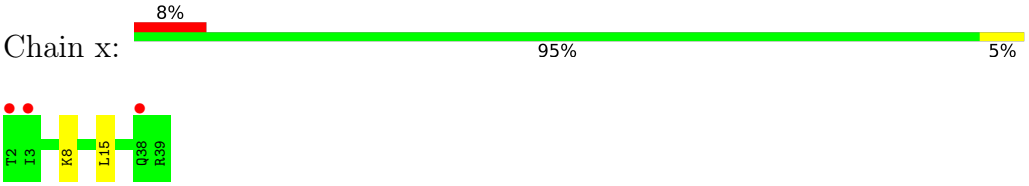
• Molecule 18: Photosystem II reaction center X protein

Chain X:



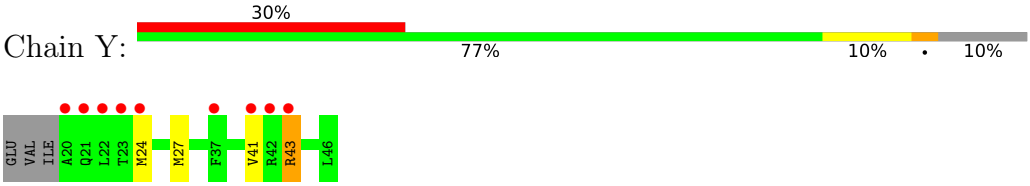
• Molecule 18: Photosystem II reaction center X protein

Chain x:



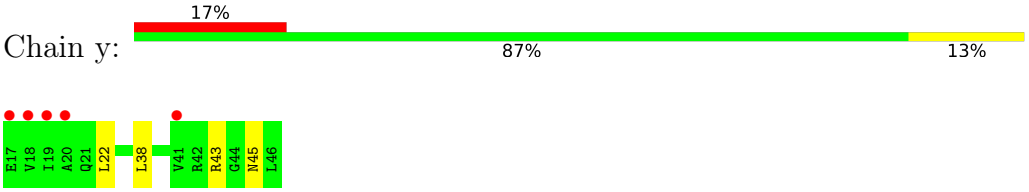
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



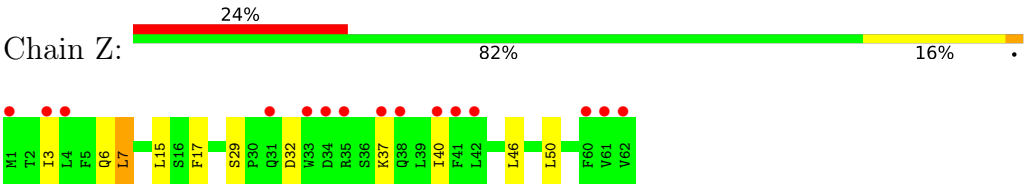
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:



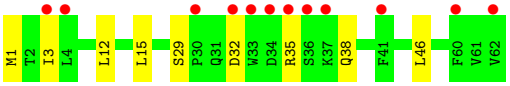
• Molecule 20: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.86Å 221.19Å 307.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.04 31.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.00-2.04) 88.5 (31.00-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.59 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.186 , 0.248 0.186 , 0.248	Depositor DCC
R_{free} test set	4461 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	105751	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: OEX, HEC, OEY, HEM, FE2, PL9, BCR, CLA, SQD, UNL, BCT, LHG, CL, LMG, DGD, FME, PHO

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	0.69	1/3179 (0.0%)	0.74	0/4331
1	a	0.65	0/3176	0.71	0/4327
2	B	0.70	0/4160	0.73	3/5668 (0.1%)
2	b	0.69	1/4118 (0.0%)	0.73	3/5611 (0.1%)
3	C	0.67	1/3593 (0.0%)	0.71	2/4891 (0.0%)
3	c	0.62	0/3673	0.70	1/4998 (0.0%)
4	D	0.75	1/2820 (0.0%)	0.74	0/3840
4	d	0.70	2/2829 (0.1%)	0.73	2/3852 (0.1%)
5	E	0.61	0/684	0.68	0/935
5	e	0.52	0/683	0.59	0/932
6	F	0.57	0/284	0.62	0/387
6	f	0.49	0/284	0.59	0/387
7	H	0.72	0/520	0.76	0/709
7	h	0.61	0/511	0.70	0/697
8	I	0.72	0/293	0.67	0/396
8	i	0.73	0/293	0.80	0/396
9	J	0.62	0/263	0.70	0/356
9	j	0.54	0/261	0.65	0/353
10	K	0.49	0/314	0.71	0/427
10	k	0.50	0/303	0.65	0/416
11	L	0.69	0/311	0.75	0/422
11	l	0.71	0/303	0.74	0/412
12	M	0.70	0/249	0.70	0/341
12	m	0.73	0/244	0.69	0/334
13	O	0.60	0/1914	0.77	1/2596 (0.0%)
13	o	0.62	0/1905	0.75	1/2583 (0.0%)
14	R	0.44	0/277	0.64	0/380
14	r	0.37	0/233	0.49	0/323
15	T	0.80	0/257	0.90	2/349 (0.6%)
15	t	0.75	0/255	0.69	0/346
16	U	0.63	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	u	0.63	0/785	0.75	0/1064
17	V	0.65	0/1085	0.68	0/1473
17	v	0.55	0/1085	0.70	0/1473
18	X	0.56	0/284	0.68	0/384
18	x	0.39	0/284	0.56	0/384
19	Y	0.39	0/197	0.65	0/264
19	y	0.35	0/219	0.54	0/294
20	Z	0.51	0/490	0.61	0/669
20	z	0.46	0/488	0.57	0/666
All	All	0.65	6/43891 (0.0%)	0.71	15/59730 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	u	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	105	CYS	CB-SG	-6.62	1.71	1.82
4	d	71	CYS	CB-SG	-6.40	1.71	1.82
4	D	76	VAL	CB-CG2	-5.99	1.40	1.52
1	A	132	GLU	CB-CG	5.81	1.63	1.52
3	C	468	SER	C-N	-5.57	1.21	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	396	MET	CG-SD-CE	-7.82	87.69	100.20
2	b	57	ARG	NE-CZ-NH1	-7.60	116.50	120.30
15	T	24	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	B	422	ARG	NE-CZ-NH1	-7.26	116.67	120.30
2	b	385	ARG	NE-CZ-NH2	-6.26	117.17	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	u	52	ASN	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	390/334 (117%)	380 (97%)	9 (2%)	1 (0%)	41	31
1	a	390/334 (117%)	383 (98%)	7 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	491 (98%)	11 (2%)	1 (0%)	47	39
3	C	447/451 (99%)	435 (97%)	10 (2%)	2 (0%)	34	24
3	c	457/451 (101%)	439 (96%)	17 (4%)	1 (0%)	47	39
4	D	339/341 (99%)	329 (97%)	10 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	32 (94%)	1 (3%)	1 (3%)	4	0
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	4	0
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	30 (100%)	0	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	34	24
13	o	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	19	10
14	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
14	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	0
15	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
17	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Y	25/30 (83%)	17 (68%)	6 (24%)	2 (8%)	1	0
19	y	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	3	0
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	0
20	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	9	2
All	All	5365/5326 (101%)	5165 (96%)	183 (3%)	17 (0%)	41	31

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
19	Y	41	VAL
19	Y	43	ARG

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	319/270 (118%)	310 (97%)	9 (3%)	43	37
1	a	318/270 (118%)	306 (96%)	12 (4%)	33	26
2	B	407/403 (101%)	387 (95%)	20 (5%)	25	17
2	b	402/403 (100%)	391 (97%)	11 (3%)	44	38
3	C	351/352 (100%)	343 (98%)	8 (2%)	50	44
3	c	360/352 (102%)	340 (94%)	20 (6%)	21	12
4	D	277/276 (100%)	272 (98%)	5 (2%)	59	55
4	d	278/276 (101%)	274 (99%)	4 (1%)	67	65
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	1
5	e	71/72 (99%)	63 (89%)	8 (11%)	6	1
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	24 (86%)	4 (14%)	3	1
7	H	53/54 (98%)	50 (94%)	3 (6%)	20	12
7	h	53/54 (98%)	48 (91%)	5 (9%)	8	3
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	1
8	i	32/32 (100%)	31 (97%)	1 (3%)	40	33
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10	4
10	K	31/30 (103%)	29 (94%)	2 (6%)	17	9
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	4
12	M	28/29 (97%)	26 (93%)	2 (7%)	14	7
12	m	28/29 (97%)	27 (96%)	1 (4%)	35	28
13	O	208/207 (100%)	195 (94%)	13 (6%)	18	9
13	o	207/207 (100%)	195 (94%)	12 (6%)	20	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	28/29 (97%)	22 (79%)	6 (21%)	1	0
14	r	19/29 (66%)	14 (74%)	5 (26%)	0	0
15	T	26/26 (100%)	22 (85%)	4 (15%)	2	0
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/84 (100%)	81 (96%)	3 (4%)	35	28
16	u	84/84 (100%)	84 (100%)	0	100	100
17	V	117/117 (100%)	111 (95%)	6 (5%)	24	15
17	v	117/117 (100%)	113 (97%)	4 (3%)	37	30
18	X	31/31 (100%)	30 (97%)	1 (3%)	39	32
18	x	31/31 (100%)	29 (94%)	2 (6%)	17	9
19	Y	19/23 (83%)	16 (84%)	3 (16%)	2	0
19	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
20	z	51/52 (98%)	43 (84%)	8 (16%)	2	0
All	All	4435/4348 (102%)	4218 (95%)	217 (5%)	25	17

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	231	GLU
3	c	213	LEU
14	r	23	ILE
1	a	305	SER
2	b	486	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	25	ASN
3	c	418	ASN
20	z	38	GLN
13	o	58	ASN
13	O	88	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)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	FME	t	1	15	8,9,10	1.15	1 (12%)	7,9,11	1.08	0
12	FME	m	1	12	8,9,10	0.87	0	7,9,11	0.73	0
8	FME	i	1	8	8,9,10	1.08	0	7,9,11	1.63	2 (28%)
8	FME	I	1	8	8,9,10	0.87	0	7,9,11	1.49	1 (14%)
12	FME	M	1	12	8,9,10	0.96	0	7,9,11	0.77	0
15	FME	T	1	15	8,9,10	1.24	1 (12%)	7,9,11	1.93	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	t	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.65	1.42	1.46
15	T	1	FME	CB-CA	2.16	1.57	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	2.90	114.96	109.73
15	T	1	FME	CA-N-CN	-2.81	118.50	122.82
15	T	1	FME	C-CA-N	2.76	114.72	109.73
8	I	1	FME	C-CA-N	2.64	114.50	109.73
15	T	1	FME	O1-CN-N	-2.19	119.50	125.27

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
8	I	1	FME	CA-CB-CG-SD
8	I	1	FME	C-CA-CB-CG
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 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	$\#\|Z\| > 2$
23	CLA	C	503	-	65,73,73	1.57	10 (15%)	76,113,113	1.66	13 (17%)
28	LMG	B	620	-	51,51,55	1.10	4 (7%)	59,59,63	1.48	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	LHG	l	101	-	48,48,48	0.75	2 (4%)	51,54,54	1.31	8 (15%)
23	CLA	c	510	-	65,73,73	1.51	7 (10%)	76,113,113	1.53	13 (17%)
25	BCR	C	514	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
25	BCR	t	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.61	13 (23%)
30	LHG	A	615	-	48,48,48	0.95	3 (6%)	51,54,54	1.15	3 (5%)
30	LHG	a	614	-	41,41,48	0.80	0	44,47,54	1.29	4 (9%)
31	DGD	A	617	-	67,67,67	1.46	9 (13%)	81,81,81	1.46	12 (14%)
21	OEX	A	601[A]	37,3,1	0,15,15	-	-	-		
31	DGD	c	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.44	15 (19%)
28	LMG	b	621	-	55,55,55	0.89	2 (3%)	63,63,63	1.38	7 (11%)
23	CLA	c	504	37	60,68,73	1.67	7 (11%)	70,107,113	1.49	10 (14%)
23	CLA	B	610	37	65,73,73	1.66	8 (12%)	76,113,113	1.63	12 (15%)
23	CLA	B	601	37	65,73,73	1.98	9 (13%)	76,113,113	1.80	12 (15%)
23	CLA	B	605	-	65,73,73	1.36	7 (10%)	76,113,113	1.47	12 (15%)
23	CLA	c	508	-	64,72,73	1.47	9 (14%)	74,111,113	1.31	10 (13%)
23	CLA	a	604	37	65,73,73	1.66	9 (13%)	76,113,113	1.45	13 (17%)
23	CLA	A	613	37	65,73,73	1.72	8 (12%)	76,113,113	1.43	9 (11%)
23	CLA	b	609	-	65,73,73	1.66	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	B	613	-	65,73,73	1.60	10 (15%)	76,113,113	1.41	12 (15%)
34	BCT	D	401	22	2,3,3	1.06	0	2,3,3	3.24	2 (100%)
25	BCR	d	404	-	41,41,41	1.27	3 (7%)	56,56,56	1.24	5 (8%)
29	SQD	a	615	-	35,35,54	1.12	2 (5%)	37,37,65	1.45	7 (18%)
30	LHG	D	408	-	46,46,48	1.05	3 (6%)	49,52,54	1.35	6 (12%)
24	PHO	d	401	-	51,69,69	1.01	3 (5%)	47,99,99	1.52	10 (21%)
28	LMG	A	612	-	48,48,55	1.01	4 (8%)	56,56,63	1.42	11 (19%)
23	CLA	b	603	-	65,73,73	1.58	8 (12%)	76,113,113	1.57	11 (14%)
28	LMG	d	406	-	44,44,55	1.23	4 (9%)	52,52,63	1.34	8 (15%)
23	CLA	B	614	-	65,73,73	1.83	9 (13%)	76,113,113	1.47	9 (11%)
25	BCR	A	608	-	41,41,41	1.18	2 (4%)	56,56,56	1.48	11 (19%)
23	CLA	B	616	-	60,68,73	1.76	11 (18%)	70,107,113	1.54	13 (18%)
23	CLA	b	607	37	65,73,73	1.28	7 (10%)	76,113,113	1.45	9 (11%)
23	CLA	C	509	-	65,73,73	1.48	7 (10%)	76,113,113	1.25	7 (9%)
28	LMG	c	521	-	48,48,55	1.18	6 (12%)	56,56,63	1.33	6 (10%)
23	CLA	b	611	-	65,73,73	1.55	8 (12%)	76,113,113	1.74	21 (27%)
23	CLA	c	501	-	65,73,73	1.63	9 (13%)	76,113,113	1.78	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	SQD	f	101	-	40,41,54	1.17	5 (12%)	49,52,65	1.65	9 (18%)
23	CLA	A	603	-	65,73,73	1.56	13 (20%)	76,113,113	1.37	12 (15%)
23	CLA	b	606	-	65,73,73	1.78	11 (16%)	76,113,113	1.55	13 (17%)
23	CLA	C	502	-	65,73,73	1.52	8 (12%)	76,113,113	1.32	7 (9%)
23	CLA	B	607	37	65,73,73	1.70	13 (20%)	76,113,113	1.25	7 (9%)
31	DGD	a	616	-	43,43,67	1.29	4 (9%)	45,45,81	1.42	5 (11%)
25	BCR	B	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.50	10 (17%)
31	DGD	C	518	-	63,63,67	0.89	3 (4%)	77,77,81	1.37	9 (11%)
30	LHG	d	409	-	38,38,48	0.96	1 (2%)	41,44,54	1.25	4 (9%)
23	CLA	c	506	-	65,73,73	2.06	11 (16%)	76,113,113	1.48	14 (18%)
30	LHG	D	406	-	48,48,48	0.85	1 (2%)	51,54,54	1.28	8 (15%)
23	CLA	C	504	37	59,67,73	1.65	11 (18%)	68,105,113	1.42	9 (13%)
25	BCR	H	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.50	9 (16%)
28	LMG	B	622	-	26,26,55	0.88	2 (7%)	26,26,63	1.12	2 (7%)
25	BCR	c	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.36	9 (16%)
23	CLA	b	610	37	65,73,73	1.47	12 (18%)	76,113,113	1.38	11 (14%)
23	CLA	C	501	-	65,73,73	1.77	10 (15%)	76,113,113	1.59	11 (14%)
28	LMG	D	409	-	31,31,55	1.43	5 (16%)	33,33,63	1.10	4 (12%)
23	CLA	C	512	-	65,73,73	1.65	11 (16%)	76,113,113	1.50	10 (13%)
23	CLA	c	511	3	65,73,73	1.82	9 (13%)	76,113,113	1.33	10 (13%)
31	DGD	C	517	-	63,63,67	1.23	6 (9%)	77,77,81	1.60	13 (16%)
23	CLA	c	505	-	65,73,73	1.57	8 (12%)	76,113,113	1.48	14 (18%)
31	DGD	C	516	-	63,63,67	1.28	9 (14%)	77,77,81	1.33	8 (10%)
23	CLA	C	507	37	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
23	CLA	C	508	-	65,73,73	1.38	9 (13%)	76,113,113	1.45	11 (14%)
23	CLA	b	613	-	65,73,73	1.62	11 (16%)	76,113,113	1.67	14 (18%)
23	CLA	d	402	-	65,73,73	1.55	10 (15%)	76,113,113	1.42	7 (9%)
28	LMG	c	522	-	49,49,55	1.04	2 (4%)	57,57,63	1.30	4 (7%)
25	BCR	T	101	-	41,41,41	1.17	5 (12%)	56,56,56	1.40	8 (14%)
25	BCR	k	101	-	41,41,41	1.03	3 (7%)	56,56,56	1.08	4 (7%)
23	CLA	b	602	-	65,73,73	1.49	7 (10%)	76,113,113	1.68	9 (11%)
23	CLA	A	604	37	65,73,73	1.53	10 (15%)	76,113,113	1.42	12 (15%)
23	CLA	B	608	-	65,73,73	1.32	7 (10%)	76,113,113	1.54	12 (15%)
23	CLA	c	503	-	65,73,73	1.62	9 (13%)	76,113,113	1.53	14 (18%)
23	CLA	B	611	-	65,73,73	1.67	10 (15%)	76,113,113	1.52	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	HEM	f	102	5,6	41,50,50	1.46	4 (9%)	45,82,82	1.48	8 (17%)
25	BCR	b	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	8 (14%)
23	CLA	b	608	-	65,73,73	1.47	9 (13%)	76,113,113	1.36	13 (17%)
29	SQD	b	601	-	48,49,54	0.98	4 (8%)	57,60,65	2.07	13 (22%)
23	CLA	b	614	-	65,73,73	1.50	8 (12%)	76,113,113	1.57	11 (14%)
24	PHO	A	606	-	51,69,69	1.19	6 (11%)	47,99,99	1.26	4 (8%)
23	CLA	a	606	-	65,73,73	1.64	13 (20%)	76,113,113	1.65	11 (14%)
23	CLA	B	615	-	65,73,73	1.73	15 (23%)	76,113,113	1.49	10 (13%)
35	HEM	F	102	5,6	41,50,50	1.49	4 (9%)	45,82,82	1.49	9 (20%)
23	CLA	D	403	-	65,73,73	1.83	10 (15%)	76,113,113	1.24	11 (14%)
34	BCT	a	610	22	2,3,3	1.53	0	2,3,3	2.60	1 (50%)
31	DGD	H	102	-	63,63,67	1.53	10 (15%)	77,77,81	1.54	13 (16%)
32	OEY	A	618[B]	37,3,1	0,16,16	-	-	-		
23	CLA	B	604	-	65,73,73	1.62	9 (13%)	76,113,113	1.75	10 (13%)
30	LHG	d	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.15	3 (5%)
25	BCR	C	515	-	41,41,41	1.25	4 (9%)	56,56,56	1.22	5 (8%)
23	CLA	c	513	-	65,73,73	1.54	9 (13%)	76,113,113	1.11	6 (7%)
25	BCR	B	617	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	5 (8%)
23	CLA	b	615	-	65,73,73	1.98	12 (18%)	76,113,113	1.51	14 (18%)
27	PL9	a	611	-	55,55,55	1.11	6 (10%)	68,69,69	1.61	14 (20%)
23	CLA	c	509	-	65,73,73	1.43	6 (9%)	76,113,113	1.57	11 (14%)
25	BCR	C	520	-	41,41,41	1.07	4 (9%)	56,56,56	1.21	3 (5%)
25	BCR	b	617	-	41,41,41	1.14	3 (7%)	56,56,56	1.39	6 (10%)
25	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	5 (8%)
30	LHG	L	101	-	48,48,48	0.86	1 (2%)	51,54,54	1.12	3 (5%)
27	PL9	d	408	-	55,55,55	1.52	9 (16%)	68,69,69	1.80	20 (29%)
23	CLA	h	101	37	65,73,73	1.71	11 (16%)	76,113,113	1.58	15 (19%)
25	BCR	B	618	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	c	507	37	65,73,73	1.59	11 (16%)	76,113,113	1.63	12 (15%)
24	PHO	a	605	-	51,69,69	1.10	5 (9%)	47,99,99	1.35	5 (10%)
27	PL9	A	611	-	55,55,55	1.01	2 (3%)	68,69,69	1.66	16 (23%)
31	DGD	c	517	-	63,63,67	1.31	11 (17%)	77,77,81	1.46	12 (15%)
29	SQD	F	101	-	35,36,54	1.08	3 (8%)	42,45,65	1.98	9 (21%)
23	CLA	b	612	-	65,73,73	1.53	8 (12%)	76,113,113	1.69	15 (19%)
36	HEC	v	201	17	32,50,50	2.04	4 (12%)	24,82,82	1.56	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	B	602	-	65,73,73	1.45	9 (13%)	76,113,113	1.36	13 (17%)
36	HEC	V	201	17	32,50,50	2.25	6 (18%)	24,82,82	1.28	3 (12%)
29	SQD	B	624	-	53,54,54	0.92	3 (5%)	62,65,65	1.78	13 (20%)
28	LMG	d	410	-	21,21,55	0.71	0	20,20,63	1.02	0
23	CLA	C	506	-	65,73,73	1.64	9 (13%)	76,113,113	1.29	9 (11%)
24	PHO	A	605	-	51,69,69	1.02	3 (5%)	47,99,99	1.44	6 (12%)
28	LMG	D	405	-	51,51,55	1.10	3 (5%)	59,59,63	1.17	5 (8%)
28	LMG	c	519	-	37,37,55	1.21	4 (10%)	45,45,63	1.21	4 (8%)
30	LHG	B	623	-	48,48,48	0.86	1 (2%)	51,54,54	1.44	9 (17%)
31	DGD	h	103	-	63,63,67	1.02	2 (3%)	77,77,81	1.42	9 (11%)
23	CLA	B	609	-	65,73,73	1.69	12 (18%)	76,113,113	1.46	8 (10%)
32	OEY	a	618[B]	37,3,1	0,16,16	-	-	-		
25	BCR	a	607	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	9 (16%)
23	CLA	C	510	-	65,73,73	1.54	13 (20%)	76,113,113	1.43	8 (10%)
23	CLA	D	402	-	65,73,73	1.48	10 (15%)	76,113,113	1.33	11 (14%)
23	CLA	C	511	3	65,73,73	1.93	8 (12%)	76,113,113	1.49	5 (6%)
28	LMG	m	101	-	51,51,55	0.84	2 (3%)	59,59,63	1.56	12 (20%)
30	LHG	d	405	-	48,48,48	0.66	0	51,54,54	1.27	4 (7%)
29	SQD	A	614	-	51,52,54	1.09	4 (7%)	60,63,65	2.46	13 (21%)
23	CLA	B	606	-	65,73,73	1.84	11 (16%)	76,113,113	1.65	12 (15%)
23	CLA	d	403	-	65,73,73	1.44	7 (10%)	76,113,113	1.35	12 (15%)
23	CLA	C	513	-	65,73,73	1.56	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	b	604	-	65,73,73	1.54	8 (12%)	76,113,113	1.57	12 (15%)
23	CLA	B	612	-	65,73,73	1.40	6 (9%)	76,113,113	1.53	11 (14%)
23	CLA	b	605	-	65,73,73	1.48	8 (12%)	76,113,113	1.76	17 (22%)
25	BCR	h	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.48	13 (23%)
25	BCR	Y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	8 (14%)
23	CLA	a	612	37	65,73,73	1.65	9 (13%)	76,113,113	1.55	10 (13%)
23	CLA	c	502	-	65,73,73	1.28	7 (10%)	76,113,113	1.79	11 (14%)
23	CLA	c	512	-	65,73,73	1.50	9 (13%)	76,113,113	1.50	10 (13%)
25	BCR	k	102	-	41,41,41	0.98	0	56,56,56	1.27	6 (10%)
25	BCR	b	618	-	41,41,41	1.37	4 (9%)	56,56,56	1.33	8 (14%)
23	CLA	A	607	-	54,62,73	1.95	8 (14%)	62,99,113	1.89	12 (19%)
23	CLA	B	603	-	65,73,73	1.42	9 (13%)	76,113,113	1.57	14 (18%)
31	DGD	c	516	-	63,63,67	1.18	6 (9%)	77,77,81	1.36	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	PL9	D	407	-	55,55,55	1.70	12 (21%)	68,69,69	1.56	15 (22%)
29	SQD	A	616	-	38,38,54	1.03	3 (7%)	40,40,65	1.63	3 (7%)
23	CLA	a	603	-	65,73,73	1.53	7 (10%)	76,113,113	1.68	13 (17%)
29	SQD	a	613	-	53,54,54	0.95	3 (5%)	62,65,65	1.93	12 (19%)
23	CLA	C	505	-	65,73,73	1.39	6 (9%)	76,113,113	1.40	10 (13%)
28	LMG	C	519	-	48,48,55	1.18	5 (10%)	56,56,63	1.29	5 (8%)
25	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.57	14 (25%)
23	CLA	b	616	-	60,68,73	1.56	11 (18%)	70,107,113	1.63	9 (12%)
21	OEX	a	601[A]	37,3,1	0,15,15	-	-	-		

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
23	CLA	C	503	-	1/1/20/20	6/37/115/115	-
28	LMG	B	620	-	-	21/46/66/70	0/1/1/1
30	LHG	l	101	-	-	19/53/53/53	-
23	CLA	c	510	-	1/1/20/20	12/37/115/115	-
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	BCR	t	101	-	-	9/29/63/63	0/2/2/2
30	LHG	A	615	-	-	27/53/53/53	-
30	LHG	a	614	-	-	28/46/46/53	-
31	DGD	A	617	-	-	24/55/95/95	0/2/2/2
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
28	LMG	b	621	-	-	16/50/70/70	0/1/1/1
23	CLA	c	504	37	1/1/19/20	9/31/109/115	-
23	CLA	B	610	37	1/1/20/20	5/37/115/115	-
23	CLA	B	601	37	1/1/20/20	15/37/115/115	-
23	CLA	B	605	-	-	10/37/115/115	-
23	CLA	c	508	-	1/1/19/20	11/36/114/115	-
23	CLA	a	604	37	-	10/37/115/115	-
23	CLA	A	613	37	-	6/37/115/115	-
23	CLA	b	609	-	1/1/20/20	13/37/115/115	-
23	CLA	B	613	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	d	404	-	-	8/29/63/63	0/2/2/2
29	SQD	a	615	-	-	18/37/37/69	-
30	LHG	D	408	-	-	22/51/51/53	-
24	PHO	d	401	-	-	6/37/103/103	0/5/6/6
28	LMG	A	612	-	-	21/43/63/70	0/1/1/1
23	CLA	b	603	-	1/1/20/20	7/37/115/115	-
28	LMG	d	406	-	-	13/39/59/70	0/1/1/1
23	CLA	B	614	-	1/1/20/20	14/37/115/115	-
25	BCR	A	608	-	-	6/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/19/20	7/31/109/115	-
23	CLA	b	607	37	1/1/20/20	14/37/115/115	-
23	CLA	C	509	-	1/1/20/20	15/37/115/115	-
28	LMG	c	521	-	-	20/43/63/70	0/1/1/1
23	CLA	b	611	-	1/1/20/20	7/37/115/115	-
23	CLA	c	501	-	1/1/20/20	6/37/115/115	-
29	SQD	f	101	-	-	18/36/56/69	0/1/1/1
23	CLA	A	603	-	1/1/20/20	1/37/115/115	-
23	CLA	b	606	-	1/1/20/20	13/37/115/115	-
23	CLA	C	502	-	1/1/20/20	6/37/115/115	-
23	CLA	B	607	37	1/1/20/20	12/37/115/115	-
31	DGD	a	616	-	-	26/45/45/95	-
25	BCR	B	619	-	-	8/29/63/63	0/2/2/2
31	DGD	C	518	-	-	17/51/91/95	0/2/2/2
30	LHG	d	409	-	-	13/43/43/53	-
23	CLA	c	506	-	1/1/20/20	19/37/115/115	-
30	LHG	D	406	-	-	20/53/53/53	-
23	CLA	C	504	37	1/1/18/20	9/30/108/115	-
25	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	LMG	B	622	-	-	11/22/22/70	-
25	BCR	c	514	-	-	15/29/63/63	0/2/2/2
23	CLA	b	610	37	1/1/20/20	7/37/115/115	-
23	CLA	C	501	-	1/1/20/20	4/37/115/115	-
28	LMG	D	409	-	-	17/33/33/70	-
23	CLA	C	512	-	1/1/20/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	511	3	1/1/20/20	10/37/115/115	-
31	DGD	C	517	-	-	23/51/91/95	0/2/2/2
23	CLA	c	505	-	1/1/20/20	9/37/115/115	-
31	DGD	C	516	-	-	19/51/91/95	0/2/2/2
23	CLA	C	507	37	1/1/20/20	9/37/115/115	-
23	CLA	b	613	-	1/1/20/20	8/37/115/115	-
23	CLA	C	508	-	-	11/37/115/115	-
23	CLA	d	402	-	1/1/20/20	9/37/115/115	-
28	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	BCR	T	101	-	-	10/29/63/63	0/2/2/2
25	BCR	k	101	-	-	9/29/63/63	0/2/2/2
23	CLA	b	602	-	1/1/20/20	7/37/115/115	-
23	CLA	A	604	37	-	5/37/115/115	-
23	CLA	B	608	-	-	1/37/115/115	-
23	CLA	c	503	-	1/1/20/20	7/37/115/115	-
23	CLA	B	611	-	-	10/37/115/115	-
35	HEM	f	102	5,6	-	3/12/54/54	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	b	608	-	-	8/37/115/115	-
29	SQD	b	601	-	-	17/44/64/69	0/1/1/1
23	CLA	b	614	-	1/1/20/20	18/37/115/115	-
24	PHO	A	606	-	-	5/37/103/103	0/5/6/6
23	CLA	a	606	-	1/1/20/20	11/37/115/115	-
23	CLA	B	615	-	1/1/20/20	9/37/115/115	-
35	HEM	F	102	5,6	-	2/12/54/54	-
23	CLA	D	403	-	1/1/20/20	15/37/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/20/20	10/37/115/115	-
30	LHG	d	407	-	-	20/53/53/53	-
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/20/20	4/37/115/115	-
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
23	CLA	b	615	-	1/1/20/20	8/37/115/115	-
27	PL9	a	611	-	-	25/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	509	-	1/1/20/20	13/37/115/115	-
25	BCR	C	520	-	-	7/29/63/63	0/2/2/2
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	D	404	-	-	7/29/63/63	0/2/2/2
30	LHG	L	101	-	-	18/53/53/53	-
27	PL9	d	408	-	-	21/53/73/73	0/1/1/1
23	CLA	h	101	37	1/1/20/20	18/37/115/115	-
25	BCR	B	618	-	-	6/29/63/63	0/2/2/2
23	CLA	c	507	37	1/1/20/20	9/37/115/115	-
24	PHO	a	605	-	-	10/37/103/103	0/5/6/6
27	PL9	A	611	-	-	26/53/73/73	0/1/1/1
31	DGD	c	517	-	-	20/51/91/95	0/2/2/2
29	SQD	F	101	-	-	16/28/48/69	0/1/1/1
23	CLA	b	612	-	1/1/20/20	7/37/115/115	-
36	HEC	v	201	17	-	2/10/54/54	-
23	CLA	B	602	-	1/1/20/20	4/37/115/115	-
36	HEC	V	201	17	-	2/10/54/54	-
29	SQD	B	624	-	-	24/49/69/69	0/1/1/1
28	LMG	d	410	-	-	10/17/17/70	-
23	CLA	C	506	-	-	14/37/115/115	-
24	PHO	A	605	-	-	8/37/103/103	0/5/6/6
28	LMG	D	405	-	-	17/46/66/70	0/1/1/1
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
30	LHG	B	623	-	-	15/53/53/53	-
31	DGD	h	103	-	-	18/51/91/95	0/2/2/2
23	CLA	B	609	-	-	7/37/115/115	-
25	BCR	a	607	-	-	4/29/63/63	0/2/2/2
23	CLA	C	510	-	1/1/20/20	7/37/115/115	-
23	CLA	D	402	-	-	5/37/115/115	-
23	CLA	C	511	3	1/1/20/20	8/37/115/115	-
28	LMG	m	101	-	-	20/46/66/70	0/1/1/1
30	LHG	d	405	-	-	24/53/53/53	-
29	SQD	A	614	-	-	23/47/67/69	0/1/1/1
23	CLA	B	606	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	403	-	-	6/37/115/115	-
23	CLA	C	513	-	1/1/20/20	8/37/115/115	-
23	CLA	b	604	-	1/1/20/20	11/37/115/115	-
23	CLA	B	612	-	1/1/20/20	12/37/115/115	-
23	CLA	b	605	-	1/1/20/20	6/37/115/115	-
25	BCR	h	102	-	-	11/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	12/29/63/63	0/2/2/2
23	CLA	a	612	37	1/1/20/20	3/37/115/115	-
23	CLA	c	502	-	-	6/37/115/115	-
23	CLA	c	512	-	1/1/20/20	18/37/115/115	-
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
25	BCR	b	618	-	-	7/29/63/63	0/2/2/2
23	CLA	A	607	-	1/1/17/20	3/24/102/115	-
23	CLA	B	603	-	1/1/20/20	15/37/115/115	-
31	DGD	c	516	-	-	28/51/91/95	0/2/2/2
27	PL9	D	407	-	-	10/53/73/73	0/1/1/1
29	SQD	A	616	-	-	17/39/39/69	-
23	CLA	a	603	-	1/1/20/20	1/37/115/115	-
29	SQD	a	613	-	-	25/49/69/69	0/1/1/1
23	CLA	C	505	-	1/1/20/20	11/37/115/115	-
28	LMG	C	519	-	-	17/43/63/70	0/1/1/1
25	BCR	c	515	-	-	4/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/19/20	7/31/109/115	-

The worst 5 of 914 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-10.99	1.84	2.05
23	b	615	CLA	MG-NA	9.73	2.29	2.06
23	C	511	CLA	MG-NA	9.42	2.28	2.06
23	b	609	CLA	C4B-NB	8.45	1.42	1.35
23	B	610	CLA	C4B-NB	8.22	1.42	1.35

The worst 5 of 1395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C4A-NA-C1A	11.08	111.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	C4A-NA-C1A	10.09	111.24	106.71
29	A	614	SQD	O6-C1-C2	9.95	123.84	108.30
29	A	614	SQD	O7-S-C6	9.86	118.66	106.94
23	c	502	CLA	C4A-NA-C1A	9.67	111.05	106.71

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	603	CLA	ND
23	A	607	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

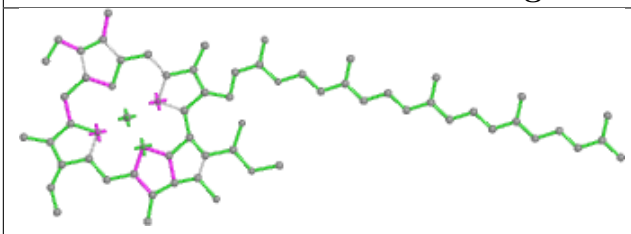
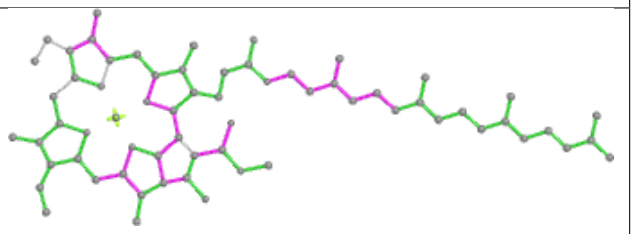
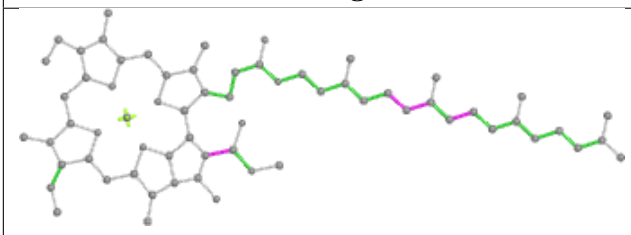
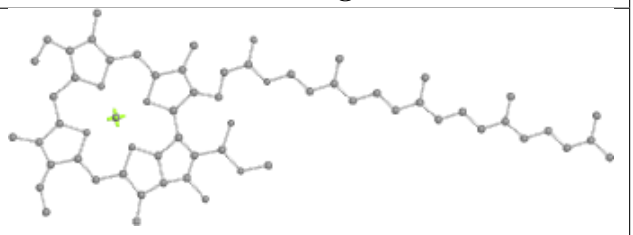
5 of 1698 torsion outliers are listed below:

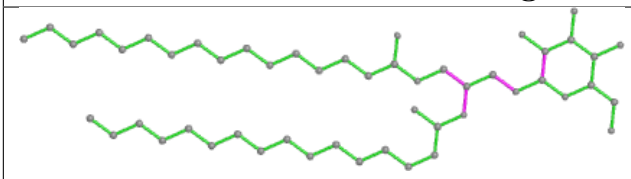
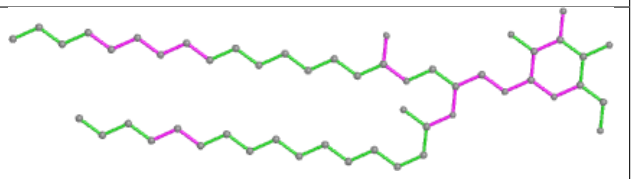
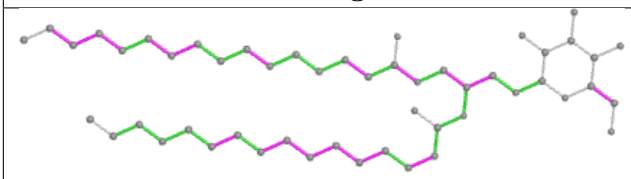
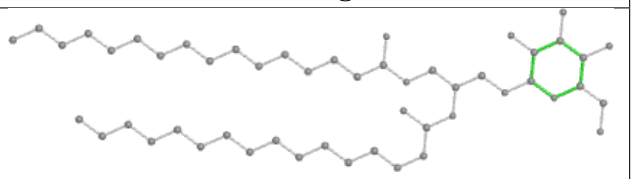
Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

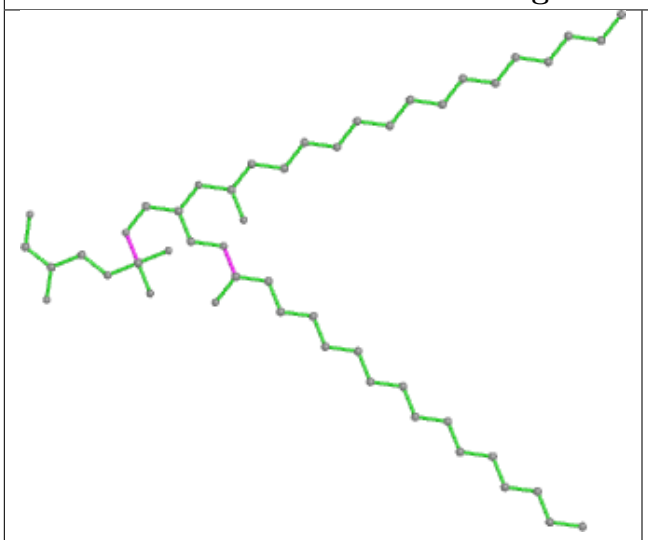
No monomer is involved in short contacts.

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.

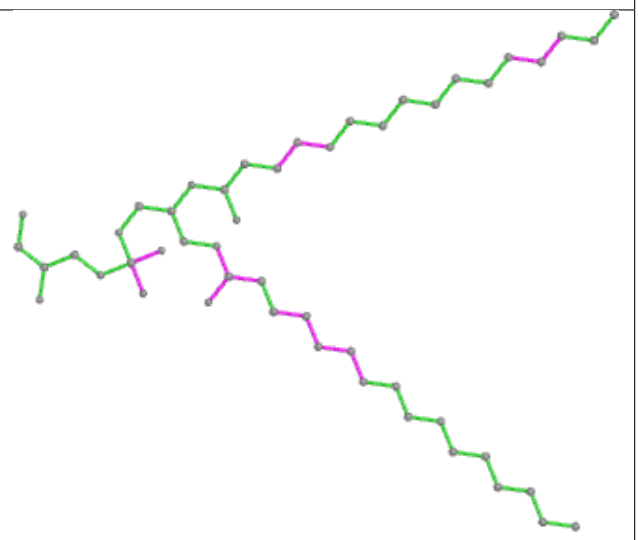
Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

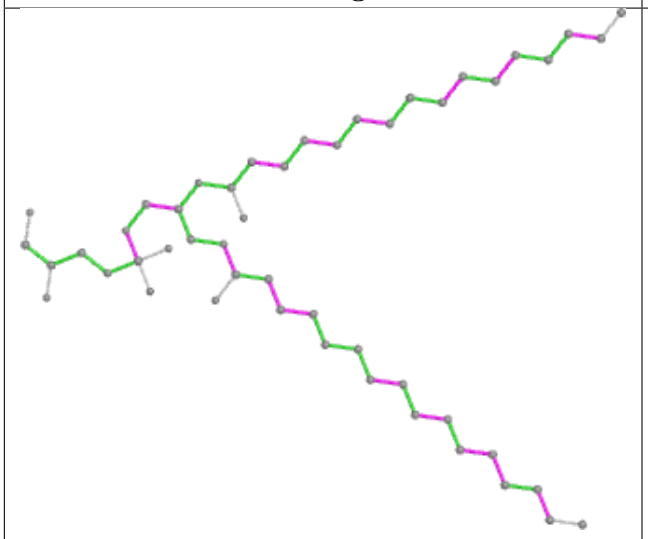
Ligand LHG l 101



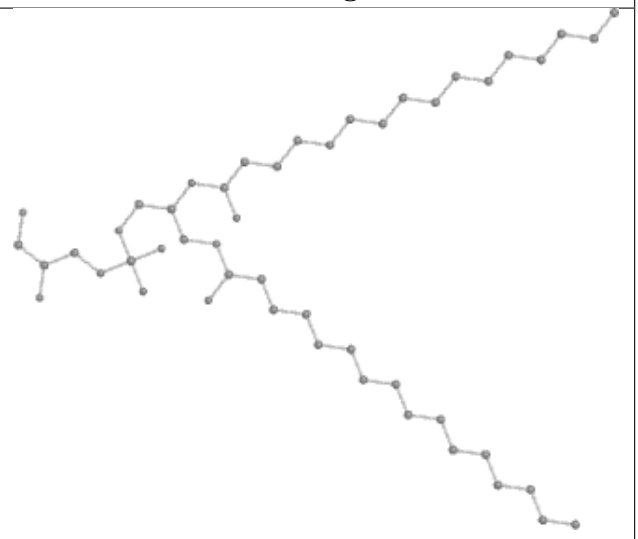
Bond lengths



Bond angles

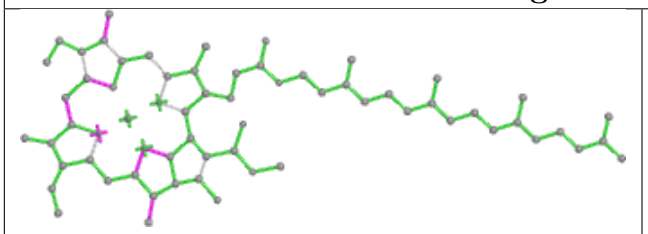


Torsions

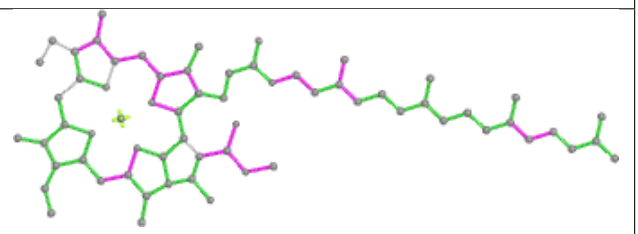


Rings

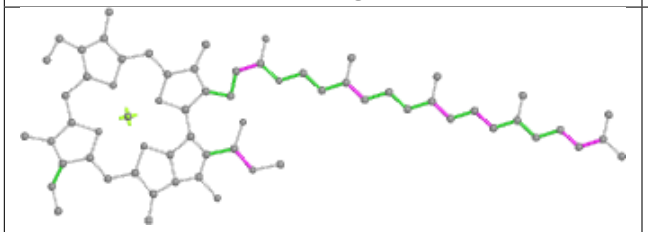
Ligand CLA c 510



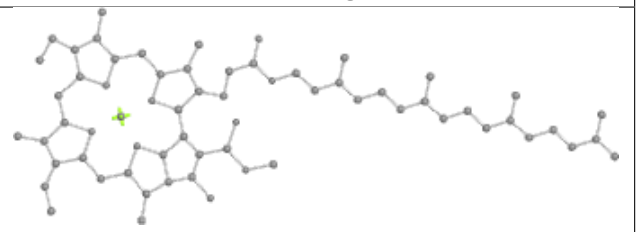
Bond lengths



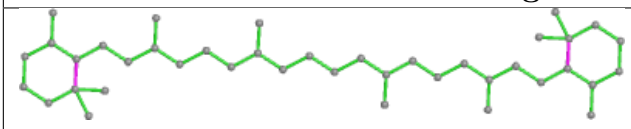
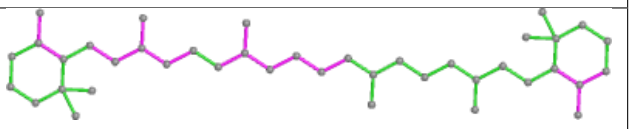
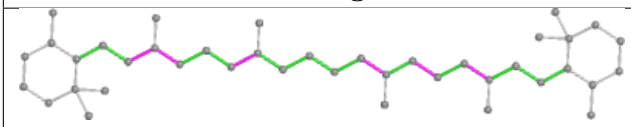
Bond angles

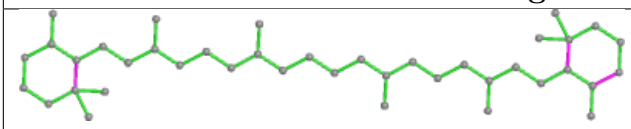
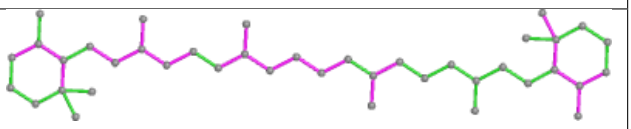
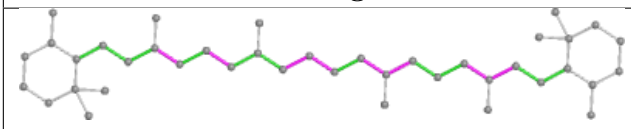
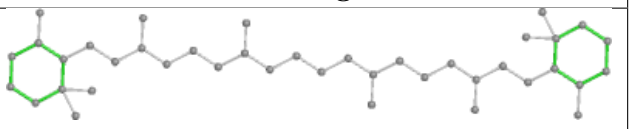


Torsions

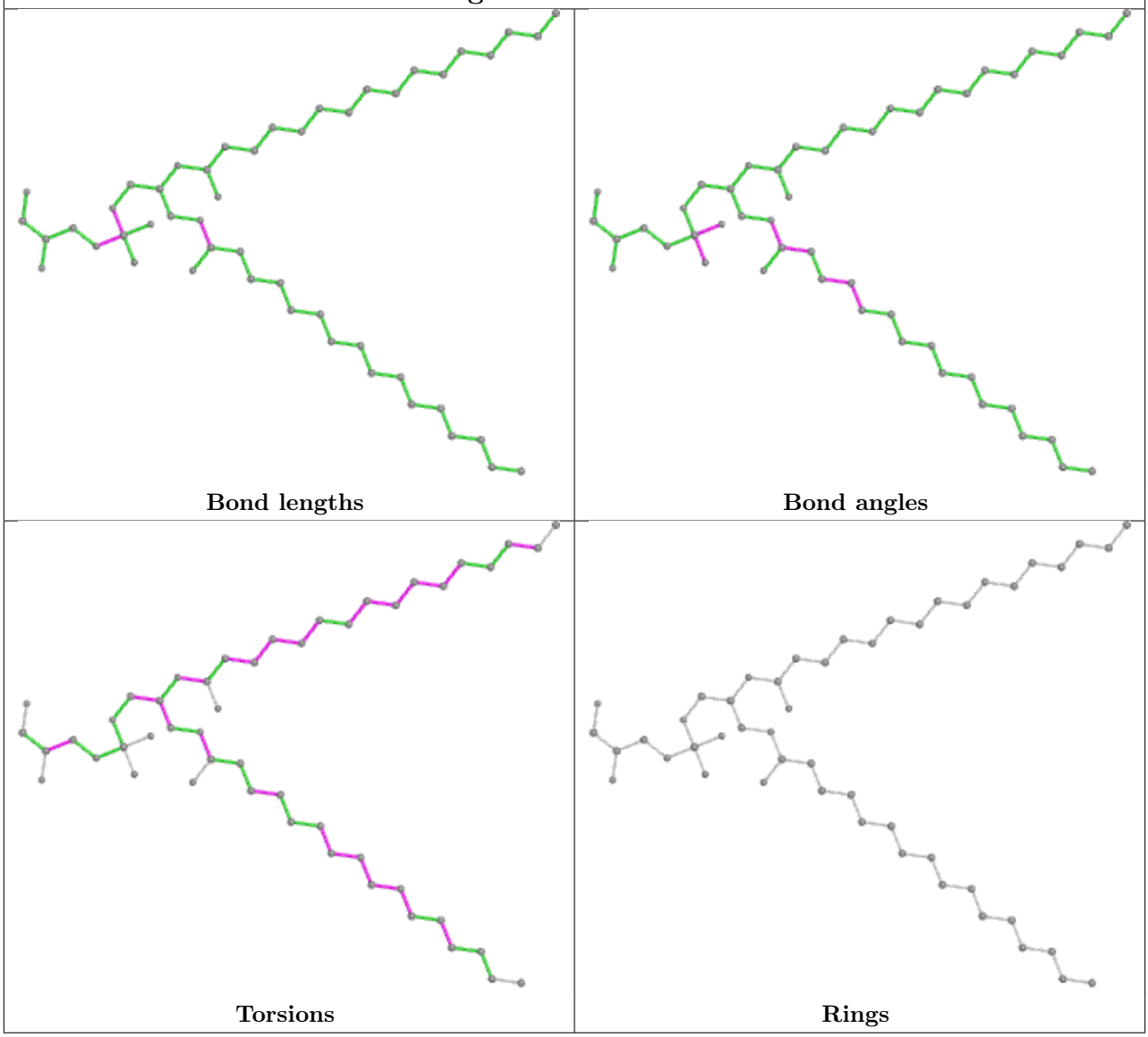


Rings

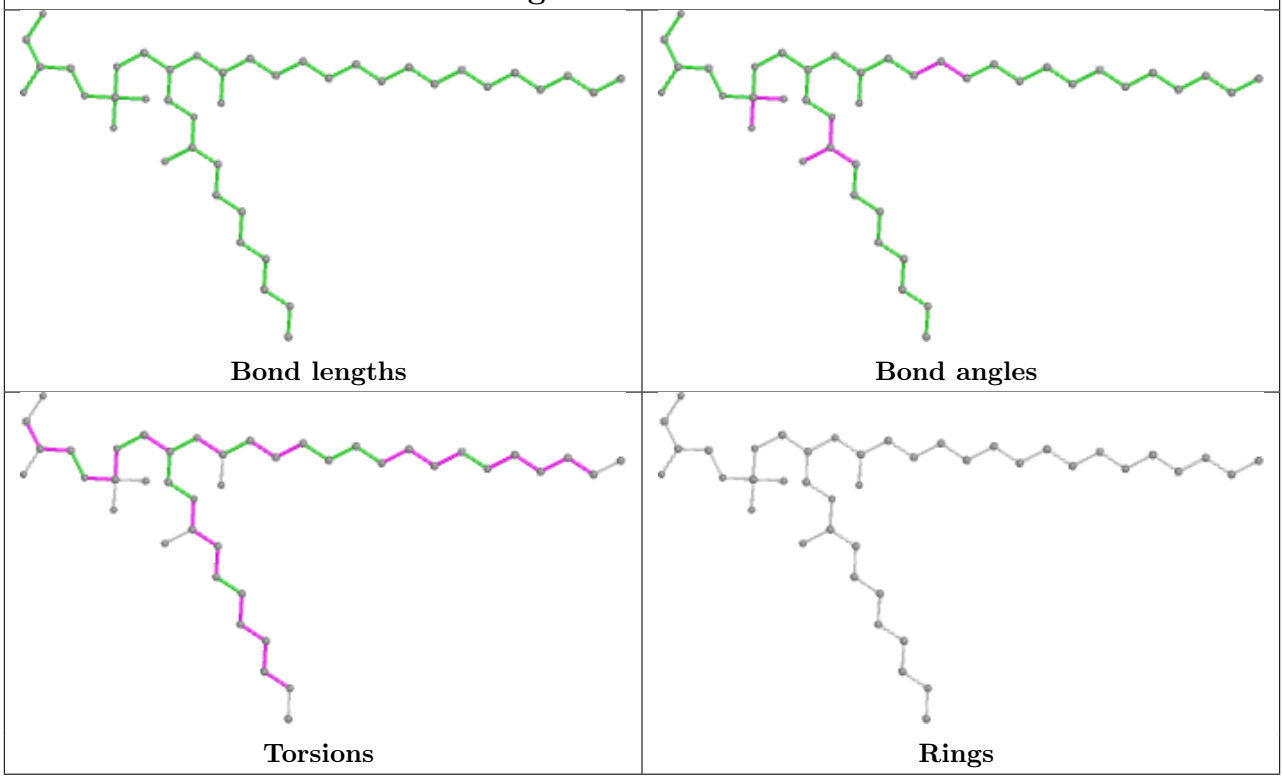
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 615



Ligand LHG a 614



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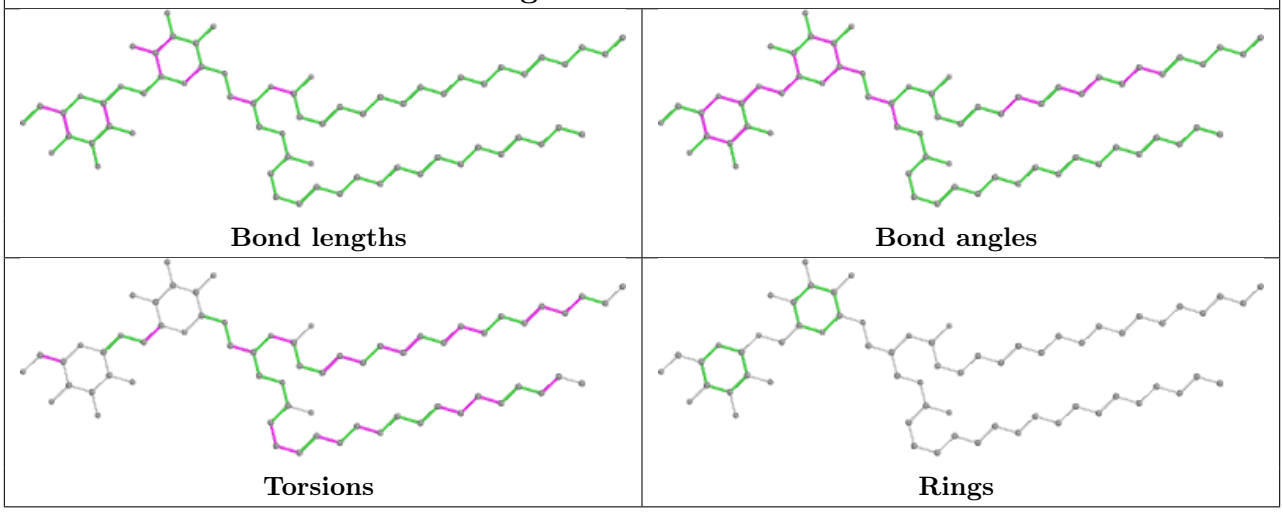
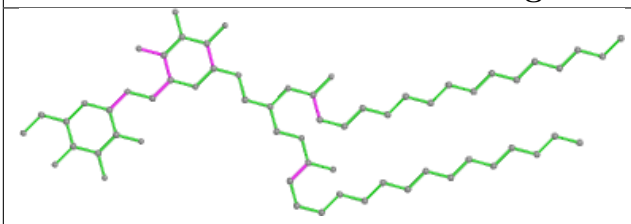
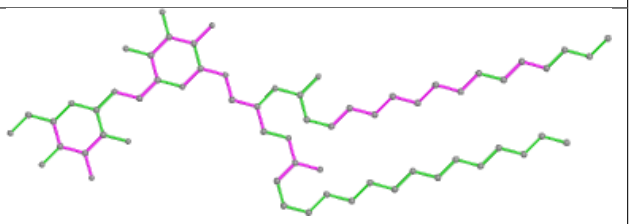


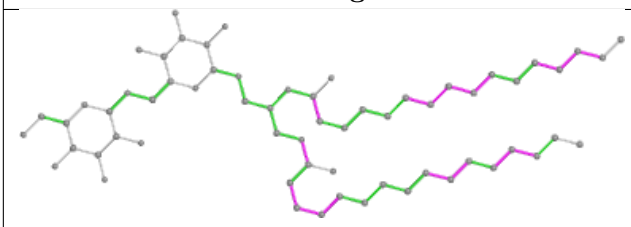
Ligand DGD c 518



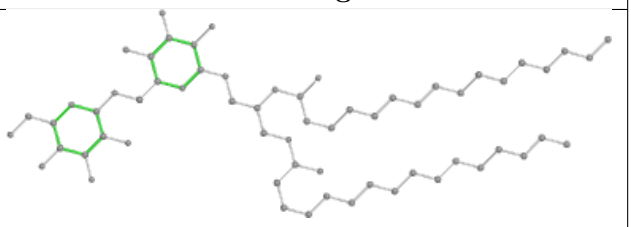
Bond lengths



Bond angles

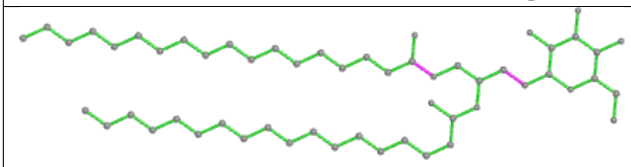


Torsions



Rings

Ligand LMG b 621



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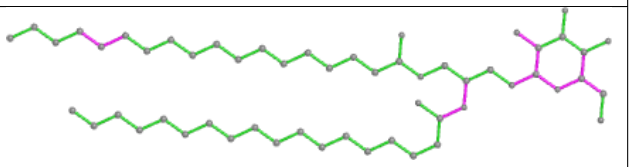
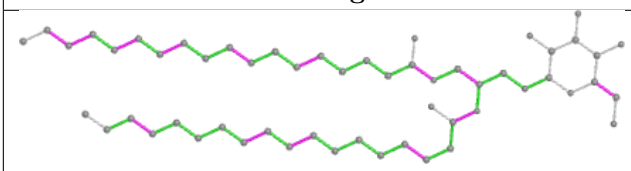


Bond angles



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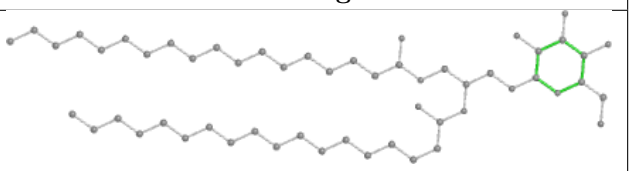
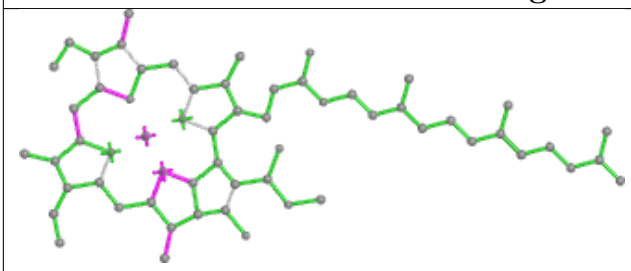
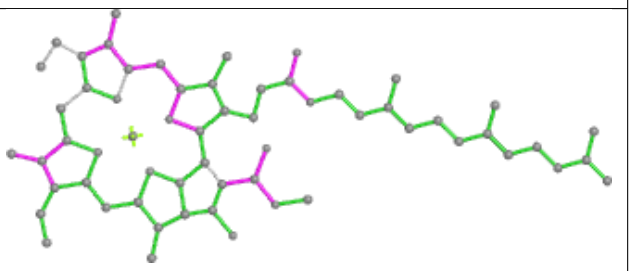


Rings

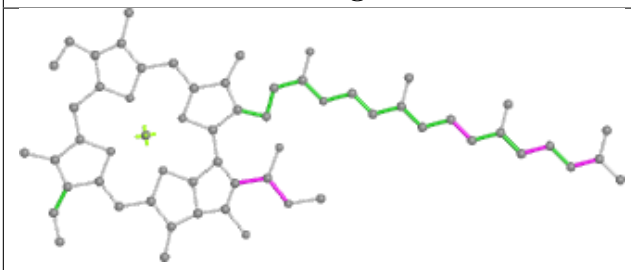
Ligand CLA c 504



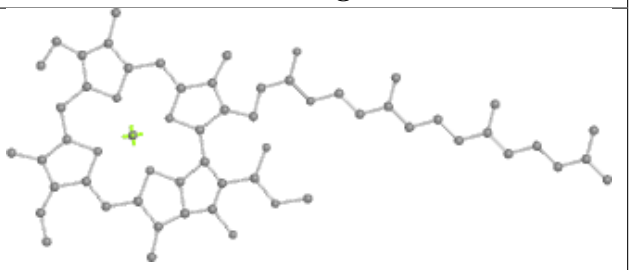
Bond lengths



Bond angles

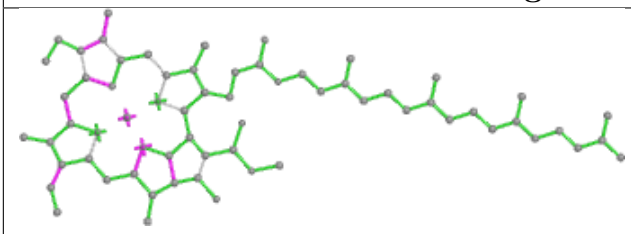


Torsions

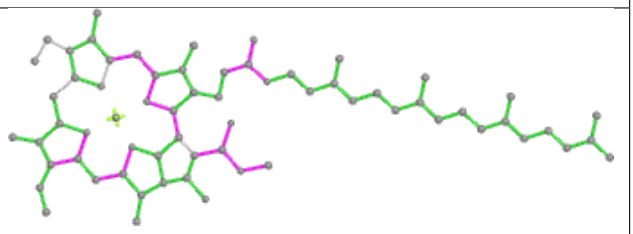


Rings

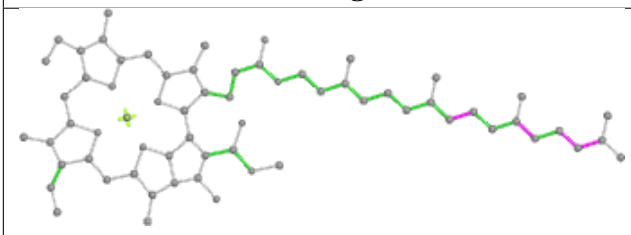
Ligand CLA B 610



Bond lengths



Bond angles



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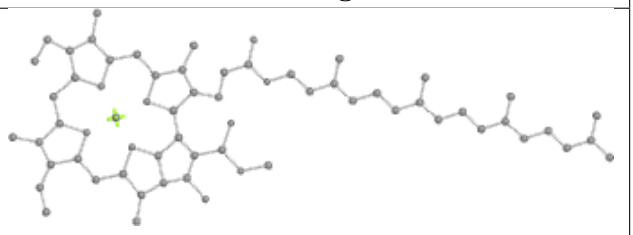
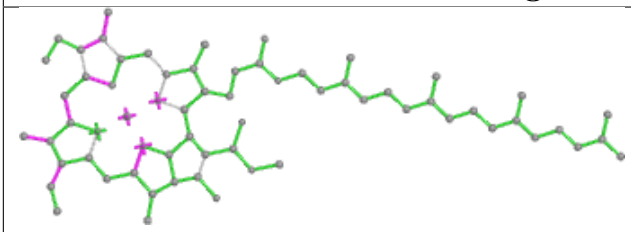


Rings

Ligand CLA B 601



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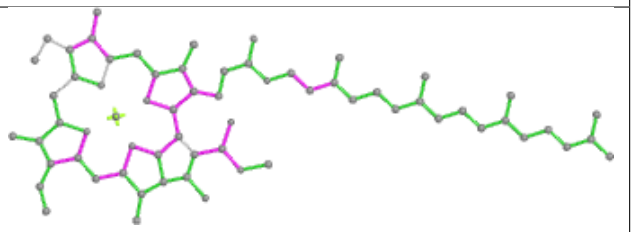
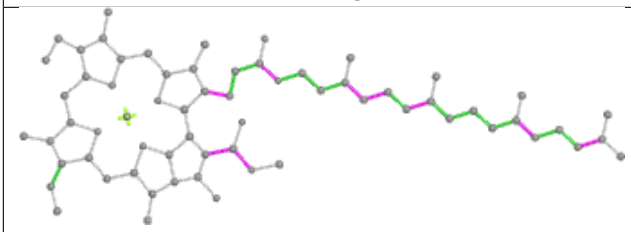
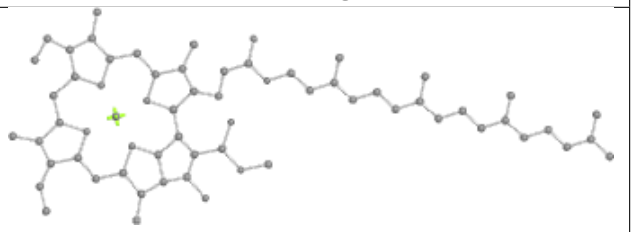


Bond angles

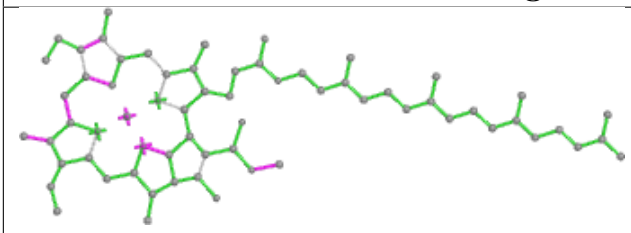


Torsions



Rings

Ligand CLA B 605



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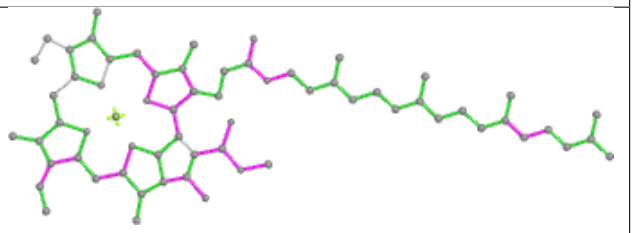
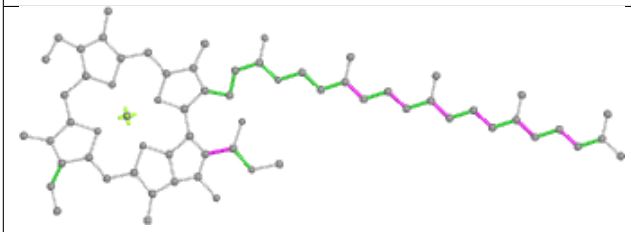
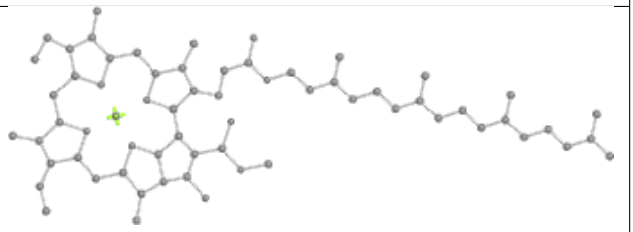


Bond angles

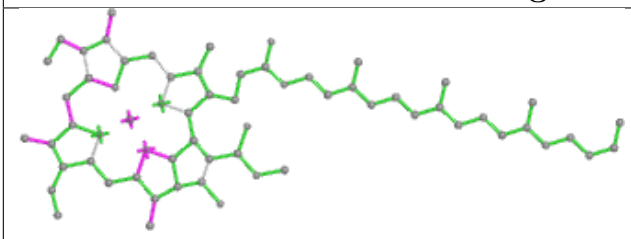


Torsions

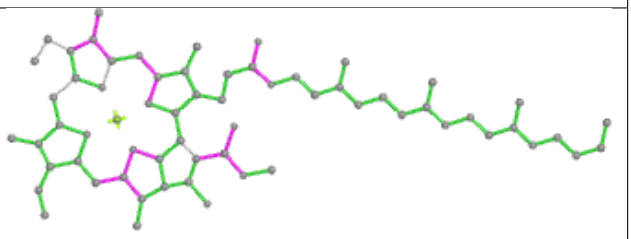


Rings

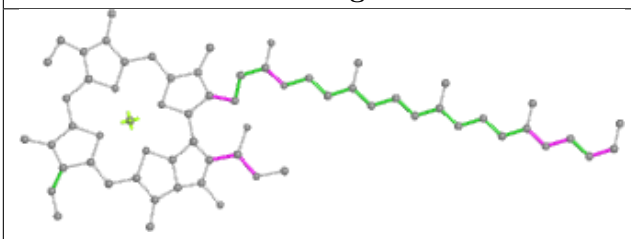
Ligand CLA c 508



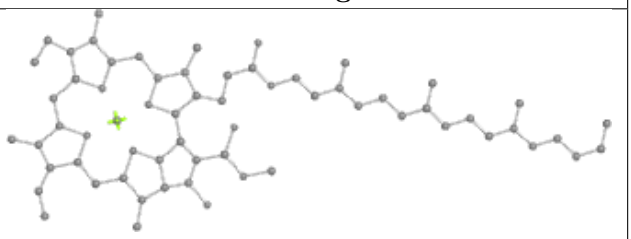
Bond lengths



Bond angles

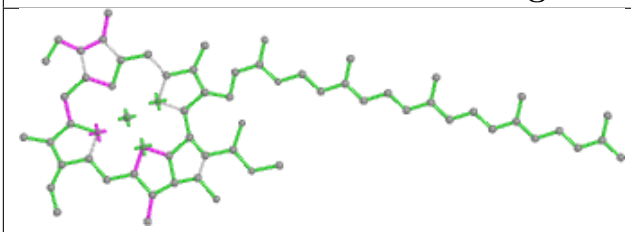


Torsions

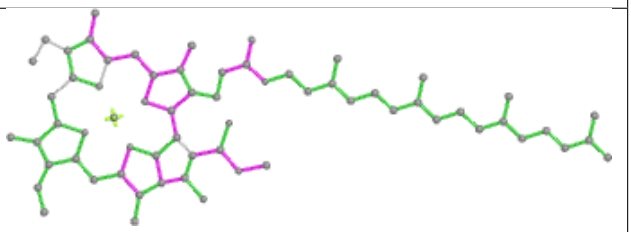


Rings

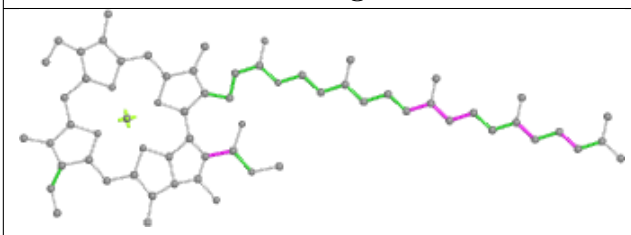
Ligand CLA a 604



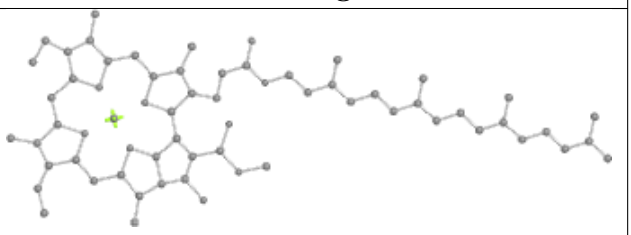
Bond lengths



Bond angles

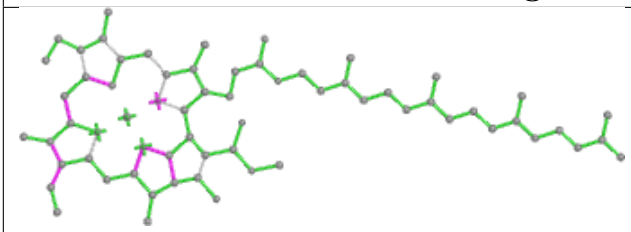


Torsions

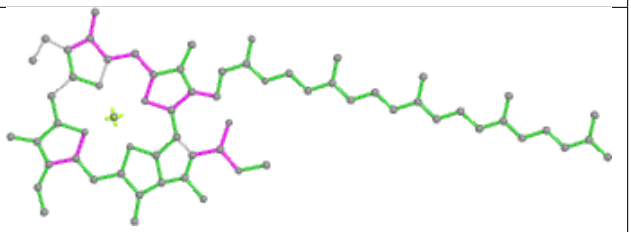


Rings

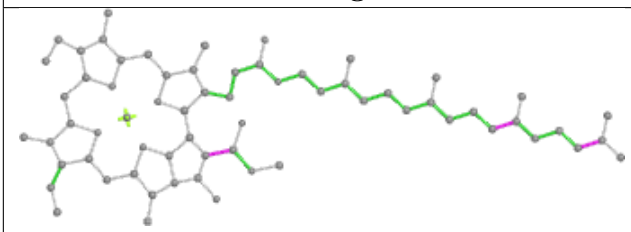
Ligand CLA A 613



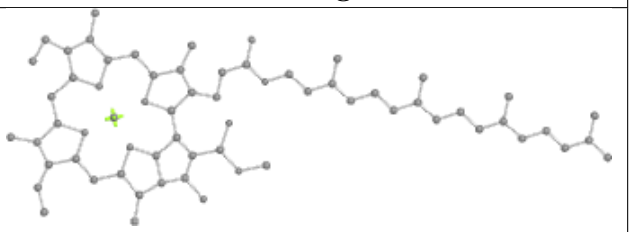
Bond lengths



Bond angles

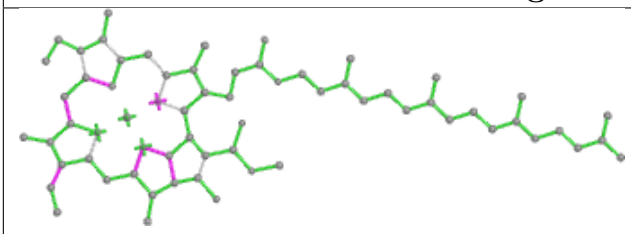


Torsions

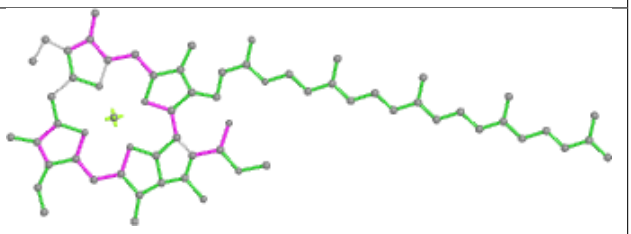


Rings

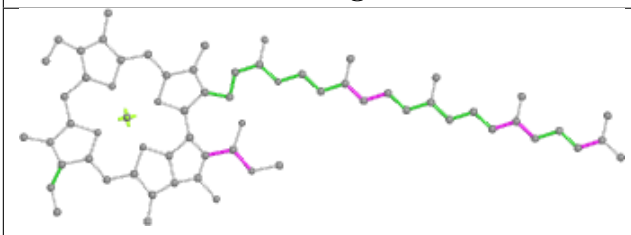
Ligand CLA b 609



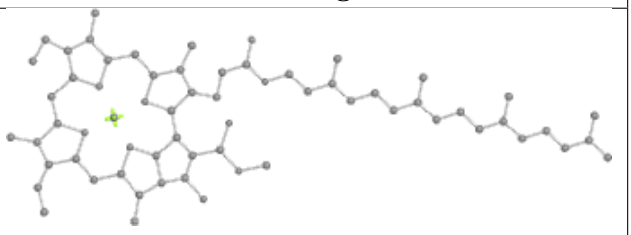
Bond lengths



Bond angles

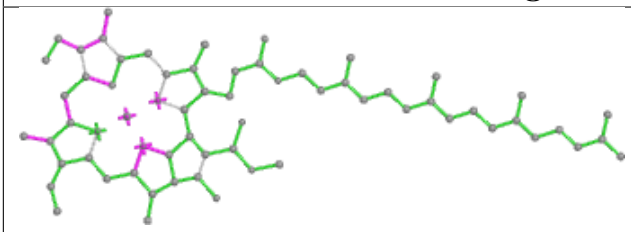


Torsions



Rings

Ligand CLA B 613



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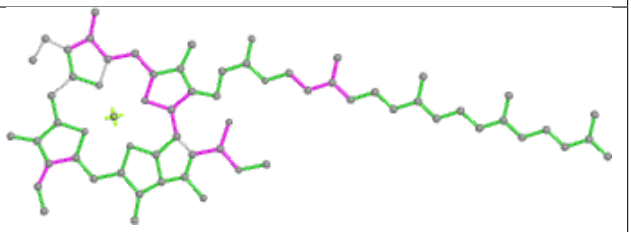
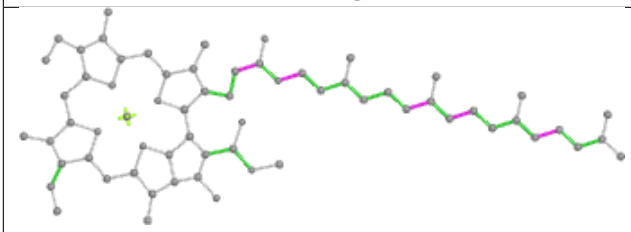
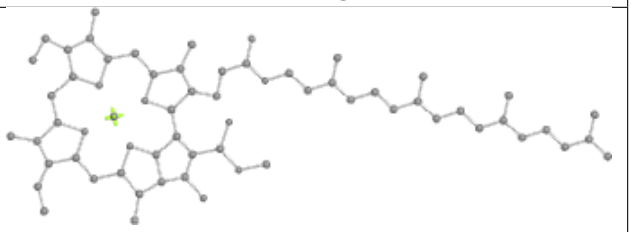


Bond angles

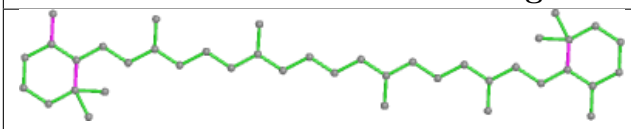


Torsions



Rings

Ligand BCR d 404



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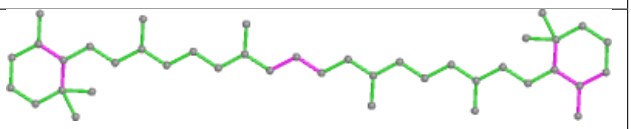
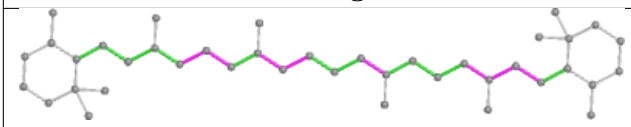


