wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 09:27 PM EDT

PDB ID	:	6W1P
Title	:	RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 Angstrom resolution
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Deposited on	:	2020-03-04
Resolution	:	2.26 Å(reported)

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

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

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

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

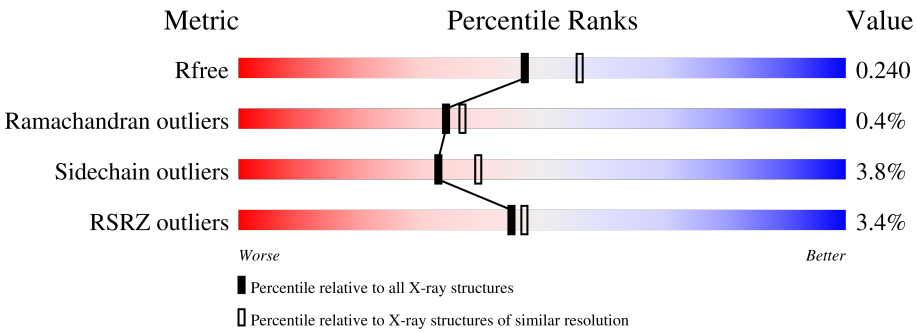
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 2.26 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	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	% 99% .
1	a	334	96% .
2	B	506	% 98% .

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Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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Mol	Chain	Length	Quality of chain
2	b	506	3% 98%
3	C	461	.% 94%
3	c	461	.% 95%
4	D	352	96%
4	d	352	.% 93%
5	E	84	2% 94%
5	e	84	6% 93% 5%
6	F	45	2% 73% 24%
6	f	45	2% 71% 24%
7	H	66	2% 92% 6%
7	h	66	6% 88% 8% 5%
8	I	38	5% 89% 5% 5%
8	i	38	8% 89% 5% 5%
9	J	40	10% 88% 10%
9	j	40	10% 88% 10%
10	K	46	4% 74% 7% 20%
10	k	46	74% 7% 20%
11	L	37	100%
11	l	37	8% 86% 11%
12	M	36	3% 89% 8%
12	m	36	81% 8% 11%
13	O	272	4% 85% 5% 10%
13	o	272	5% 86% 10%
14	R	40	28% 70% 15% 15%
14	r	40	58% 60% 18% 22%

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Mol	Chain	Length	Quality of chain
15	T	30	3% 97%
15	t	30	10% 93% 7%
16	U	134	2% 69% 28%
16	u	134	70% 28%
17	V	163	79% 16%
17	v	163	2% 82% 16%
18	X	41	7% 90% 7%
18	x	41	12% 90% 5% 5%
19	Y	46	20% 54% 41%
19	y	46	9% 59% 7% 35%
20	Z	62	18% 89% 11%
20	z	62	18% 87% 13%

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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 103385 atoms, of which 51555 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	5130	1717	2508	431	459	15	0	0	0
1	a	334	5118	1714	2499	431	459	15	0	0	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	7864	2631	3859	666	695	13	0	5	0
2	b	505	7800	2610	3822	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	6768	2249	3342	571	593	13	0	2	0
3	c	451	6913	2290	3413	587	610	13	0	2	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	5330	1800	2613	444	461	12	0	0	0
4	d	341	5342	1804	2619	444	463	12	0	1	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	82	1316	436	650	107	123	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	1042	341	532	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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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	525	174	268	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	598	204	305	43	46	0	0	0
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
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
12	m	32	518	168	267	36	46	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

- 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	3698	1168	1828	313	385	4	0	1	0
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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
14	r	31	493	162	253	42	36	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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- 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
			Total	C	H	N	O			
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	2132	675	1068	177	208	4	0	0	0
			Total	C	H	N	O	S			
17	v	137	2132	675	1068	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
			Total	C	H	N	O			
18	x	39	602	191	316	46	49	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	413	128	217	35	30	3	0	0	0
19	y	30	459	144	241	35	36	3	0	0	0

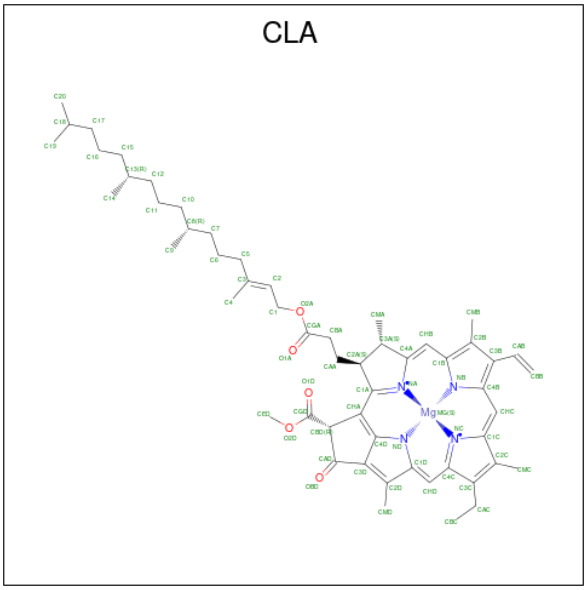
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
20	Z	62	995	328	516	72	77	2	0	0	0
20	z	62	986	326	509	72	77	2	0	0	0

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	A	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		
22	A	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	A	1	102	44	48	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	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		
22	C	1	117	49	58	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	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		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	132	54	68	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0

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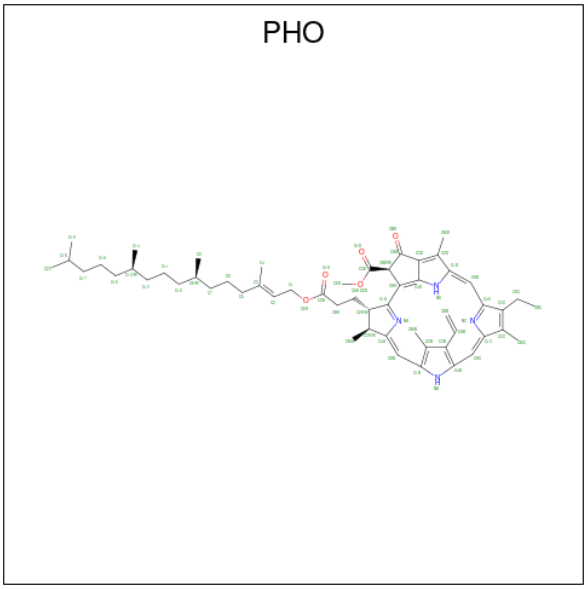
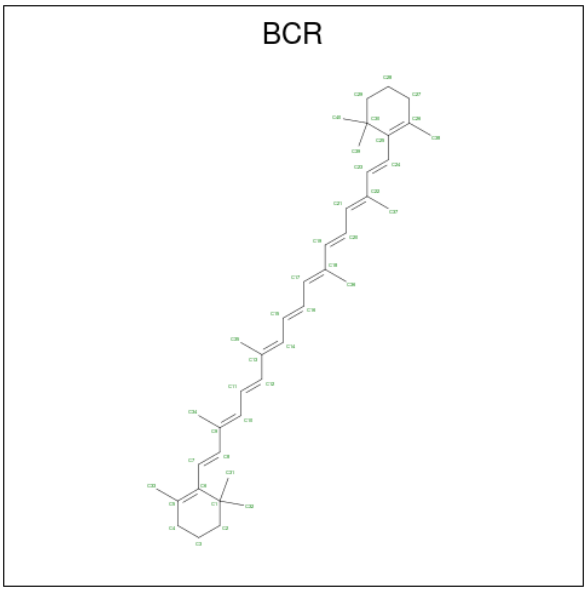
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	d	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	d	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	d	1	137	55	72	1	4	5	0	0

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
24	A	1	96	40	56	0	0
24	B	1	96	40	56	0	0
24	B	1	96	40	56	0	0
24	B	1	96	40	56	0	0
24	C	1	96	40	56	0	0
24	C	1	96	40	56	0	0
24	D	1	96	40	56	0	0
24	H	1	96	40	56	0	0
24	K	1	96	40	56	0	0
24	T	1	96	40	56	0	0
24	Z	1	96	40	56	0	0
24	a	1	96	40	56	0	0
24	b	1	96	40	56	0	0
24	b	1	96	40	56	0	0

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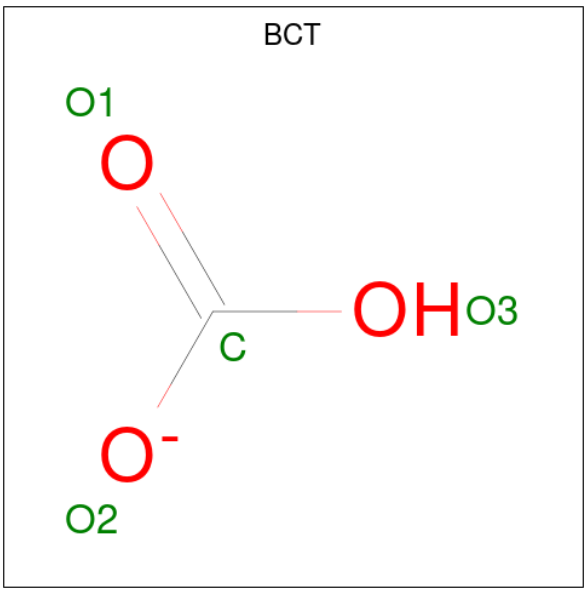
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
24	b	1	96	40	56	0	0
24	c	1	96	40	56	0	0
24	c	1	96	40	56	0	0
24	d	1	96	40	56	0	0
24	k	1	96	40	56	0	0
24	k	1	96	40	56	0	0
24	t	1	96	40	56	0	0
24	x	1	96	40	56	0	0

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

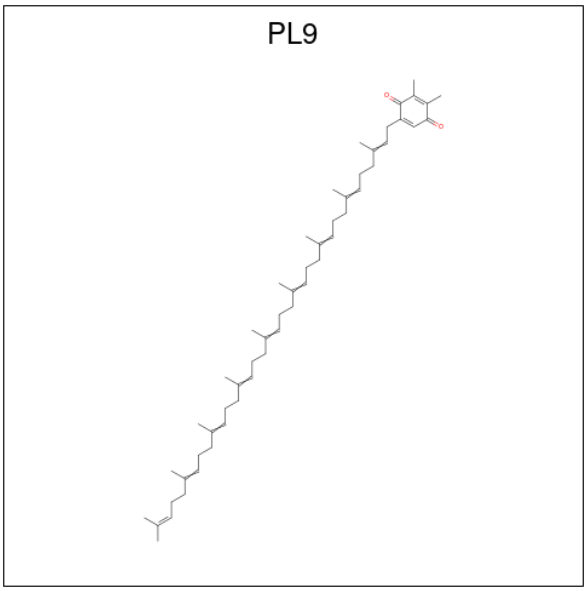
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
25	A	2	2	2	0	0
25	a	2	2	2	0	0

- Molecule 26 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



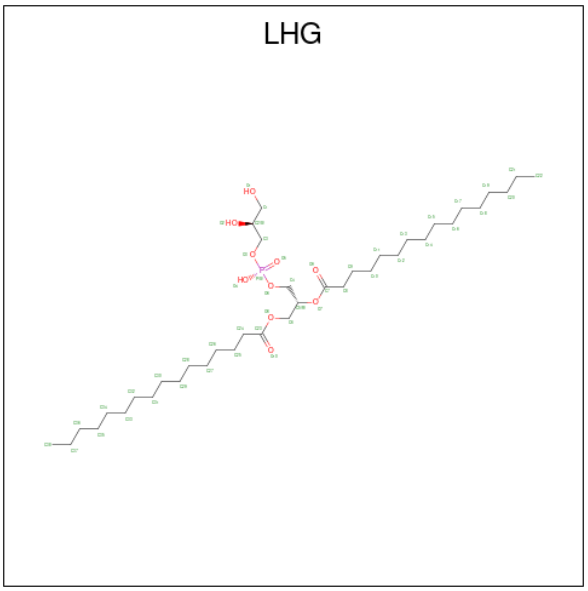
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	5	1	1	3	0	0
26	a	1	5	1	1	3	0	0

- 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



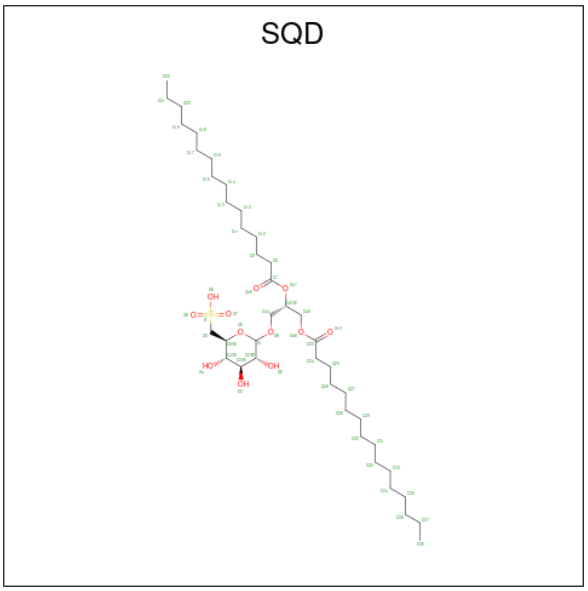
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	A	1	135	53	80	2	0	0
27	D	1	135	53	80	2	0	0
27	a	1	135	53	80	2	0	0
27	d	1	135	53	80	2	0	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	A	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

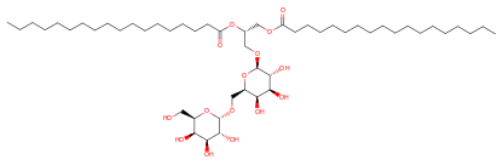
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 121 39 69 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	L	1	Total C H O S 113 36 64 12 1	0	0
29	a	1	Total C H O S 131 41 77 12 1	0	0
29	a	1	Total C H O 92 31 56 5	0	0
29	f	1	Total C H O S 89 28 48 12 1	0	0

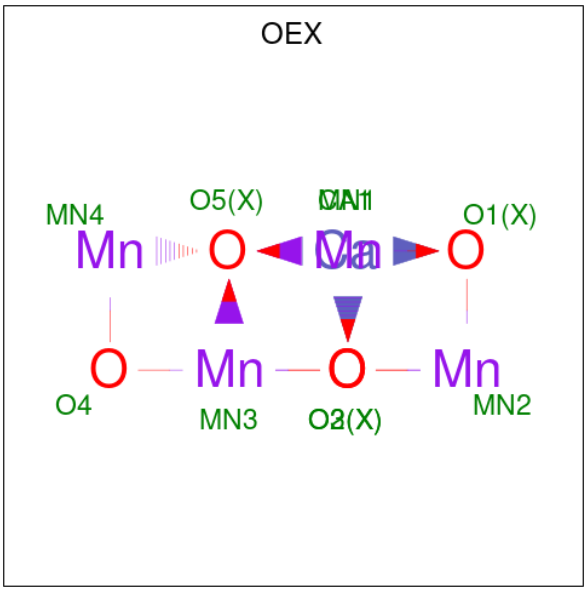
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



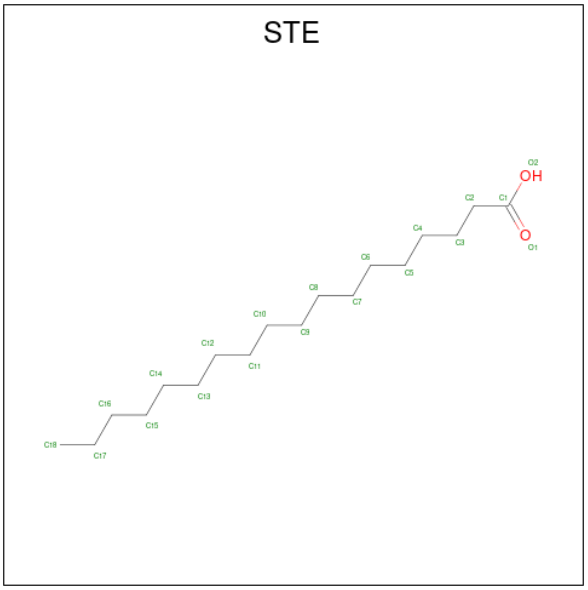
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
30	A	1	161	51	95	15	0	0
			Total	C	H	O		
30	C	1	141	47	79	15	0	0
			Total	C	H	O		
30	C	1	141	47	79	15	0	0
			Total	C	H	O		
30	C	1	141	47	79	15	0	0
			Total	C	H	O		
30	H	1	141	47	79	15	0	0
			Total	C	H	O		
30	c	1	141	47	79	15	0	0
			Total	C	H	O		
30	c	1	139	47	77	15	0	0
			Total	C	H	O		
30	c	1	139	47	77	15	0	0
			Total	C	H	O		
30	h	1	140	47	78	15	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
32	B	1	28	10	16	2	0	0
			Total	C	H	O		
32	B	1	43	15	26	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H 41 15 26	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0

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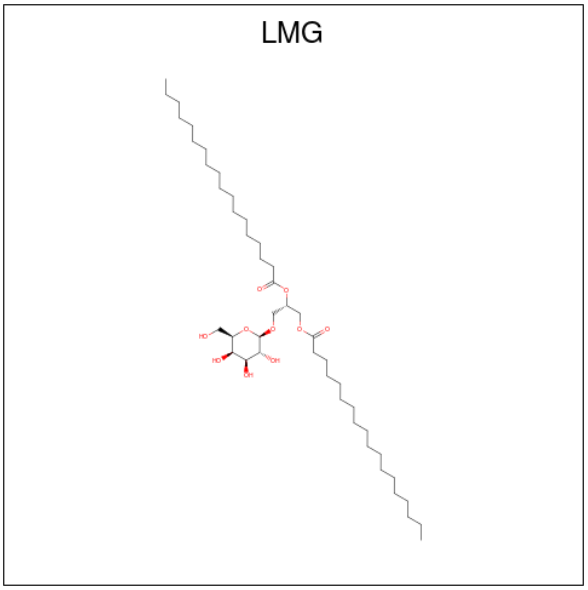
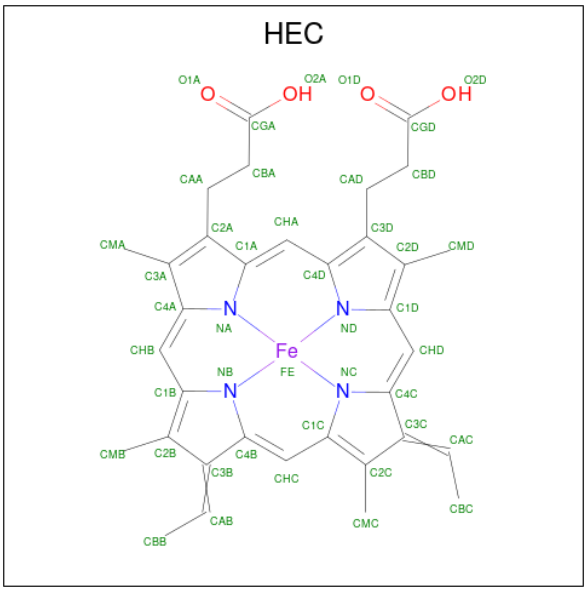
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	h	1	Total C H 41 14 27	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	k	1	Total C H O 28 10 16 2	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	t	1	Total C H O 46 16 28 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 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		
33	B	1	141	45	86	10	0	0
			Total	C	H	O		
33	C	1	112	38	64	10	0	0
			Total	C	H	O		
33	D	1	122	41	71	10	0	0
			Total	C	H	O		
33	D	1	78	27	45	6	0	0
			Total	C	H	O		
33	D	1	68	24	40	4	0	0
			Total	C	H	O		
33	M	1	122	41	71	10	0	0
			Total	C	H	O		
33	Y	1	114	38	66	10	0	0
			Total	C	H	O		
33	b	1	140	45	85	10	0	0
			Total	C	H	O		
33	c	1	80	27	43	10	0	0
			Total	C	H	O		
33	c	1	117	38	69	10	0	0
			Total	C	H	O		
33	c	1	116	39	67	10	0	0
			Total	C	H	O		
33	d	1	100	34	56	10	0	0
			Total	C	H	O		
33	m	1	122	41	71	10	0	0

- Molecule 34 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		
34	E	1	75	34	1	32	4	4	0	0
34	V	1	73	34	1	30	4	4	0	0
34	e	1	75	34	1	32	4	4	0	0
34	v	1	73	34	1	30	4	4	0	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
35	A	132	132	132	0	0
35	B	174	174	174	0	0
35	C	139	139	139	0	0
35	D	116	116	116	0	0
35	E	26	26	26	0	0
35	F	4	4	4	0	0
35	H	16	16	16	0	0
35	I	14	14	14	0	0
35	J	9	9	9	0	0
35	K	7	7	7	0	0
35	L	9	9	9	0	0
35	M	5	5	5	0	0
35	O	78	78	78	0	0
35	R	1	1	1	0	0
35	T	9	9	9	0	0
35	U	34	34	34	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	V	53	Total O 53 53	0	0
35	X	12	Total O 12 12	0	0
35	Y	6	Total O 6 6	0	0
35	Z	1	Total O 1 1	0	0
35	a	109	Total O 109 109	0	0
35	b	134	Total O 134 134	0	0
35	c	130	Total O 130 130	0	0
35	d	91	Total O 91 91	0	0
35	e	15	Total O 15 15	0	0
35	f	8	Total O 8 8	0	0
35	h	26	Total O 26 26	0	0
35	i	7	Total O 7 7	0	0
35	j	9	Total O 9 9	0	0
35	k	6	Total O 6 6	0	0
35	l	10	Total O 10 10	0	0
35	m	3	Total O 3 3	0	0
35	o	81	Total O 81 81	0	0
35	r	7	Total O 7 7	0	0
35	t	11	Total O 11 11	0	0
35	u	43	Total O 43 43	0	0
35	v	37	Total O 37 37	0	0

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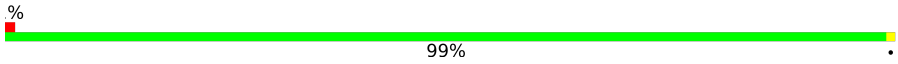
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
35	x	4	4	4	0	0
			Total	O		
35	y	2	2	2	0	0
			Total	O		
35	z	4	4	4	0	0

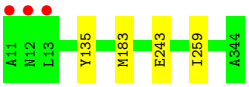
3 Residue-property plots (i)

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

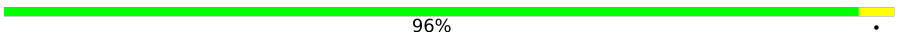
Chain A:

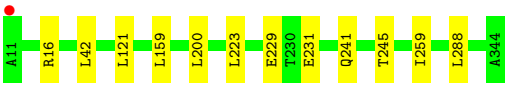




• Molecule 1: Photosystem II protein D1 1

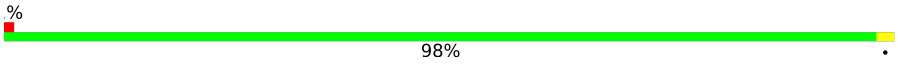
Chain a:

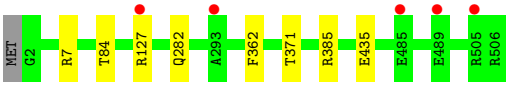




• Molecule 2: Photosystem II CP47 reaction center protein

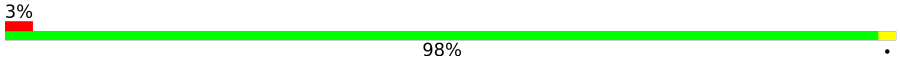
Chain B:

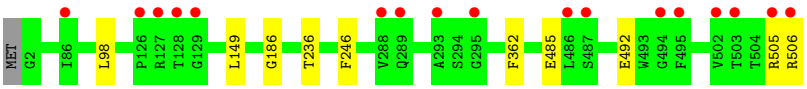




• Molecule 2: Photosystem II CP47 reaction center protein

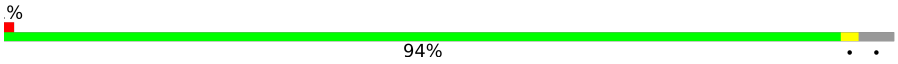
Chain b:

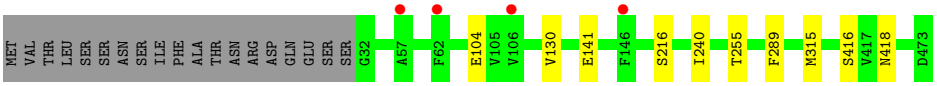




• Molecule 3: Photosystem II CP43 reaction center protein

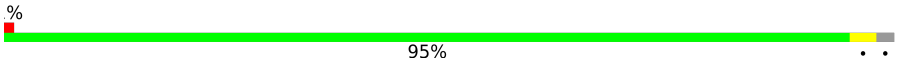
Chain C:

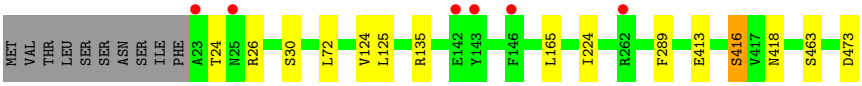




• Molecule 3: Photosystem II CP43 reaction center protein

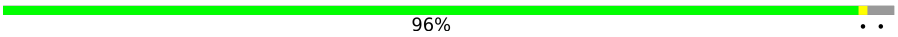
Chain c:

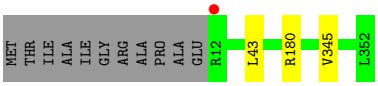




• Molecule 4: Photosystem II D2 protein

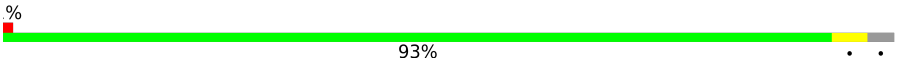
Chain D:

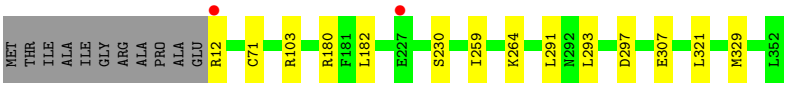




• Molecule 4: Photosystem II D2 protein

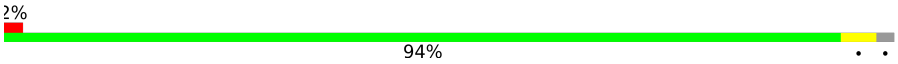
Chain d:

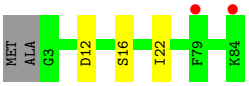




• Molecule 5: Cytochrome b559 subunit alpha

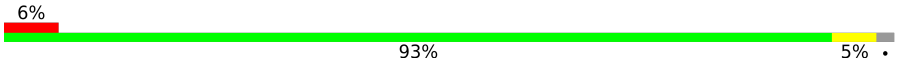
Chain E:

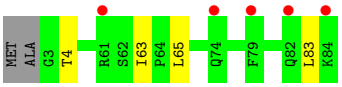




• Molecule 5: Cytochrome b559 subunit alpha

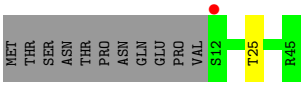
Chain e:





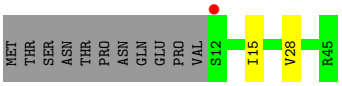
• Molecule 6: Cytochrome b559 subunit beta

Chain F:

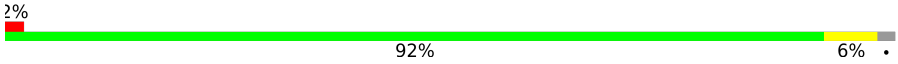


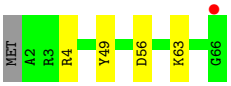
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



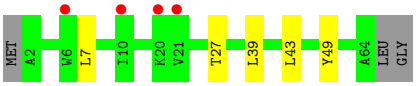
• Molecule 7: Photosystem II reaction center protein H

Chain H: 

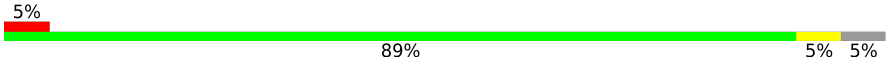


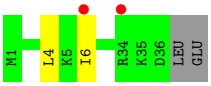
• Molecule 7: Photosystem II reaction center protein H

Chain h:

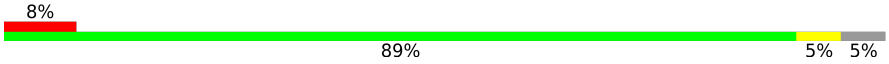


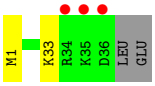
• Molecule 8: Photosystem II reaction center protein I

Chain I: 



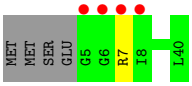
• Molecule 8: Photosystem II reaction center protein I

Chain i: 



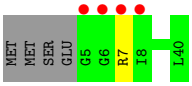
• Molecule 9: Photosystem II reaction center protein J

Chain J:



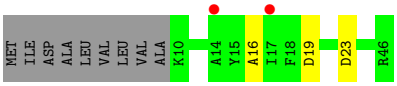
• Molecule 9: Photosystem II reaction center protein J

Chain j:



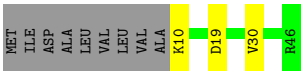
• Molecule 10: Photosystem II reaction center protein K

Chain K:

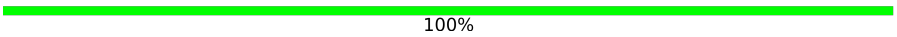


• Molecule 10: Photosystem II reaction center protein K

Chain k:



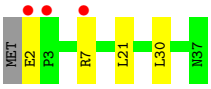
• Molecule 11: Photosystem II reaction center protein L

Chain L: 

There are no outlier residues recorded for this chain.

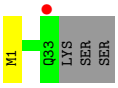
• Molecule 11: Photosystem II reaction center protein L

Chain l:



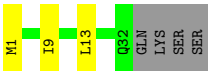
• Molecule 12: Photosystem II reaction center protein M

Chain M:



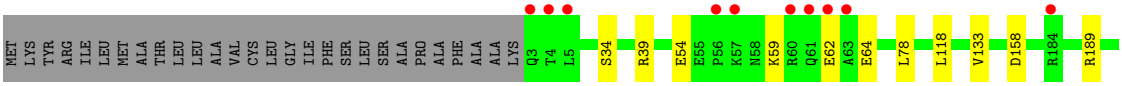
• Molecule 12: Photosystem II reaction center protein M

Chain m:



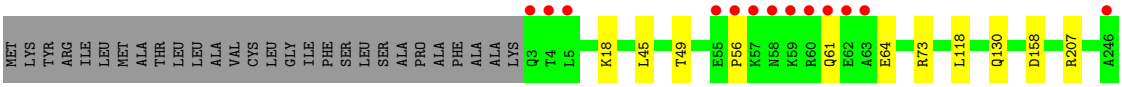
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



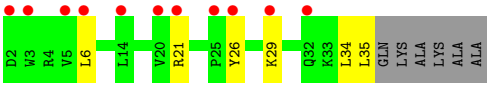
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



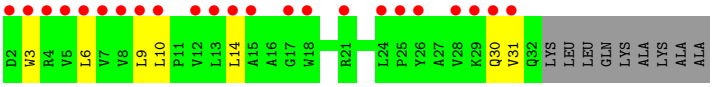
• Molecule 14: Photosystem II protein Y

Chain R:



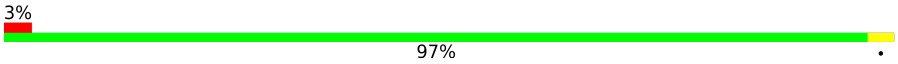
• Molecule 14: Photosystem II protein Y

Chain r:



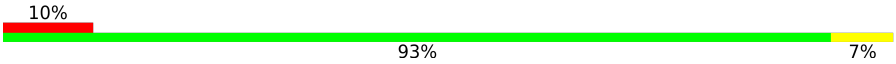
• Molecule 15: Photosystem II reaction center protein T

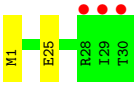
Chain T:



• Molecule 15: Photosystem II reaction center protein T

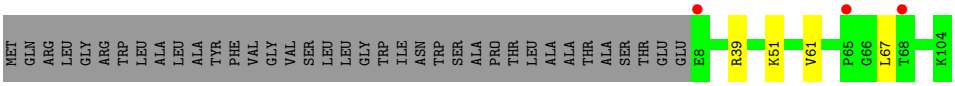
Chain t:





• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:

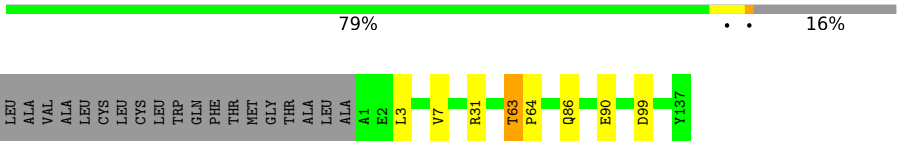


• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:

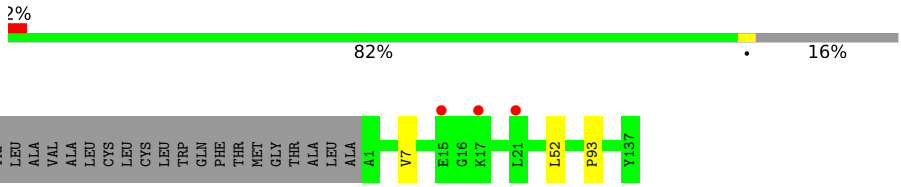
• Molecule 17: Cytochrome c-550

Chain V:



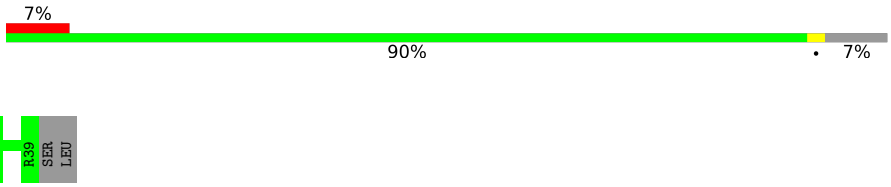
• Molecule 17: Cytochrome c-550

Chain v:



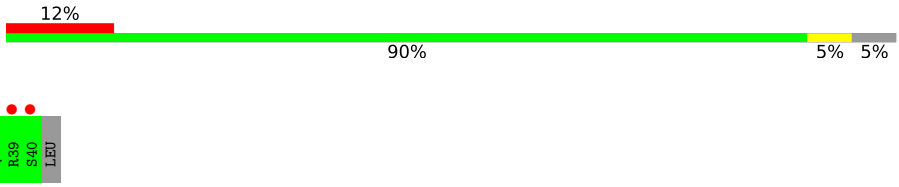
• Molecule 18: Photosystem II reaction center X protein

Chain X:



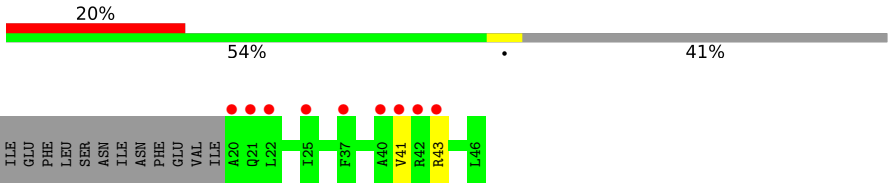
• Molecule 18: Photosystem II reaction center X protein

Chain x:



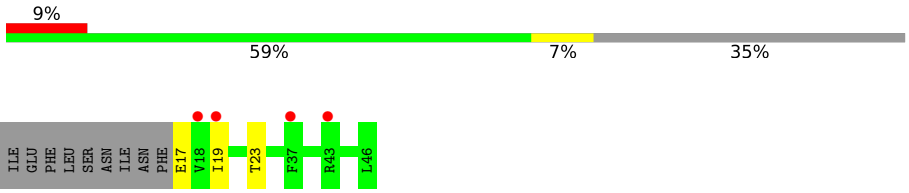
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



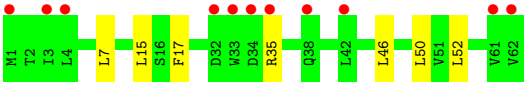
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:



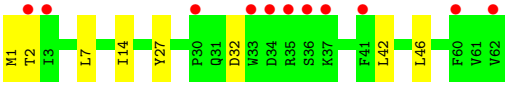
• Molecule 20: Photosystem II reaction center protein Z

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	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26 33.54 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.54-2.26) 86.8 (33.54-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.173 , 0.241 0.173 , 0.240	Depositor DCC
R_{free} test set	3302 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	103385	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: CL, PL9, OEX, DGD, CLA, FME, SQD, LMG, HEC, STE, PHO, BCT, BCR, FE2, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.70	1/2707 (0.0%)	0.72	1/3692 (0.0%)
1	a	0.67	0/2704	0.70	0/3688
2	B	0.68	0/4161	0.71	2/5669 (0.0%)
2	b	0.65	0/4118	0.69	0/5611
3	C	0.64	0/3547	0.68	0/4830
3	c	0.61	0/3619	0.69	1/4926 (0.0%)
4	D	0.67	0/2812	0.70	0/3832
4	d	0.66	1/2821 (0.0%)	0.72	1/3844 (0.0%)
5	E	0.56	0/688	0.65	0/940
5	e	0.59	0/683	0.65	0/932
6	F	0.54	0/284	0.58	0/387
6	f	0.62	0/284	0.62	0/387
7	H	0.74	0/523	0.72	0/713
7	h	0.61	0/511	0.75	0/697
8	I	0.66	0/293	0.68	0/396
8	i	0.69	0/293	0.68	0/396
9	J	0.59	0/263	0.66	0/356
9	j	0.57	0/263	0.65	0/356
10	K	0.52	0/303	0.70	1/416 (0.2%)
10	k	0.55	0/303	0.65	0/416
11	L	0.70	0/311	0.68	0/422
11	l	0.66	0/303	0.76	0/412
12	M	0.72	0/249	0.74	0/341
12	m	0.71	0/244	0.75	0/334
13	O	0.63	0/1904	0.76	2/2585 (0.1%)
13	o	0.63	0/1905	0.76	1/2583 (0.0%)
14	R	0.51	0/277	0.61	0/380
14	r	0.44	0/246	0.59	0/339
15	T	0.69	0/257	0.67	0/349
15	t	0.68	0/255	0.66	0/346
16	U	0.60	0/785	0.69	0/1064
16	u	0.64	0/785	0.76	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	V	0.62	0/1085	0.72	1/1473 (0.1%)
17	v	0.60	0/1085	0.68	0/1473
18	X	0.52	0/284	0.63	0/384
18	x	0.47	0/289	0.61	0/391
19	Y	0.51	0/197	0.61	0/264
19	y	0.43	0/219	0.52	0/294
20	Z	0.54	0/490	0.60	0/669
20	z	0.48	0/488	0.59	0/666
All	All	0.64	2/42838 (0.0%)	0.70	10/58317 (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
2	b	0	1
17	V	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	71	CYS	CB-SG	-5.34	1.73	1.81
1	A	135	TYR	CD1-CE1	-5.24	1.31	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	63	THR	C-N-CD	-7.40	104.32	120.60
4	d	297	ASP	CB-CG-OD1	6.41	124.06	118.30
1	A	183	MET	CA-CB-CG	6.01	123.52	113.30
2	B	385	ARG	NE-CZ-NH2	-5.96	117.32	120.30
13	o	158	ASP	CB-CG-OD1	5.91	123.62	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
2	b	186	GLY	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	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	41	46
1	a	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	41	46
2	B	508/506 (100%)	497 (98%)	11 (2%)	0	100	100
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	442/461 (96%)	428 (97%)	13 (3%)	1 (0%)	47	55
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	47	55
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	29 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	4	2
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	4	2
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	12 (5%)	3 (1%)	13	9
13	o	242/272 (89%)	231 (96%)	9 (4%)	2 (1%)	19	17
14	R	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	1
14	r	29/40 (72%)	26 (90%)	1 (3%)	2 (7%)	1	0
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	2 (2%)	2 (2%)	7	3
17	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	22	21
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	5240/5666 (92%)	5062 (97%)	159 (3%)	19 (0%)	34	37

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/270 (100%)	269 (100%)	1 (0%)	91	94
1	a	269/270 (100%)	258 (96%)	11 (4%)	30	36
2	B	408/404 (101%)	402 (98%)	6 (2%)	65	75
2	b	402/404 (100%)	393 (98%)	9 (2%)	52	61
3	C	346/362 (96%)	337 (97%)	9 (3%)	46	55
3	c	354/362 (98%)	339 (96%)	15 (4%)	30	34
4	D	276/283 (98%)	273 (99%)	3 (1%)	73	82
4	d	277/283 (98%)	265 (96%)	12 (4%)	29	33
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	21
5	e	71/73 (97%)	67 (94%)	4 (6%)	21	21
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	42
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	13
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	12
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	6
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	17
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	49
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	34
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	46
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	13
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	32
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	38
14	R	28/32 (88%)	23 (82%)	5 (18%)	2	0
14	r	23/32 (72%)	18 (78%)	5 (22%)	1	0
15	T	26/26 (100%)	25 (96%)	1 (4%)	33	39
15	t	25/26 (96%)	24 (96%)	1 (4%)	31	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	28
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	58
17	V	117/138 (85%)	111 (95%)	6 (5%)	24	25
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	55
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	47
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	16
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	23
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	2
All	All	4328/4622 (94%)	4163 (96%)	165 (4%)	33	39

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	83	LEU
14	r	6	LEU
7	h	27	THR
11	l	21	LEU
17	v	7	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
14	r	30	GLN
20	z	31	GLN
20	z	38	GLN
16	u	78	ASN
17	V	86	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.87	0	7,9,11	1.19	1 (14%)
12	FME	M	1	12	8,9,10	1.03	0	7,9,11	1.16	1 (14%)
8	FME	I	1	8	8,9,10	1.12	0	7,9,11	0.78	0
15	FME	T	1	15	8,9,10	0.88	0	7,9,11	1.09	0
15	FME	t	1	15	8,9,10	1.20	1 (12%)	7,9,11	0.63	0
12	FME	m	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.62	0

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
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
15	FME	T	1	15	-	3/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.58	1.42	1.46
12	m	1	FME	CA-N	-2.03	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-2.37	119.17	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	1	FME	C-CA-N	-2.07	105.99	109.73