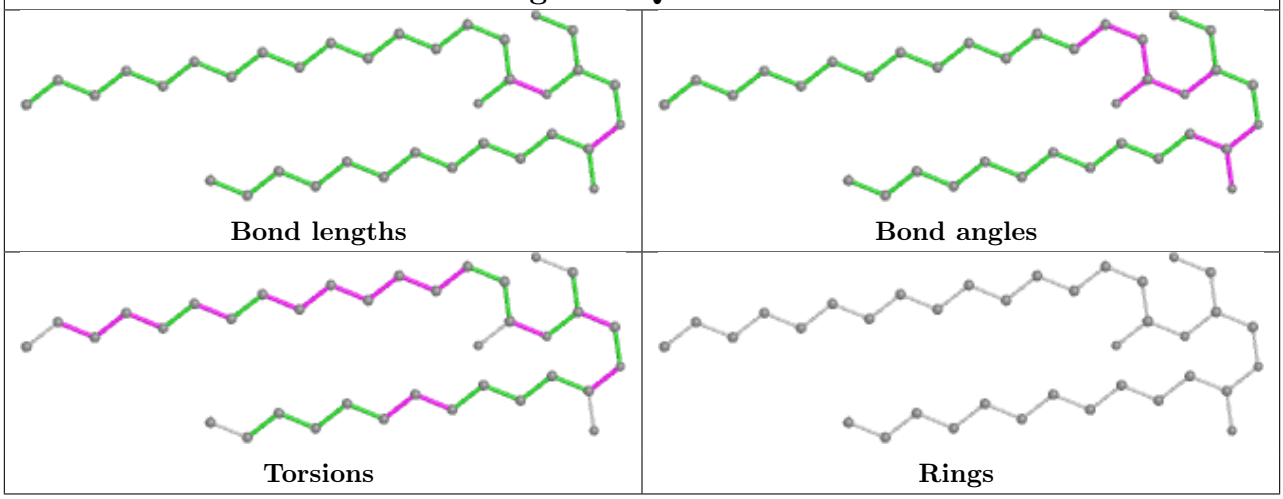
Bond angles



Torsions

Rings

Ligand SQD a 615



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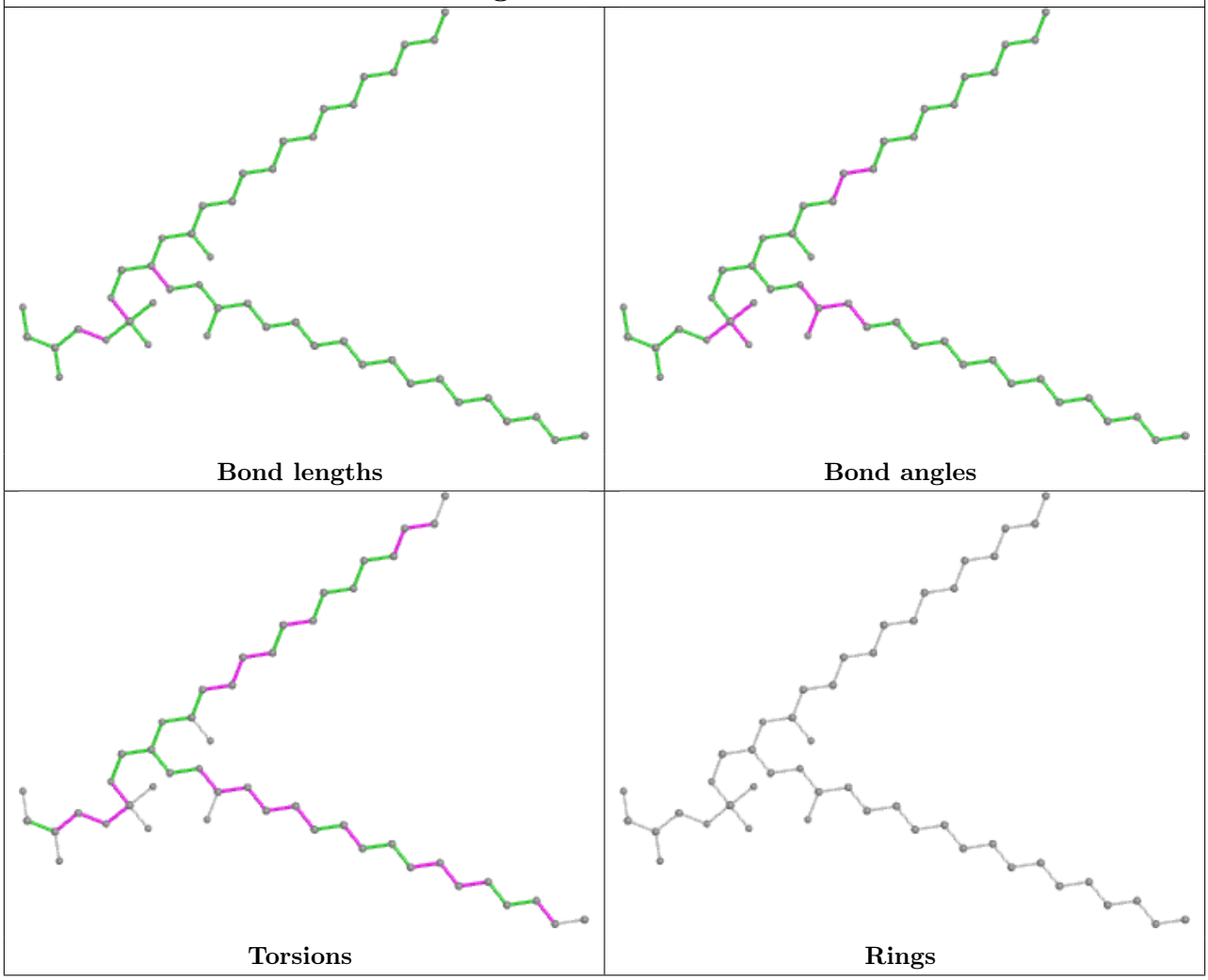
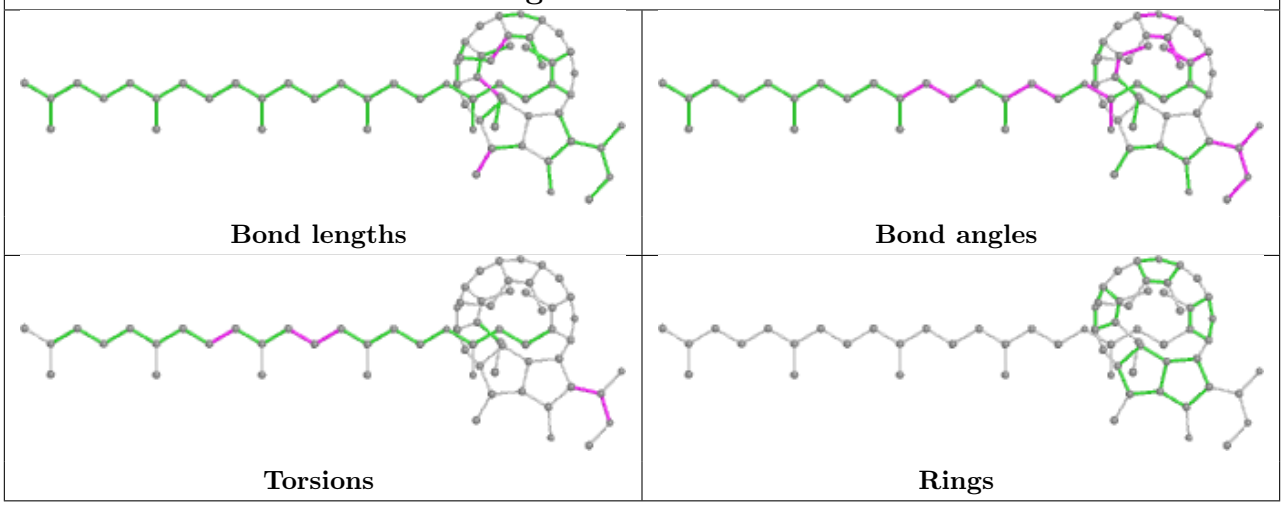
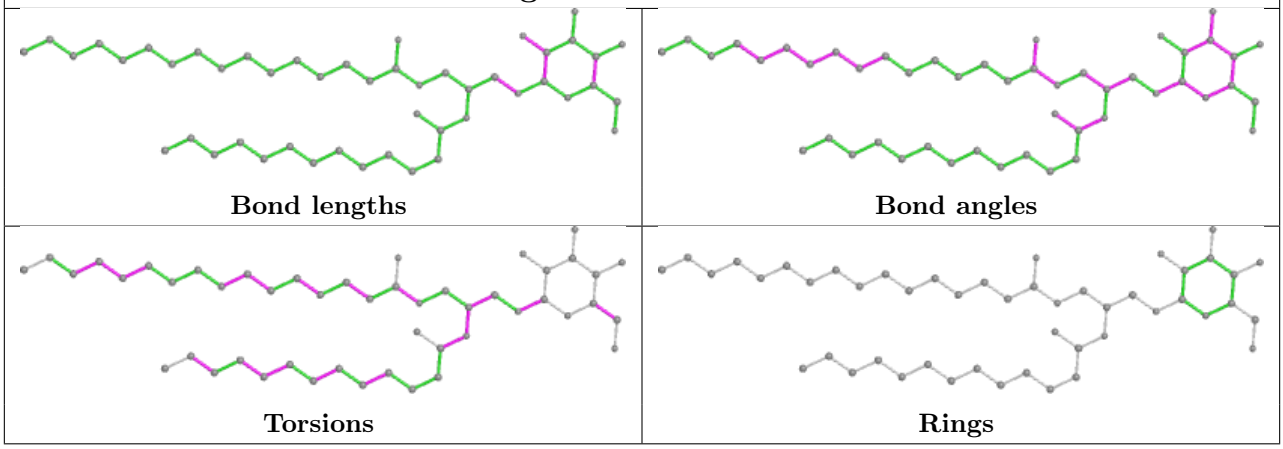


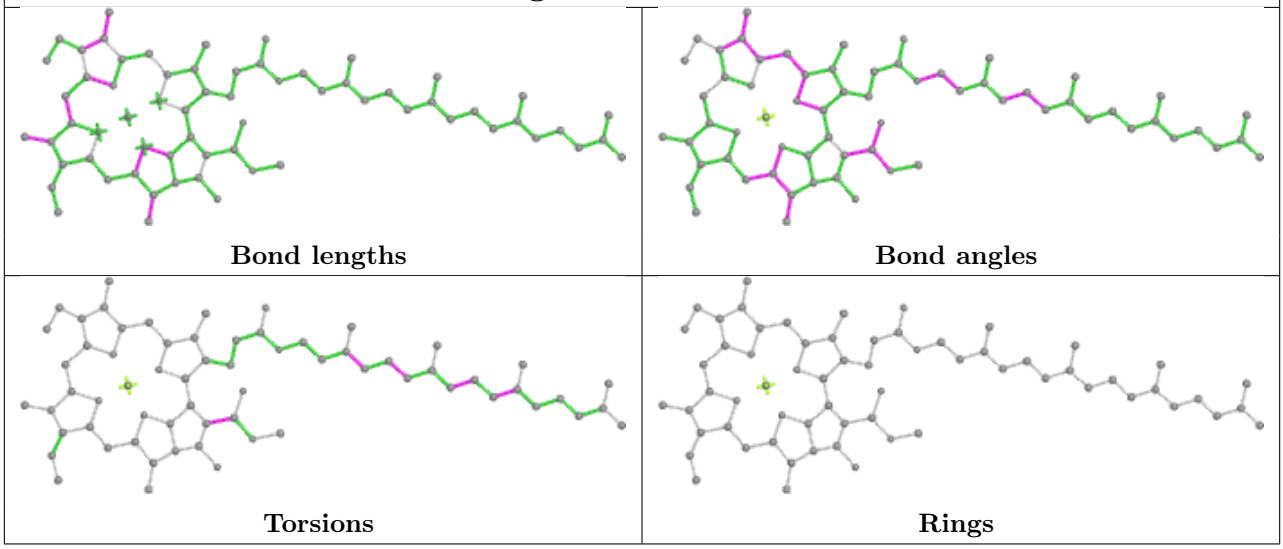
Ligand PHO d 401



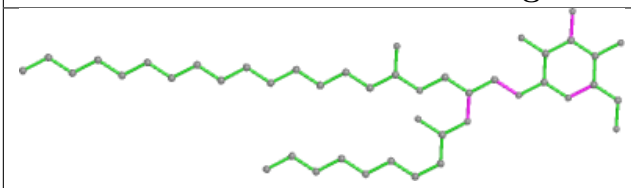
Ligand LMG A 612



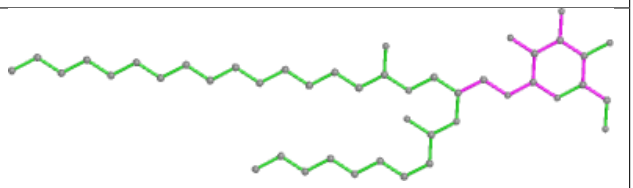
Ligand CLA b 603



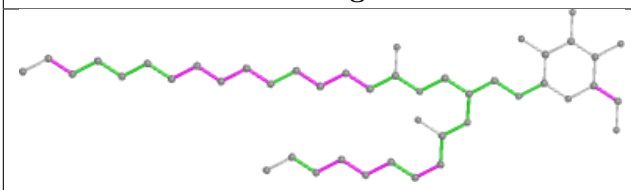
Ligand LMG d 406



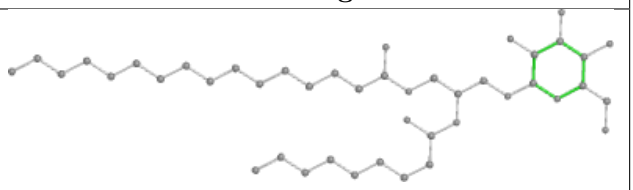
Bond lengths



Bond angles

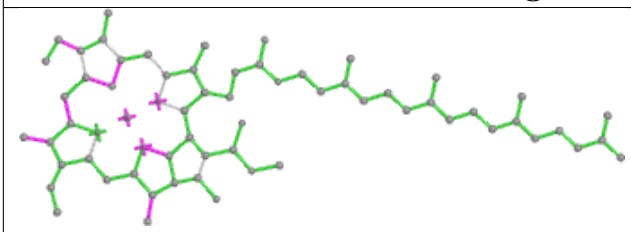


Torsions



Rings

Ligand CLA B 614



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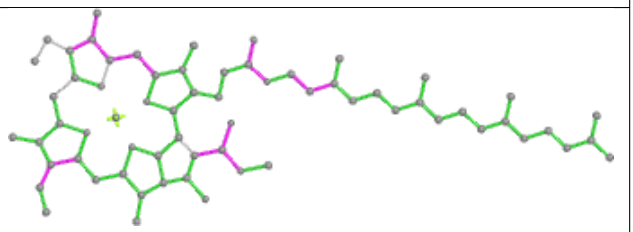
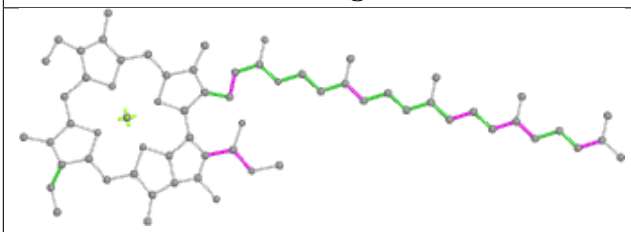
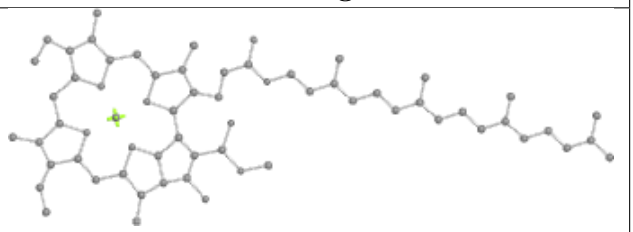


Bond angles

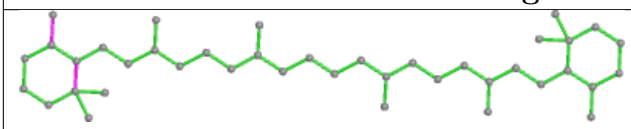


Torsions

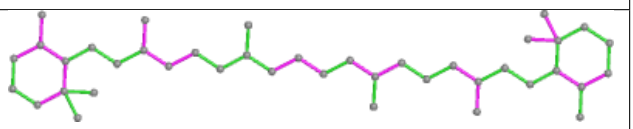


Rings

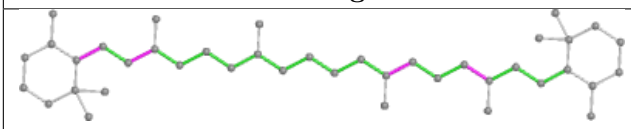
Ligand BCR A 608



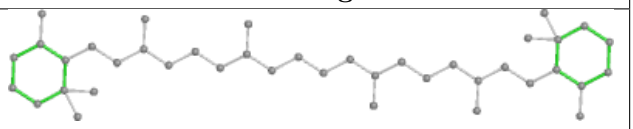
Bond lengths



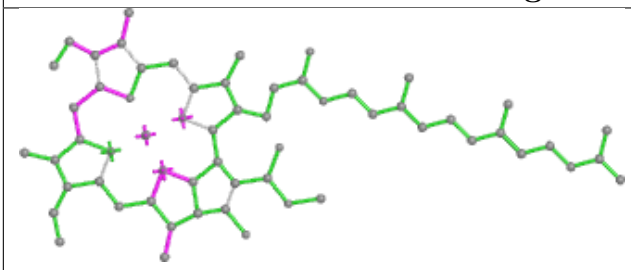
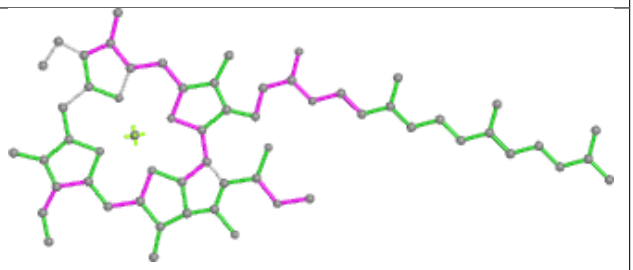
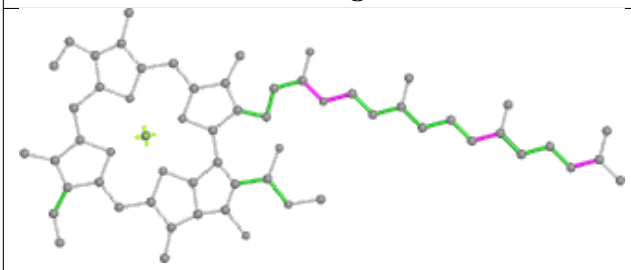
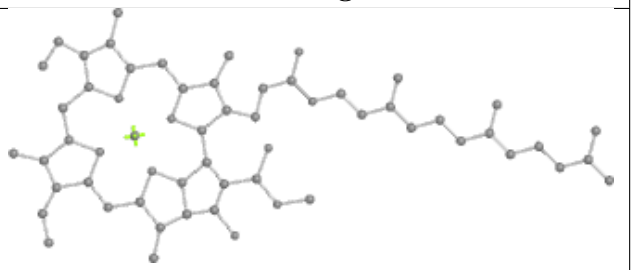
Bond angles

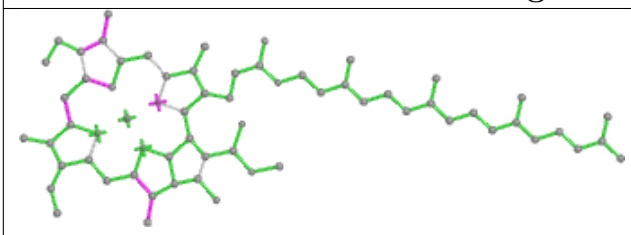
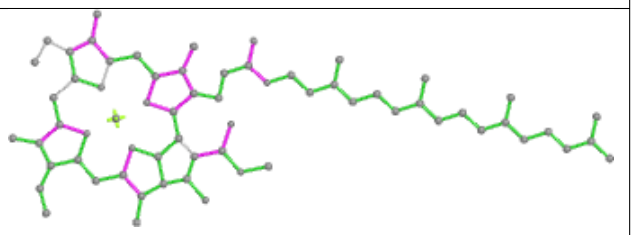
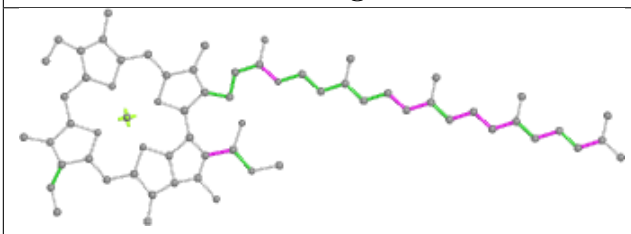
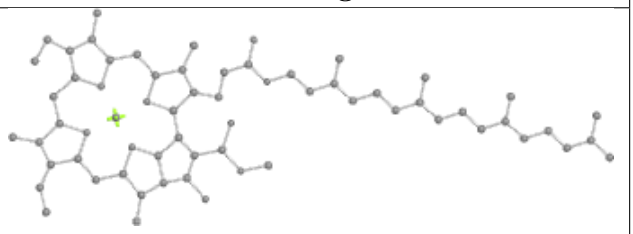


Torsions

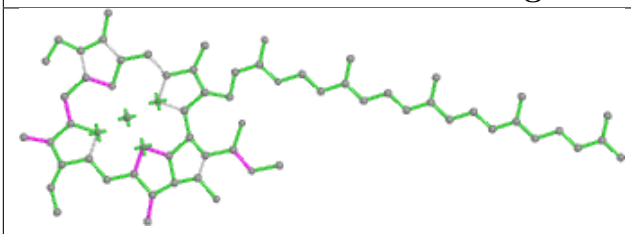


Rings

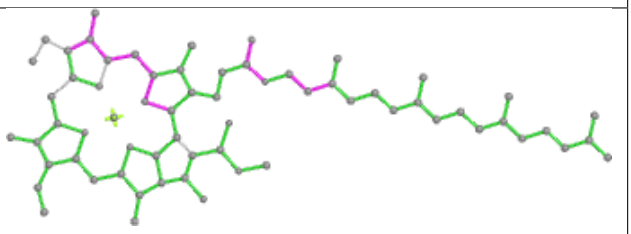
Ligand CLA B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

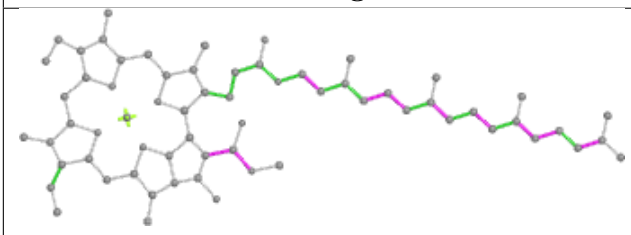
Ligand CLA C 509



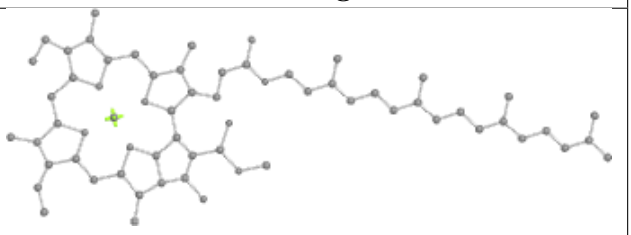
Bond lengths



Bond angles

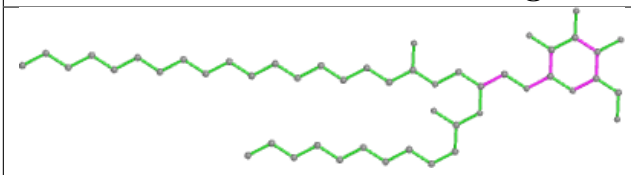


Torsions

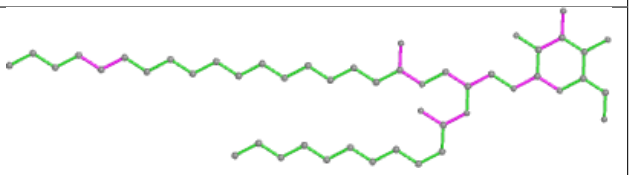


Rings

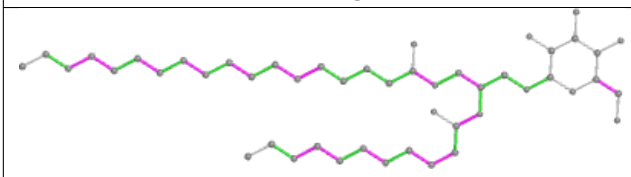
Ligand LMG c 521



Bond lengths



Bond angles



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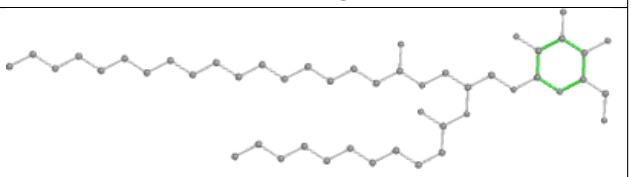
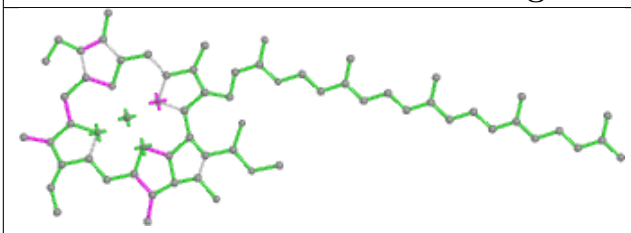
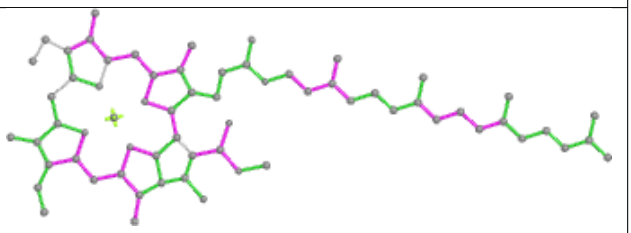


Rings

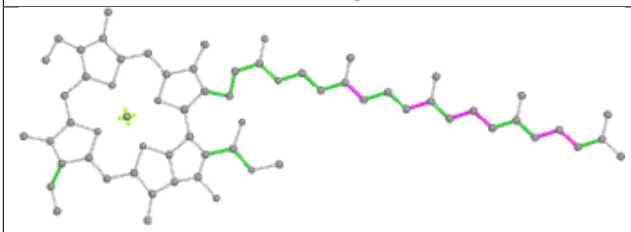
Ligand CLA b 611



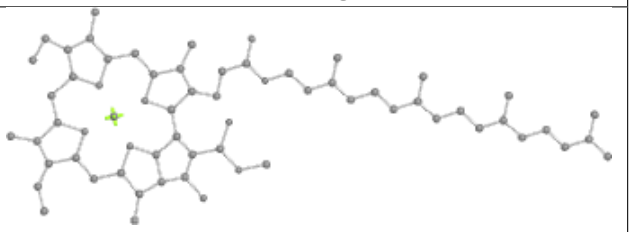
Bond lengths



Bond angles

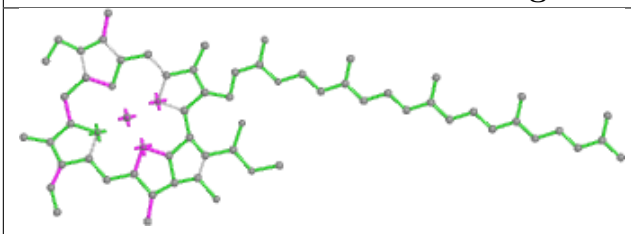


Torsions

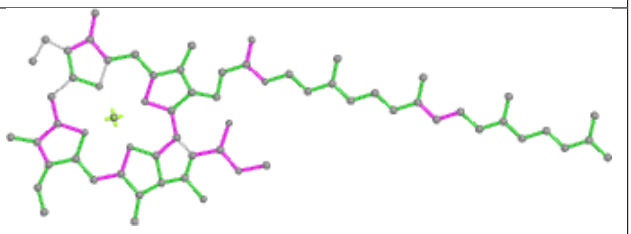


Rings

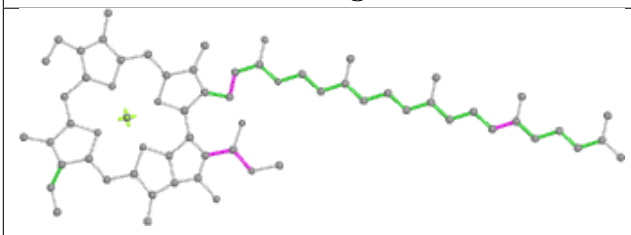
Ligand CLA c 501



Bond lengths



Bond angles



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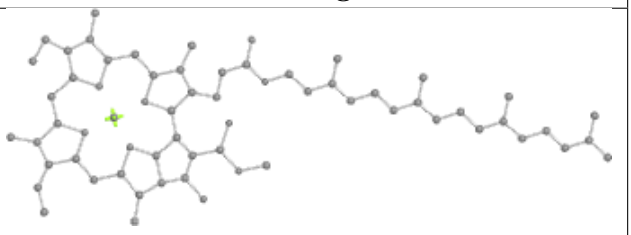
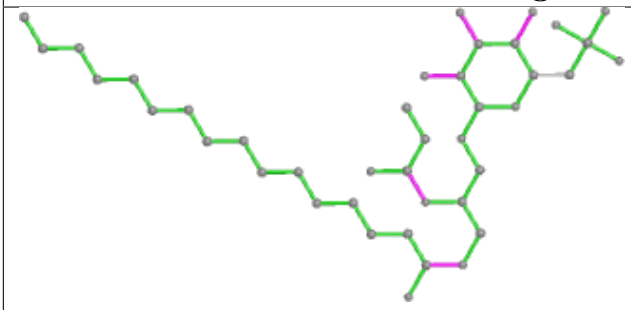


Rings

Ligand SQD f 101



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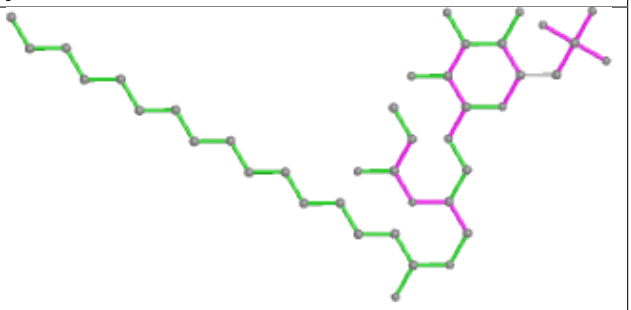

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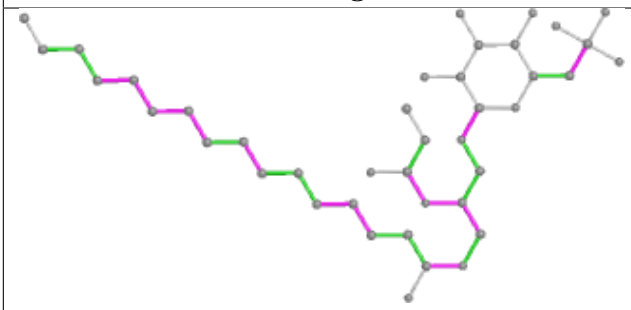

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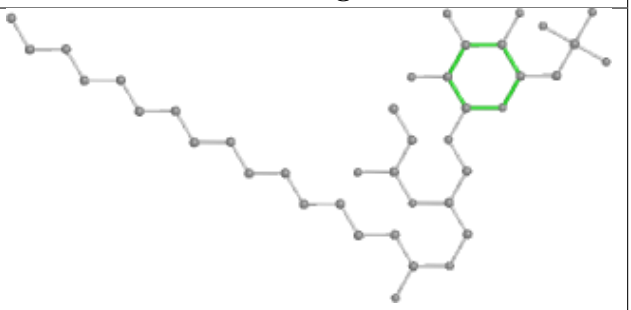
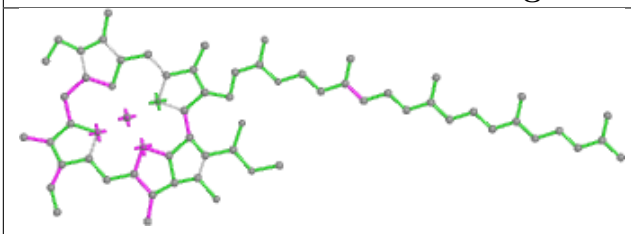


Rings

Ligand CLA A 603



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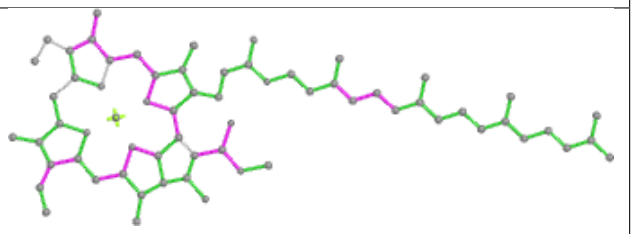

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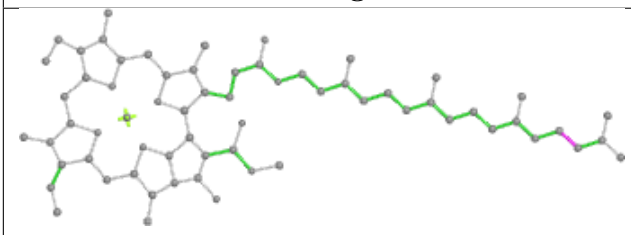

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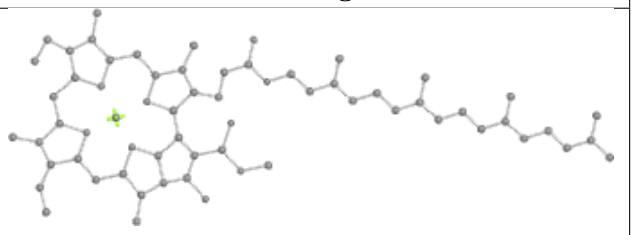
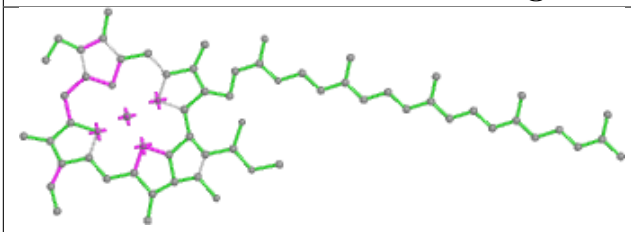


Rings

Ligand CLA b 606



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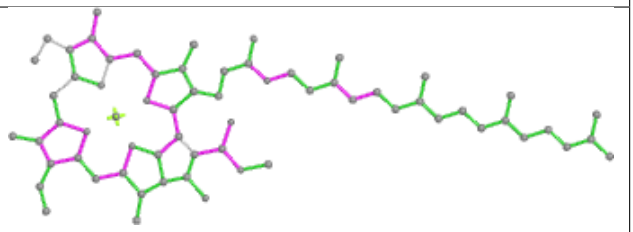
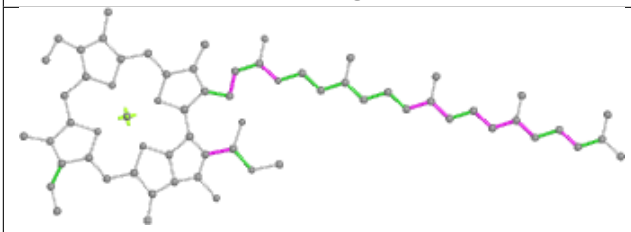


Bond angles



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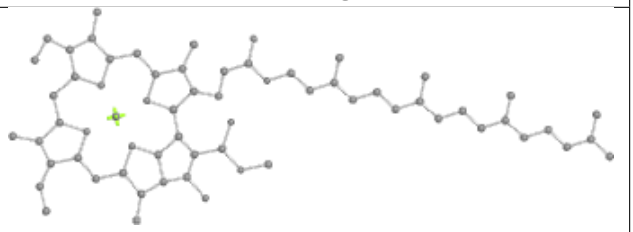
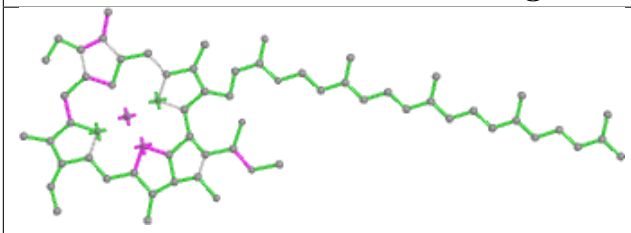


Rings

Ligand CLA C 502



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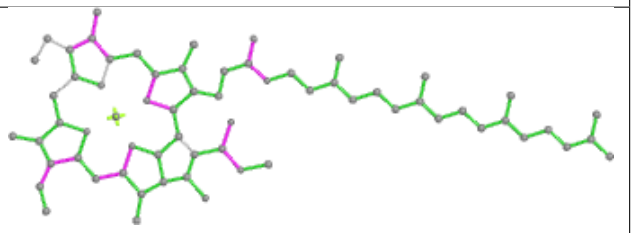

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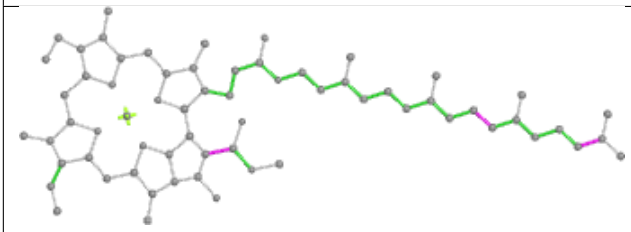

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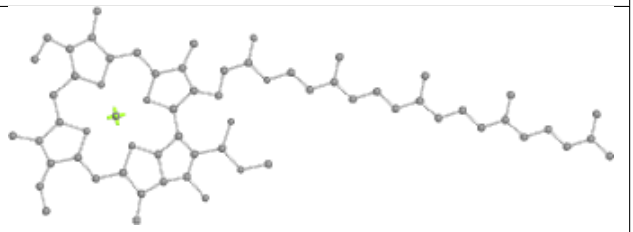

Rings

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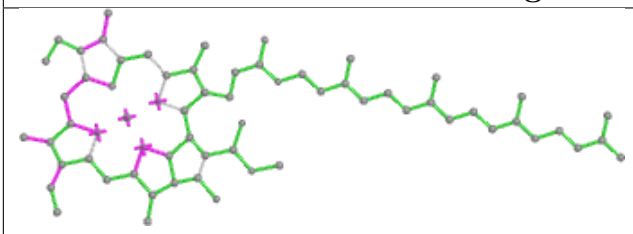

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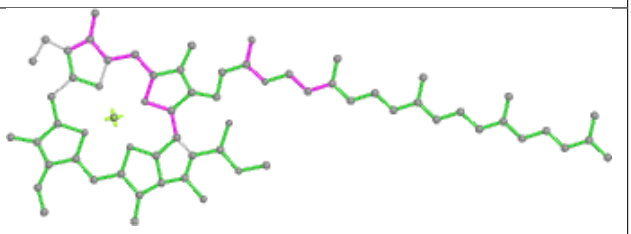

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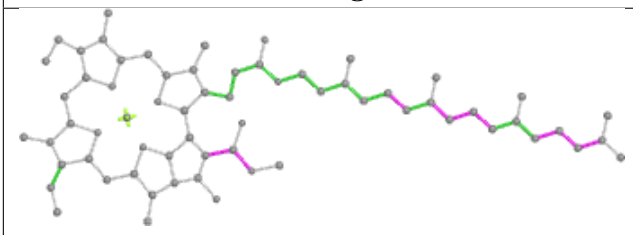

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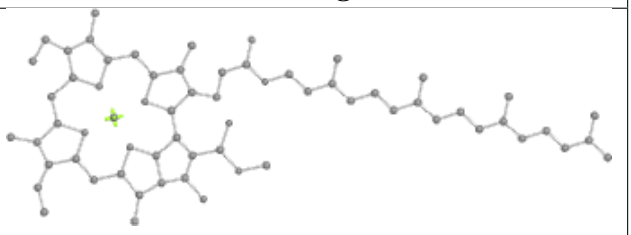
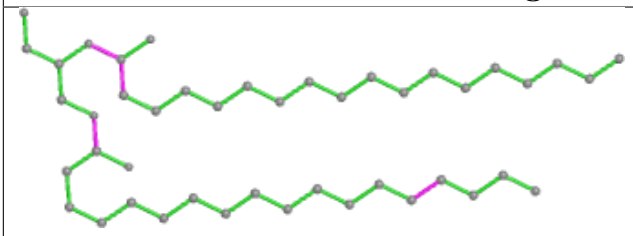


Rings

Ligand DGD a 616



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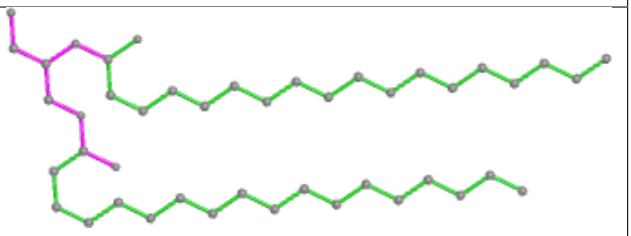
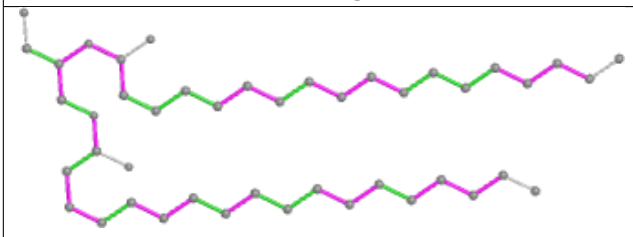


Bond angles



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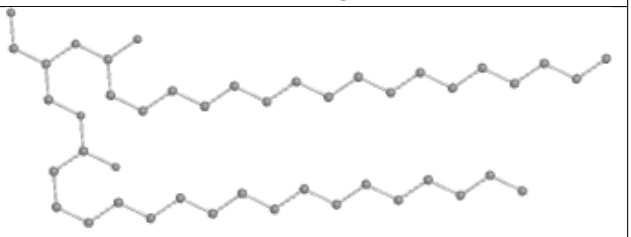
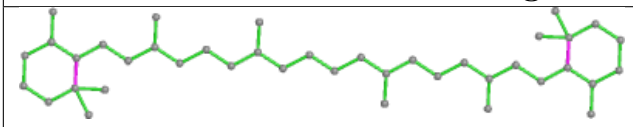


Rings

Ligand BCR B 619



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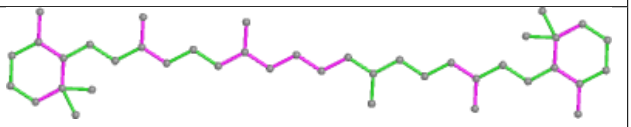
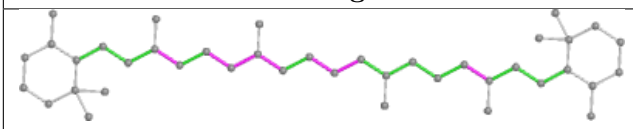


Bond angles



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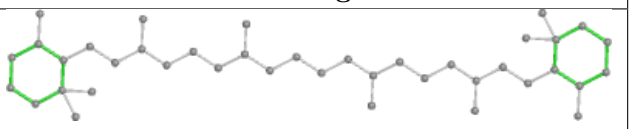
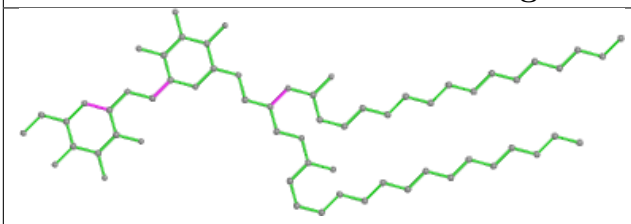


Rings

Ligand DGD C 518



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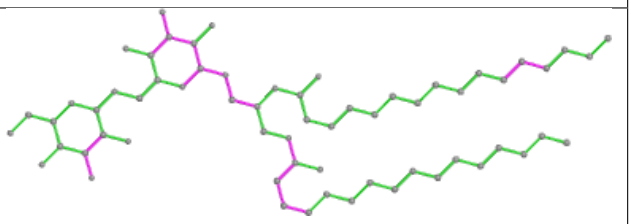
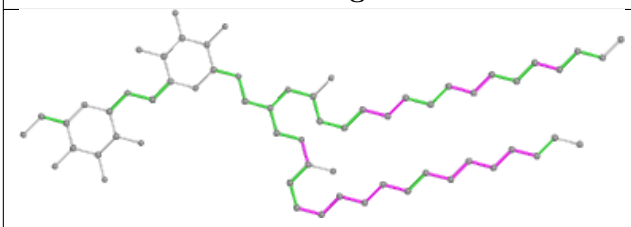


Bond angles



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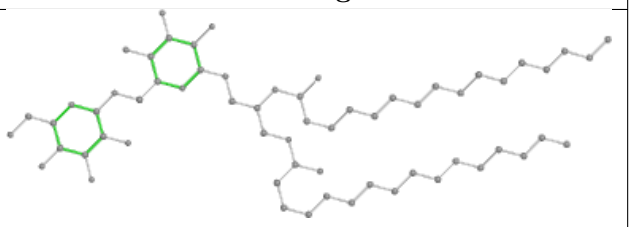
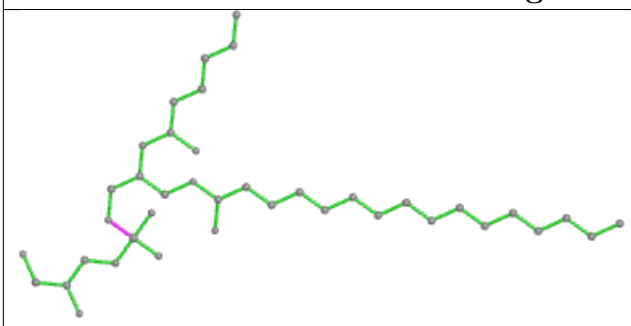


Rings

Ligand LHG d 409



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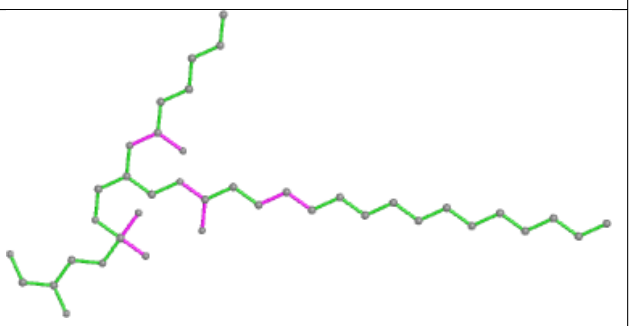

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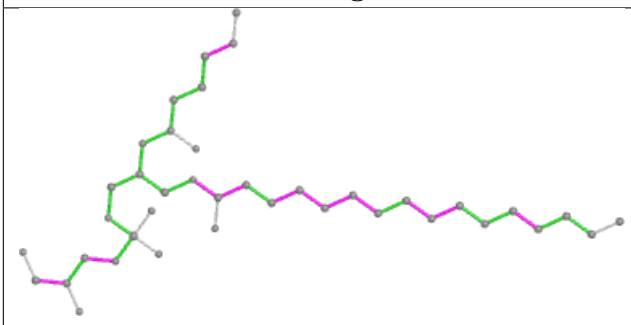

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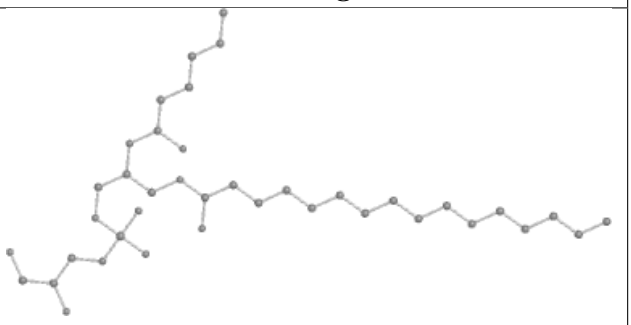

Rings

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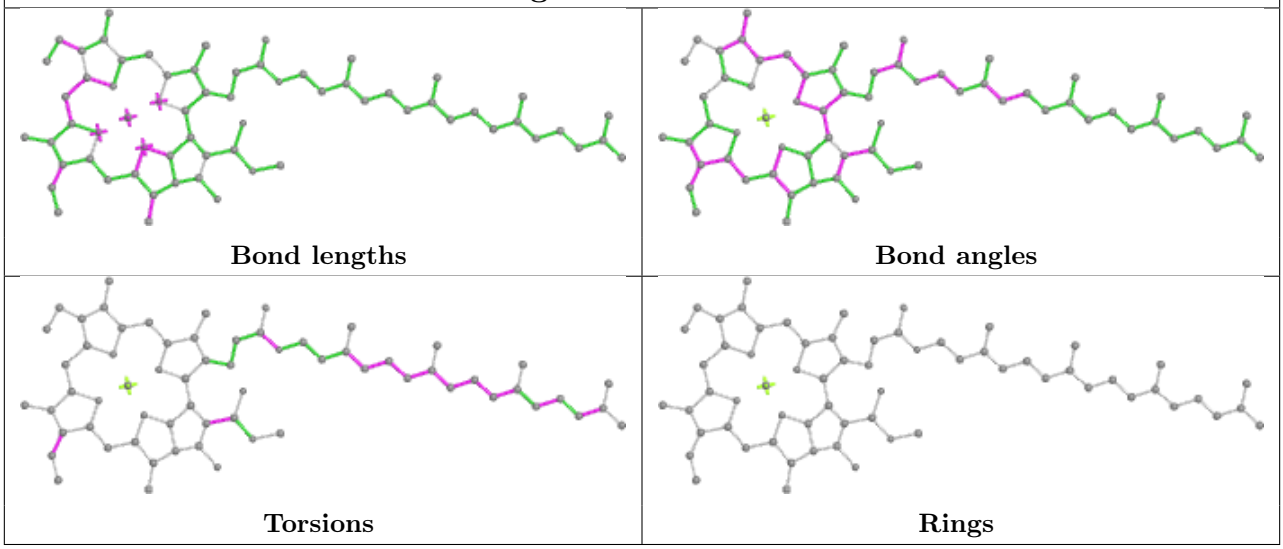

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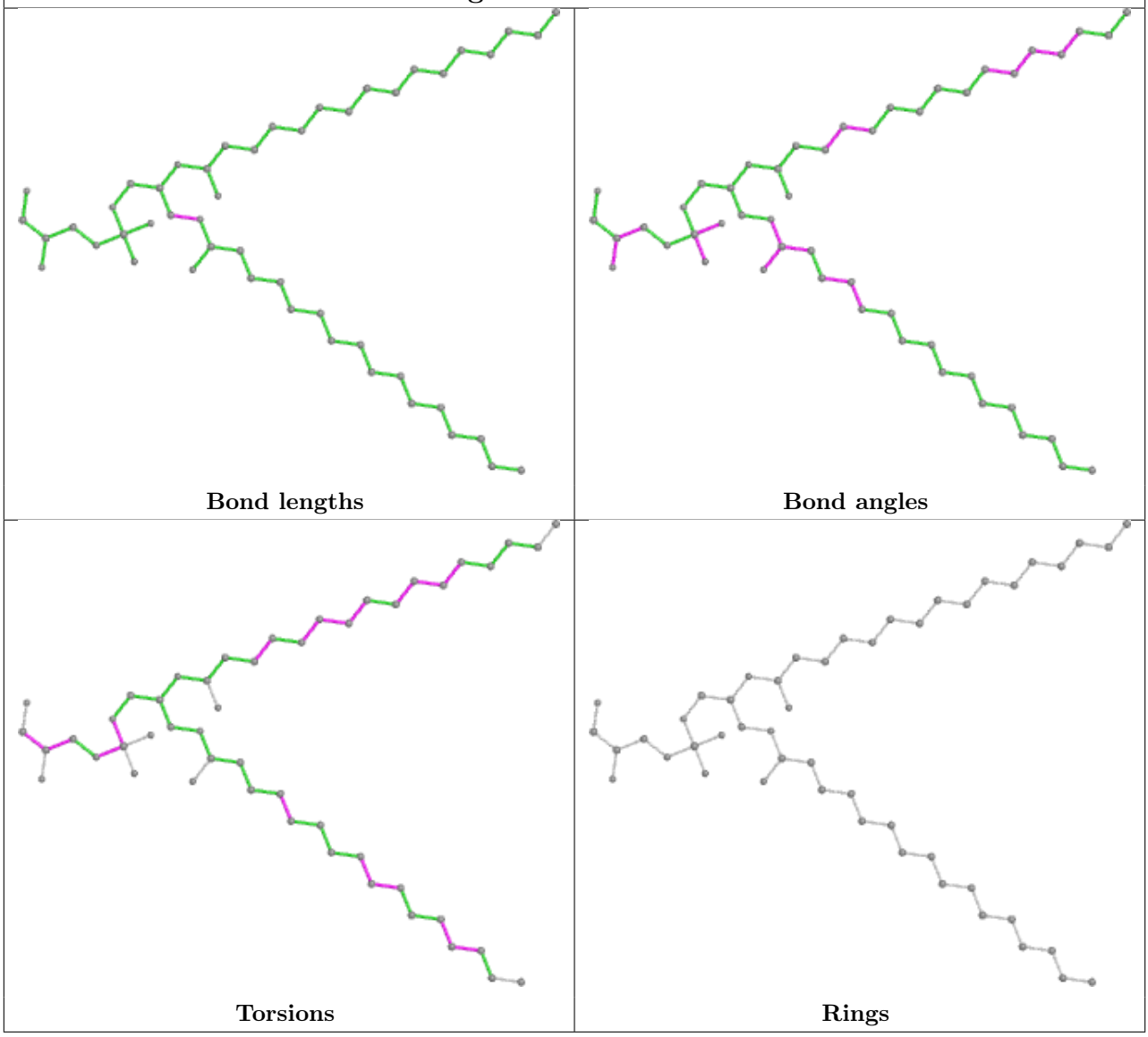

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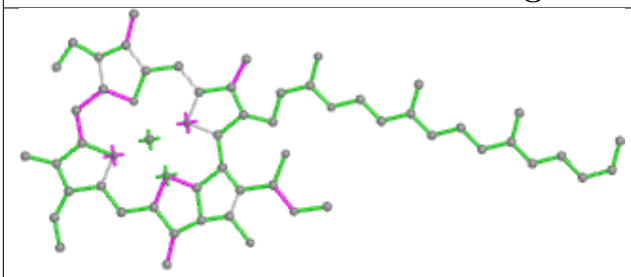
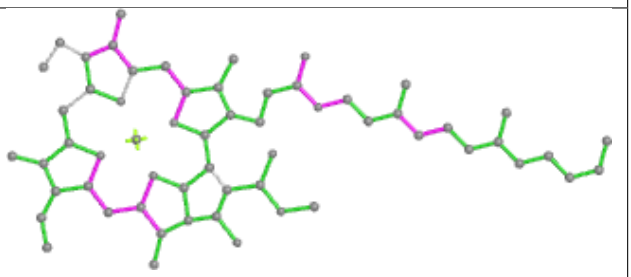
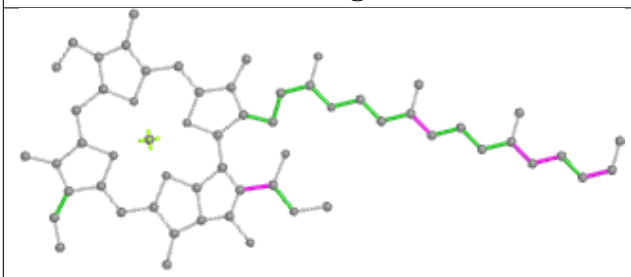


Bond lengths



Bond angles



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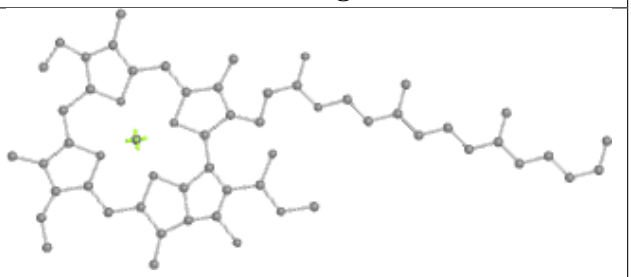
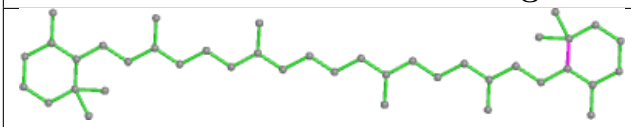


Rings

Ligand BCR H 101



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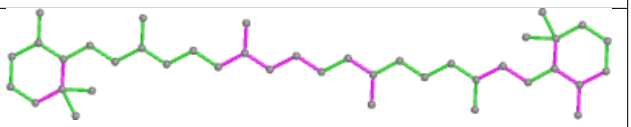
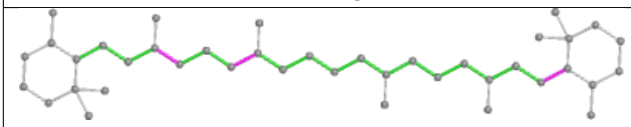
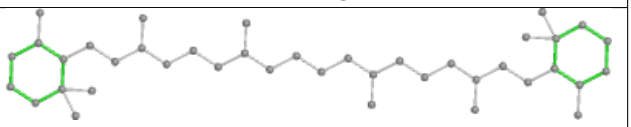


Bond angles

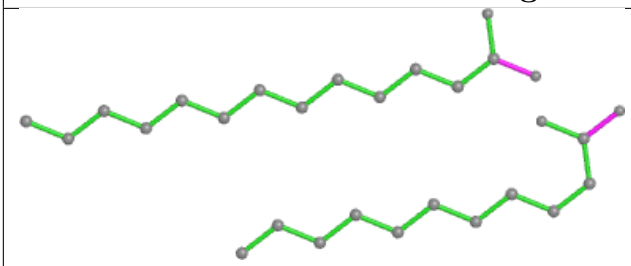


Torsions



Rings

Ligand LMG B 622



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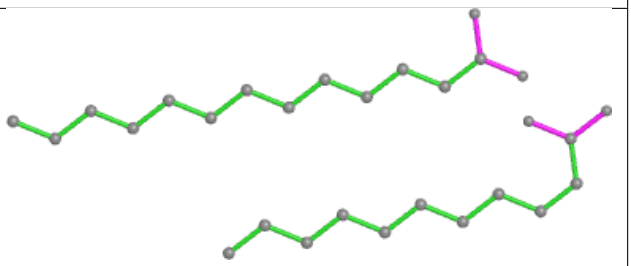
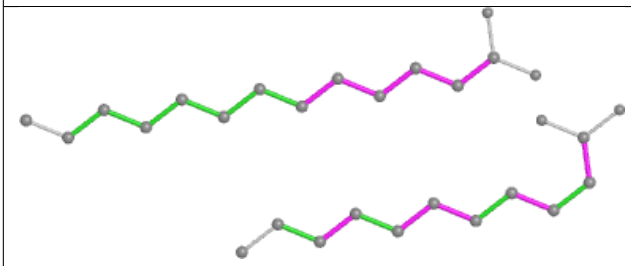
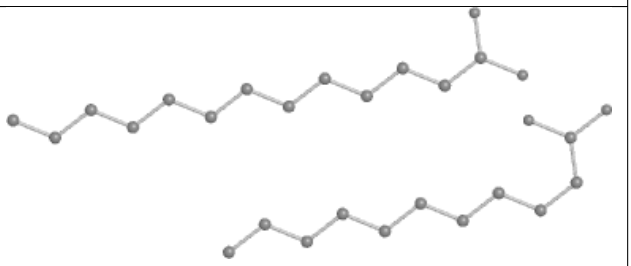


Bond angles

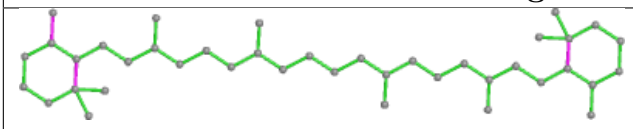


Torsions

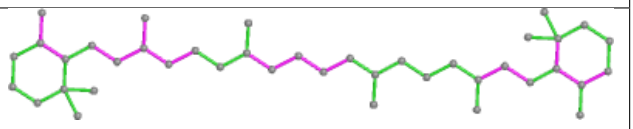


Rings

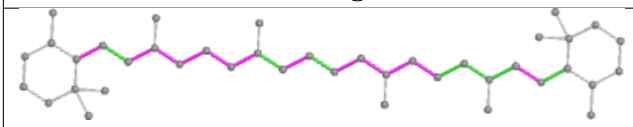
Ligand BCR c 514



Bond lengths



Bond angles



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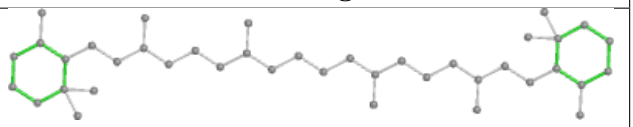
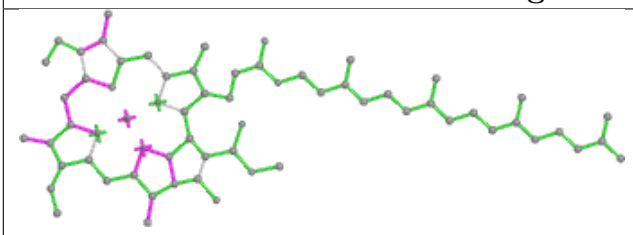


Rings

Ligand CLA b 610



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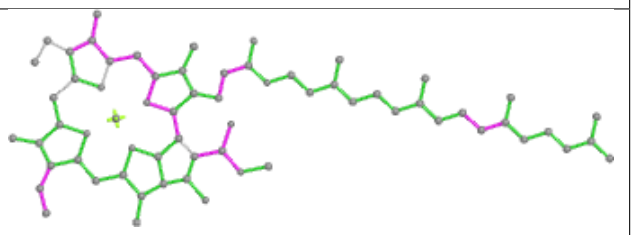
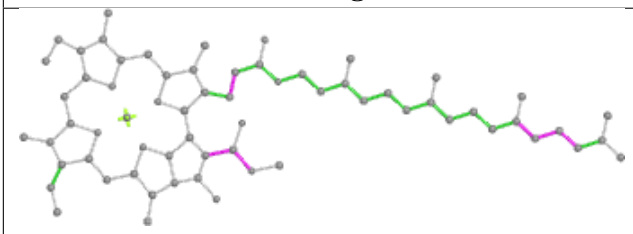


Bond angles



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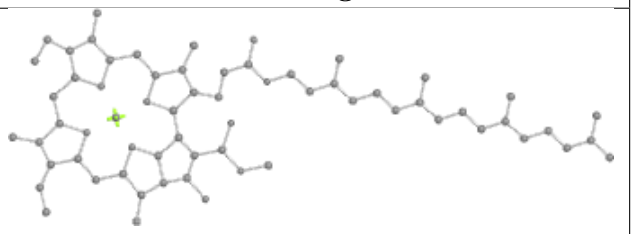
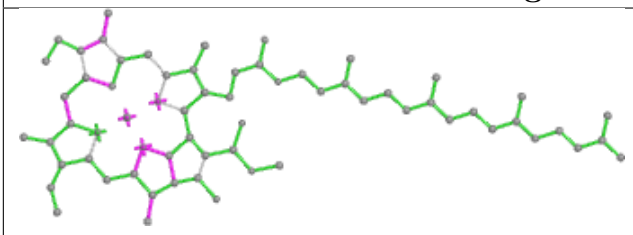


Rings

Ligand CLA C 501



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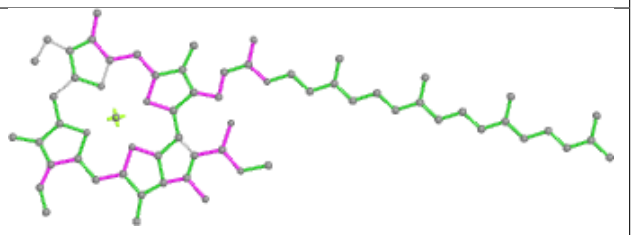
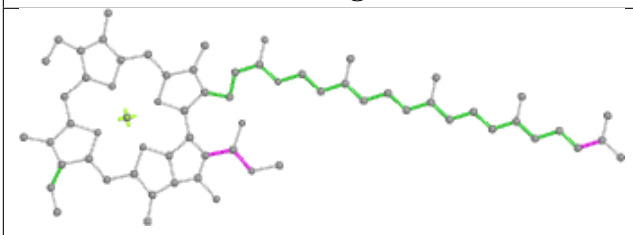


Bond angles



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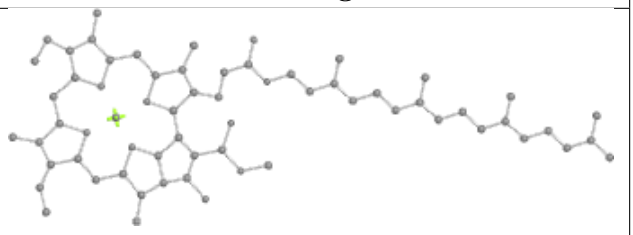
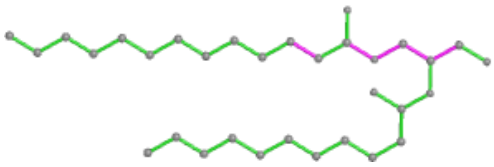
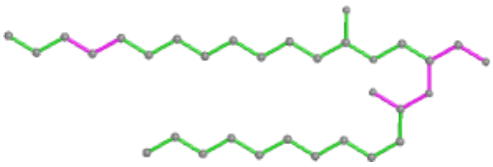


Rings

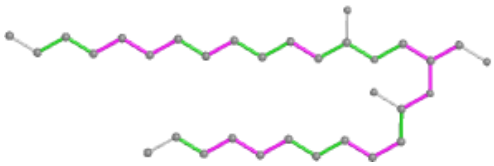
Ligand LMG D 409



Bond lengths



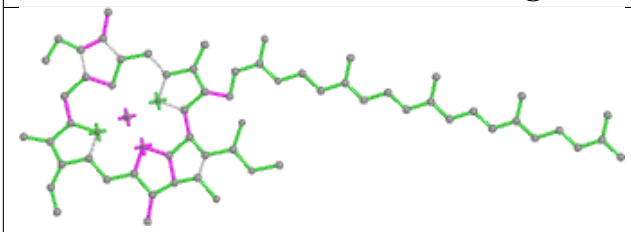
Bond angles



Torsions

Rings

Ligand CLA C 512



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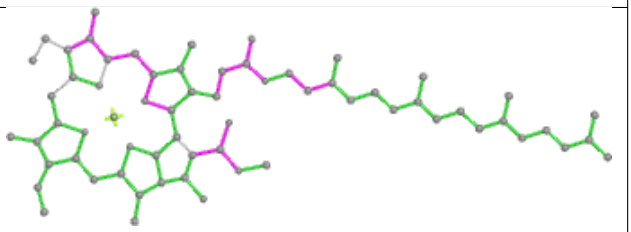
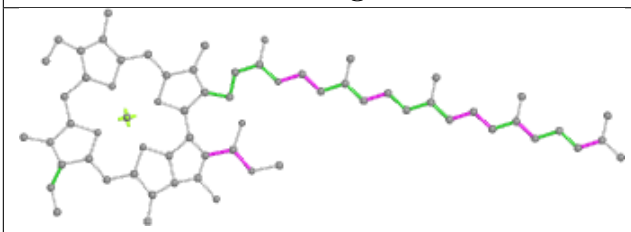
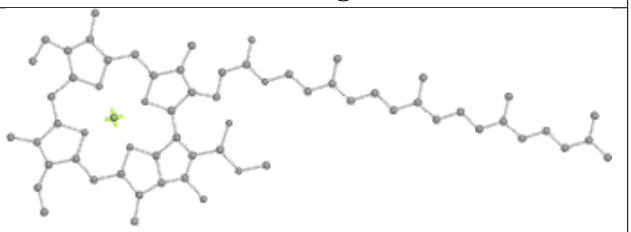


Bond angles

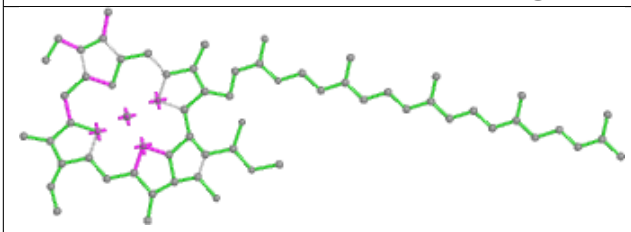


Torsions

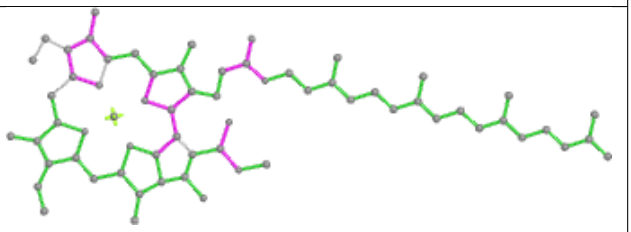


Rings

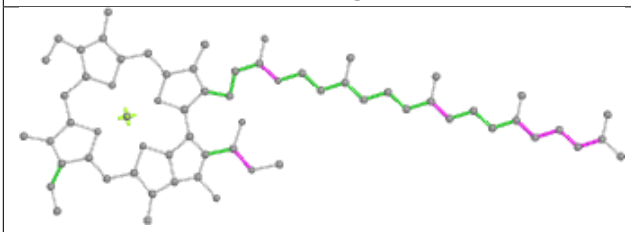
Ligand CLA c 511



Bond lengths



Bond angles



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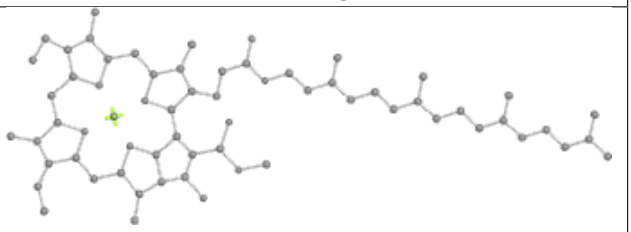
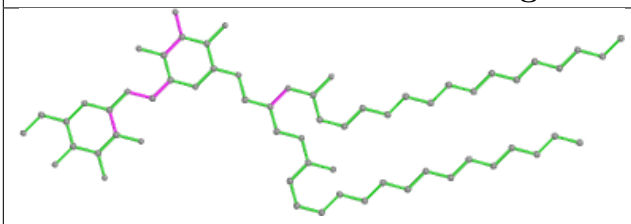


Rings

Ligand DGD C 517



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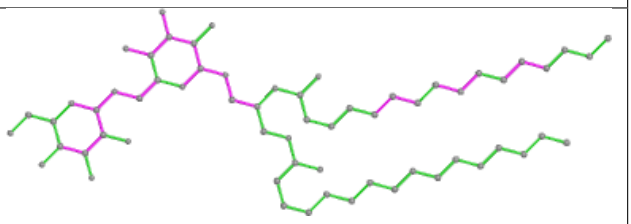
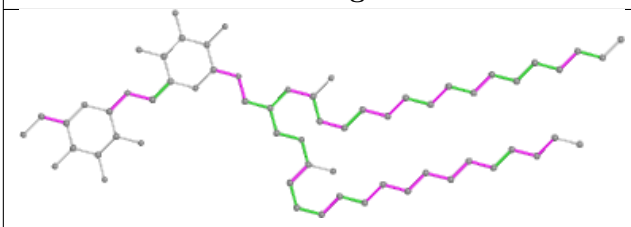


Bond angles



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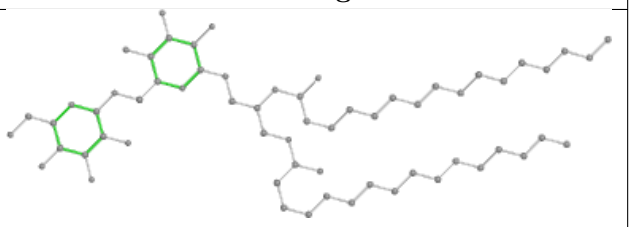
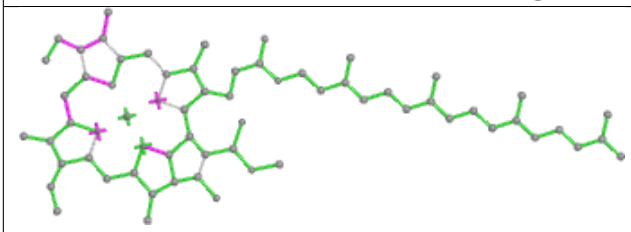


Rings

Ligand CLA c 505



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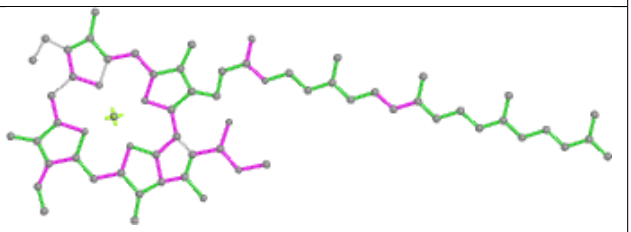
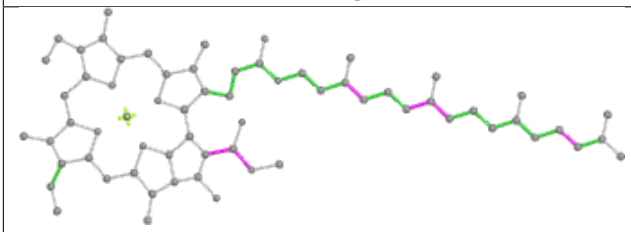
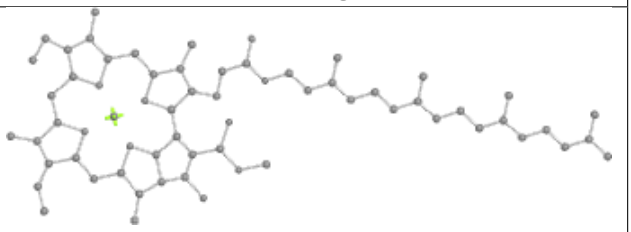


Bond angles

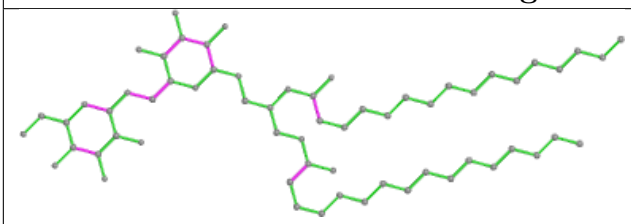


Torsions



Rings

Ligand DGD C 516



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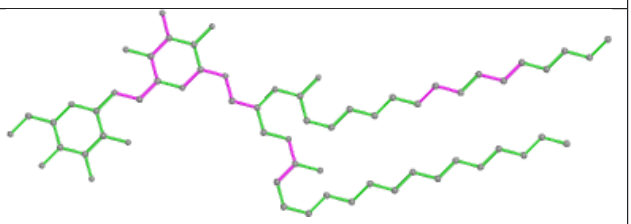
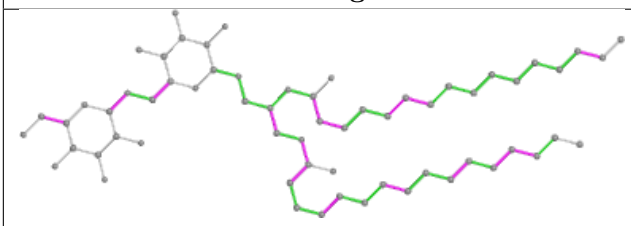


Bond angles



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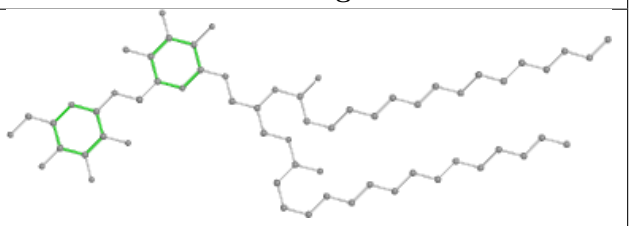
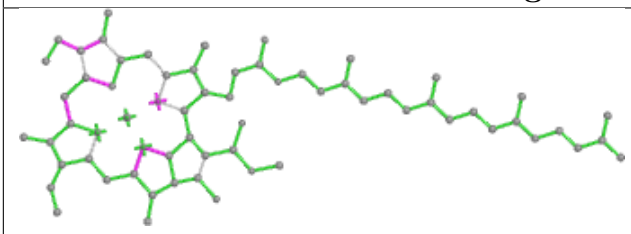


Rings

Ligand CLA C 507



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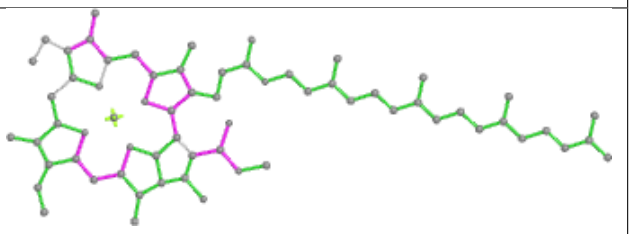

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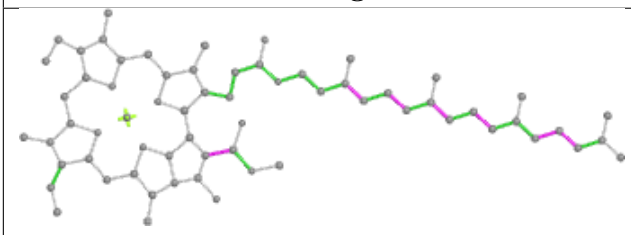

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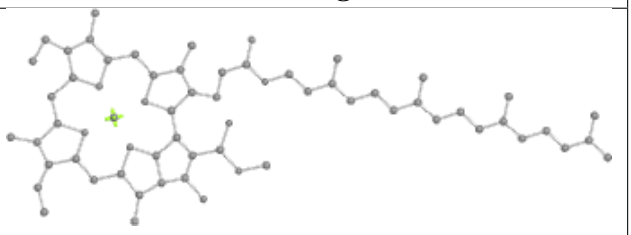

Rings

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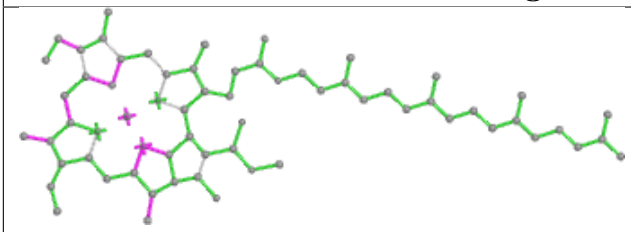

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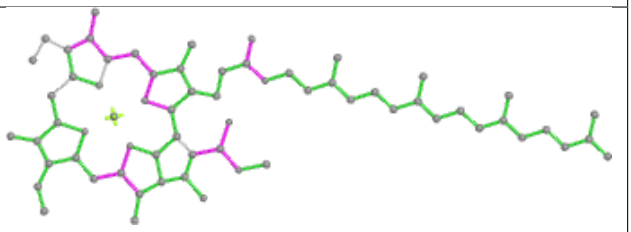
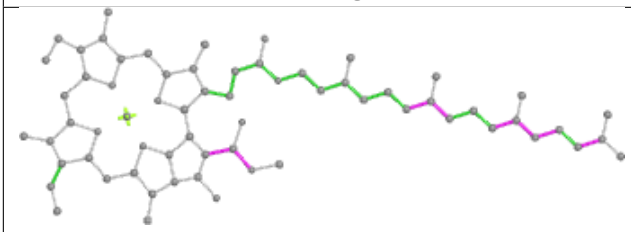


Bond angles



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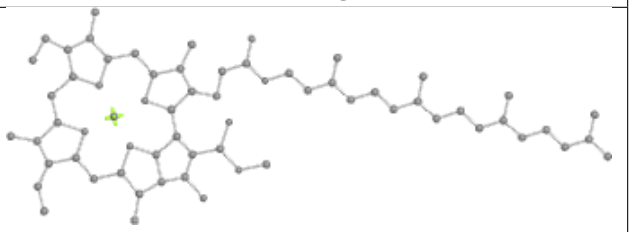
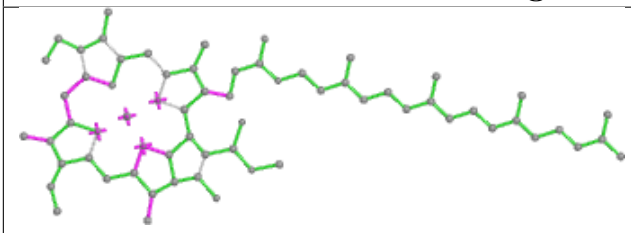


Rings

Ligand CLA b 613



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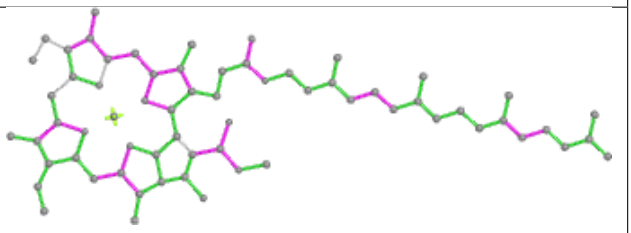
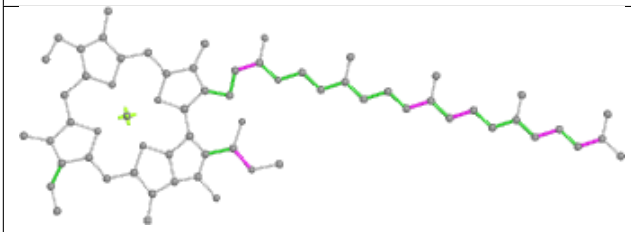


Bond angles



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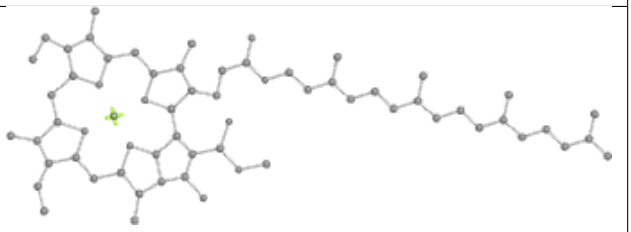
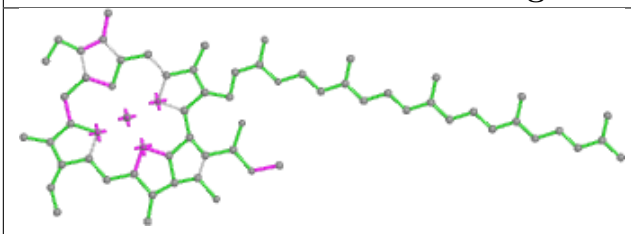
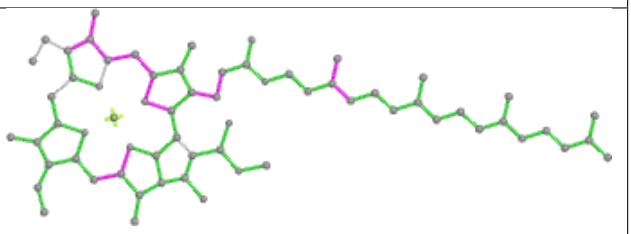


Rings

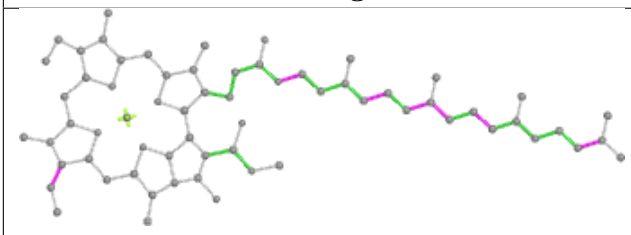
Ligand CLA d 402



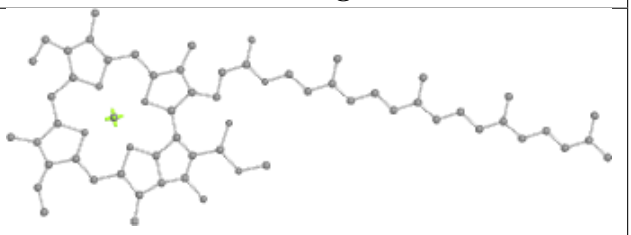
Bond lengths



Bond angles

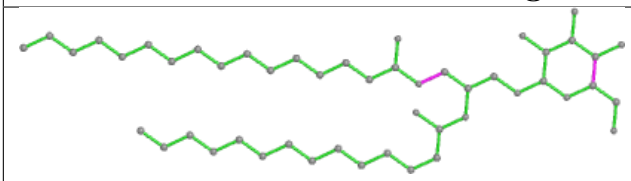


Torsions

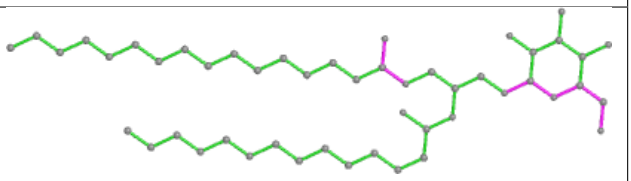


Rings

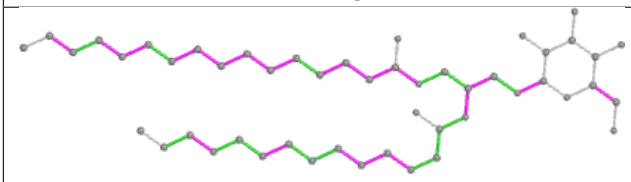
Ligand LMG c 522



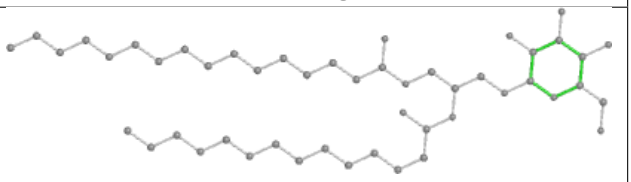
Bond lengths



Bond angles

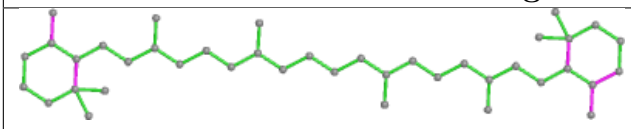


Torsions



Rings

Ligand BCR T 101



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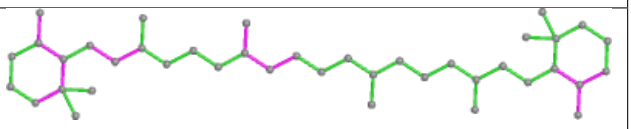

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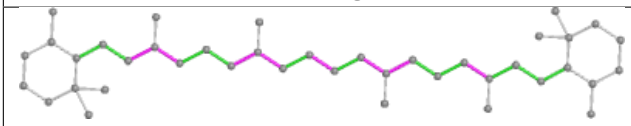
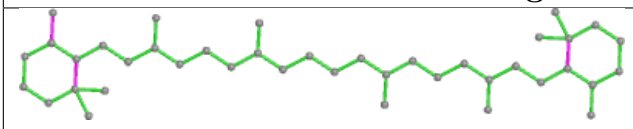


Torsions

Rings

Ligand BCR k 101



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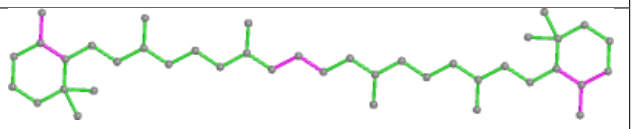