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
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 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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	$\#\|Z\| > 2$
29	SQD	B	623	-	53,54,54	0.96	2 (3%)	62,65,65	1.89	11 (17%)
32	STE	B	626	-	14,14,19	0.55	0	13,13,19	0.40	0
33	LMG	M	101	-	51,51,55	0.98	4 (7%)	59,59,63	1.42	8 (13%)
22	CLA	C	513	-	65,73,73	1.59	7 (10%)	76,113,113	1.57	13 (17%)
32	STE	D	411	-	19,19,19	0.76	1 (5%)	19,19,19	1.27	3 (15%)
22	CLA	b	605	-	65,73,73	1.36	10 (15%)	76,113,113	1.54	14 (18%)
34	HEC	v	201	17	32,50,50	2.42	4 (12%)	24,82,82	1.65	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	A	402	-	65,73,73	1.42	9 (13%)	76,113,113	1.30	9 (11%)
22	CLA	B	612	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	10 (13%)
22	CLA	c	512	-	65,73,73	1.61	9 (13%)	76,113,113	1.52	13 (17%)
30	DGD	A	415	-	67,67,67	1.32	8 (11%)	81,81,81	1.40	14 (17%)
32	STE	b	625	-	9,9,19	0.52	0	8,8,19	0.50	0
24	BCR	c	514	-	41,41,41	0.99	2 (4%)	56,56,56	1.37	9 (16%)
33	LMG	D	409	-	31,31,55	1.05	3 (9%)	33,33,63	1.07	0
32	STE	d	411	-	16,16,19	0.78	0	16,16,19	1.00	1 (6%)
27	PL9	a	410	-	55,55,55	0.92	3 (5%)	68,69,69	1.60	10 (14%)
29	SQD	f	101	-	40,41,54	1.12	4 (10%)	49,52,65	1.92	12 (24%)
31	OEX	a	415	1,35,3	0,15,15	-	-	-		
32	STE	B	621	-	16,16,19	0.79	1 (6%)	16,16,19	0.91	1 (6%)
27	PL9	d	406	-	55,55,55	1.60	9 (16%)	68,69,69	1.85	16 (23%)
22	CLA	B	610	-	65,73,73	1.52	10 (15%)	76,113,113	1.39	11 (14%)
32	STE	M	104	-	17,17,19	0.42	0	16,16,19	0.84	0
29	SQD	a	413	-	35,35,54	1.18	2 (5%)	37,37,65	1.38	7 (18%)
22	CLA	B	613	-	65,73,73	1.30	6 (9%)	76,113,113	1.50	12 (15%)
22	CLA	b	604	-	65,73,73	1.51	7 (10%)	76,113,113	1.65	15 (19%)
32	STE	B	624	-	11,11,19	1.00	1 (9%)	11,11,19	0.87	0
22	CLA	B	603	-	65,73,73	1.63	9 (13%)	76,113,113	1.43	11 (14%)
22	CLA	c	510	-	65,73,73	1.66	12 (18%)	76,113,113	1.45	9 (11%)
32	STE	k	101	-	11,11,19	0.82	0	11,11,19	0.87	0
32	STE	L	103	-	11,11,19	0.79	0	11,11,19	1.25	1 (9%)
22	CLA	b	601	35	65,73,73	1.82	12 (18%)	76,113,113	1.40	10 (13%)
22	CLA	a	403	35	65,73,73	1.63	7 (10%)	76,113,113	1.58	14 (18%)
24	BCR	b	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	10 (17%)
23	PHO	a	404	-	51,69,69	1.10	3 (5%)	47,99,99	1.40	8 (17%)
24	BCR	b	618	-	41,41,41	1.26	3 (7%)	56,56,56	1.33	10 (17%)
32	STE	M	103	-	9,9,19	0.44	0	8,8,19	0.73	0
33	LMG	m	101	-	51,51,55	1.17	6 (11%)	59,59,63	1.49	8 (13%)
22	CLA	b	615	-	65,73,73	1.82	12 (18%)	76,113,113	1.34	6 (7%)
32	STE	h	102	-	13,13,19	0.49	0	12,12,19	0.53	0
22	CLA	C	510	-	65,73,73	1.34	8 (12%)	76,113,113	1.48	9 (11%)
22	CLA	c	506	-	65,73,73	1.52	10 (15%)	76,113,113	1.34	11 (14%)
24	BCR	C	515	-	41,41,41	1.22	5 (12%)	56,56,56	1.34	6 (10%)
30	DGD	C	517	-	63,63,67	1.39	9 (14%)	77,77,81	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	STE	a	414	-	11,11,19	0.92	0	11,11,19	1.04	0
24	BCR	b	617	-	41,41,41	1.13	3 (7%)	56,56,56	1.45	9 (16%)
22	CLA	B	609	-	65,73,73	1.72	10 (15%)	76,113,113	1.49	12 (15%)
22	CLA	B	617	-	60,68,73	1.65	11 (18%)	70,107,113	1.77	12 (17%)
28	LHG	d	407	-	48,48,48	1.04	3 (6%)	51,54,54	1.30	5 (9%)
22	CLA	a	405	-	65,73,73	1.62	11 (16%)	76,113,113	1.52	9 (11%)
22	CLA	B	607	-	65,73,73	1.75	8 (12%)	76,113,113	1.62	11 (14%)
31	OEX	A	416	1,35,3	0,15,15	-	-	-		
30	DGD	c	516	-	63,63,67	1.15	6 (9%)	77,77,81	1.40	9 (11%)
26	BCT	A	409	21	2,3,3	1.22	0	2,3,3	2.65	1 (50%)
22	CLA	d	404	-	65,73,73	1.58	11 (16%)	76,113,113	1.47	10 (13%)
32	STE	c	520	-	19,19,19	0.75	0	19,19,19	1.02	1 (5%)
28	LHG	D	408	-	48,48,48	0.77	1 (2%)	51,54,54	1.34	6 (11%)
24	BCR	x	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
24	BCR	T	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	4 (7%)
22	CLA	C	514	-	65,73,73	1.54	11 (16%)	76,113,113	1.56	14 (18%)
24	BCR	C	501	-	41,41,41	1.01	3 (7%)	56,56,56	1.26	7 (12%)
32	STE	I	101	-	14,14,19	0.60	0	13,13,19	0.45	0
24	BCR	D	405	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
32	STE	b	621	-	19,19,19	0.77	1 (5%)	19,19,19	1.06	2 (10%)
22	CLA	C	503	-	65,73,73	1.52	13 (20%)	76,113,113	1.55	12 (15%)
27	PL9	D	406	-	55,55,55	1.85	7 (12%)	68,69,69	1.80	18 (26%)
22	CLA	A	403	35	65,73,73	1.65	9 (13%)	76,113,113	1.32	7 (9%)
22	CLA	B	611	35	65,73,73	1.80	10 (15%)	76,113,113	1.33	9 (11%)
22	CLA	b	614	-	65,73,73	1.74	11 (16%)	76,113,113	1.41	14 (18%)
22	CLA	c	511	3	65,73,73	1.93	11 (16%)	76,113,113	1.45	10 (13%)
22	CLA	b	603	-	65,73,73	1.52	10 (15%)	76,113,113	1.55	14 (18%)
24	BCR	d	405	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
34	HEC	E	101	5,6	32,50,50	2.39	4 (12%)	24,82,82	2.04	5 (20%)
30	DGD	c	517	-	63,63,67	1.20	7 (11%)	77,77,81	1.38	9 (11%)
28	LHG	A	411	-	46,46,48	1.05	3 (6%)	49,52,54	1.19	3 (6%)
30	DGD	H	102	-	63,63,67	1.48	13 (20%)	77,77,81	1.42	11 (14%)
32	STE	C	520	-	11,11,19	0.77	0	11,11,19	1.37	2 (18%)
32	STE	T	102	-	14,14,19	0.43	0	13,13,19	0.78	0
23	PHO	D	401	-	51,69,69	1.26	9 (17%)	47,99,99	1.26	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	BCT	a	409	21	2,3,3	1.29	0	2,3,3	4.06	2 (100%)
22	CLA	b	606	-	65,73,73	1.74	8 (12%)	76,113,113	1.60	9 (11%)
24	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	8 (14%)
22	CLA	c	503	-	65,73,73	1.63	11 (16%)	76,113,113	1.55	11 (14%)
22	CLA	b	608	-	65,73,73	1.53	9 (13%)	76,113,113	1.20	6 (7%)
22	CLA	c	513	-	65,73,73	1.58	9 (13%)	76,113,113	1.37	8 (10%)
28	LHG	a	412	-	41,41,48	1.06	4 (9%)	44,47,54	1.29	3 (6%)
32	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.33	2 (18%)
22	CLA	c	501	-	65,73,73	1.38	9 (13%)	76,113,113	1.54	9 (11%)
32	STE	b	624	-	19,19,19	0.90	0	19,19,19	0.82	1 (5%)
24	BCR	A	406	-	41,41,41	1.02	3 (7%)	56,56,56	1.49	11 (19%)
32	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.53	0
32	STE	C	522	-	11,11,19	0.84	0	11,11,19	0.85	0
32	STE	j	101	-	11,11,19	1.05	0	11,11,19	0.80	1 (9%)
22	CLA	D	402	-	65,73,73	1.55	8 (12%)	76,113,113	1.53	9 (11%)
33	LMG	Y	101	-	48,48,55	1.04	4 (8%)	56,56,63	1.37	8 (14%)
28	LHG	l	101	-	48,48,48	0.77	0	51,54,54	1.26	4 (7%)
33	LMG	D	410	-	26,26,55	1.03	1 (3%)	26,26,63	1.14	2 (7%)
24	BCR	t	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	5 (8%)
22	CLA	c	508	-	64,72,73	1.56	9 (14%)	74,111,113	1.52	10 (13%)
22	CLA	B	604	-	65,73,73	1.68	8 (12%)	76,113,113	1.53	13 (17%)
22	CLA	B	614	-	65,73,73	1.67	6 (9%)	76,113,113	1.50	11 (14%)
32	STE	t	104	-	17,17,19	0.73	0	17,17,19	1.16	1 (5%)
28	LHG	d	408	-	48,48,48	0.72	1 (2%)	51,54,54	1.18	4 (7%)
33	LMG	d	410	-	44,44,55	1.01	3 (6%)	52,52,63	1.46	7 (13%)
33	LMG	c	519	-	37,37,55	1.18	4 (10%)	45,45,63	1.31	6 (13%)
33	LMG	b	622	-	55,55,55	1.42	7 (12%)	63,63,63	1.51	8 (12%)
22	CLA	b	616	-	60,68,73	1.41	9 (15%)	70,107,113	1.57	8 (11%)
22	CLA	B	616	-	65,73,73	1.53	6 (9%)	76,113,113	1.41	10 (13%)
22	CLA	C	508	35	65,73,73	1.36	7 (10%)	76,113,113	1.37	7 (9%)
32	STE	B	601	-	11,11,19	0.79	0	11,11,19	1.31	1 (9%)
28	LHG	d	409	-	38,38,48	0.92	1 (2%)	41,44,54	1.26	3 (7%)
32	STE	C	521	-	15,15,19	0.66	0	14,14,19	0.39	0
29	SQD	F	101	-	35,36,54	1.04	2 (5%)	42,45,65	1.82	9 (21%)
22	CLA	B	615	-	65,73,73	1.91	13 (20%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	b	610	35	65,73,73	1.54	10 (15%)	76,113,113	1.39	11 (14%)
32	STE	Z	102	-	7,7,19	0.50	0	6,6,19	0.56	0
22	CLA	B	606	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	11 (14%)
24	BCR	c	515	-	41,41,41	1.08	4 (9%)	56,56,56	1.42	6 (10%)
32	STE	t	102	-	13,13,19	0.66	0	13,13,19	1.30	1 (7%)
32	STE	b	620	-	15,15,19	0.60	0	14,14,19	0.62	0
22	CLA	c	504	35	60,68,73	1.59	9 (15%)	70,107,113	1.50	9 (12%)
23	PHO	d	401	-	51,69,69	1.09	5 (9%)	47,99,99	1.42	9 (19%)
32	STE	t	103	-	9,9,19	0.51	0	8,8,19	0.45	0
29	SQD	a	411	-	53,54,54	0.96	5 (9%)	62,65,65	1.89	13 (20%)
32	STE	M	102	-	14,14,19	0.78	0	14,14,19	0.95	0
22	CLA	B	605	-	65,73,73	1.37	7 (10%)	76,113,113	1.83	13 (17%)
29	SQD	L	101	-	48,49,54	0.98	2 (4%)	57,60,65	2.29	15 (26%)
22	CLA	b	612	-	65,73,73	1.34	5 (7%)	76,113,113	1.40	11 (14%)
33	LMG	c	521	-	48,48,55	1.16	5 (10%)	56,56,63	1.25	6 (10%)
22	CLA	B	602	35	65,73,73	1.89	11 (16%)	76,113,113	1.32	6 (7%)
22	CLA	D	404	-	65,73,73	1.46	8 (12%)	76,113,113	1.60	13 (17%)
32	STE	b	626	-	19,19,19	0.73	0	19,19,19	1.12	1 (5%)
22	CLA	a	402	-	65,73,73	1.59	9 (13%)	76,113,113	1.36	10 (13%)
24	BCR	a	406	-	41,41,41	1.02	2 (4%)	56,56,56	1.15	5 (8%)
22	CLA	b	613	-	65,73,73	1.48	11 (16%)	76,113,113	1.58	14 (18%)
22	CLA	C	509	-	65,73,73	1.68	7 (10%)	76,113,113	1.45	12 (15%)
24	BCR	Z	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.46	10 (17%)
22	CLA	b	611	-	65,73,73	1.49	8 (12%)	76,113,113	1.59	12 (15%)
22	CLA	C	504	-	65,73,73	1.65	11 (16%)	76,113,113	1.82	9 (11%)
29	SQD	A	414	-	38,38,54	1.16	3 (7%)	40,40,65	1.39	4 (10%)
22	CLA	b	607	35	65,73,73	1.54	8 (12%)	76,113,113	1.46	9 (11%)
24	BCR	K	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.26	4 (7%)
28	LHG	B	622	-	48,48,48	1.01	3 (6%)	51,54,54	1.33	6 (11%)
22	CLA	A	405	-	54,62,73	1.76	9 (16%)	62,99,113	1.61	12 (19%)
22	CLA	c	509	-	65,73,73	1.60	7 (10%)	76,113,113	1.50	9 (11%)
22	CLA	c	502	-	65,73,73	1.39	6 (9%)	76,113,113	1.39	9 (11%)
32	STE	b	623	-	15,15,19	0.76	0	15,15,19	0.86	0
33	LMG	c	522	-	49,49,55	0.98	3 (6%)	57,57,63	1.36	5 (8%)
33	LMG	D	407	-	51,51,55	1.14	4 (7%)	59,59,63	1.31	6 (10%)
22	CLA	d	403	35	65,73,73	1.51	10 (15%)	76,113,113	1.61	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	c	505	-	65,73,73	1.43	7 (10%)	76,113,113	1.33	7 (9%)
24	BCR	k	102	-	41,41,41	1.08	4 (9%)	56,56,56	1.20	6 (10%)
22	CLA	C	505	35	59,67,73	1.59	10 (16%)	68,105,113	1.49	10 (14%)
30	DGD	h	101	-	63,63,67	1.22	9 (14%)	77,77,81	1.50	14 (18%)
22	CLA	c	507	35	65,73,73	1.51	12 (18%)	76,113,113	1.43	8 (10%)
28	LHG	A	413	-	48,48,48	1.09	5 (10%)	51,54,54	1.24	6 (11%)
22	CLA	b	609	-	65,73,73	1.87	11 (16%)	76,113,113	1.51	12 (15%)
23	PHO	A	404	-	51,69,69	1.24	6 (11%)	47,99,99	1.36	9 (19%)
22	CLA	C	512	3	65,73,73	1.63	10 (15%)	76,113,113	1.40	8 (10%)
22	CLA	B	608	35	65,73,73	1.47	12 (18%)	76,113,113	1.65	10 (13%)
22	CLA	D	403	35	65,73,73	1.30	7 (10%)	76,113,113	1.32	10 (13%)
22	CLA	C	506	-	65,73,73	1.54	8 (12%)	76,113,113	1.41	7 (9%)
22	CLA	C	507	-	65,73,73	1.49	4 (6%)	76,113,113	1.16	6 (7%)
22	CLA	C	502	-	65,73,73	1.72	10 (15%)	76,113,113	1.39	14 (18%)
24	BCR	B	620	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	7 (12%)
33	LMG	B	627	-	55,55,55	1.48	7 (12%)	63,63,63	1.61	9 (14%)
30	DGD	C	519	-	63,63,67	1.14	7 (11%)	77,77,81	1.35	9 (11%)
32	STE	E	102	-	11,11,19	0.94	0	11,11,19	1.05	0
32	STE	x	102	-	19,19,19	0.70	0	19,19,19	0.81	1 (5%)
28	LHG	L	102	-	48,48,48	0.87	2 (4%)	51,54,54	1.23	3 (5%)
24	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.48	9 (16%)
30	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.40	9 (11%)
33	LMG	C	516	-	48,48,55	0.95	2 (4%)	56,56,63	1.26	6 (10%)
22	CLA	b	602	-	65,73,73	1.66	10 (15%)	76,113,113	1.59	11 (14%)
22	CLA	d	402	-	65,73,73	1.65	7 (10%)	76,113,113	1.49	11 (14%)
34	HEC	e	101	5,6	32,50,50	2.40	5 (15%)	24,82,82	2.10	3 (12%)
32	STE	B	625	-	15,15,19	0.56	0	14,14,19	0.48	0
22	CLA	C	511	-	65,73,73	1.68	10 (15%)	76,113,113	1.43	8 (10%)
27	PL9	A	410	-	55,55,55	1.20	3 (5%)	68,69,69	1.49	13 (19%)
34	HEC	V	201	17	32,50,50	1.93	3 (9%)	24,82,82	2.26	7 (29%)
24	BCR	k	103	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	7 (12%)
29	SQD	A	412	-	51,52,54	1.08	5 (9%)	60,63,65	1.99	13 (21%)
30	DGD	C	518	-	63,63,67	1.38	8 (12%)	77,77,81	1.45	10 (12%)
24	BCR	B	618	-	41,41,41	1.25	3 (7%)	56,56,56	1.30	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	B	623	-	-	20/49/69/69	0/1/1/1
32	STE	B	626	-	-	11/12/12/17	-
33	LMG	M	101	-	-	23/46/66/70	0/1/1/1
22	CLA	C	513	-	1/1/20/20	20/37/115/115	-
32	STE	D	411	-	-	11/17/17/17	-
22	CLA	b	605	-	1/1/20/20	11/37/115/115	-
34	HEC	v	201	17	-	2/10/54/54	-
22	CLA	A	402	-	1/1/20/20	3/37/115/115	-
22	CLA	B	612	-	1/1/20/20	7/37/115/115	-
22	CLA	c	512	-	1/1/20/20	22/37/115/115	-
30	DGD	A	415	-	-	27/55/95/95	0/2/2/2
32	STE	b	625	-	-	3/7/7/17	-
24	BCR	c	514	-	-	16/29/63/63	0/2/2/2
33	LMG	D	409	-	-	16/33/33/70	-
32	STE	d	411	-	-	8/14/14/17	-
27	PL9	a	410	-	-	25/53/73/73	0/1/1/1
29	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	STE	B	621	-	-	6/14/14/17	-
27	PL9	d	406	-	-	17/53/73/73	0/1/1/1
22	CLA	B	610	-	-	4/37/115/115	-
32	STE	M	104	-	-	8/15/15/17	-
29	SQD	a	413	-	-	12/37/37/69	-
22	CLA	B	613	-	1/1/20/20	6/37/115/115	-
22	CLA	b	604	-	1/1/20/20	5/37/115/115	-
32	STE	B	624	-	-	5/9/9/17	-
22	CLA	B	603	-	1/1/20/20	13/37/115/115	-
22	CLA	c	510	-	1/1/20/20	13/37/115/115	-
32	STE	k	101	-	-	3/9/9/17	-
32	STE	L	103	-	-	5/9/9/17	-
22	CLA	b	601	35	1/1/20/20	17/37/115/115	-
22	CLA	a	403	35	-	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	619	-	-	11/29/63/63	0/2/2/2
23	PHO	a	404	-	-	8/37/103/103	0/5/6/6
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
32	STE	M	103	-	-	3/7/7/17	-
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
22	CLA	b	615	-	1/1/20/20	8/37/115/115	-
32	STE	h	102	-	-	7/11/11/17	-
22	CLA	C	510	-	1/1/20/20	18/37/115/115	-
22	CLA	c	506	-	1/1/20/20	19/37/115/115	-
24	BCR	C	515	-	-	8/29/63/63	0/2/2/2
30	DGD	C	517	-	-	21/51/91/95	0/2/2/2
32	STE	a	414	-	-	3/9/9/17	-
24	BCR	b	617	-	-	6/29/63/63	0/2/2/2
22	CLA	B	609	-	-	5/37/115/115	-
22	CLA	B	617	-	1/1/19/20	9/31/109/115	-
28	LHG	d	407	-	-	18/53/53/53	-
22	CLA	a	405	-	1/1/20/20	11/37/115/115	-
22	CLA	B	607	-	1/1/20/20	8/37/115/115	-
30	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	d	404	-	-	5/37/115/115	-
32	STE	c	520	-	-	7/17/17/17	-
28	LHG	D	408	-	-	16/53/53/53	-
24	BCR	x	101	-	-	3/29/63/63	0/2/2/2
24	BCR	T	101	-	-	9/29/63/63	0/2/2/2
22	CLA	C	514	-	-	14/37/115/115	-
24	BCR	C	501	-	-	7/29/63/63	0/2/2/2
32	STE	I	101	-	-	6/12/12/17	-
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2
32	STE	b	621	-	-	7/17/17/17	-
22	CLA	C	503	-	1/1/20/20	8/37/115/115	-
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
22	CLA	A	403	35	1/1/20/20	3/37/115/115	-
22	CLA	B	611	35	1/1/20/20	3/37/115/115	-
22	CLA	b	614	-	1/1/20/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	511	3	1/1/20/20	14/37/115/115	-
22	CLA	b	603	-	1/1/20/20	11/37/115/115	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
34	HEC	E	101	5,6	-	2/10/54/54	-
30	DGD	c	517	-	-	18/51/91/95	0/2/2/2
28	LHG	A	411	-	-	24/51/51/53	-
30	DGD	H	102	-	-	18/51/91/95	0/2/2/2
32	STE	C	520	-	-	4/9/9/17	-
32	STE	T	102	-	-	8/12/12/17	-
23	PHO	D	401	-	-	4/37/103/103	0/5/6/6
22	CLA	b	606	-	1/1/20/20	8/37/115/115	-
24	BCR	B	619	-	-	9/29/63/63	0/2/2/2
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
22	CLA	b	608	-	-	4/37/115/115	-
22	CLA	c	513	-	1/1/20/20	10/37/115/115	-
28	LHG	a	412	-	-	25/46/46/53	-
32	STE	J	101	-	-	8/9/9/17	-
22	CLA	c	501	-	1/1/20/20	3/37/115/115	-
32	STE	b	624	-	-	7/17/17/17	-
24	BCR	A	406	-	-	11/29/63/63	0/2/2/2
32	STE	H	103	-	-	10/15/15/17	-
32	STE	C	522	-	-	3/9/9/17	-
32	STE	j	101	-	-	1/9/9/17	-
22	CLA	D	402	-	1/1/20/20	5/37/115/115	-
33	LMG	Y	101	-	-	20/43/63/70	0/1/1/1
28	LHG	l	101	-	-	20/53/53/53	-
33	LMG	D	410	-	-	8/22/22/70	-
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
22	CLA	c	508	-	1/1/19/20	18/36/114/115	-
22	CLA	B	604	-	1/1/20/20	13/37/115/115	-
22	CLA	B	614	-	1/1/20/20	16/37/115/115	-
32	STE	t	104	-	-	8/15/15/17	-
28	LHG	d	408	-	-	20/53/53/53	-
33	LMG	d	410	-	-	14/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	519	-	-	7/31/51/70	0/1/1/1
33	LMG	b	622	-	-	28/50/70/70	0/1/1/1
22	CLA	b	616	-	1/1/19/20	7/31/109/115	-
22	CLA	B	616	-	1/1/20/20	9/37/115/115	-
22	CLA	C	508	35	1/1/20/20	7/37/115/115	-
32	STE	B	601	-	-	2/9/9/17	-
28	LHG	d	409	-	-	12/43/43/53	-
32	STE	C	521	-	-	5/13/13/17	-
29	SQD	F	101	-	-	10/28/48/69	0/1/1/1
22	CLA	B	615	-	1/1/20/20	12/37/115/115	-
22	CLA	b	610	35	1/1/20/20	5/37/115/115	-
32	STE	Z	102	-	-	3/5/5/17	-
22	CLA	B	606	-	1/1/20/20	11/37/115/115	-
24	BCR	c	515	-	-	5/29/63/63	0/2/2/2
32	STE	t	102	-	-	5/11/11/17	-
32	STE	b	620	-	-	6/13/13/17	-
22	CLA	c	504	35	1/1/19/20	10/31/109/115	-
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
32	STE	t	103	-	-	5/7/7/17	-
29	SQD	a	411	-	-	21/49/69/69	0/1/1/1
32	STE	M	102	-	-	5/12/12/17	-
22	CLA	B	605	-	1/1/20/20	10/37/115/115	-
29	SQD	L	101	-	-	21/44/64/69	0/1/1/1
22	CLA	b	612	-	1/1/20/20	10/37/115/115	-
33	LMG	c	521	-	-	23/43/63/70	0/1/1/1
22	CLA	B	602	35	1/1/20/20	22/37/115/115	-
22	CLA	D	404	-	1/1/20/20	10/37/115/115	-
32	STE	b	626	-	-	8/17/17/17	-
22	CLA	a	402	-	1/1/20/20	4/37/115/115	-
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	b	613	-	1/1/20/20	7/37/115/115	-
22	CLA	C	509	-	1/1/20/20	6/37/115/115	-
24	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
22	CLA	b	611	-	1/1/20/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	504	-	1/1/20/20	4/37/115/115	-
29	SQD	A	414	-	-	14/39/39/69	-
22	CLA	b	607	35	1/1/20/20	13/37/115/115	-
24	BCR	K	101	-	-	13/29/63/63	0/2/2/2
28	LHG	B	622	-	-	20/53/53/53	-
22	CLA	A	405	-	1/1/17/20	4/24/102/115	-
22	CLA	c	509	-	1/1/20/20	15/37/115/115	-
22	CLA	c	502	-	1/1/20/20	7/37/115/115	-
32	STE	b	623	-	-	5/13/13/17	-
33	LMG	c	522	-	-	16/44/64/70	0/1/1/1
33	LMG	D	407	-	-	15/46/66/70	0/1/1/1
22	CLA	d	403	35	1/1/20/20	11/37/115/115	-
22	CLA	c	505	-	1/1/20/20	13/37/115/115	-
24	BCR	k	102	-	-	10/29/63/63	0/2/2/2
22	CLA	C	505	35	1/1/18/20	8/30/108/115	-
30	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	c	507	35	1/1/20/20	12/37/115/115	-
28	LHG	A	413	-	-	29/53/53/53	-
22	CLA	b	609	-	1/1/20/20	6/37/115/115	-
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
22	CLA	C	512	3	1/1/20/20	6/37/115/115	-
22	CLA	B	608	35	1/1/20/20	8/37/115/115	-
22	CLA	D	403	35	1/1/20/20	7/37/115/115	-
22	CLA	C	506	-	1/1/20/20	8/37/115/115	-
22	CLA	C	507	-	1/1/20/20	12/37/115/115	-
22	CLA	C	502	-	1/1/20/20	4/37/115/115	-
24	BCR	B	620	-	-	4/29/63/63	0/2/2/2
33	LMG	B	627	-	-	28/50/70/70	0/1/1/1
30	DGD	C	519	-	-	12/51/91/95	0/2/2/2
32	STE	E	102	-	-	5/9/9/17	-
32	STE	x	102	-	-	14/17/17/17	-
28	LHG	L	102	-	-	21/53/53/53	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	516	-	-	23/43/63/70	0/1/1/1
22	CLA	b	602	-	1/1/20/20	11/37/115/115	-
22	CLA	d	402	-	-	6/37/115/115	-
34	HEC	e	101	5,6	-	2/10/54/54	-
32	STE	B	625	-	-	6/13/13/17	-
22	CLA	C	511	-	1/1/20/20	11/37/115/115	-
27	PL9	A	410	-	-	24/53/73/73	0/1/1/1
34	HEC	V	201	17	-	2/10/54/54	-
24	BCR	k	103	-	-	6/29/63/63	0/2/2/2
29	SQD	A	412	-	-	18/47/67/69	0/1/1/1
30	DGD	C	518	-	-	20/51/91/95	0/2/2/2
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2

The worst 5 of 929 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	406	PL9	C7-C3	-10.03	1.41	1.51
22	b	609	CLA	C4B-NB	8.97	1.43	1.35
22	B	607	CLA	MG-NA	8.88	2.27	2.06
22	B	604	CLA	MG-ND	8.83	2.23	2.05
22	B	611	CLA	C4B-NB	8.83	1.43	1.35

The worst 5 of 1317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C4A-NA-C1A	10.83	111.58	106.71
22	B	617	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	L	101	SQD	O6-C1-C2	9.35	122.90	108.30
29	A	412	SQD	O6-C1-C2	8.82	122.07	108.30
22	B	607	CLA	C4A-NA-C1A	8.69	110.61	106.71

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND

5 of 1906 torsion outliers are listed below:

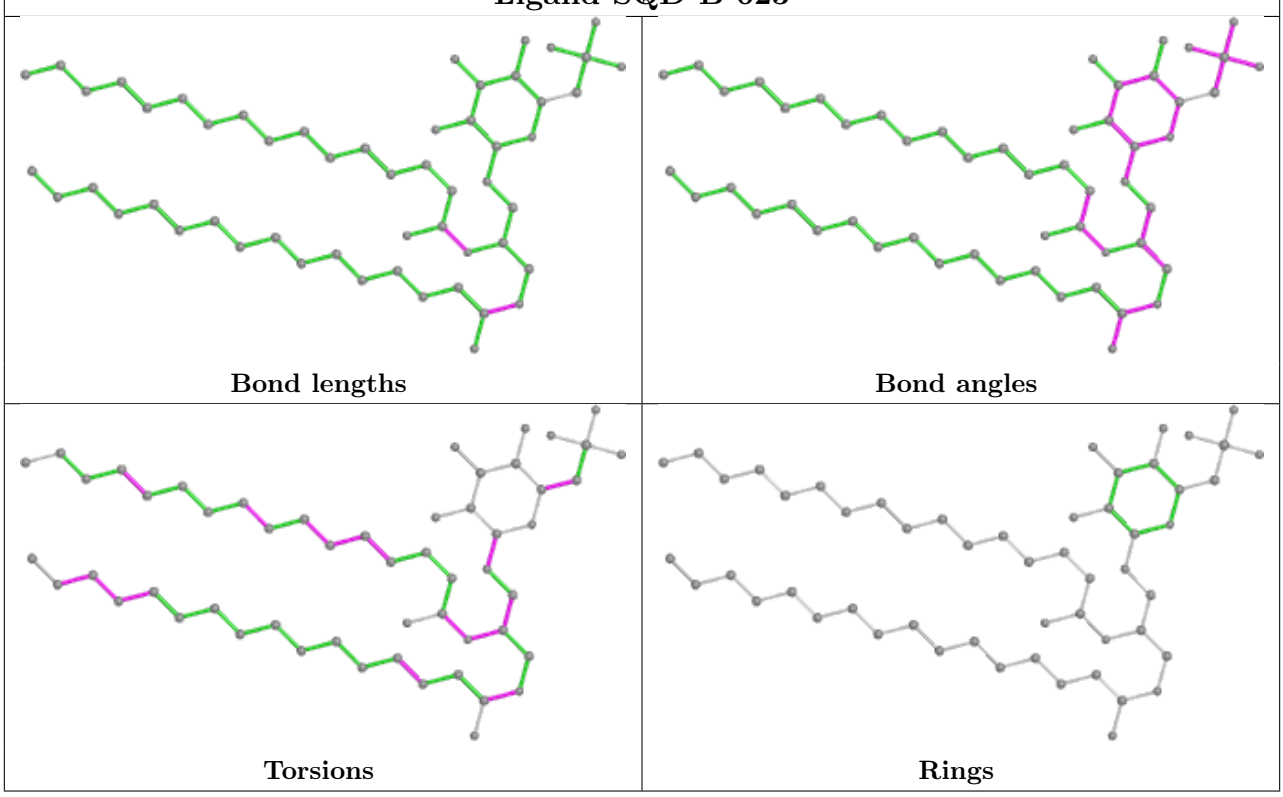
Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

No monomer is involved in short contacts.

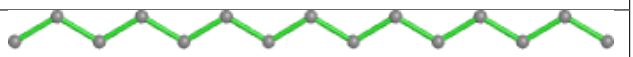
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 SQD B 623

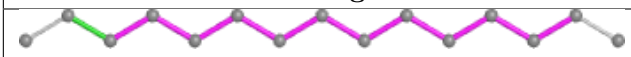


Ligand STE B 626

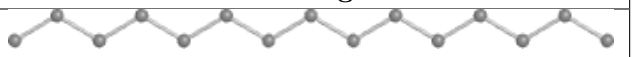
Bond lengths



Bond angles

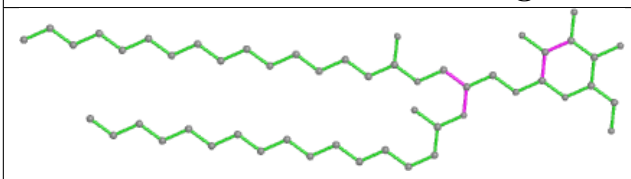


Torsions

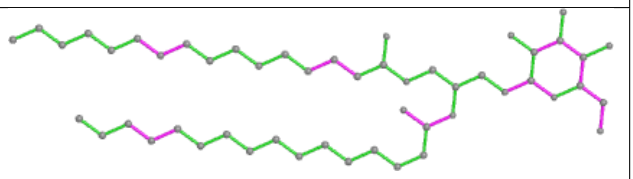


Rings

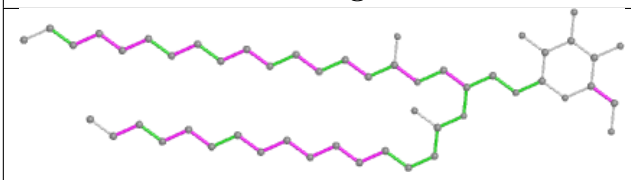
Ligand LMG M 101



Bond lengths



Bond angles



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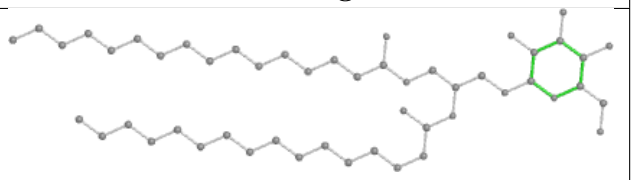
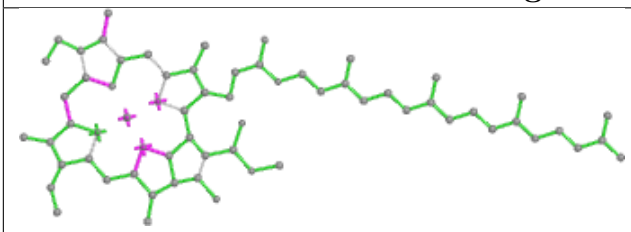
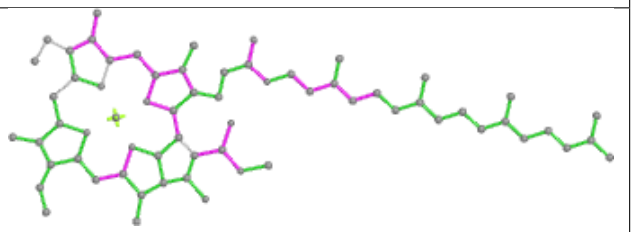


Rings

Ligand CLA C 513



Bond lengths



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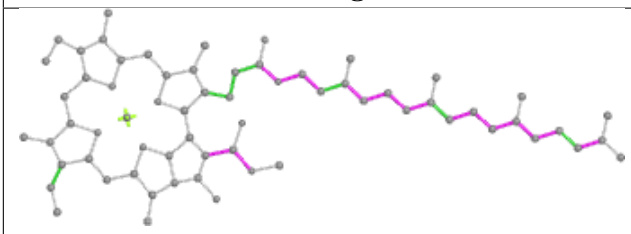
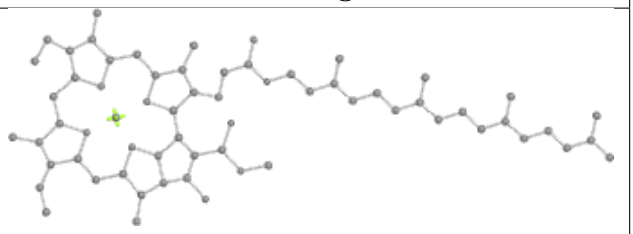
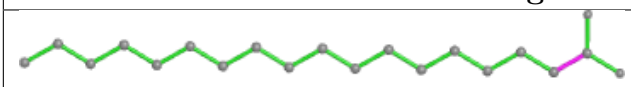


Torsions

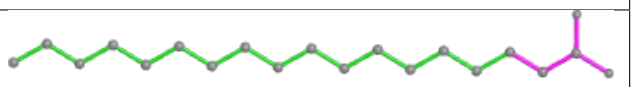


Rings

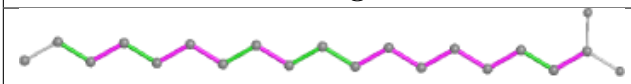
Ligand STE D 411



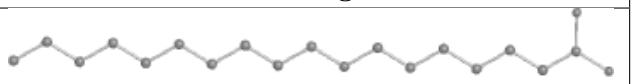
Bond lengths



Bond angles

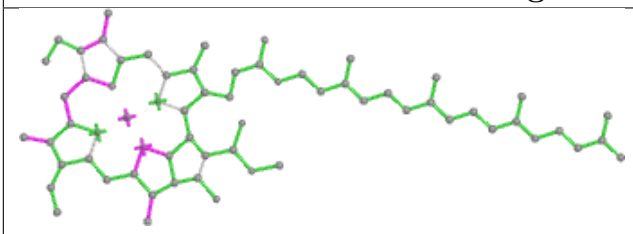


Torsions



Rings

Ligand CLA b 605



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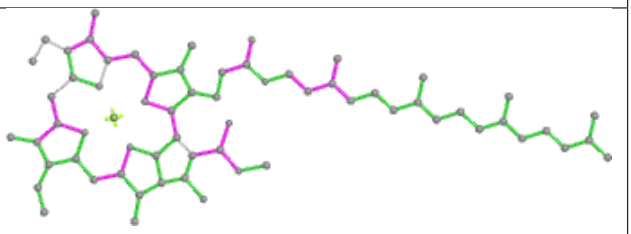
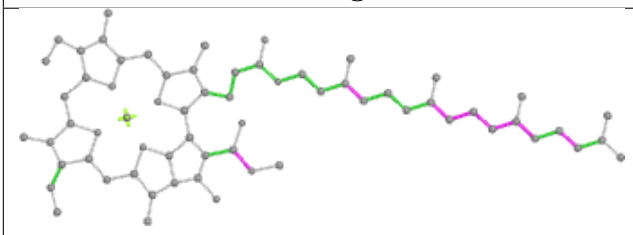


Bond angles



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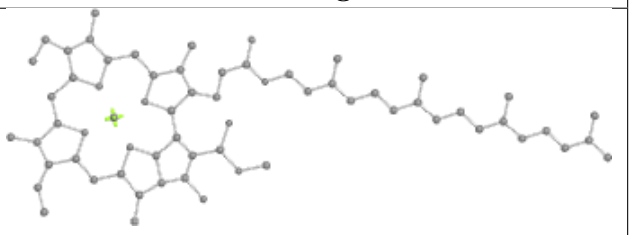
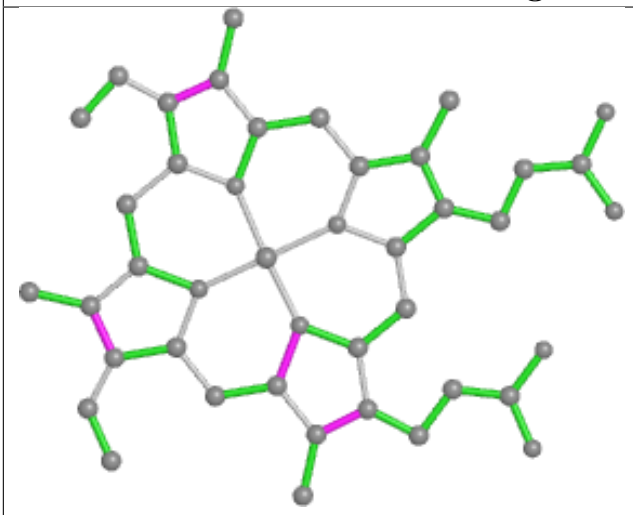


Rings

Ligand HEC v 201



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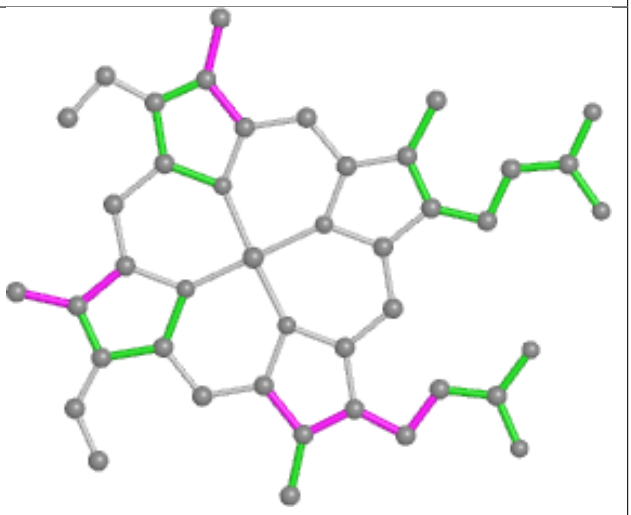
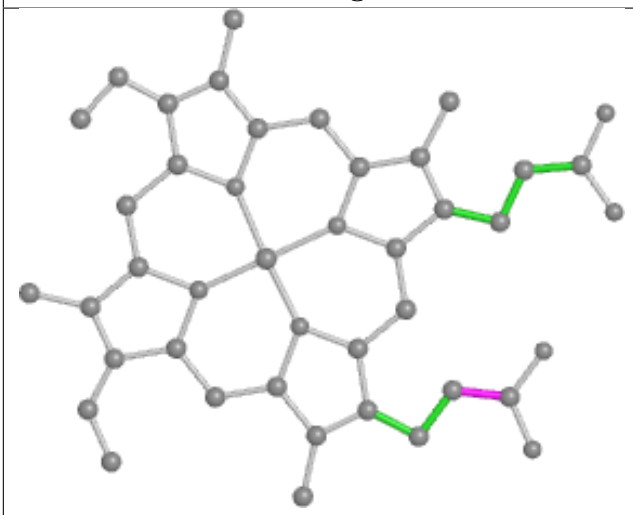


Bond angles



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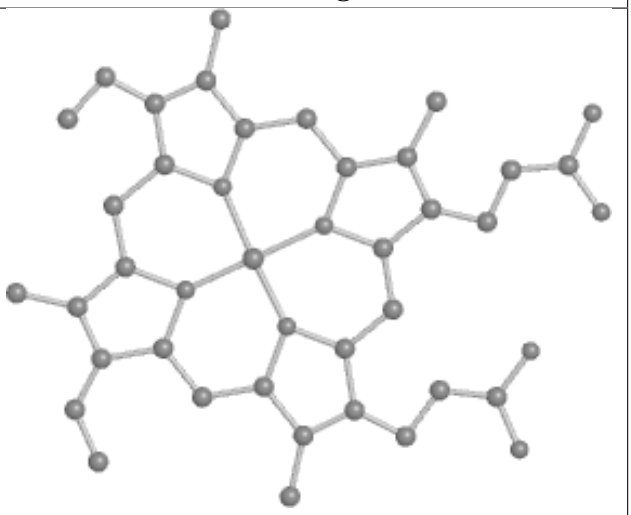
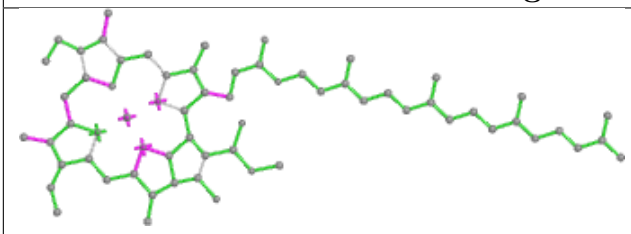


Rings

Ligand CLA A 402



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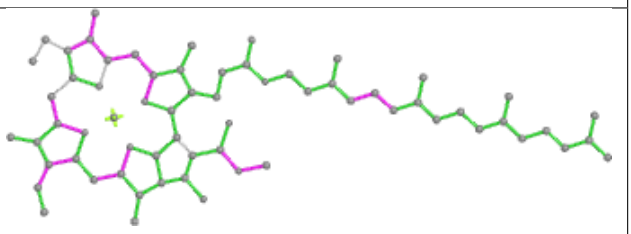
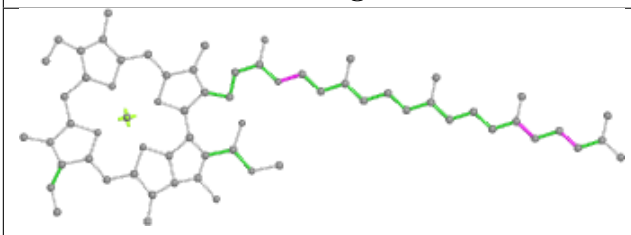


Bond angles



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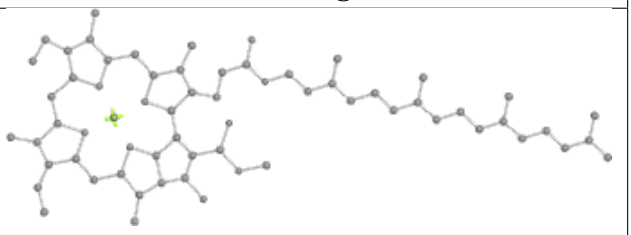
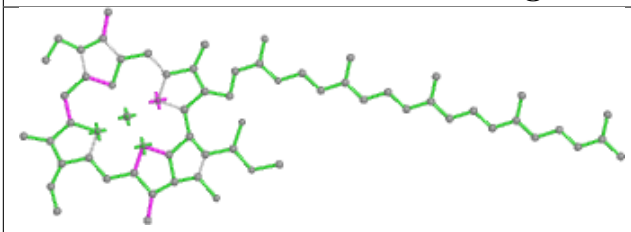


Rings

Ligand CLA B 612



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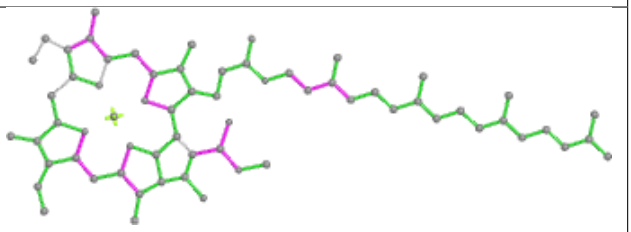
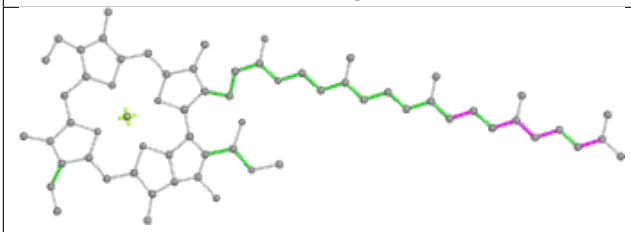
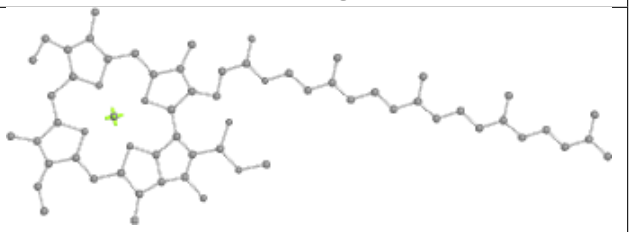


Bond angles

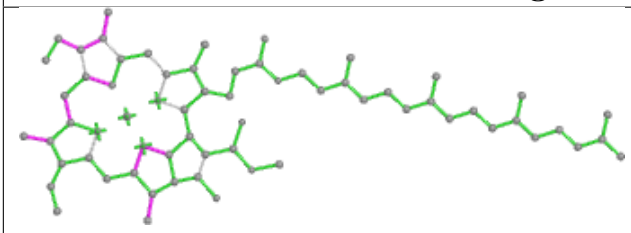


Torsions

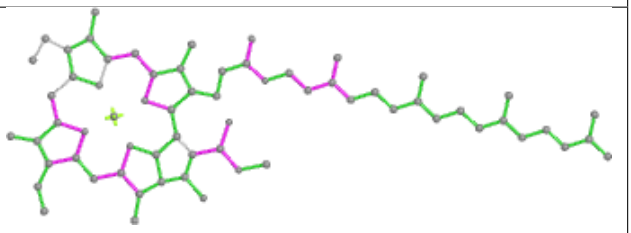


Rings

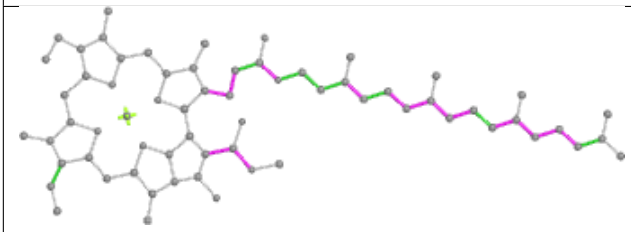
Ligand CLA c 512



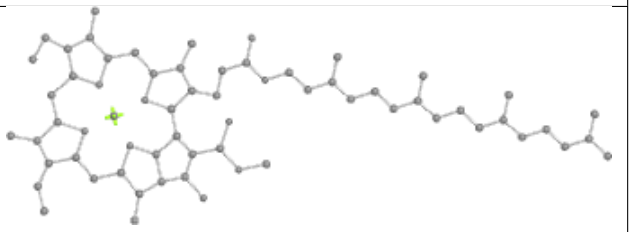
Bond lengths



Bond angles

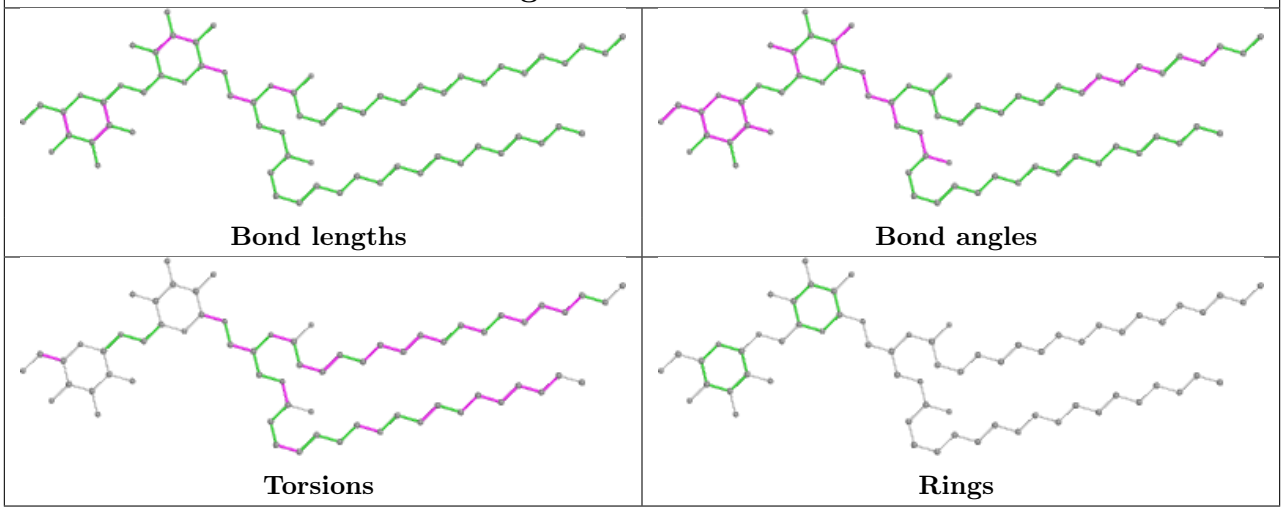


Torsions

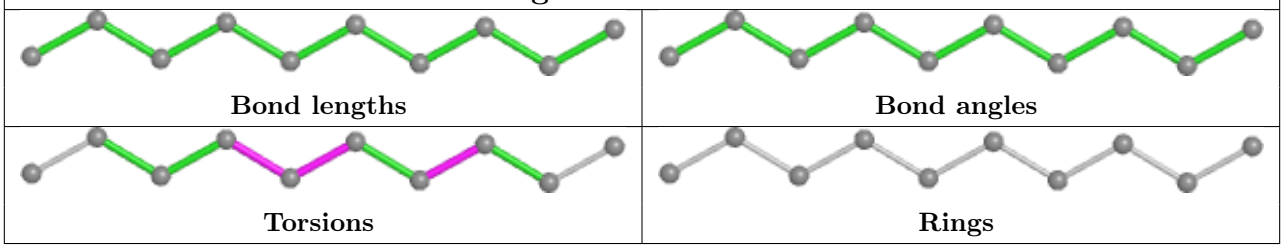


Rings

Ligand DGD A 415



Ligand STE b 625



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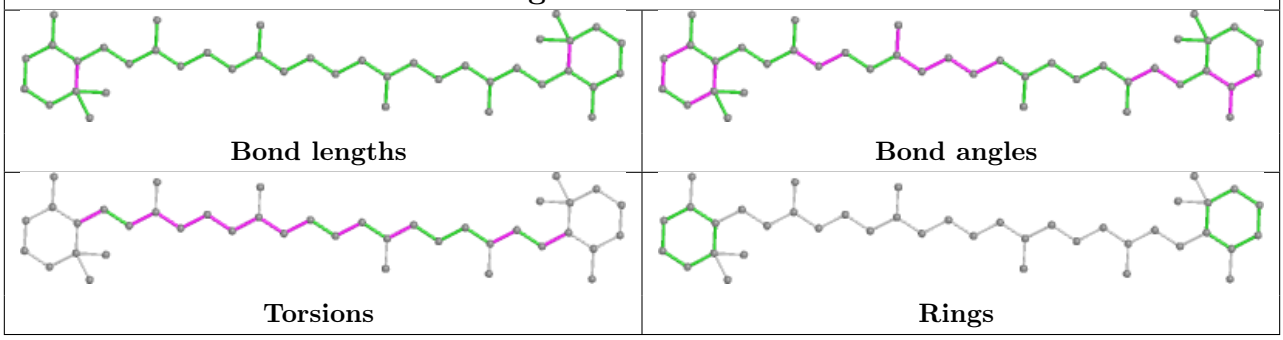

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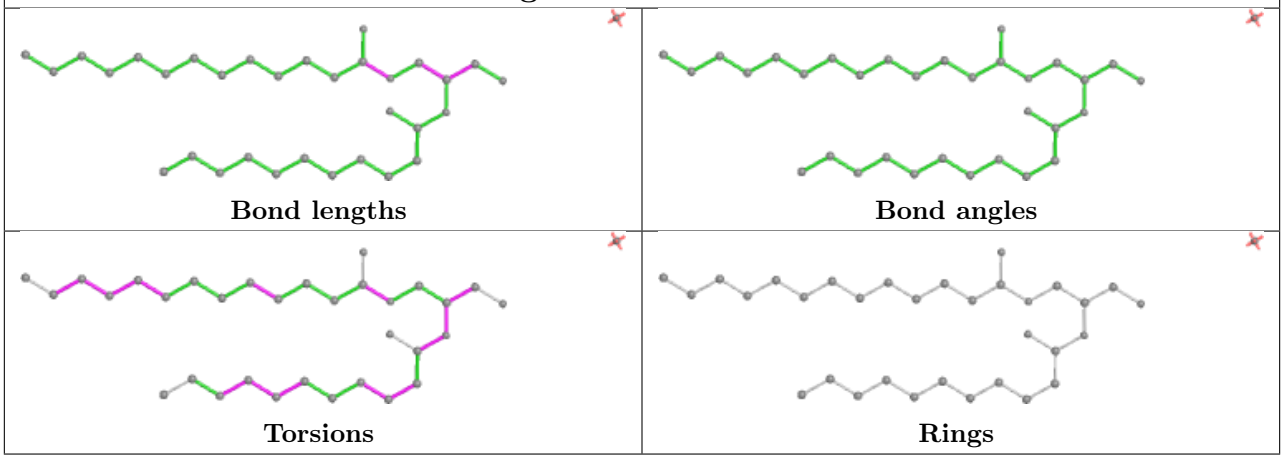

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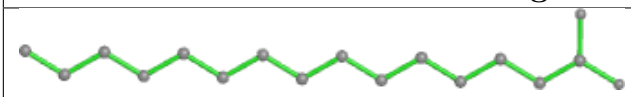
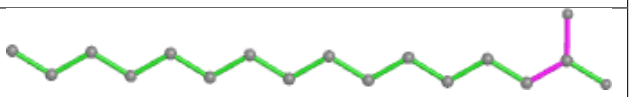
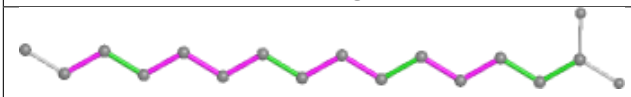


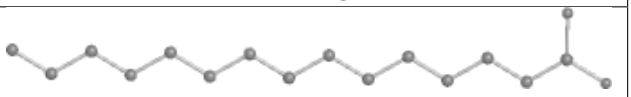
Bond lengths



Bond angles

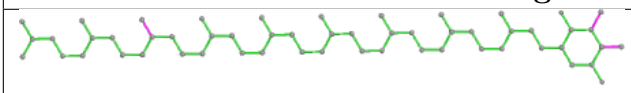


Torsions



Rings

Ligand PL9 a 410



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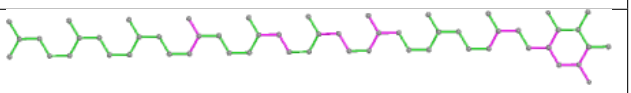
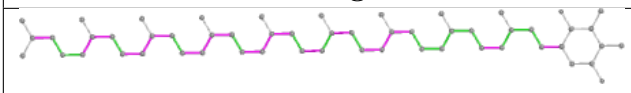