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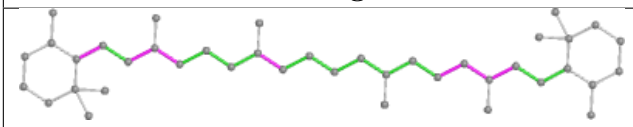

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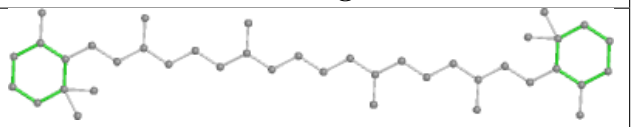
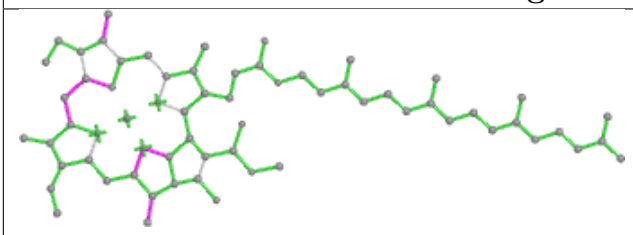


Rings

Ligand CLA b 602



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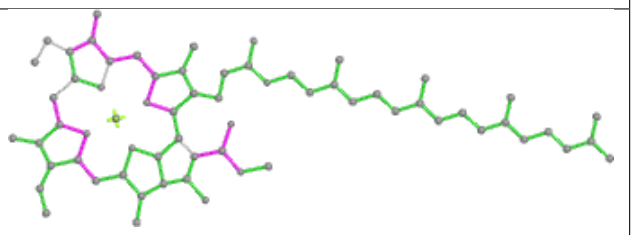

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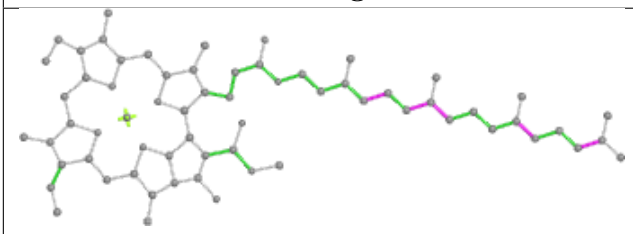

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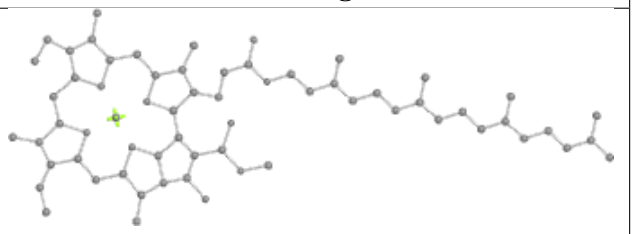
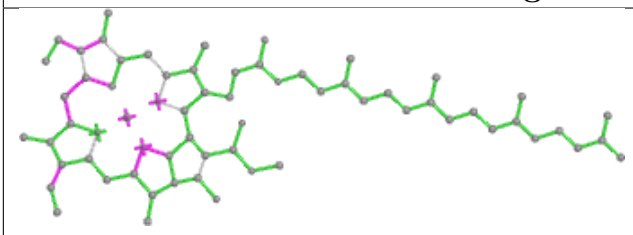


Rings

Ligand CLA A 604



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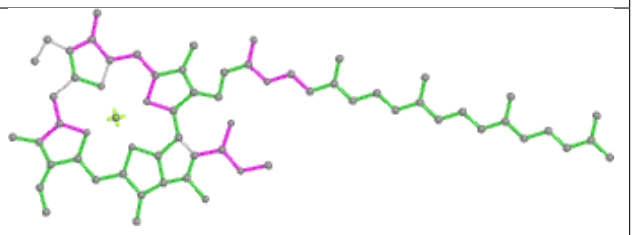

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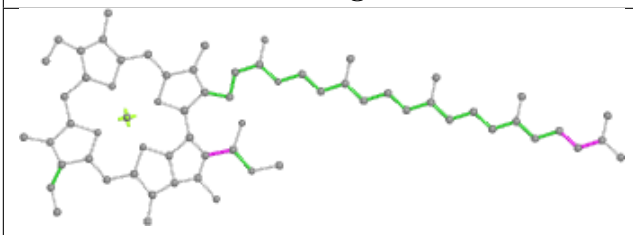

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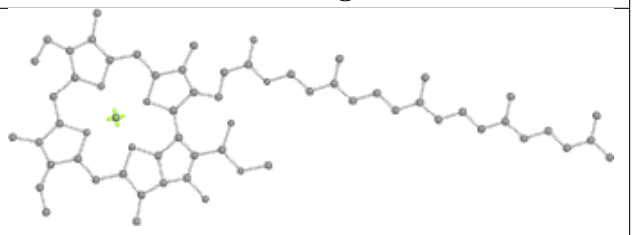
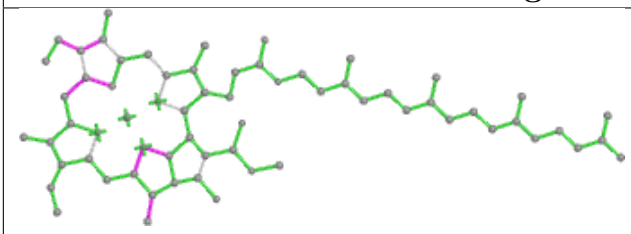


Rings

Ligand CLA B 608



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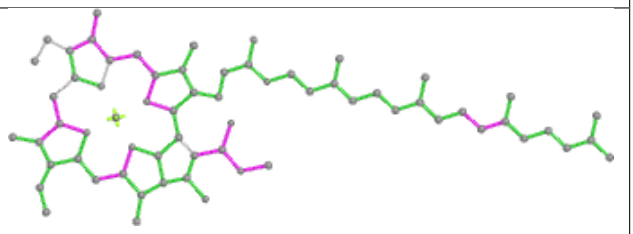

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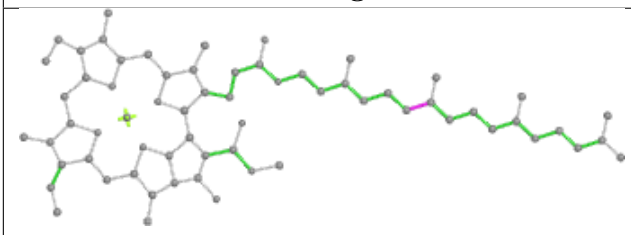

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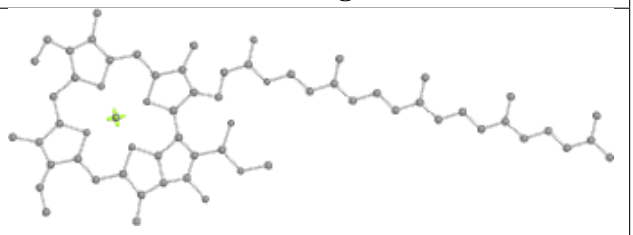
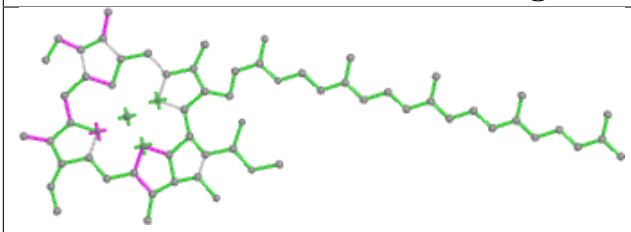


Rings

Ligand CLA c 503



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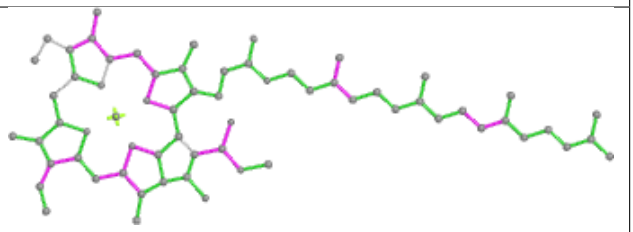

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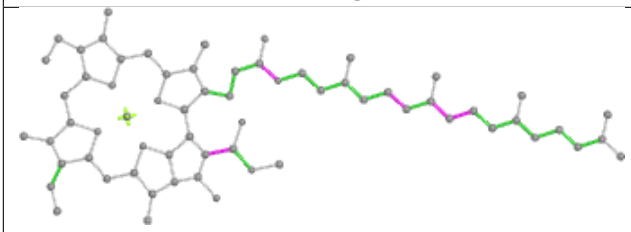

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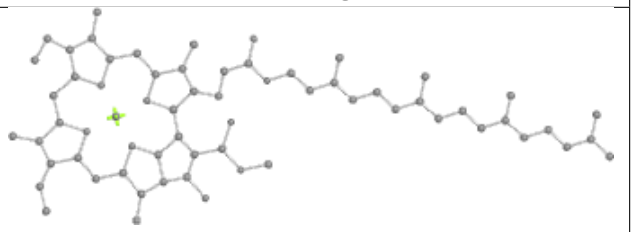

Rings

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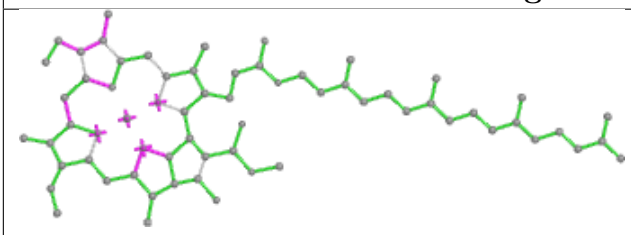

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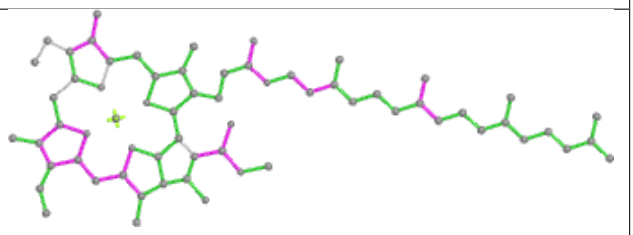

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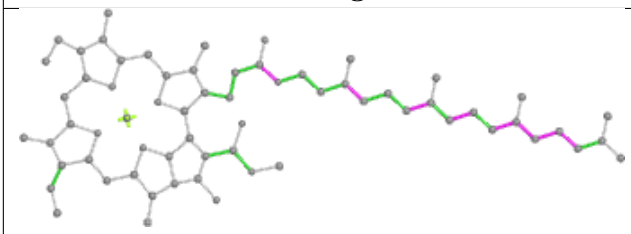

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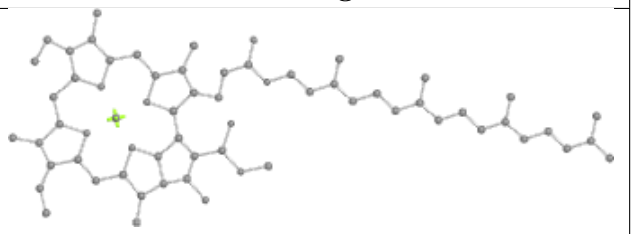
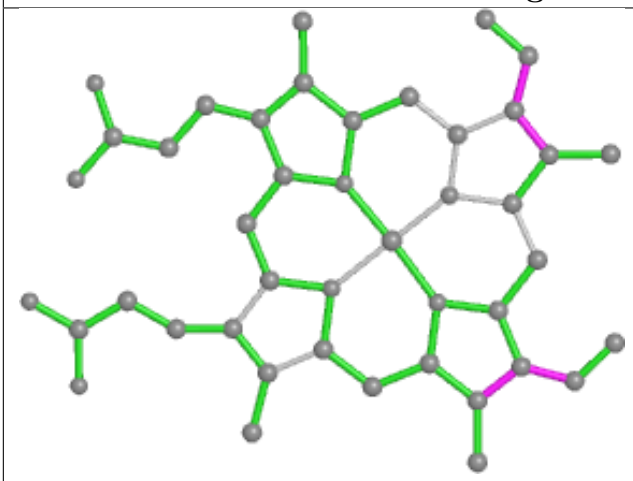


Rings

Ligand HEM f 102



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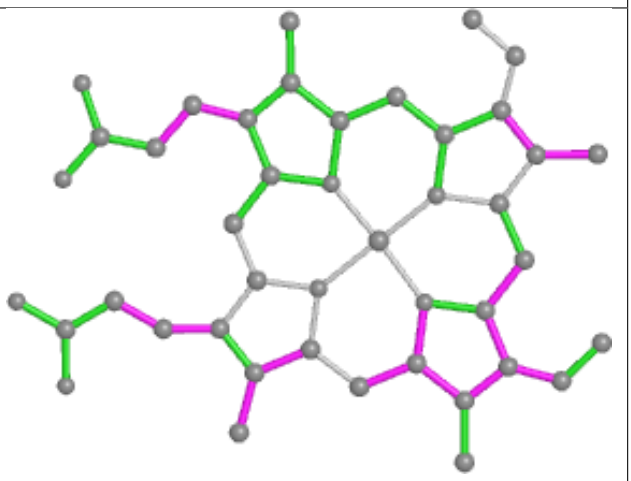
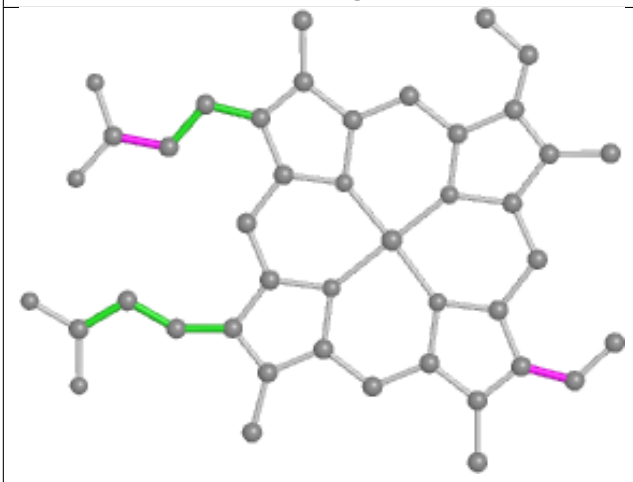


Bond angles



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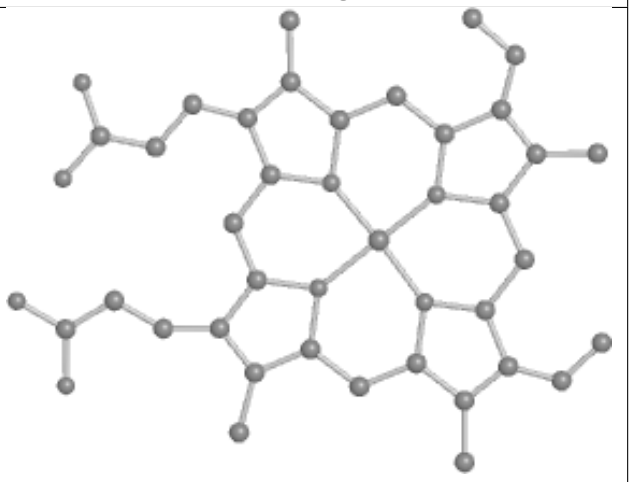
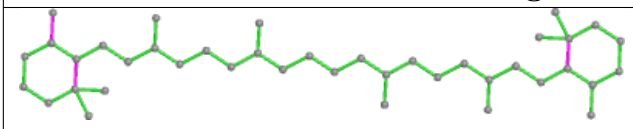


Rings

Ligand BCR b 619



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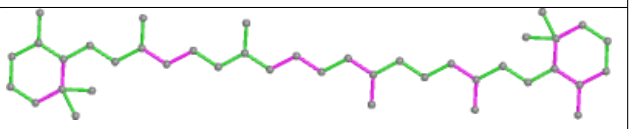

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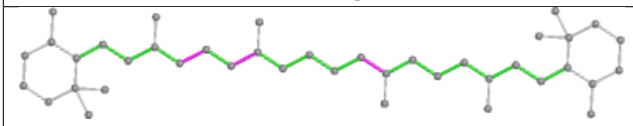
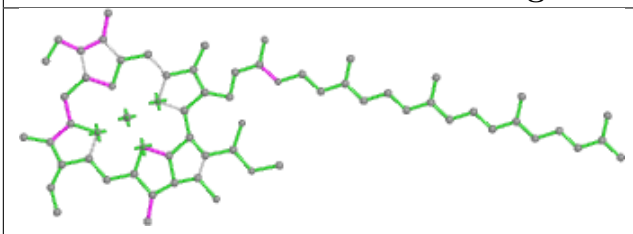


Torsions

Rings

Ligand CLA b 608



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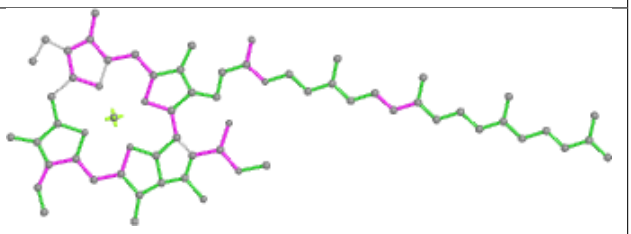

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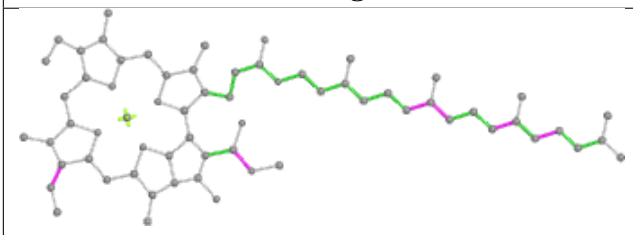

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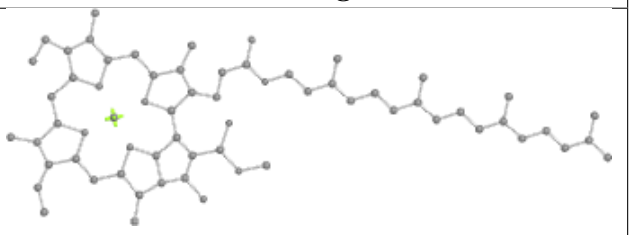
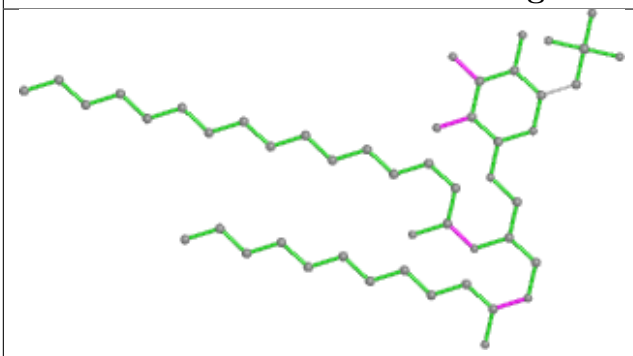


Rings

Ligand SQD b 601



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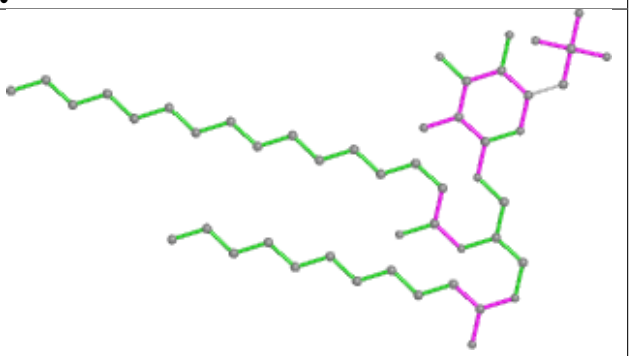
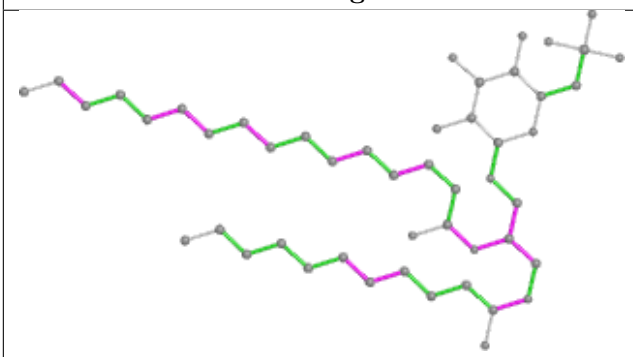


Bond angles



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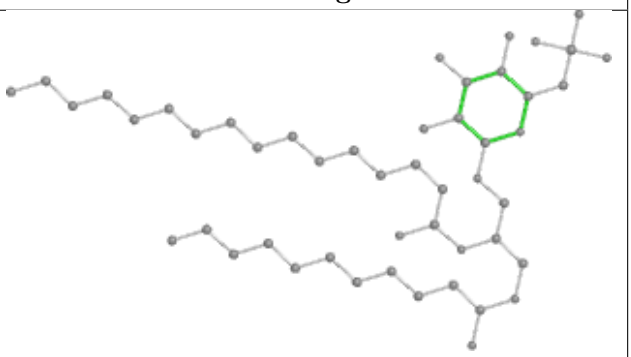

Rings

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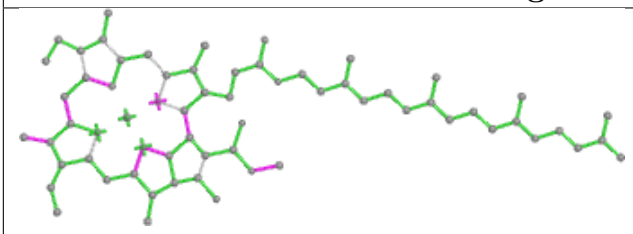

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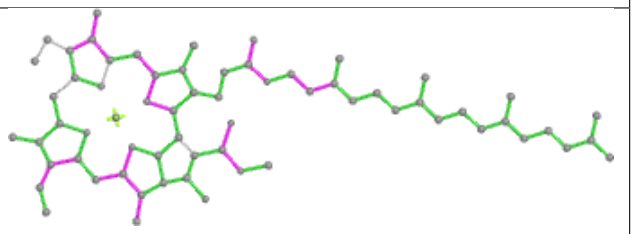
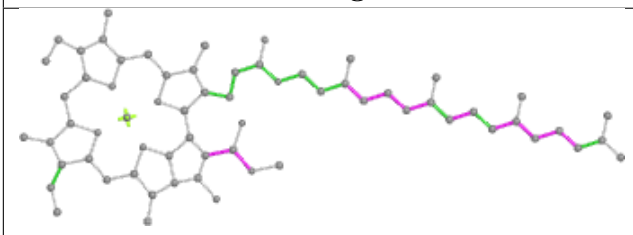


Bond angles



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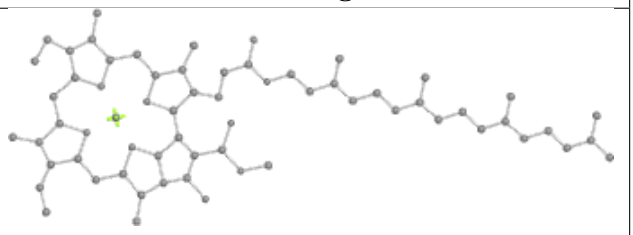
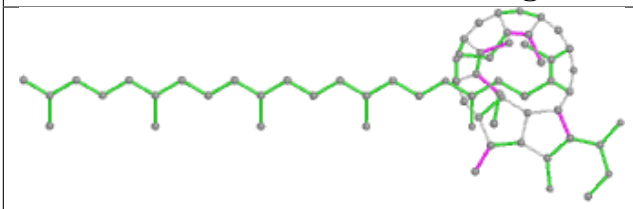


Rings

Ligand PHO A 606



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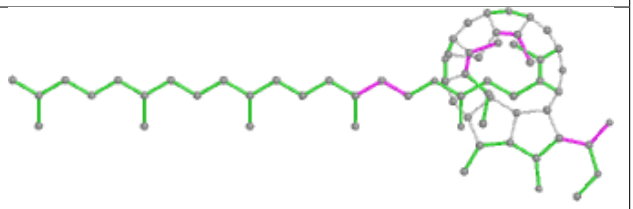
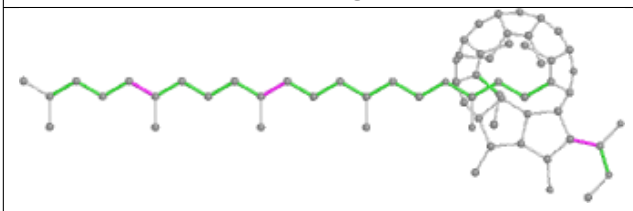


Bond angles



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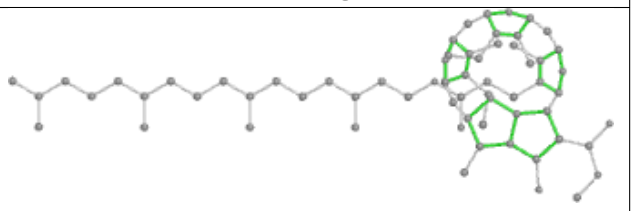
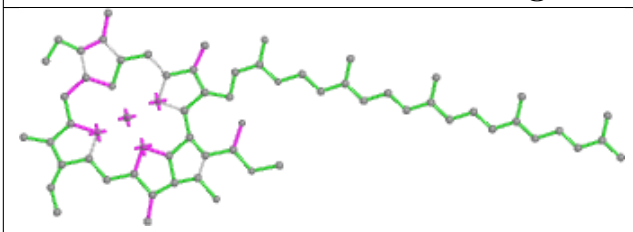
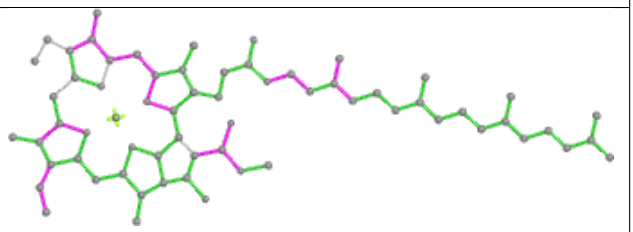


Rings

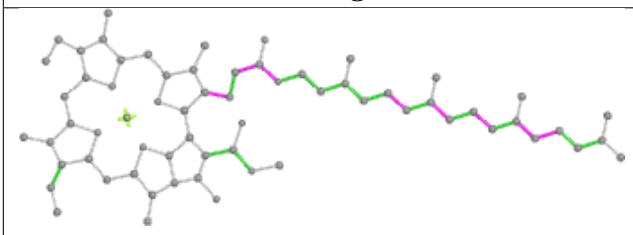
Ligand CLA a 606



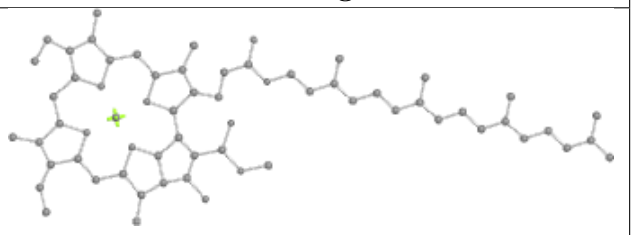
Bond lengths



Bond angles

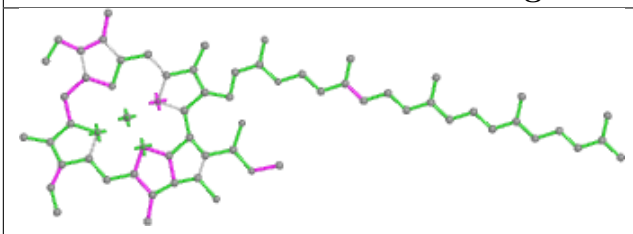


Torsions



Rings

Ligand CLA B 615



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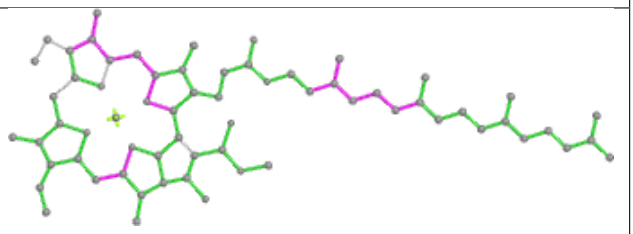

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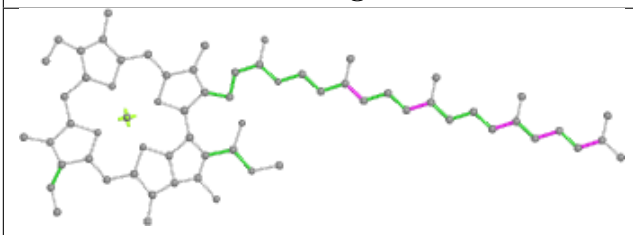
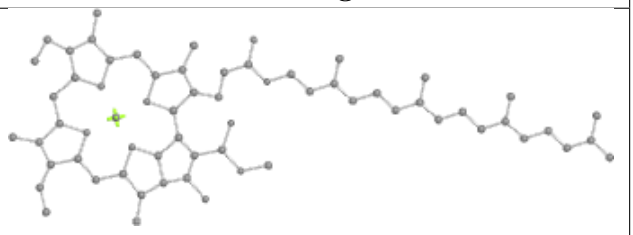
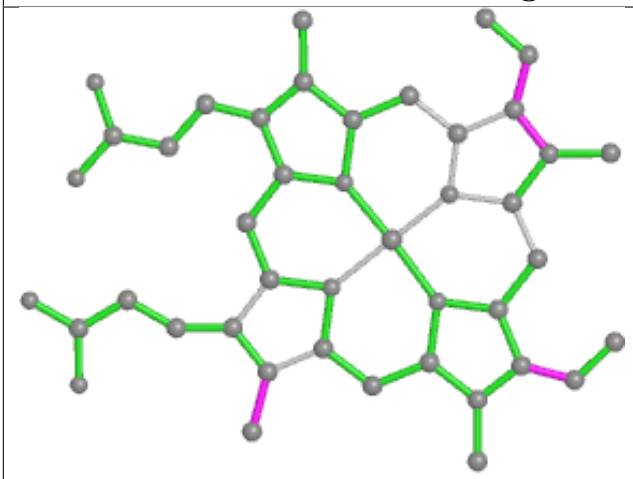


Torsions



Rings

Ligand HEM F 102



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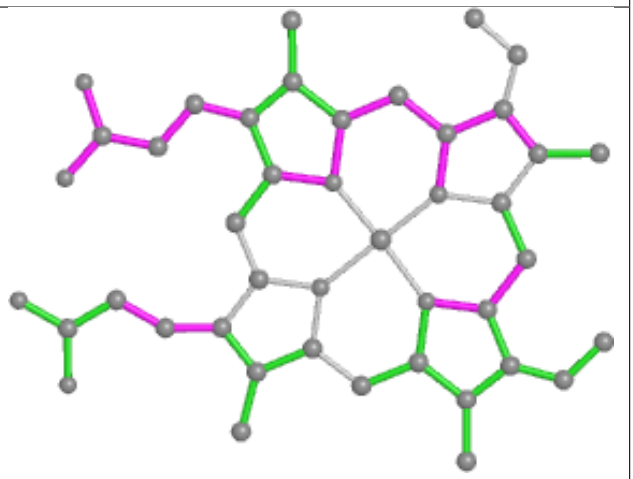
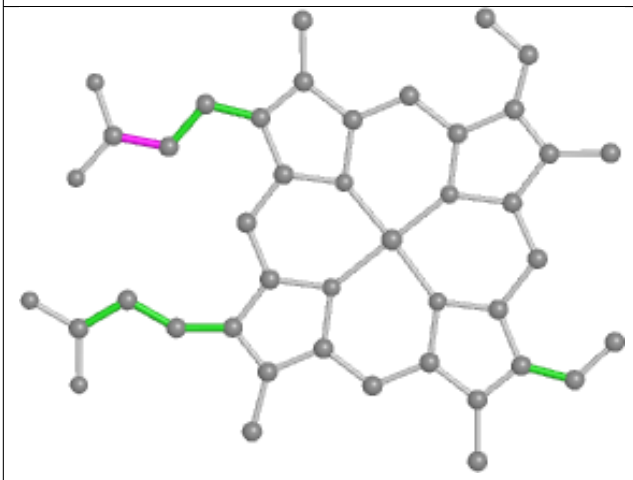
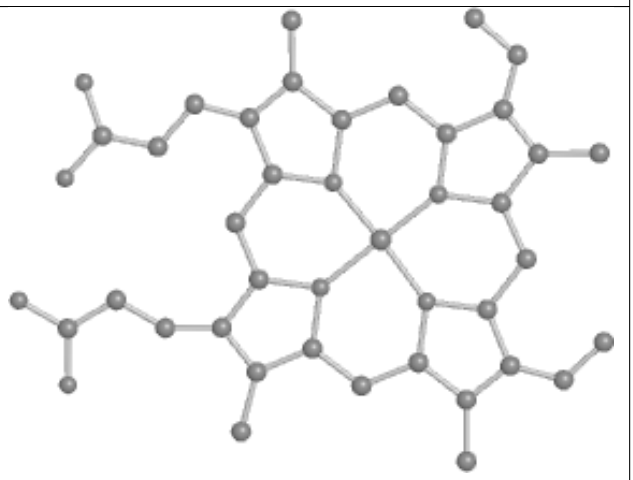


Bond angles

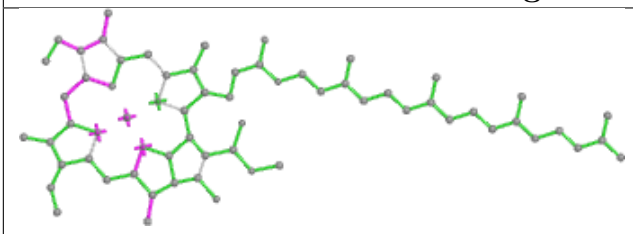


Torsions



Rings

Ligand CLA D 403



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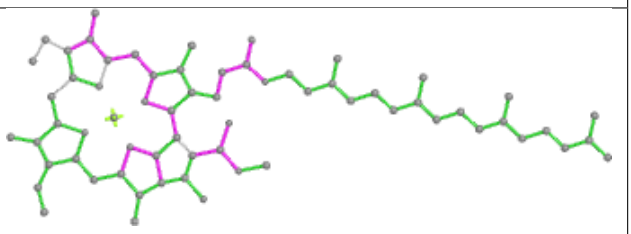
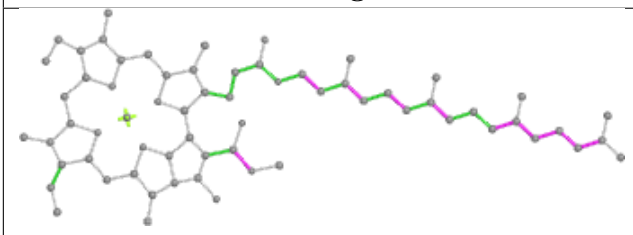
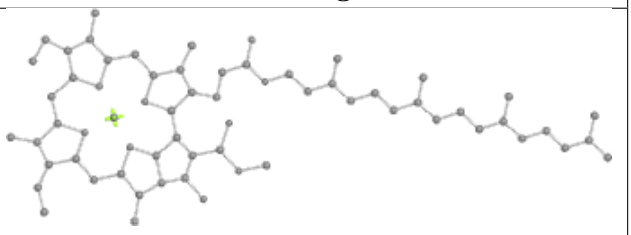


Bond angles

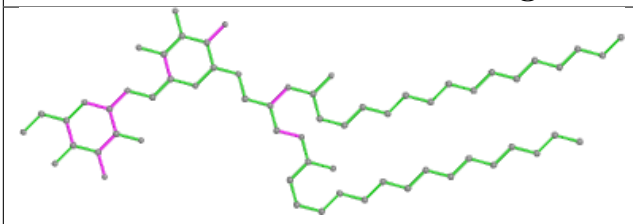


Torsions



Rings

Ligand DGD H 102



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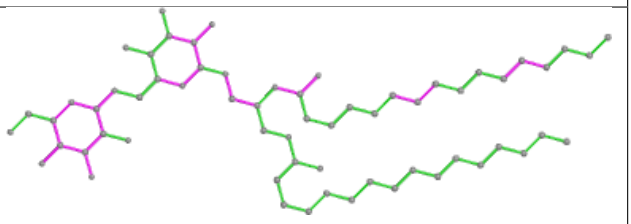
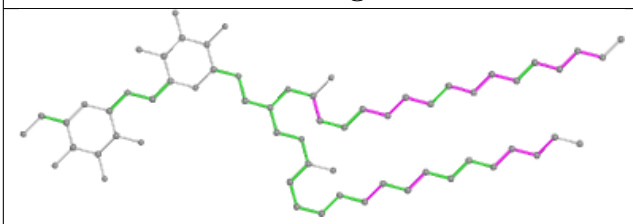


Bond angles



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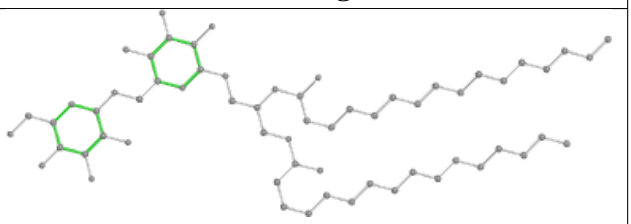
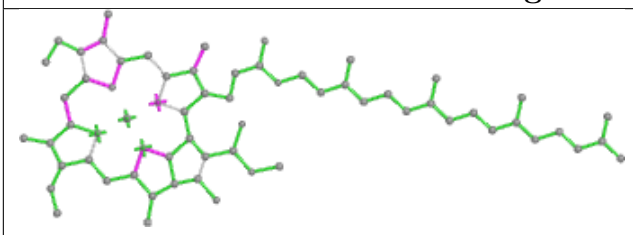


Rings

Ligand CLA B 604



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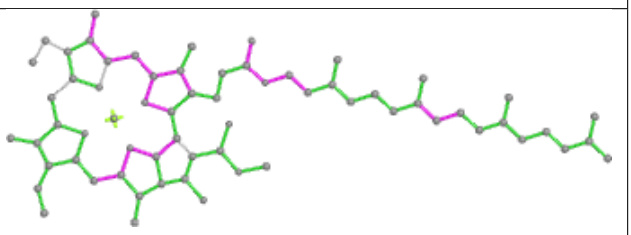
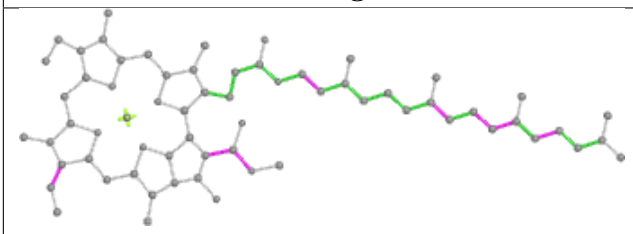


Bond angles



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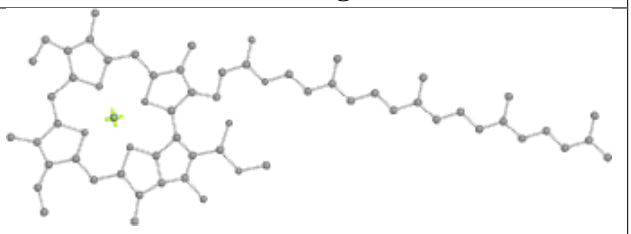
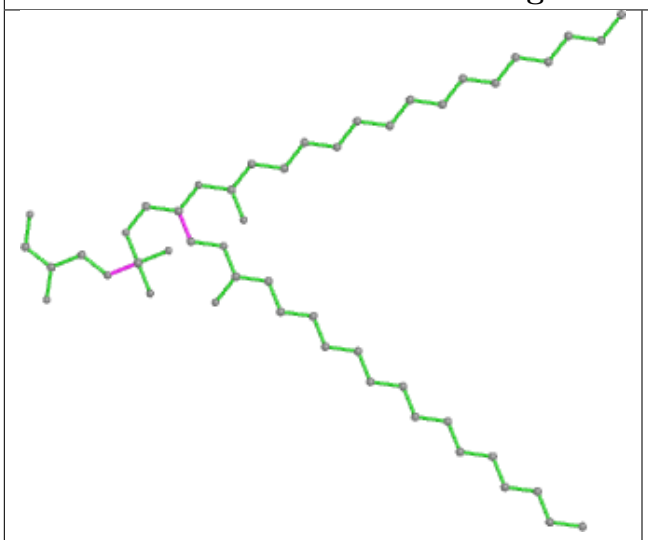


Rings

Ligand LHG d 407



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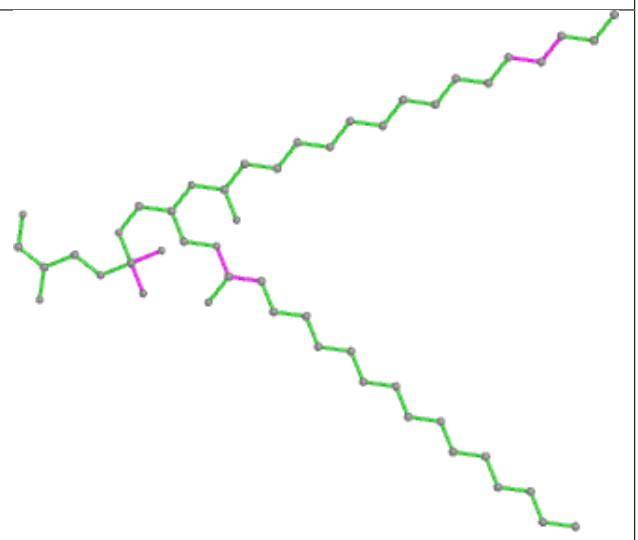
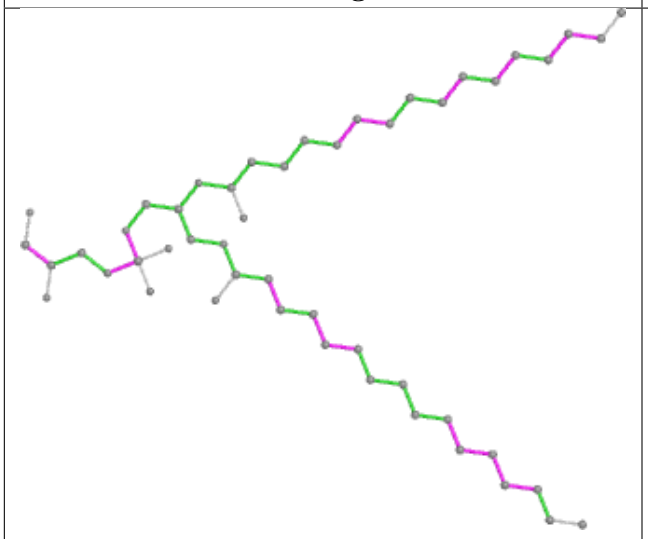


Bond angles



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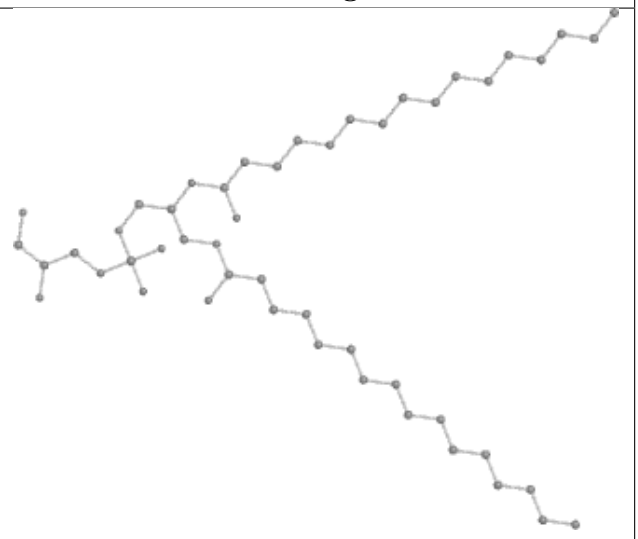
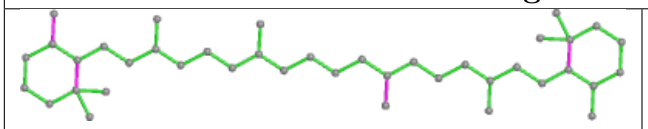


Rings

Ligand BCR C 515



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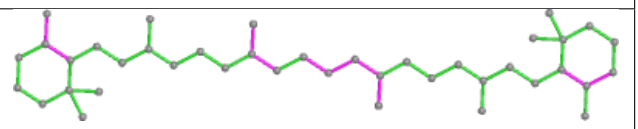
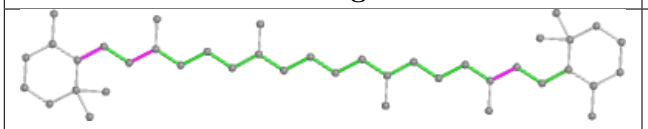


Bond angles



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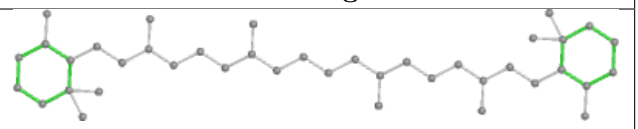
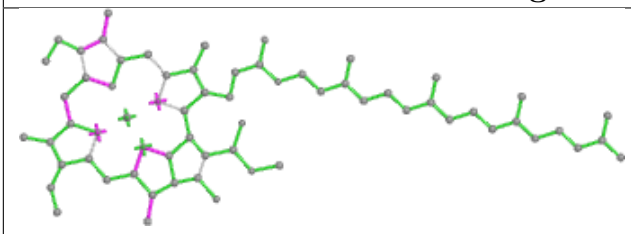


Rings

Ligand CLA c 513



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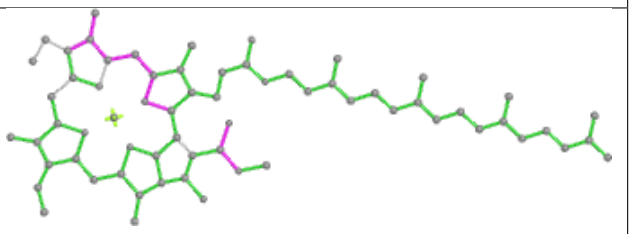
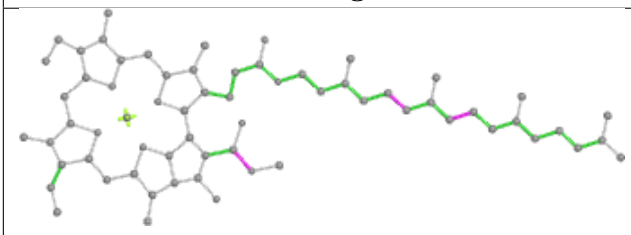
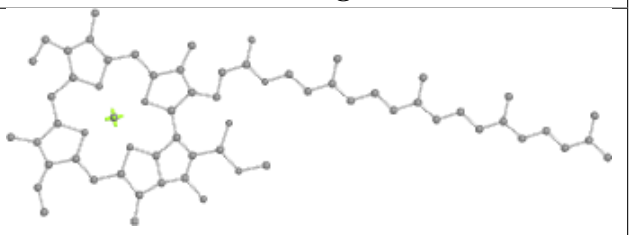


Bond angles

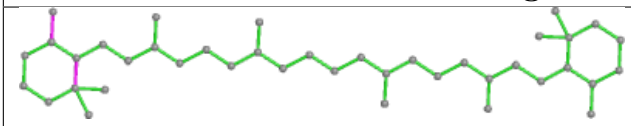


Torsions



Rings

Ligand BCR B 617



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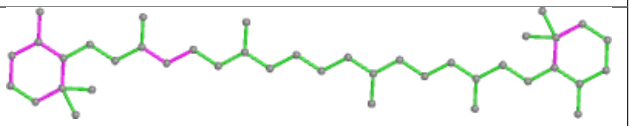
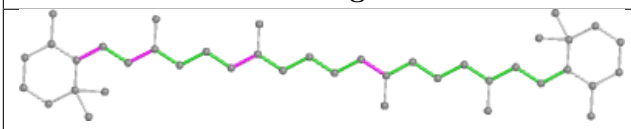


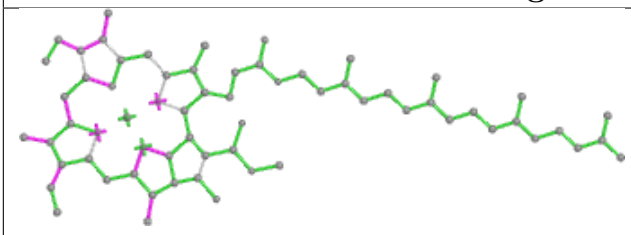
Bond angles



Torsions

Rings

Ligand CLA b 615



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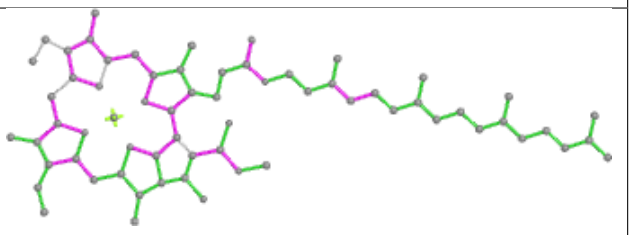
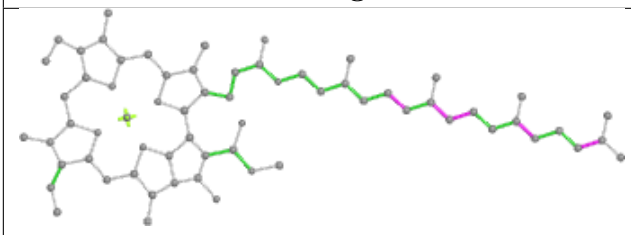
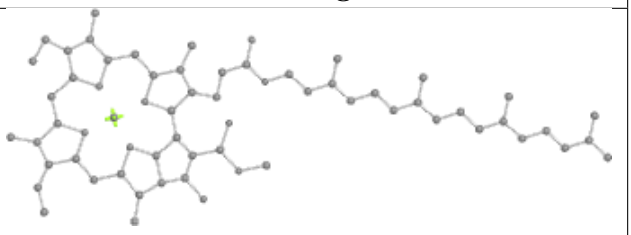


Bond angles

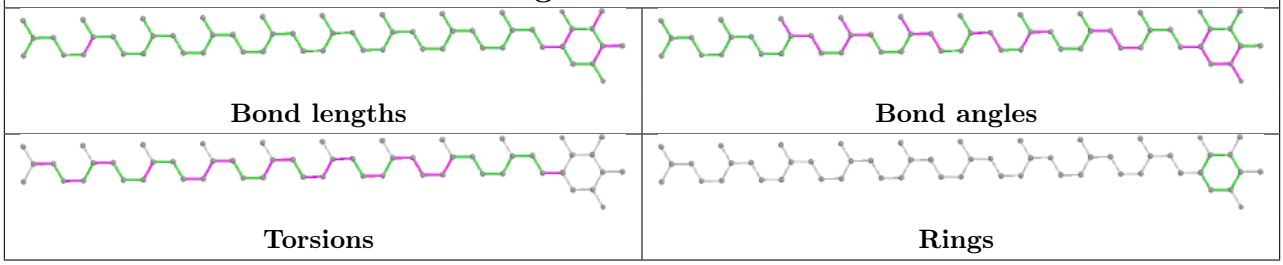


Torsions

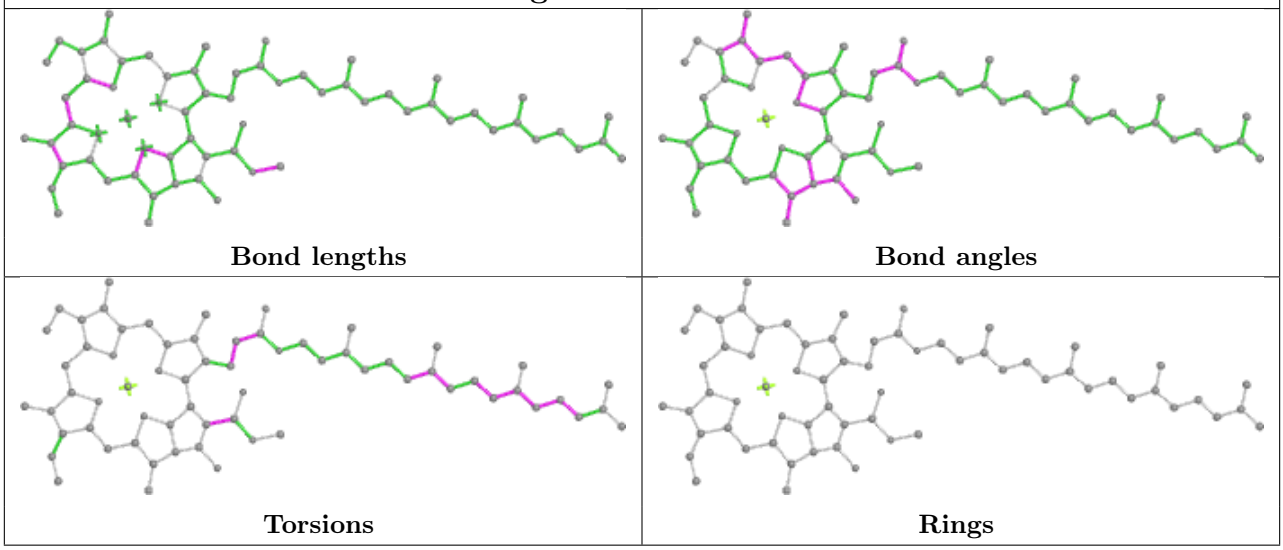


Rings

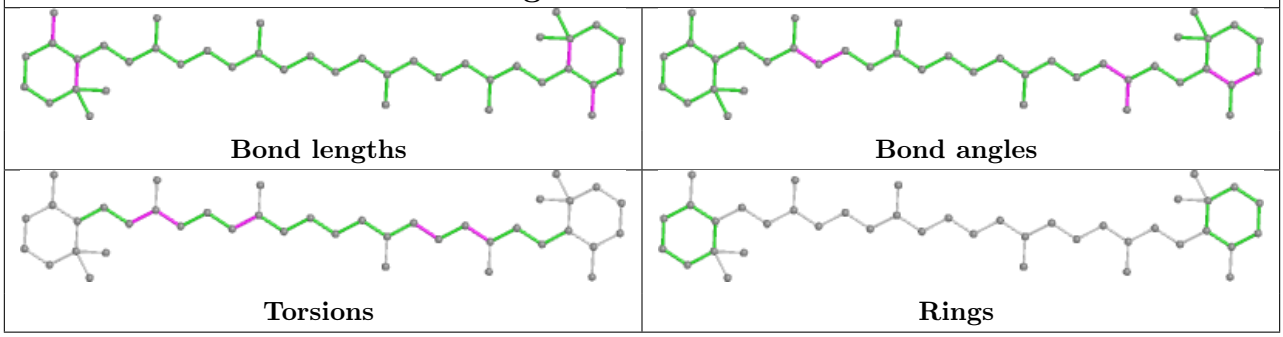
Ligand PL9 a 611



Ligand CLA c 509



Ligand BCR C 520



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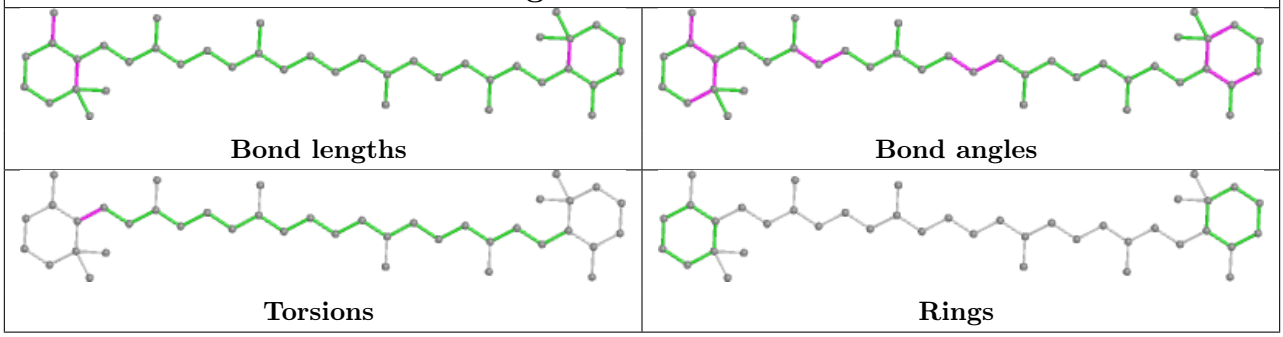
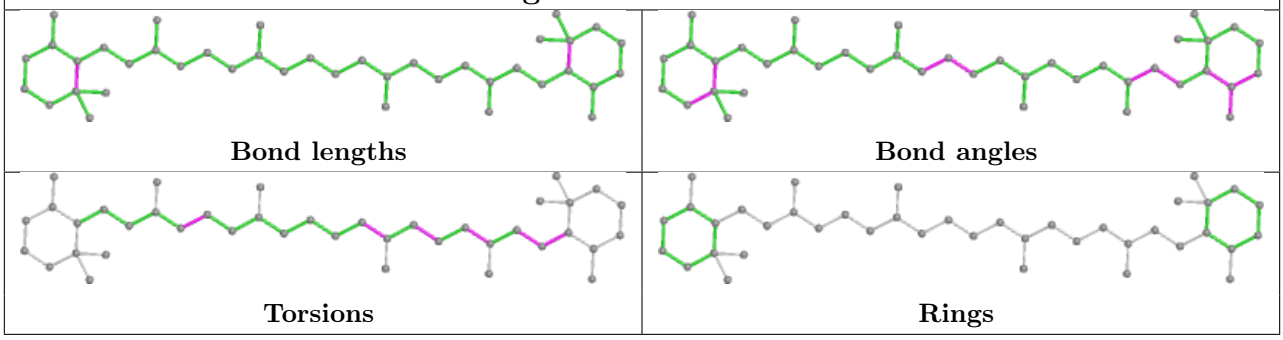
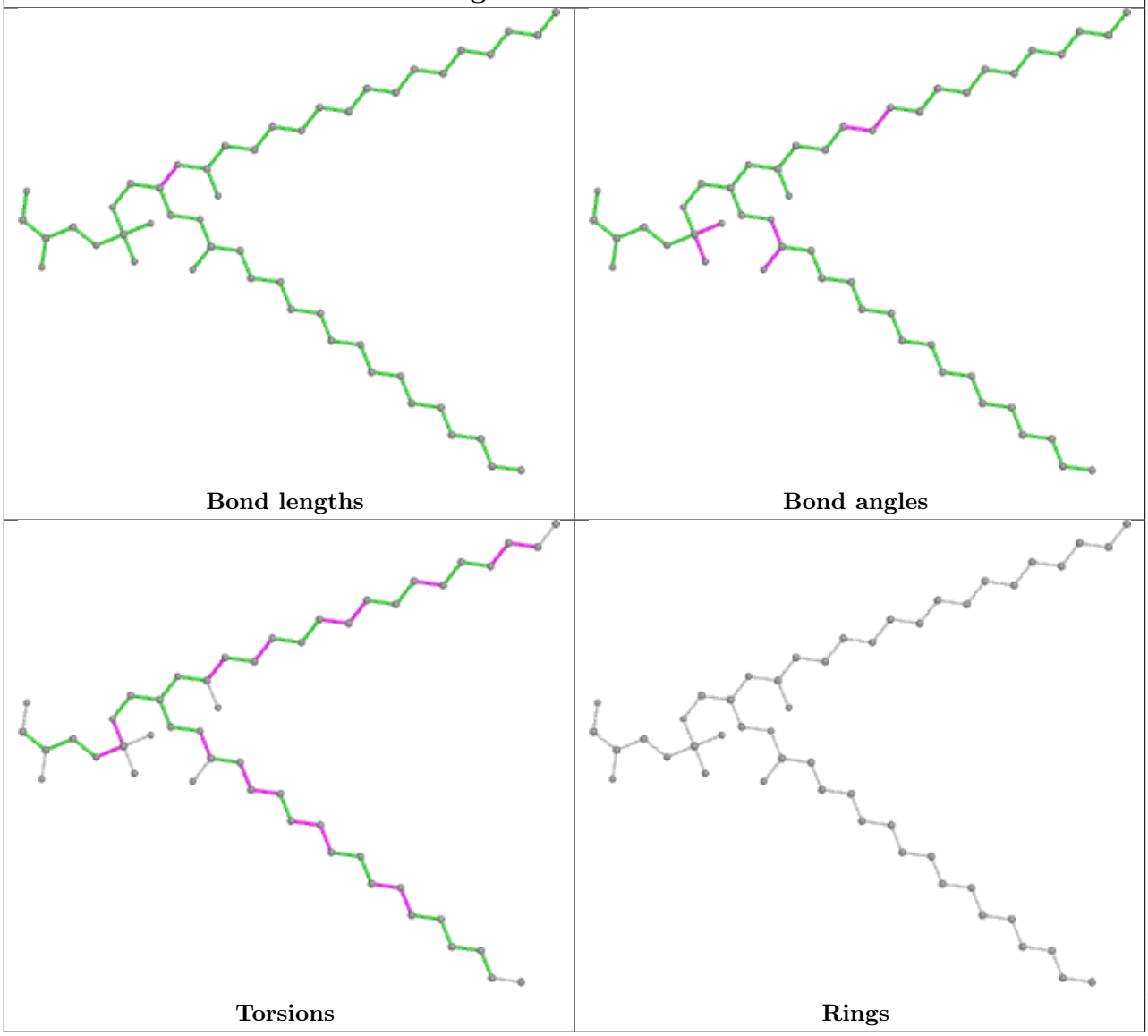


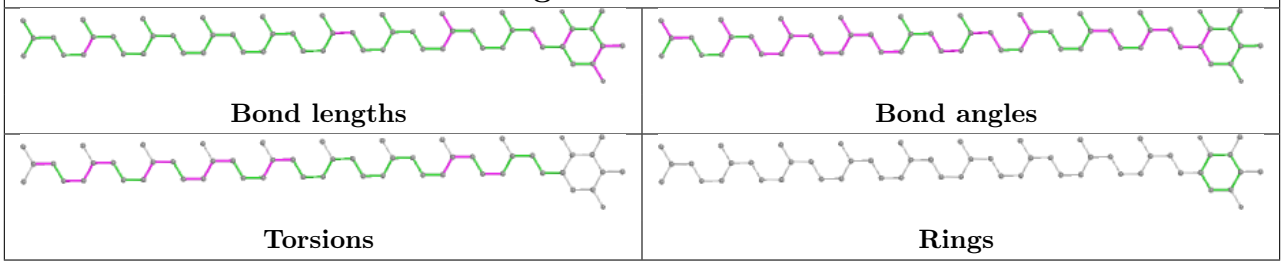
Ligand BCR D 404



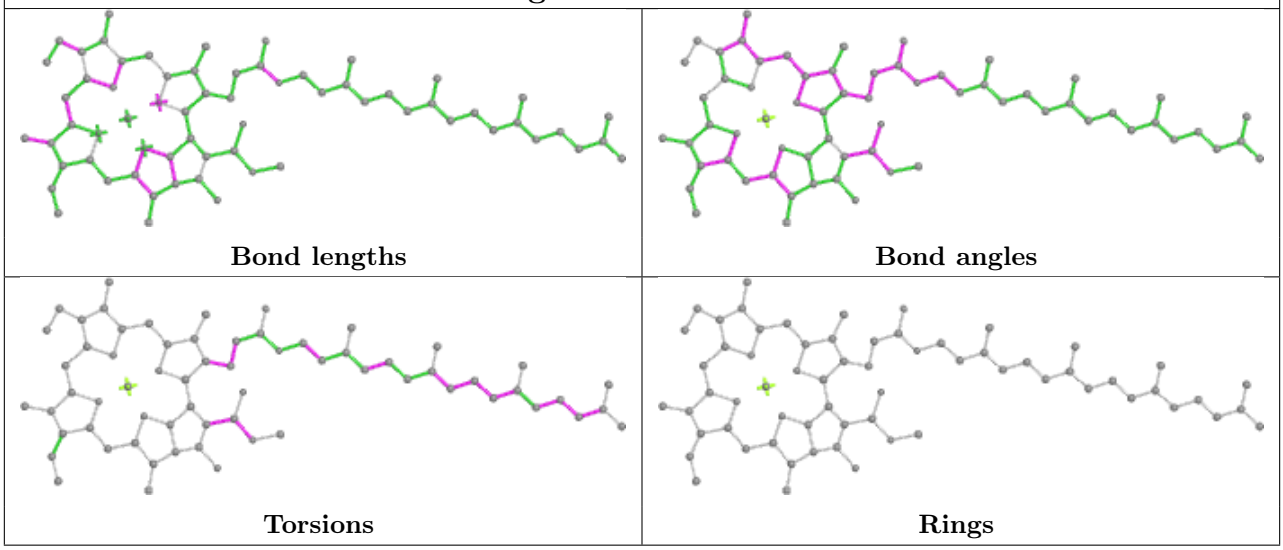
Ligand LHG L 101



Ligand PL9 d 408



Ligand CLA h 101



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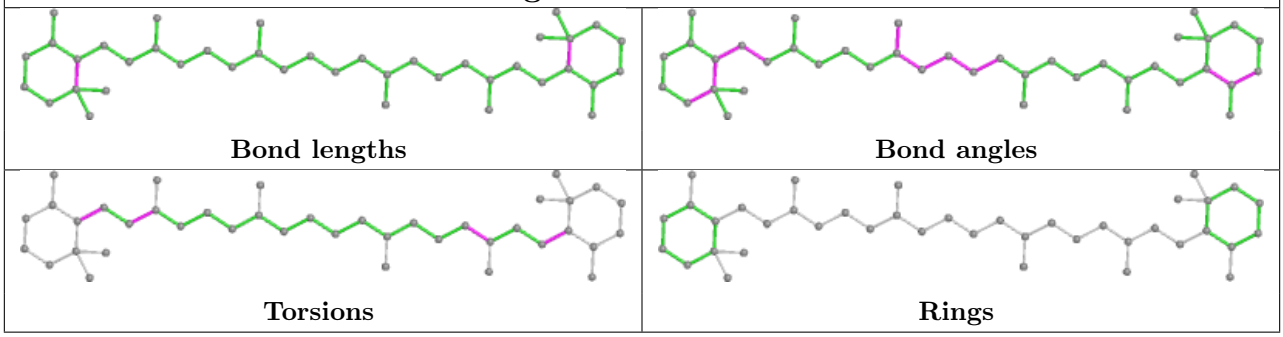

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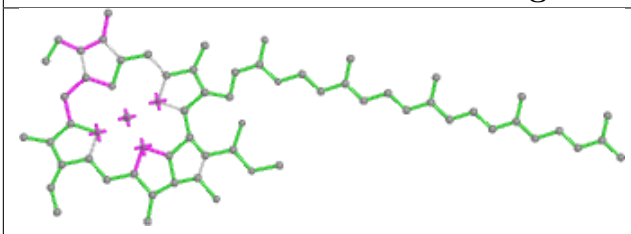
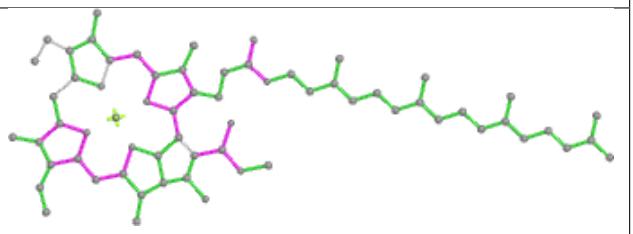
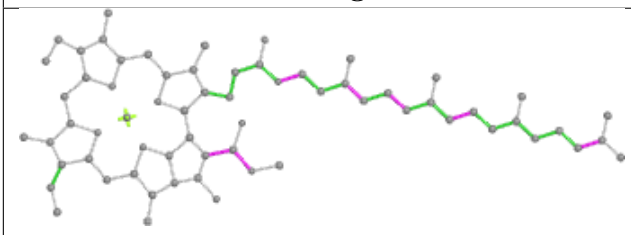


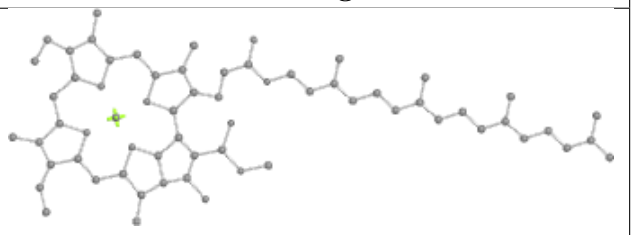
Bond lengths



Bond angles

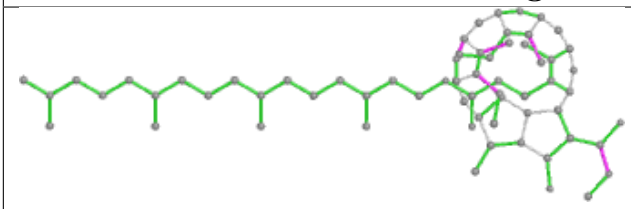


Torsions



Rings

Ligand PHO a 605



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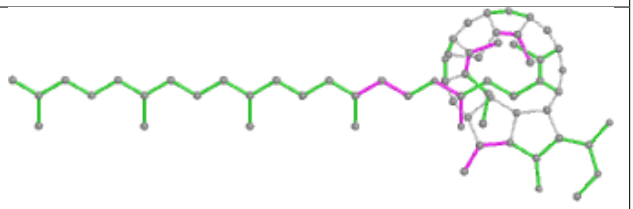

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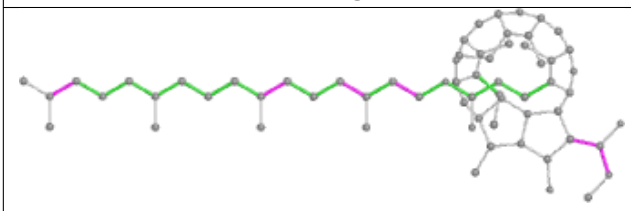

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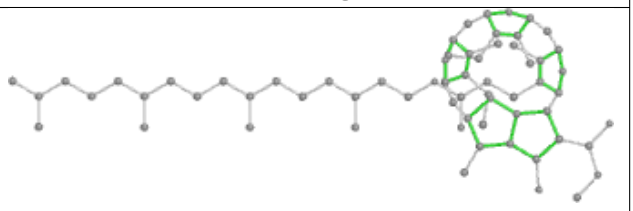
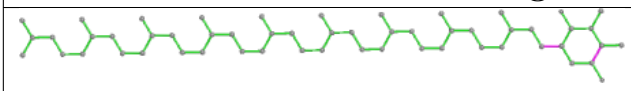


Rings

Ligand PL9 A 611



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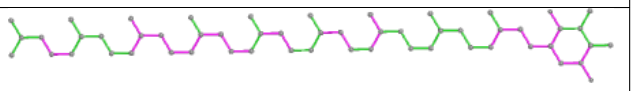
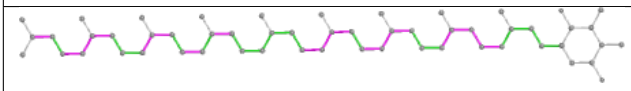


Bond angles



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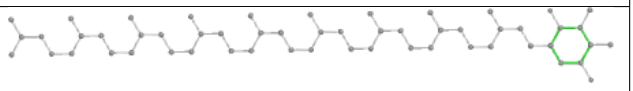
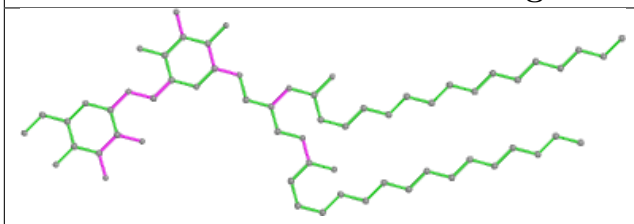


Rings

Ligand DGD c 517



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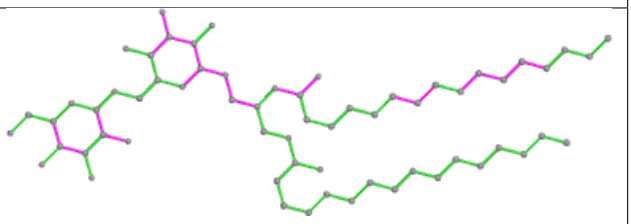

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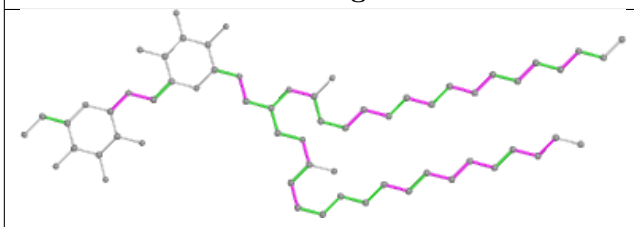

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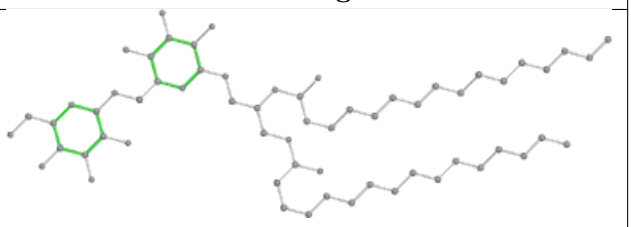
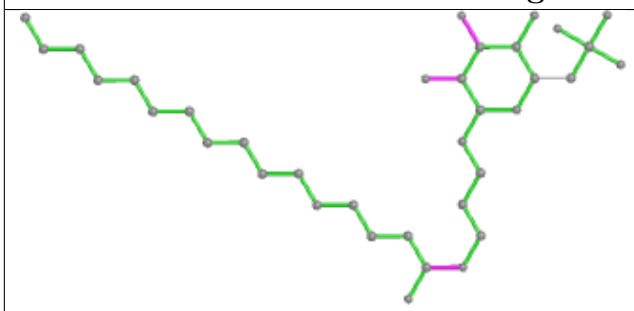


Rings

Ligand SQD F 101



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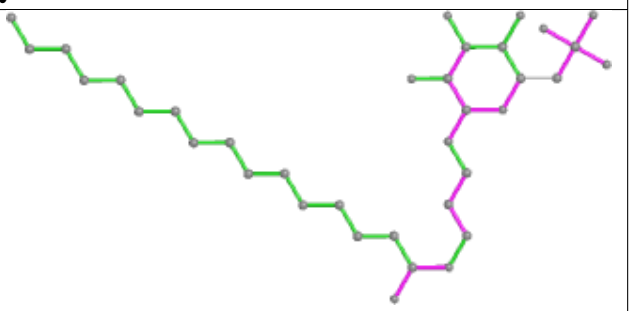

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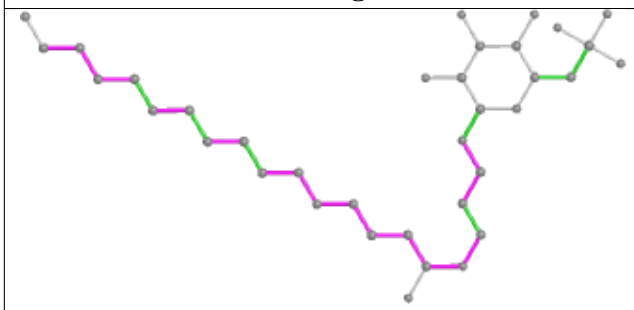

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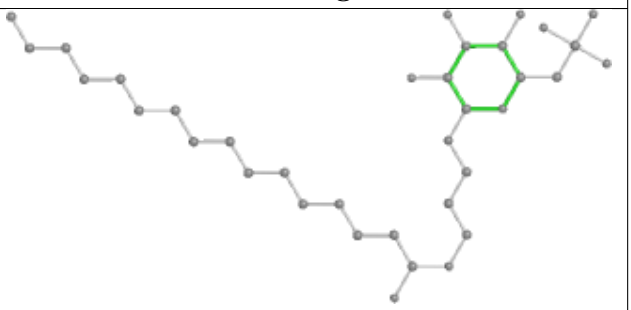
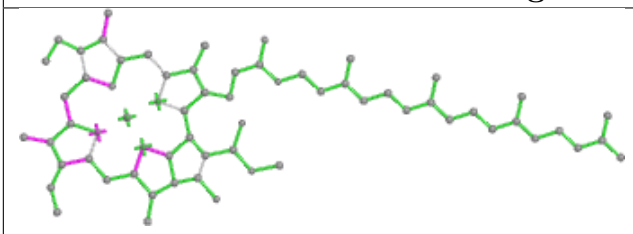


Rings

Ligand CLA b 612



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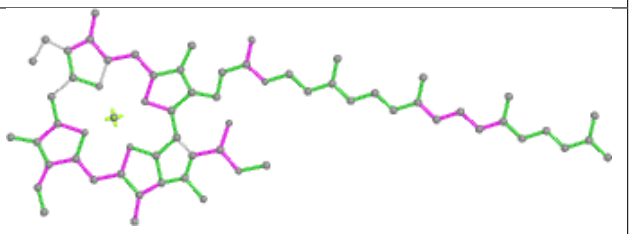
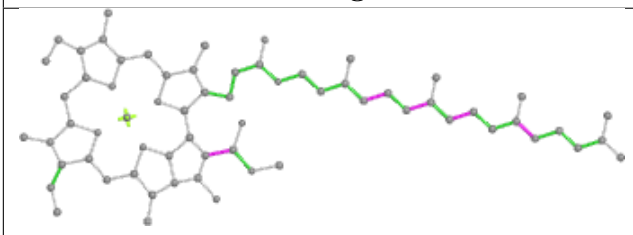


Bond angles



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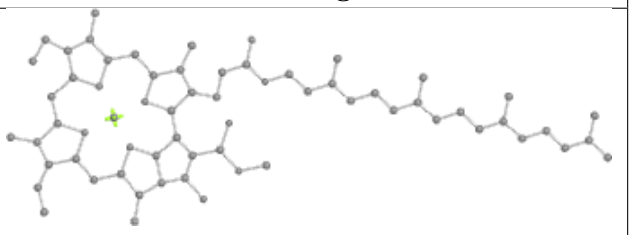
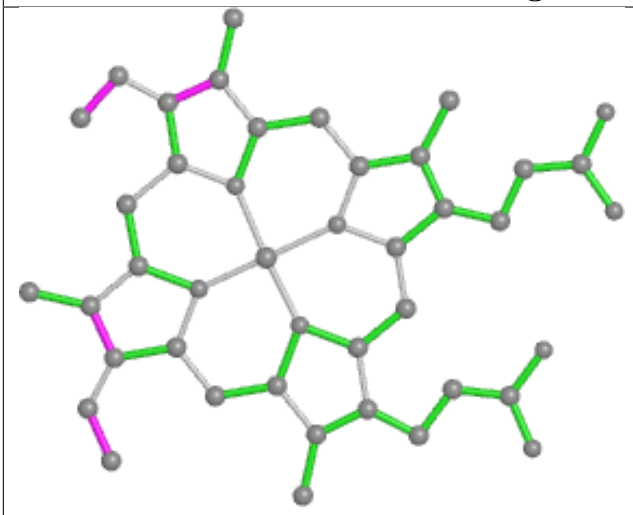


Rings

Ligand HEC v 201



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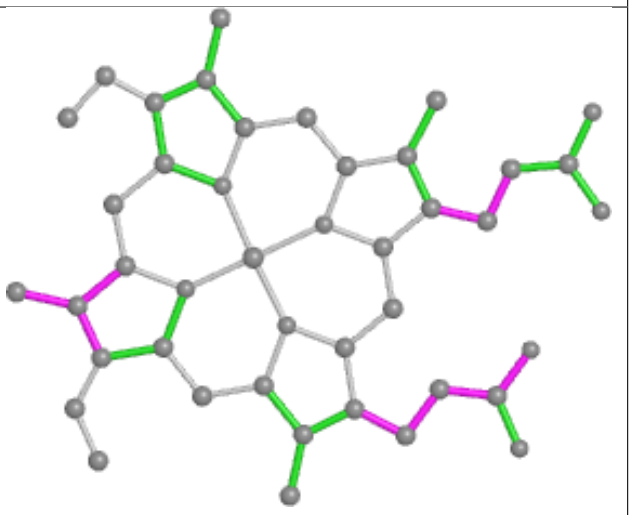
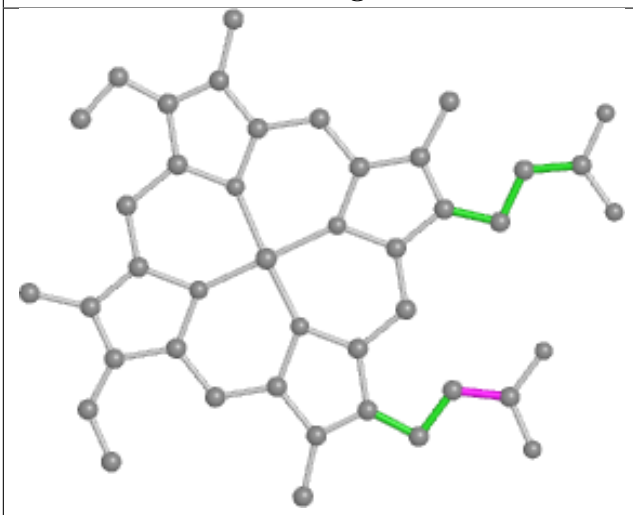


Bond angles



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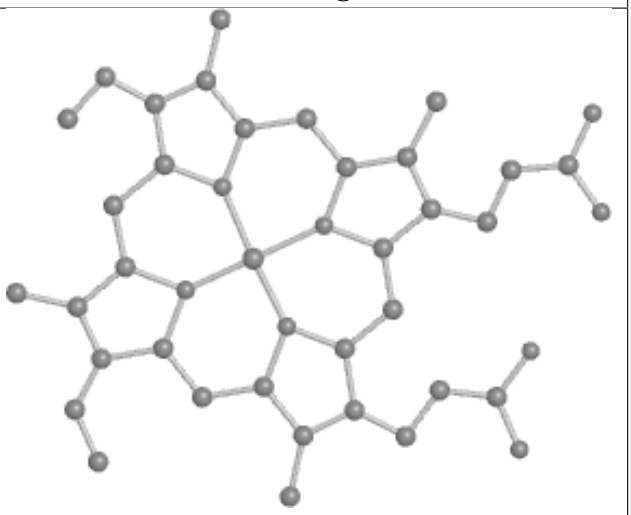
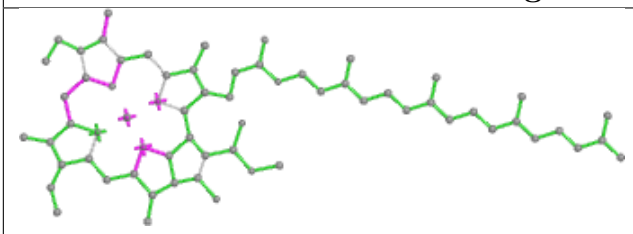


Rings

Ligand CLA B 602



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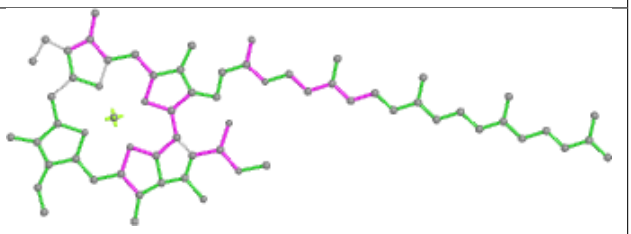

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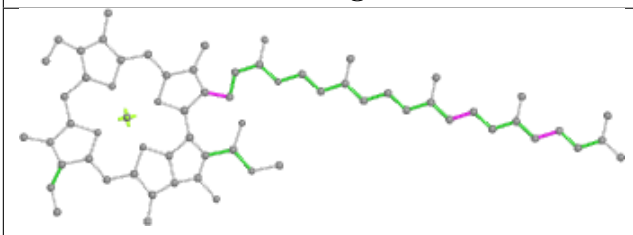