Bond angles



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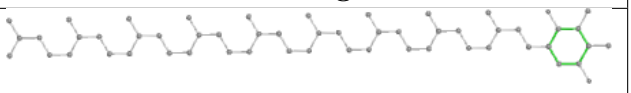
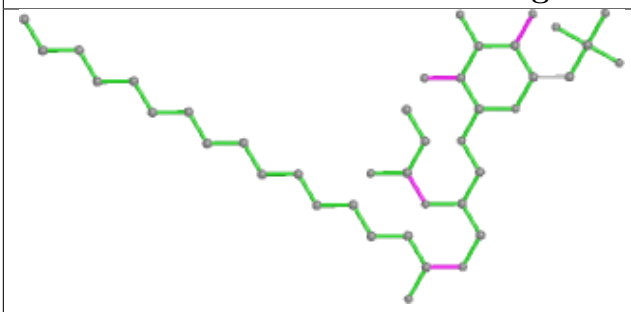
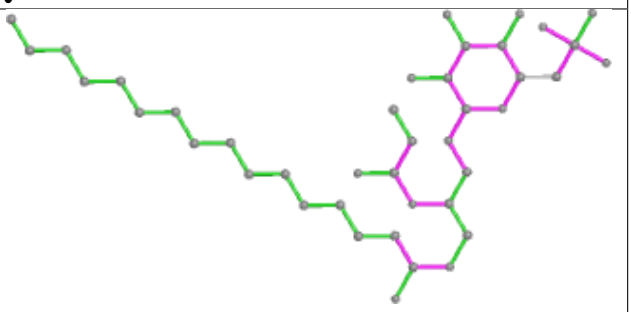


Rings

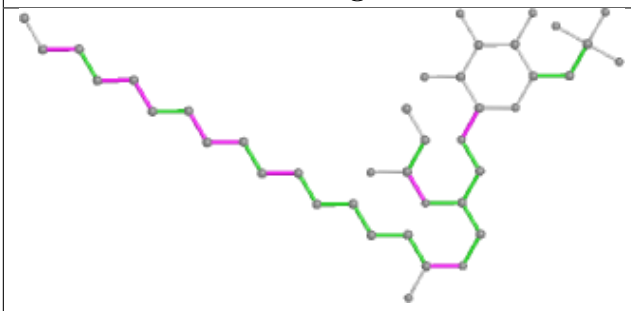
Ligand SQD f 101



Bond lengths



Bond angles



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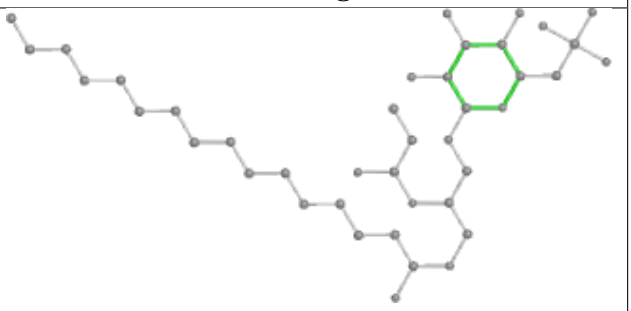
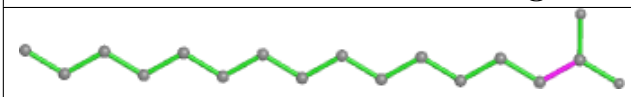
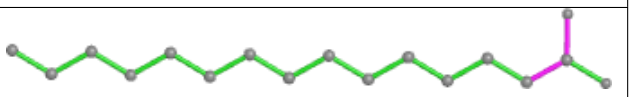


Rings

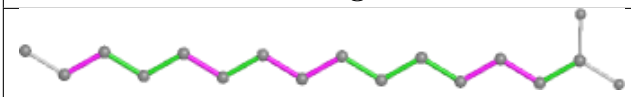
Ligand STE B 621



Bond lengths



Bond angles



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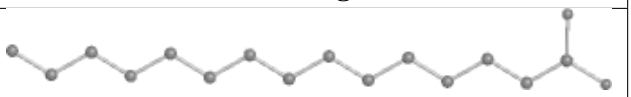
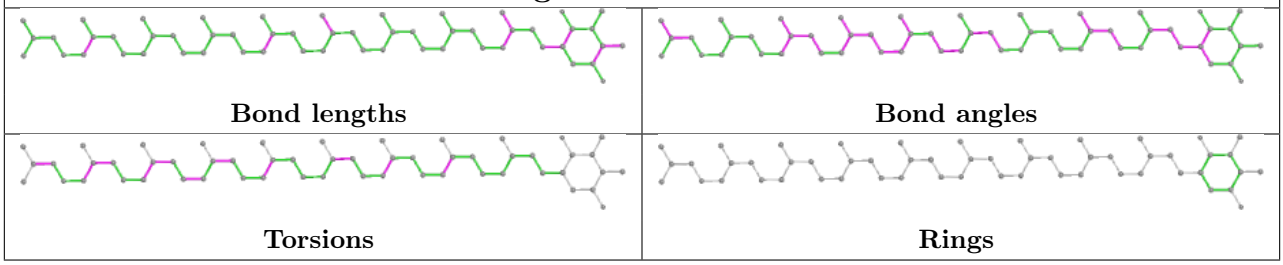
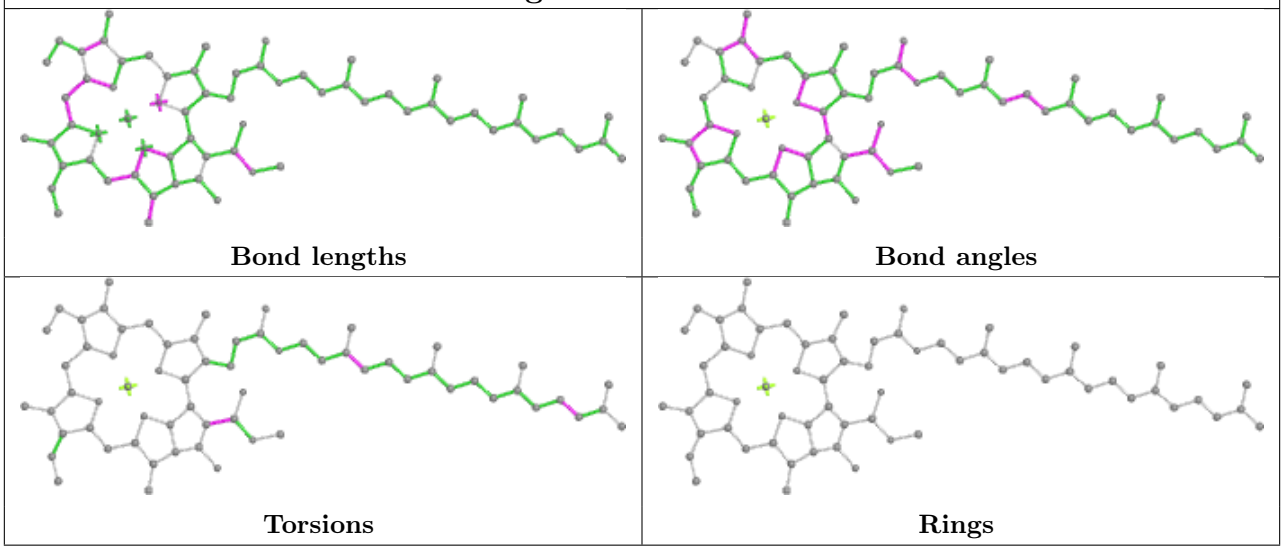


Rings

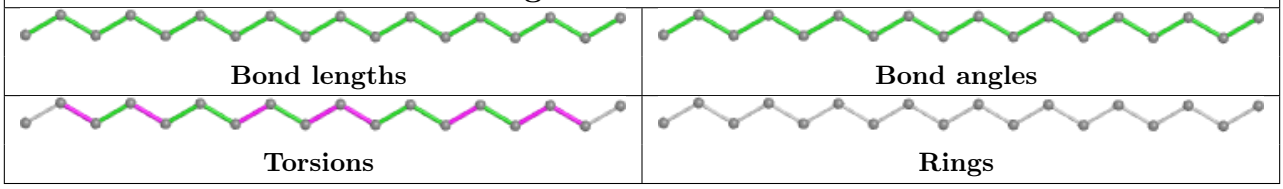
Ligand PL9 d 406



Ligand CLA B 610



Ligand STE M 104



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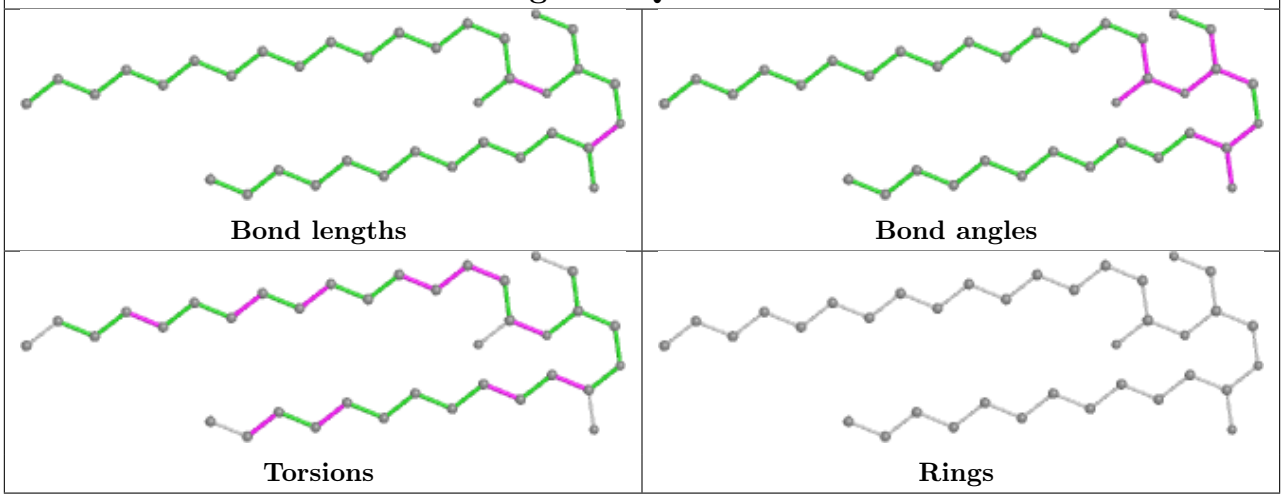

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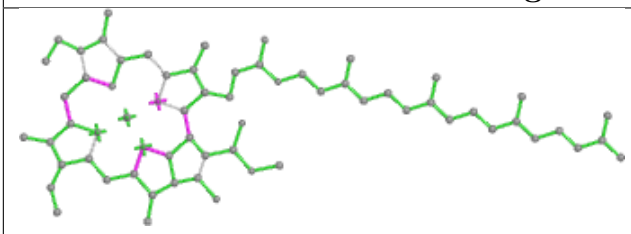
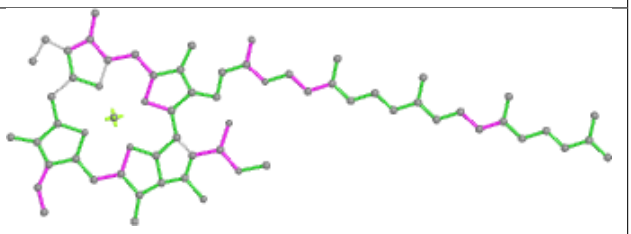
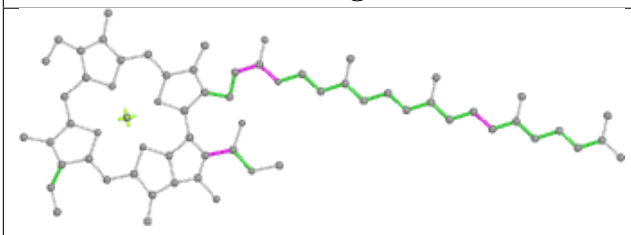


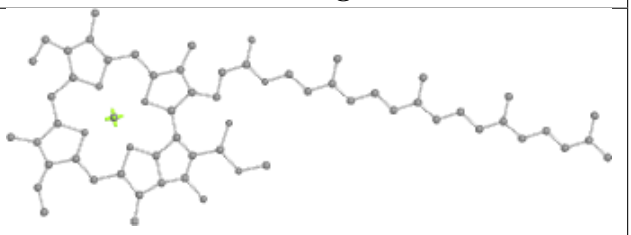
Bond lengths



Bond angles

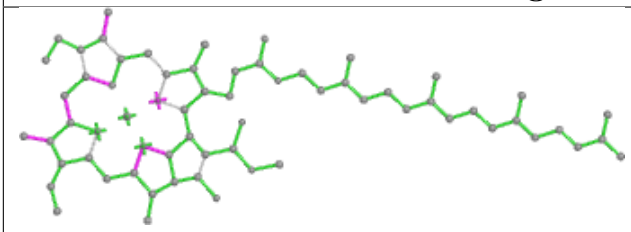


Torsions

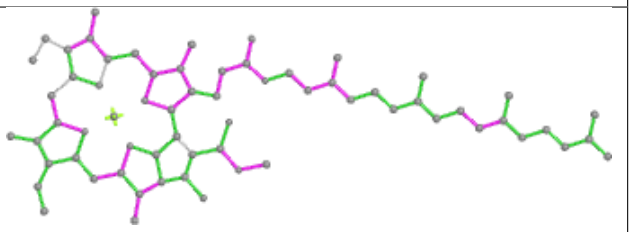


Rings

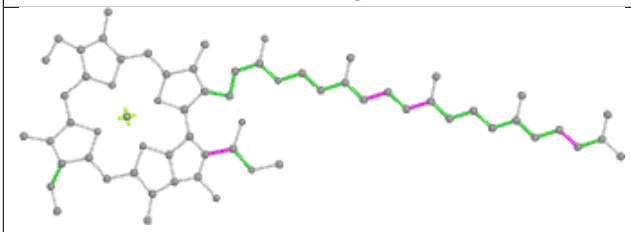
Ligand CLA b 604



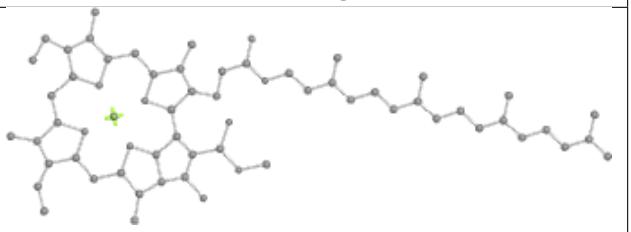
Bond lengths



Bond angles

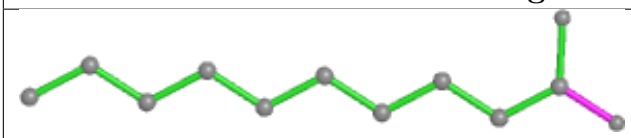


Torsions



Rings

Ligand STE B 624



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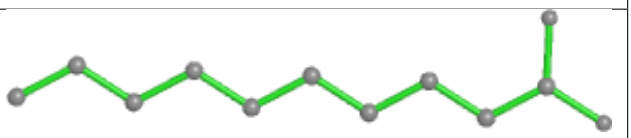
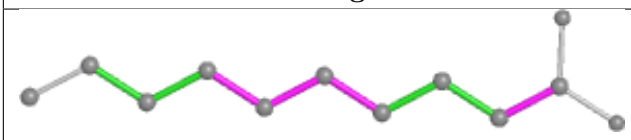


Bond angles



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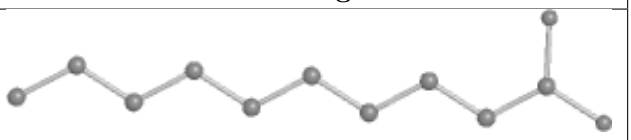

Rings

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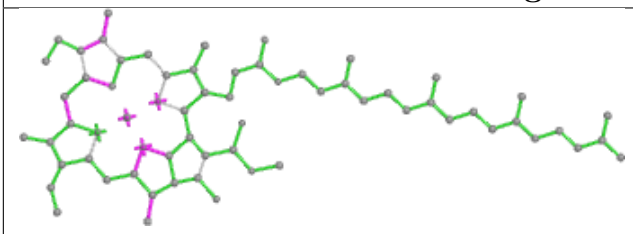

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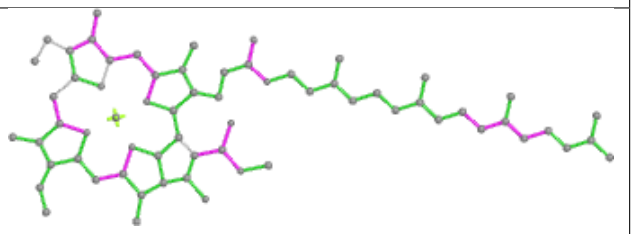
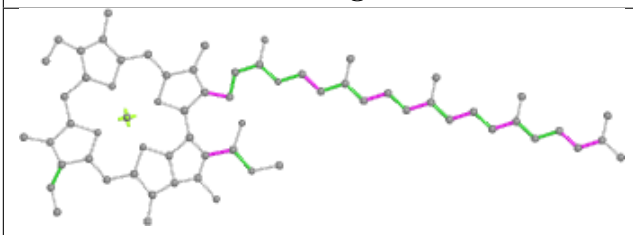


Bond angles



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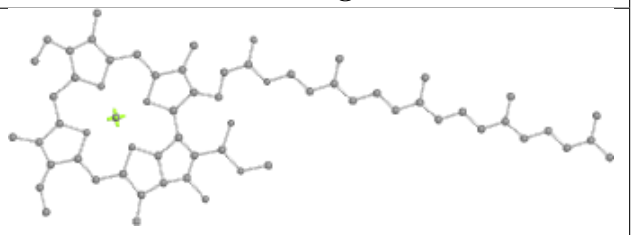
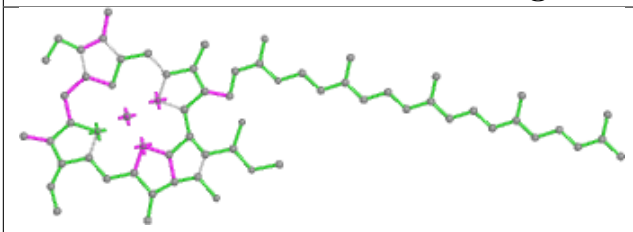


Rings

Ligand CLA c 510



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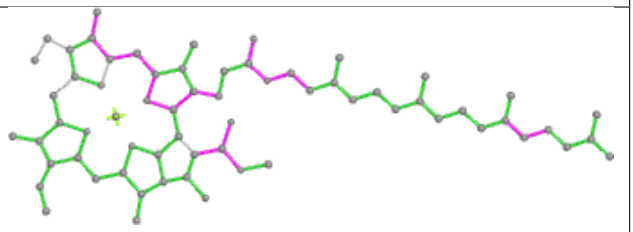
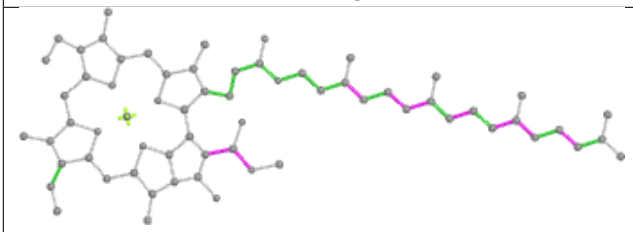


Bond angles



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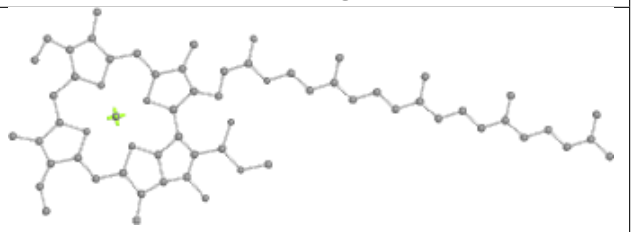
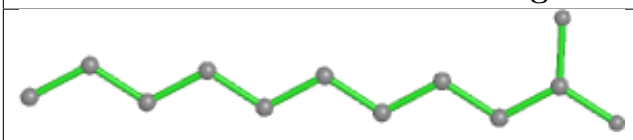


Rings

Ligand STE k 101



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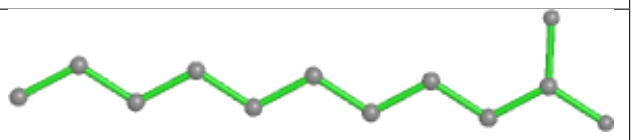
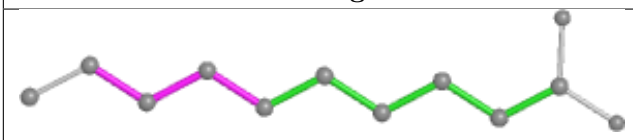


Bond angles



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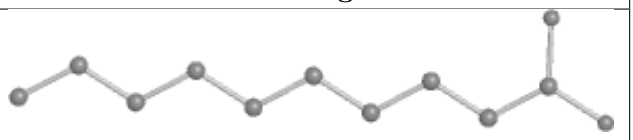

Rings

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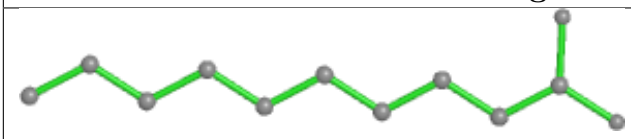
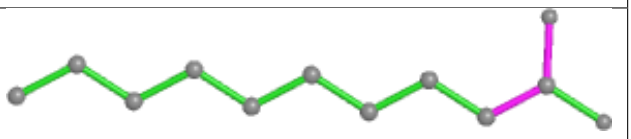
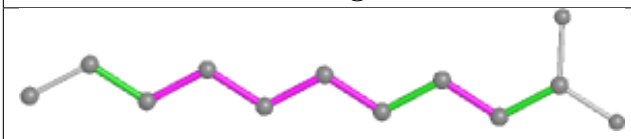


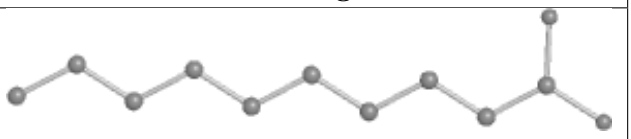
Bond lengths



Bond angles

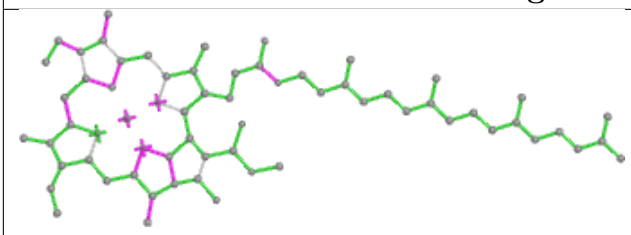


Torsions

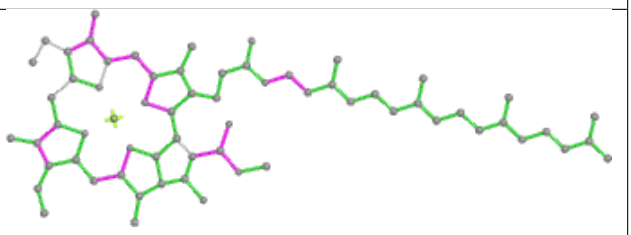


Rings

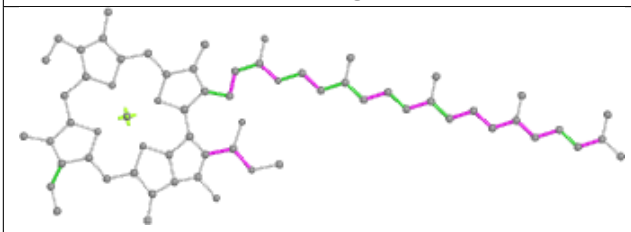
Ligand CLA b 601



Bond lengths



Bond angles



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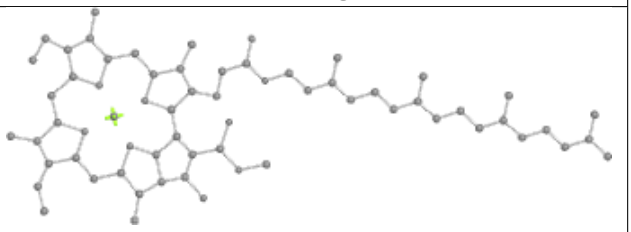
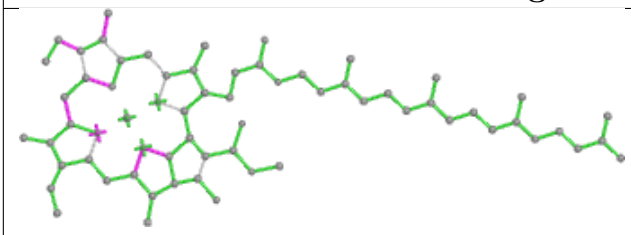
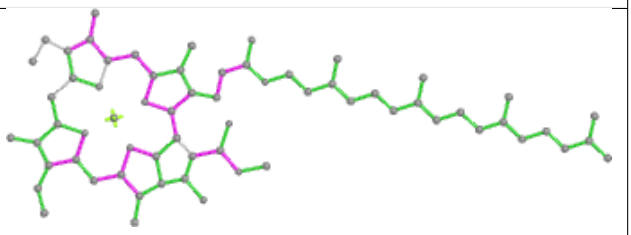