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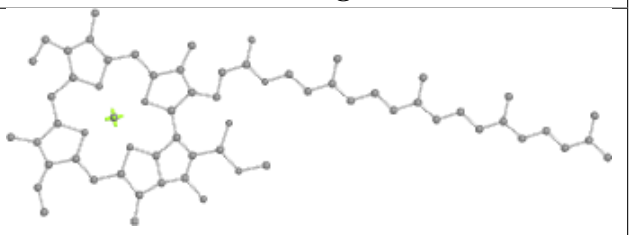

Rings

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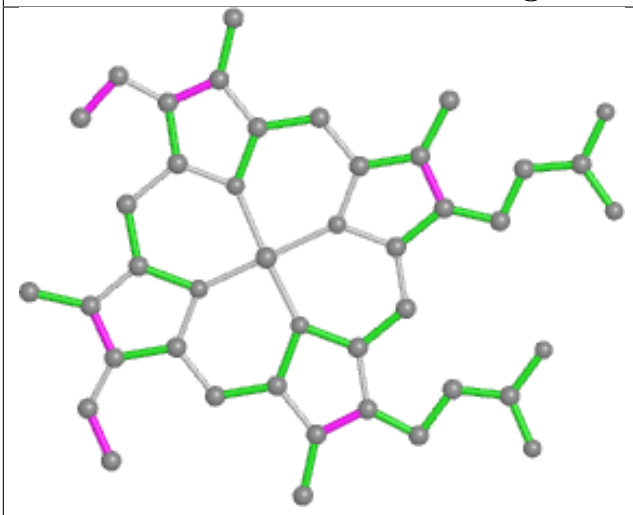

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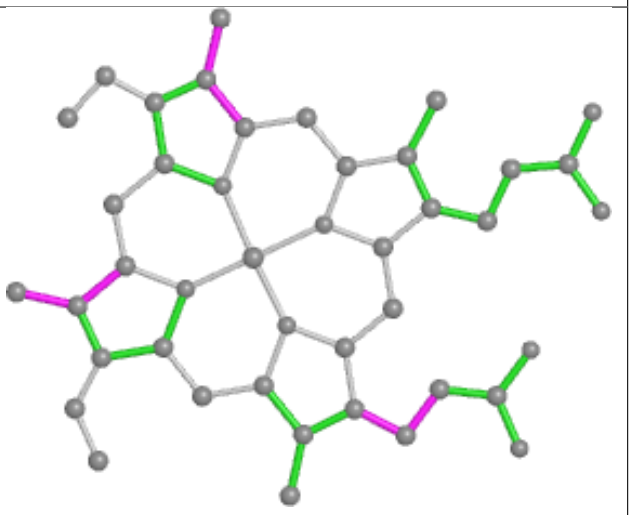
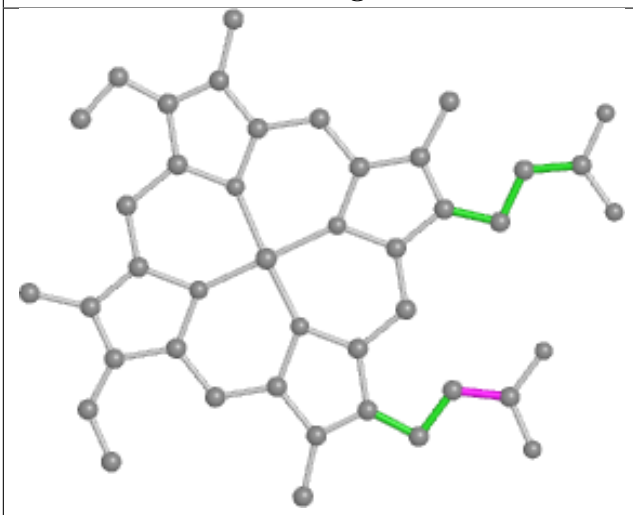


Bond angles



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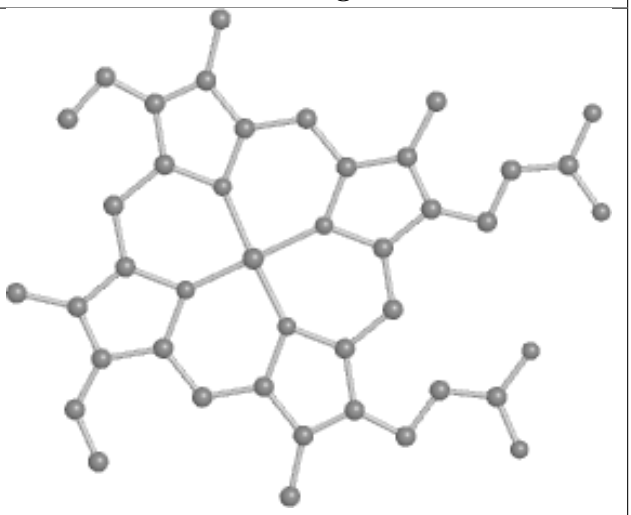
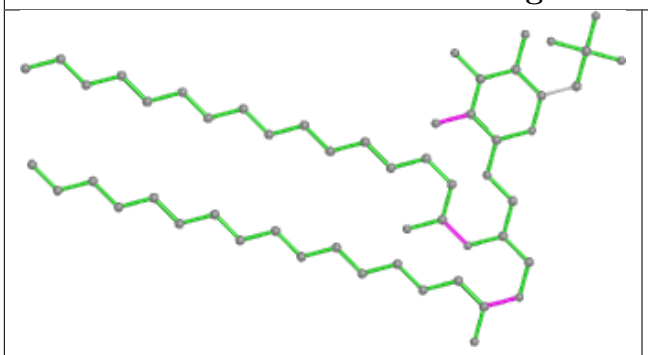


Rings

Ligand SQD B 624



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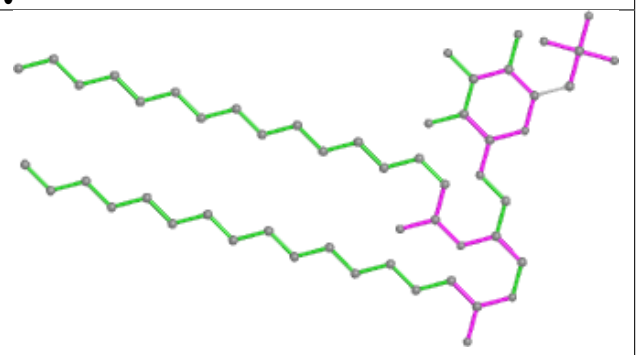

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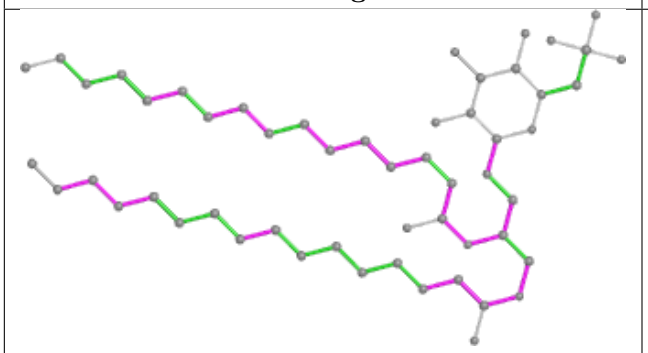

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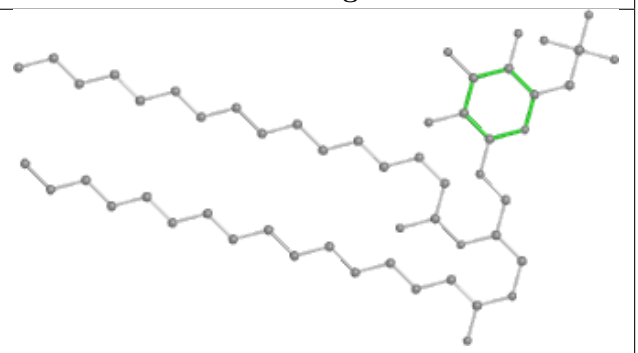
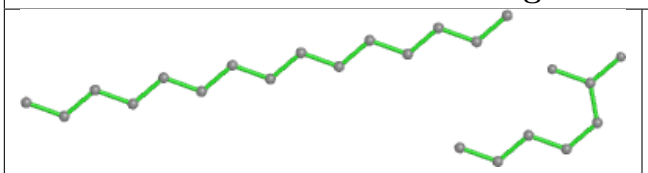


Rings

Ligand LMG d 410



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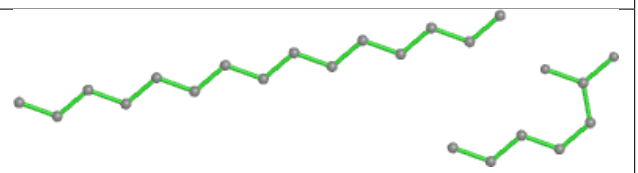
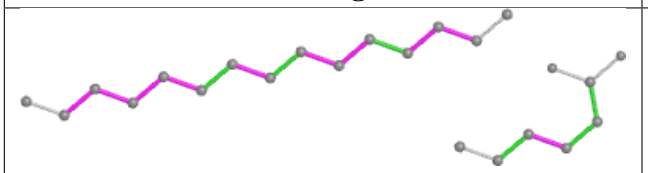


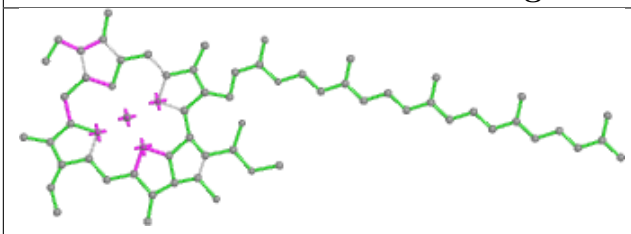
Bond angles



Torsions

Rings

Ligand CLA C 506



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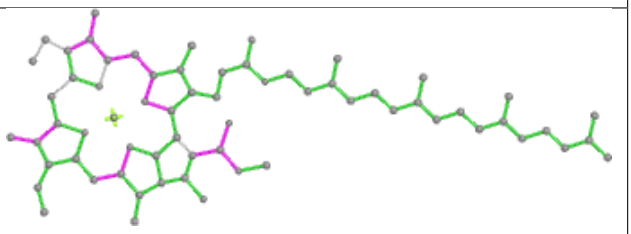
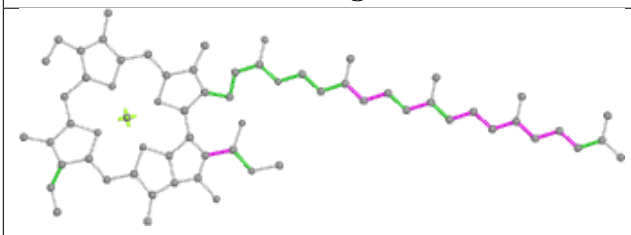


Bond angles



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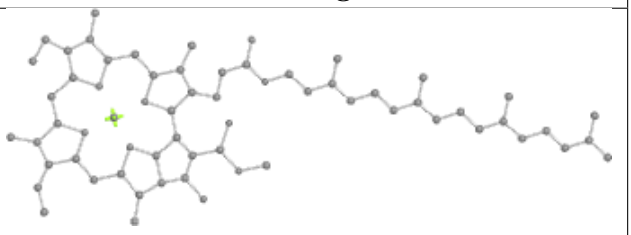
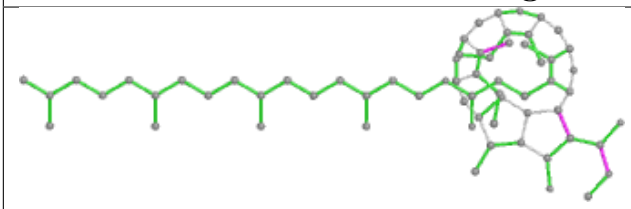


Rings

Ligand PHO A 605



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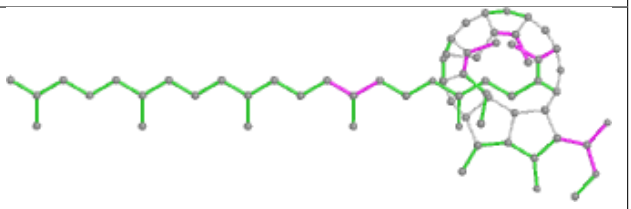
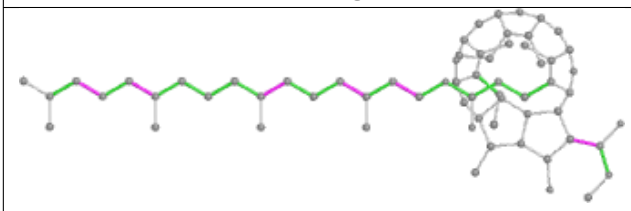


Bond angles



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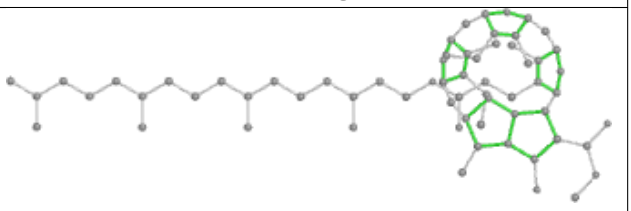
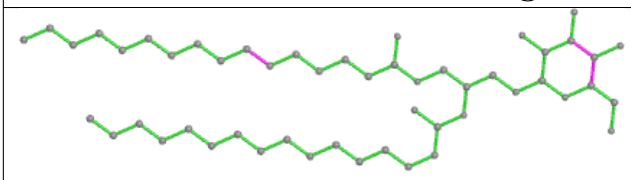


Rings

Ligand LMG D 405



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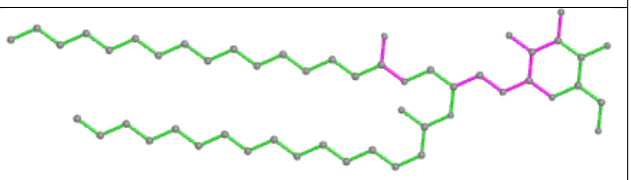
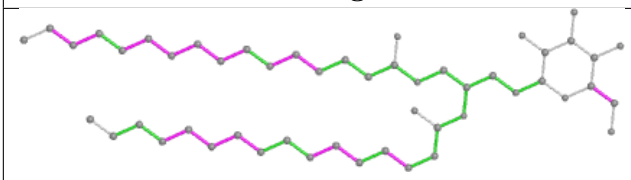


Bond angles



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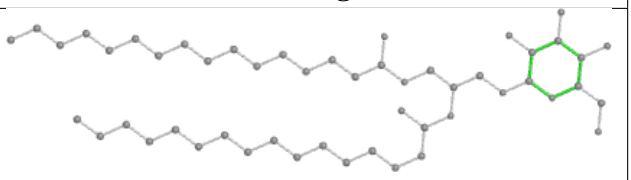
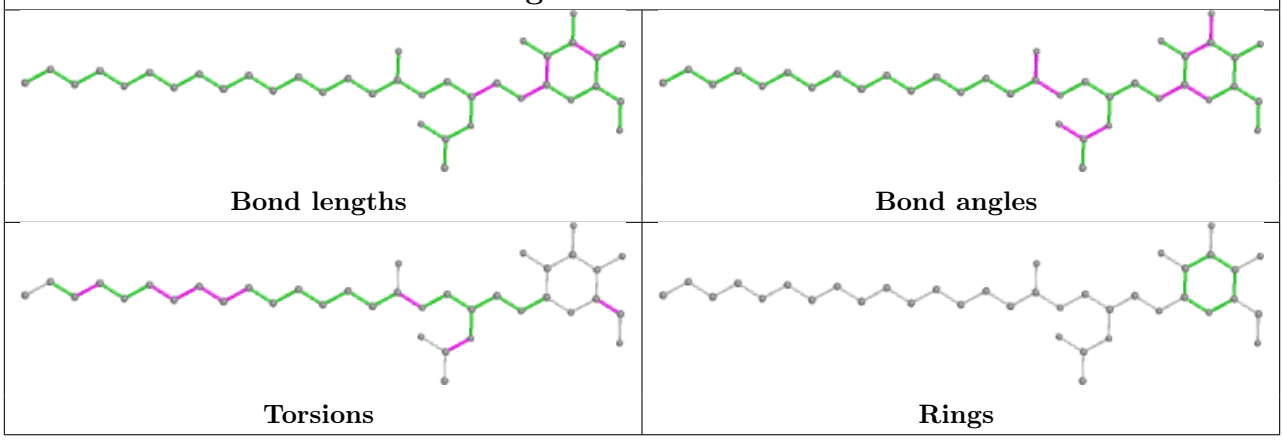
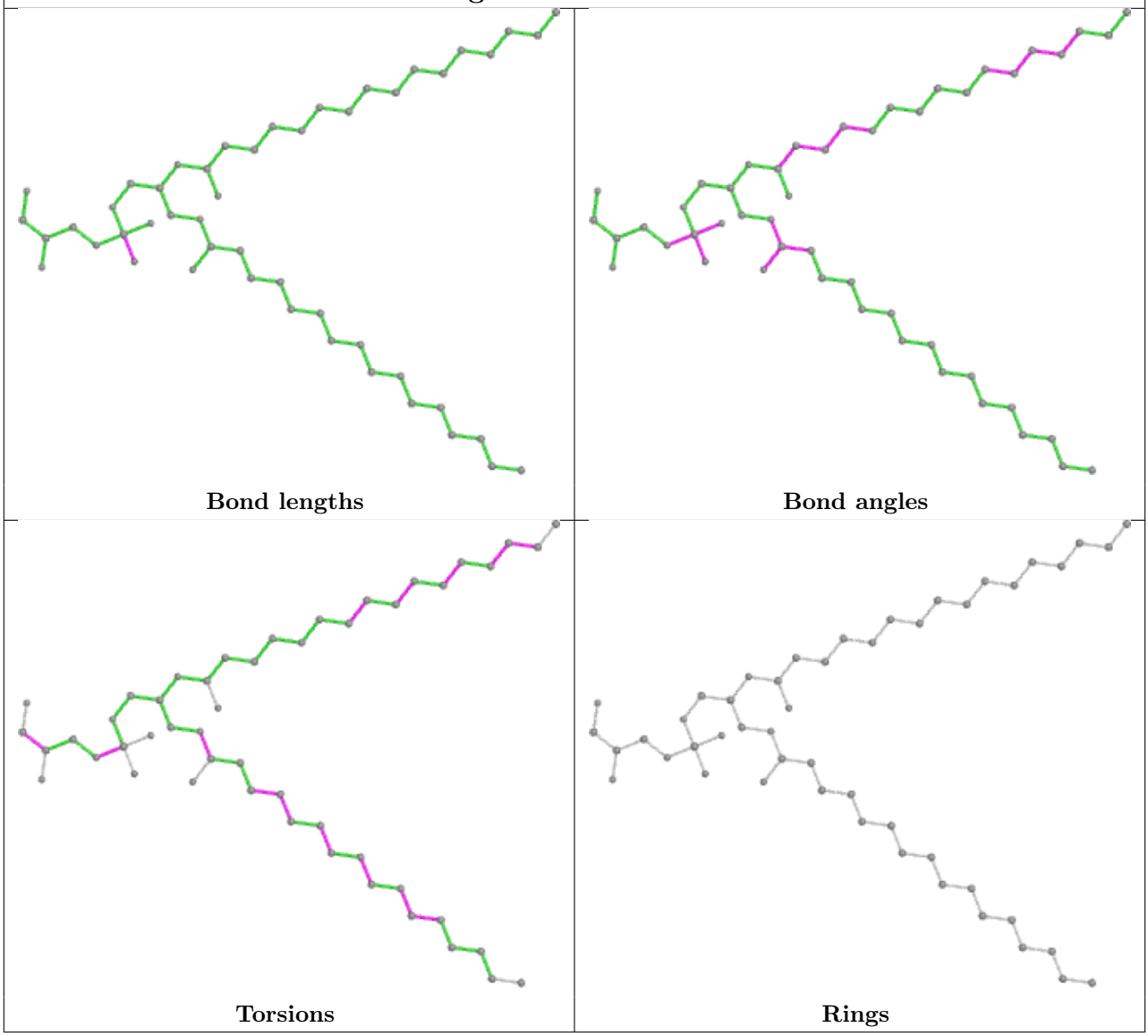


Rings

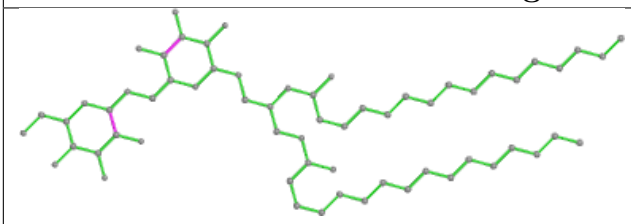
Ligand LMG c 519



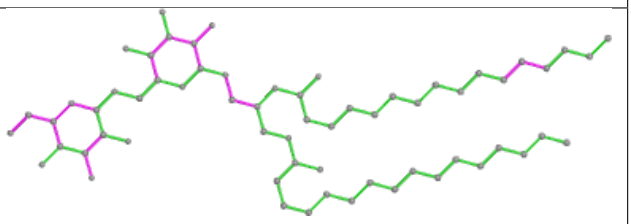
Ligand LHG B 623



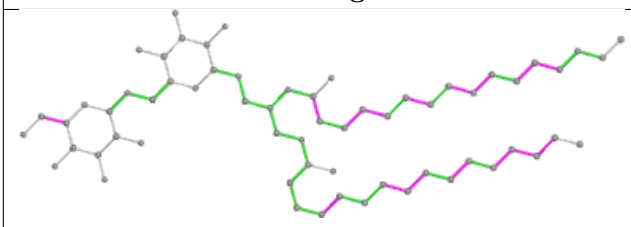
Ligand DGD h 103



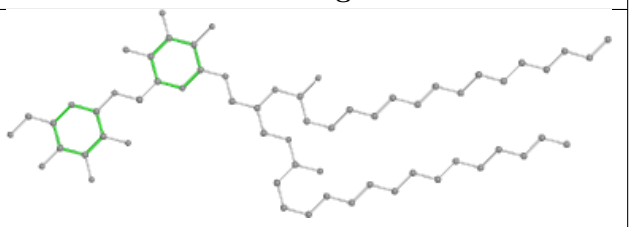
Bond lengths



Bond angles

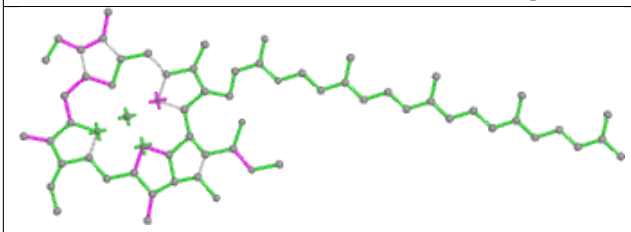


Torsions

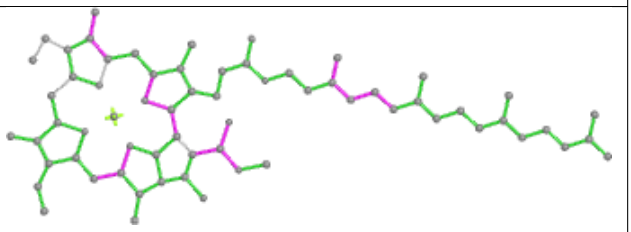


Rings

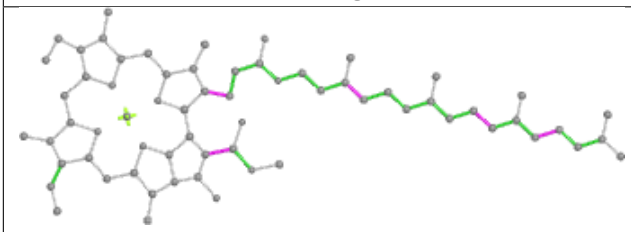
Ligand CLA B 609



Bond lengths



Bond angles



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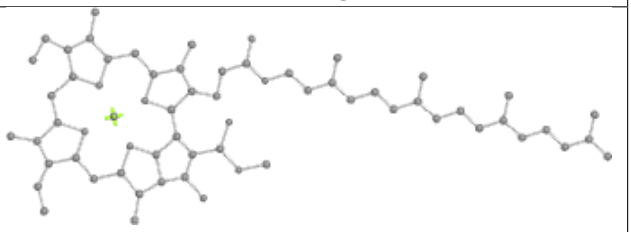
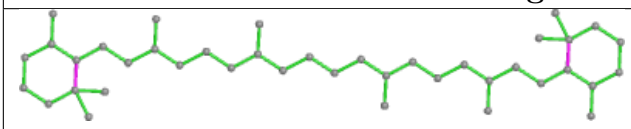
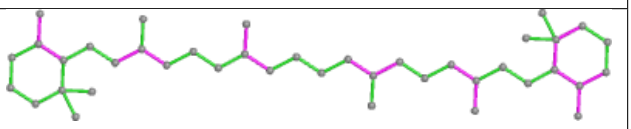


Rings

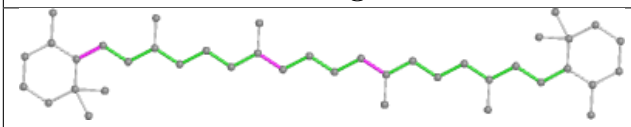
Ligand BCR a 607



Bond lengths



Bond angles



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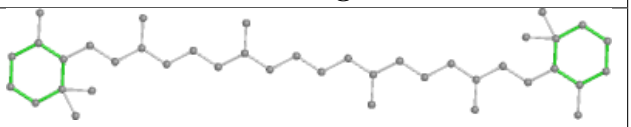
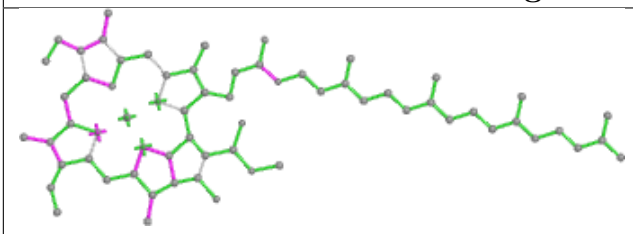
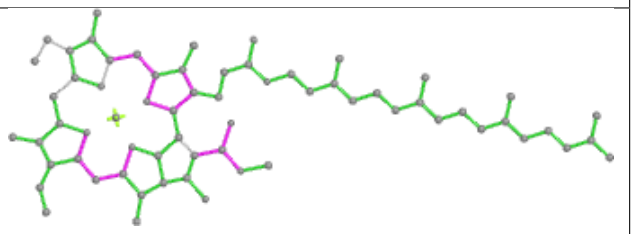


Rings

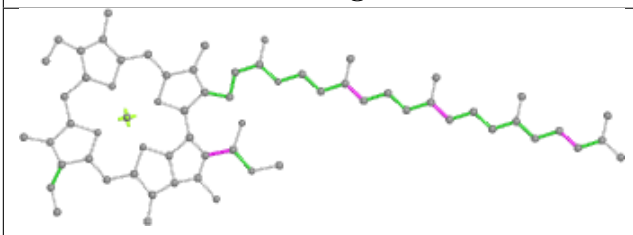
Ligand CLA C 510



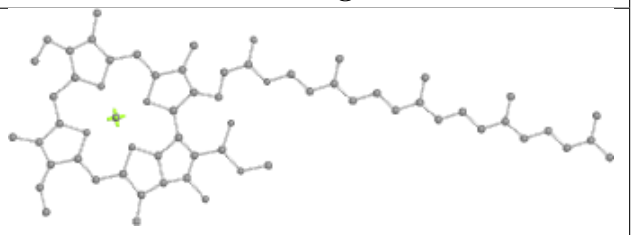
Bond lengths



Bond angles

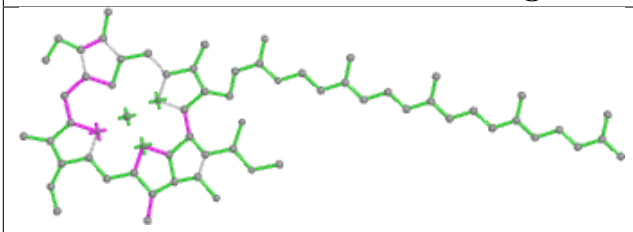


Torsions

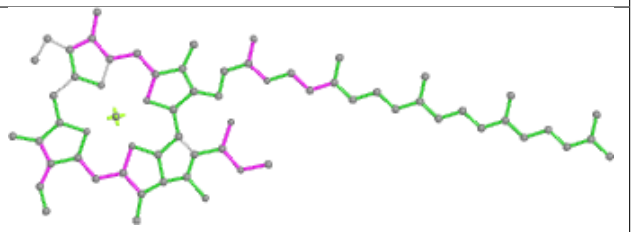


Rings

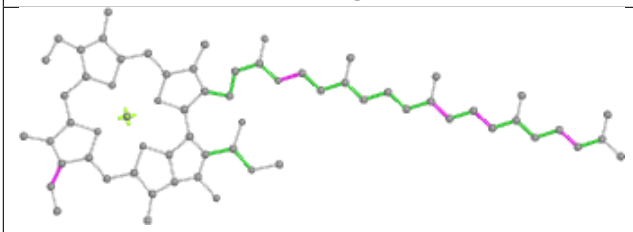
Ligand CLA D 402



Bond lengths



Bond angles



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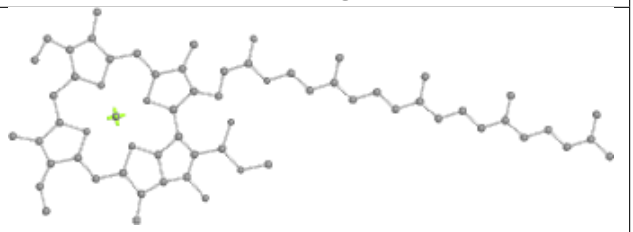
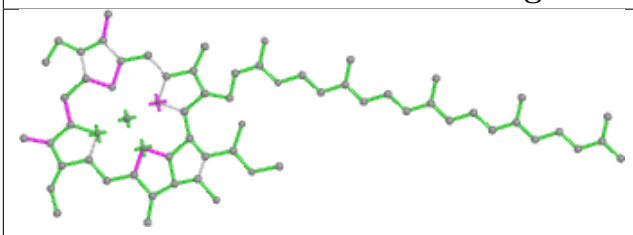
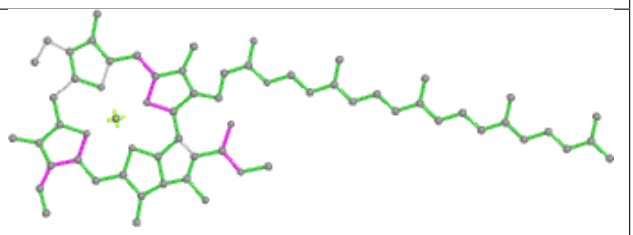


Rings

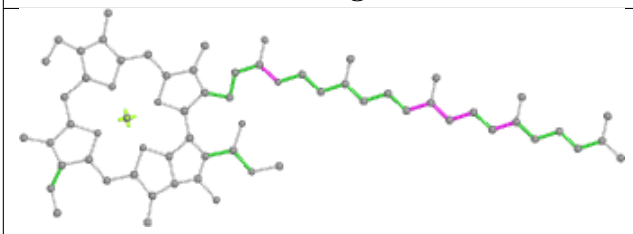
Ligand CLA C 511



Bond lengths



Bond angles



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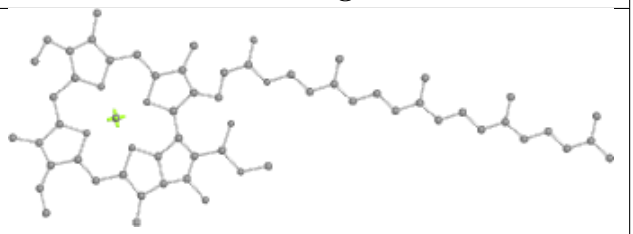
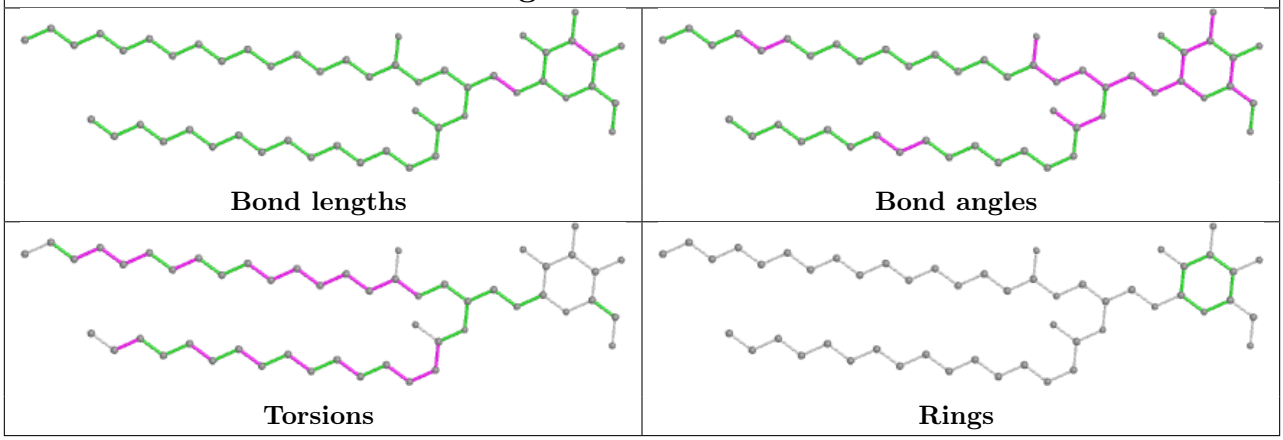
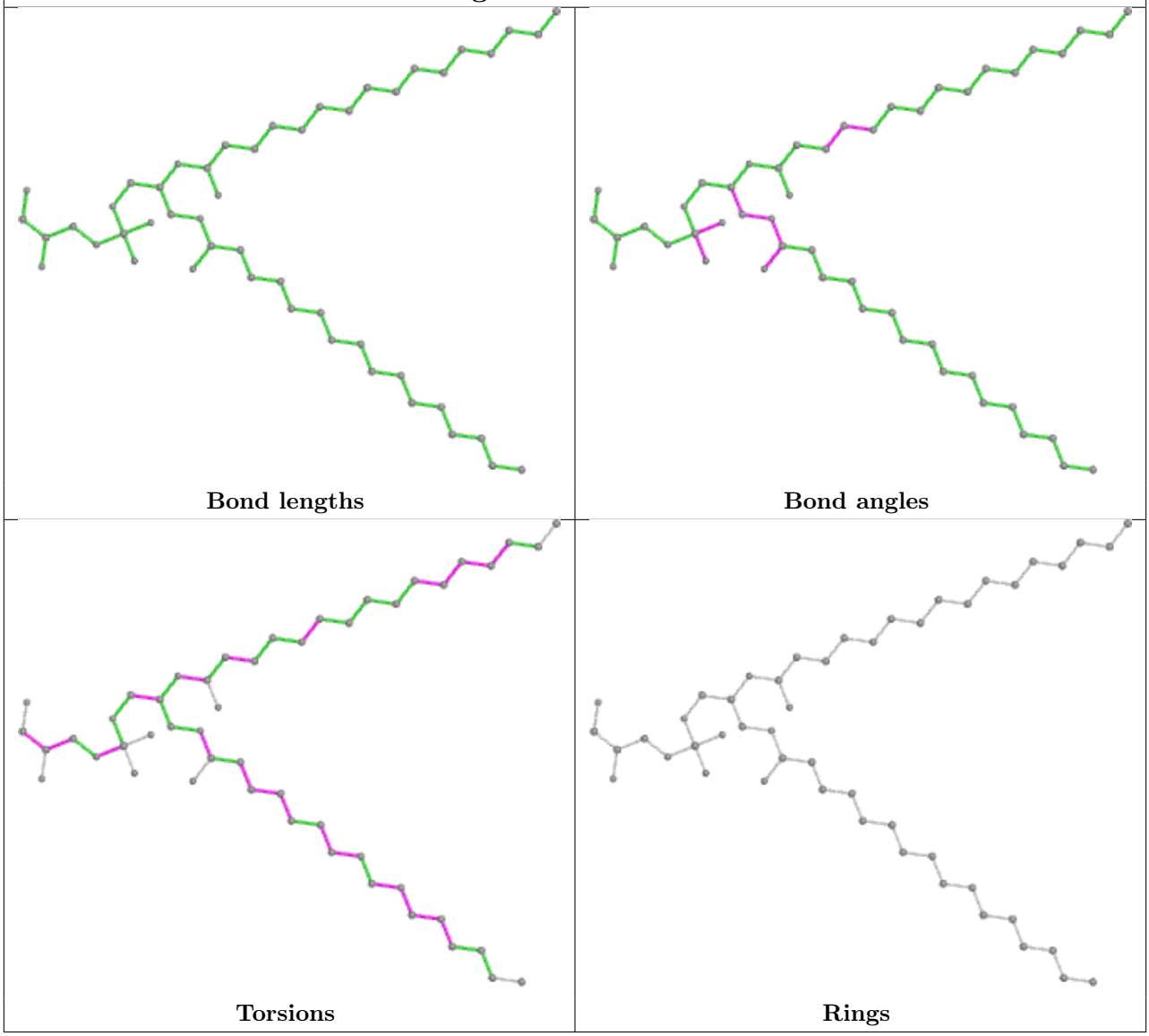


Rings

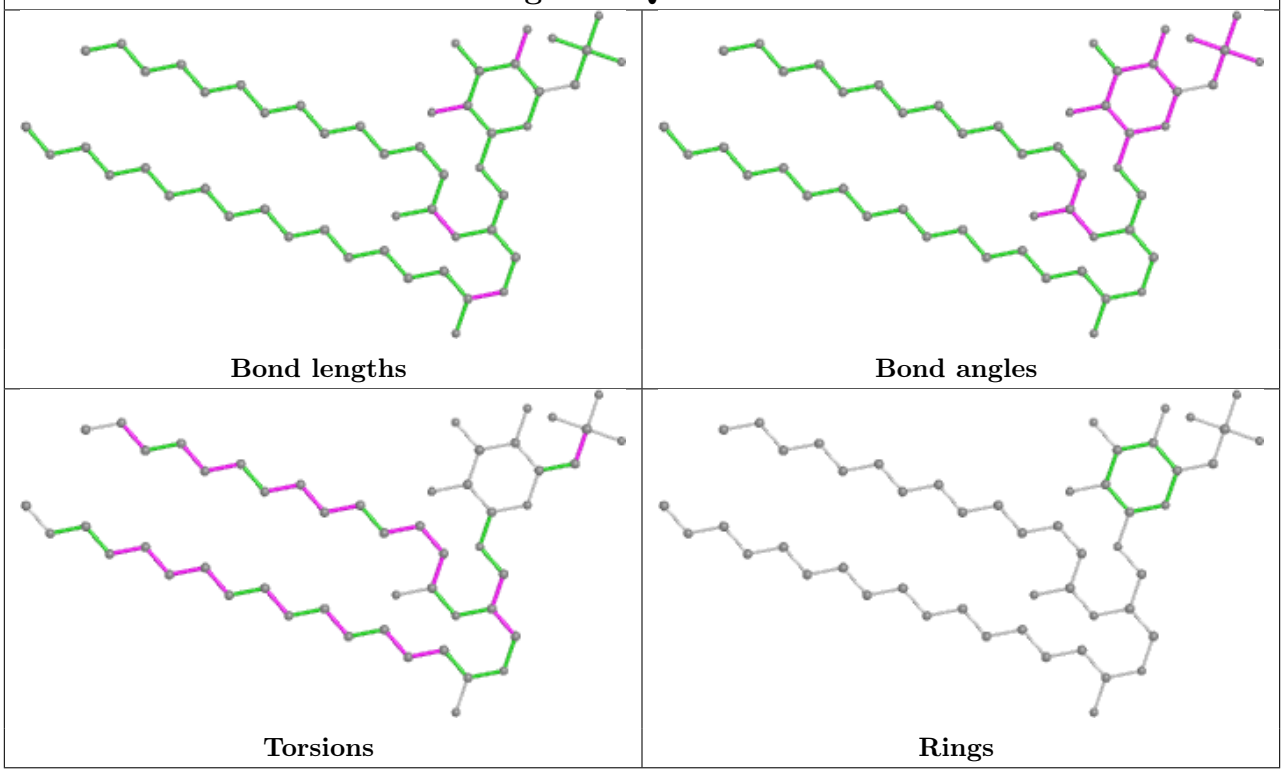
Ligand LMG m 101



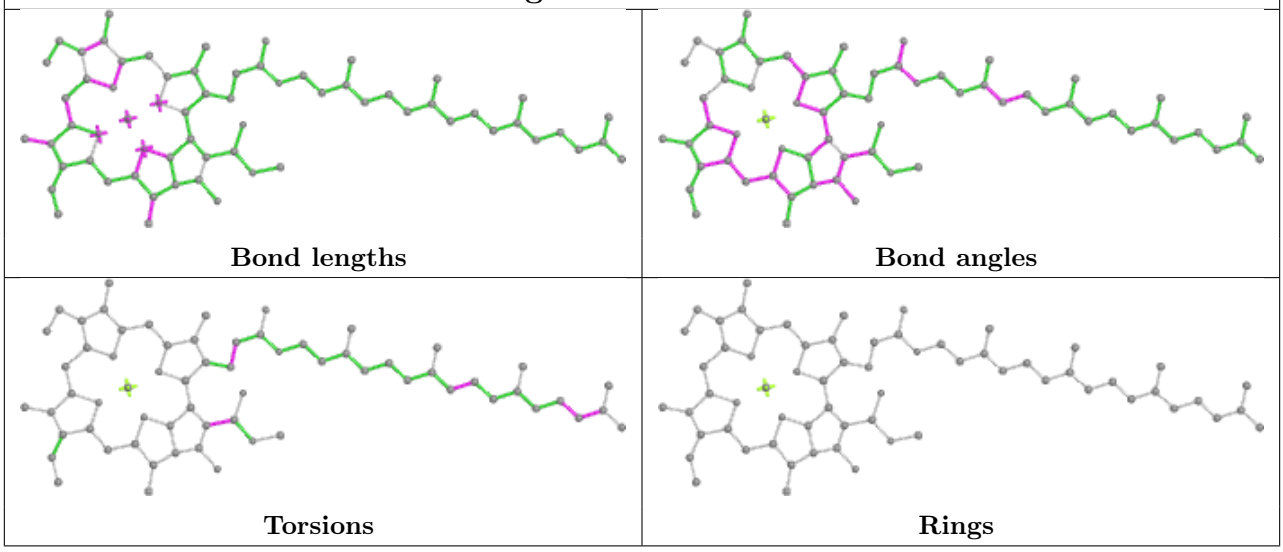
Ligand LHG d 405



Ligand SQD A 614



Ligand CLA B 606



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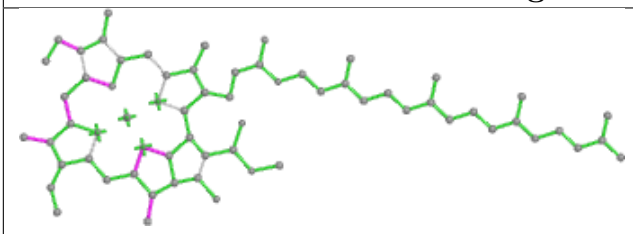
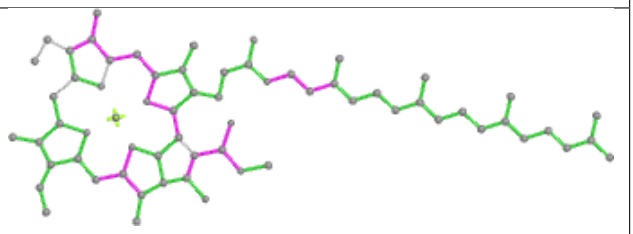
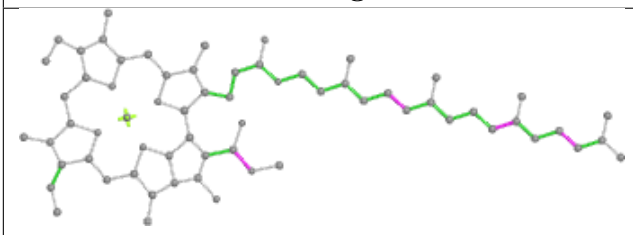


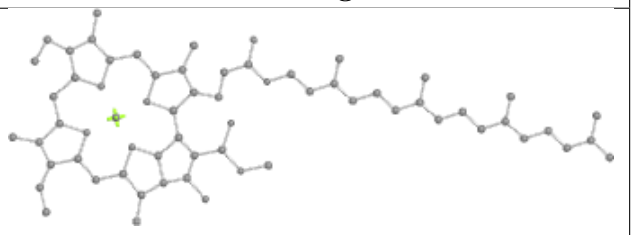
Bond lengths



Bond angles

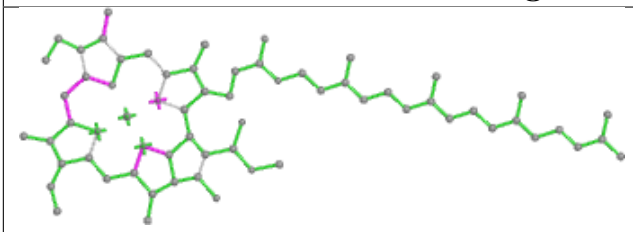


Torsions



Rings

Ligand CLA C 513



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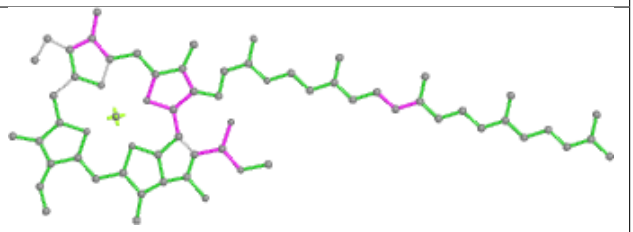
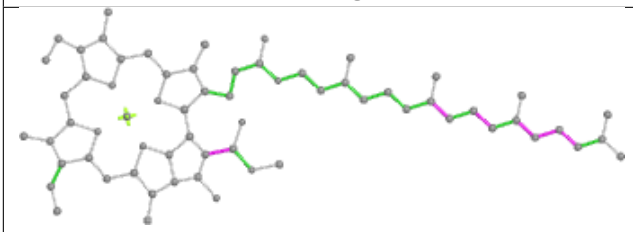
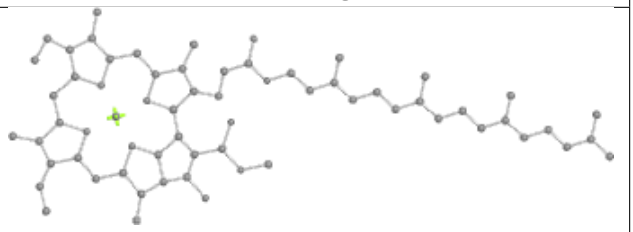


Bond angles

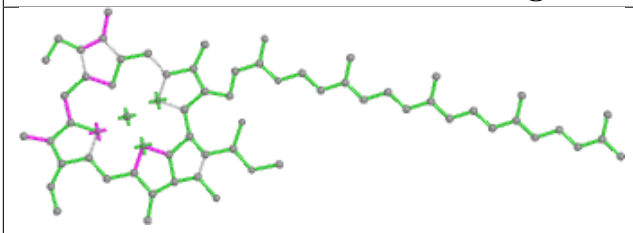


Torsions



Rings

Ligand CLA b 604



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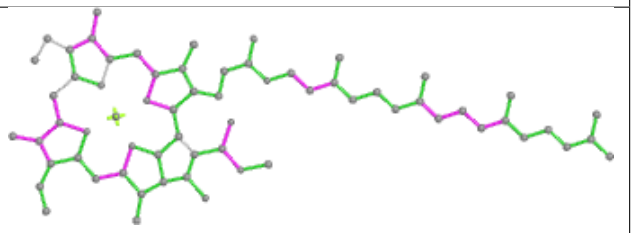
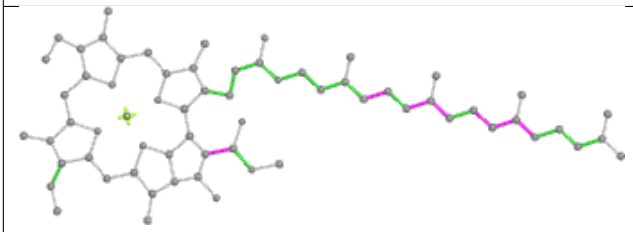


Bond angles



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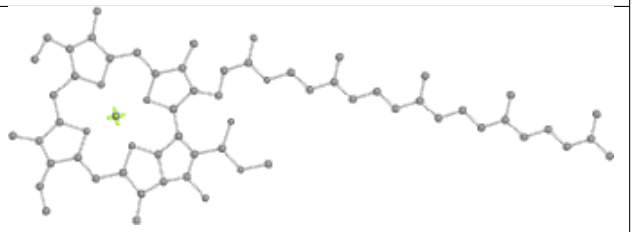
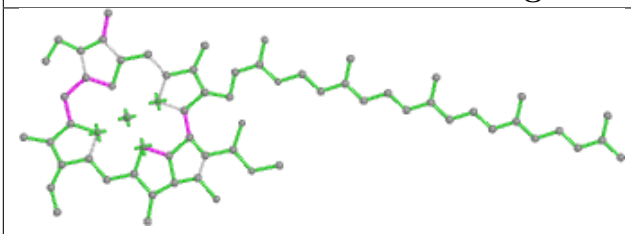


Rings

Ligand CLA B 612



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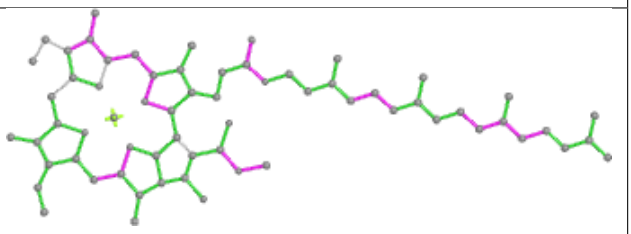
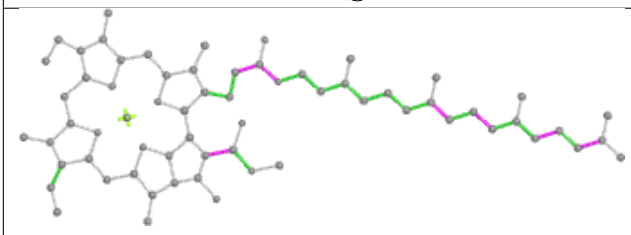
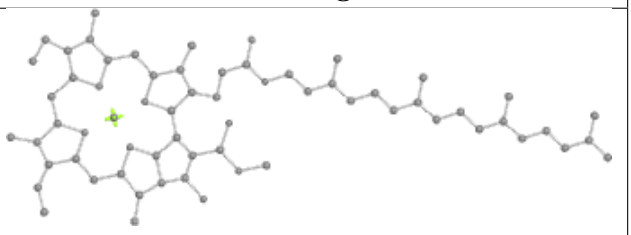


Bond angles

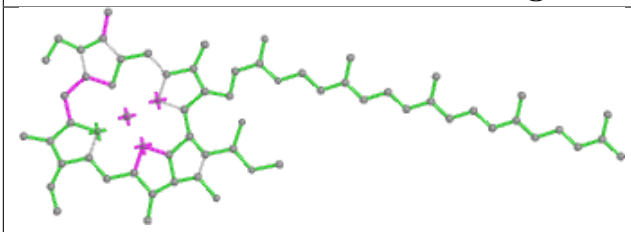


Torsions



Rings

Ligand CLA b 605



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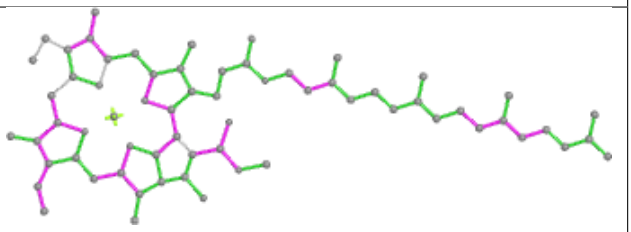
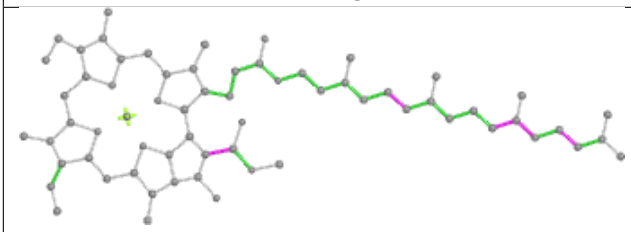


Bond angles



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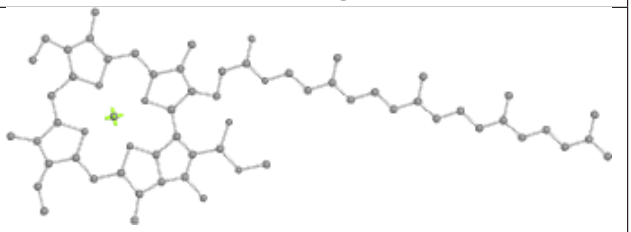
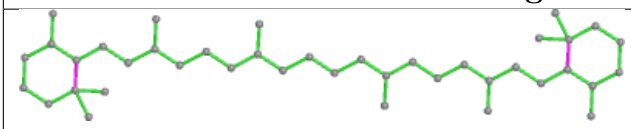
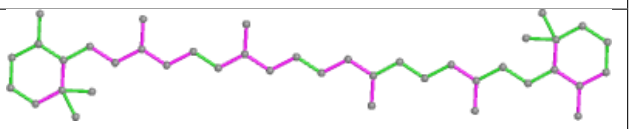


Rings

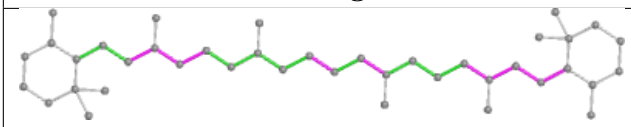
Ligand BCR h 102



Bond lengths



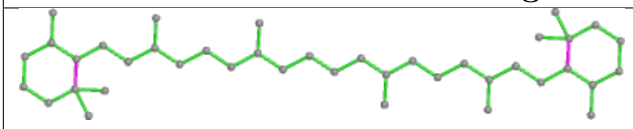
Bond angles



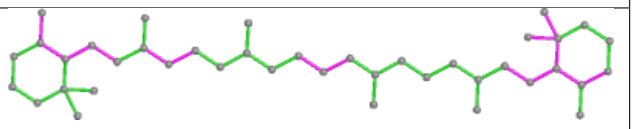
Torsions

Rings

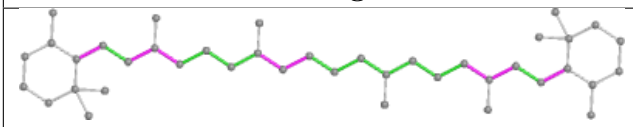
Ligand BCR Y 101



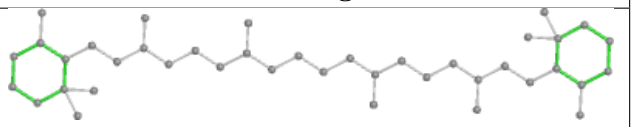
Bond lengths



Bond angles

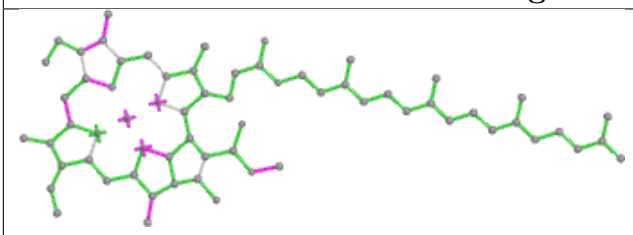


Torsions



Rings

Ligand CLA a 612



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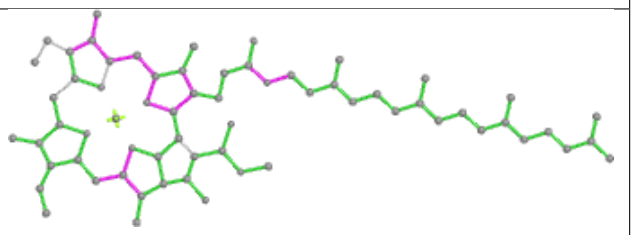

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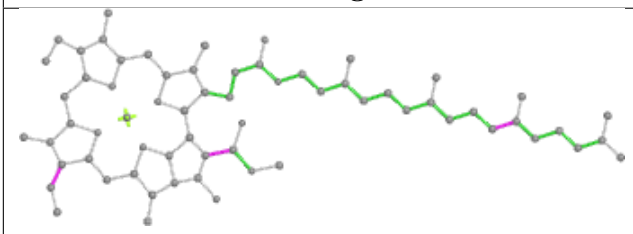

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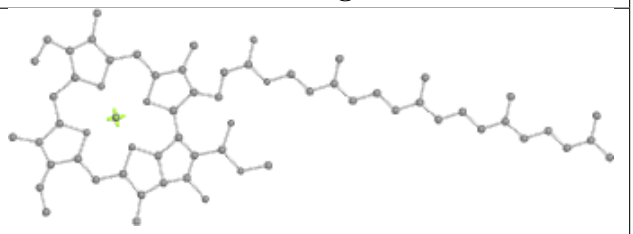
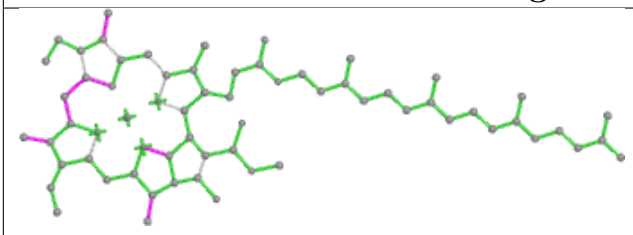


Rings

Ligand CLA c 502



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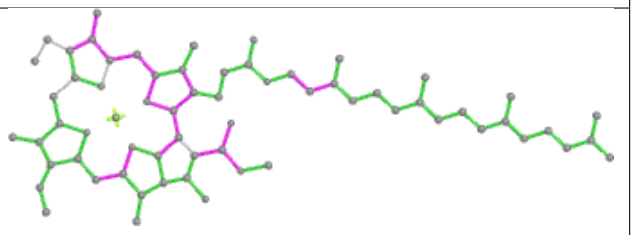

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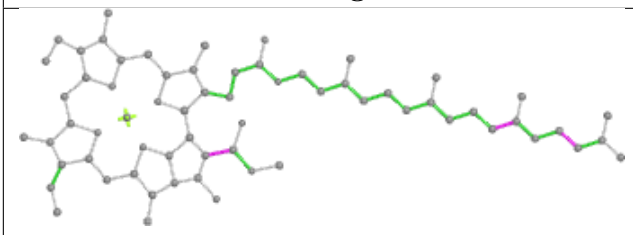

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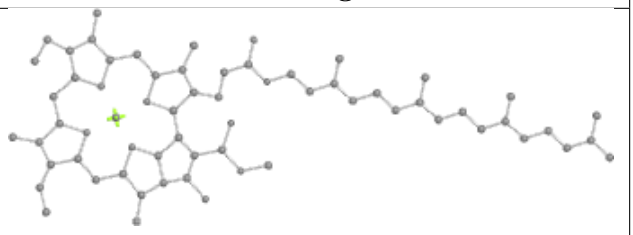
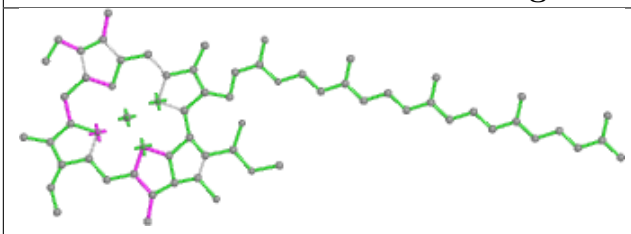


Rings

Ligand CLA c 512



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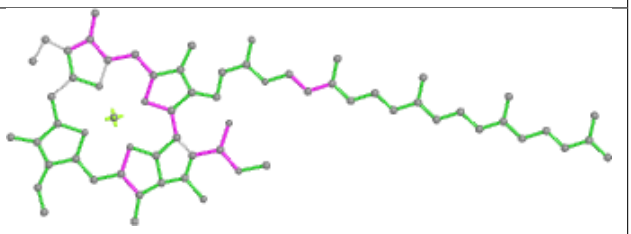

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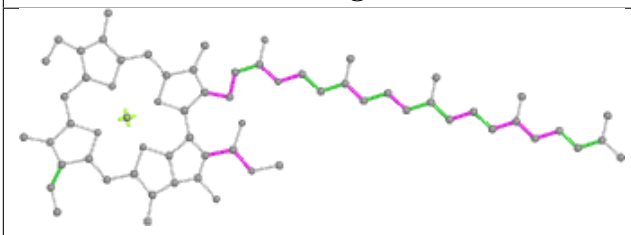

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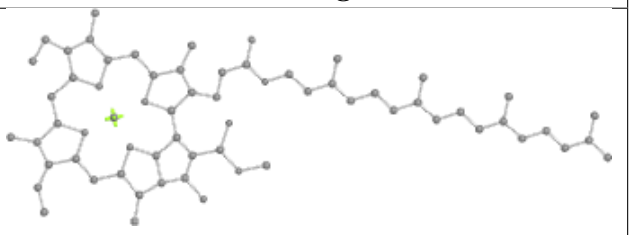
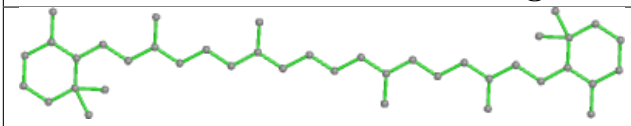


Rings

Ligand BCR k 102



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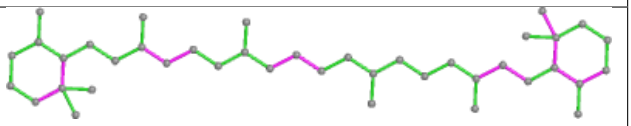
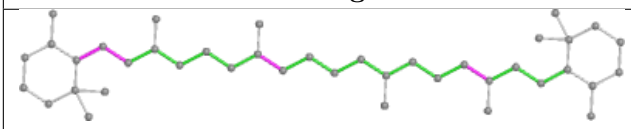


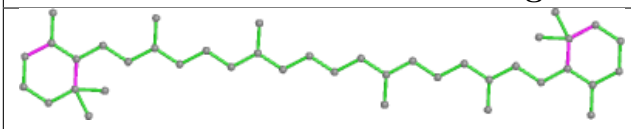
Bond angles



Torsions

Rings

Ligand BCR b 618



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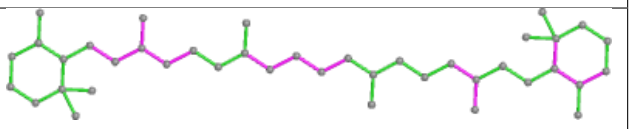
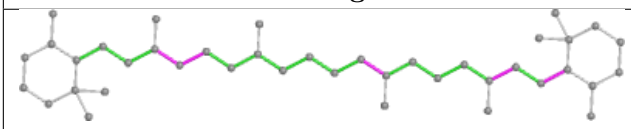


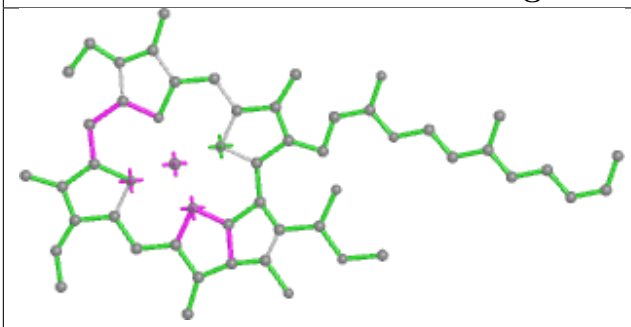
Bond angles



Torsions

Rings

Ligand CLA A 607



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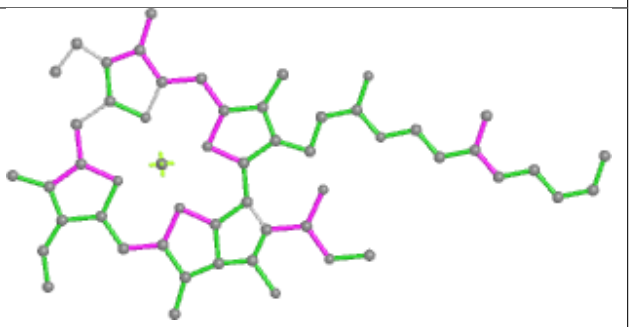
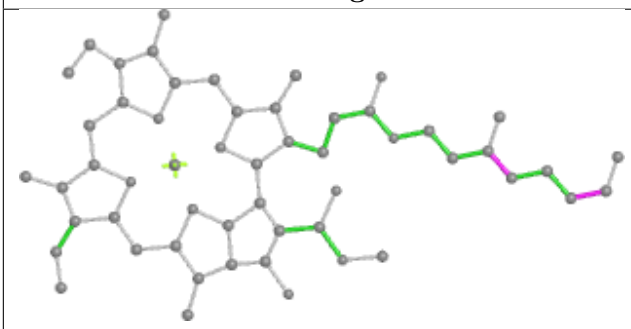


Bond angles



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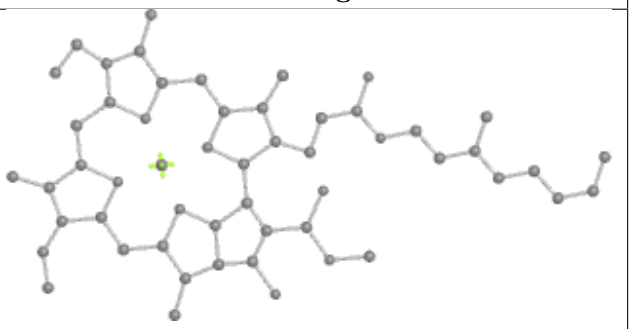
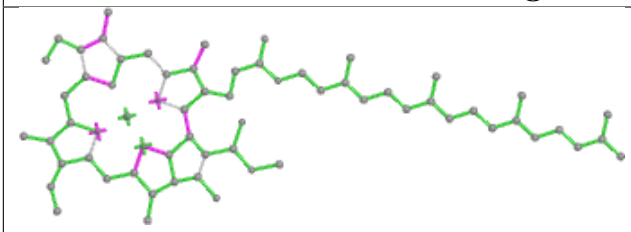


Rings

Ligand CLA B 603



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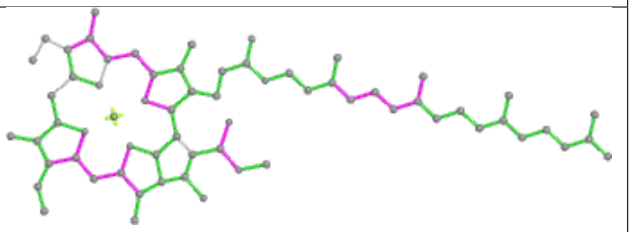

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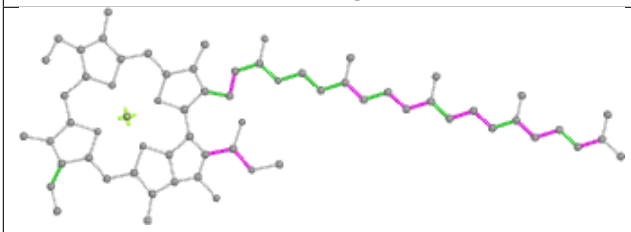

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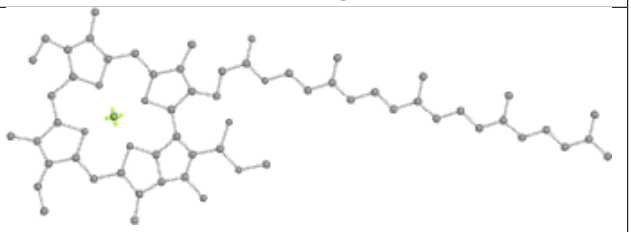
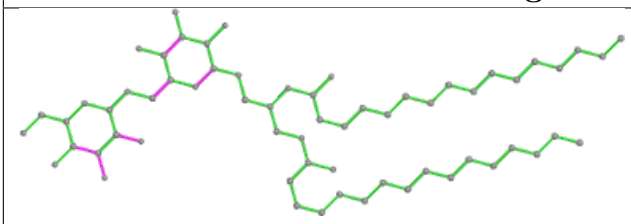


Rings

Ligand DGD c 516



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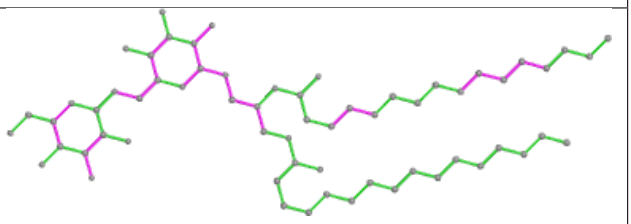
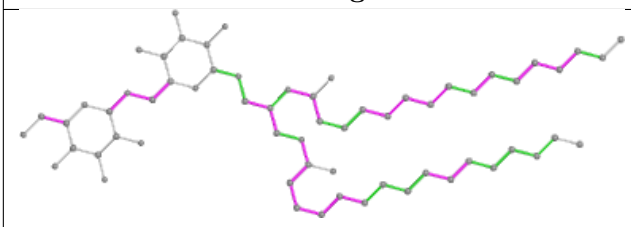
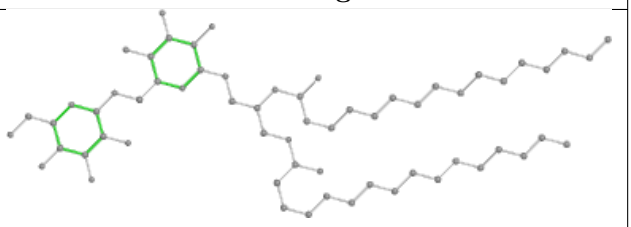


Bond angles

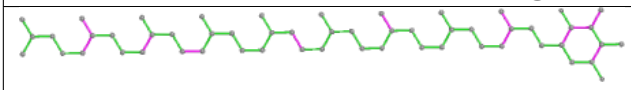


Torsions



Rings

Ligand PL9 D 407



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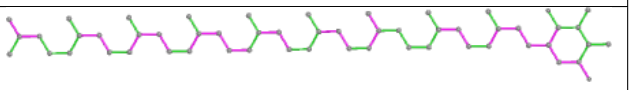
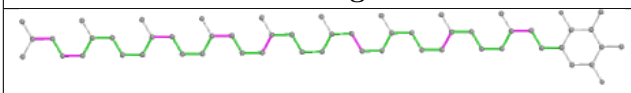


Bond angles



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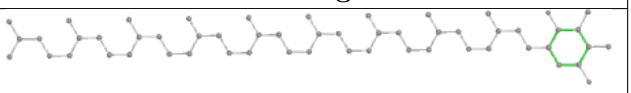
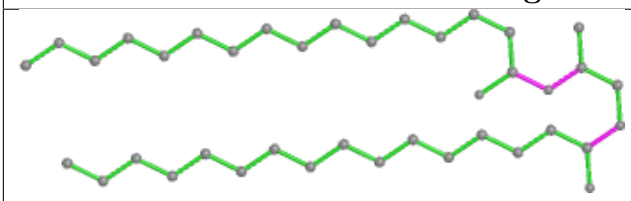


Rings

Ligand SQD A 616



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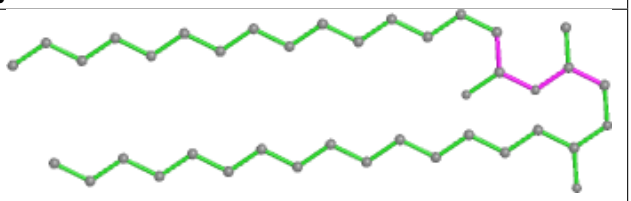
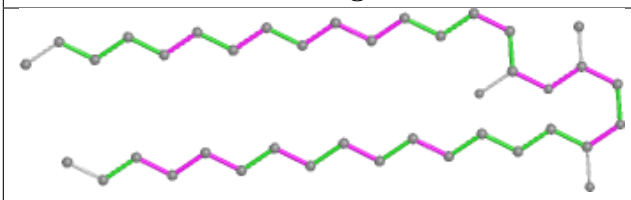
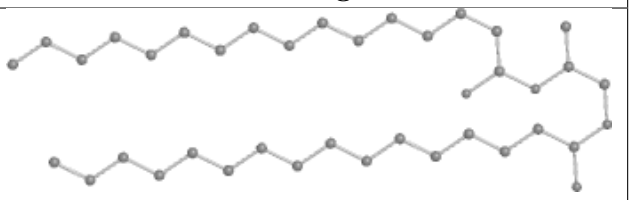


Bond angles

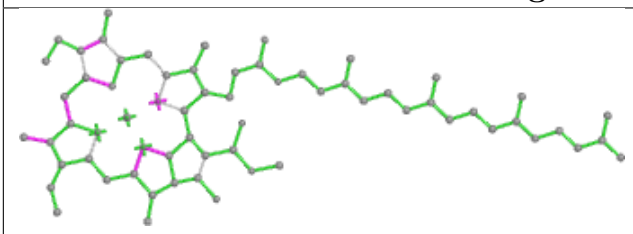


Torsions



Rings

Ligand CLA a 603



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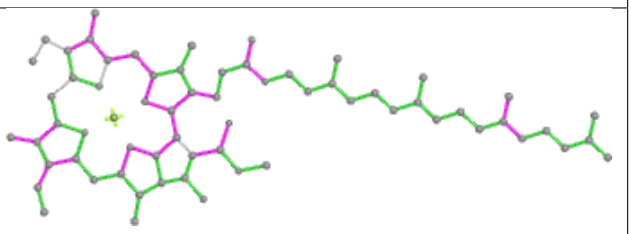
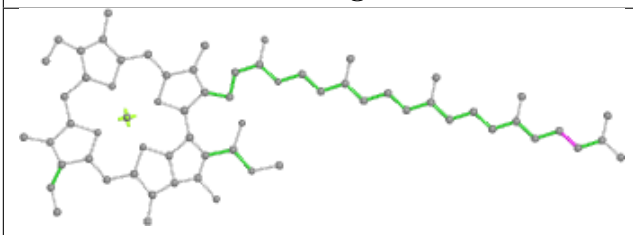


Bond angles



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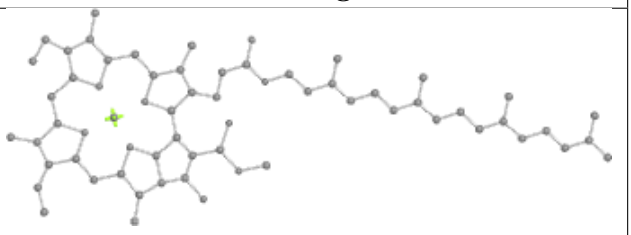
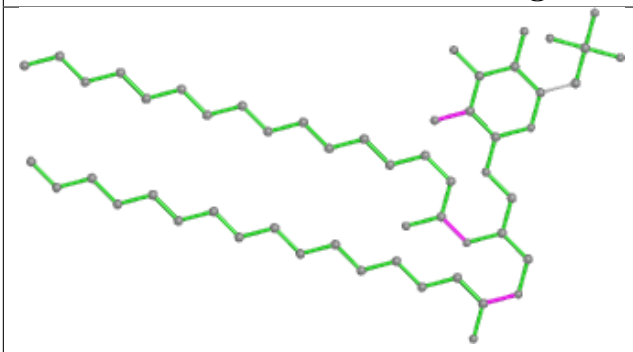


Rings

Ligand SQD a 613



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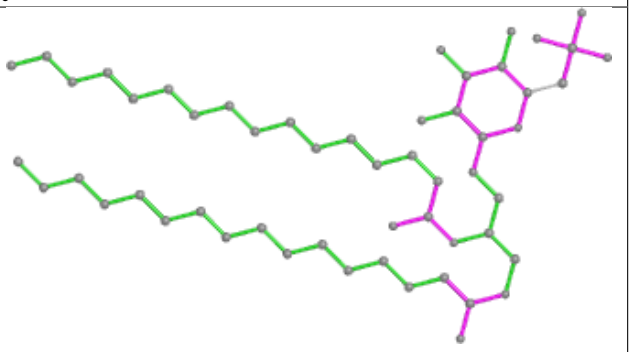
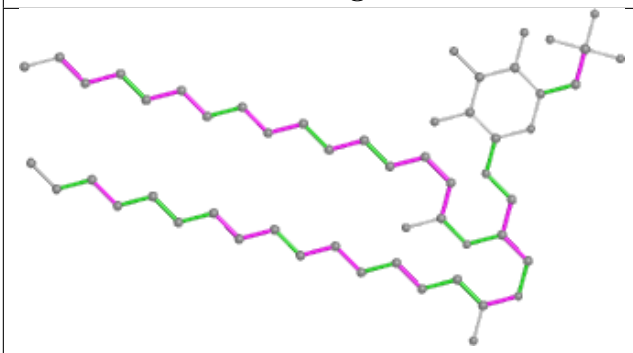
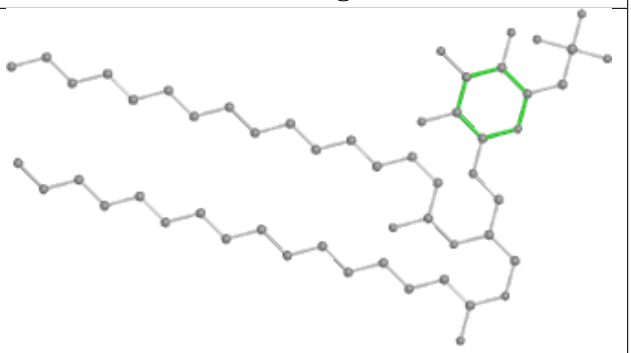


Bond angles

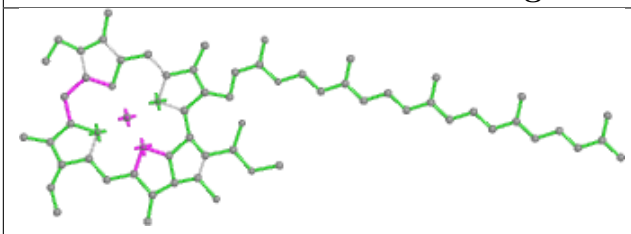


Torsions



Rings

Ligand CLA C 505



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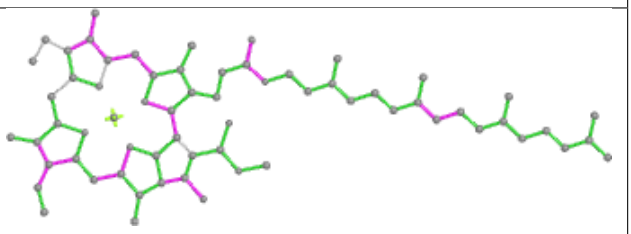
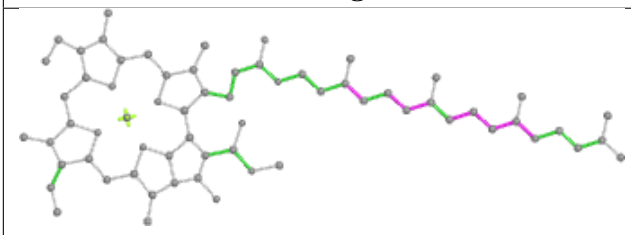
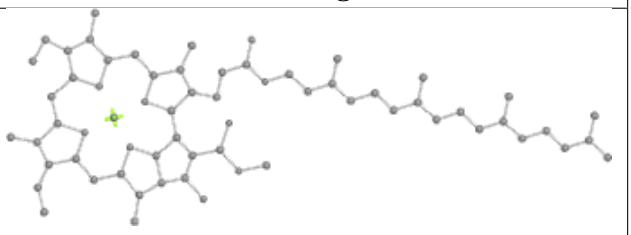