Rings

Ligand CLA a 403



Bond lengths



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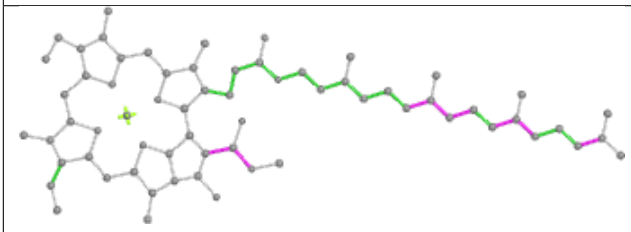

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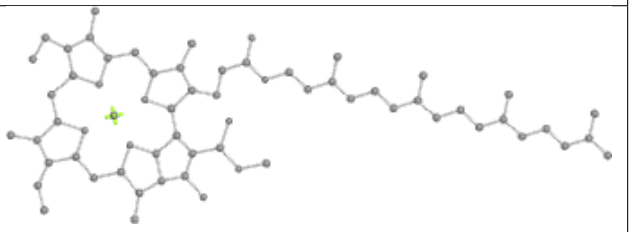
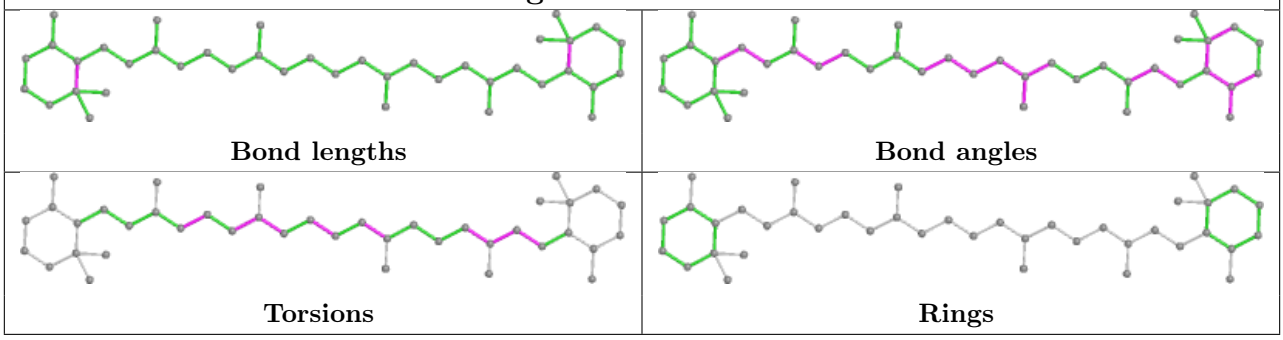
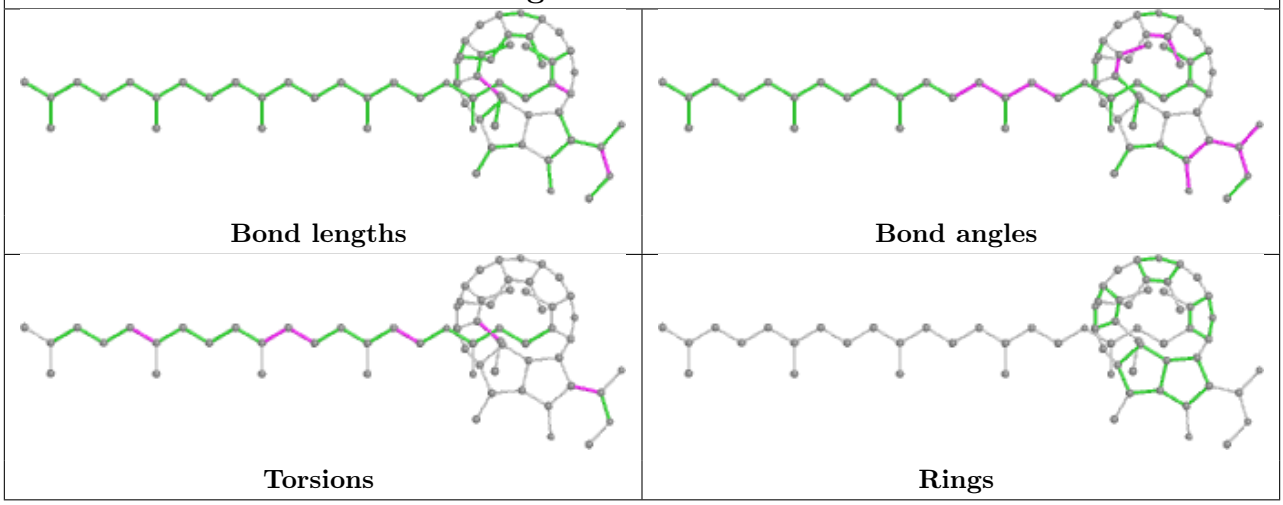


Rings

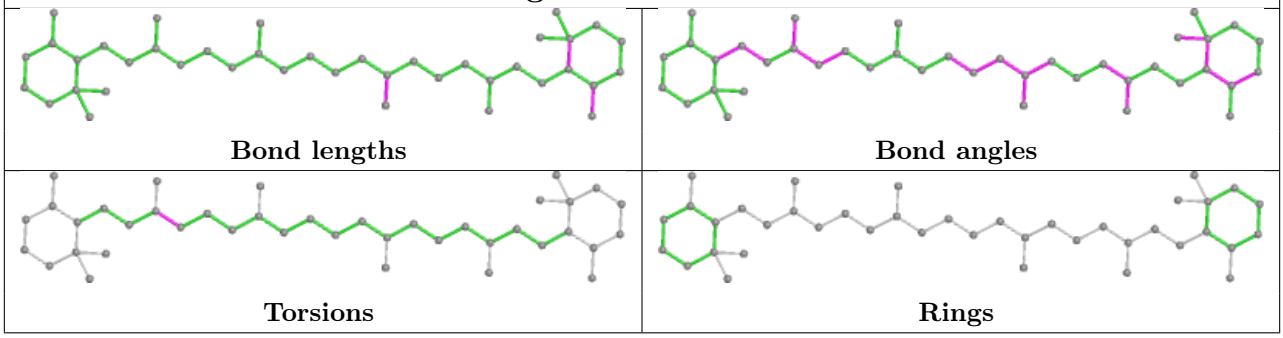
Ligand BCR b 619



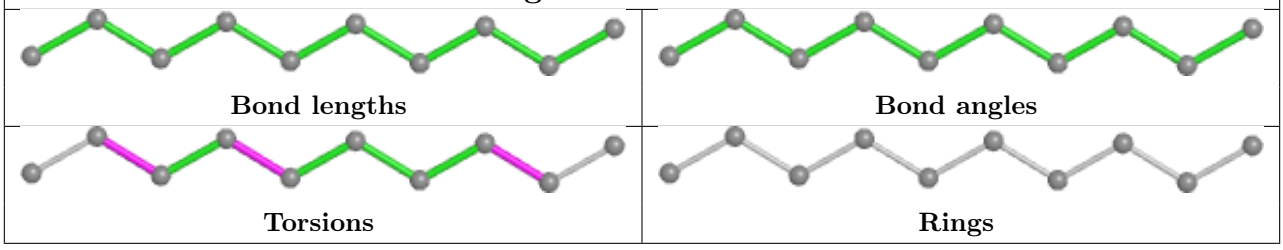
Ligand PHO a 404



Ligand BCR b 618



Ligand STE M 103



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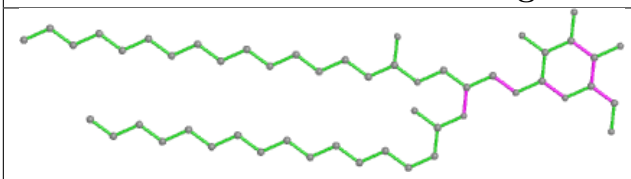
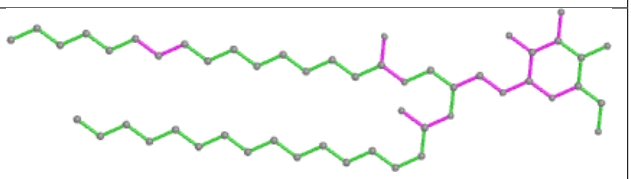
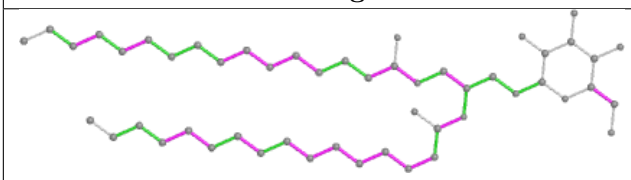


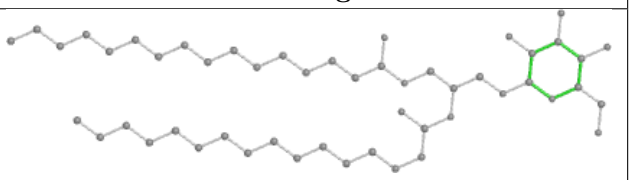
Bond lengths



Bond angles

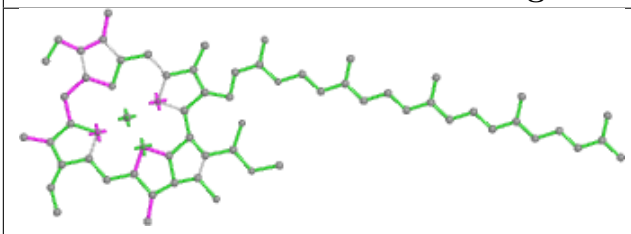


Torsions



Rings

Ligand CLA b 615



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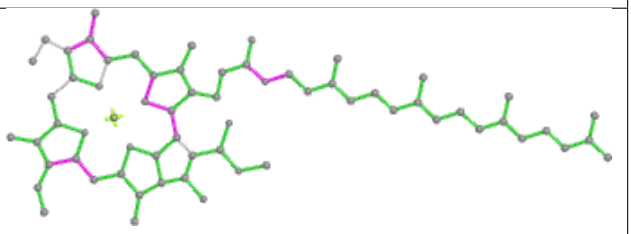
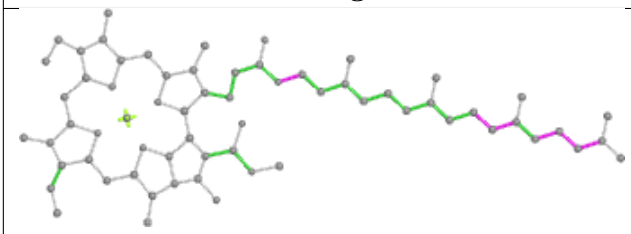


Bond angles



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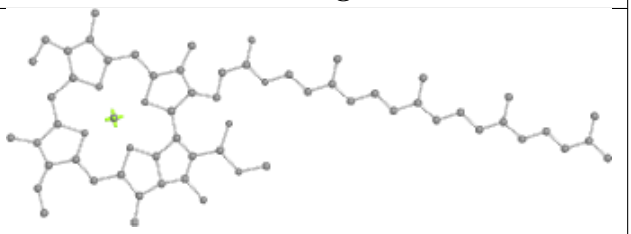
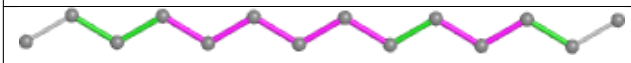


Rings

Ligand STE h 102

Bond lengths

Bond angles



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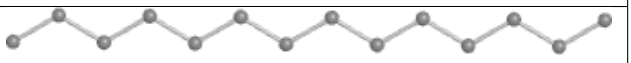
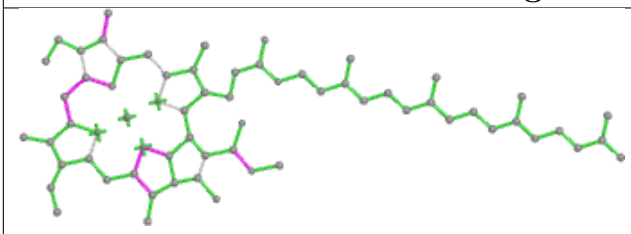


Rings

Ligand CLA C 510



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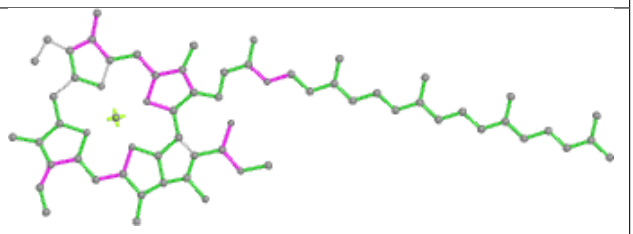

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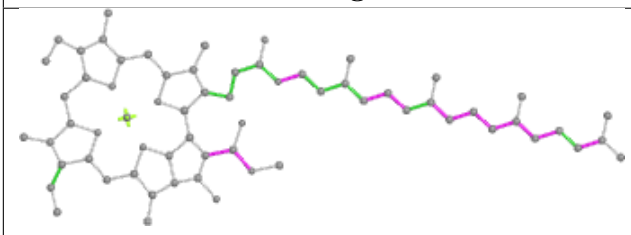

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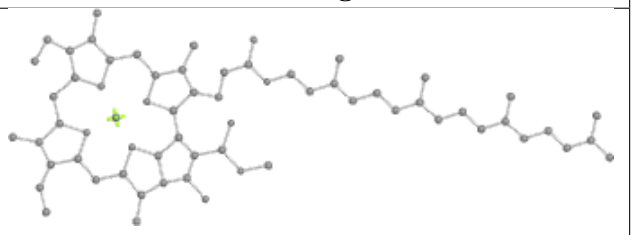
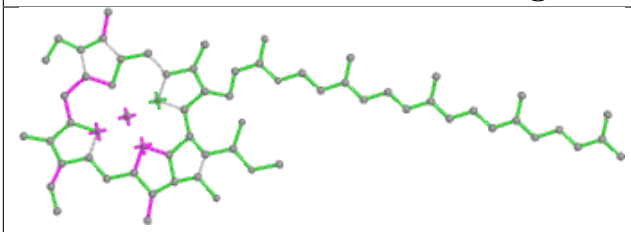


Rings

Ligand CLA c 506



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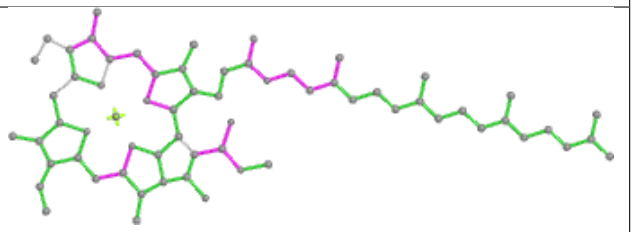
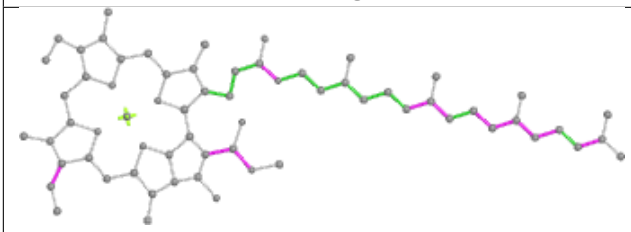


Bond angles



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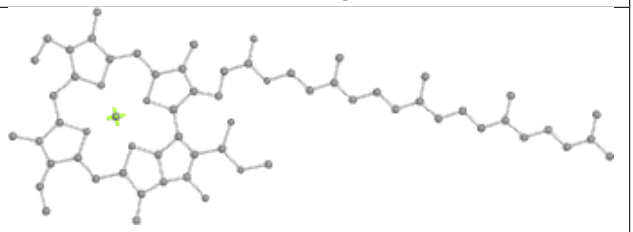
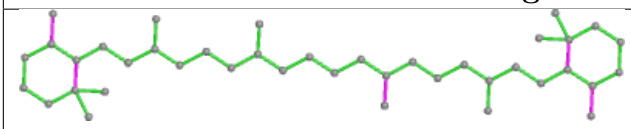


Rings

Ligand BCR C 515



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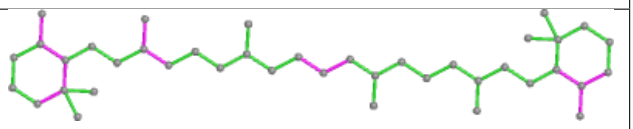

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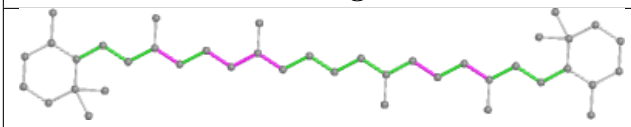
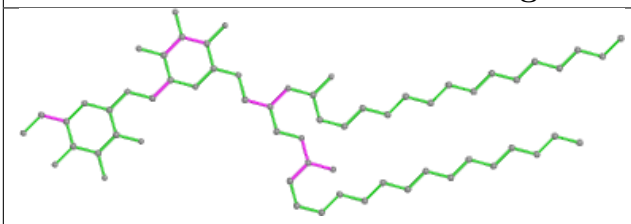


Torsions

Rings

Ligand DGD C 517



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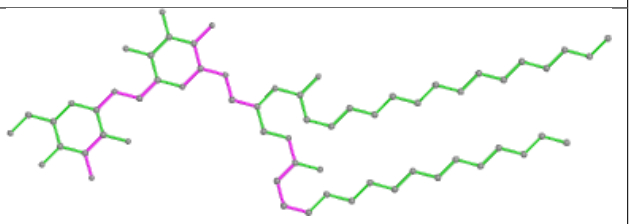

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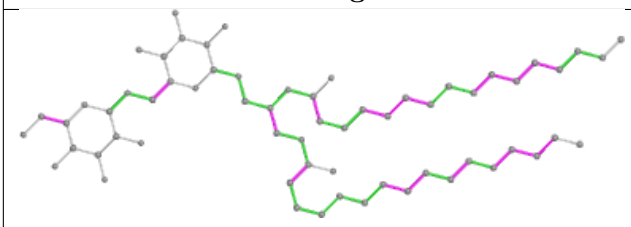

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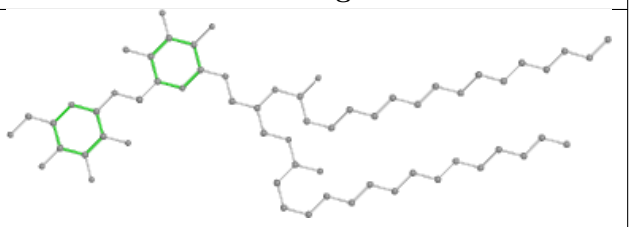
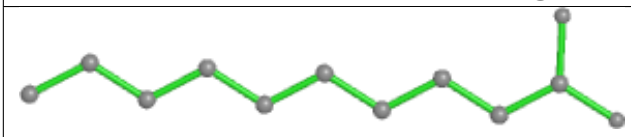


Rings

Ligand STE a 414



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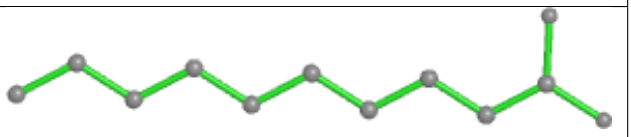

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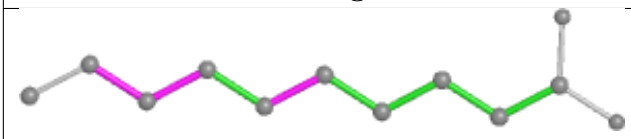

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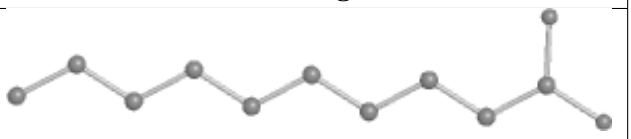
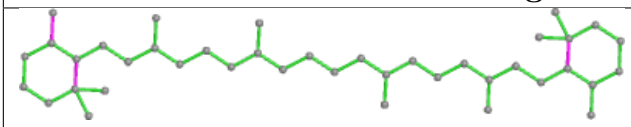


Rings

Ligand BCR b 617



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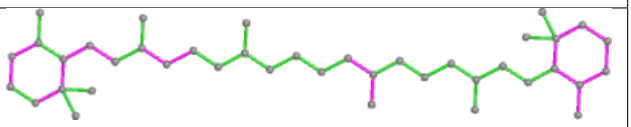
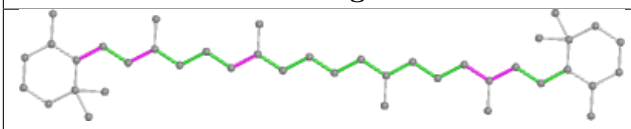


Bond angles



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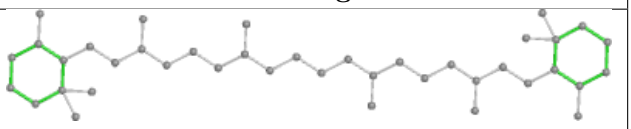
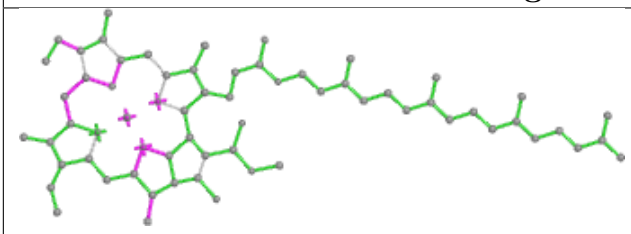
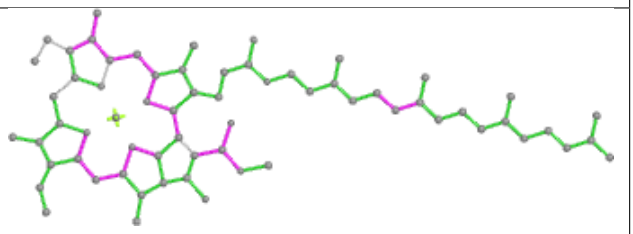
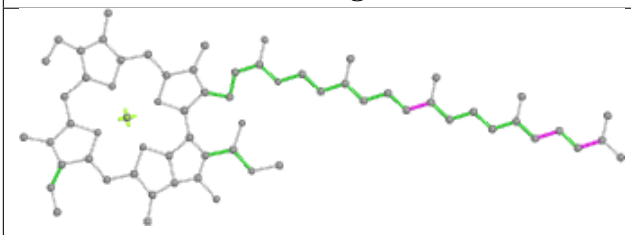
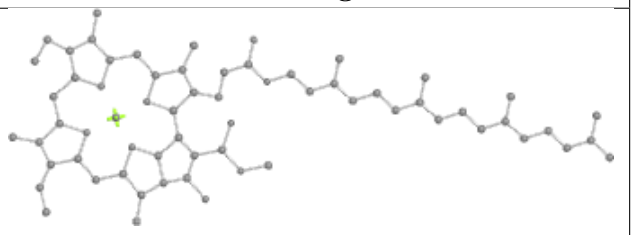
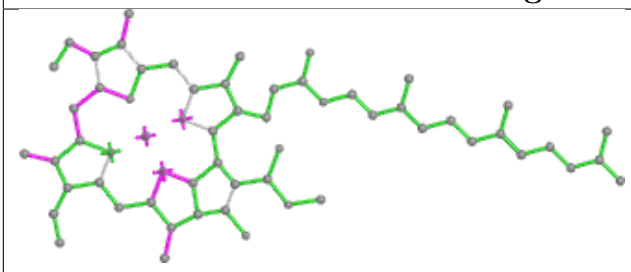
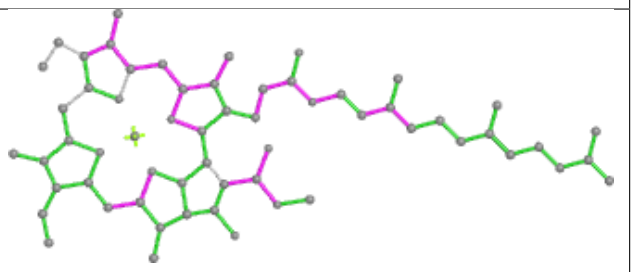
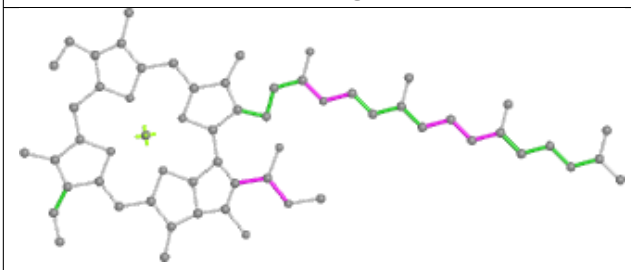
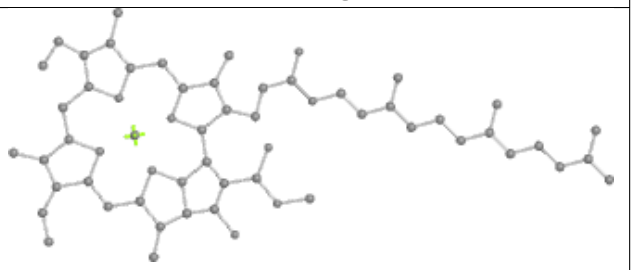
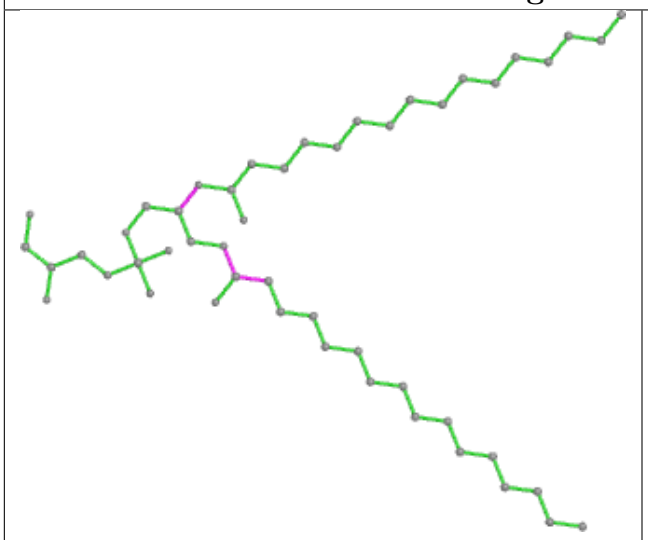


Rings

Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 407



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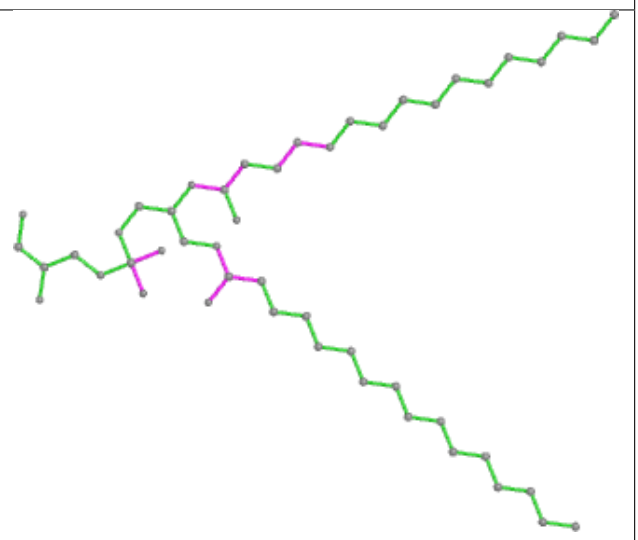
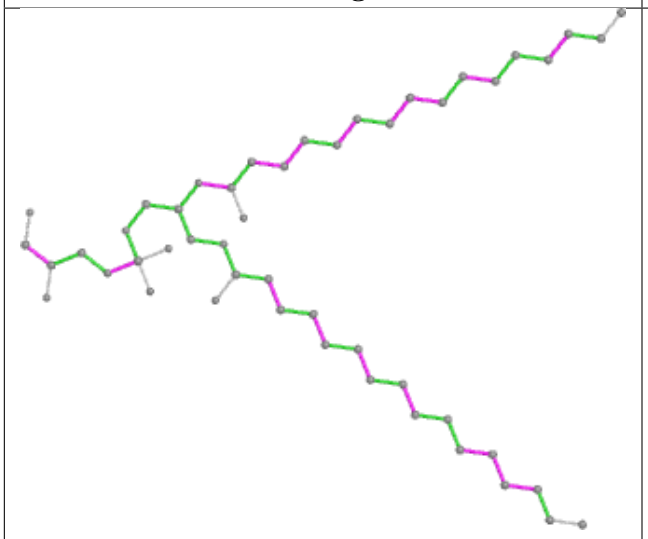
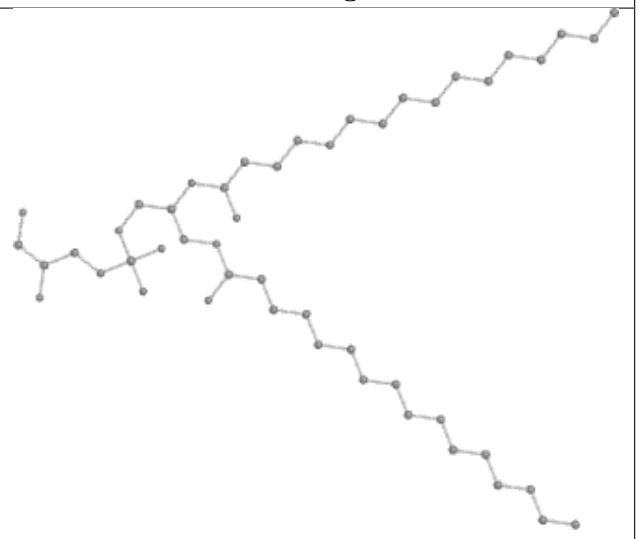


Bond angles

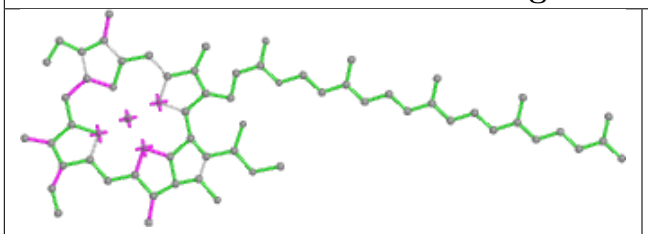


Torsions



Rings

Ligand CLA a 405



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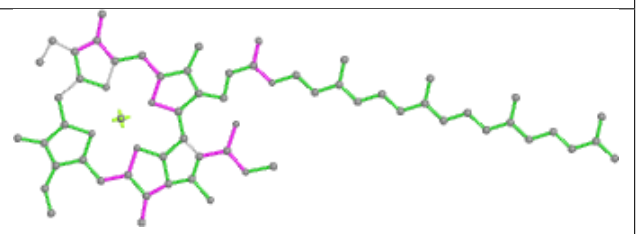

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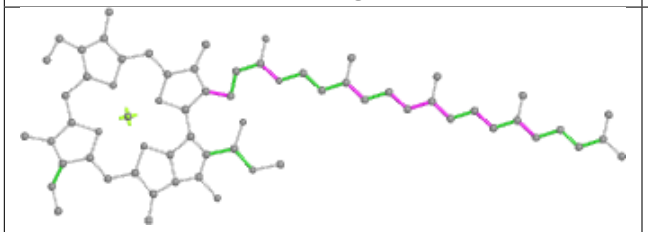

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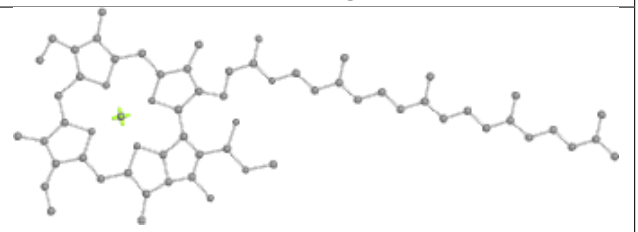
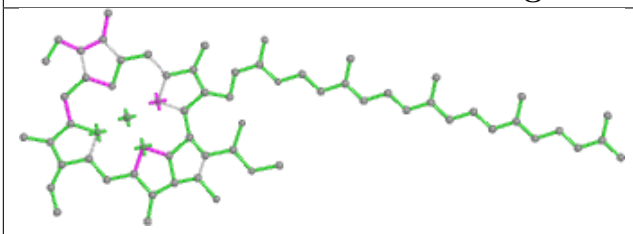


Rings

Ligand CLA B 607



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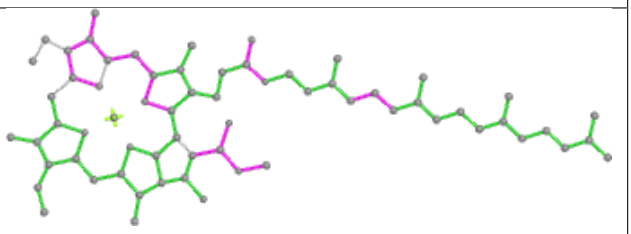

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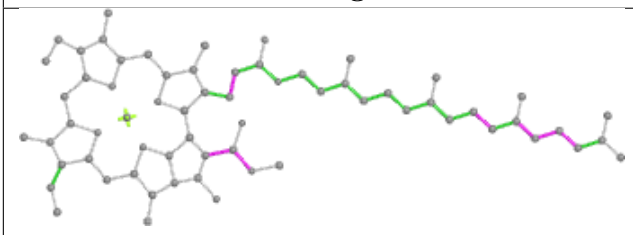

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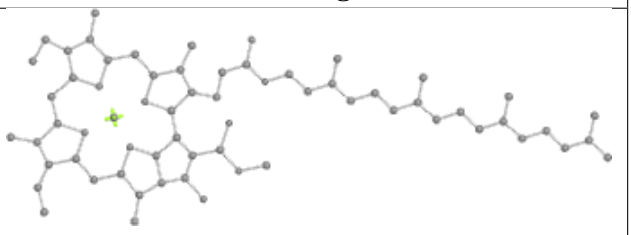
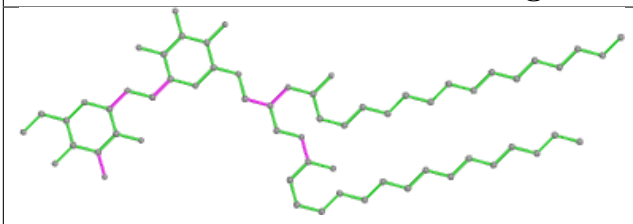


Rings

Ligand DGD c 516



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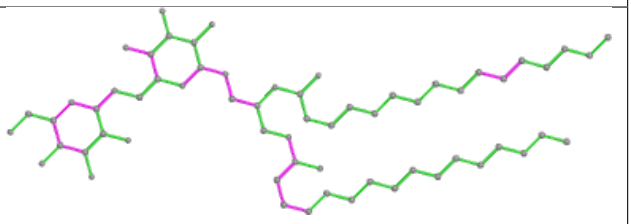
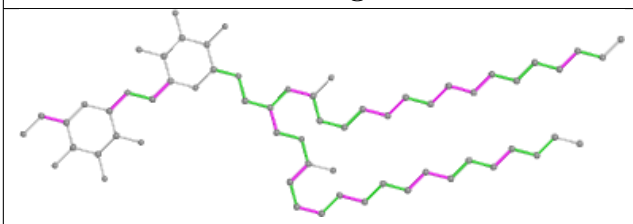


Bond angles



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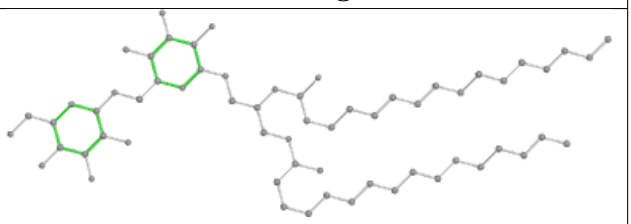
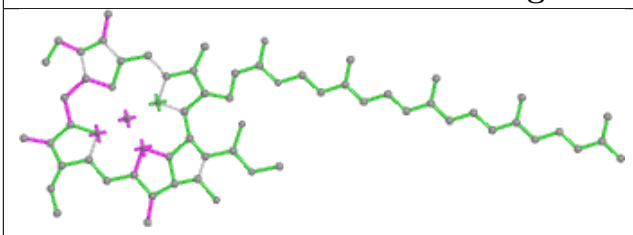


Rings

Ligand CLA d 404



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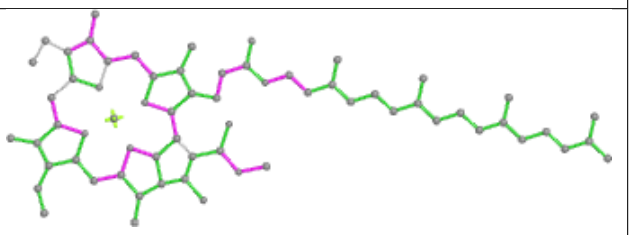

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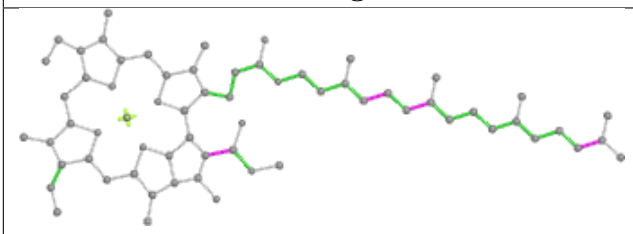

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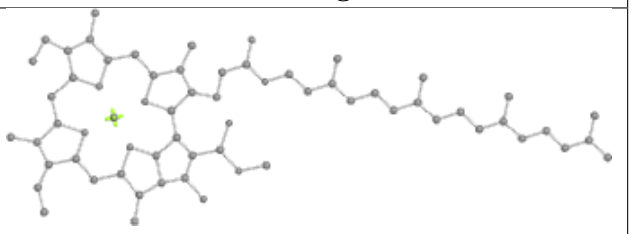
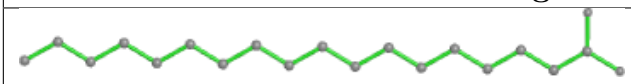


Rings

Ligand STE c 520



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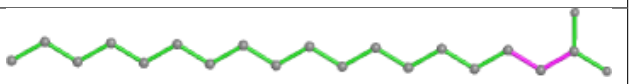

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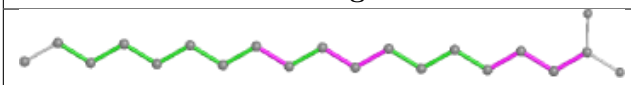

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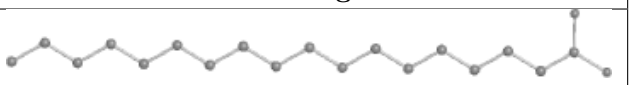
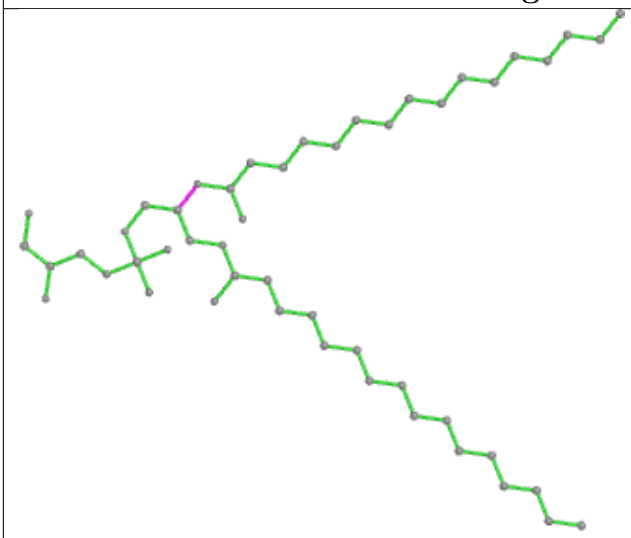


Rings

Ligand LHG D 408



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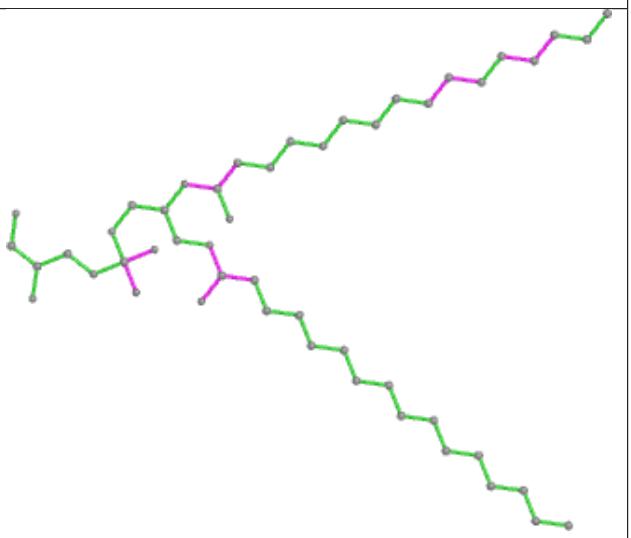

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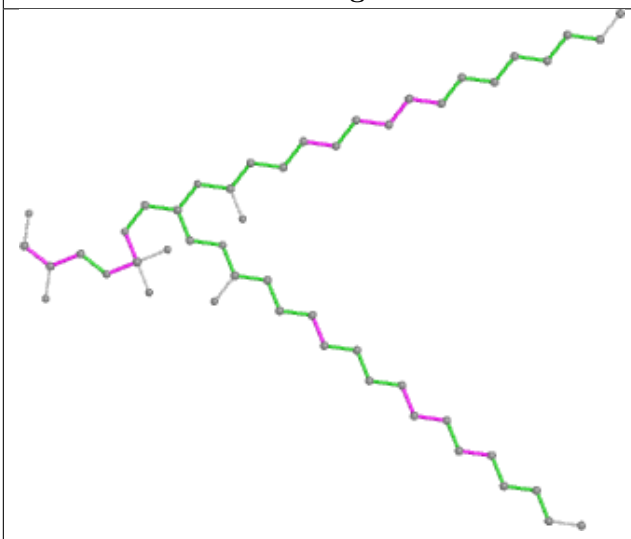

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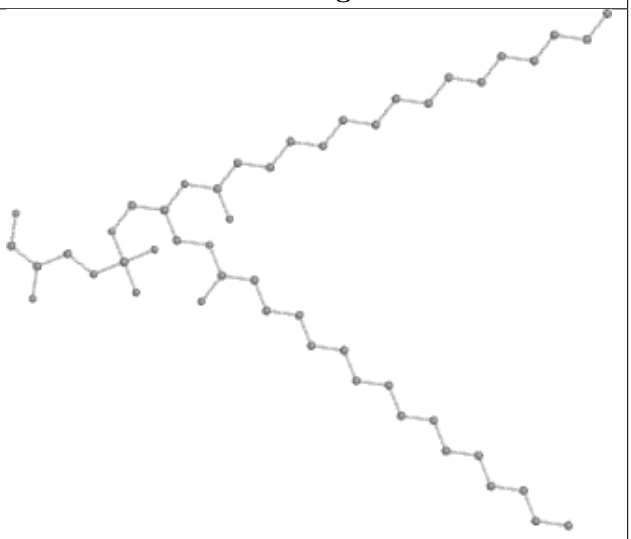
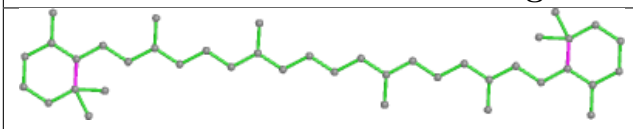


Rings

Ligand BCR x 101



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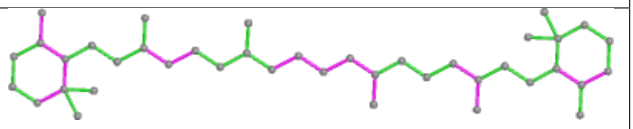

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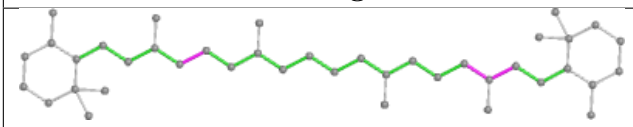

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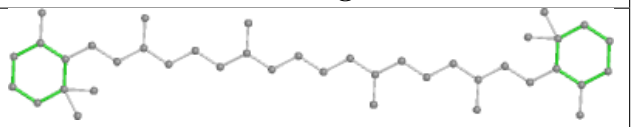

Rings

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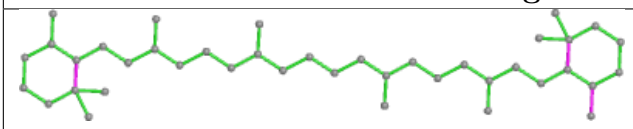

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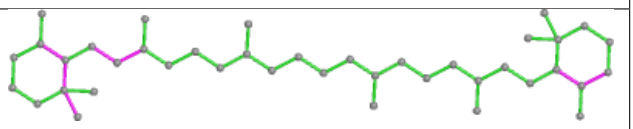
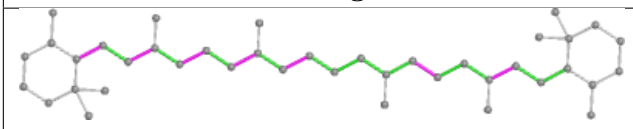


Bond angles



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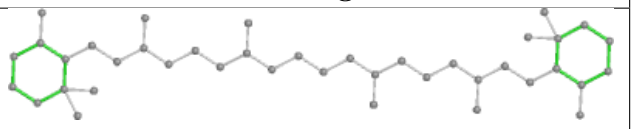
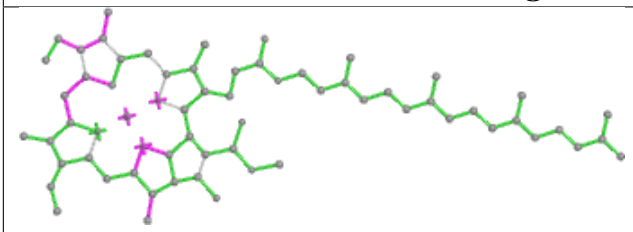


Rings

Ligand CLA C 514



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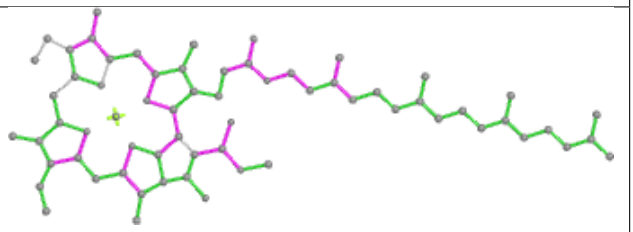

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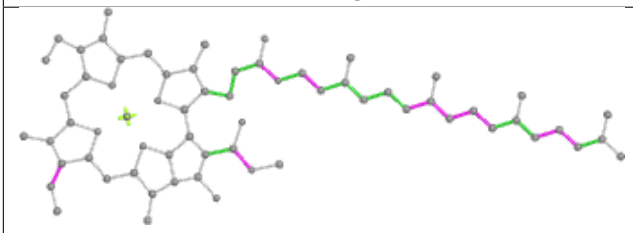

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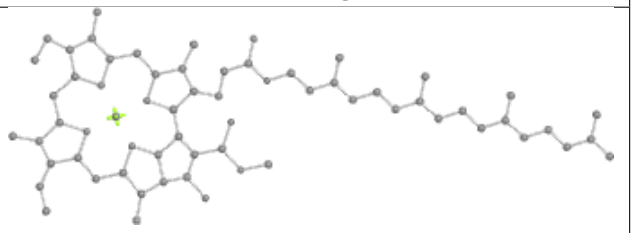

Rings

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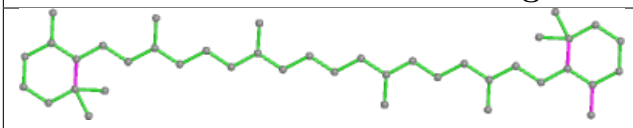

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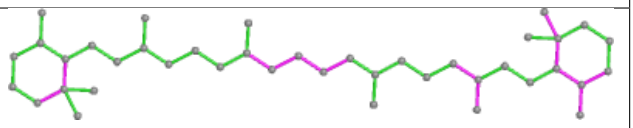

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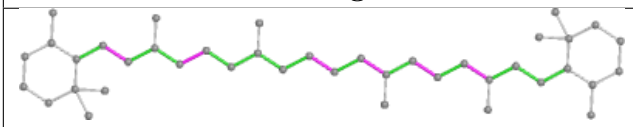
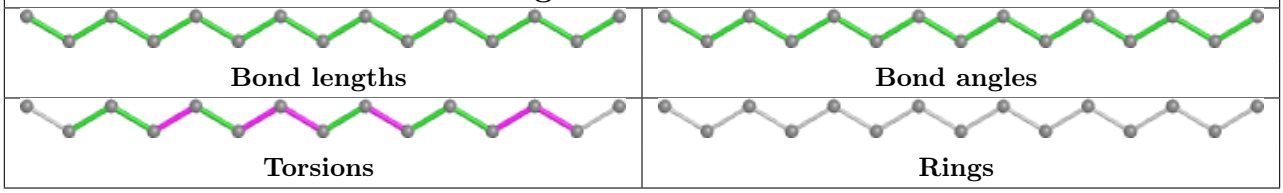