Bond angles

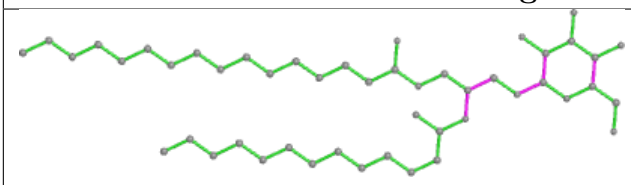


Torsions

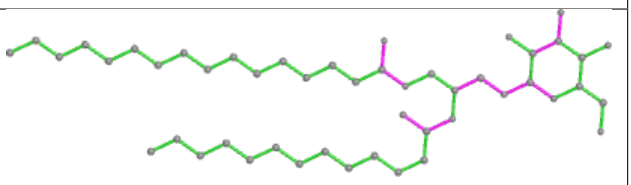


Rings

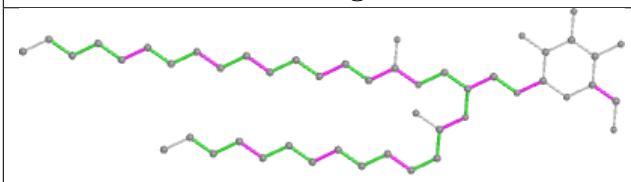
Ligand LMG C 519



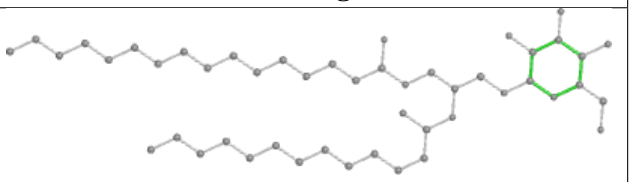
Bond lengths



Bond angles

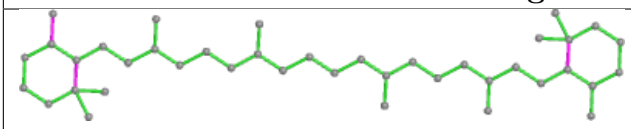


Torsions

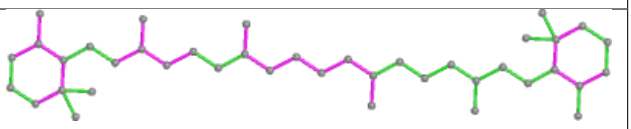


Rings

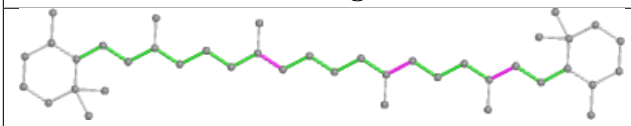
Ligand BCR c 515



Bond lengths



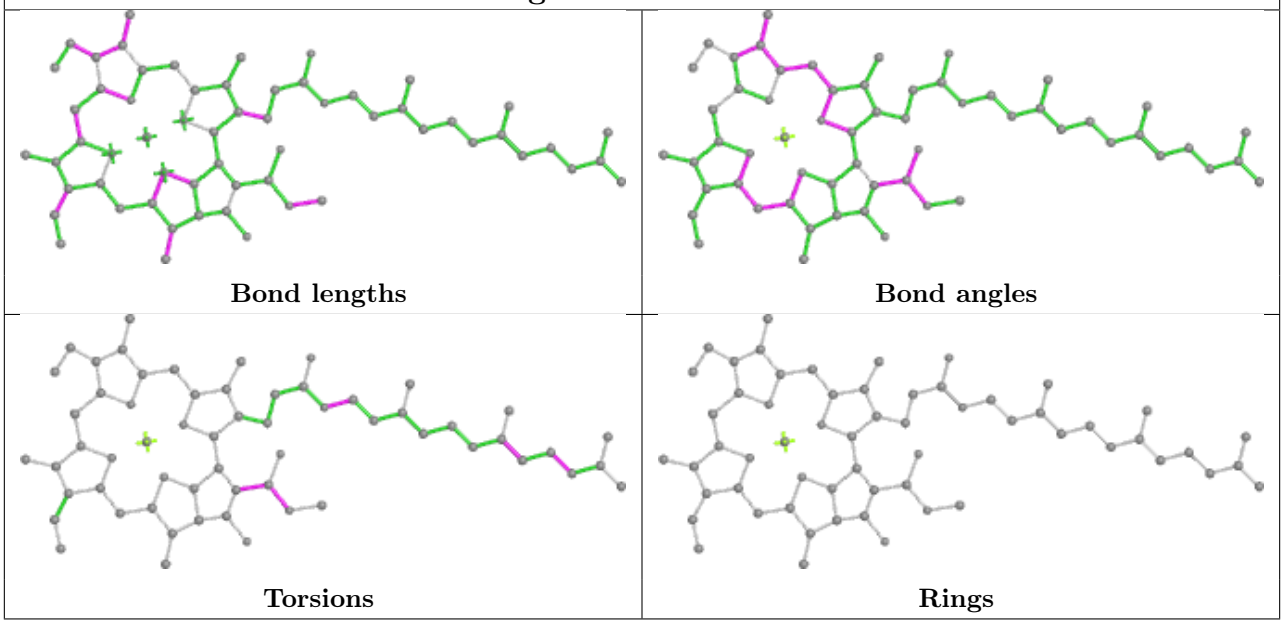
Bond angles



Torsions

Rings

Ligand CLA b 616



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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/334 (100%)	-0.49	3 (0%)	84	86	19, 26, 44, 75	0
1	a	334/334 (100%)	-0.45	2 (0%)	89	91	20, 28, 55, 78	0
2	B	505/505 (100%)	-0.42	5 (0%)	82	84	20, 30, 60, 94	0
2	b	505/505 (100%)	-0.30	13 (2%)	56	60	22, 34, 72, 106	0
3	C	442/451 (98%)	-0.36	3 (0%)	87	89	23, 34, 51, 75	0
3	c	451/451 (100%)	-0.31	5 (1%)	80	82	23, 38, 60, 101	0
4	D	341/341 (100%)	-0.39	0	100	100	20, 28, 44, 84	0
4	d	341/341 (100%)	-0.38	2 (0%)	89	91	20, 32, 57, 76	0
5	E	81/82 (98%)	0.06	4 (4%)	29	31	30, 48, 69, 87	0
5	e	82/82 (100%)	0.24	4 (4%)	29	31	36, 57, 81, 89	0
6	F	34/34 (100%)	-0.38	1 (2%)	51	56	33, 40, 57, 80	0
6	f	34/34 (100%)	-0.20	1 (2%)	51	56	41, 49, 80, 86	0
7	H	65/65 (100%)	-0.08	2 (3%)	49	53	30, 37, 58, 71	0
7	h	63/65 (96%)	0.07	1 (1%)	72	74	38, 48, 56, 70	0
8	I	35/36 (97%)	-0.28	1 (2%)	51	56	28, 35, 68, 73	0
8	i	35/36 (97%)	-0.25	1 (2%)	51	56	30, 38, 68, 73	0
9	J	36/36 (100%)	0.23	4 (11%)	5	5	32, 46, 77, 91	0
9	j	36/36 (100%)	0.31	5 (13%)	2	2	36, 49, 85, 89	0
10	K	37/37 (100%)	-0.23	0	100	100	39, 49, 63, 69	0
10	k	37/37 (100%)	0.10	1 (2%)	54	59	45, 54, 70, 75	0
11	L	37/37 (100%)	-0.42	0	100	100	22, 26, 63, 70	0
11	l	36/37 (97%)	-0.39	0	100	100	23, 27, 66, 79	0
12	M	32/33 (96%)	-0.28	1 (3%)	49	53	24, 31, 64, 72	0
12	m	31/33 (93%)	-0.29	0	100	100	26, 32, 45, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.09	11 (4%) 33 35	22, 40, 79, 136	0
13	o	244/244 (100%)	-0.18	13 (5%) 26 28	22, 38, 78, 134	0
14	R	34/34 (100%)	1.73	12 (35%) 0 0	58, 68, 84, 92	0
14	r	31/34 (91%)	2.51	18 (58%) 0 0	66, 85, 99, 104	0
15	T	29/30 (96%)	-0.67	2 (6%) 16 18	24, 28, 58, 70	0
15	t	29/30 (96%)	-0.51	2 (6%) 16 18	23, 28, 75, 90	0
16	U	97/97 (100%)	-0.29	3 (3%) 49 53	28, 40, 67, 94	0
16	u	97/97 (100%)	-0.49	1 (1%) 82 84	28, 37, 56, 88	0
17	V	137/137 (100%)	-0.57	0 100 100	25, 38, 54, 80	0
17	v	137/137 (100%)	-0.23	2 (1%) 73 76	31, 44, 67, 81	0
18	X	38/38 (100%)	0.05	3 (7%) 12 13	35, 49, 74, 82	0
18	x	38/38 (100%)	0.44	3 (7%) 12 13	45, 58, 83, 98	0
19	Y	27/30 (90%)	1.72	9 (33%) 0 0	51, 74, 114, 117	0
19	y	30/30 (100%)	0.88	5 (16%) 1 1	54, 72, 96, 103	0
20	Z	62/62 (100%)	0.74	15 (24%) 0 0	48, 62, 114, 126	0
20	z	62/62 (100%)	0.94	12 (19%) 1 0	54, 70, 109, 121	0
All	All	5300/5326 (99%)	-0.24	170 (3%) 47 52	19, 35, 72, 136	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	z	33	TRP	8.8
13	o	3	GLN	8.1
13	O	3	GLN	8.0
18	X	2	THR	7.1
19	Y	20	ALA	7.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.94	0.12	36,45,71,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	FME	T	1	10/11	0.94	0.12	27,45,71,71	0
8	FME	i	1	10/11	0.95	0.12	35,43,56,58	0
8	FME	I	1	10/11	0.96	0.12	34,47,61,64	0
15	FME	t	1	10/11	0.96	0.08	19,33,65,69	0
12	FME	m	1	10/11	0.97	0.12	26,49,72,73	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	UNL	c	523	28/-	0.72	0.20	45,67,86,88	0
33	UNL	a	617	28/-	0.75	0.30	42,65,78,78	0
33	UNL	H	103	53/-	0.78	0.22	45,74,95,103	0
30	LHG	A	615	49/49	0.78	0.22	48,80,108,117	0
33	UNL	c	520	55/-	0.78	0.17	34,54,93,94	0
33	UNL	E	101	28/-	0.78	0.31	45,71,88,95	0
33	UNL	B	628	28/-	0.80	0.39	52,70,102,107	0
28	LMG	c	521	48/55	0.80	0.25	39,81,114,121	0
28	LMG	D	409	33/55	0.80	0.16	34,53,93,95	0
29	SQD	a	615	36/54	0.81	0.18	30,66,85,87	0
33	UNL	B	627	47/-	0.81	0.32	44,63,79,79	0
33	UNL	b	620	55/-	0.82	0.20	37,60,83,90	0
33	UNL	b	623	55/-	0.82	0.17	42,64,85,85	0
33	UNL	m	102	28/-	0.82	0.16	42,63,77,78	0
33	UNL	x	101	55/-	0.82	0.19	39,58,75,75	0
27	PL9	a	611	55/55	0.83	0.20	38,69,88,94	0
28	LMG	d	410	23/55	0.83	0.19	31,71,94,98	0
33	UNL	t	103	26/-	0.83	0.20	35,59,76,83	0
28	LMG	b	621	55/55	0.83	0.27	40,76,103,112	0
31	DGD	A	617	66/66	0.84	0.18	42,64,85,111	0
33	UNL	C	523	47/-	0.84	0.11	37,53,71,75	0
27	PL9	A	611	55/55	0.84	0.23	35,58,81,84	135
23	CLA	c	513	65/65	0.85	0.19	44,69,104,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	DGD	a	616	44/66	0.85	0.15	33,56,77,89	0
33	UNL	B	621	43/-	0.85	0.13	31,50,71,76	0
25	BCR	h	102	40/40	0.85	0.14	35,54,74,82	0
23	CLA	c	512	65/65	0.86	0.14	38,55,94,108	0
33	UNL	b	622	40/-	0.86	0.14	43,59,81,83	0
30	LHG	a	614	42/49	0.86	0.26	58,86,109,122	0
23	CLA	C	513	65/65	0.86	0.16	43,62,88,97	0
23	CLA	h	101	65/65	0.86	0.15	41,62,91,97	0
25	BCR	H	101	40/40	0.86	0.11	29,45,59,68	0
33	UNL	T	102	47/-	0.86	0.17	35,51,66,74	0
33	UNL	B	626	46/-	0.86	0.14	39,59,72,77	0
29	SQD	b	601	49/54	0.87	0.13	39,58,99,111	0
25	BCR	Y	101	40/40	0.87	0.13	33,53,73,76	0
33	UNL	b	624	26/-	0.87	0.22	39,54,65,72	0
33	UNL	I	101	41/-	0.87	0.15	36,53,72,79	0
29	SQD	B	624	54/54	0.88	0.14	37,59,97,109	0
28	LMG	c	519	37/55	0.88	0.16	38,69,88,92	0
25	BCR	k	101	40/40	0.88	0.12	44,63,75,80	0
29	SQD	f	101	41/54	0.88	0.19	45,84,111,119	0
33	UNL	J	101	28/-	0.88	0.13	48,62,68,70	0
28	LMG	B	622	28/55	0.88	0.15	31,48,58,63	0
33	UNL	d	411	43/-	0.88	0.16	39,55,66,70	0
33	UNL	l	102	53/-	0.88	0.15	25,48,87,99	0
33	UNL	T	103	44/-	0.88	0.18	38,57,79,84	0
33	UNL	X	101	55/-	0.88	0.21	33,52,73,79	0
29	SQD	A	616	39/54	0.88	0.16	41,65,88,92	0
33	UNL	j	101	28/-	0.89	0.12	46,61,70,74	0
23	CLA	C	512	65/65	0.89	0.15	31,53,103,112	0
28	LMG	c	522	49/55	0.89	0.14	32,56,91,110	0
33	UNL	t	102	34/-	0.89	0.13	35,50,56,63	0
23	CLA	B	616	60/65	0.89	0.15	21,39,94,99	0
28	LMG	C	519	48/55	0.89	0.16	46,73,95,106	0
28	LMG	A	612	48/55	0.90	0.15	31,56,74,91	0
33	UNL	M	102	26/-	0.91	0.14	30,50,60,62	0
23	CLA	D	403	65/65	0.91	0.13	19,39,104,113	0
33	UNL	C	521	28/-	0.91	0.09	28,40,53,66	0
33	UNL	C	522	28/-	0.91	0.12	43,54,64,66	0
28	LMG	B	620	51/55	0.91	0.11	25,49,73,87	0
28	LMG	m	101	51/55	0.91	0.12	33,51,81,98	0
33	UNL	B	625	28/-	0.91	0.11	26,48,64,71	0
23	CLA	a	606	65/65	0.91	0.14	17,34,86,104	0
23	CLA	b	616	60/65	0.91	0.14	25,42,90,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	615	65/65	0.92	0.11	25,40,55,65	0
23	CLA	d	403	65/65	0.92	0.14	31,48,100,105	0
25	BCR	k	102	40/40	0.92	0.15	36,51,72,74	0
23	CLA	B	615	65/65	0.92	0.12	22,37,67,83	0
25	BCR	C	515	40/40	0.92	0.11	21,35,50,54	0
31	DGD	h	103	62/66	0.92	0.11	31,48,61,74	0
25	BCR	D	404	40/40	0.92	0.10	28,43,98,109	0
23	CLA	c	508	64/65	0.92	0.12	28,44,83,104	0
23	CLA	B	601	65/65	0.92	0.14	25,60,104,130	0
29	SQD	a	613	54/54	0.92	0.13	39,67,93,101	0
25	BCR	c	514	40/40	0.92	0.15	39,60,71,72	0
25	BCR	d	404	40/40	0.92	0.11	32,51,90,97	0
23	CLA	b	604	65/65	0.93	0.15	20,34,80,90	0
30	LHG	d	409	39/49	0.93	0.12	27,47,66,70	0
25	BCR	C	514	40/40	0.93	0.11	35,54,66,68	0
31	DGD	C	517	62/66	0.93	0.12	32,51,107,118	0
31	DGD	H	102	62/66	0.93	0.11	30,48,61,73	0
23	CLA	c	510	65/65	0.93	0.13	33,49,67,74	0
28	LMG	D	405	51/55	0.93	0.14	26,54,98,102	0
33	UNL	M	101	37/-	0.93	0.11	31,43,63,70	0
23	CLA	b	606	65/65	0.93	0.11	20,38,69,74	0
23	CLA	c	503	65/65	0.93	0.14	32,44,57,62	0
23	CLA	c	507	65/65	0.93	0.14	23,42,57,66	0
25	BCR	b	617	40/40	0.93	0.10	24,42,54,58	0
25	BCR	b	618	40/40	0.93	0.09	25,37,53,60	0
23	CLA	C	510	65/65	0.94	0.12	28,45,67,73	0
23	CLA	C	511	65/65	0.94	0.11	28,50,68,68	0
23	CLA	c	502	65/65	0.94	0.13	28,41,65,67	0
28	LMG	d	406	44/55	0.94	0.13	31,54,94,113	0
23	CLA	A	604	65/65	0.94	0.12	14,33,101,121	0
23	CLA	c	504	60/65	0.94	0.12	31,45,79,90	0
25	BCR	b	619	40/40	0.94	0.11	25,47,58,64	0
23	CLA	c	505	65/65	0.94	0.14	22,41,66,73	0
29	SQD	F	101	36/54	0.94	0.12	45,67,87,92	0
23	CLA	c	506	65/65	0.94	0.13	31,52,107,111	0
23	CLA	B	606	65/65	0.94	0.10	17,32,74,80	0
23	CLA	C	503	65/65	0.94	0.09	24,39,51,63	0
23	CLA	a	604	65/65	0.94	0.12	26,40,89,107	0
25	BCR	t	101	40/40	0.94	0.08	24,36,57,63	0
23	CLA	c	511	65/65	0.94	0.13	36,54,72,75	0
27	PL9	D	407	55/55	0.94	0.11	20,31,40,48	0
23	CLA	C	505	65/65	0.94	0.16	20,39,71,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	DGD	C	516	62/66	0.94	0.11	21,41,76,90	0
23	CLA	b	602	65/65	0.94	0.14	23,41,65,75	0
31	DGD	C	518	62/66	0.94	0.10	25,44,75,84	0
23	CLA	C	506	65/65	0.94	0.12	25,40,101,113	0
23	CLA	C	507	65/65	0.94	0.12	20,38,60,68	0
31	DGD	c	517	62/66	0.94	0.11	29,50,83,96	0
31	DGD	c	518	62/66	0.94	0.11	27,50,77,91	0
25	BCR	A	608	40/40	0.94	0.09	20,32,40,46	0
25	BCR	B	618	40/40	0.94	0.08	21,37,56,56	0
23	CLA	b	609	65/65	0.94	0.13	27,45,69,79	0
23	CLA	b	613	65/65	0.94	0.12	18,32,65,75	0
23	CLA	C	501	65/65	0.95	0.11	23,35,49,60	0
27	PL9	d	408	55/55	0.95	0.10	21,33,43,47	0
25	BCR	C	520	40/40	0.95	0.15	36,51,66,69	0
30	LHG	B	623	49/49	0.95	0.11	25,42,70,73	0
23	CLA	C	502	65/65	0.95	0.10	26,40,54,61	0
30	LHG	d	405	49/49	0.95	0.12	35,50,72,88	0
23	CLA	b	612	65/65	0.95	0.13	16,33,47,56	0
25	BCR	T	101	40/40	0.95	0.08	25,42,61,68	0
23	CLA	c	509	65/65	0.95	0.15	28,46,64,68	0
25	BCR	a	607	40/40	0.95	0.08	15,31,41,49	0
23	CLA	A	607	54/65	0.95	0.12	15,28,62,69	0
23	CLA	b	614	65/65	0.95	0.13	22,36,77,87	0
23	CLA	D	402	65/65	0.95	0.10	16,30,56,64	0
31	DGD	c	516	62/66	0.95	0.11	19,41,75,84	0
23	CLA	B	609	65/65	0.95	0.10	23,35,58,66	0
25	BCR	c	515	40/40	0.95	0.10	28,41,52,71	0
23	CLA	c	501	65/65	0.95	0.12	27,38,49,55	0
23	CLA	B	614	65/65	0.95	0.12	20,34,82,95	0
29	SQD	A	614	52/54	0.95	0.13	31,58,84,89	0
23	CLA	A	603	65/65	0.95	0.10	13,25,44,57	0
25	BCR	B	617	40/40	0.95	0.09	25,39,53,56	0
23	CLA	C	508	65/65	0.95	0.10	23,40,100,118	0
25	BCR	B	619	40/40	0.95	0.09	20,39,59,66	0
23	CLA	B	604	65/65	0.95	0.11	18,31,82,93	0
24	PHO	a	605	64/64	0.96	0.11	18,29,38,43	0
24	PHO	d	401	64/64	0.96	0.11	25,38,46,65	0
23	CLA	C	504	59/65	0.96	0.12	24,42,80,85	0
23	CLA	B	612	65/65	0.96	0.12	19,30,44,44	0
23	CLA	a	603	65/65	0.96	0.09	16,29,43,51	0
30	LHG	D	406	49/49	0.96	0.11	22,38,54,65	0
23	CLA	B	613	65/65	0.96	0.11	17,30,68,73	0

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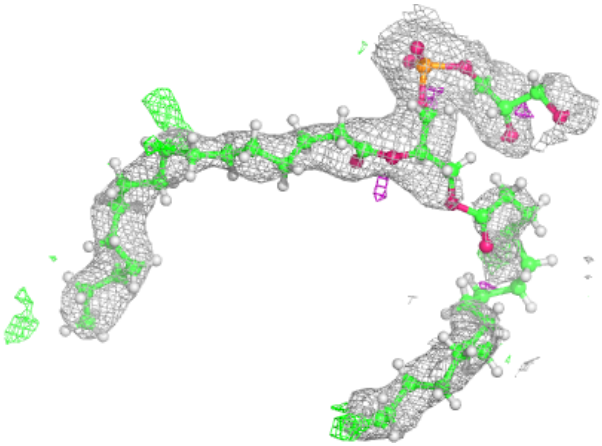
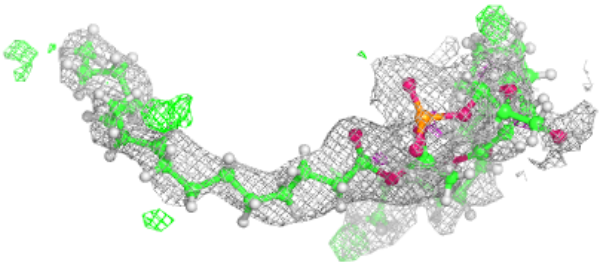
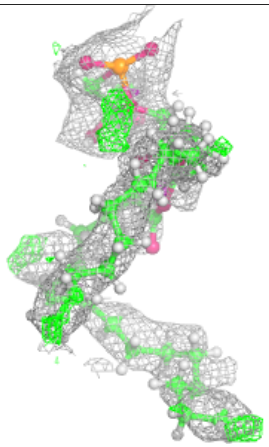
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	A	613	65/65	0.96	0.10	14,26,48,58	0
30	LHG	d	407	49/49	0.96	0.10	25,42,60,64	0
23	CLA	a	612	65/65	0.96	0.10	18,28,38,44	0
30	LHG	l	101	49/49	0.96	0.11	29,43,59,64	0
23	CLA	B	605	65/65	0.96	0.14	17,29,47,49	0
23	CLA	b	603	65/65	0.96	0.13	21,36,69,76	0
23	CLA	C	509	65/65	0.96	0.13	22,41,63,64	0
23	CLA	b	605	65/65	0.96	0.12	19,33,47,56	0
23	CLA	B	602	65/65	0.96	0.11	22,34,59,63	0
23	CLA	b	607	65/65	0.96	0.11	19,36,61,68	0
23	CLA	b	608	65/65	0.96	0.10	24,39,61,64	0
23	CLA	B	607	65/65	0.96	0.10	15,31,59,67	0
23	CLA	b	610	65/65	0.96	0.13	22,36,53,55	0
23	CLA	b	611	65/65	0.96	0.10	20,34,51,55	0
23	CLA	d	402	65/65	0.96	0.09	20,34,64,70	0
23	CLA	B	603	65/65	0.96	0.12	14,31,62,69	0
23	CLA	B	610	65/65	0.96	0.13	18,30,43,47	0
24	PHO	A	605	64/64	0.96	0.09	12,27,36,40	0
24	PHO	A	606	64/64	0.96	0.08	19,30,44,50	0
35	HEM	F	102	43/43	0.96	0.12	34,48,68,69	0
30	LHG	L	101	49/49	0.97	0.11	24,39,54,65	0
23	CLA	B	611	65/65	0.97	0.11	18,30,47,53	0
23	CLA	B	608	65/65	0.97	0.10	20,33,52,64	0
30	LHG	D	408	47/49	0.97	0.09	23,46,81,103	0
35	HEM	f	102	43/43	0.97	0.11	41,55,76,78	0
36	HEC	v	201	43/43	0.97	0.13	27,36,49,53	0
36	HEC	V	201	43/43	0.98	0.12	21,31,42,46	0
22	FE2	A	602	1/1	0.99	0.07	25,25,25,25	0
22	FE2	a	602	1/1	0.99	0.06	30,30,30,30	0
26	CL	A	609	1/1	0.99	0.05	27,27,27,27	0
32	OEY	A	618[B]	11/11	0.99	0.10	23,27,30,31	11
32	OEY	a	618[B]	11/11	0.99	0.11	22,28,30,31	11
26	CL	A	610	1/1	0.99	0.04	24,24,24,24	0
34	BCT	D	401	4/4	0.99	0.15	26,27,32,37	0
34	BCT	a	610	4/4	0.99	0.17	26,32,41,50	0
26	CL	a	608	1/1	0.99	0.06	25,25,25,25	0
26	CL	a	609	1/1	0.99	0.05	25,25,25,25	0
21	OEX	A	601[A]	10/10	0.99	0.10	21,25,28,32	10
21	OEX	a	601[A]	10/10	0.99	0.10	19,22,28,28	10

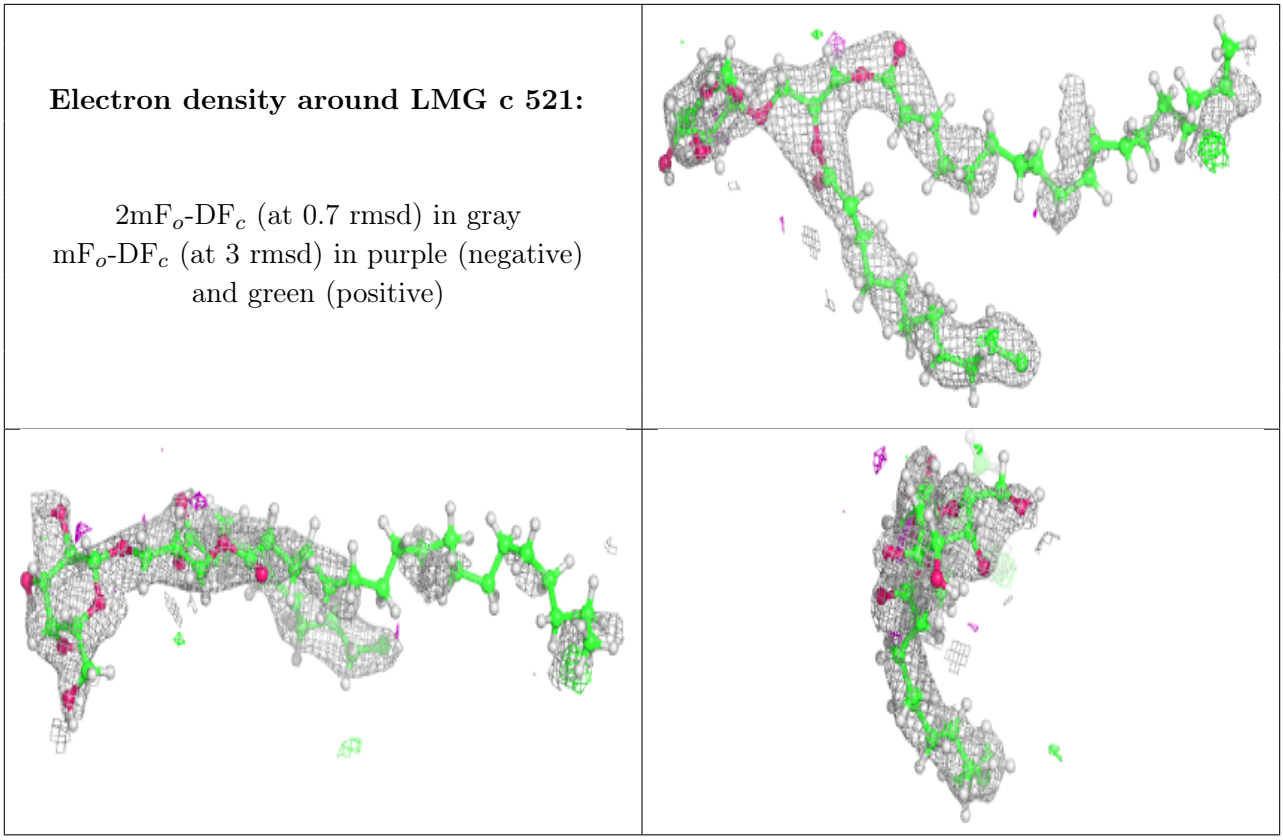
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around LHG A 615: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

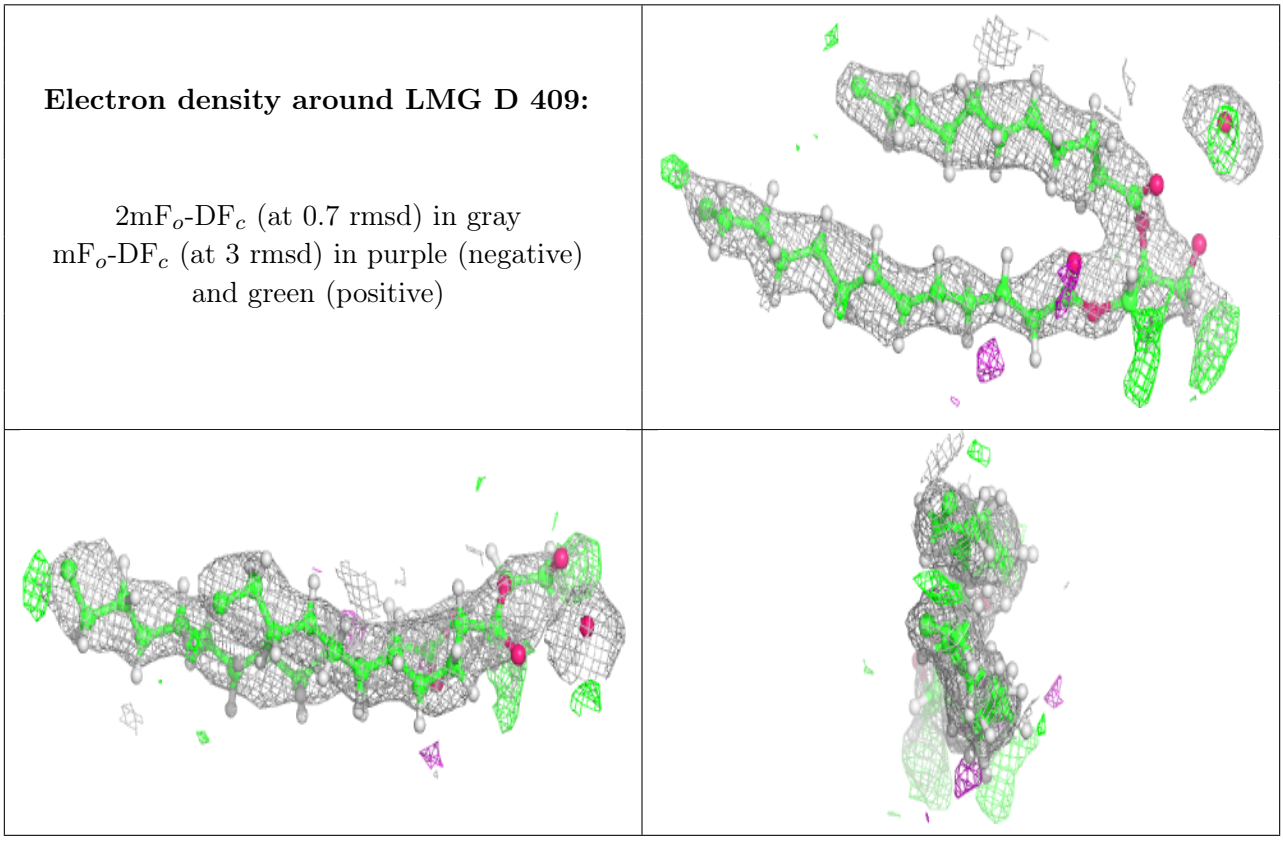
Electron density around LMG c 521:

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



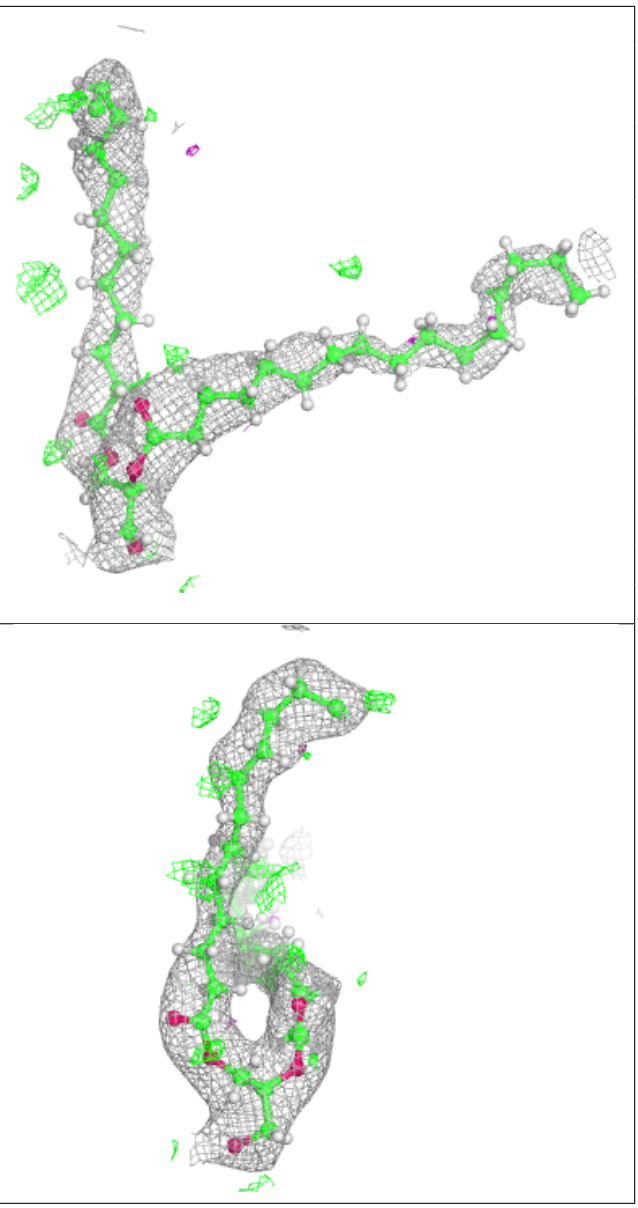
Electron density around LMG D 409:

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



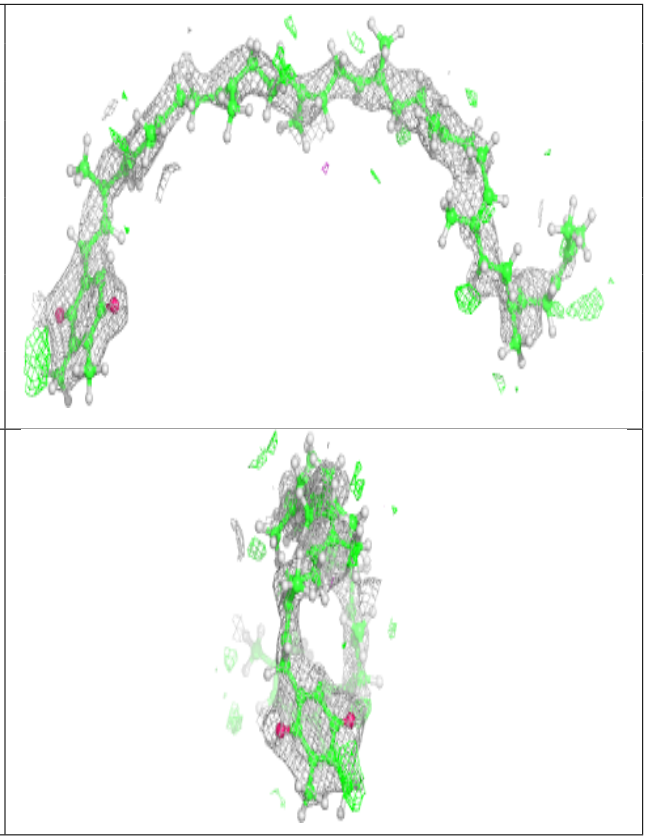
Electron density around SQD a 615:

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



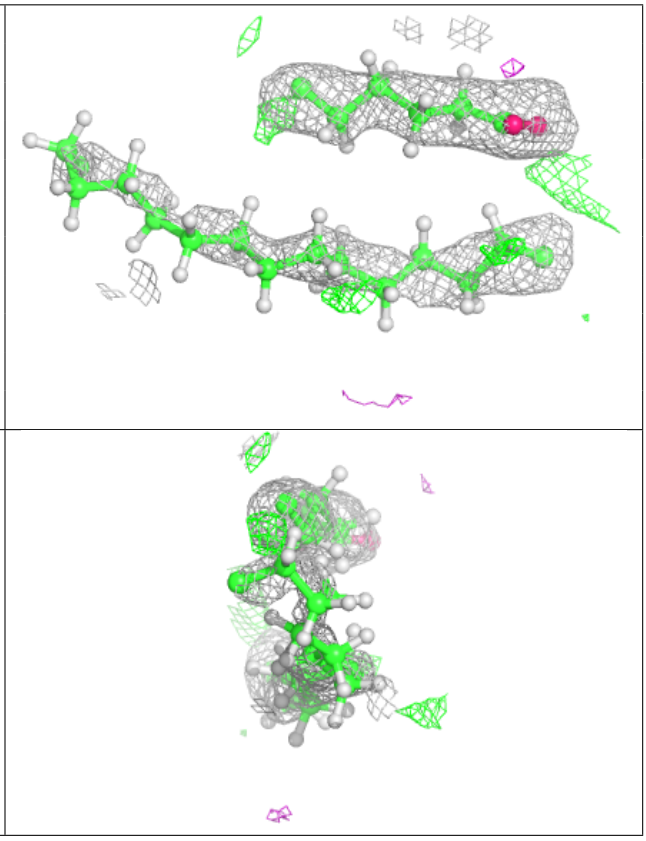
Electron density around PL9 a 611:

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



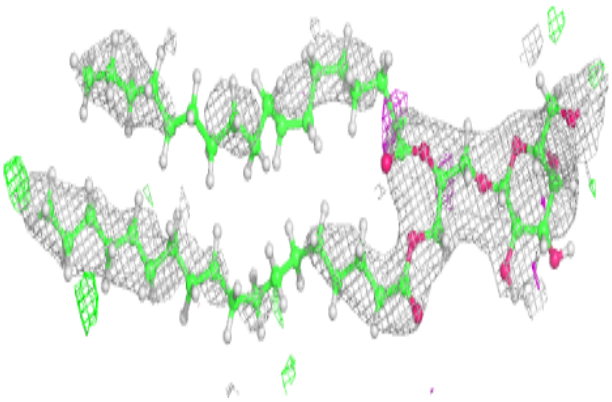
Electron density around LMG d 410:

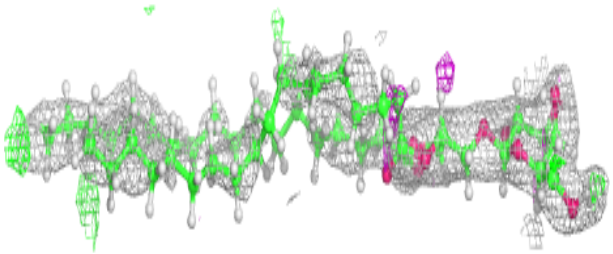
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

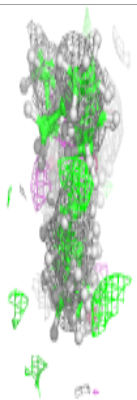


Electron density around LMG b 621:

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

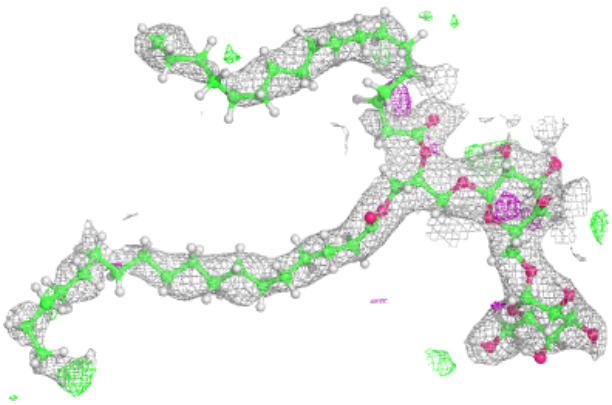


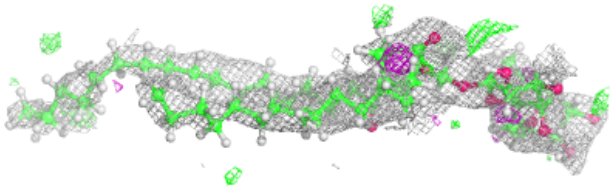




Electron density around DGD A 617:

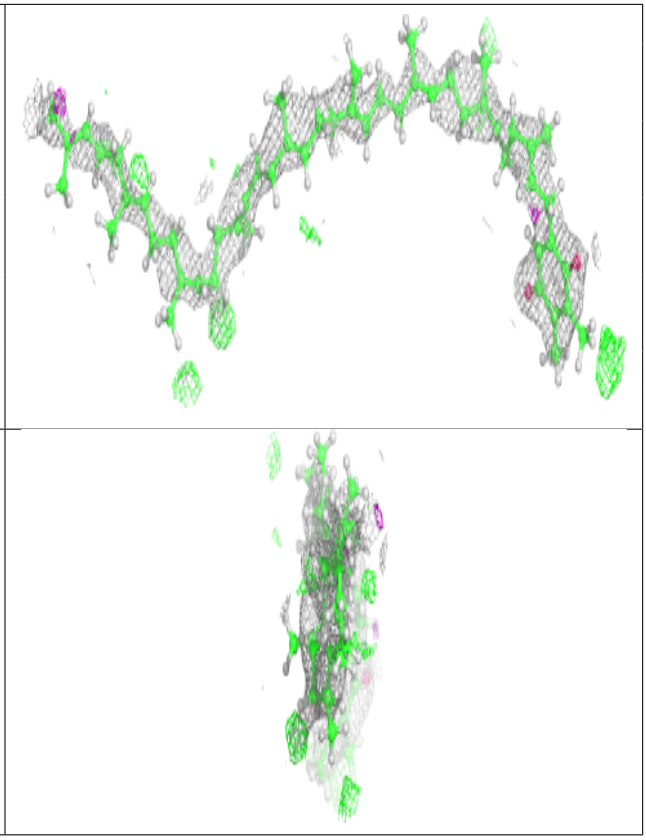
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





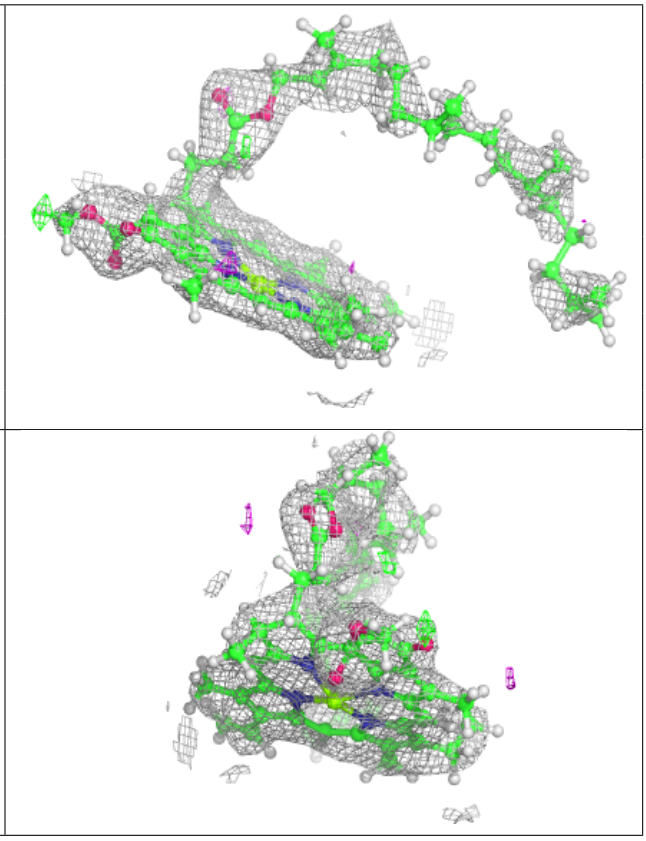
Electron density around PL9 A 611:

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



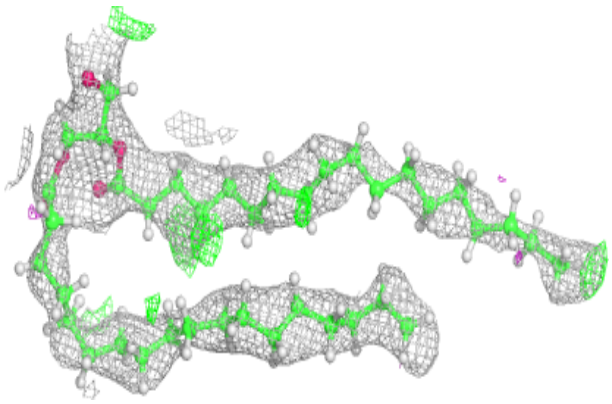
Electron density around CLA c 513:

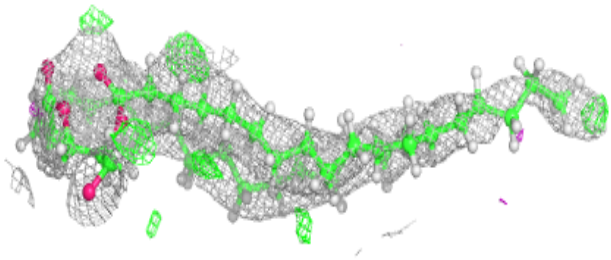
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

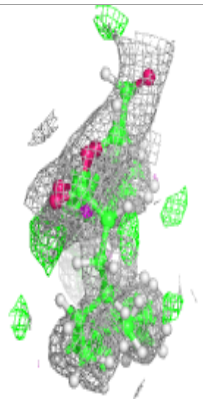


Electron density around DGD a 616:

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

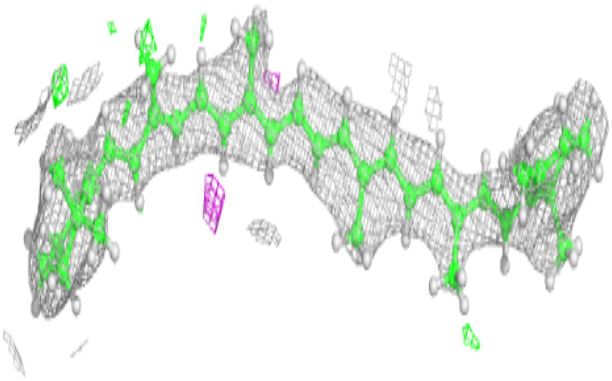


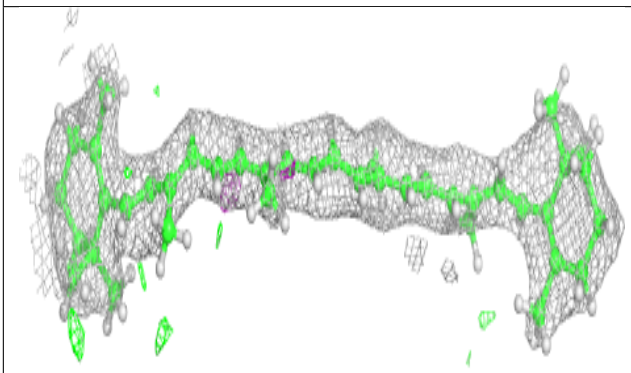


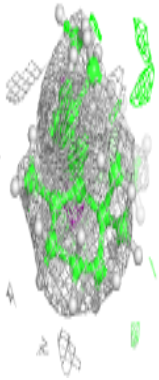


Electron density around BCR h 102:

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

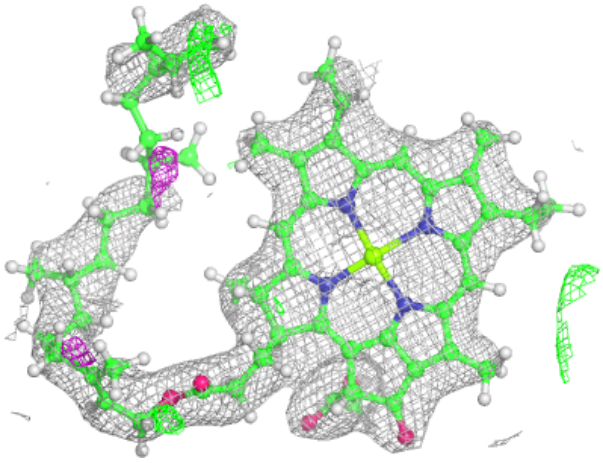


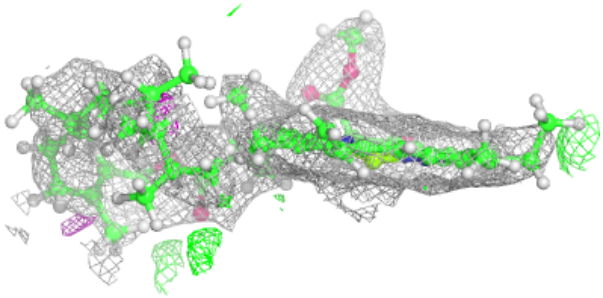


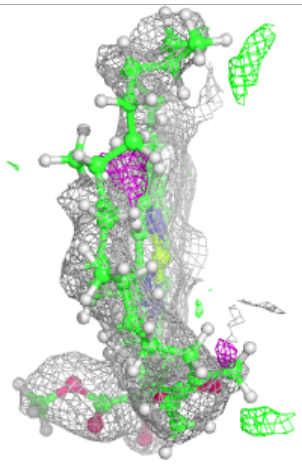


Electron density around CLA c 512:

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

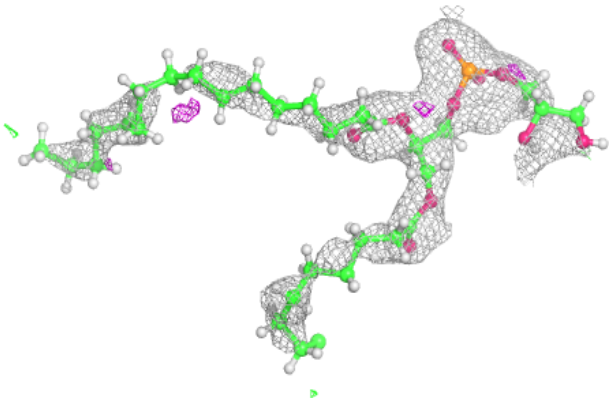


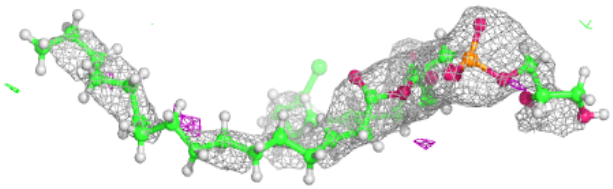


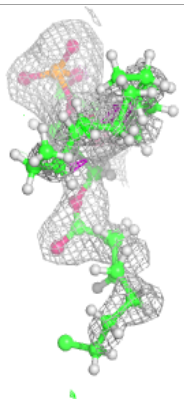


Electron density around LHG a 614:

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

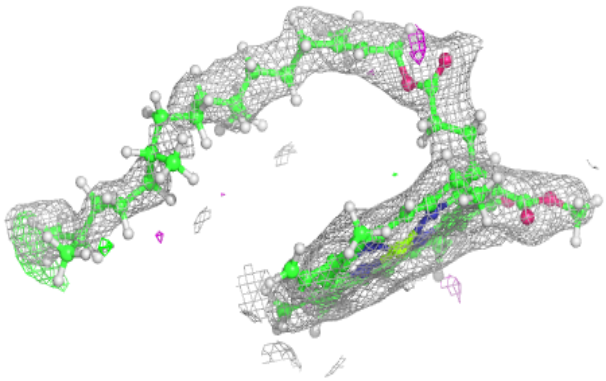


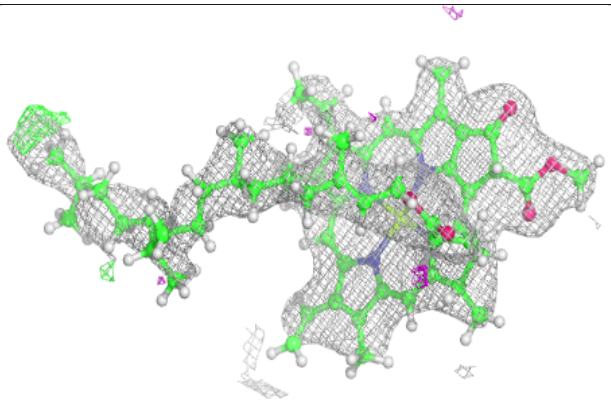


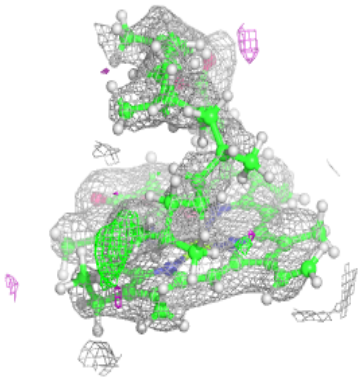


Electron density around CLA C 513:

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

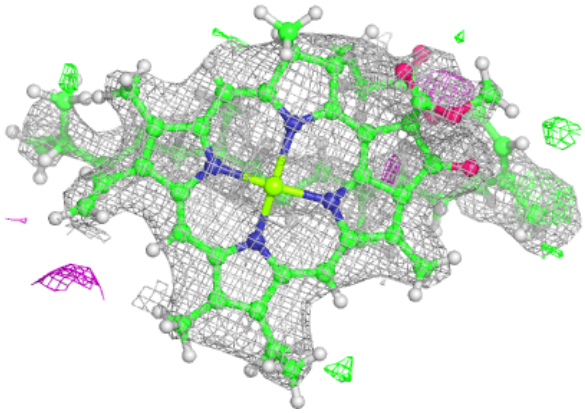


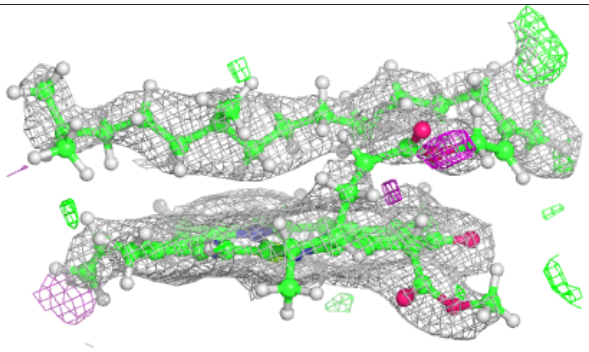




Electron density around CLA h 101:

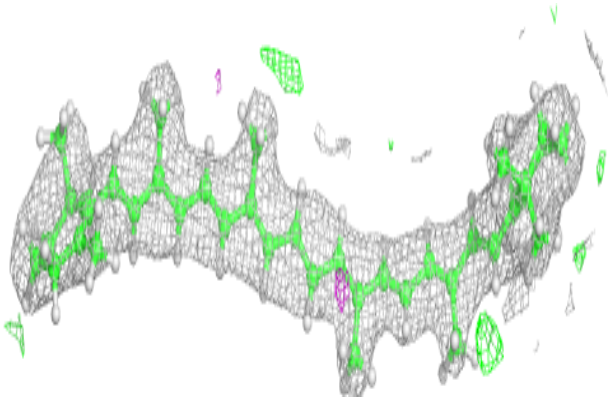
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

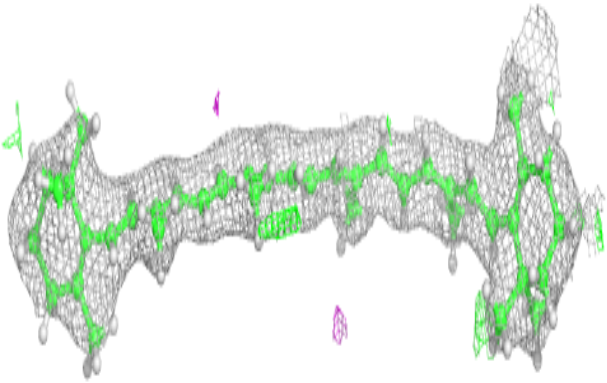


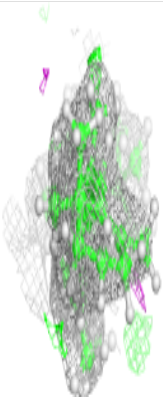


Electron density around BCR H 101:

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

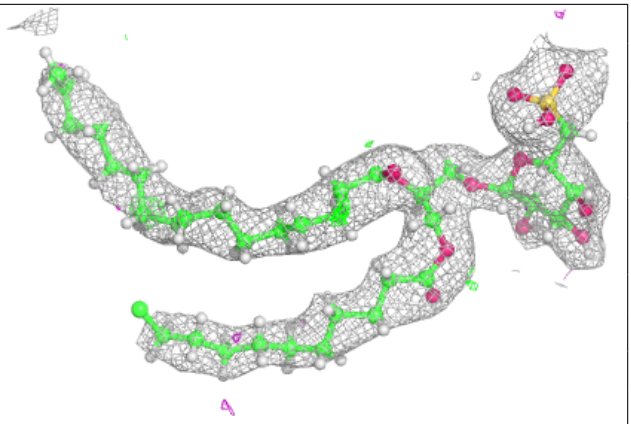


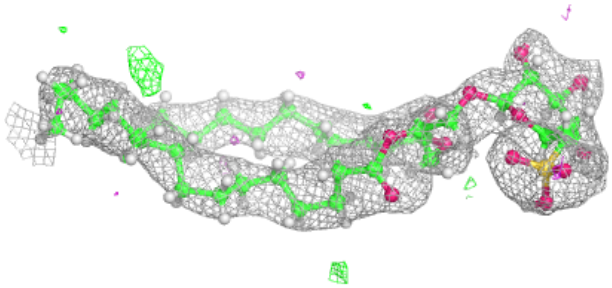


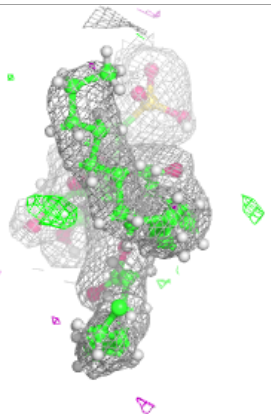


Electron density around SQD b 601:

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

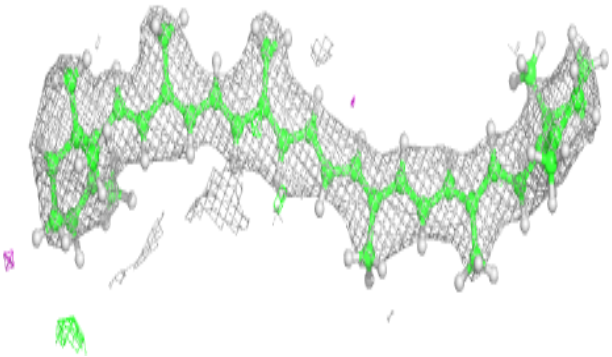


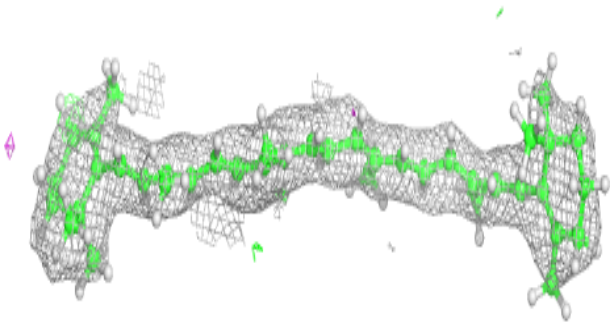


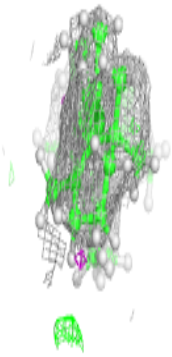


Electron density around BCR Y 101:

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

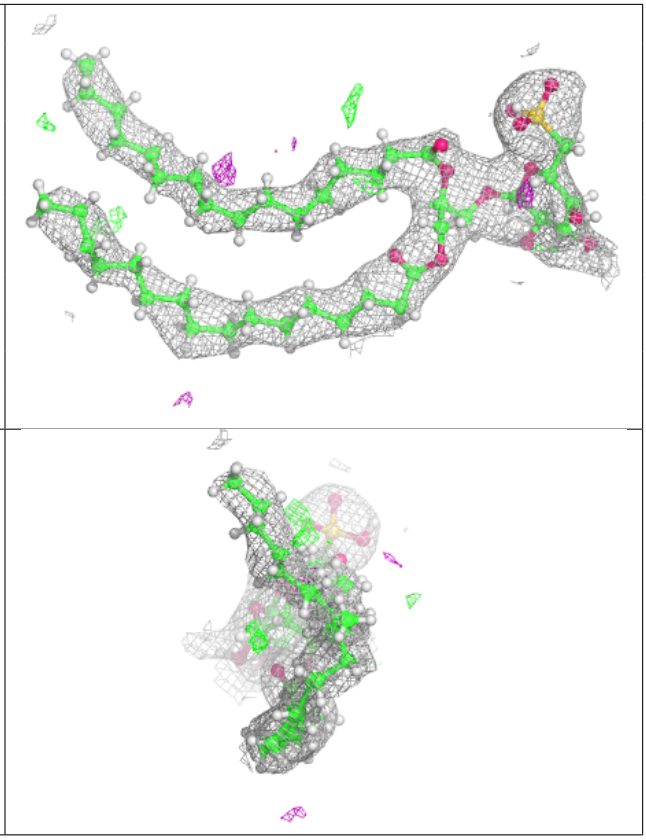






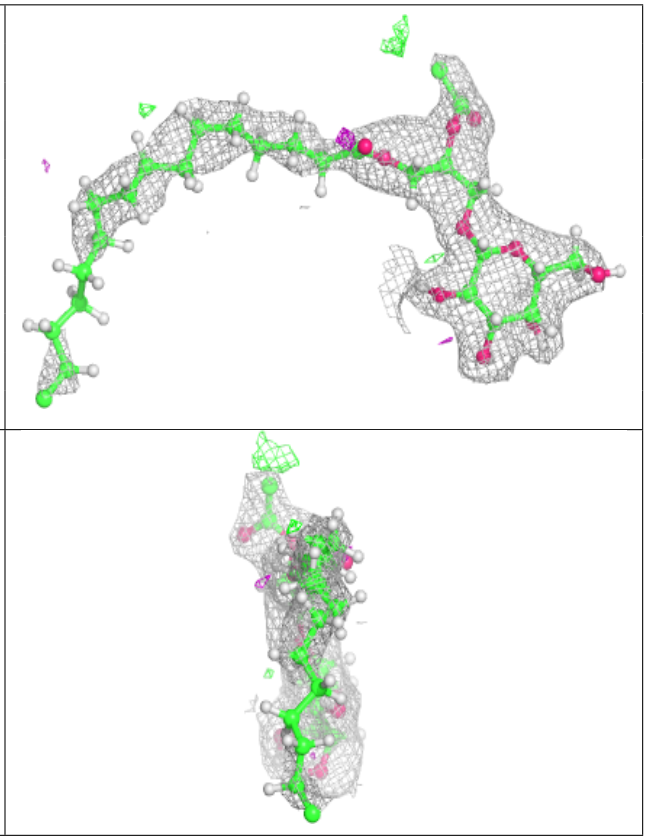
Electron density around SQD B 624:

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



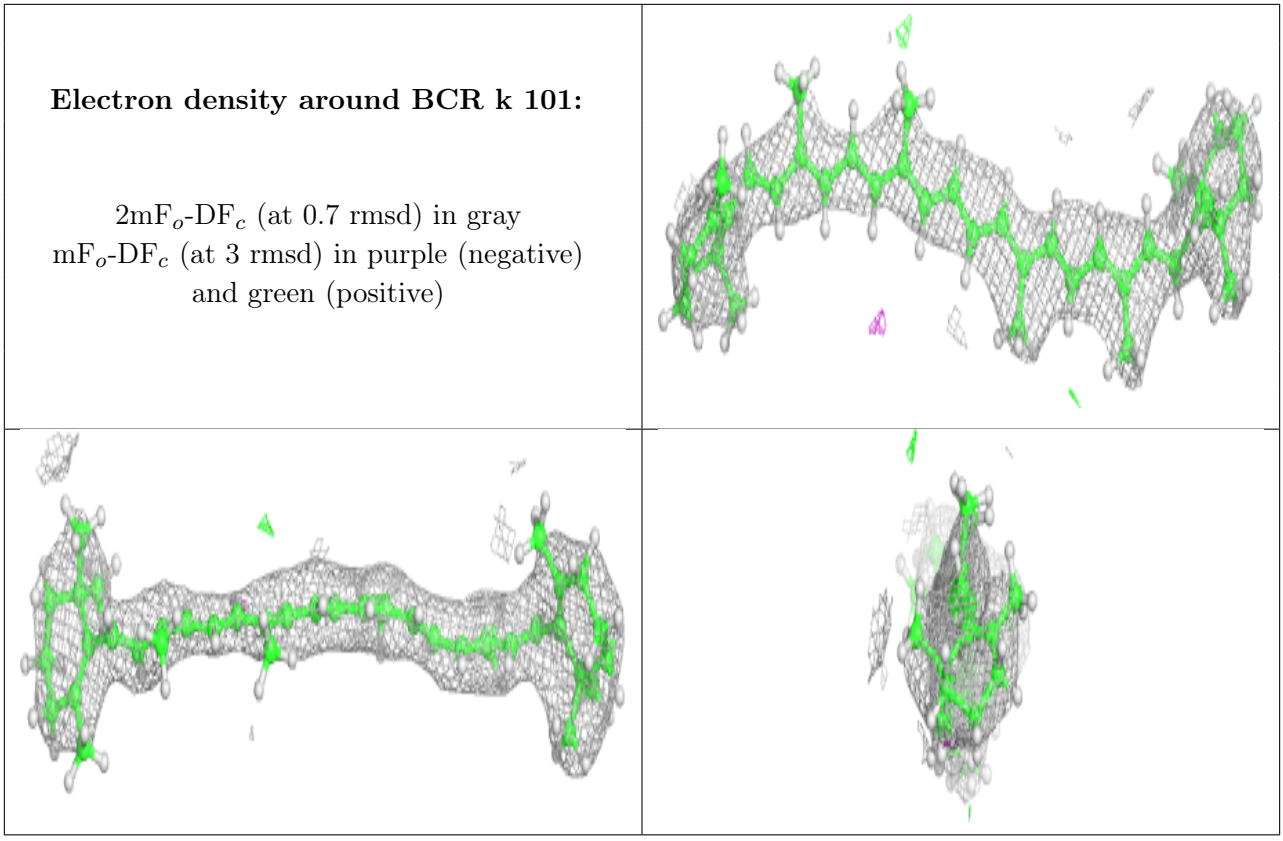
Electron density around LMG c 519:

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



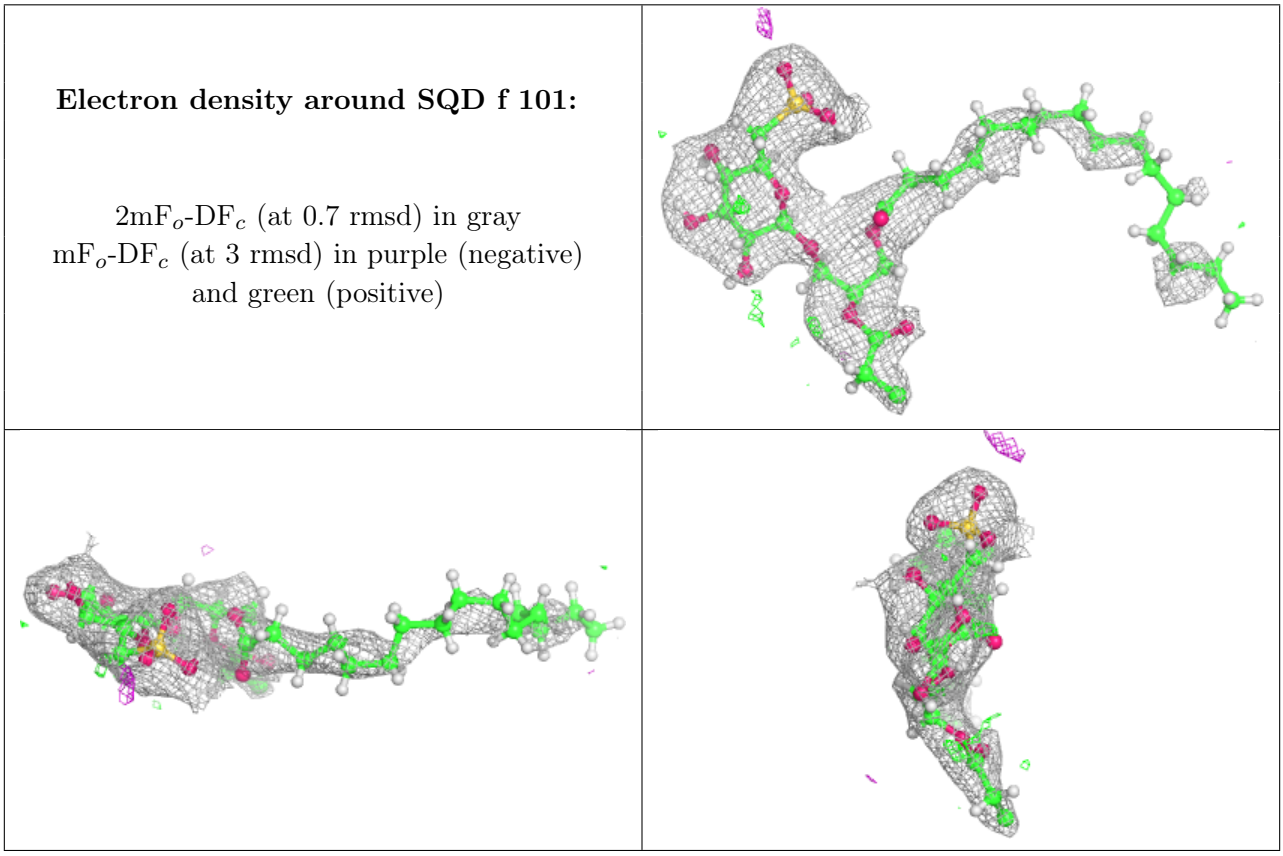
Electron density around BCR k 101:

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



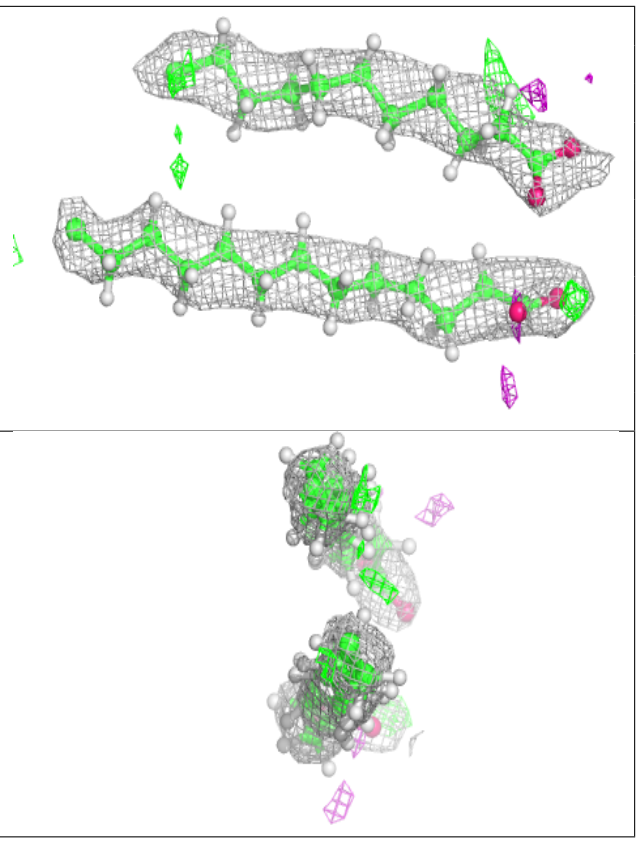
Electron density around SQD f 101:

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



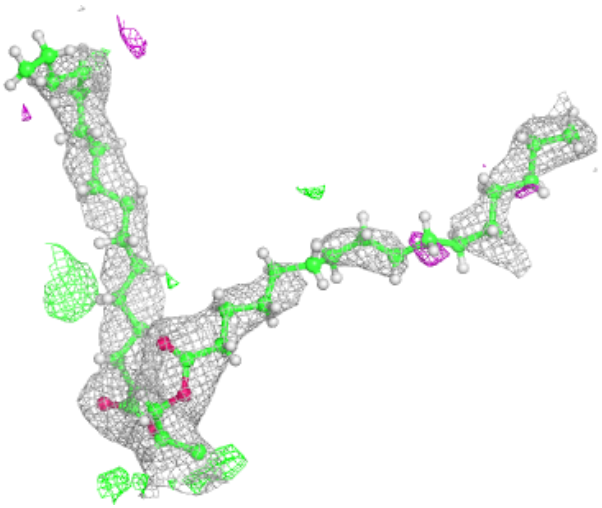
Electron density around LMG B 622:

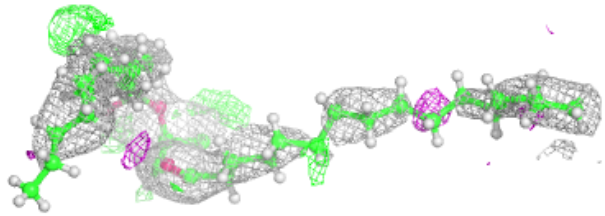
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

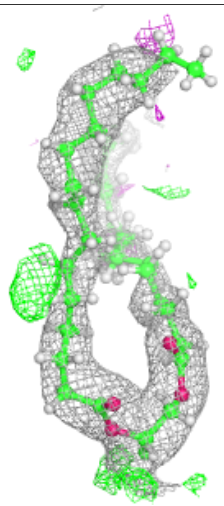


Electron density around SQD A 616:

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

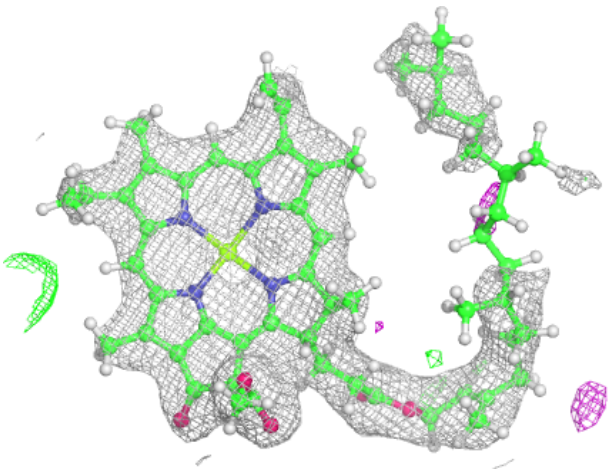


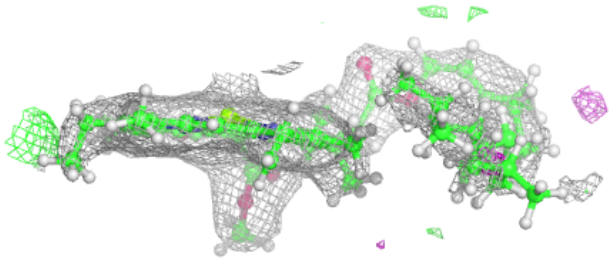


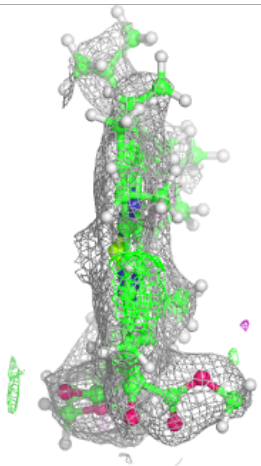


Electron density around CLA C 512:

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

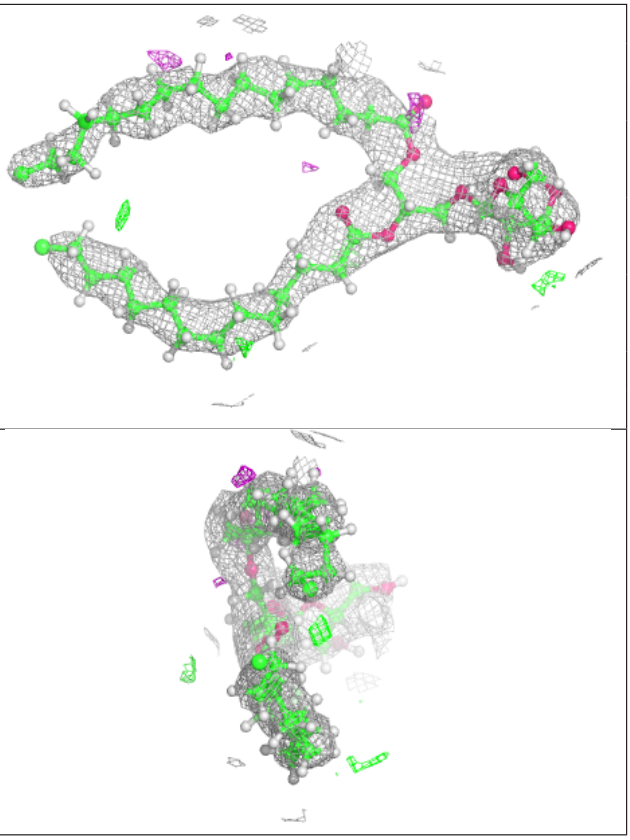


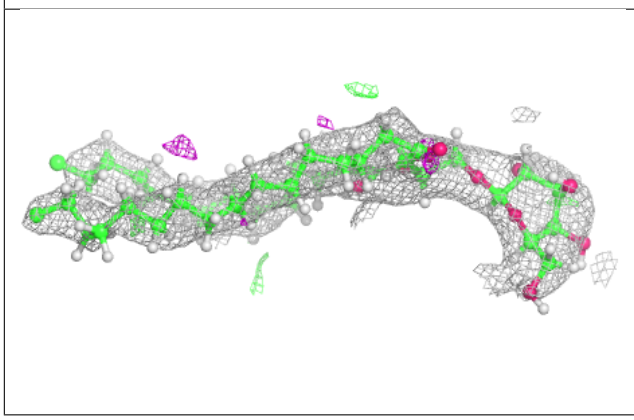




Electron density around LMG c 522:

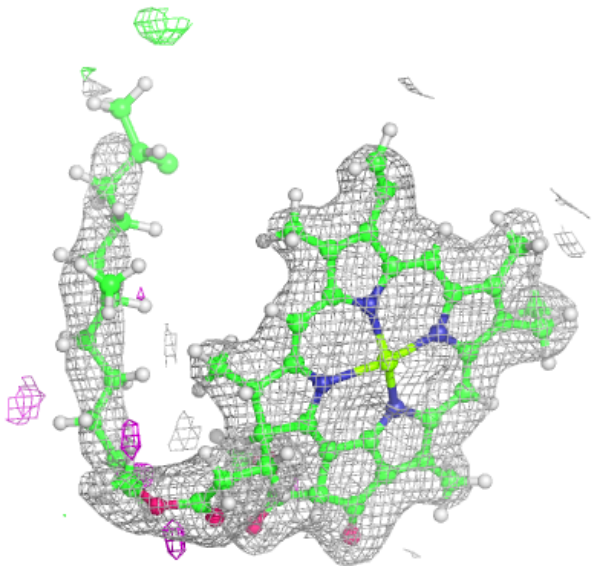
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

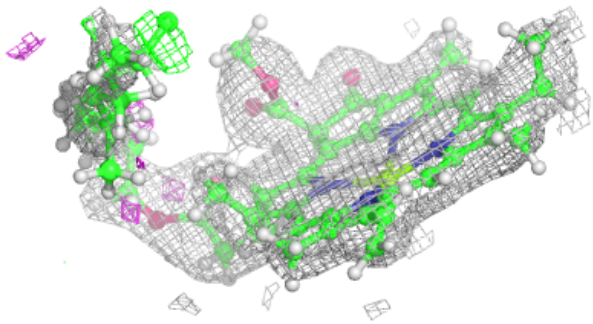


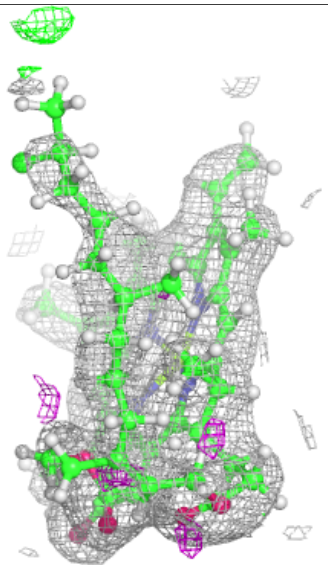


Electron density around CLA B 616:

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

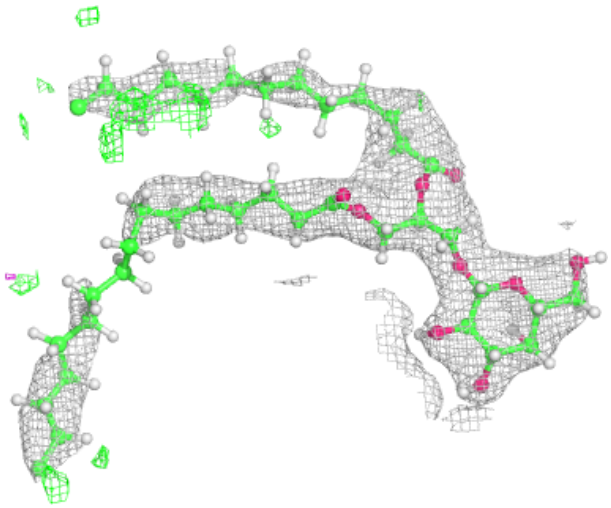


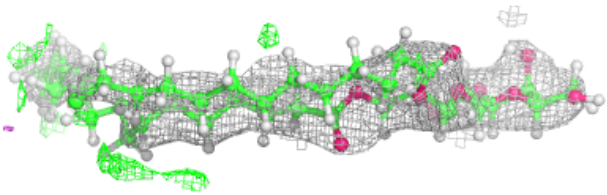


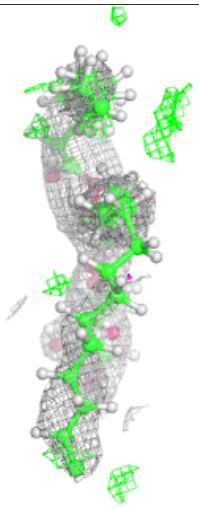


Electron density around LMG C 519:

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

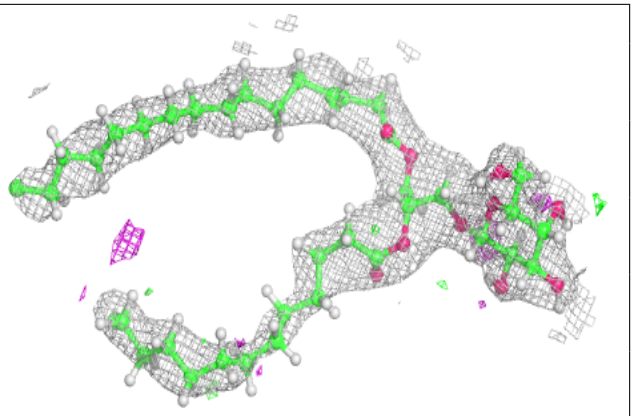


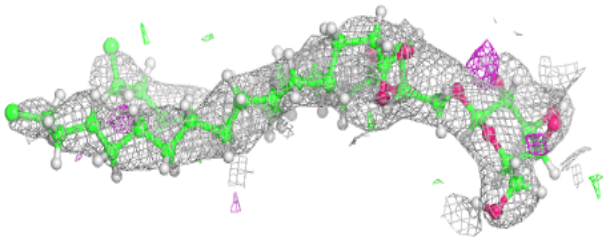


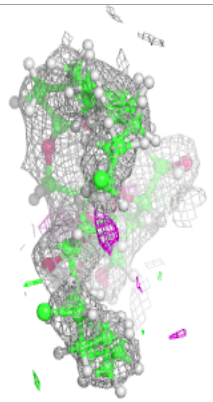


Electron density around LMG A 612:

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

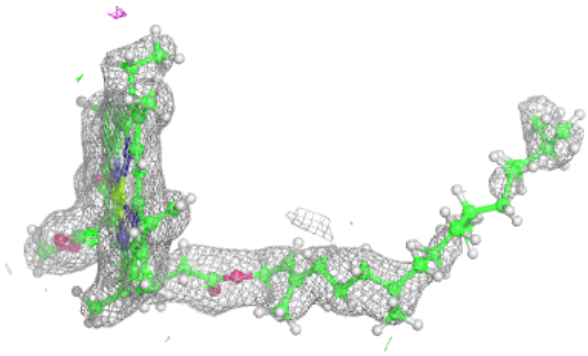


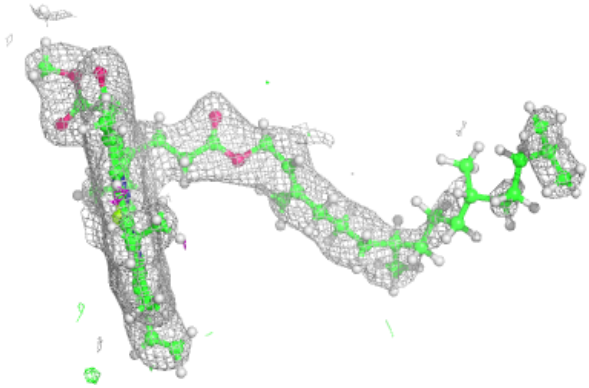


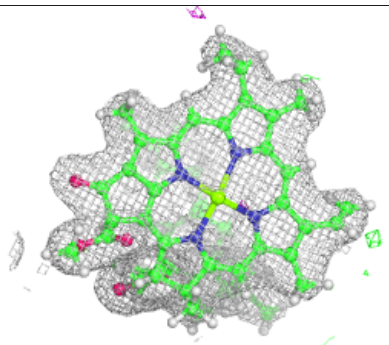


Electron density around CLA D 403:

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

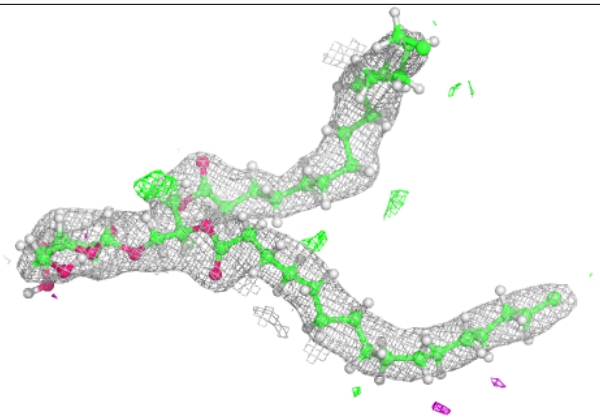


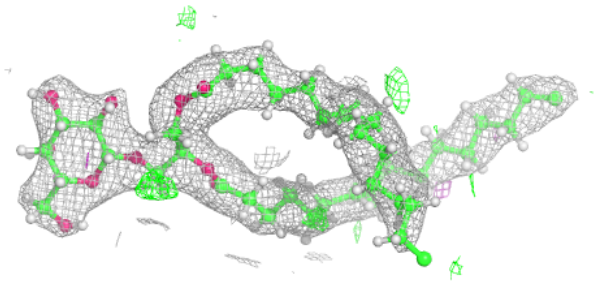


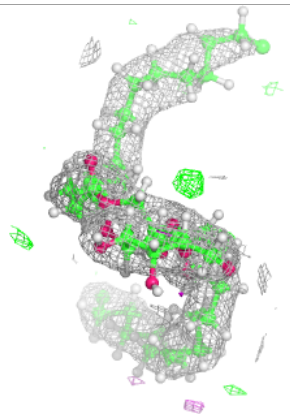


Electron density around LMG B 620:

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

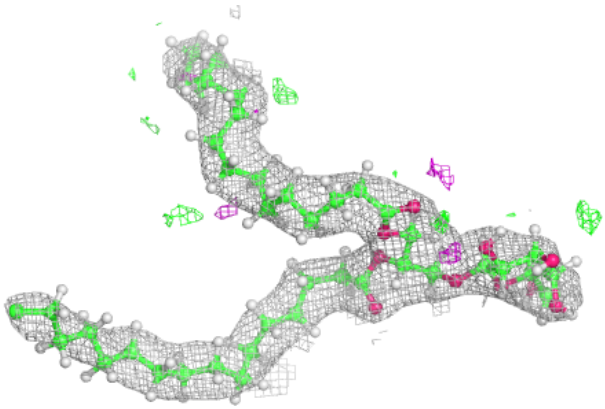


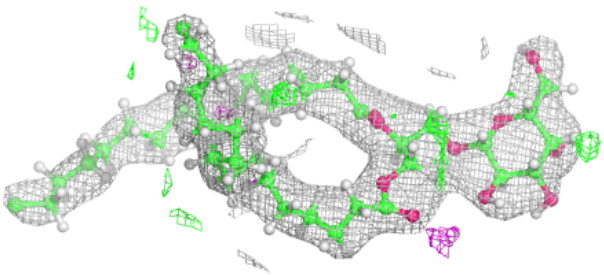


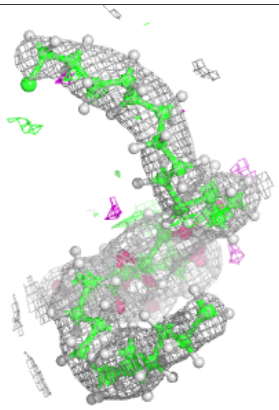


Electron density around LMG m 101:

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

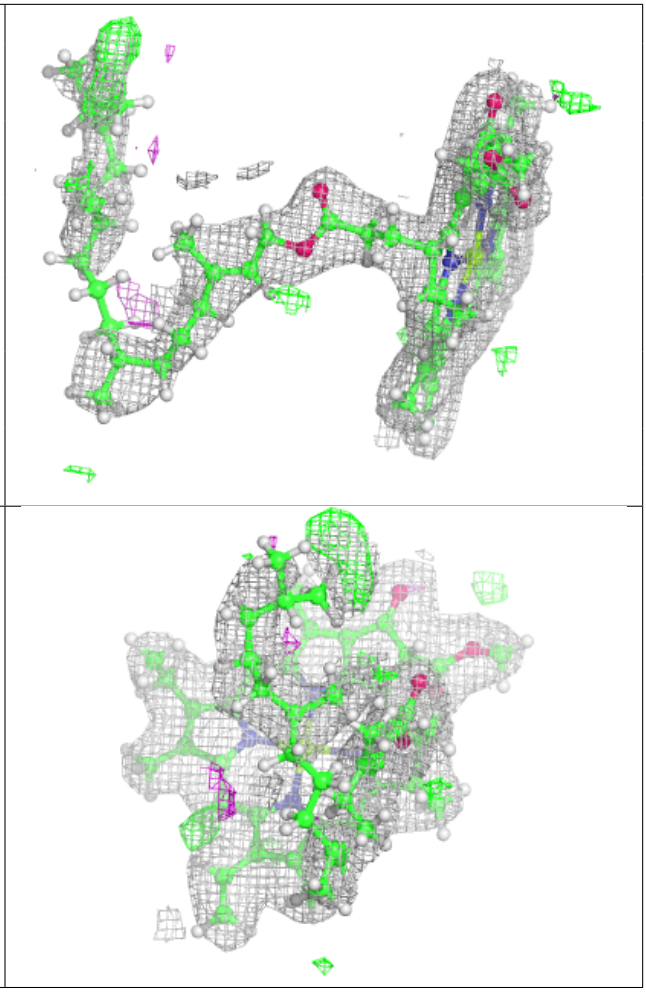






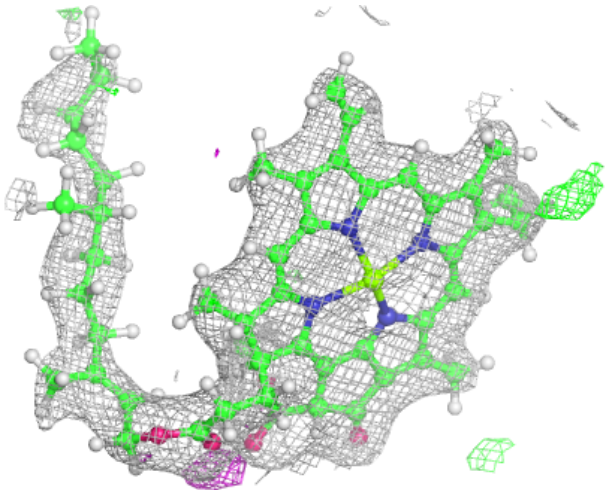
Electron density around CLA a 606:

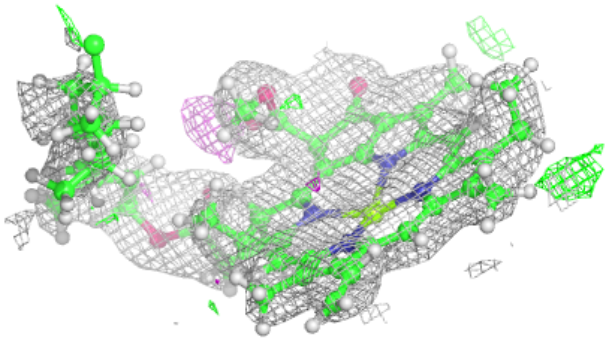
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

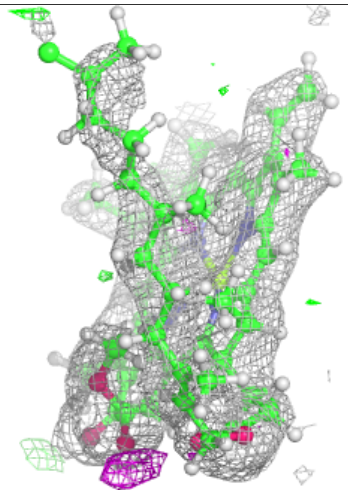


Electron density around CLA b 616:

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

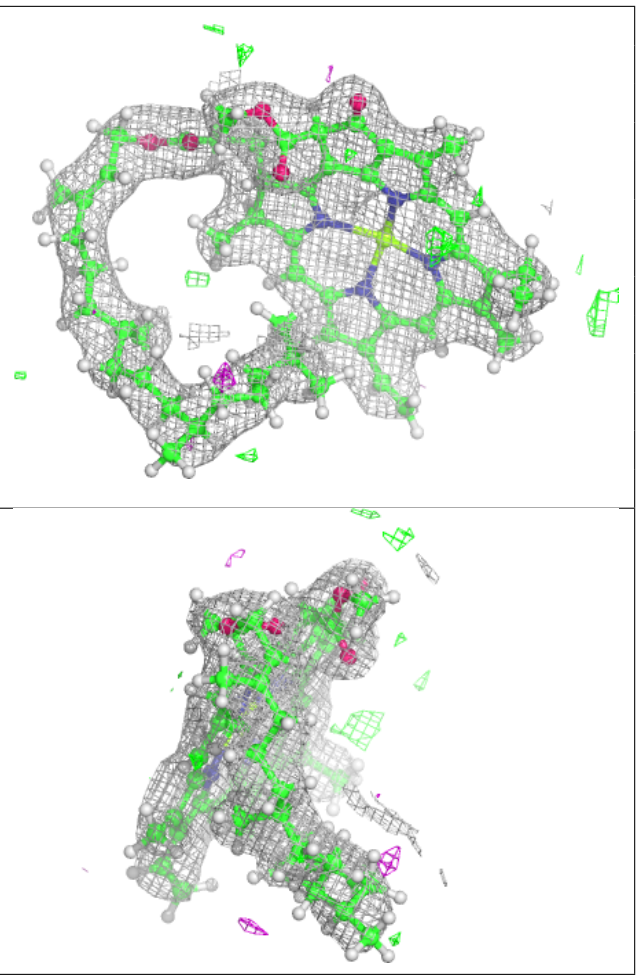






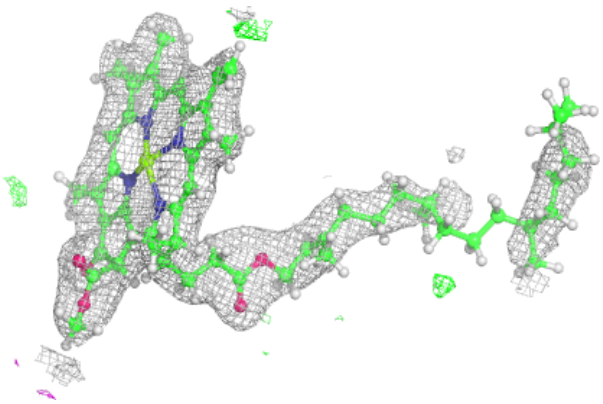
Electron density around CLA b 615:

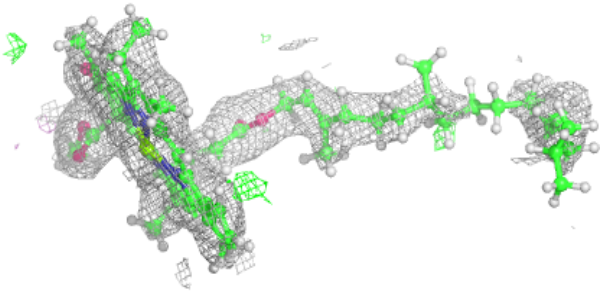
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

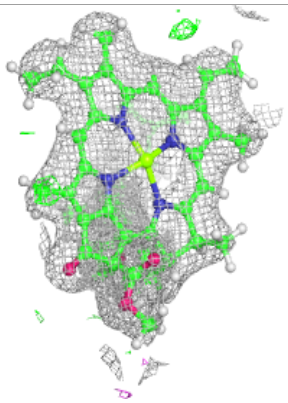


Electron density around CLA d 403:

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

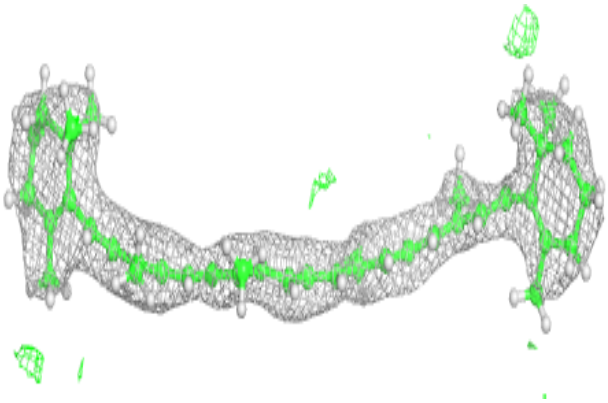


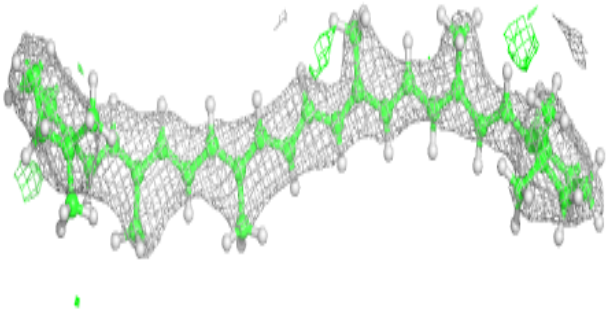


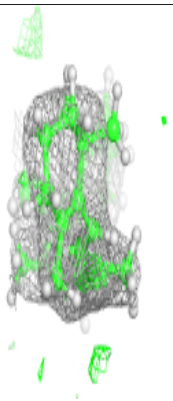


Electron density around BCR k 102:

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

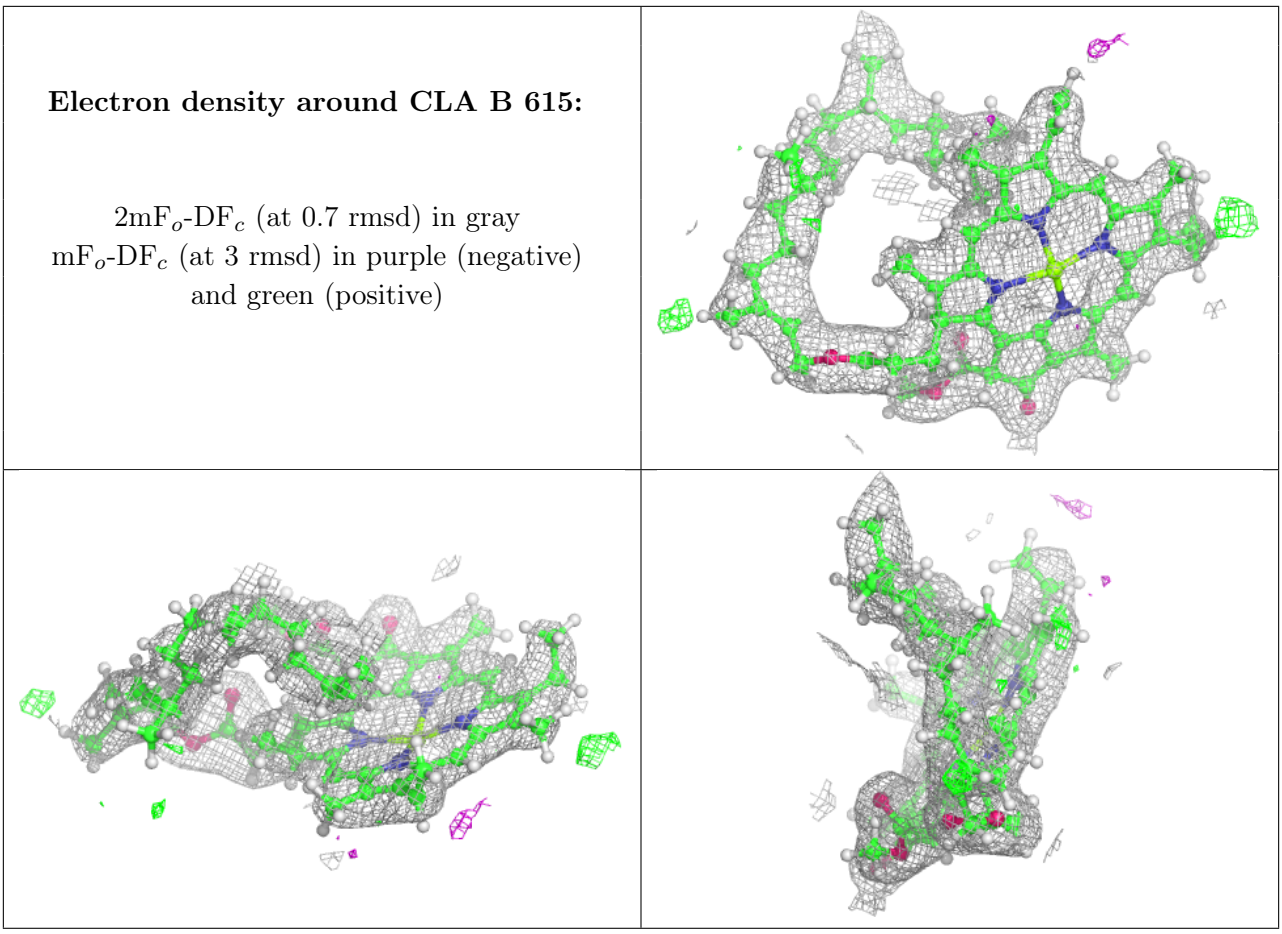






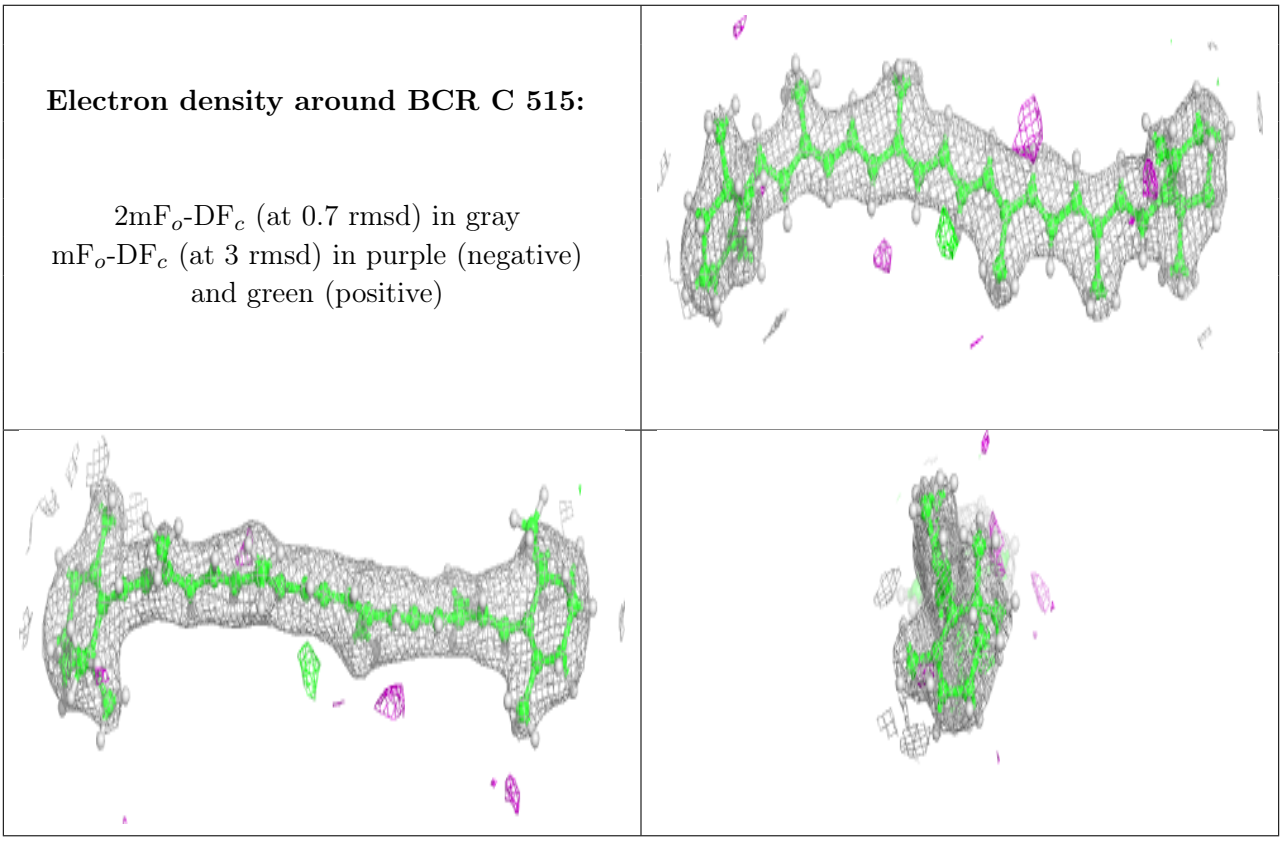
Electron density around CLA B 615:

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



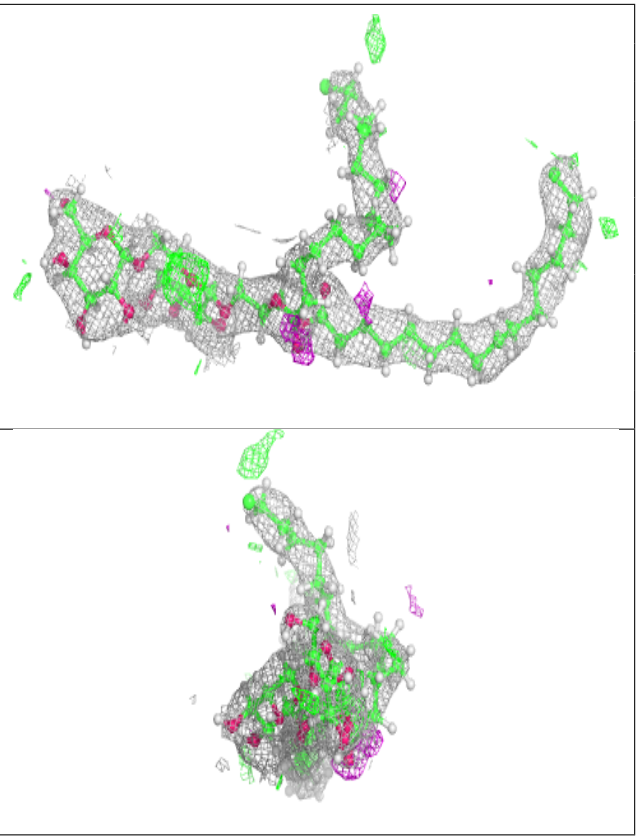
Electron density around BCR C 515:

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



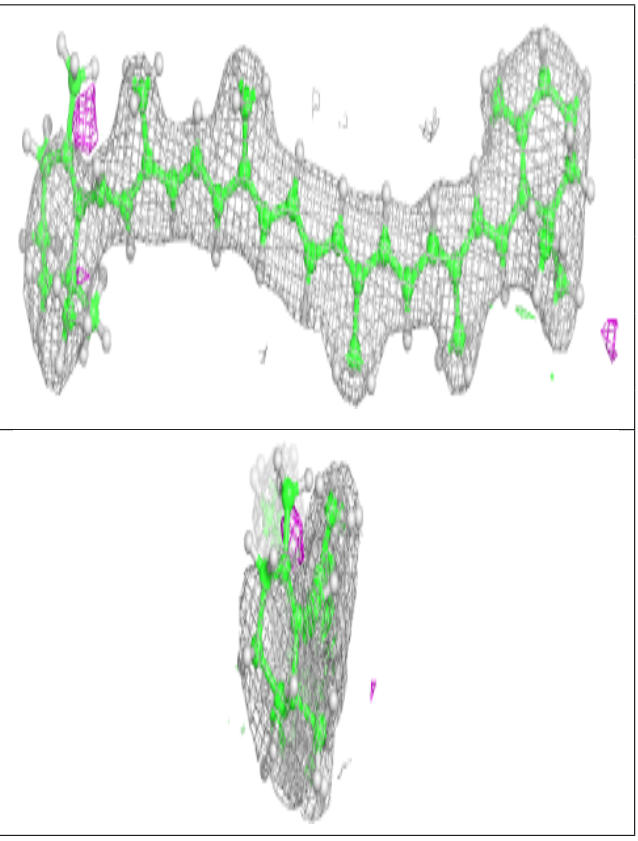
Electron density around DGD h 103:

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



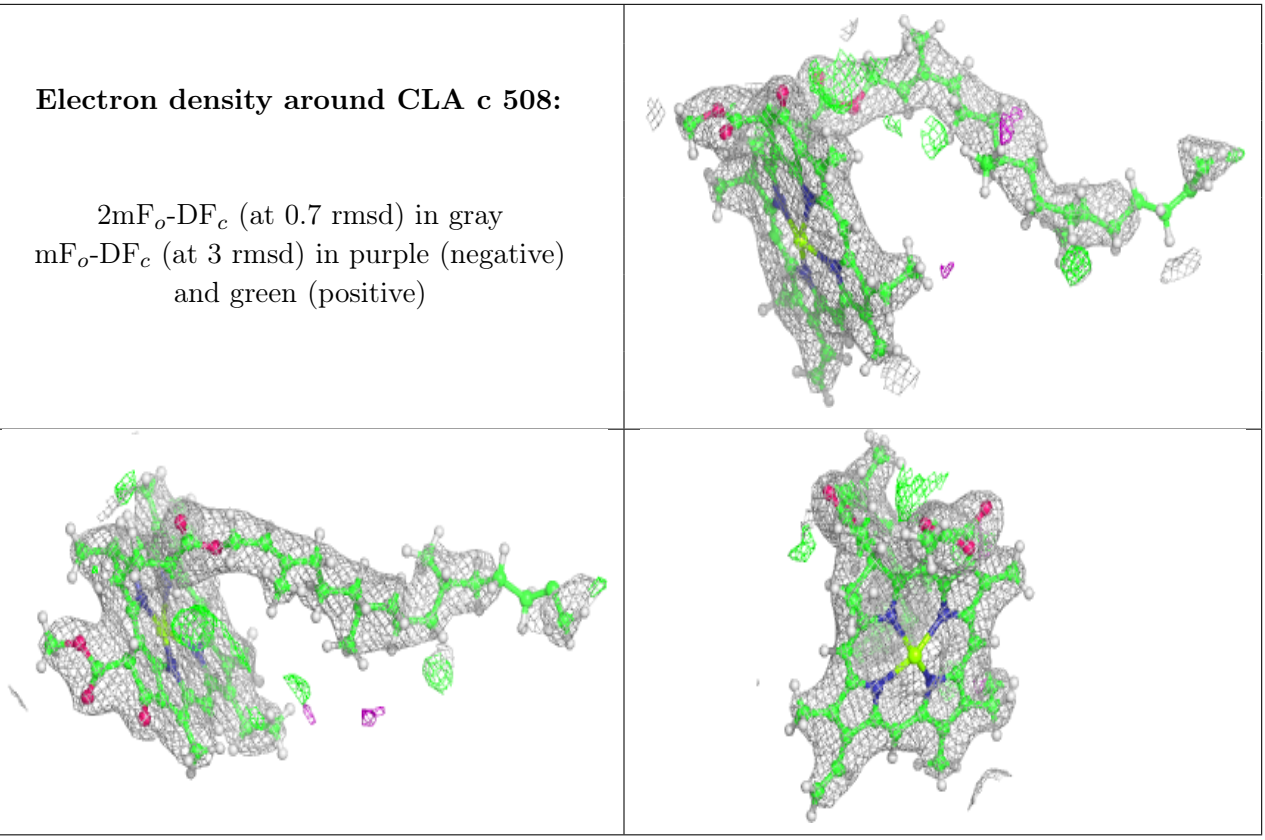
Electron density around BCR D 404:

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



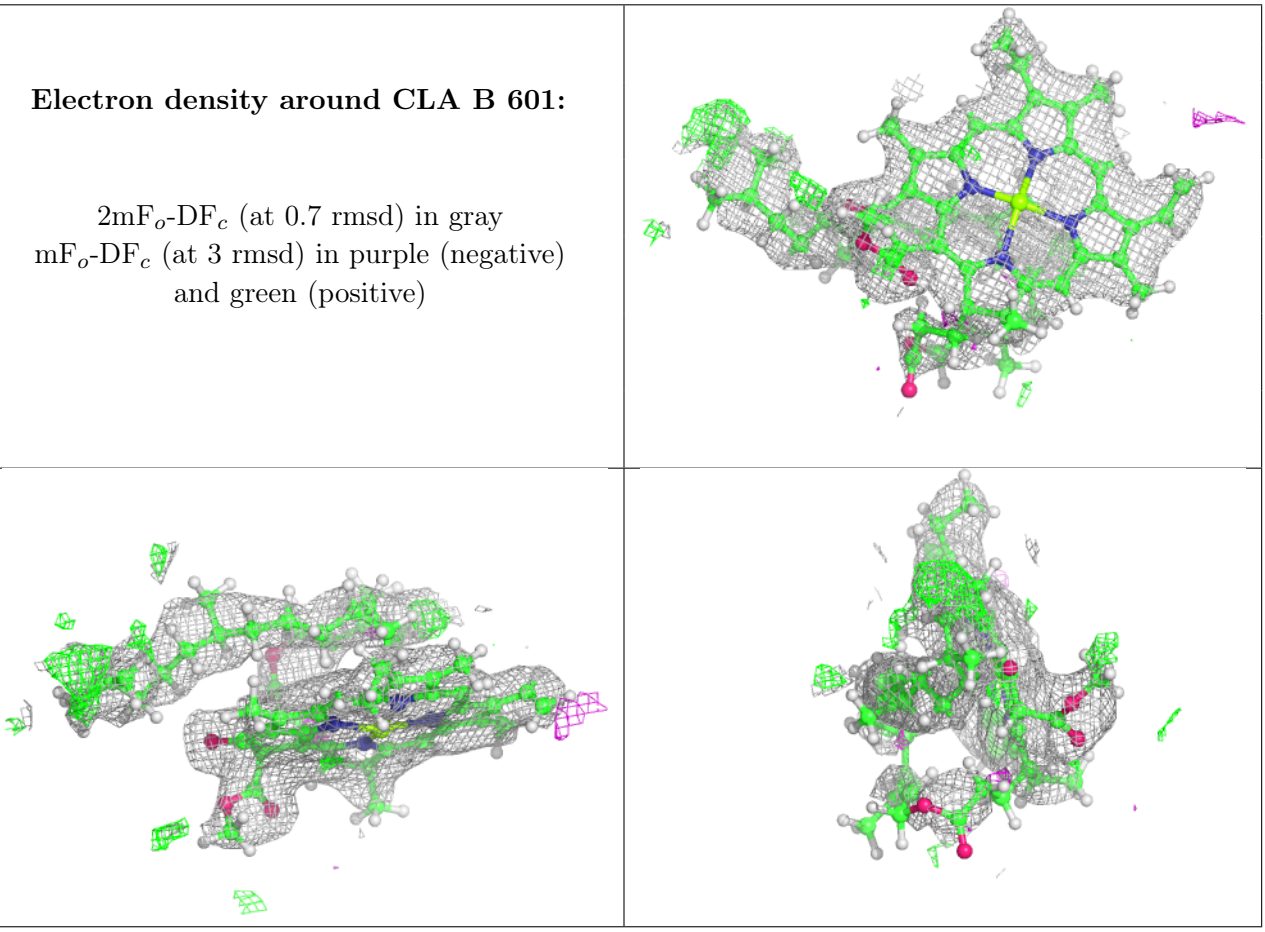
Electron density around CLA c 508:

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



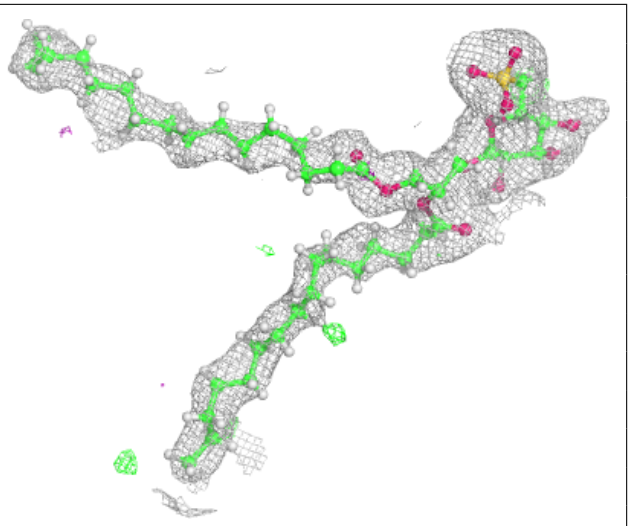
Electron density around CLA B 601:

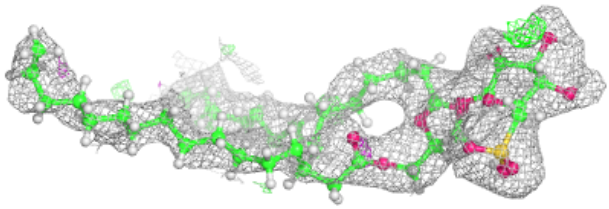
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

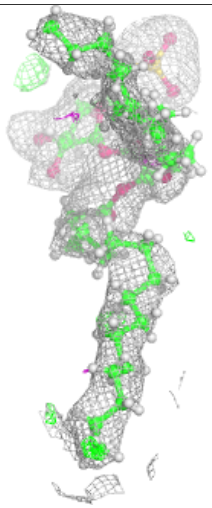


Electron density around SQD a 613:

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

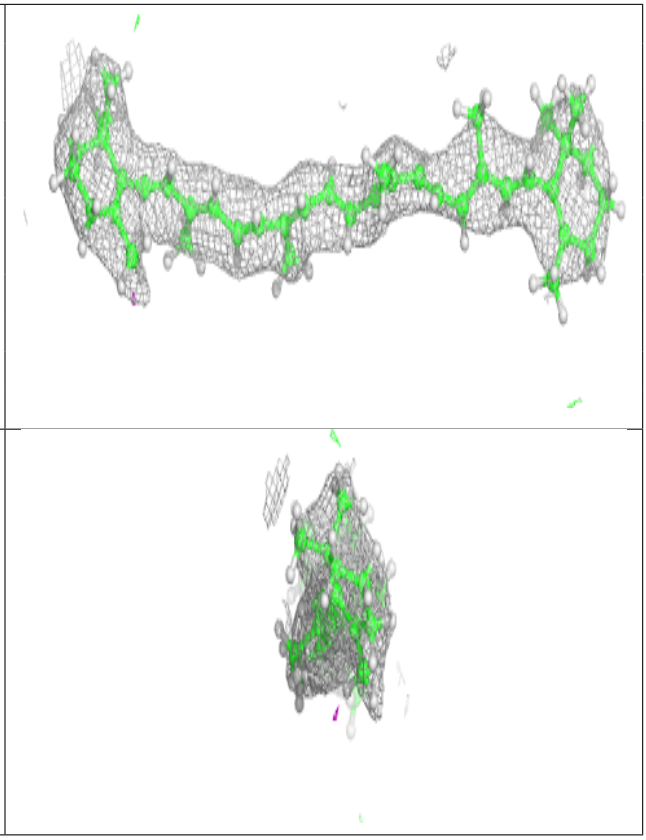






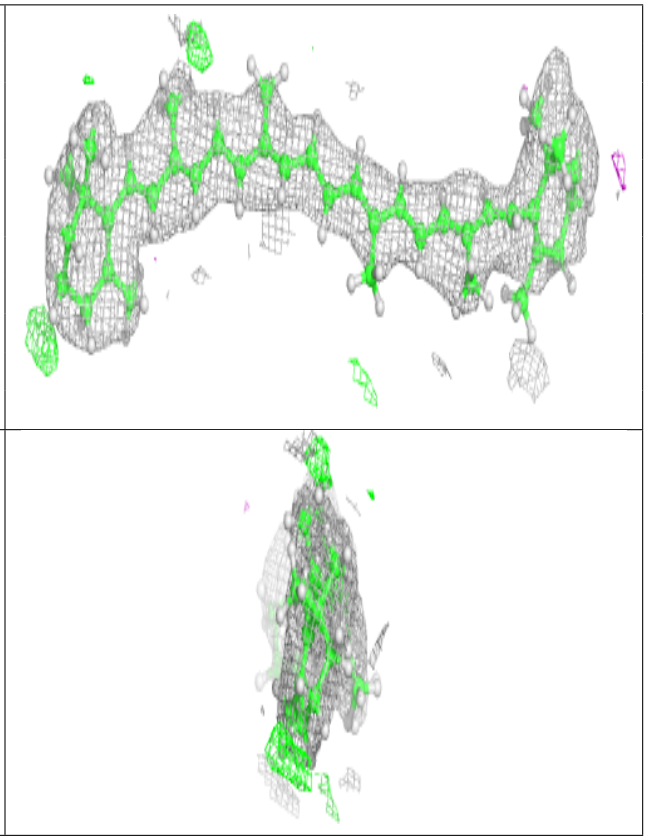
Electron density around BCR c 514:

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



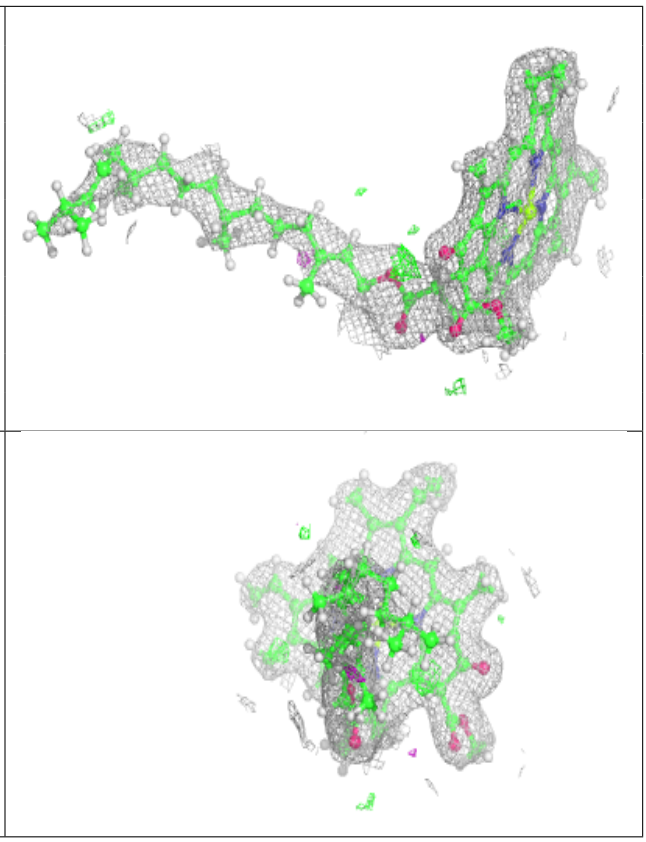
Electron density around BCR d 404:

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



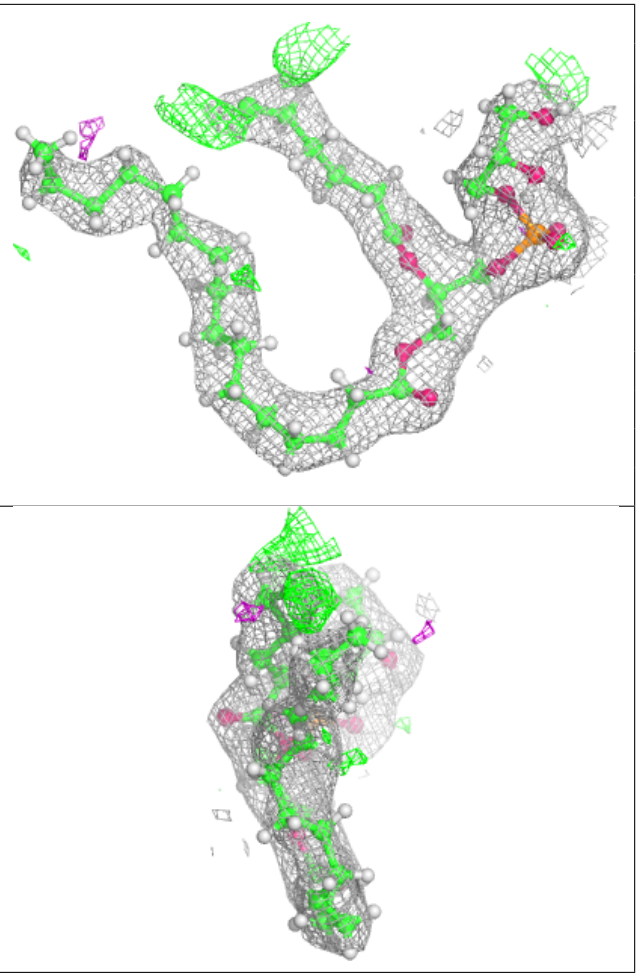
Electron density around CLA b 604:

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



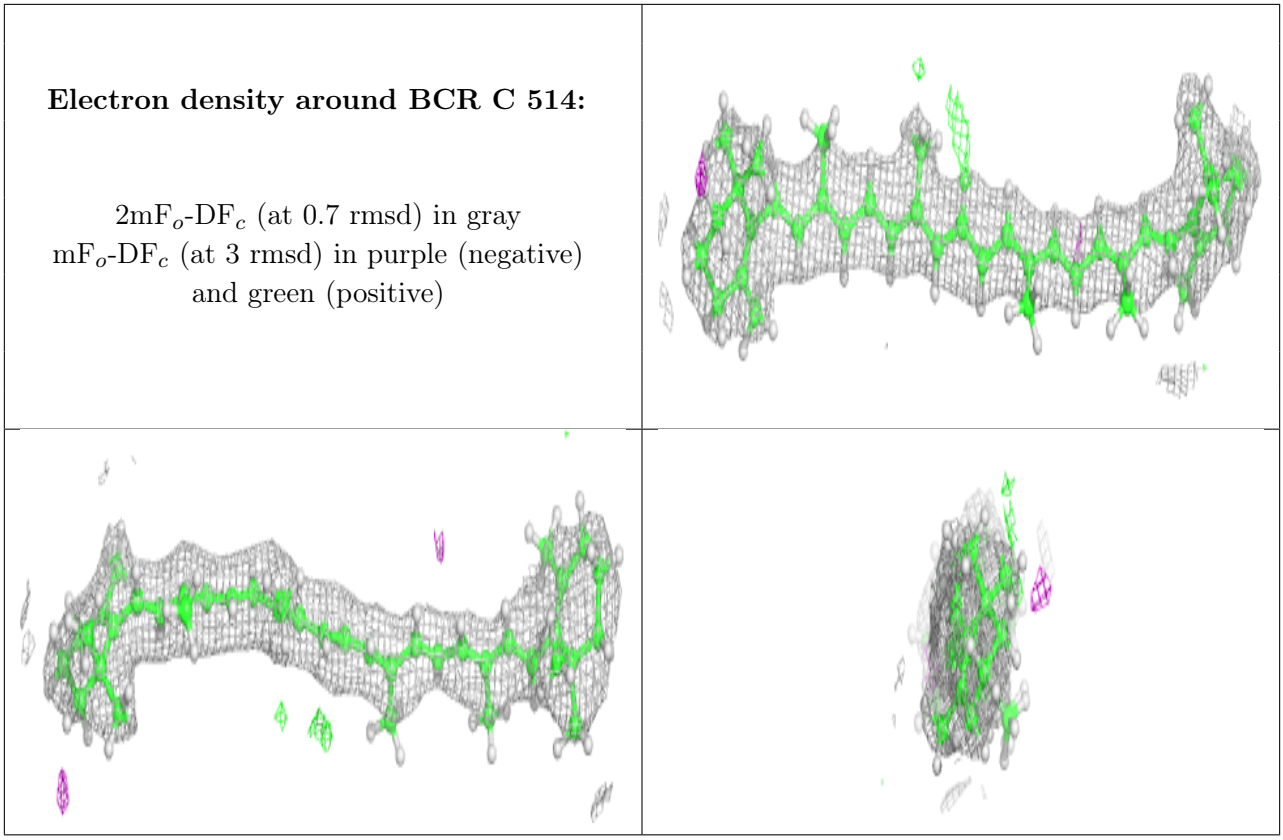
Electron density around LHG d 409:

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



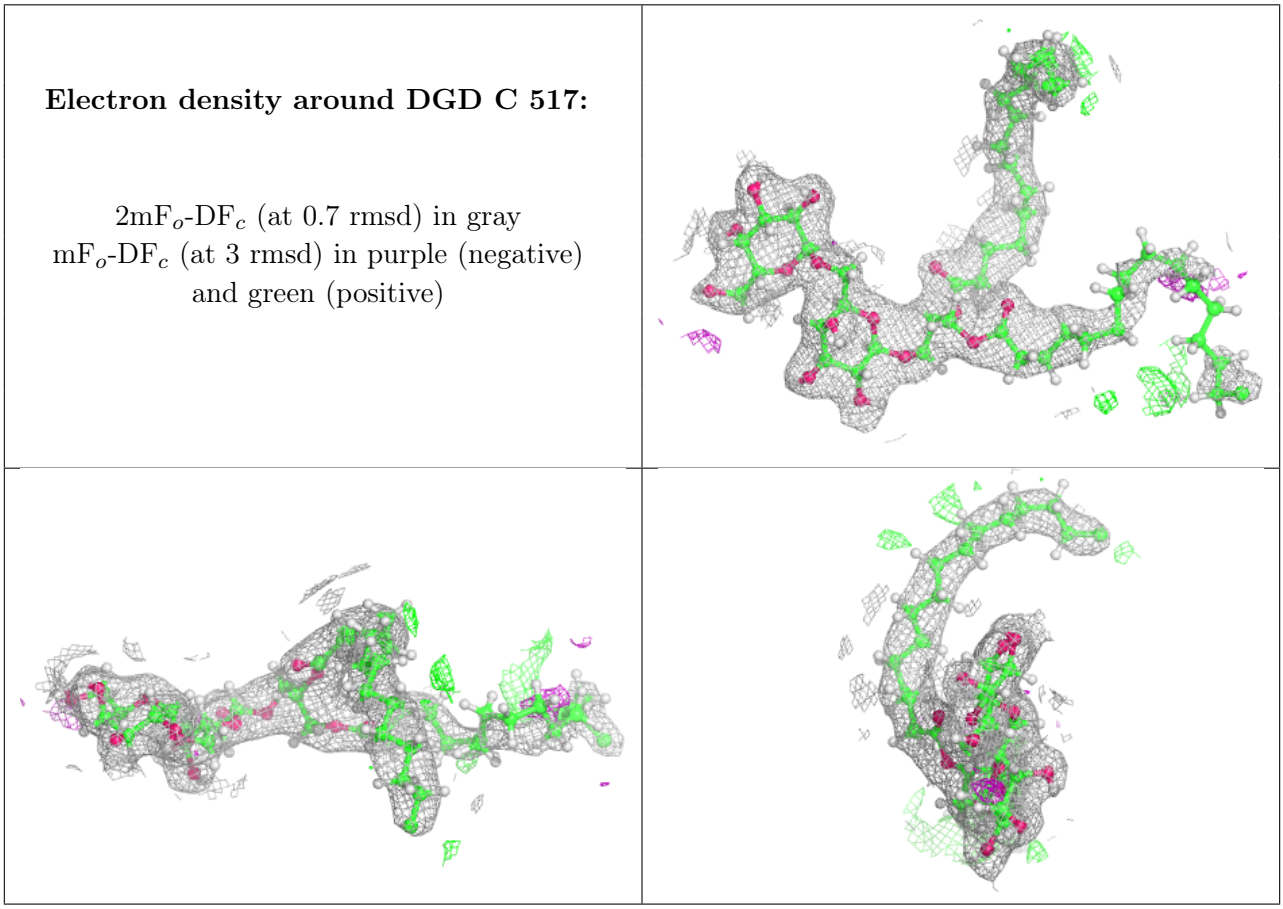
Electron density around BCR C 514:

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



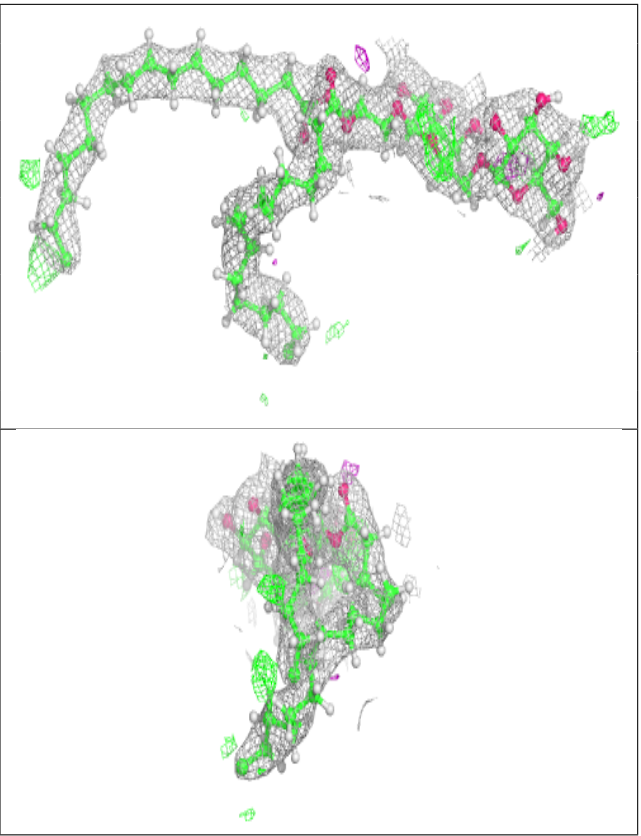
Electron density around DGD C 517:

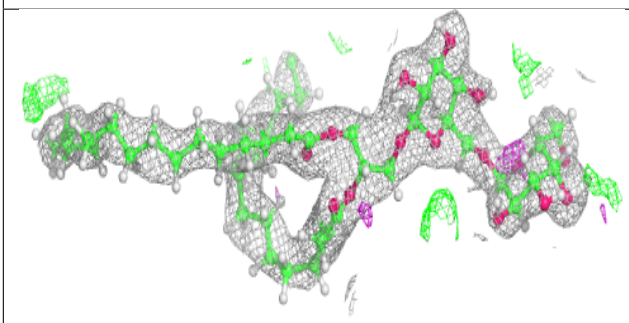
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DGD H 102:

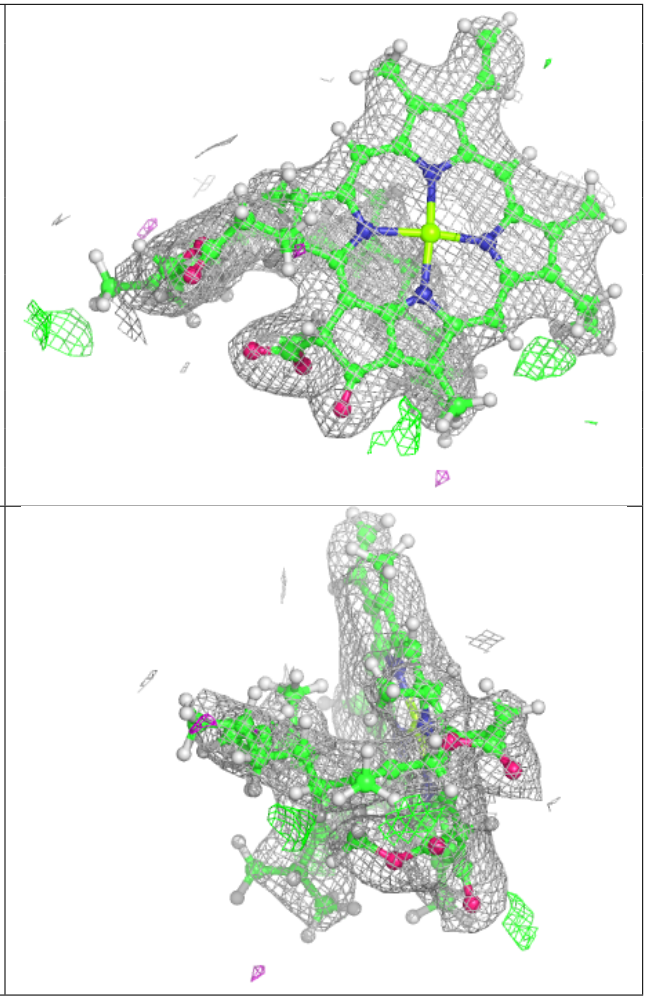
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





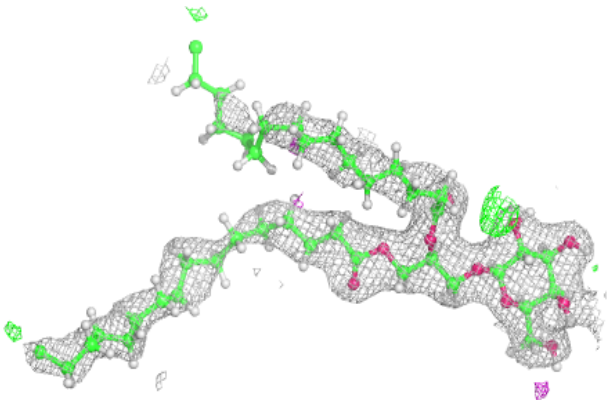
Electron density around CLA c 510:

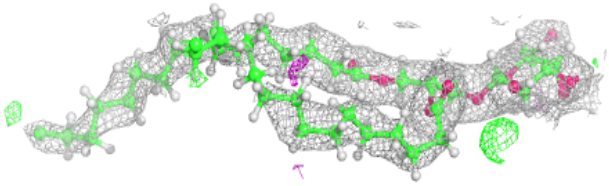
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

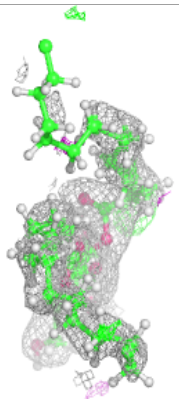


Electron density around LMG D 405:

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

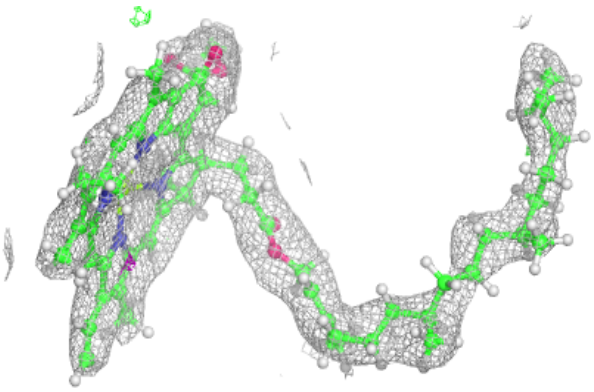


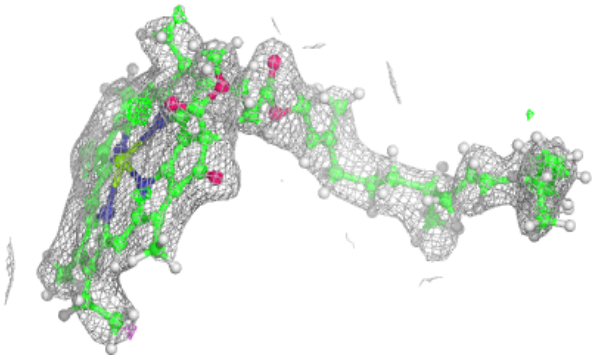


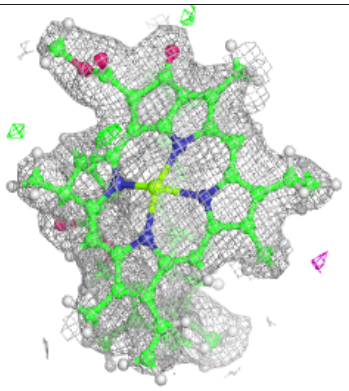


Electron density around CLA b 606:

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

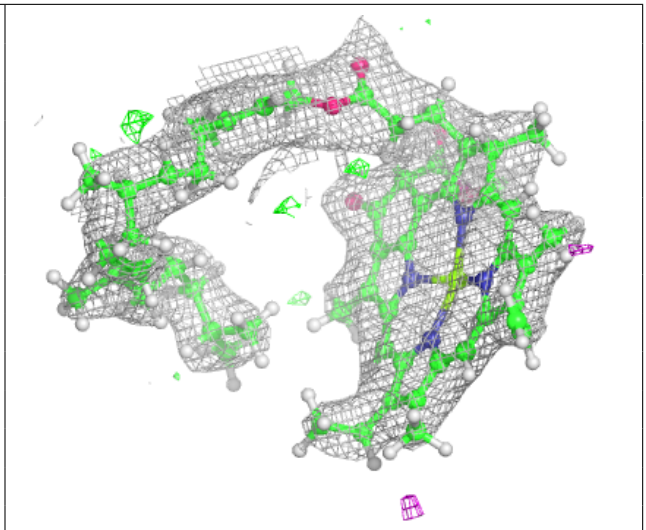


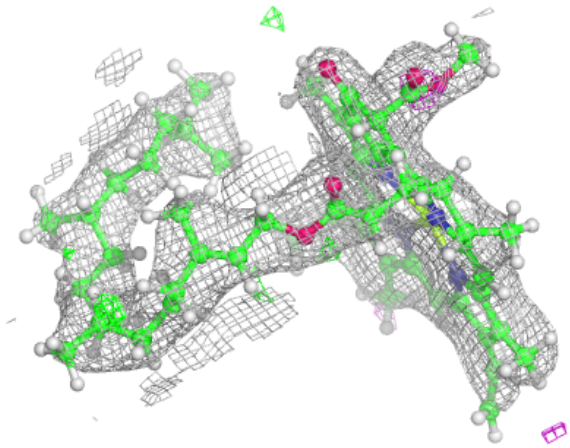


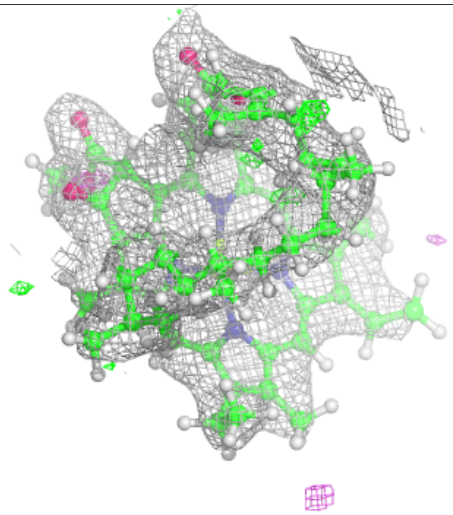


Electron density around CLA c 503:

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

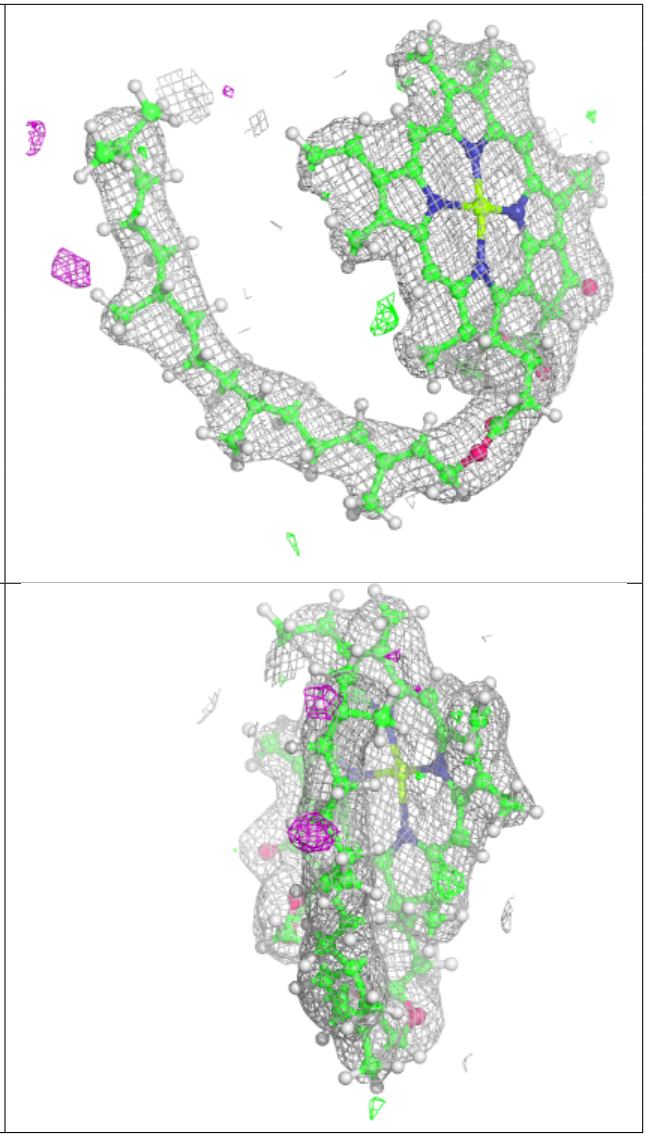






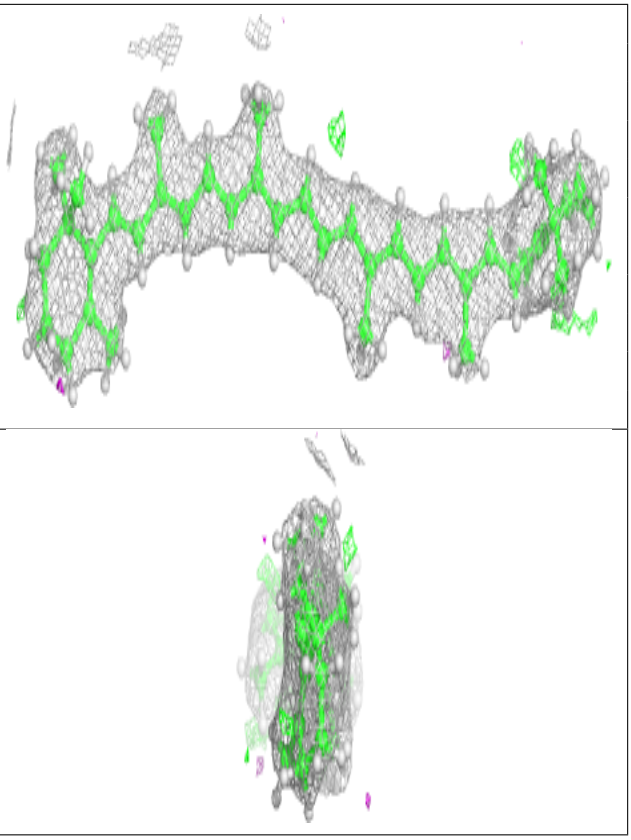
Electron density around CLA c 507:

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



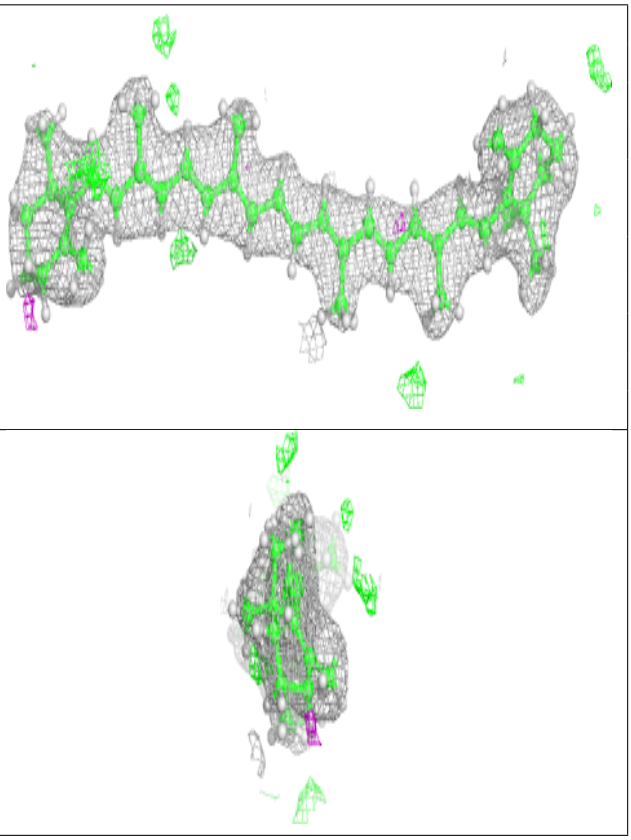
Electron density around BCR b 617:

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



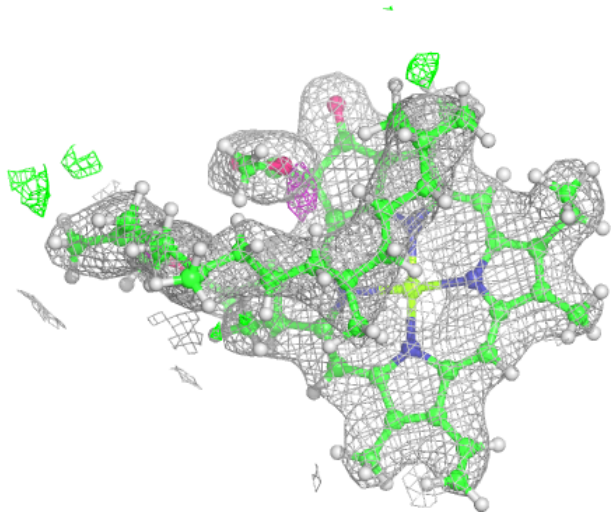
Electron density around BCR b 618:

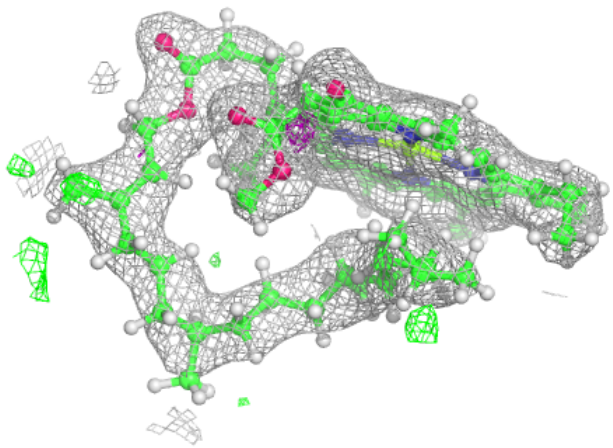
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

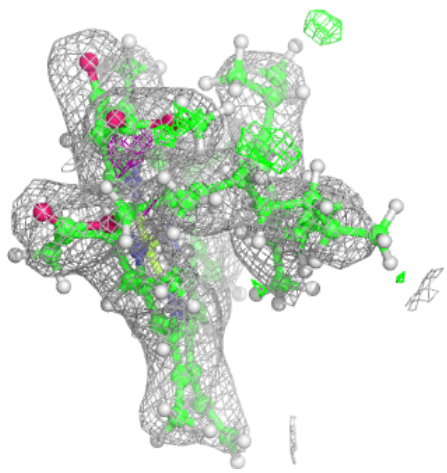


Electron density around CLA C 510:

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

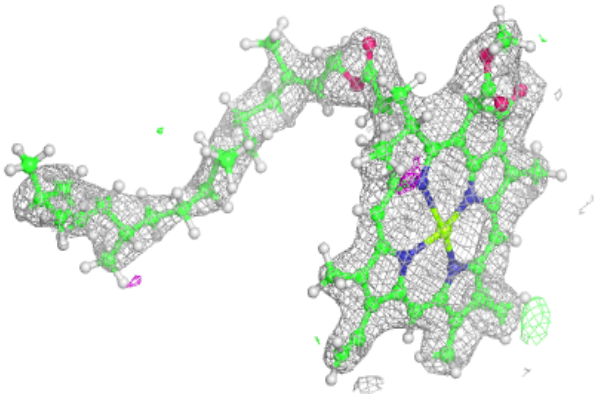


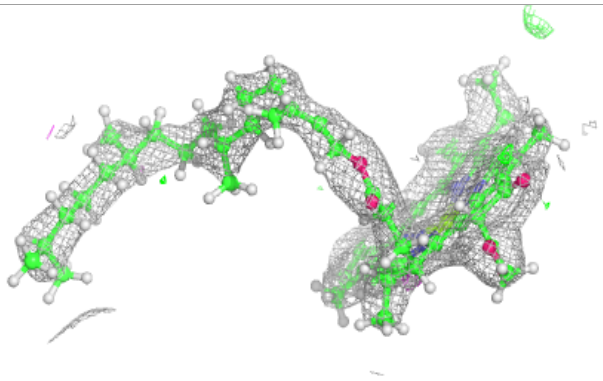


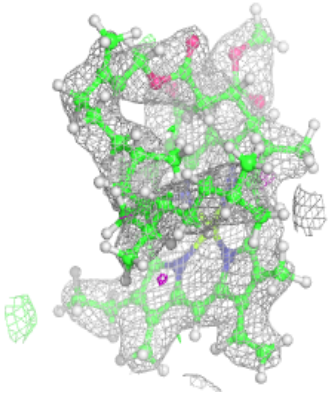


Electron density around CLA C 511:

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

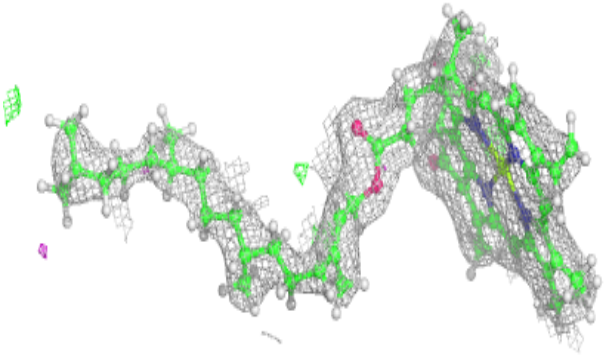


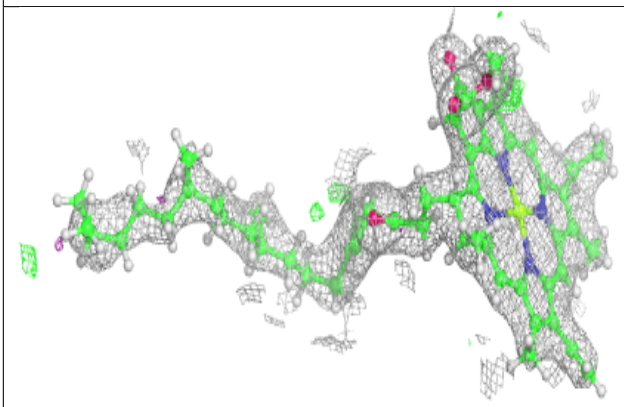


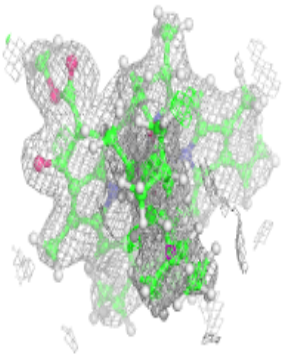


Electron density around CLA c 502:

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

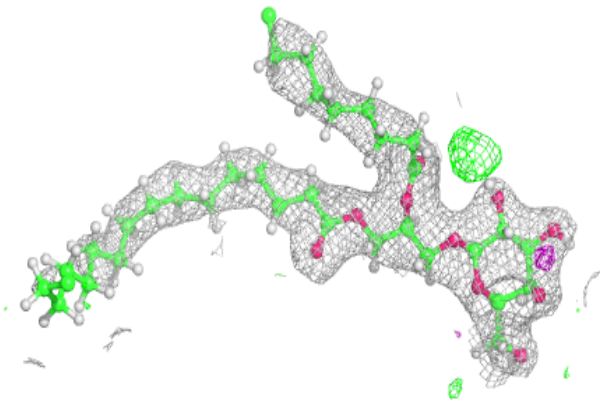


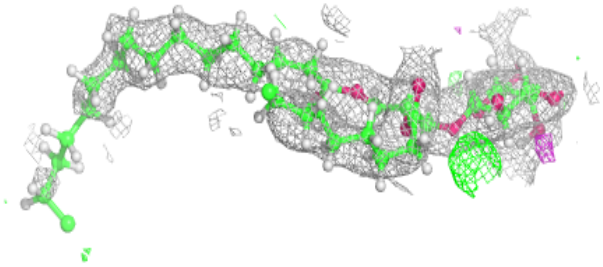


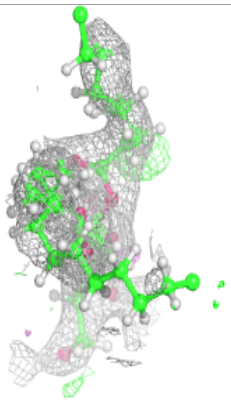


Electron density around LMG d 406:

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

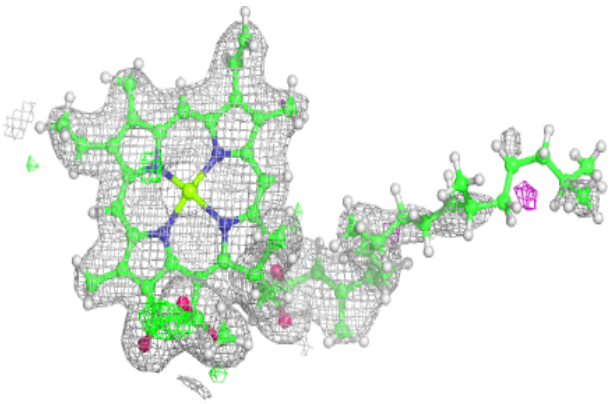


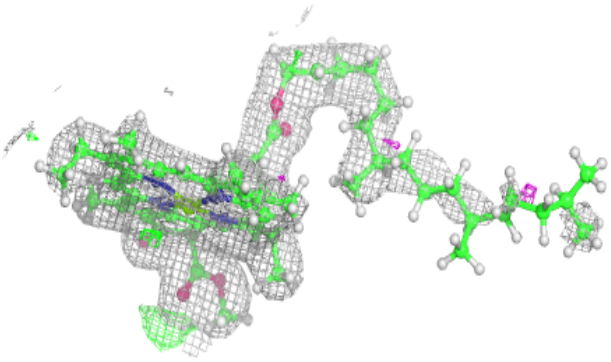


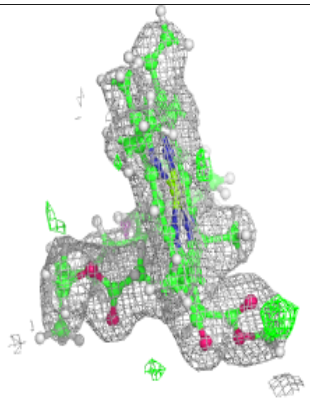


Electron density around CLA A 604:

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

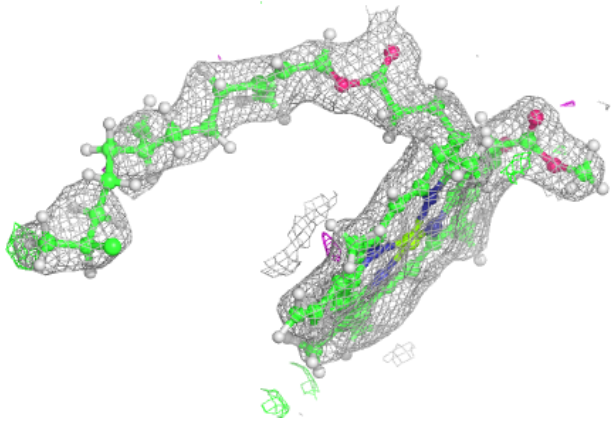


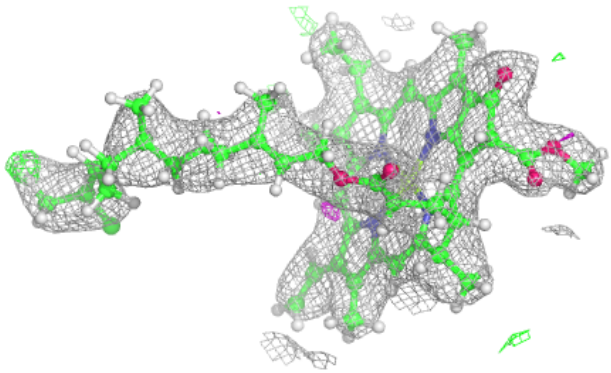


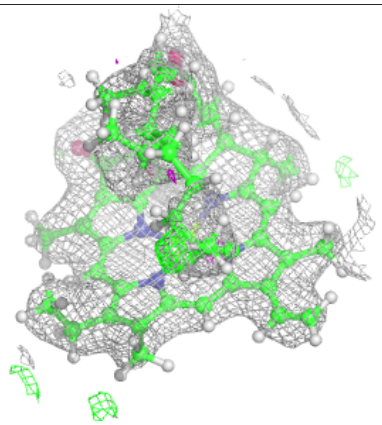


Electron density around CLA c 504:

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

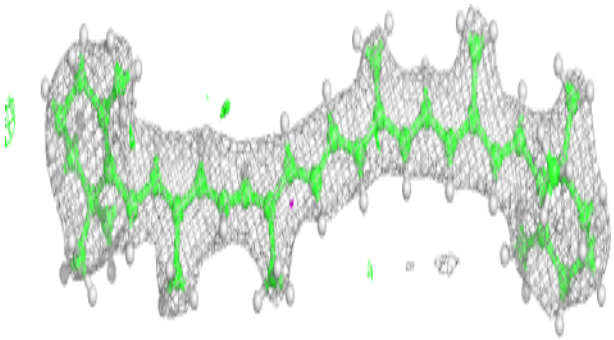


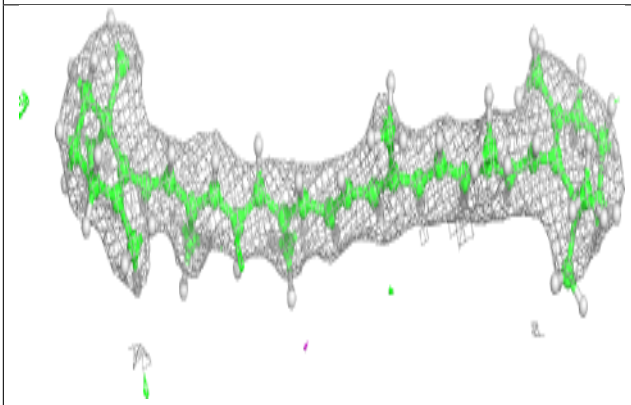


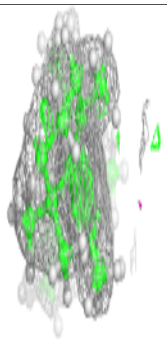


Electron density around BCR b 619:

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

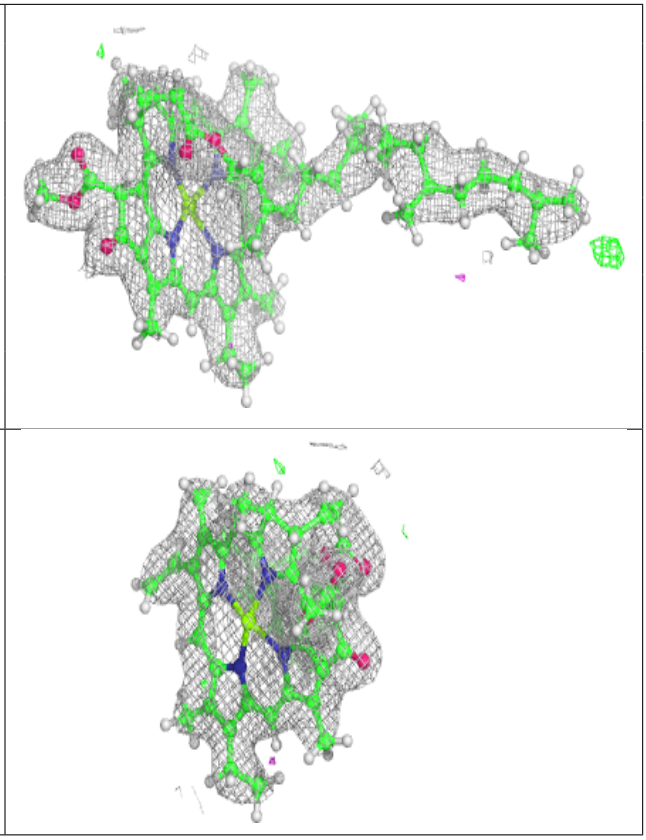






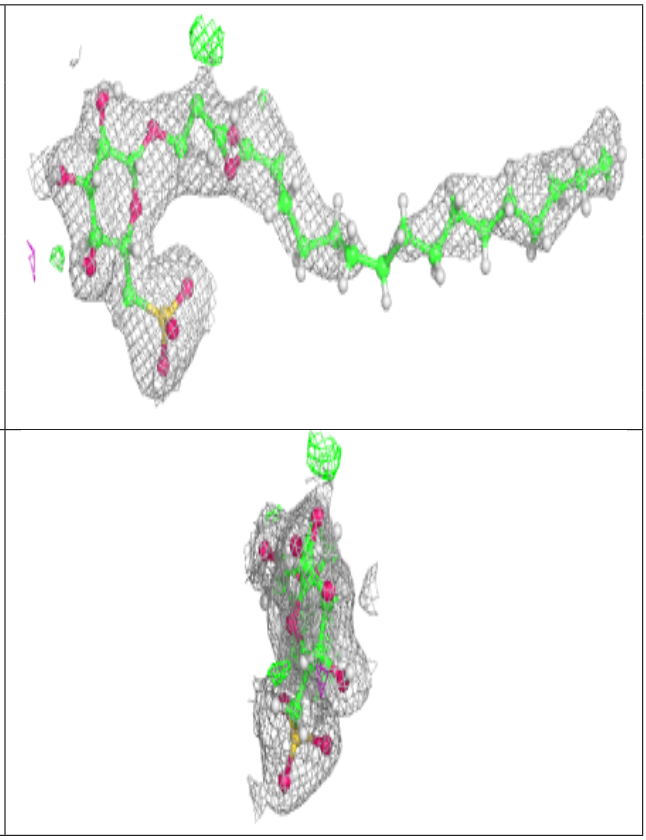
Electron density around CLA c 505:

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



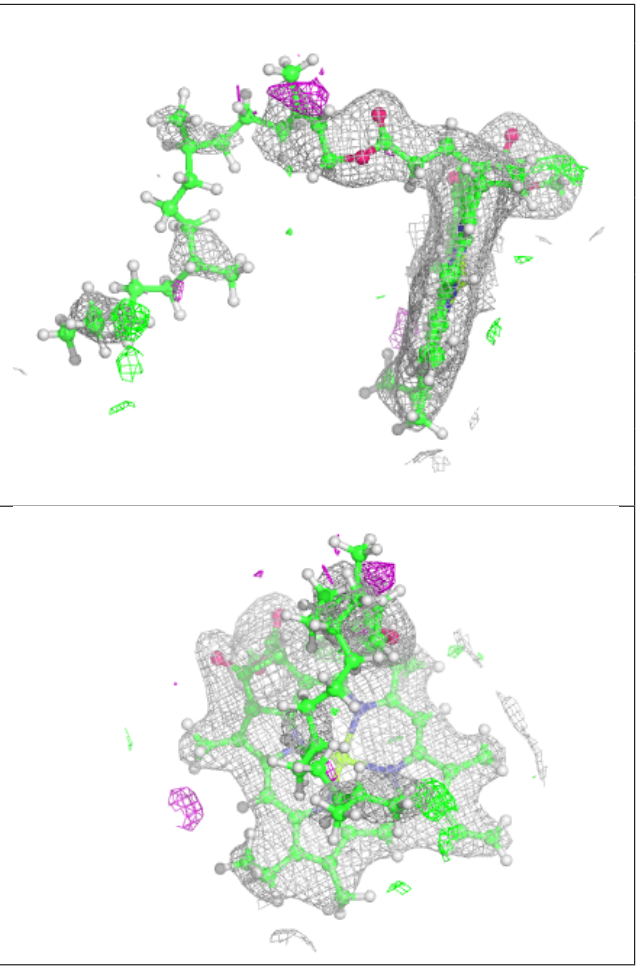
Electron density around SQD F 101:

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



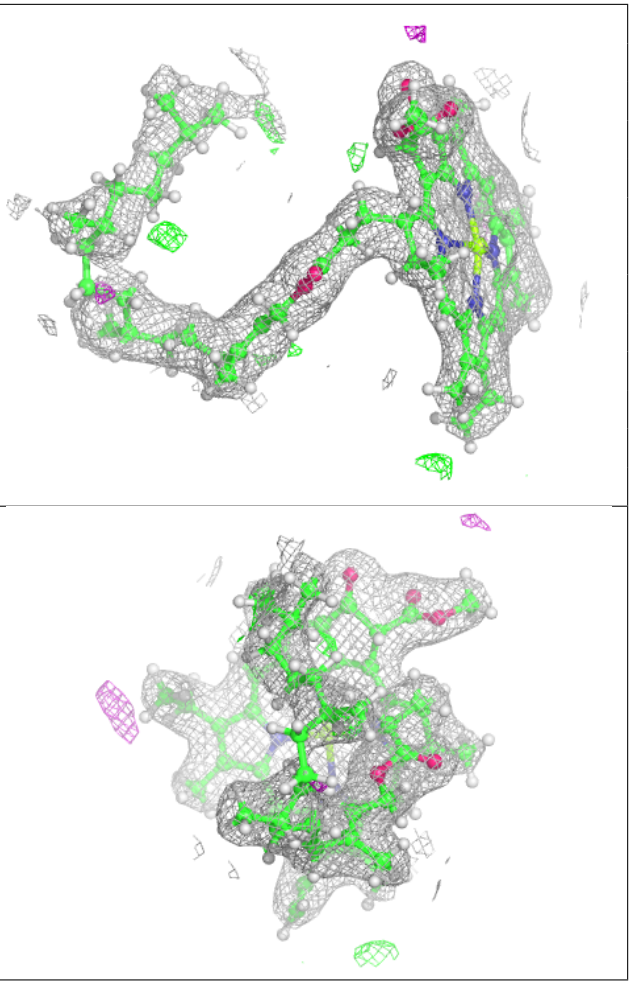
Electron density around CLA c 506:

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



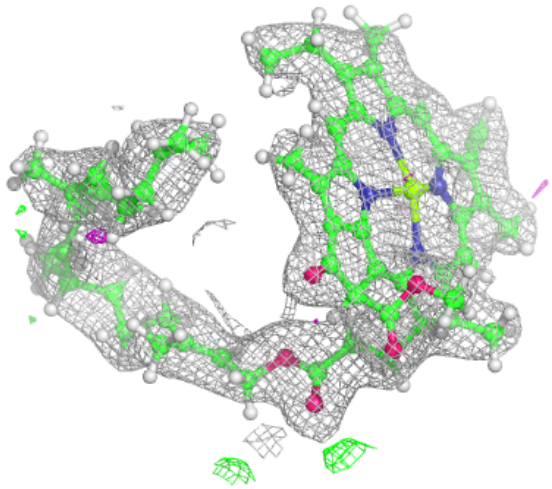
Electron density around CLA B 606:

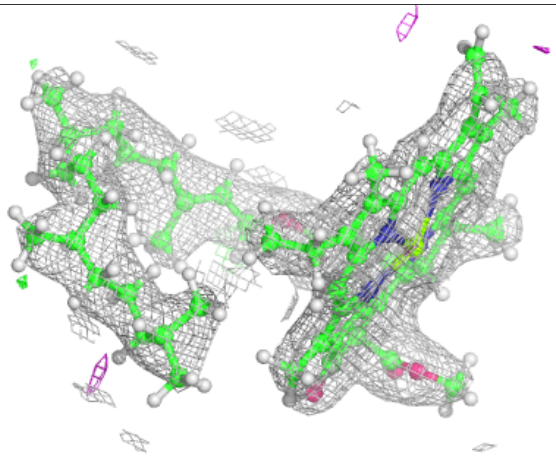
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

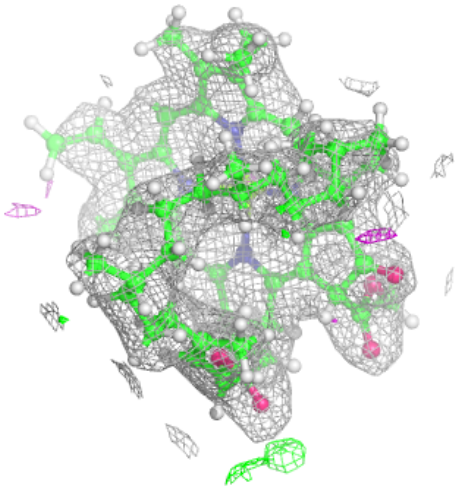


Electron density around CLA C 503:

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

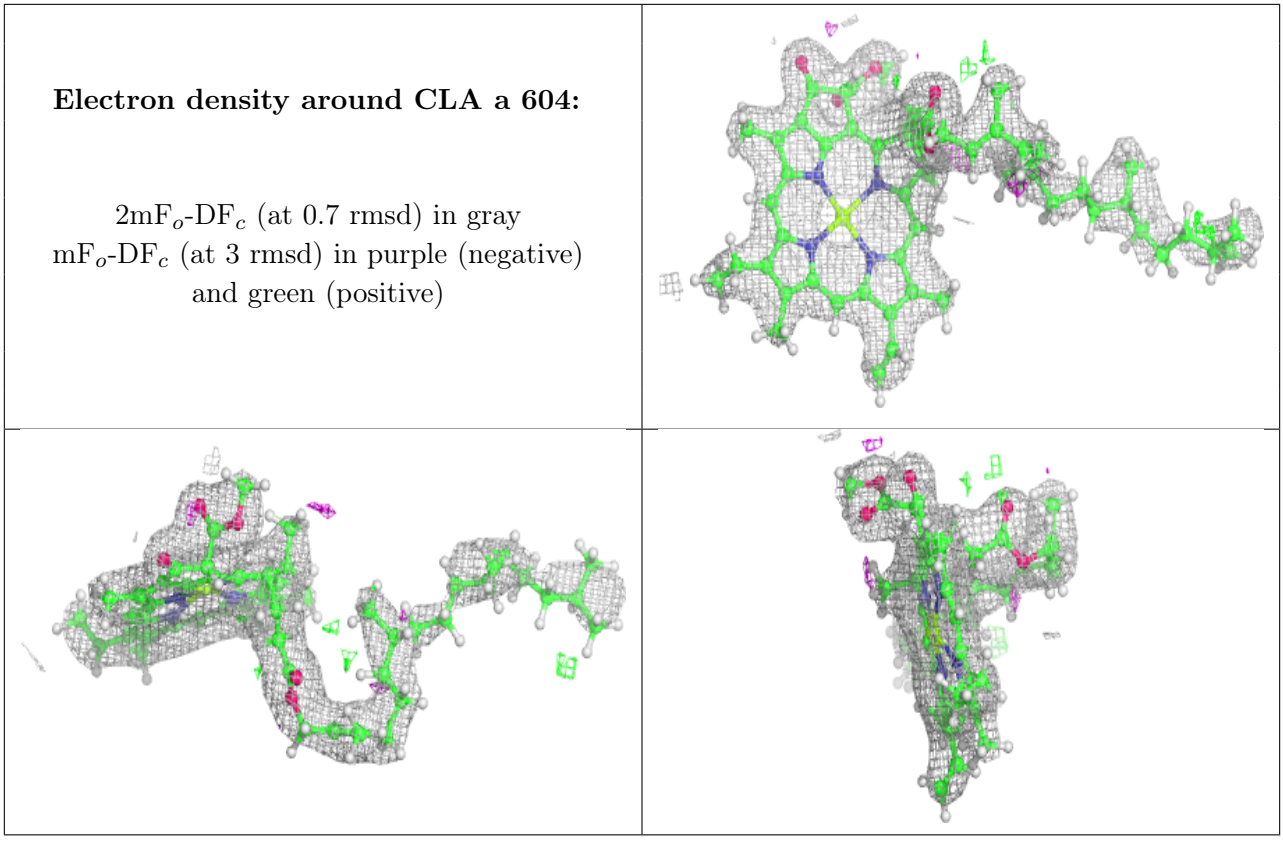






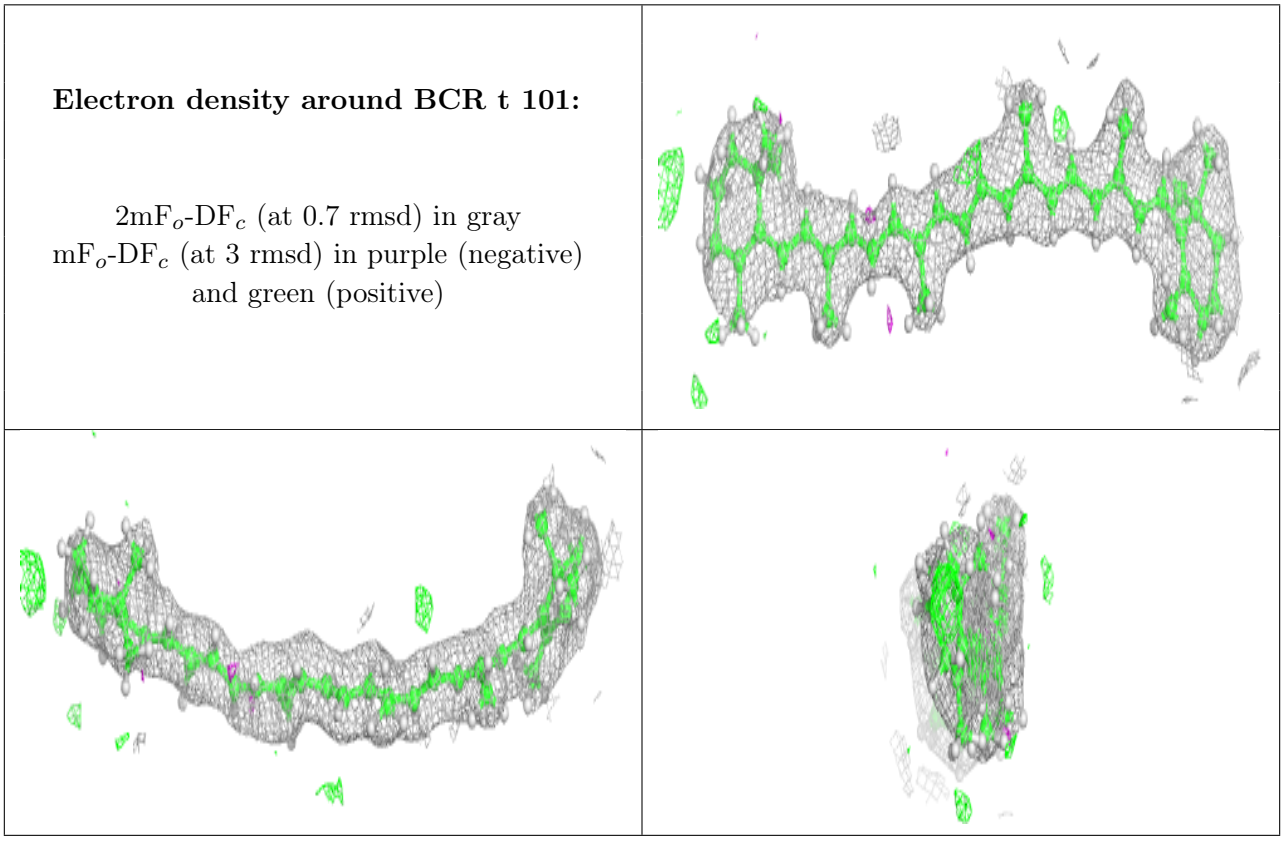
Electron density around CLA a 604:

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



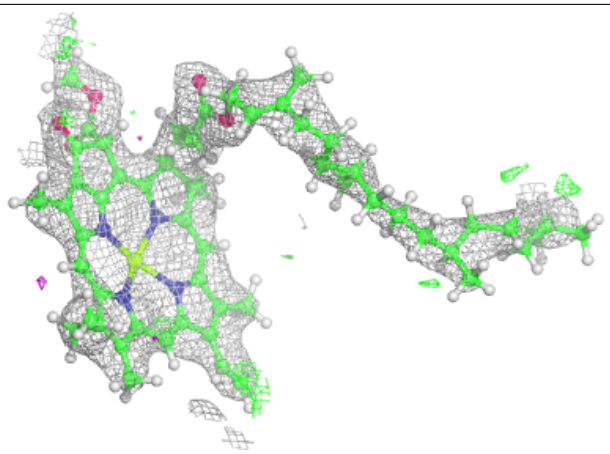
Electron density around BCR t 101:

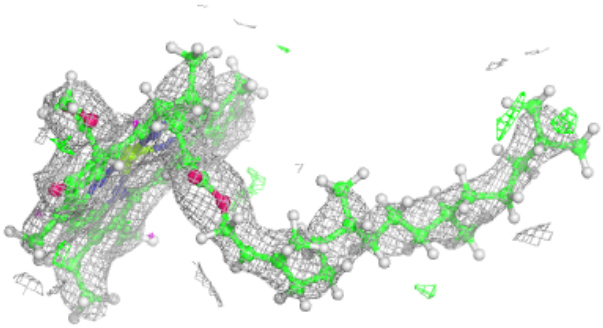
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

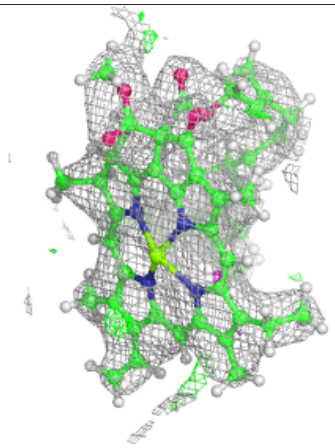


Electron density around CLA c 511:

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

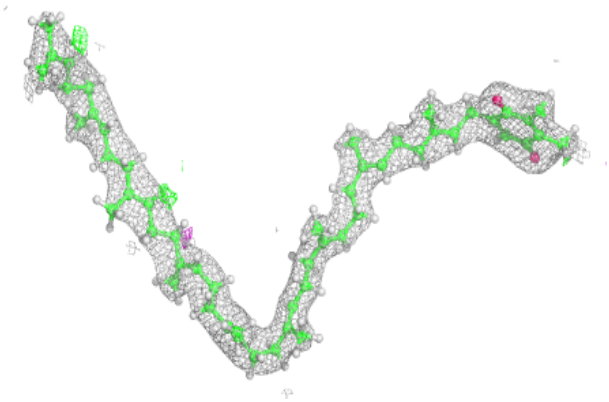


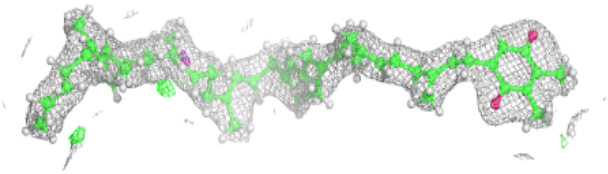


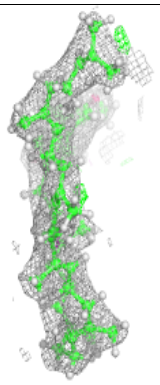


Electron density around PL9 D 407:

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

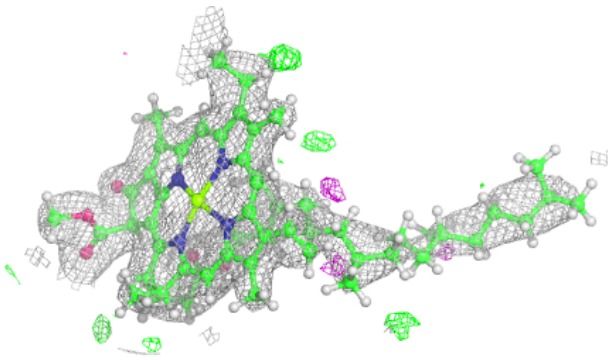


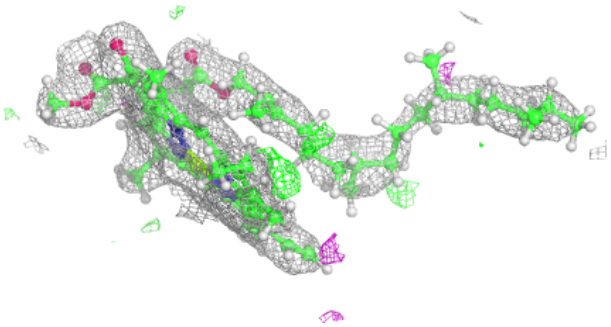


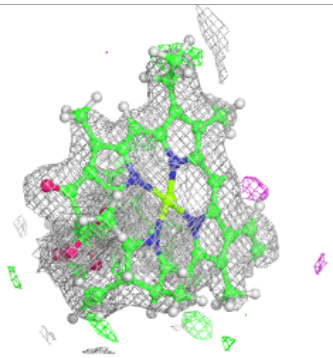


Electron density around CLA C 505:

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

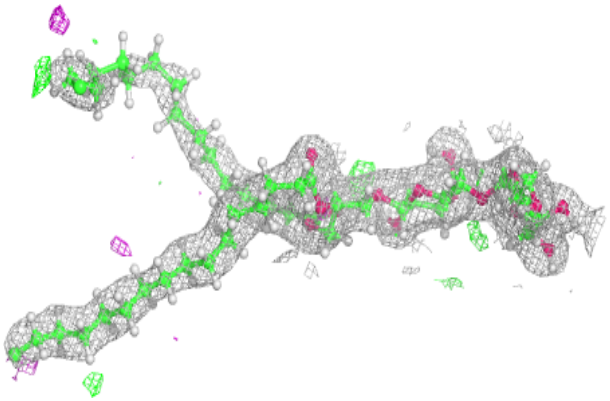


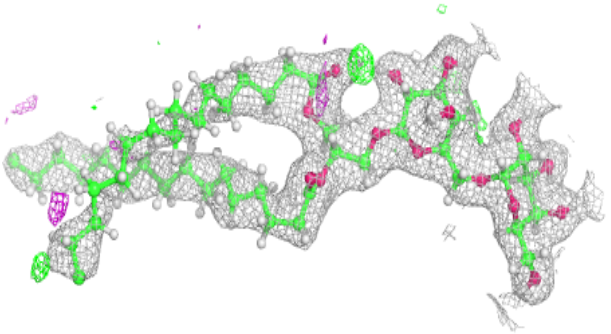


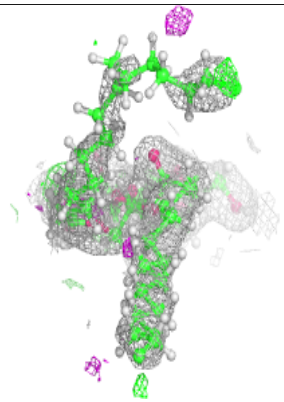


Electron density around DGD C 516:

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

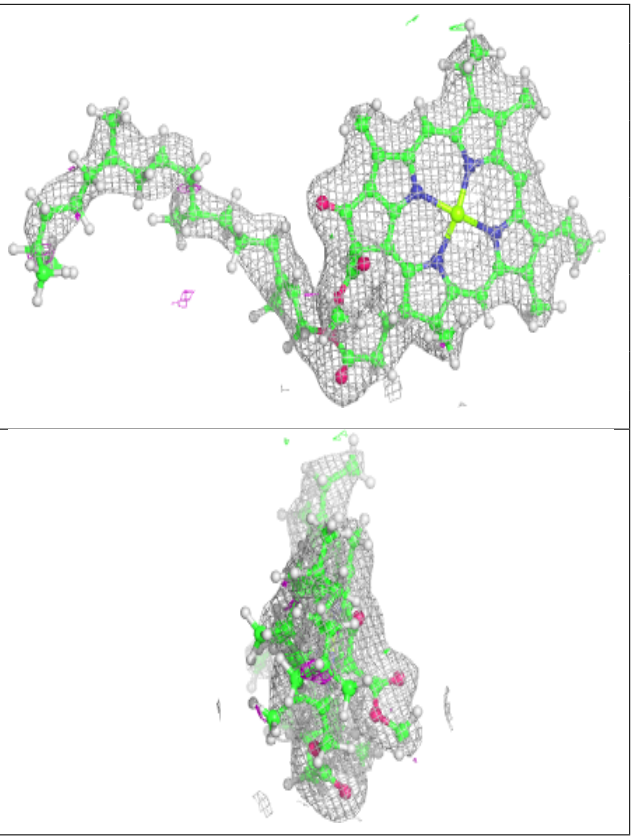






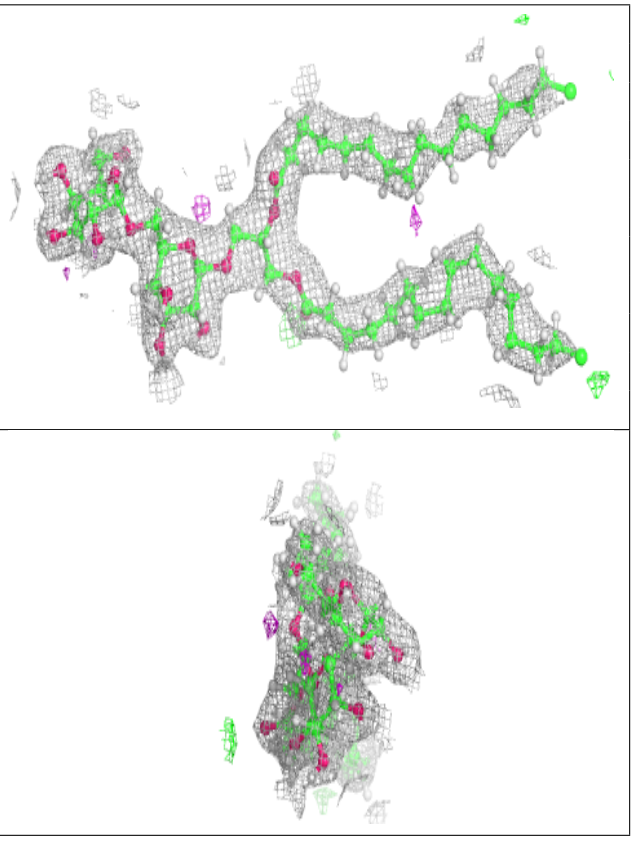
Electron density around CLA b 602:

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



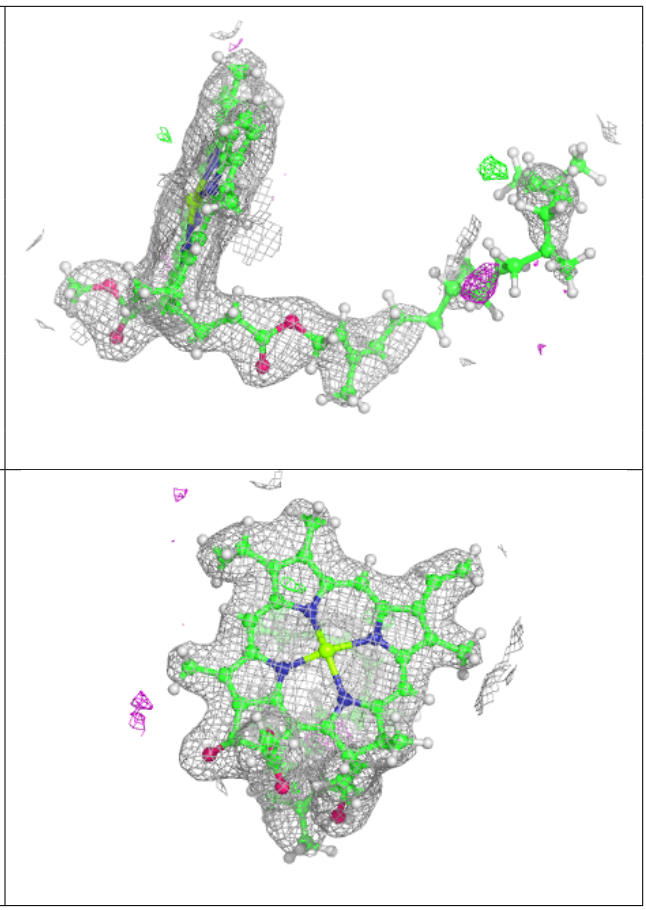
Electron density around DGD C 518:

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



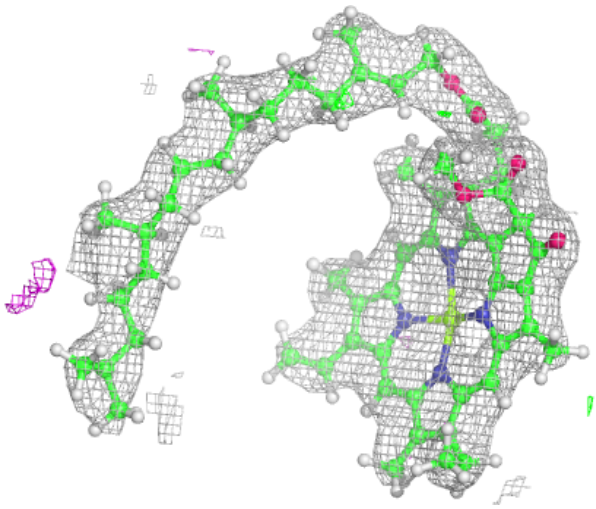
Electron density around CLA C 506:

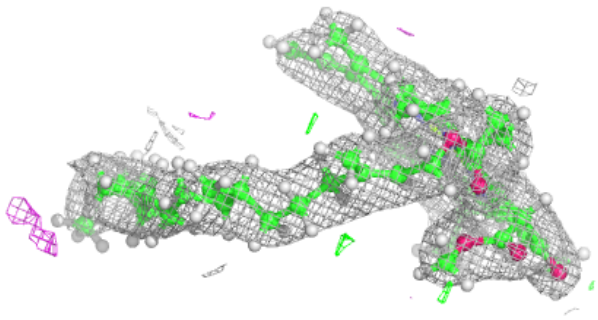
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

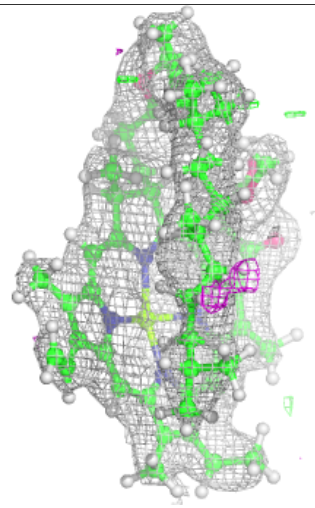


Electron density around CLA C 507:

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

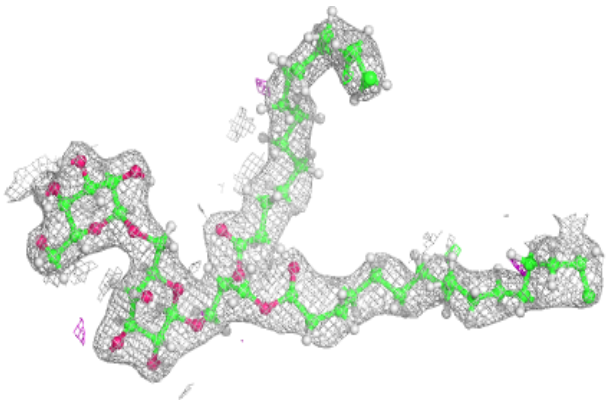


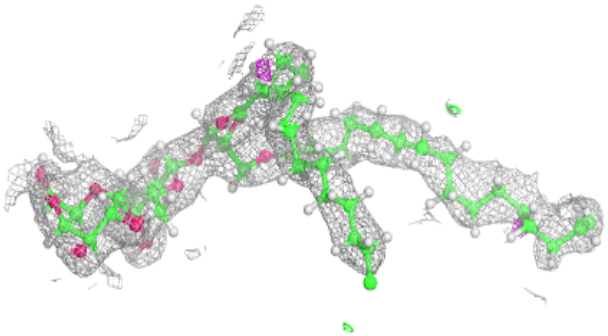


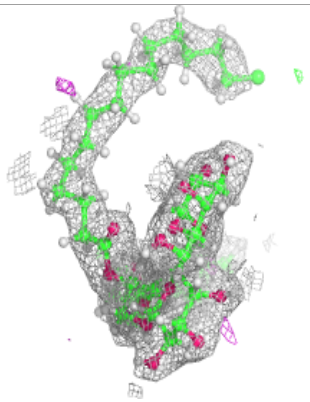


Electron density around DGD c 517:

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

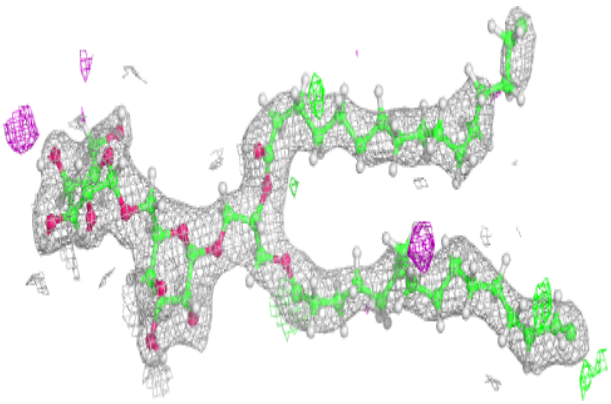


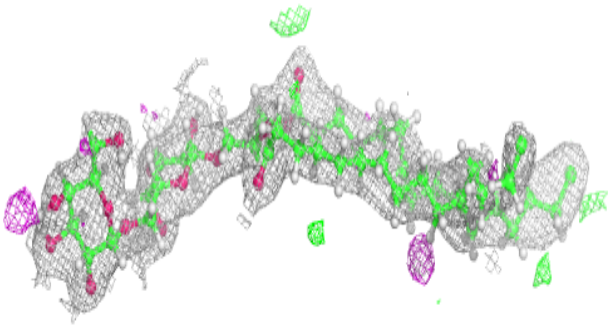


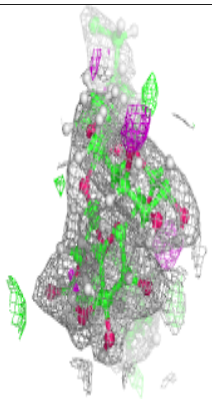


Electron density around DGD c 518:

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

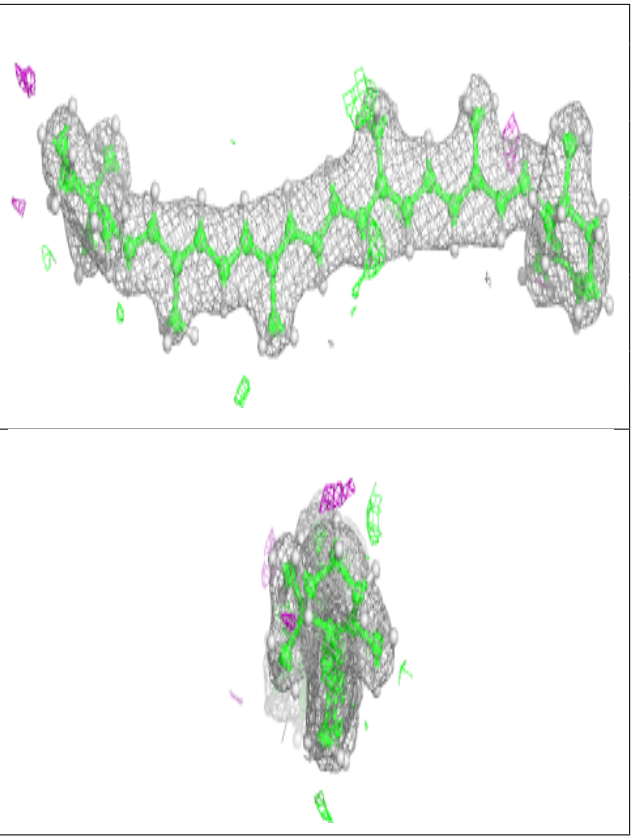






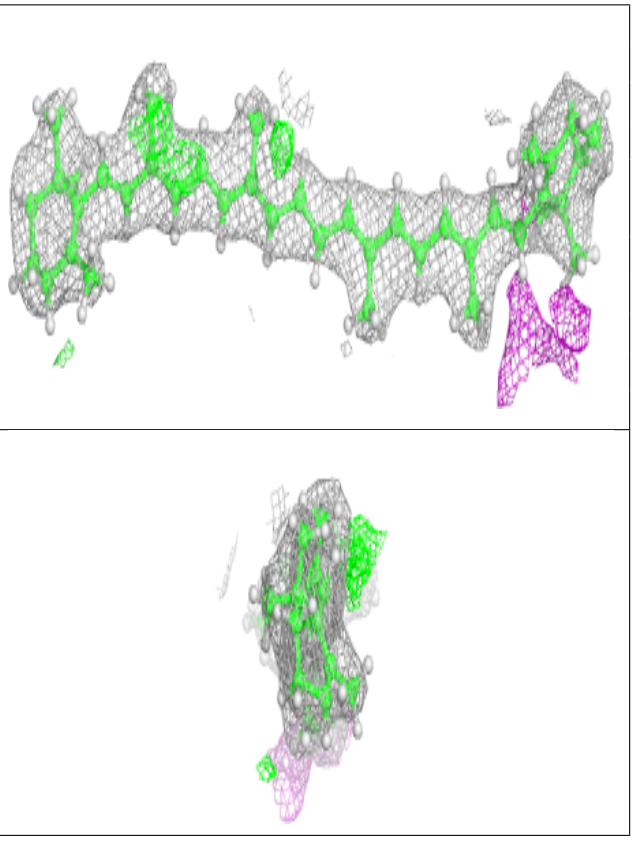
Electron density around BCR A 608:

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



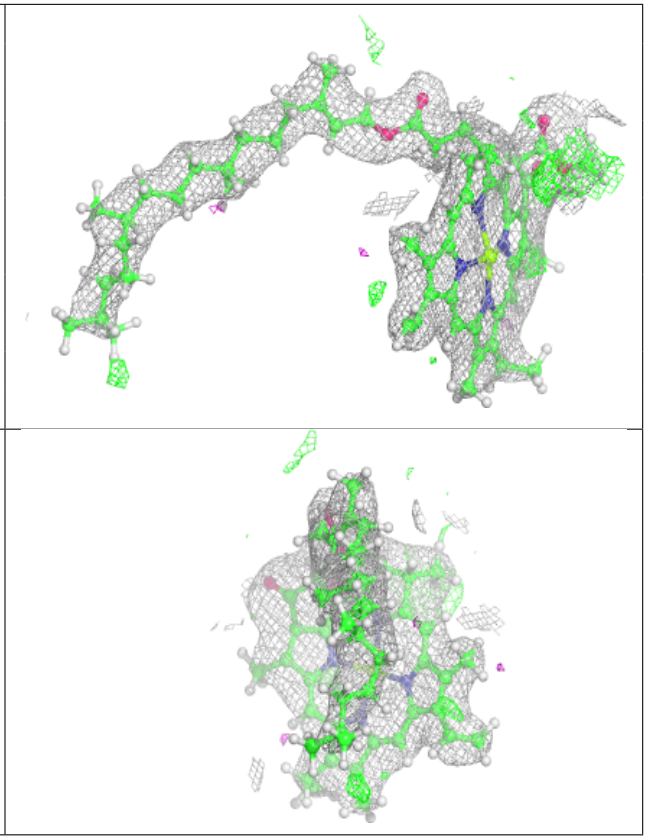
Electron density around BCR B 618:

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



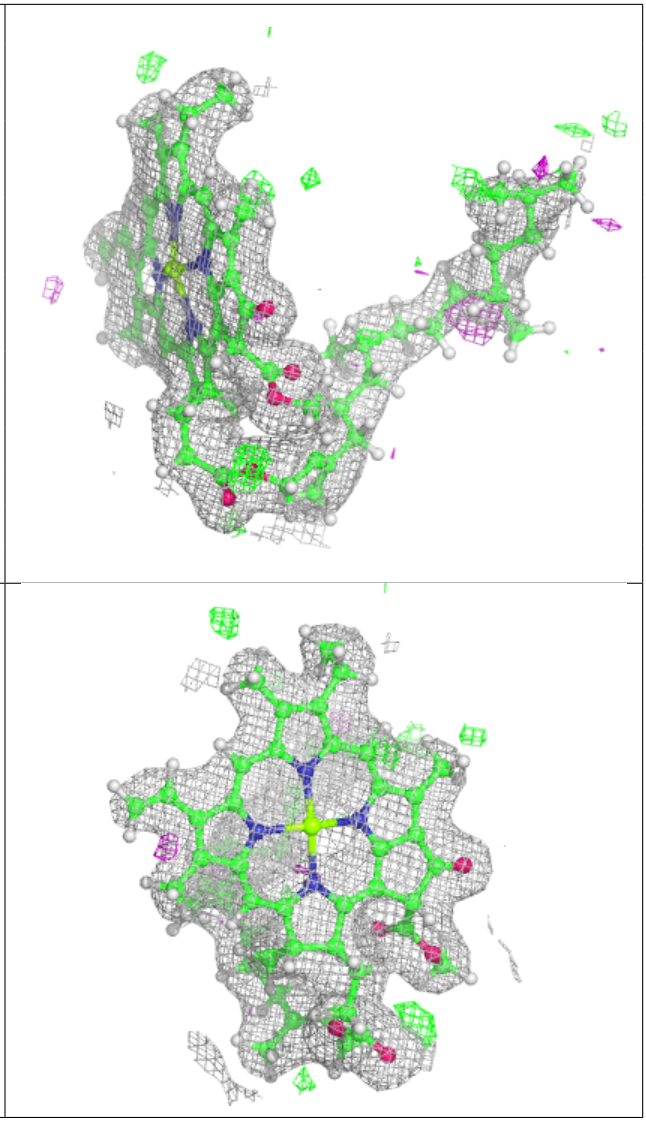
Electron density around CLA b 609:

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



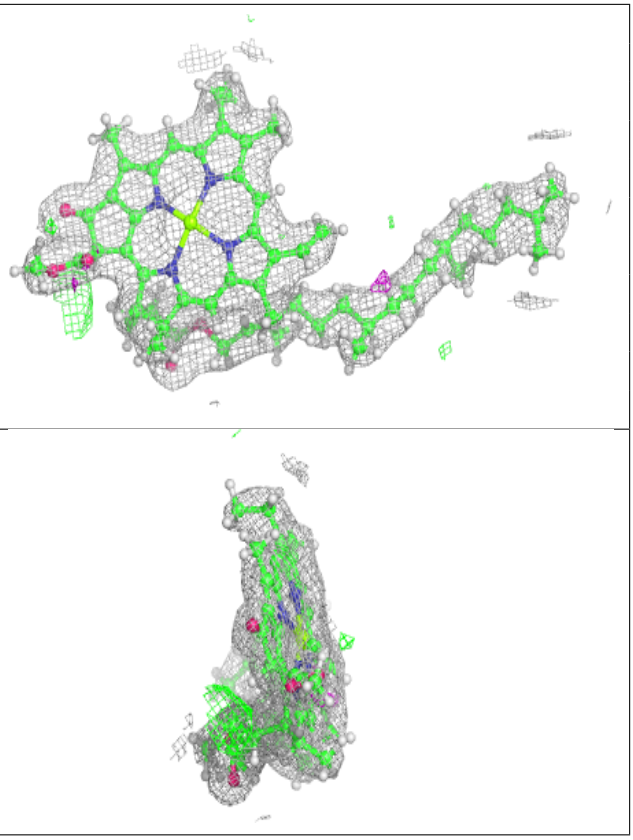
Electron density around CLA b 613:

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



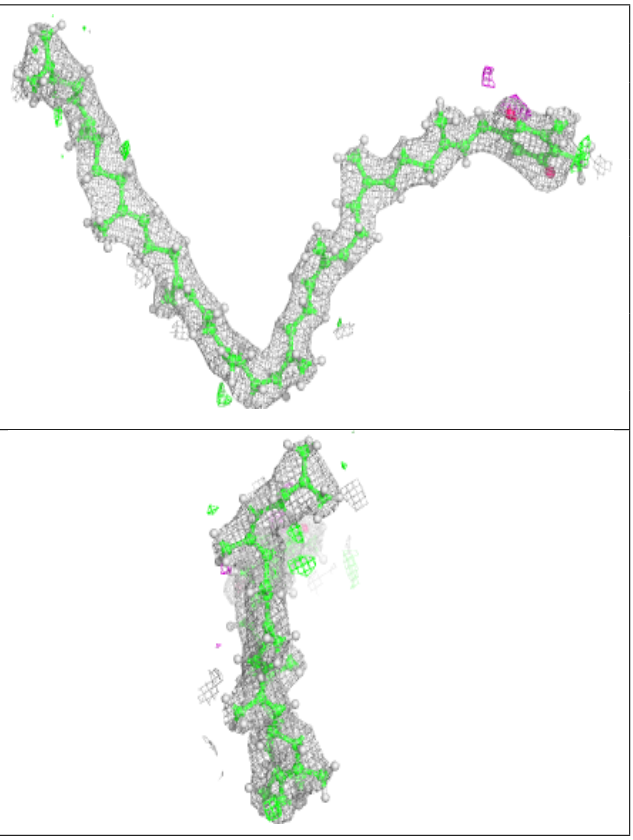
Electron density around CLA C 501:

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



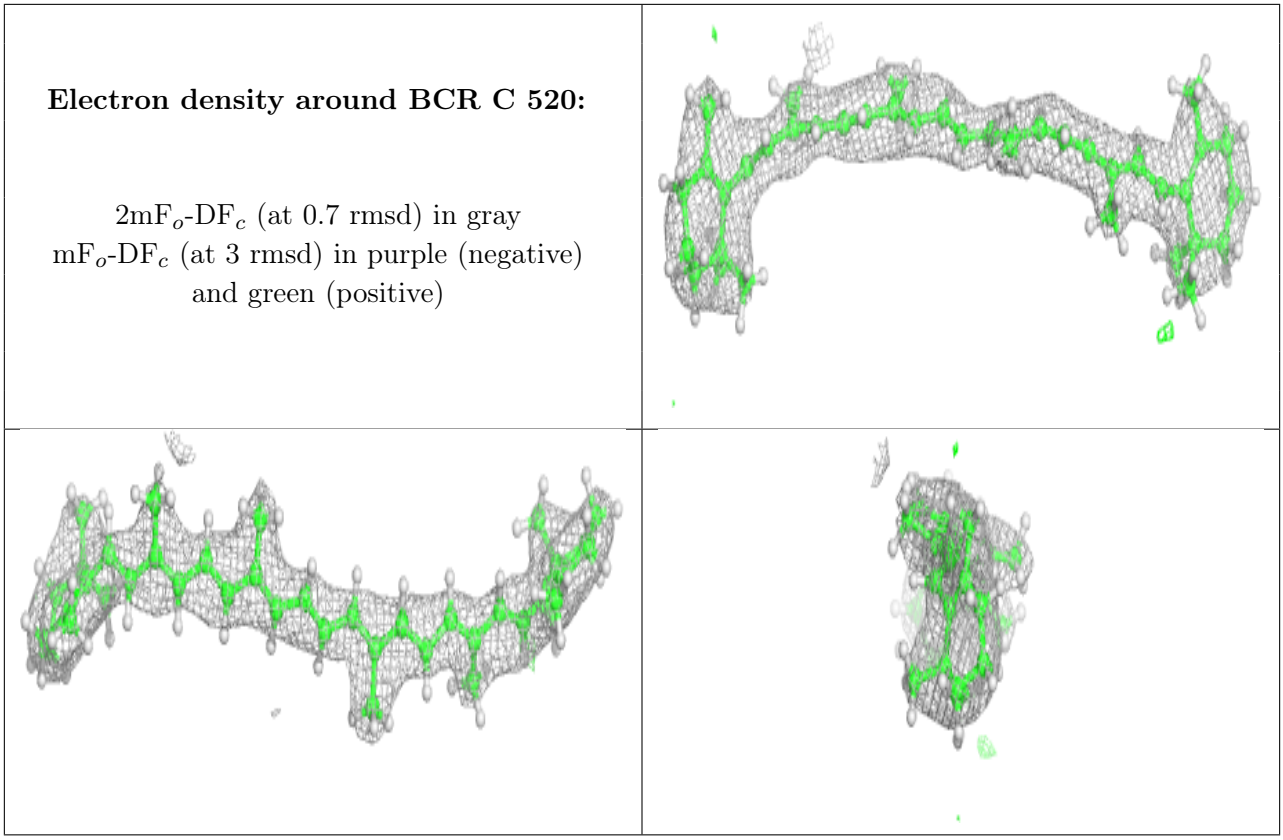
Electron density around PL9 d 408:

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



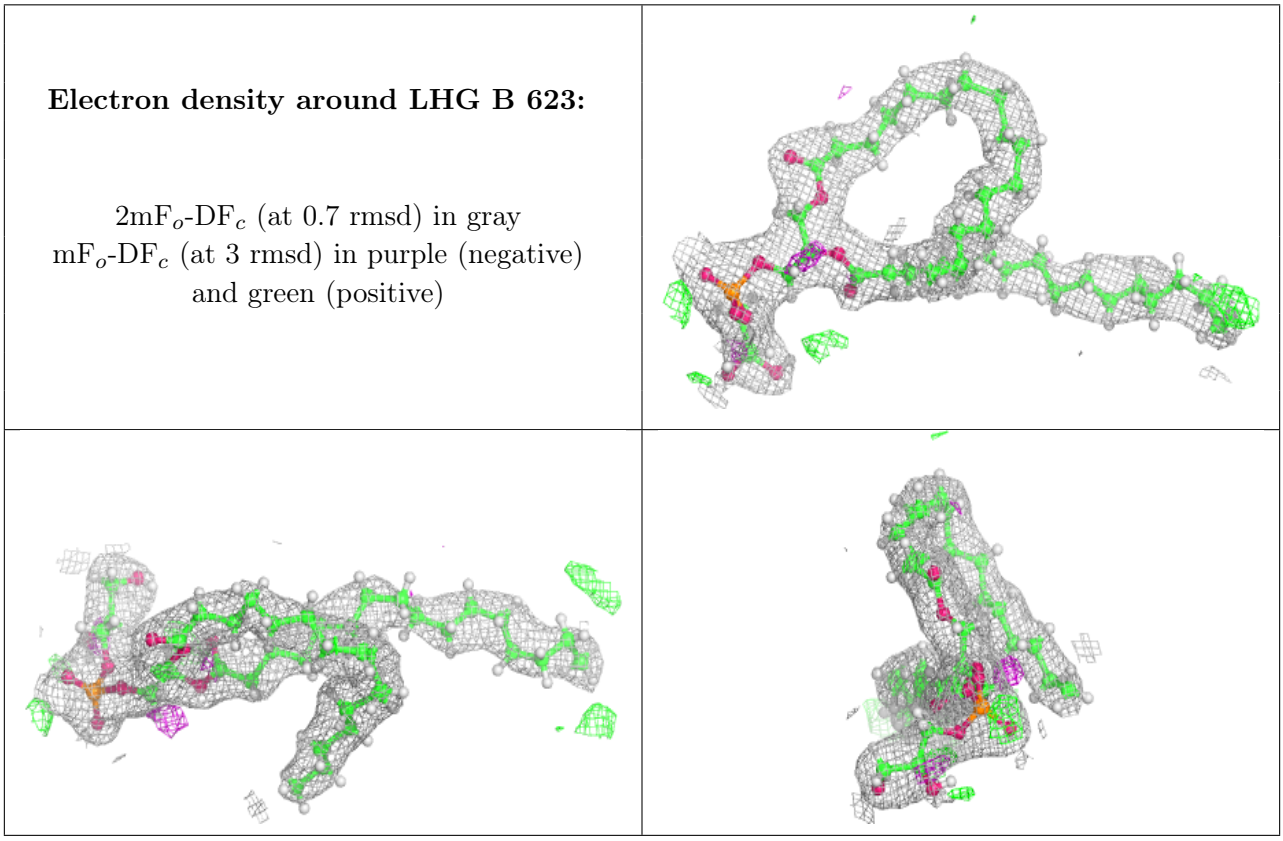
Electron density around BCR C 520:

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



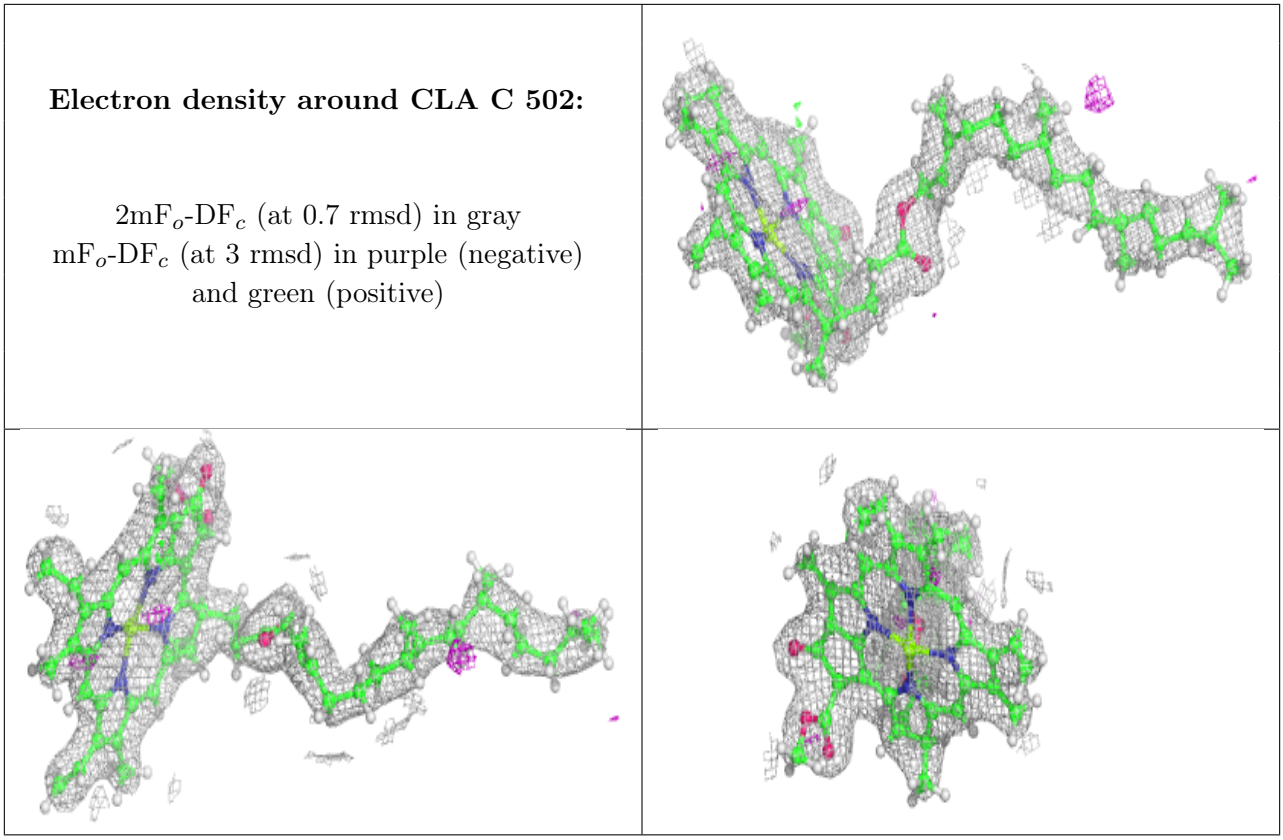
Electron density around LHG B 623:

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



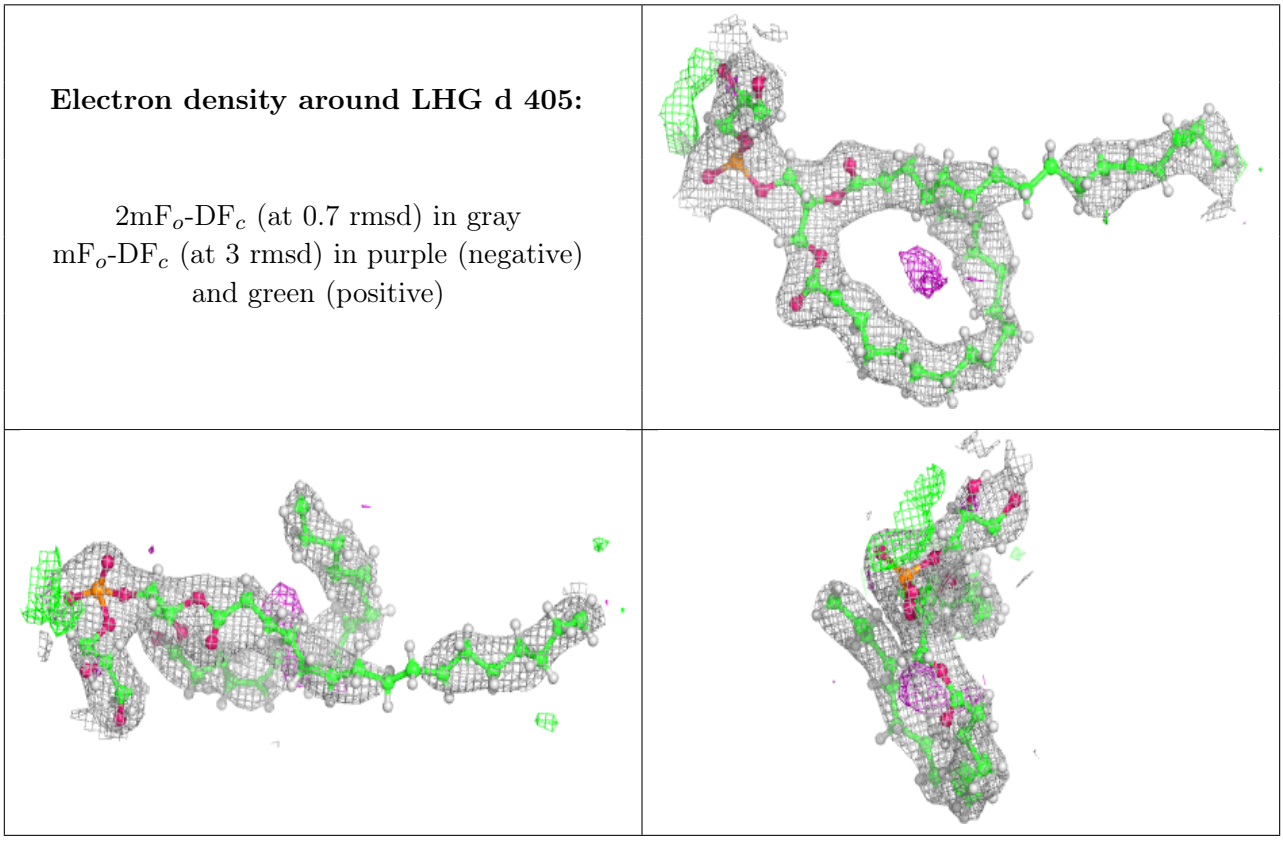
Electron density around CLA C 502:

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



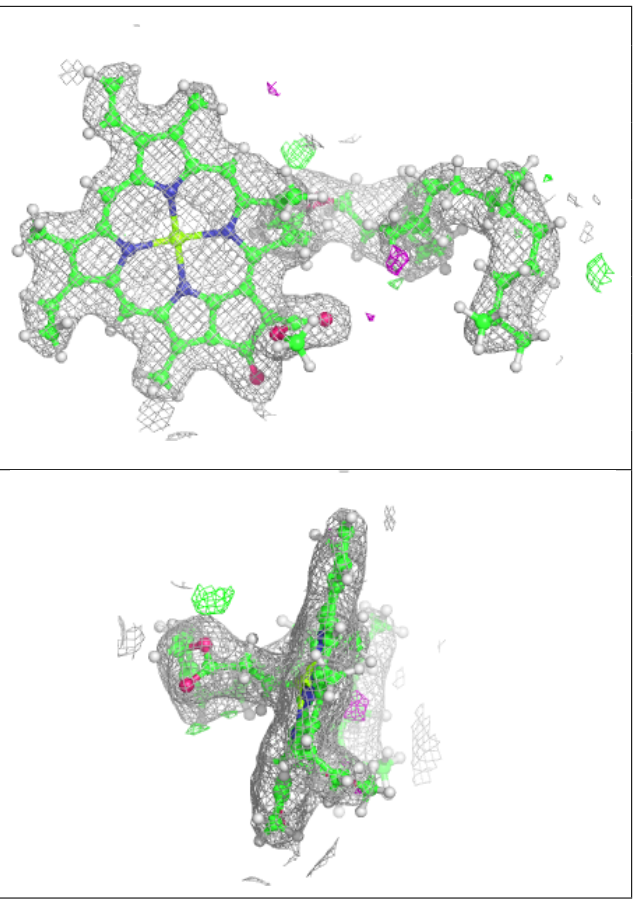
Electron density around LHG d 405:

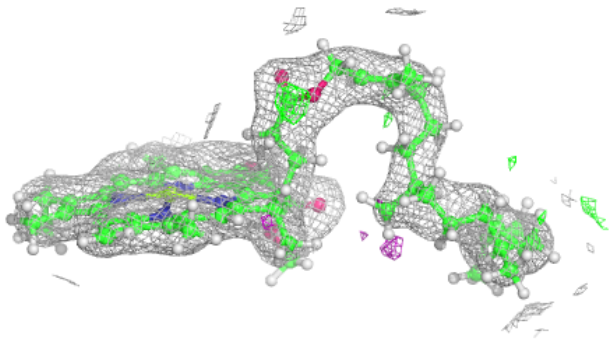
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 612:

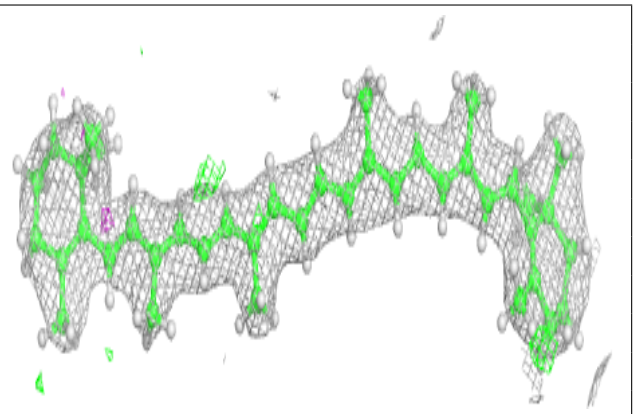
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

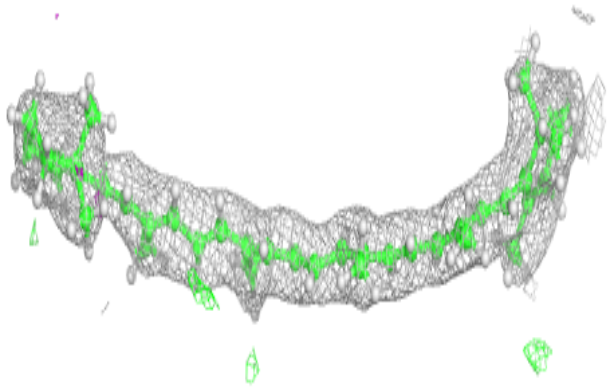


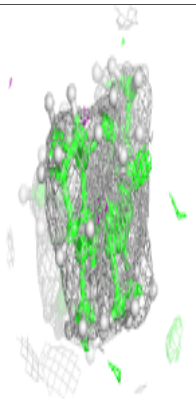


Electron density around BCR T 101:

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

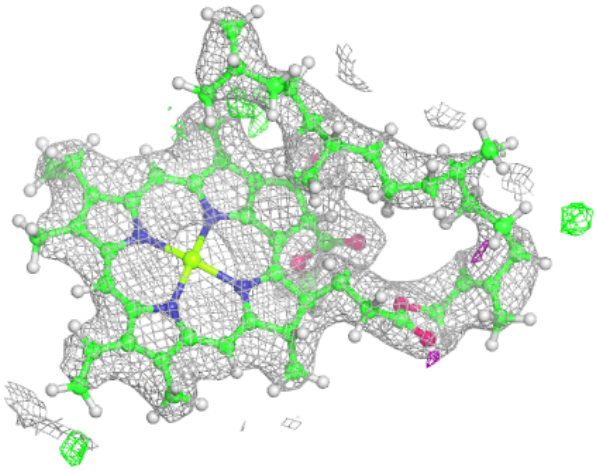


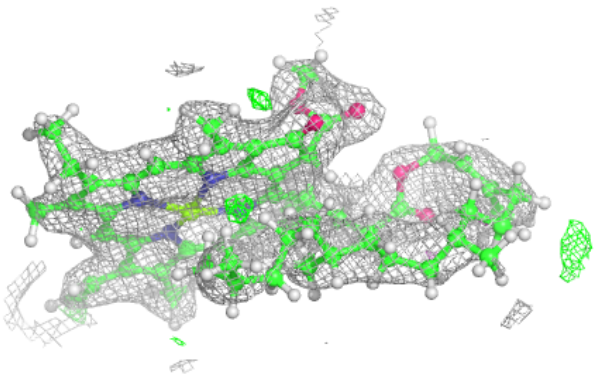


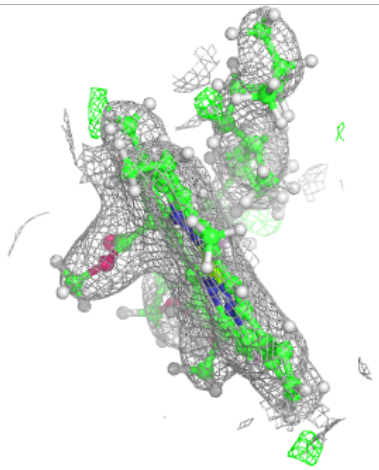


Electron density around CLA c 509:

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

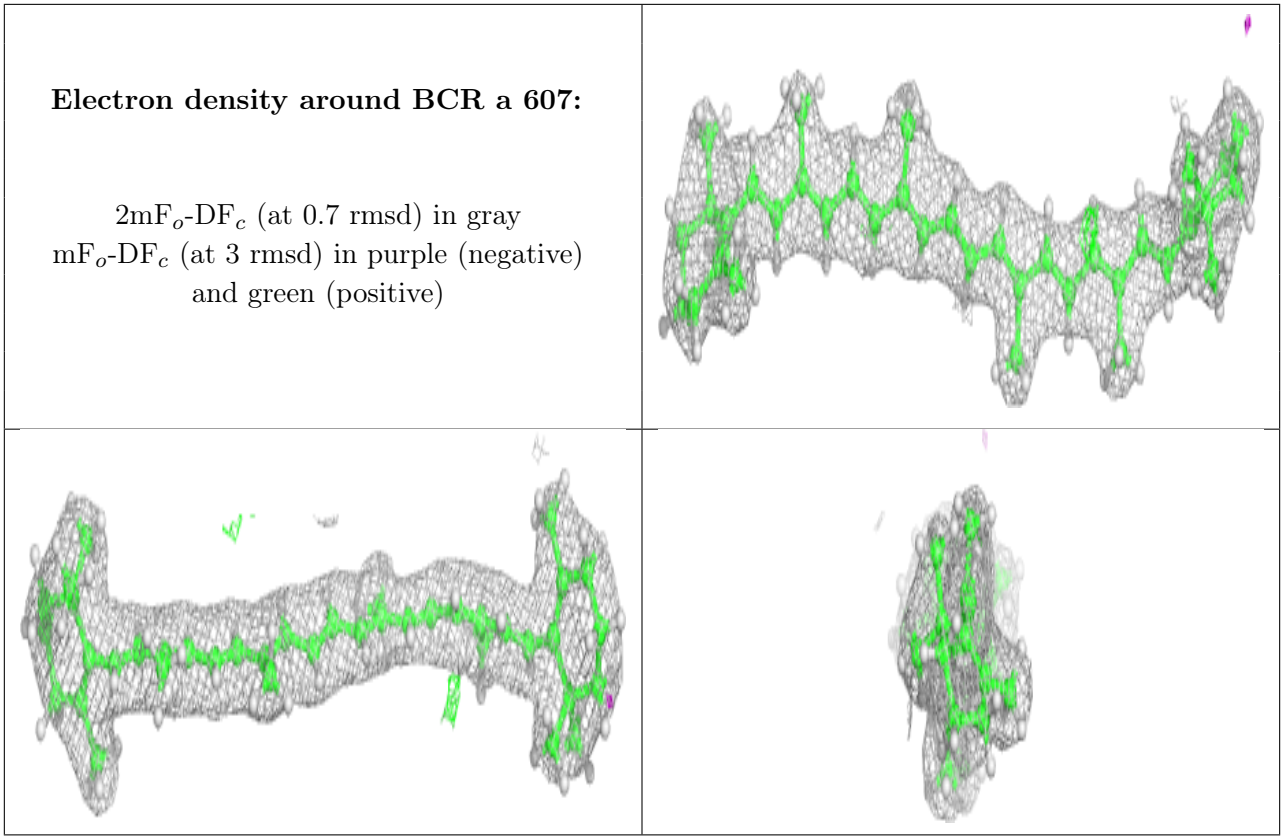






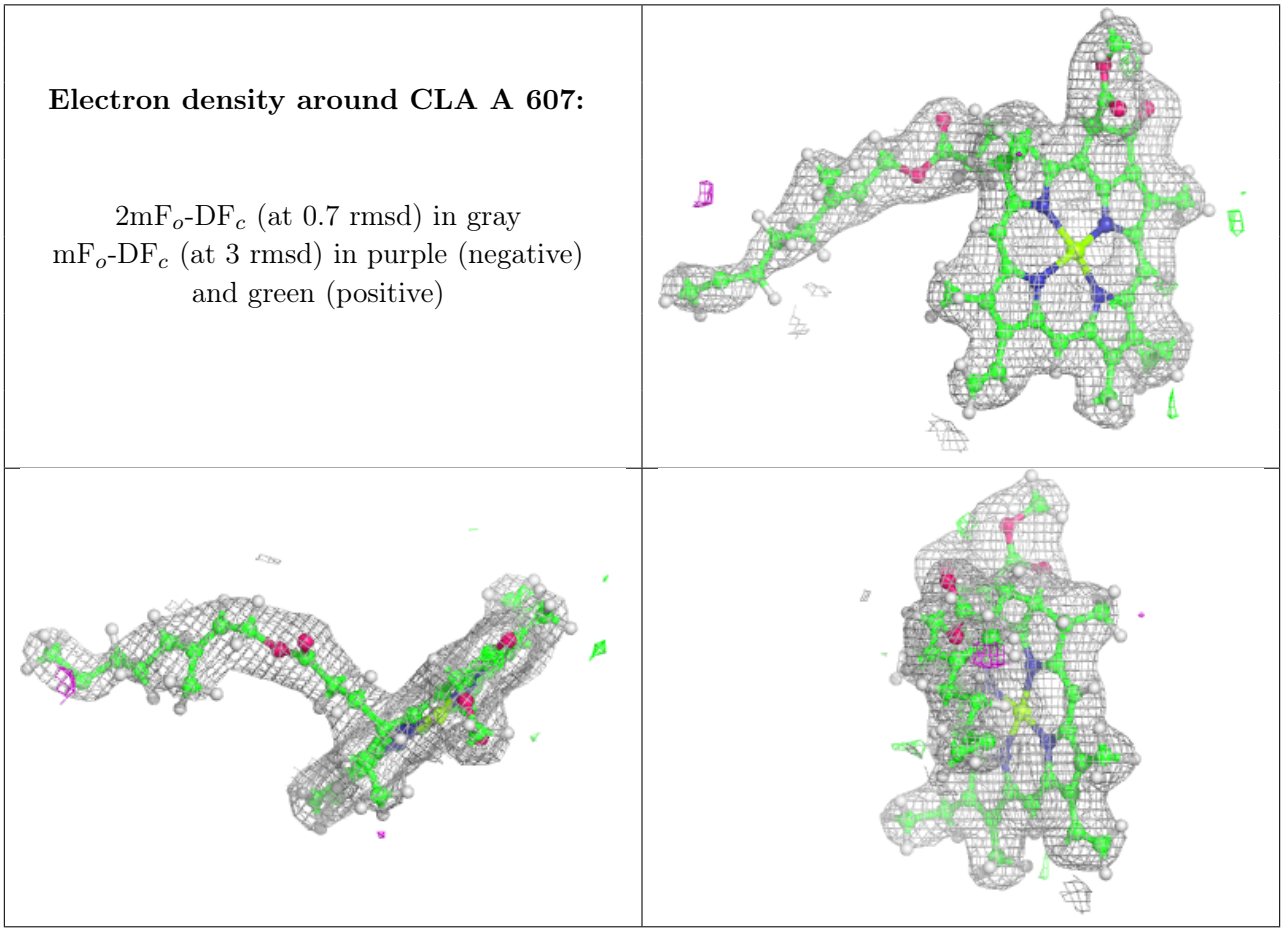
Electron density around BCR a 607:

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



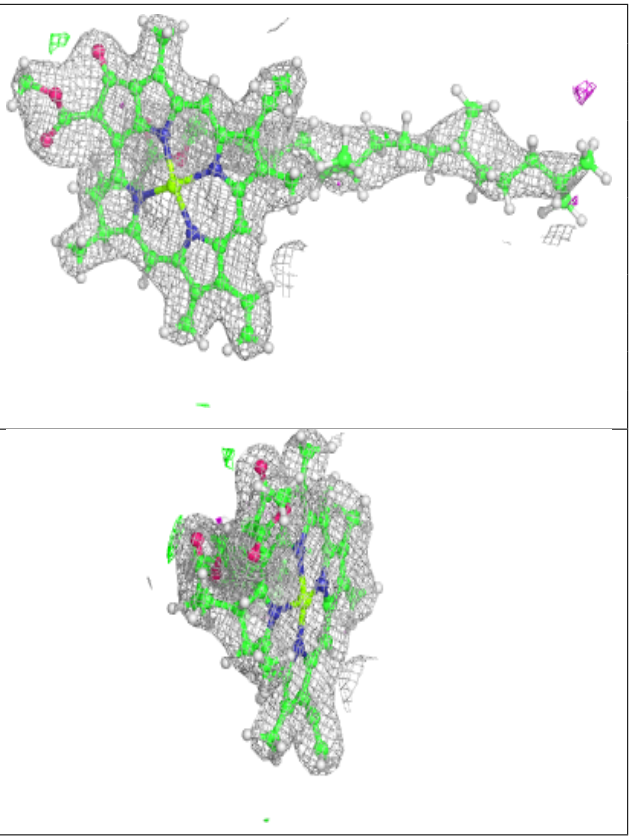
Electron density around CLA A 607:

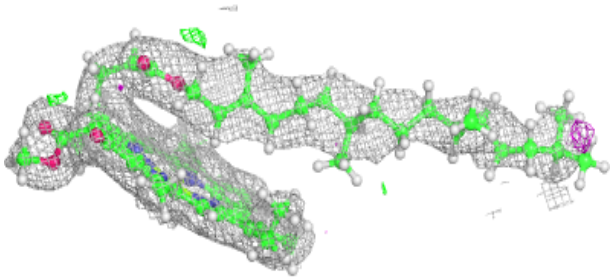
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 614:

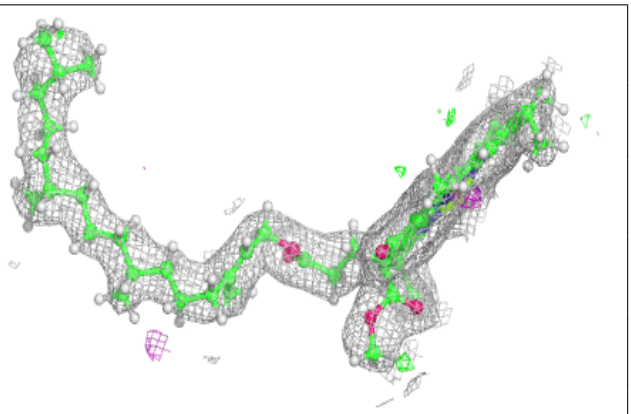
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

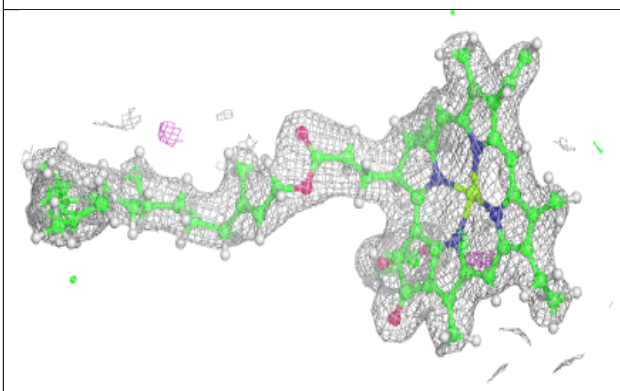


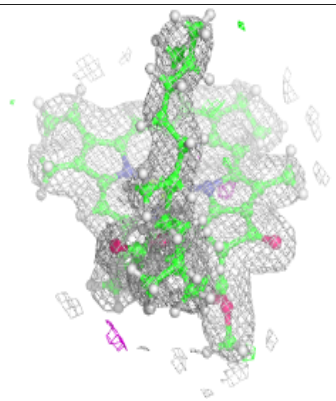


Electron density around CLA D 402:

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

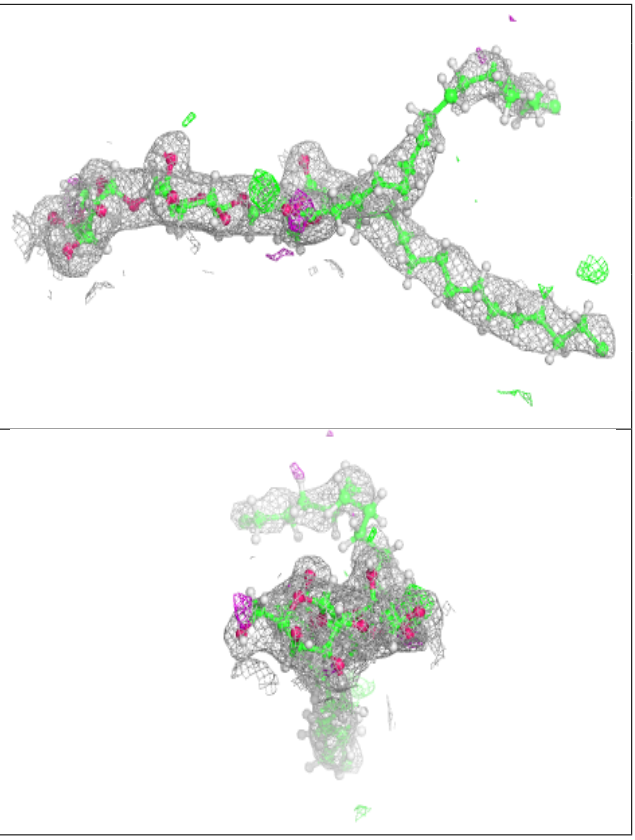


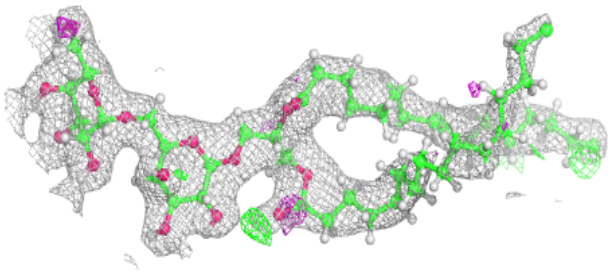




Electron density around DGD c 516:

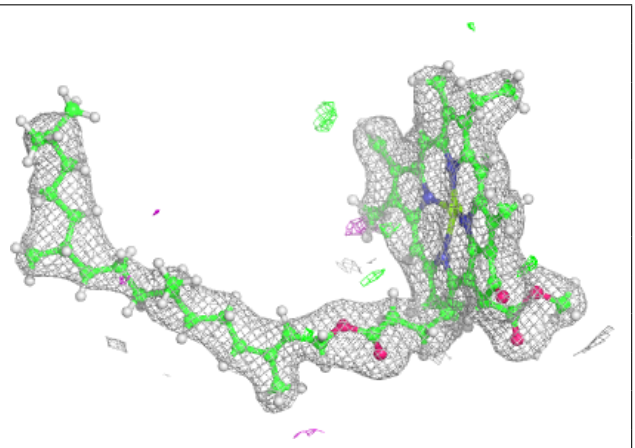
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

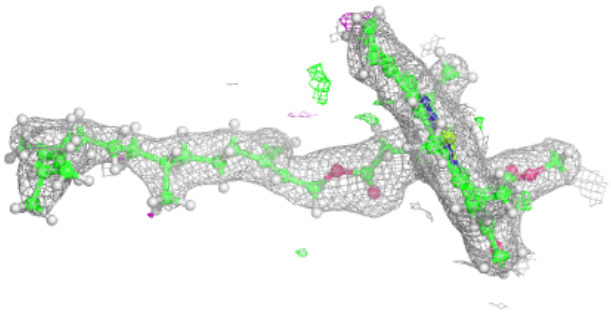


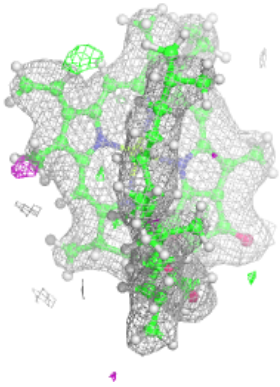


Electron density around CLA B 609:

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

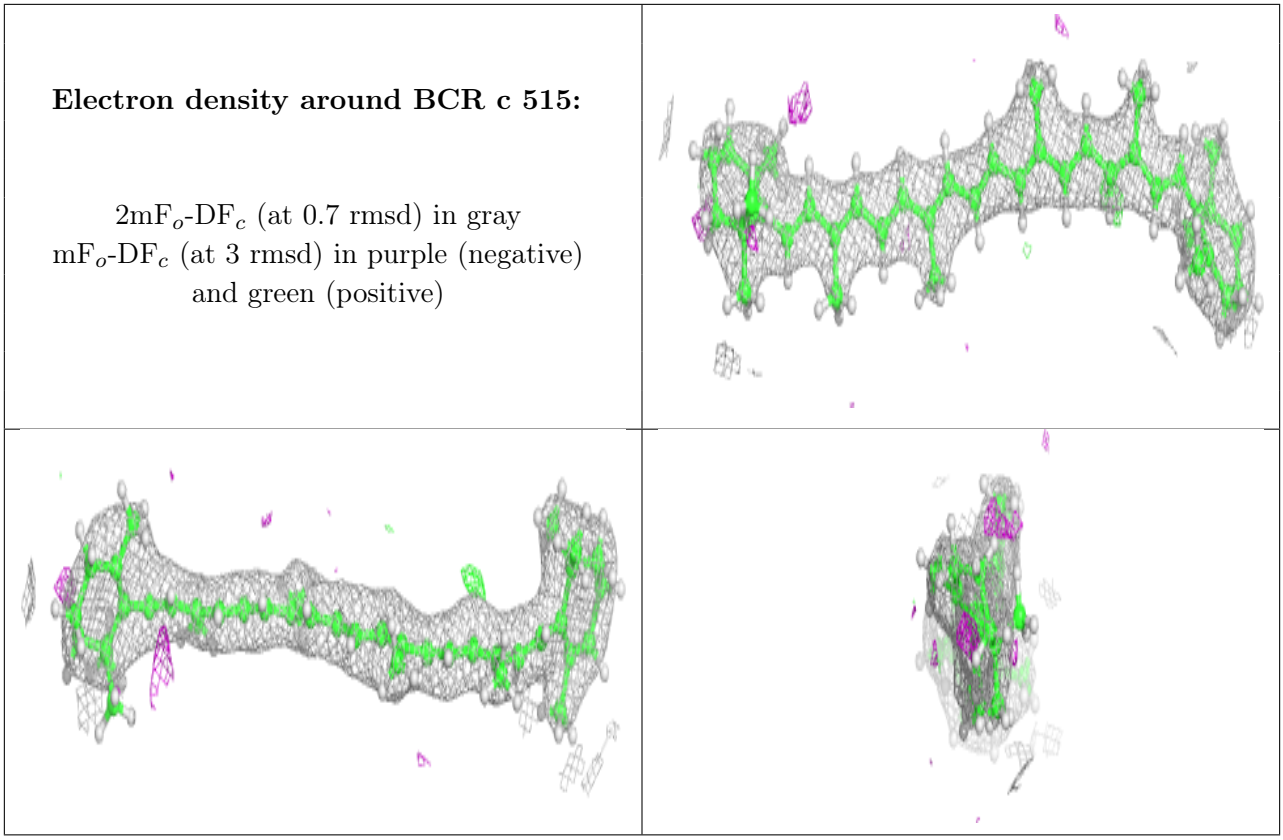






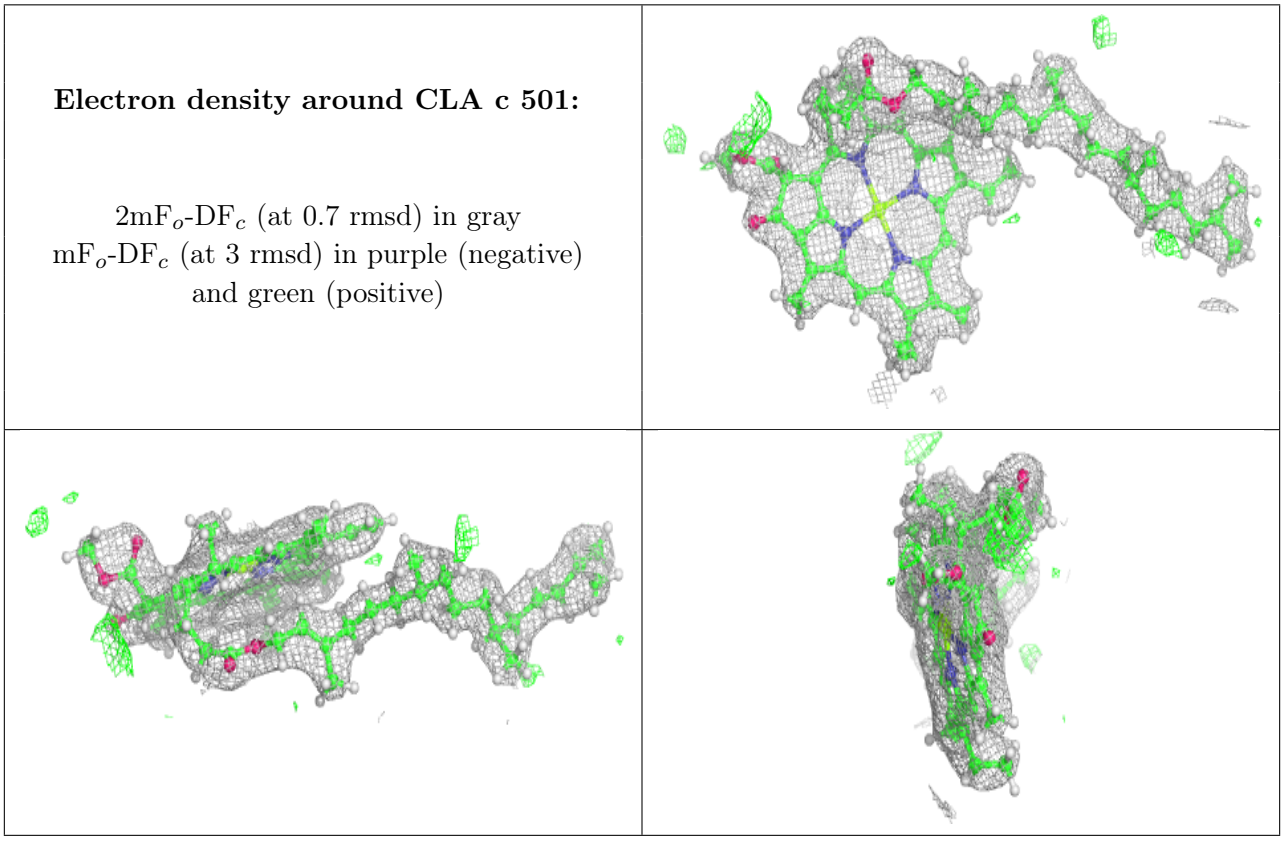
Electron density around BCR c 515:

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



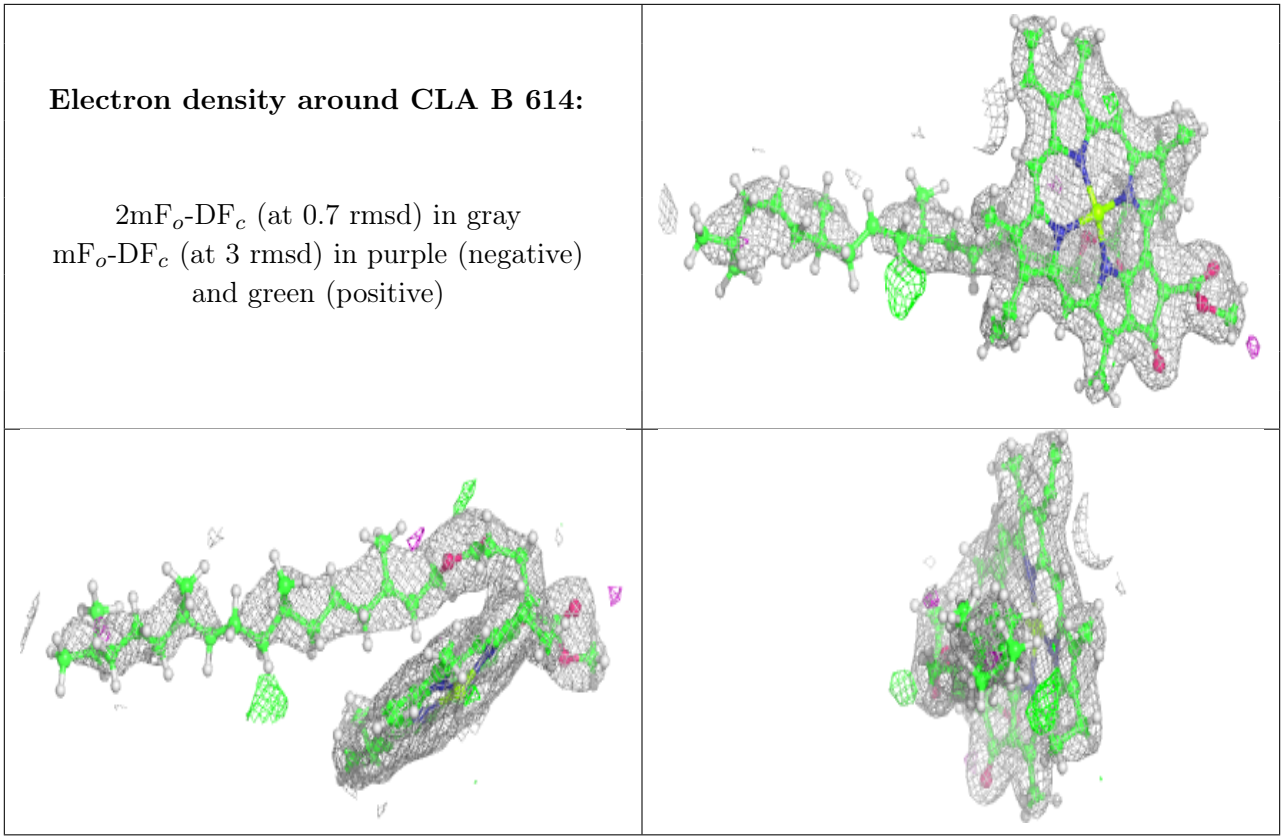
Electron density around CLA c 501:

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



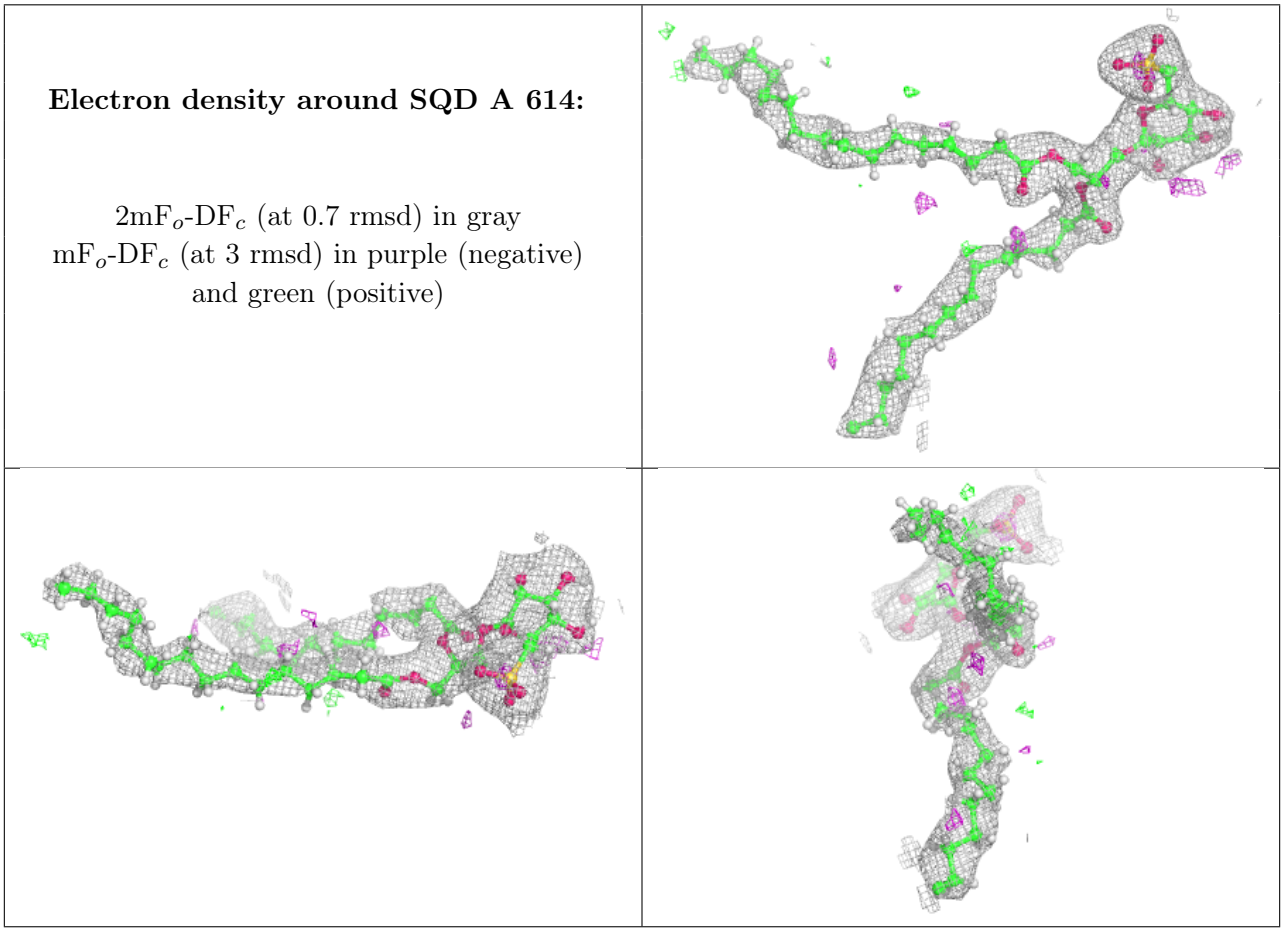
Electron density around CLA B 614:

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



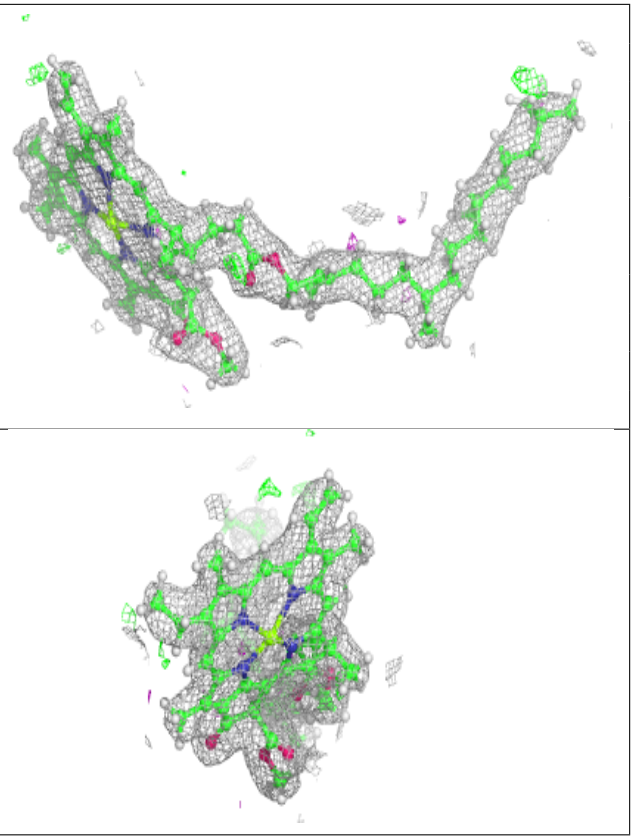
Electron density around SQD A 614:

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



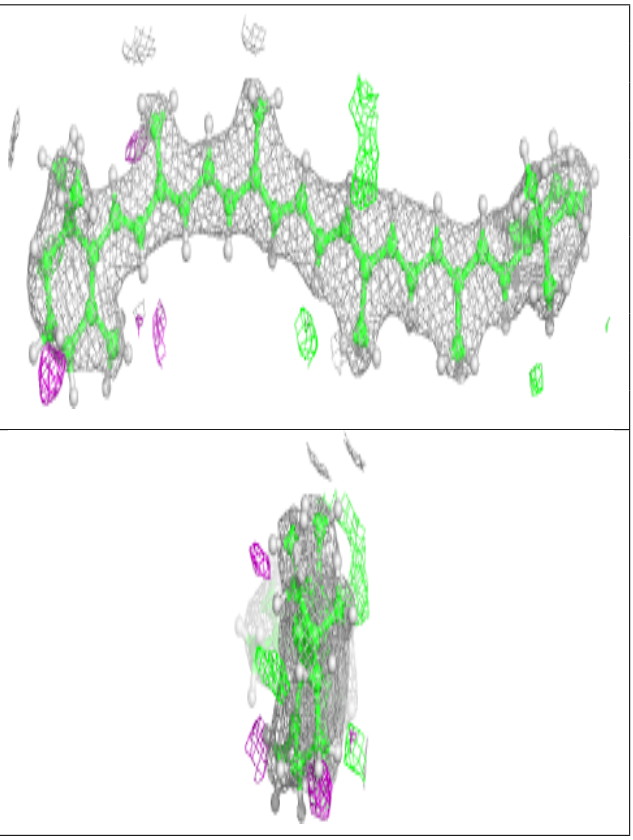
Electron density around CLA A 603:

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



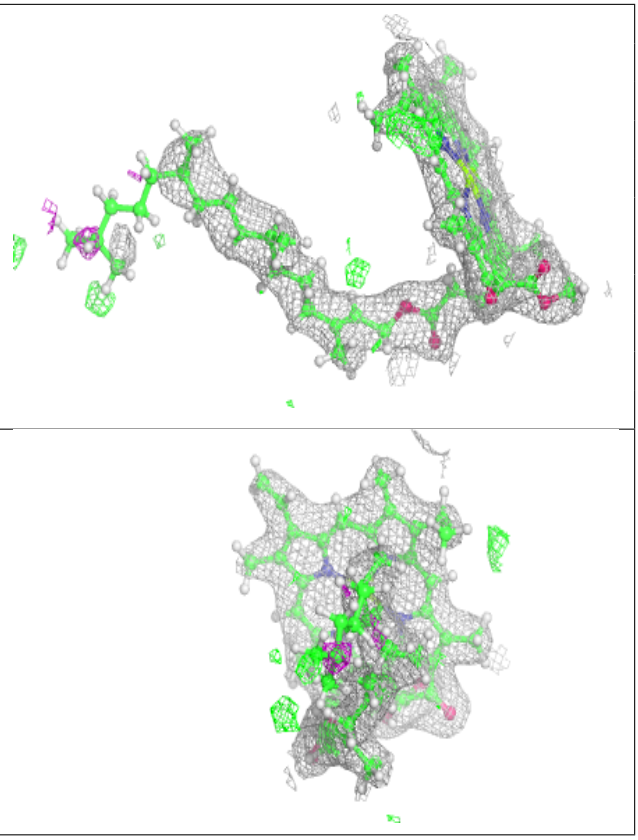
Electron density around BCR B 617:

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



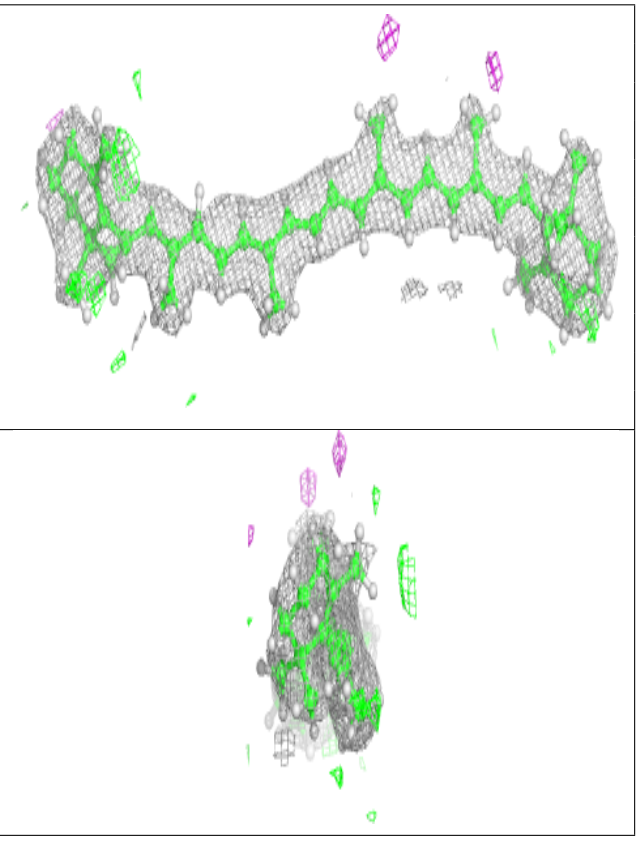
Electron density around CLA C 508:

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



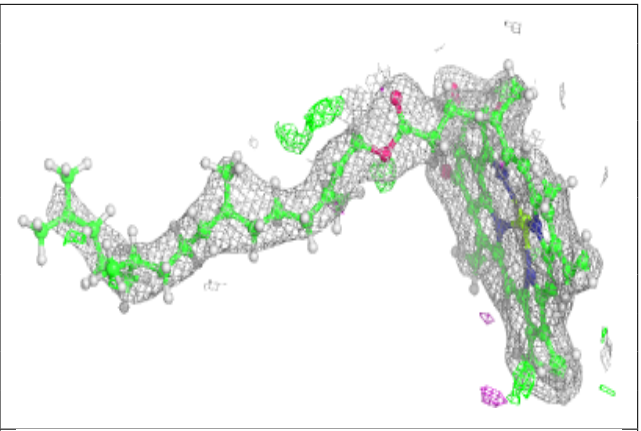
Electron density around BCR B 619:

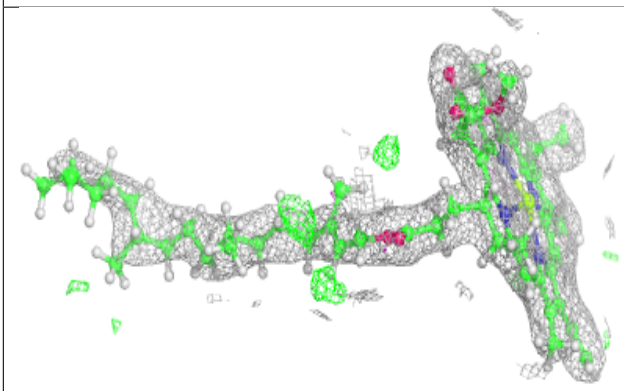
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

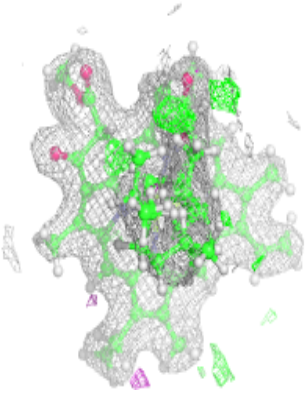


Electron density around CLA B 604:

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

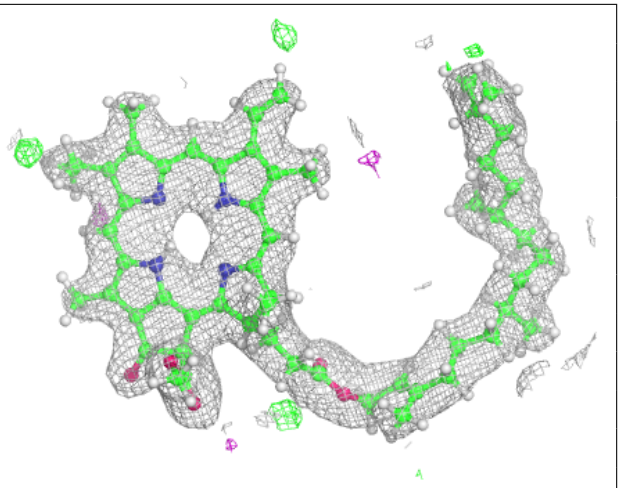


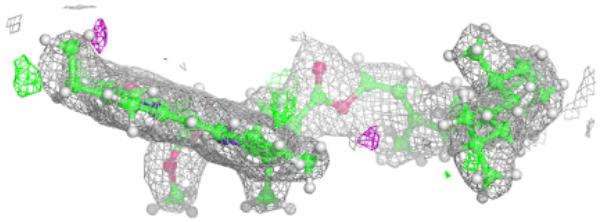


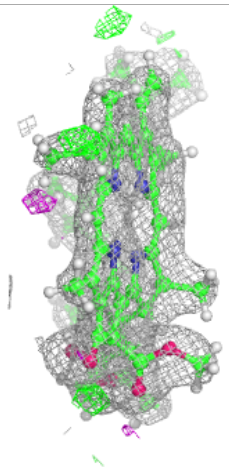


Electron density around PHO a 605:

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

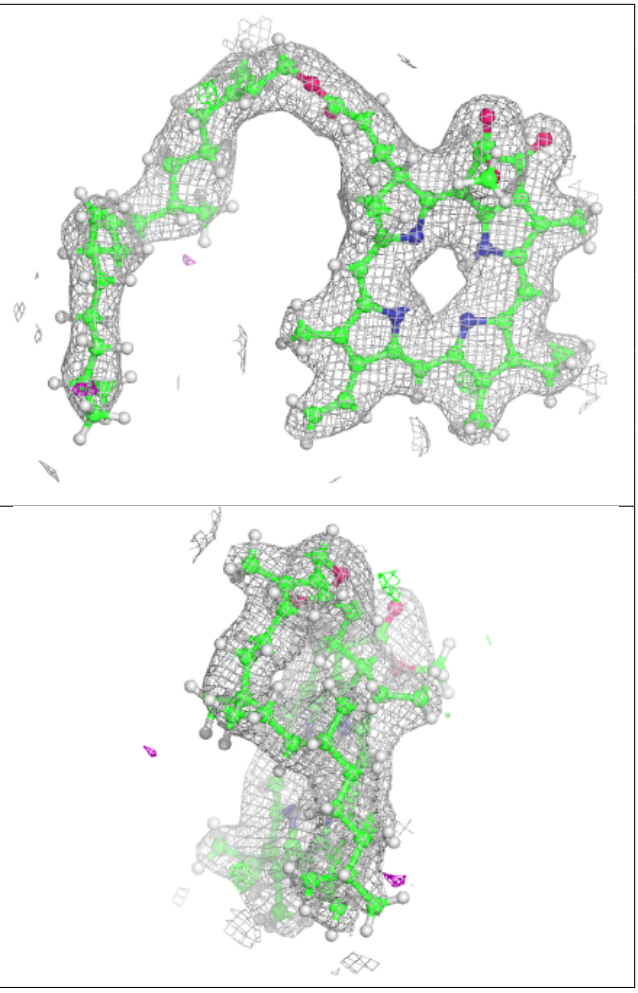






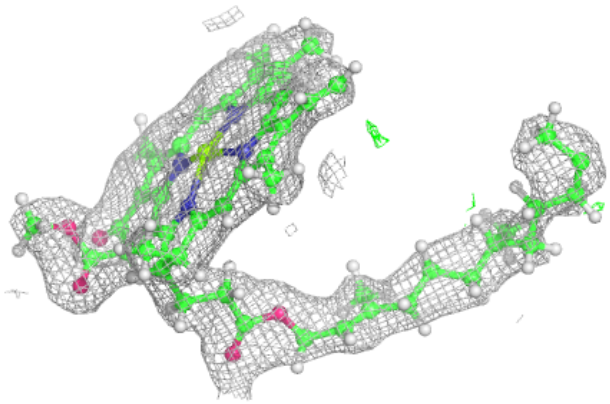
Electron density around PHO d 401:

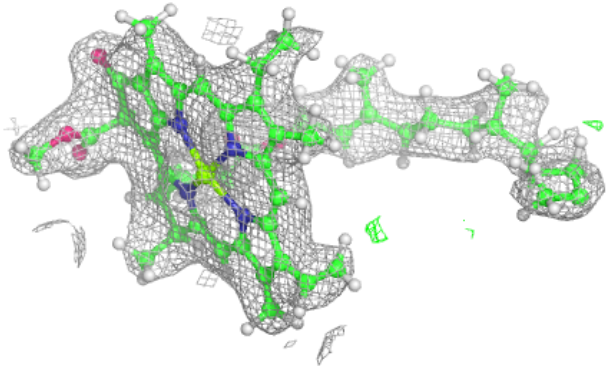
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

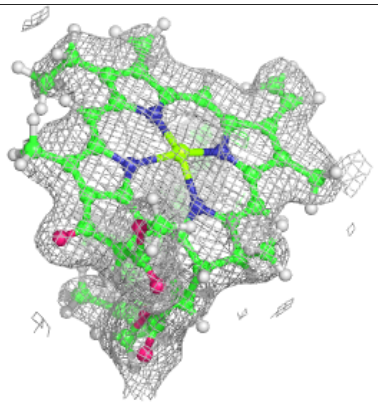


Electron density around CLA C 504:

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

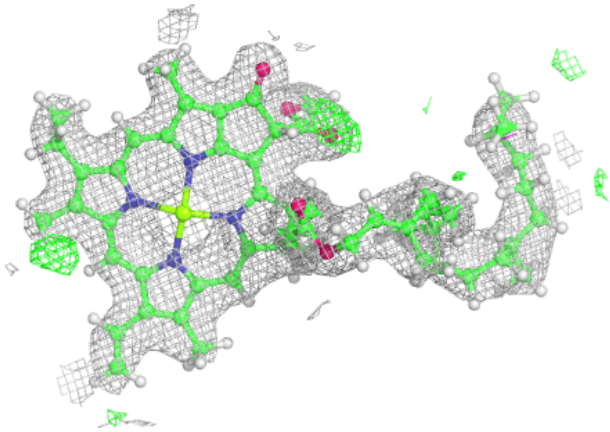


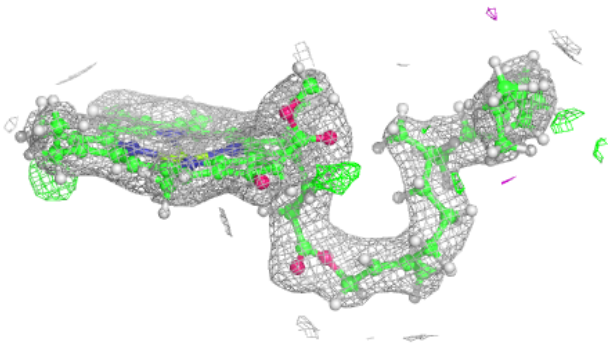


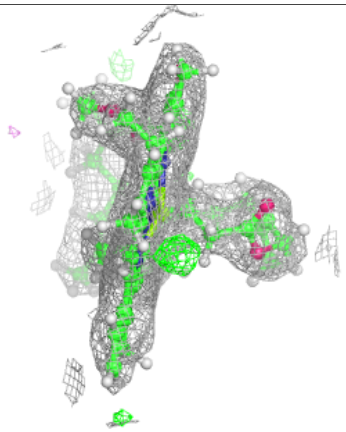


Electron density around CLA B 612:

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

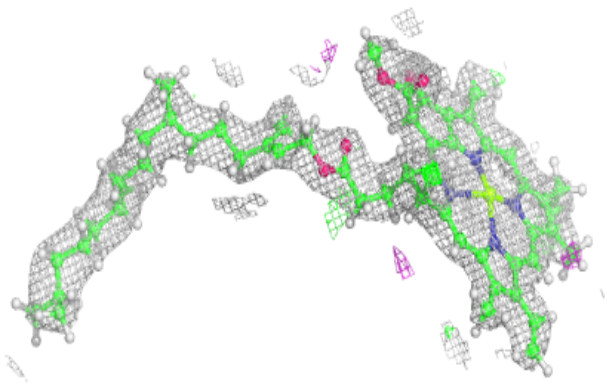


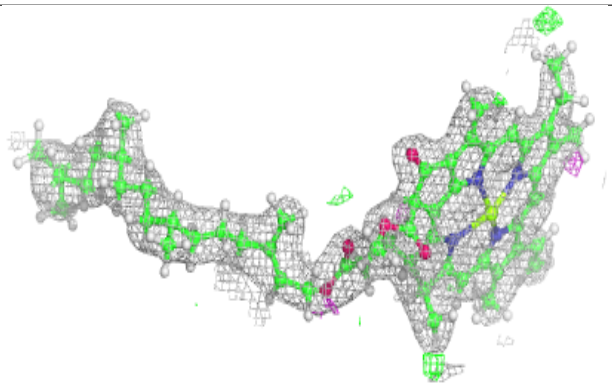


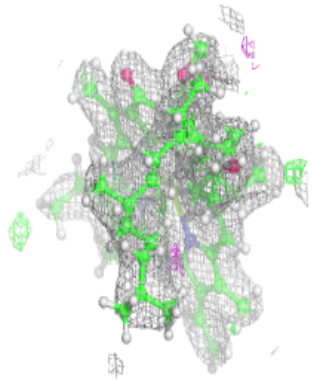


Electron density around CLA a 603:

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

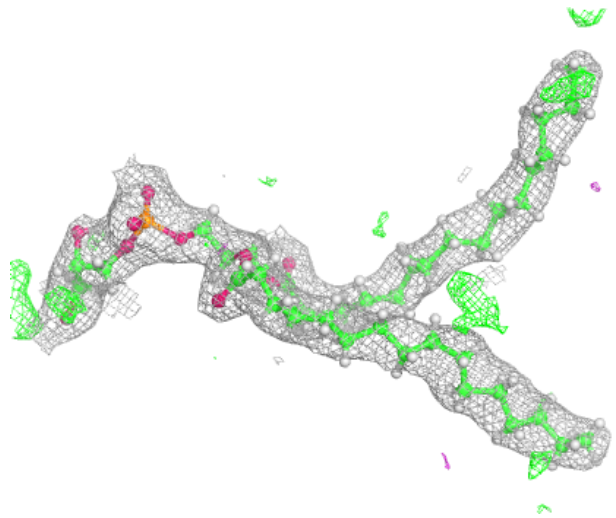


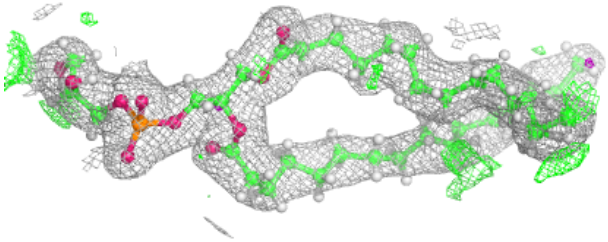


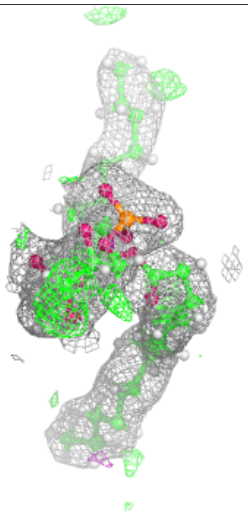


Electron density around LHG D 406:

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

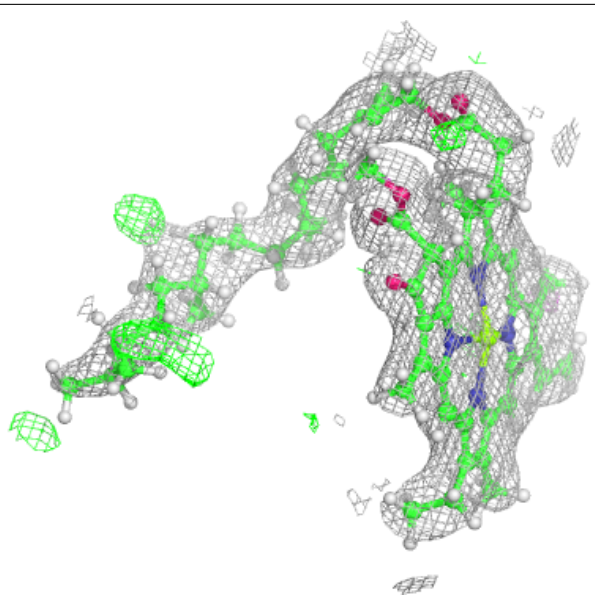


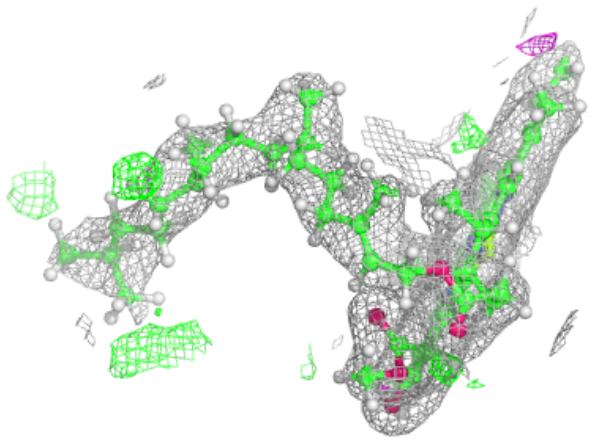


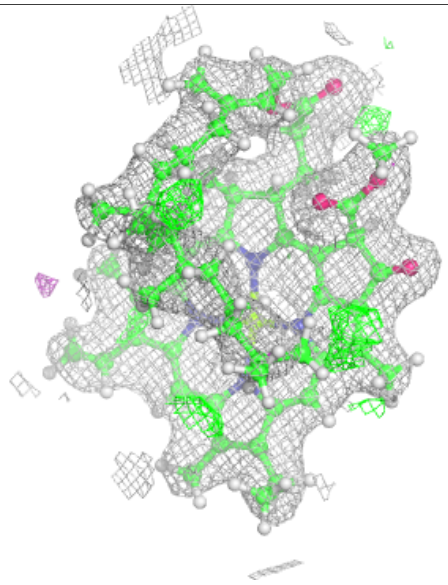


Electron density around CLA B 613:

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

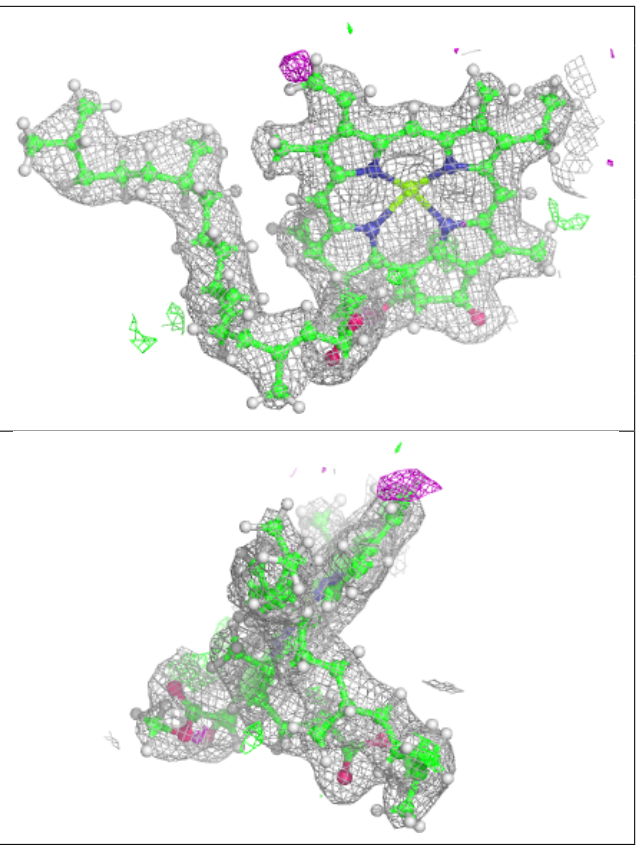






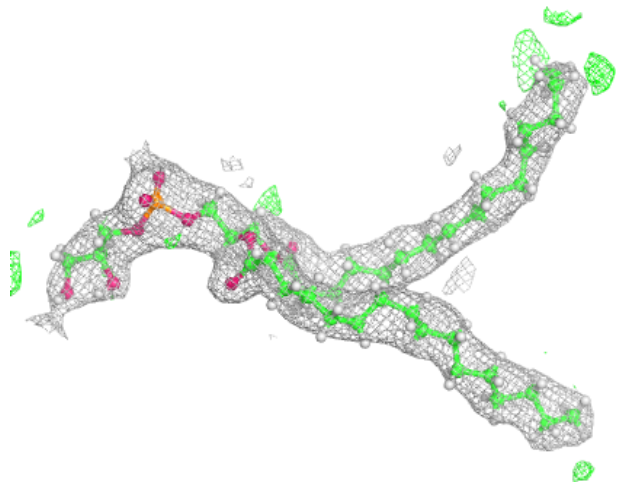
Electron density around CLA A 613:

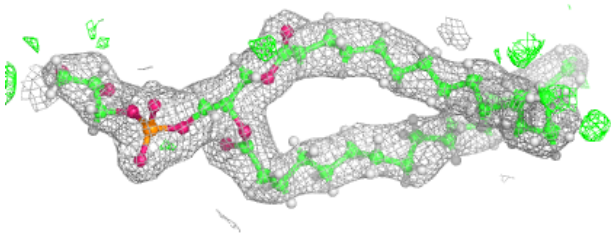
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

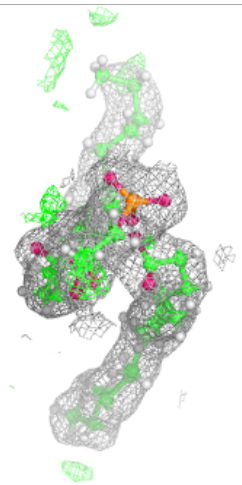


Electron density around LHG d 407:

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

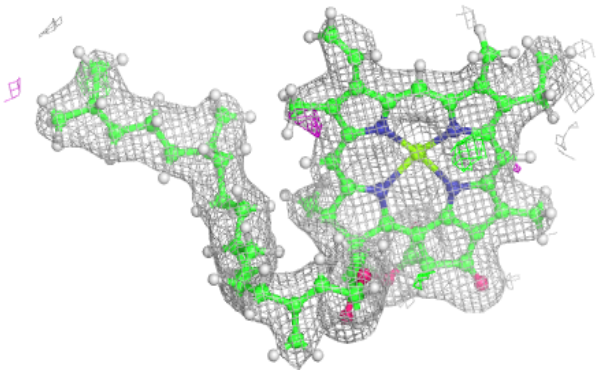


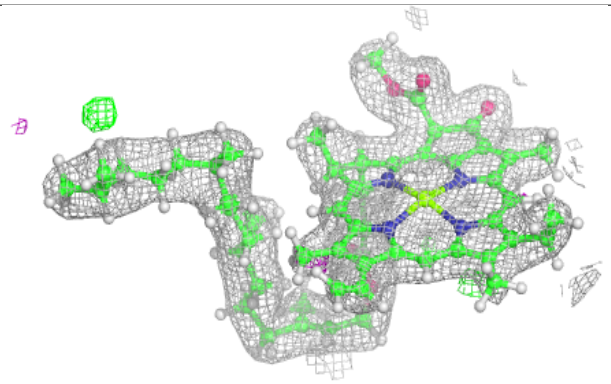


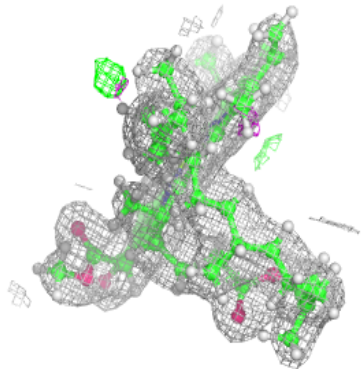


Electron density around CLA a 612:

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

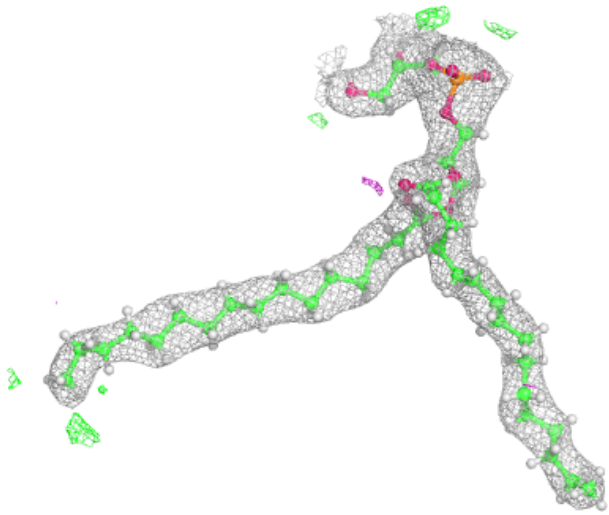


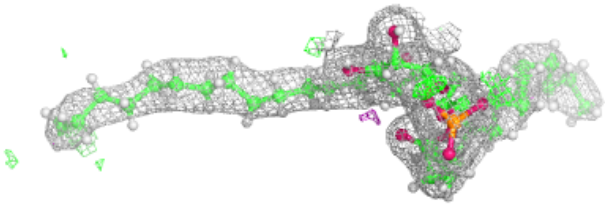


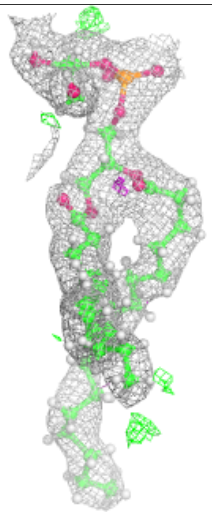


Electron density around LHG l 101:

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

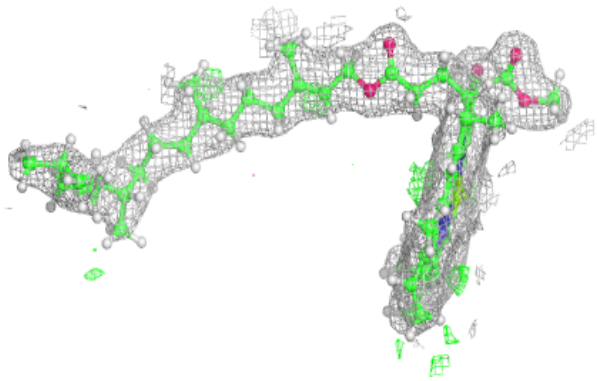


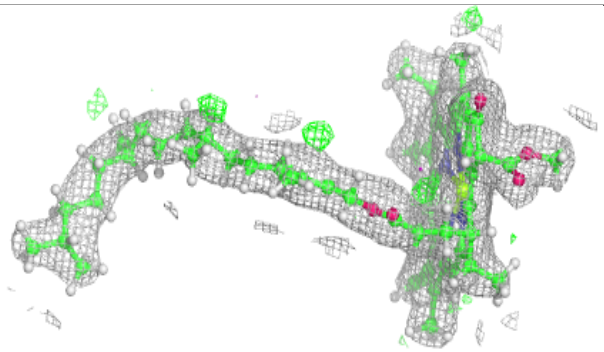


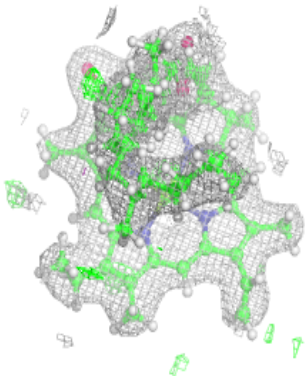


Electron density around CLA B 605:

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

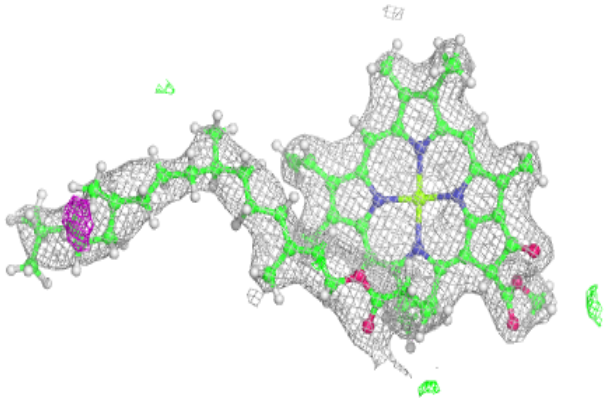


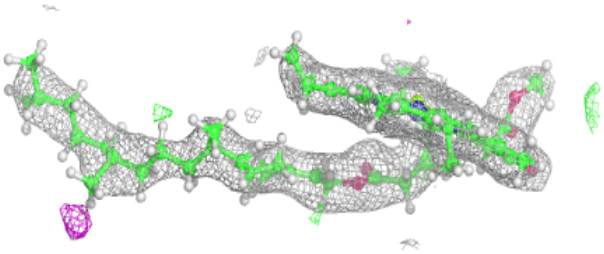


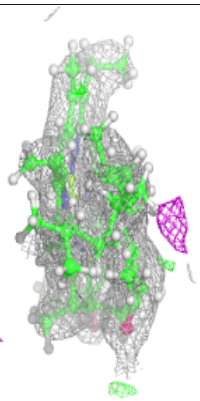


Electron density around CLA b 603:

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

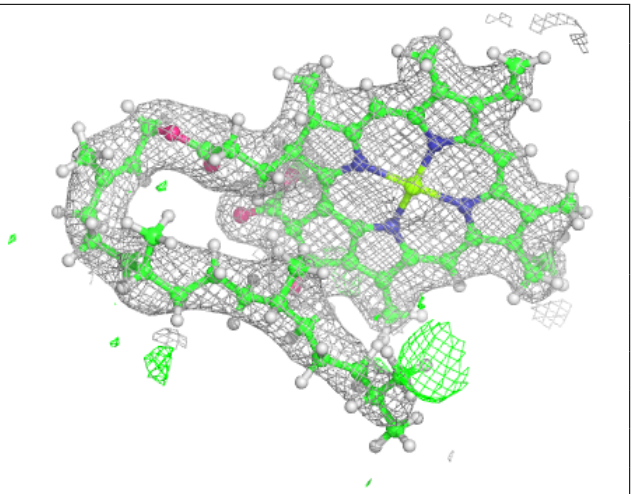


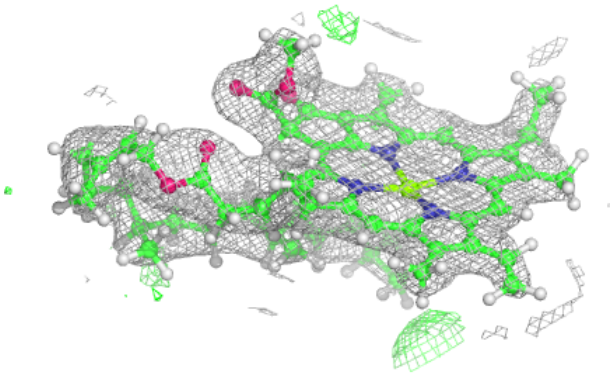


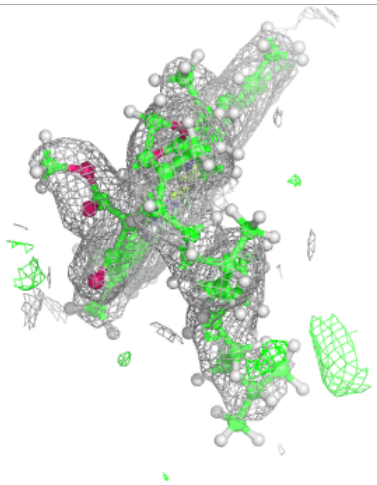


Electron density around CLA C 509:

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

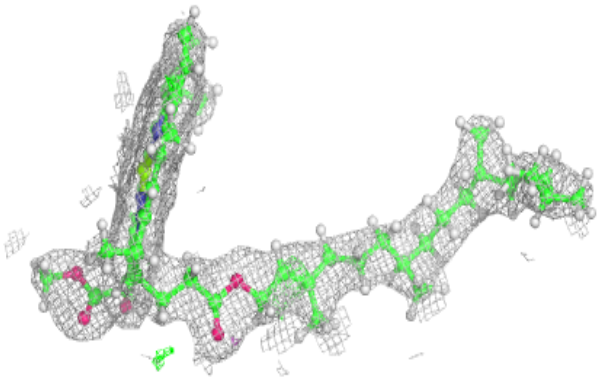


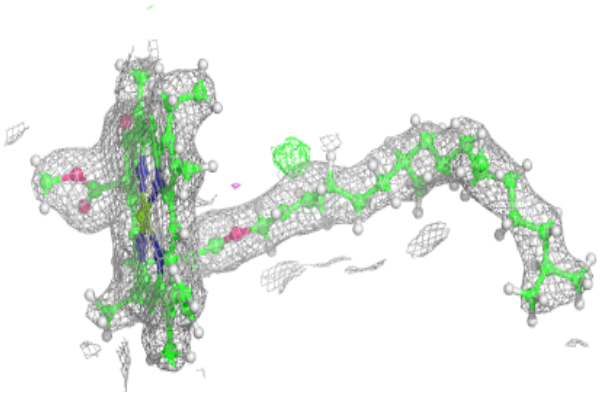


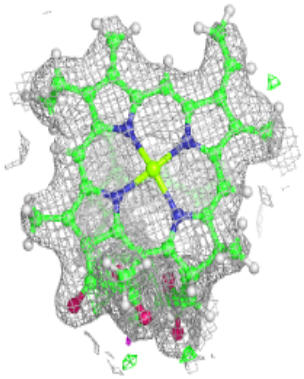


Electron density around CLA b 605:

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

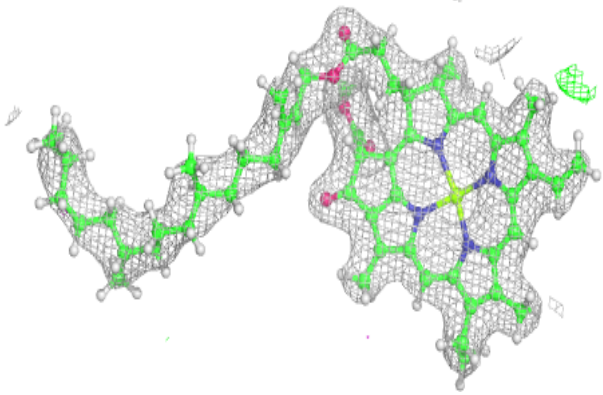


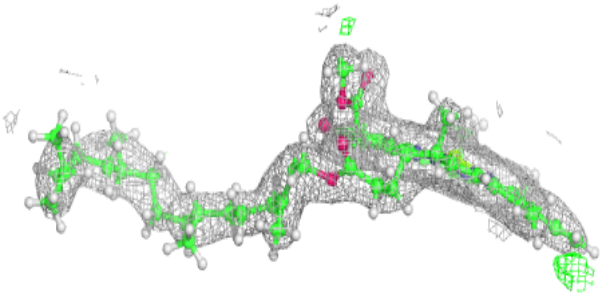


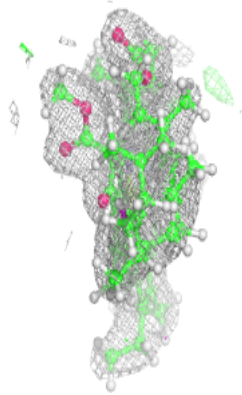


Electron density around CLA B 602:

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

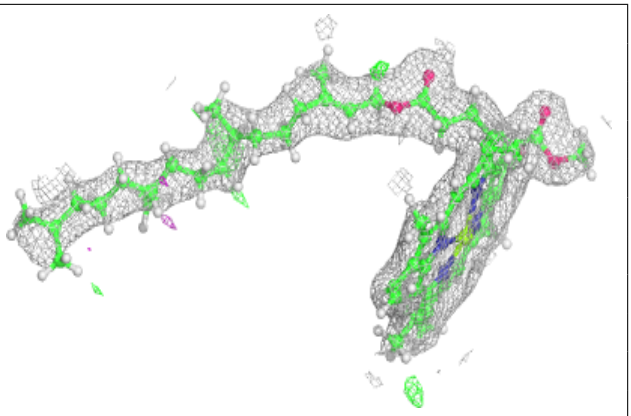


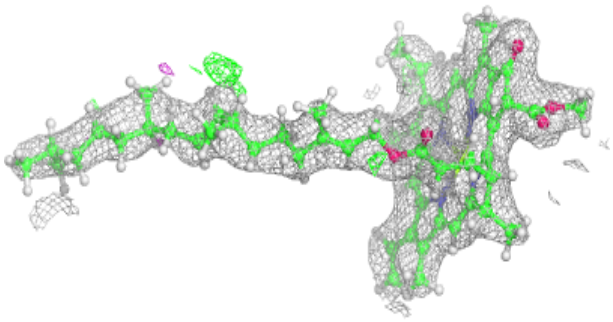


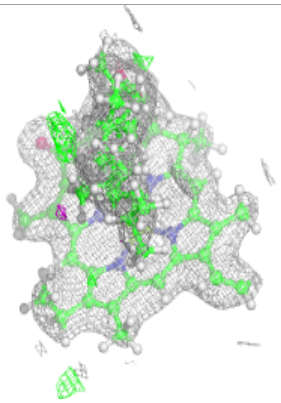


Electron density around CLA b 607:

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

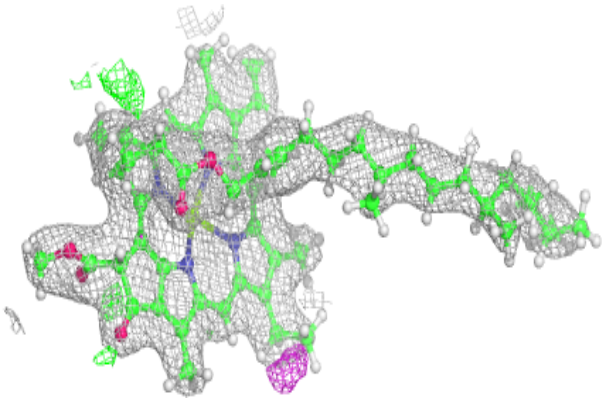


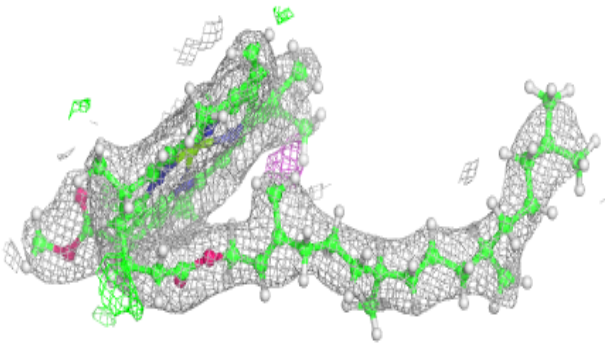


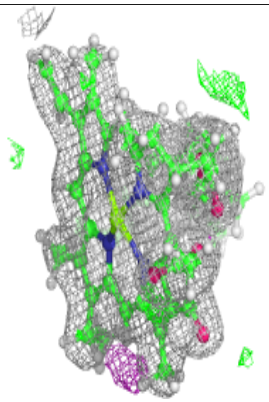


Electron density around CLA b 608:

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

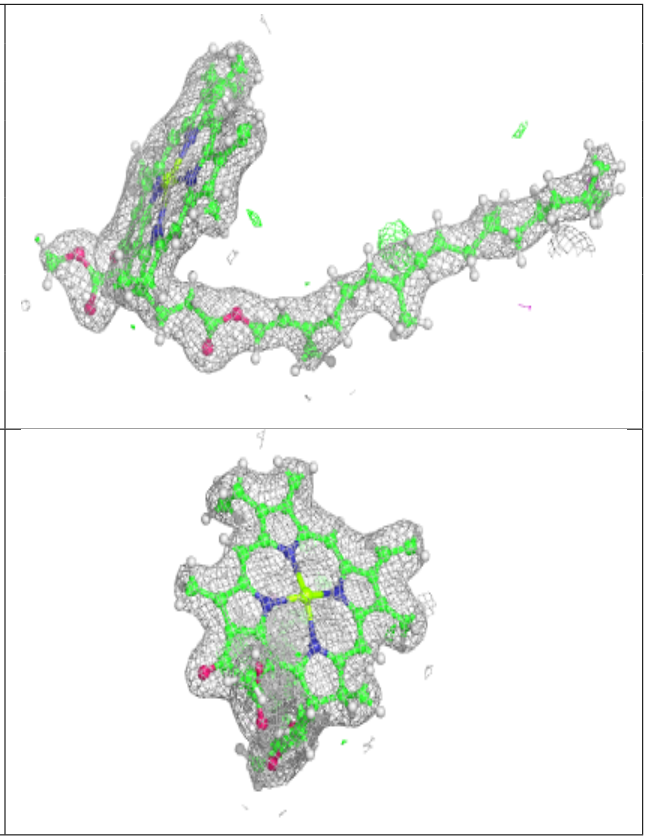






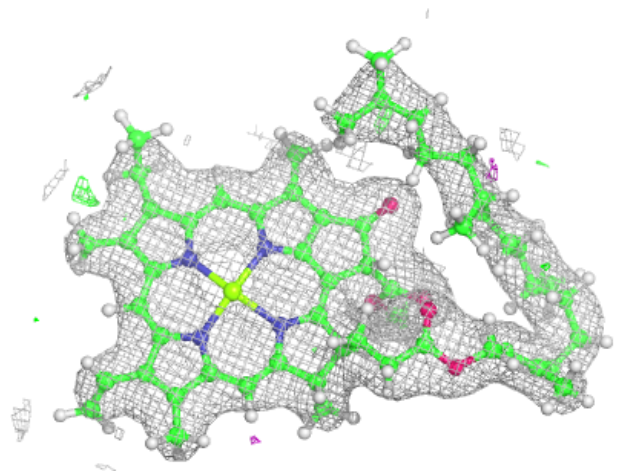
Electron density around CLA B 607:

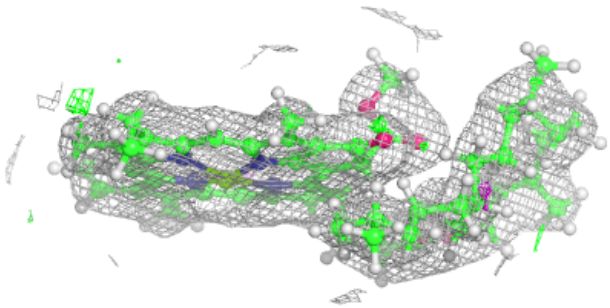
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

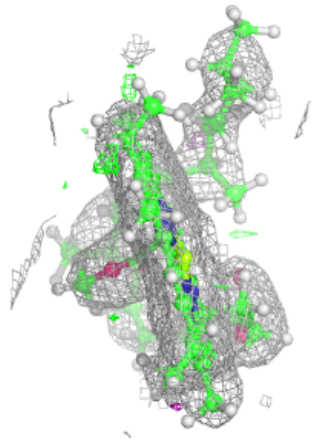


Electron density around CLA b 610:

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

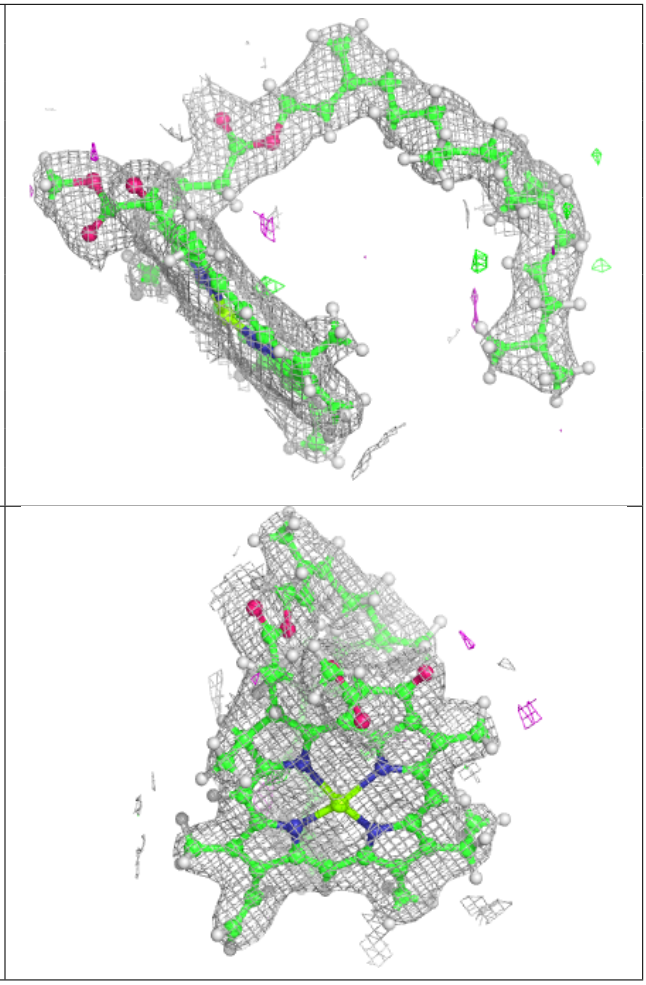






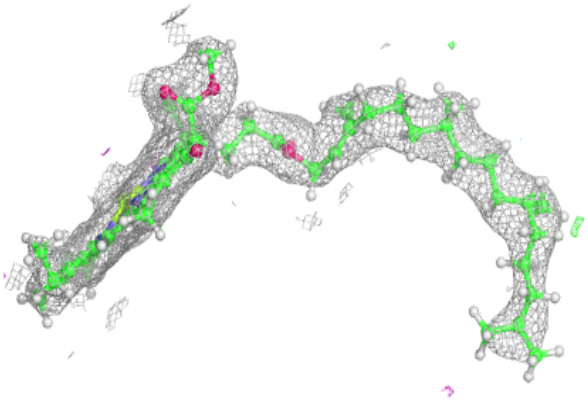
Electron density around CLA b 611:

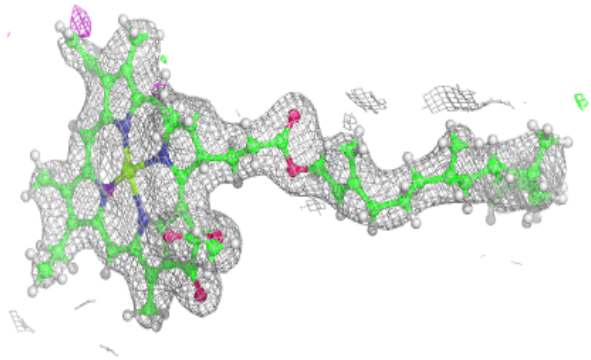
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

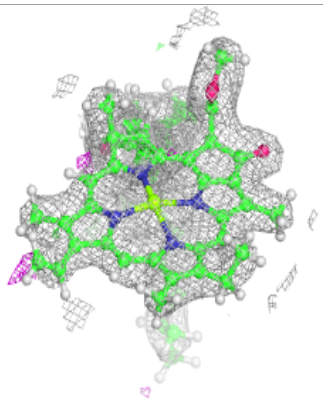


Electron density around CLA d 402:

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

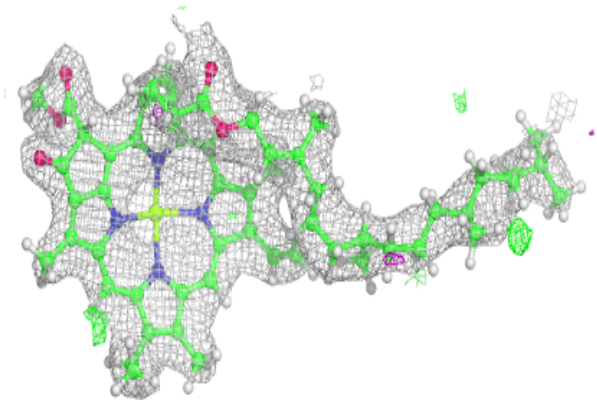


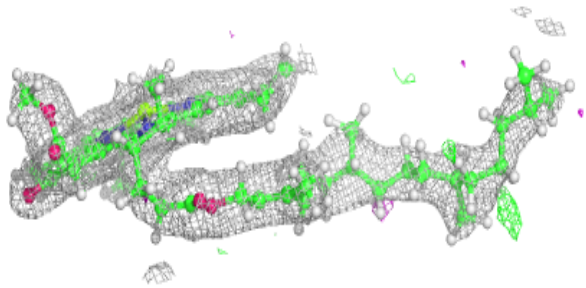


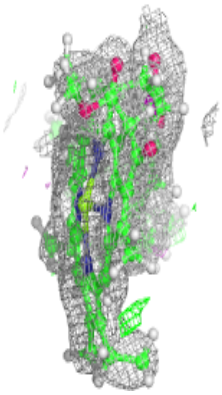


Electron density around CLA B 603:

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

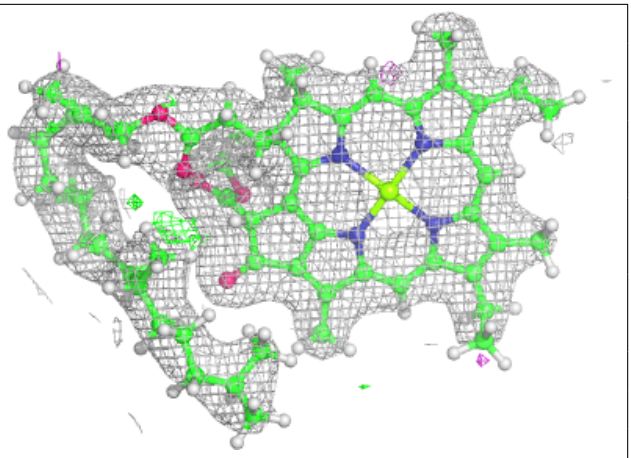


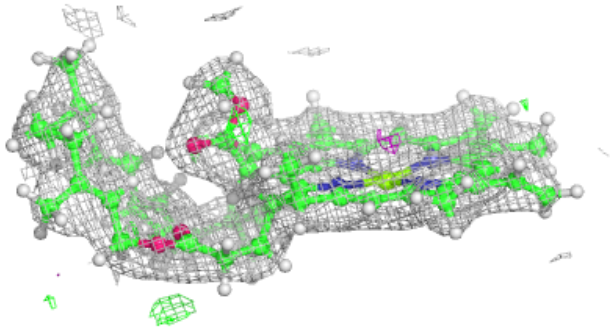


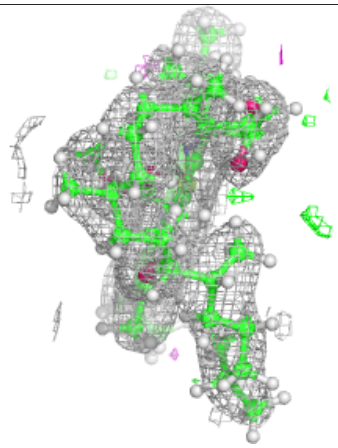


Electron density around CLA B 610:

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

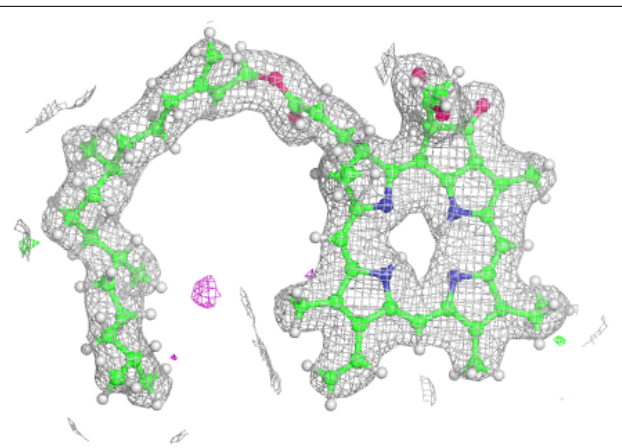


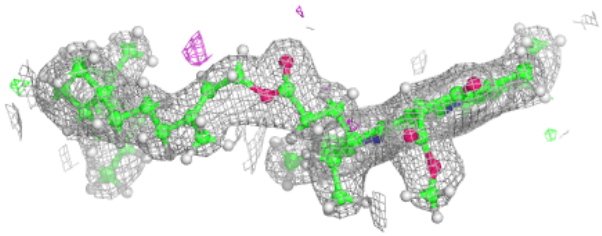




Electron density around PHO A 605:

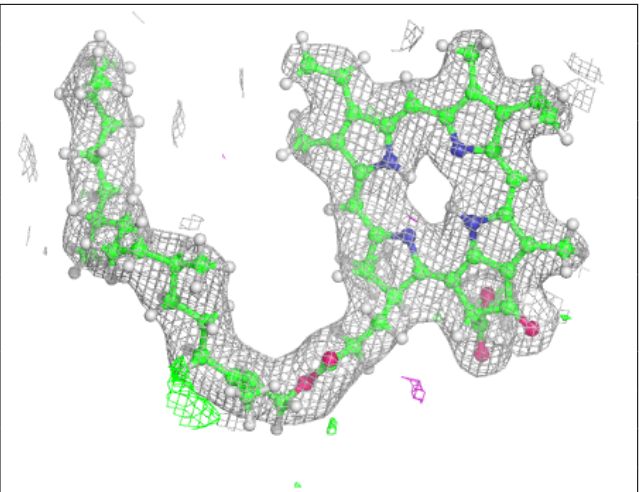
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

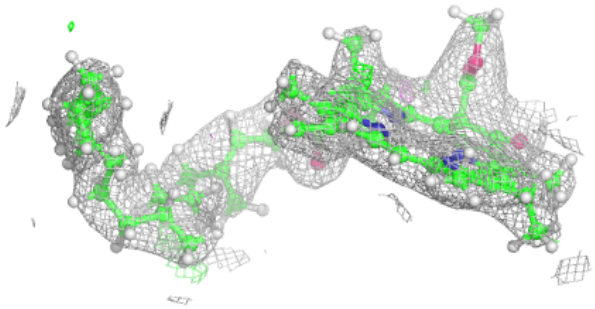


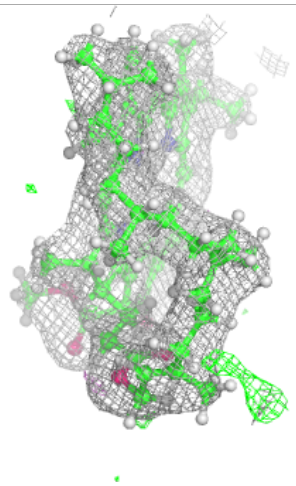


Electron density around PHO A 606:

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

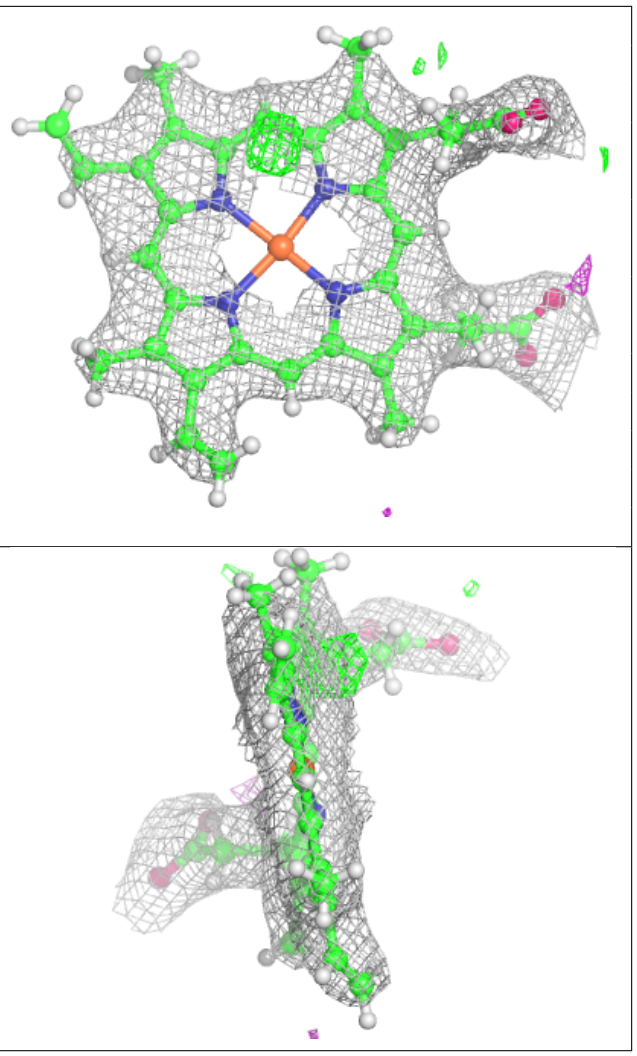






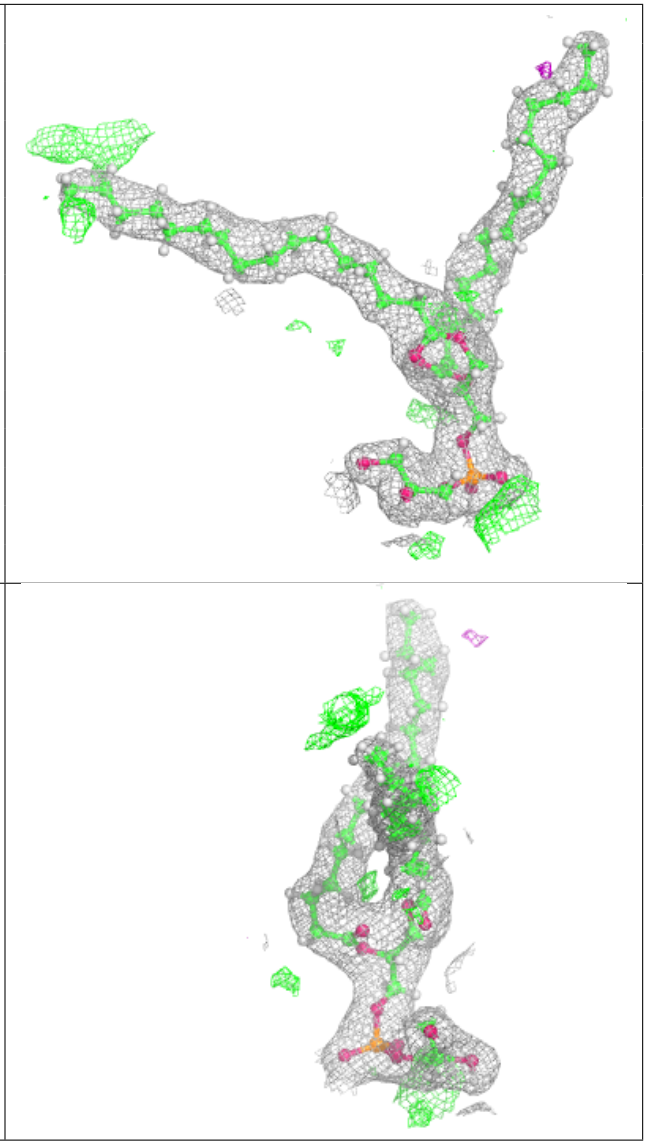
Electron density around HEM F 102:

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



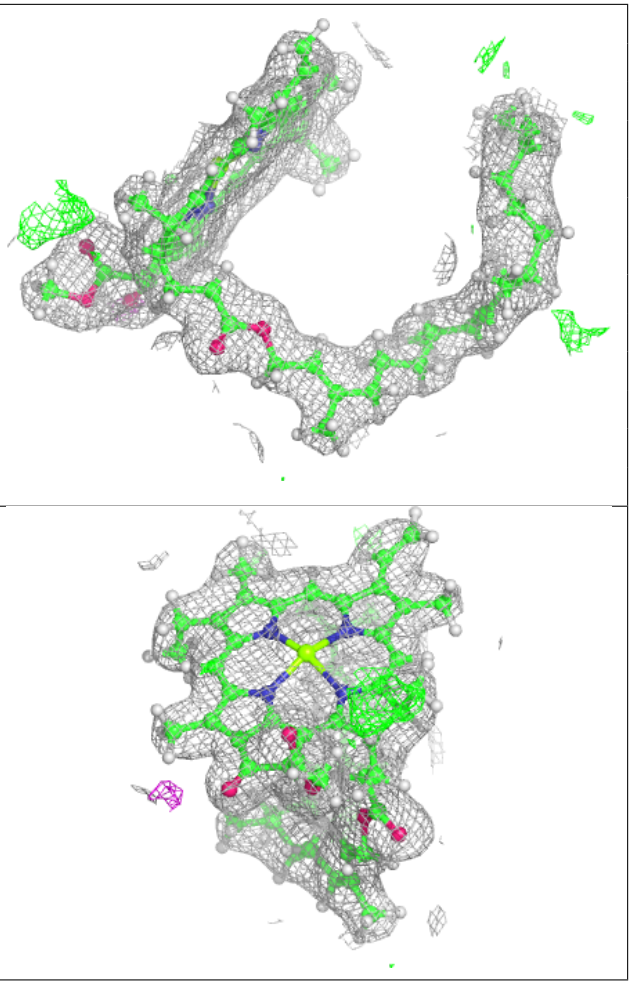
Electron density around LHG L 101:

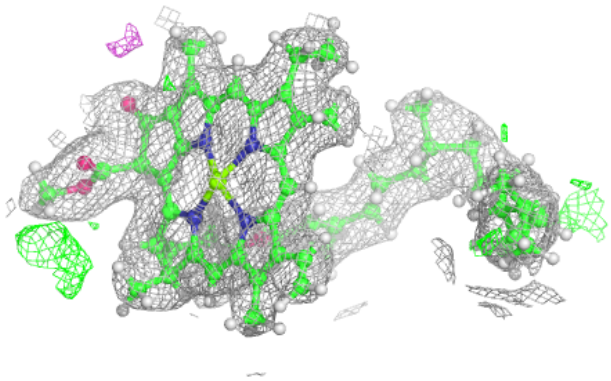
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 611:

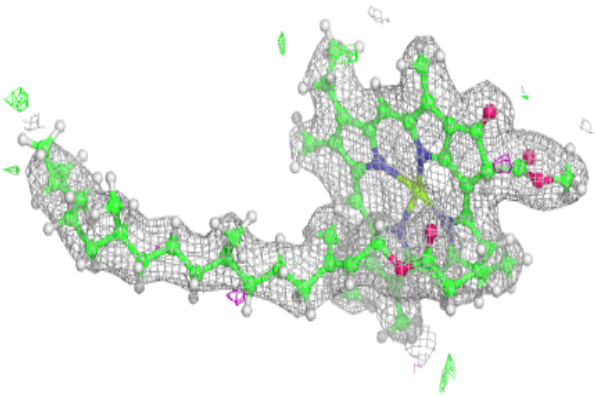
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

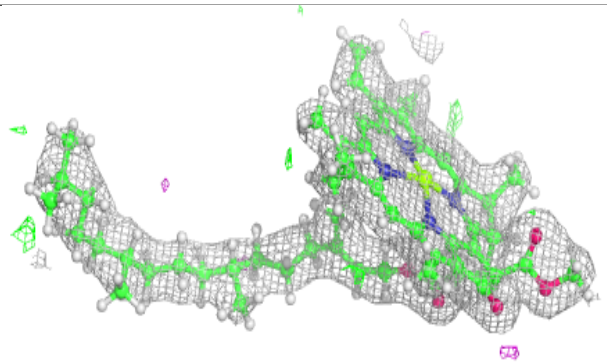


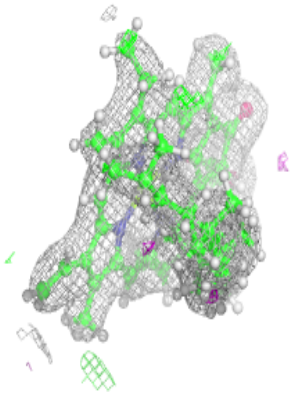


Electron density around CLA B 608:

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

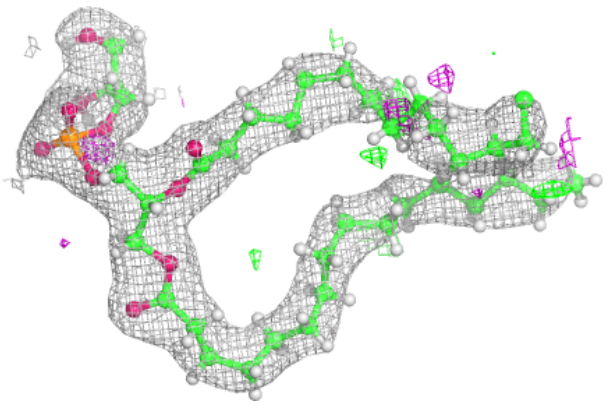


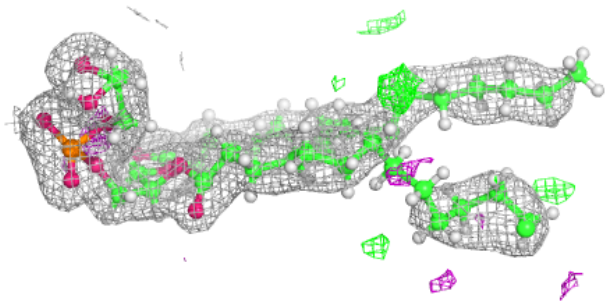


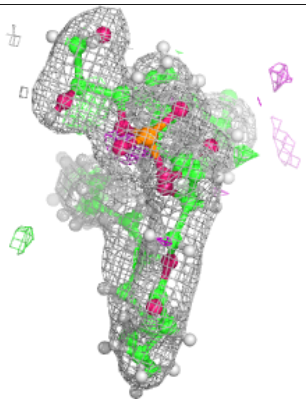


Electron density around LHG D 408:

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

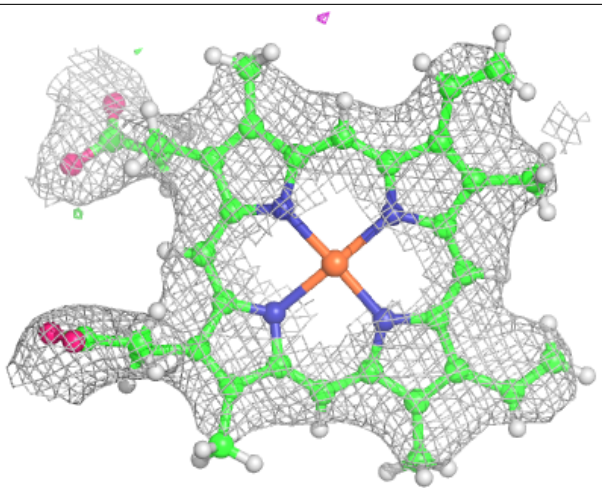


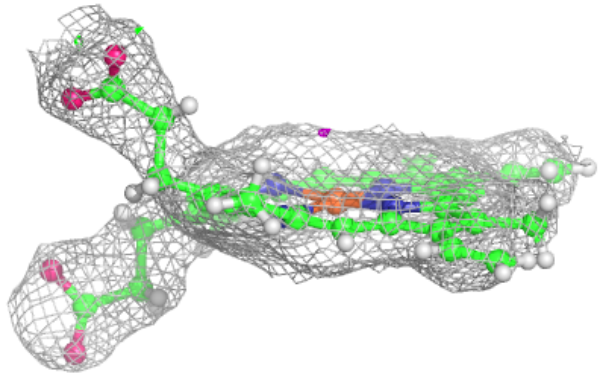


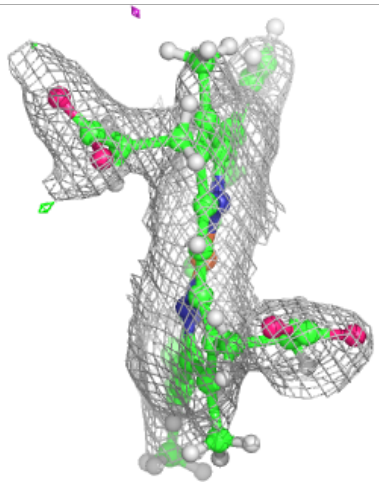


Electron density around HEM f 102:

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

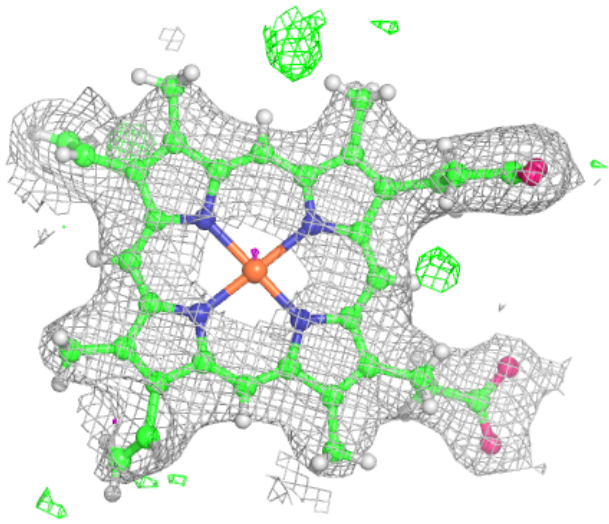


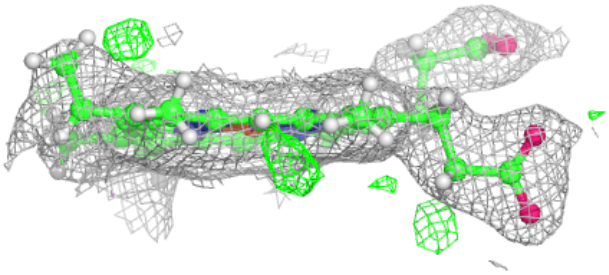


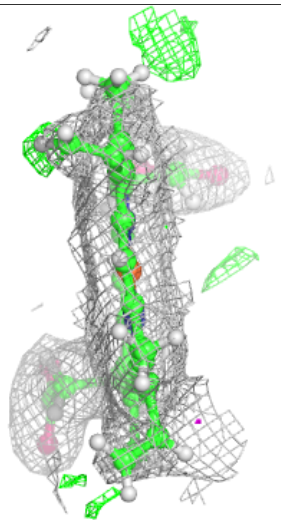


Electron density around HEC v 201:

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

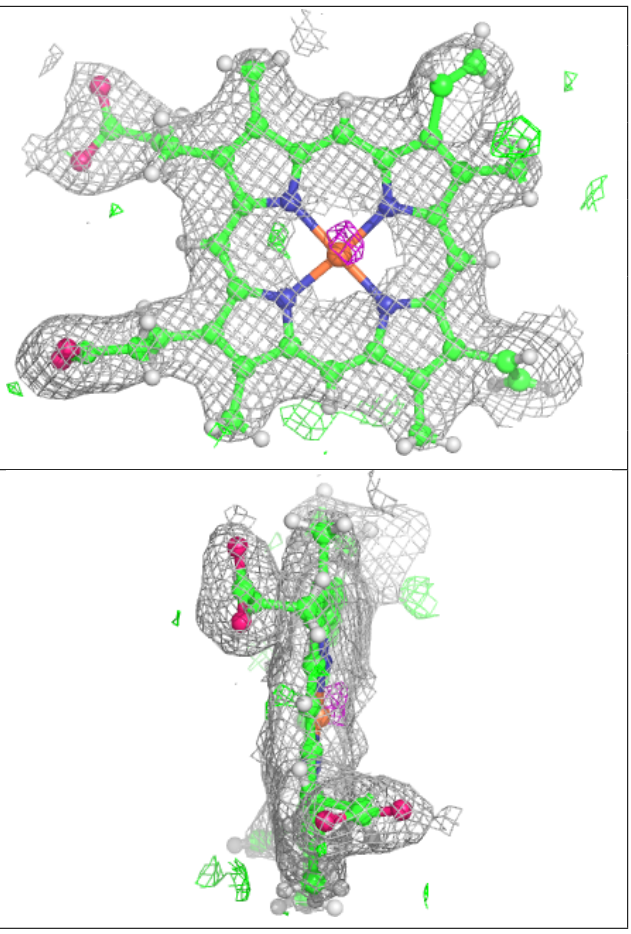






Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.