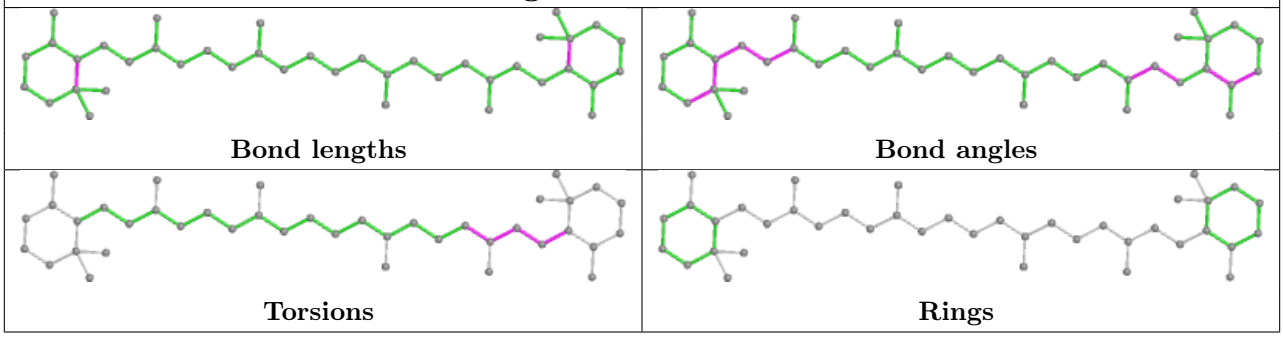
Torsions

Rings

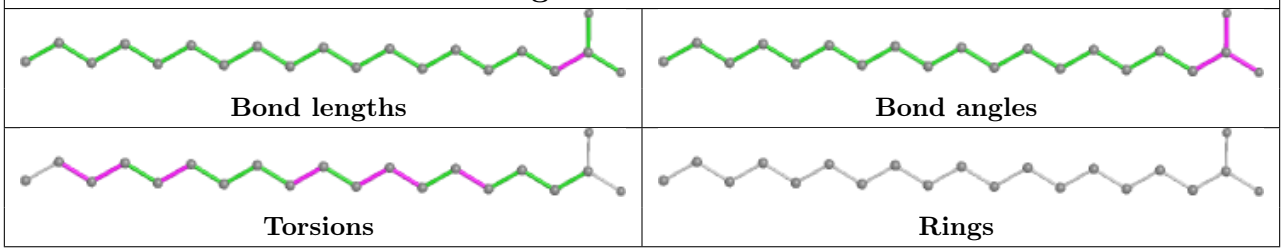
Ligand STE I 101



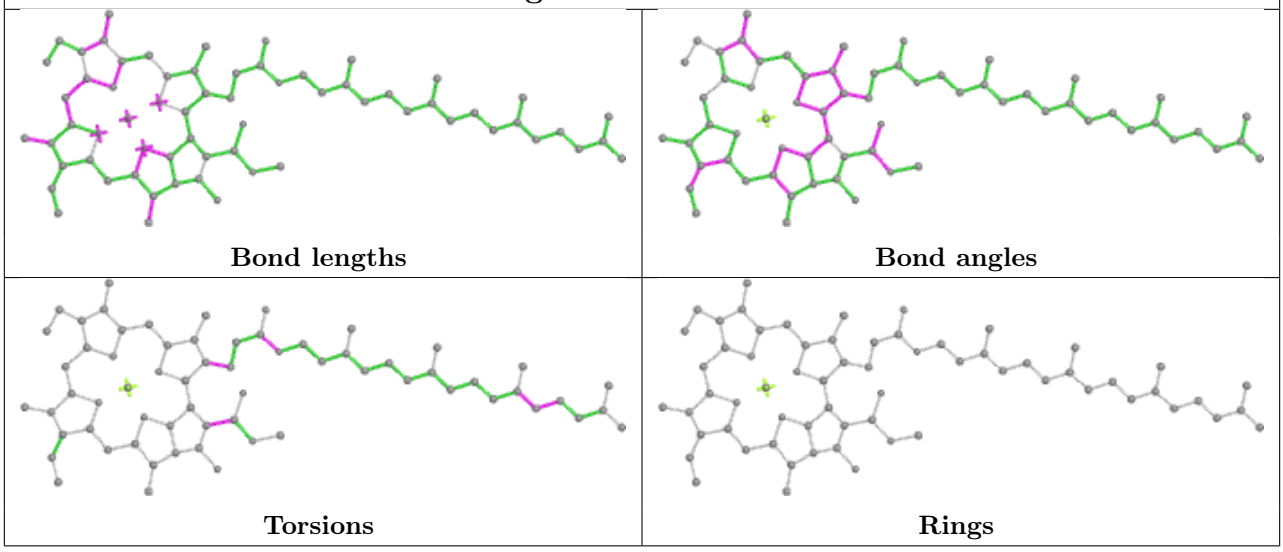
Ligand BCR D 405



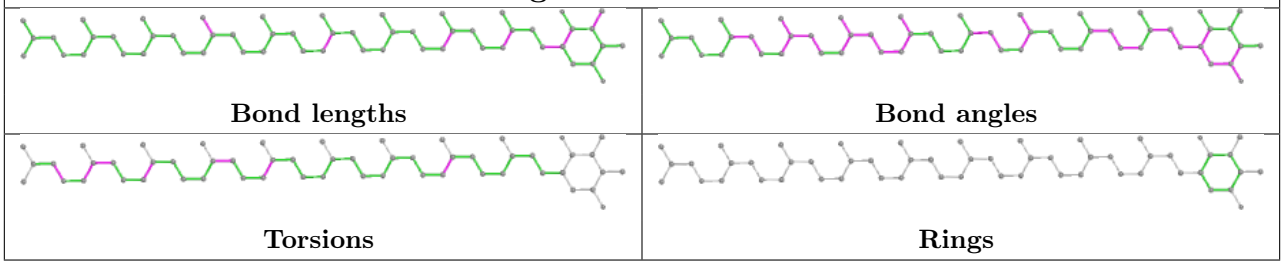
Ligand STE b 621



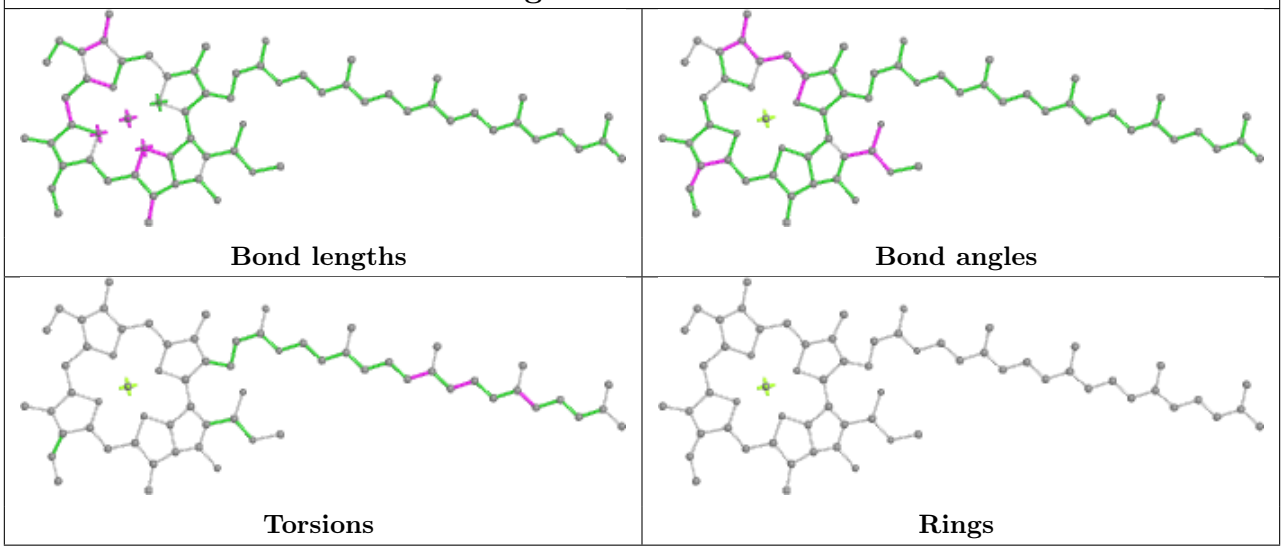
Ligand CLA C 503



Ligand PL9 D 406



Ligand CLA A 403



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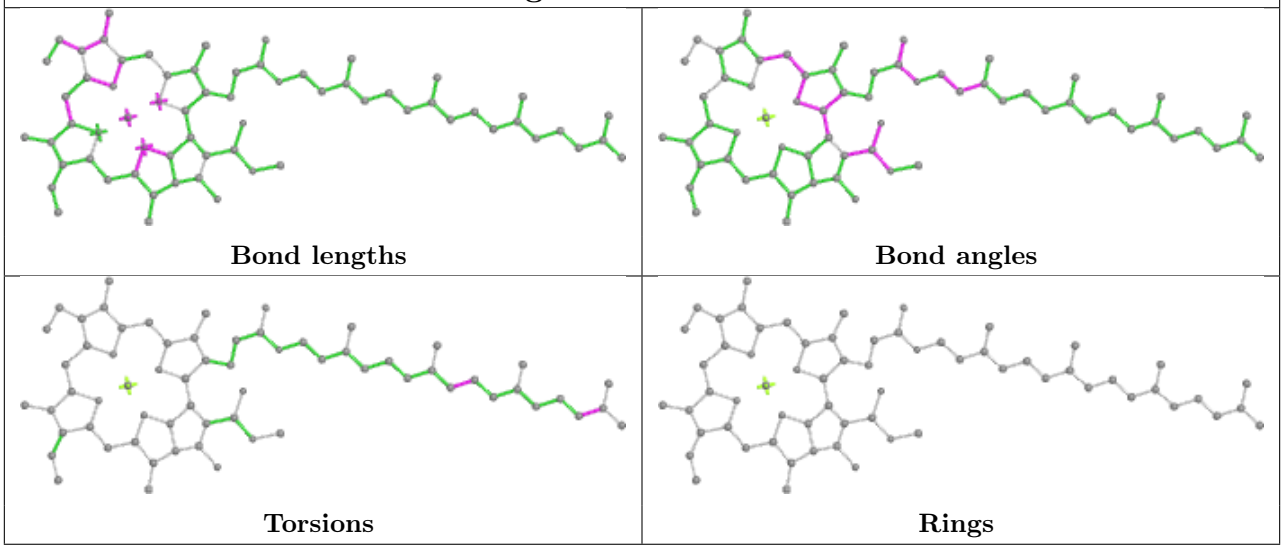
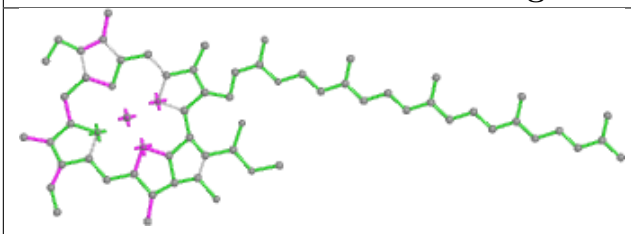
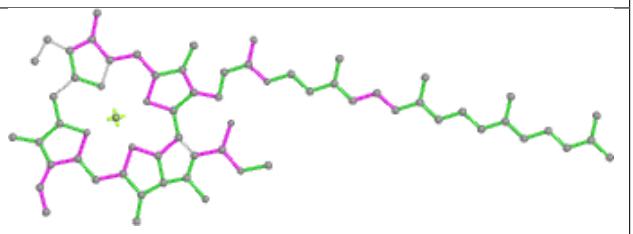


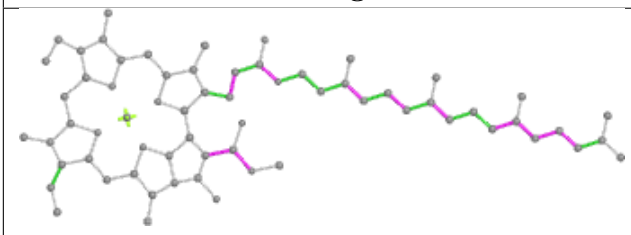
Ligand CLA b 614



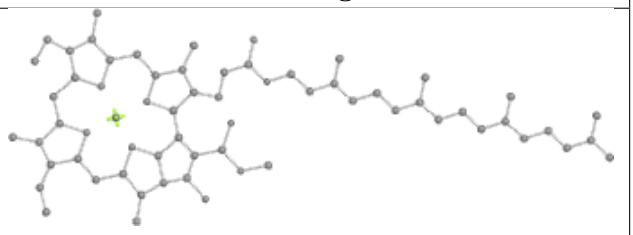
Bond lengths



Bond angles

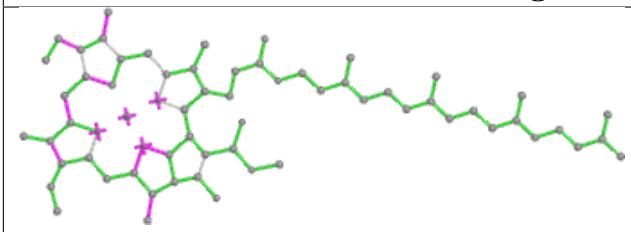


Torsions



Rings

Ligand CLA c 511



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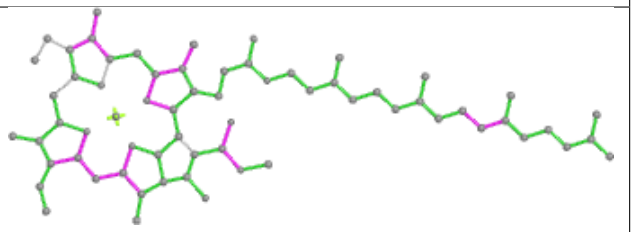

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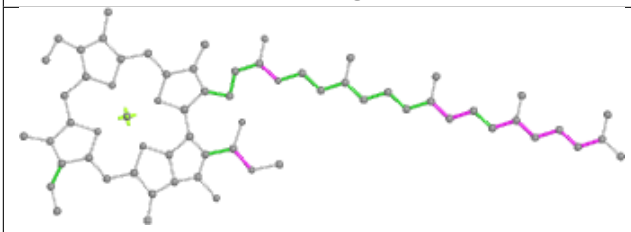

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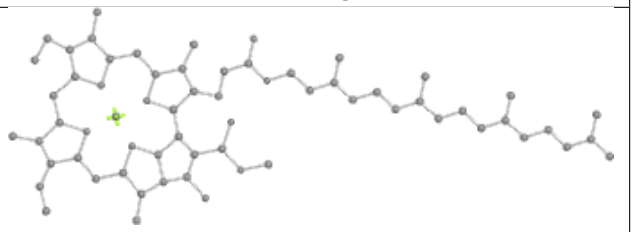
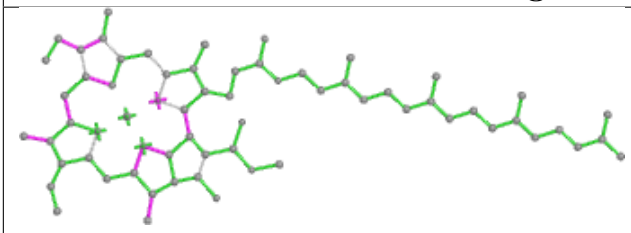


Rings

Ligand CLA b 603



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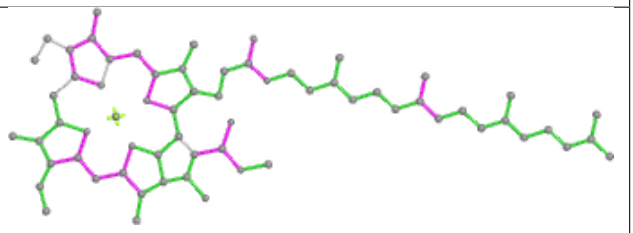
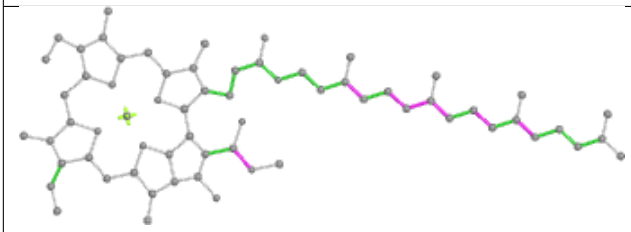


Bond angles



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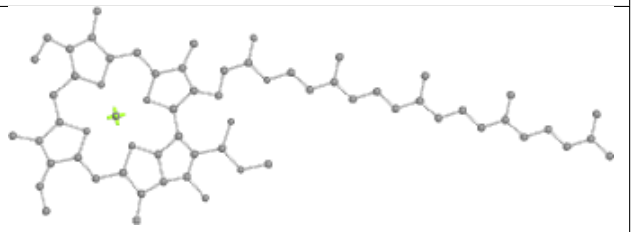
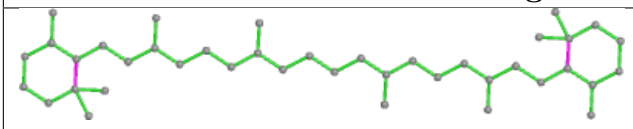


Rings

Ligand BCR d 405



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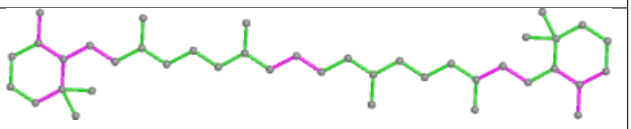
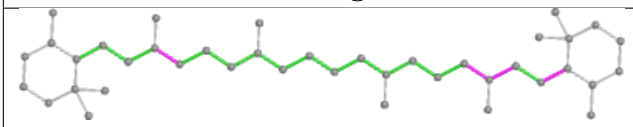


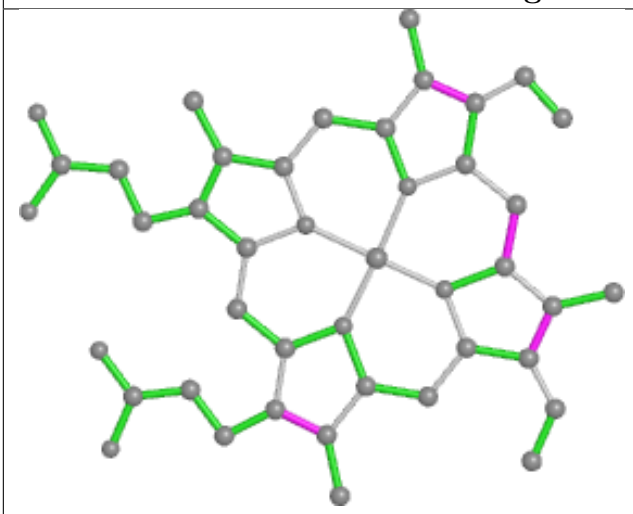
Bond angles



Torsions

Rings

Ligand HEC E 101



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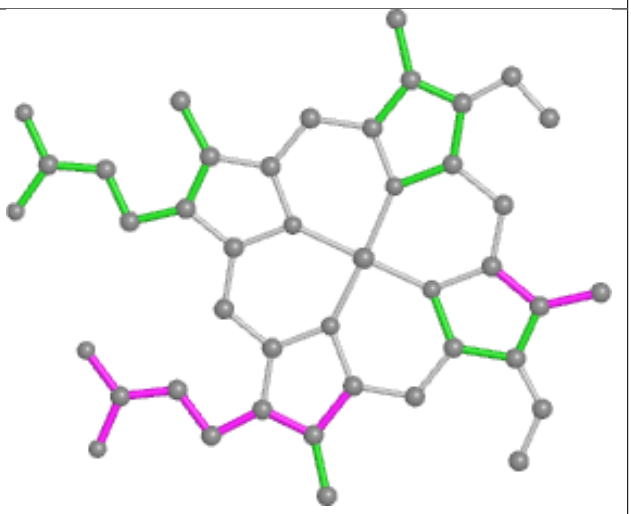
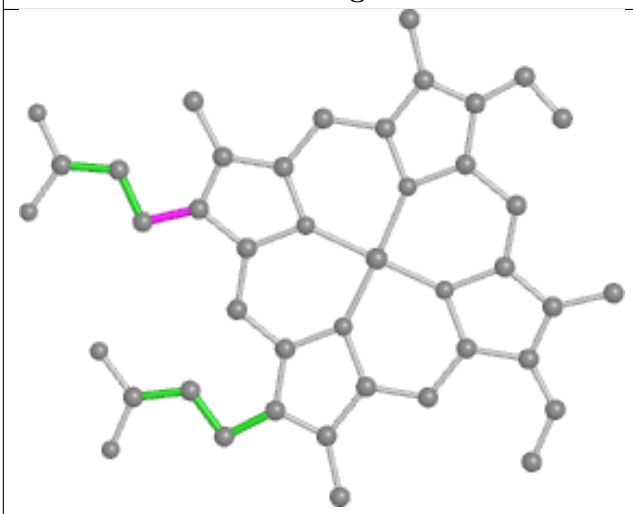
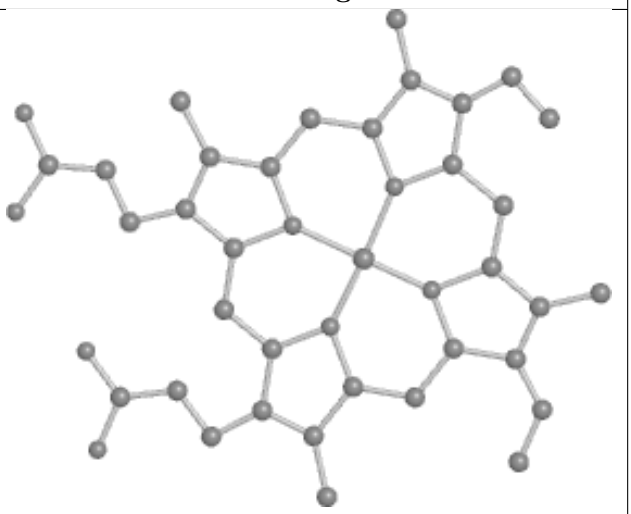


Bond angles

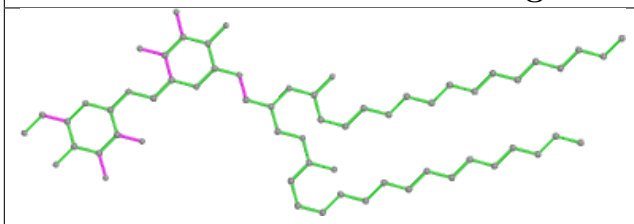


Torsions



Rings

Ligand DGD c 517



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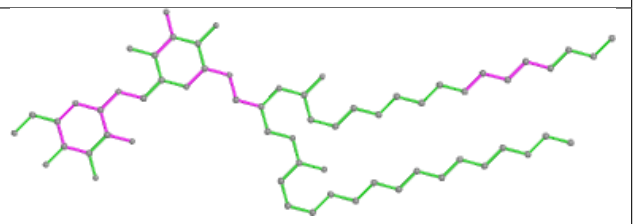
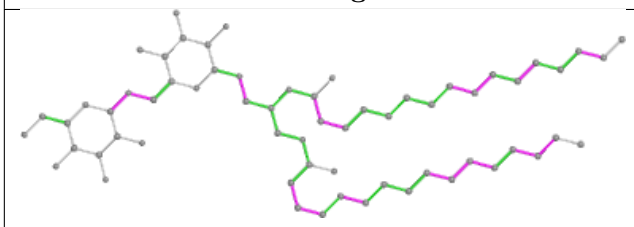


Bond angles



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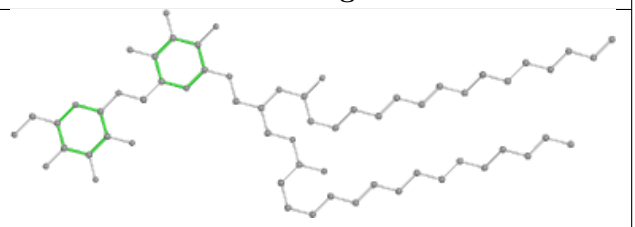
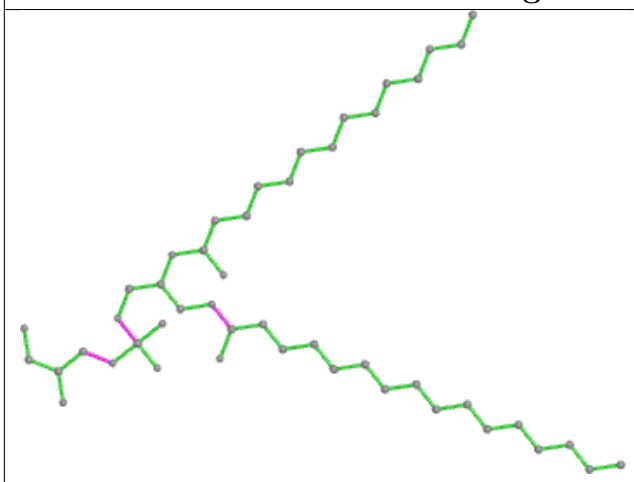


Rings

Ligand LHG A 411



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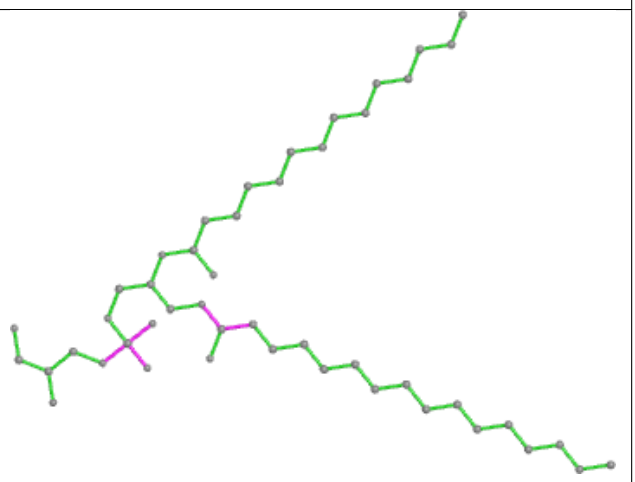
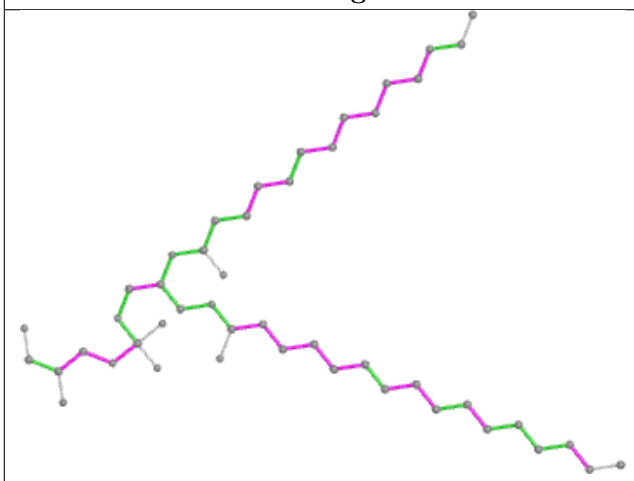


Bond angles



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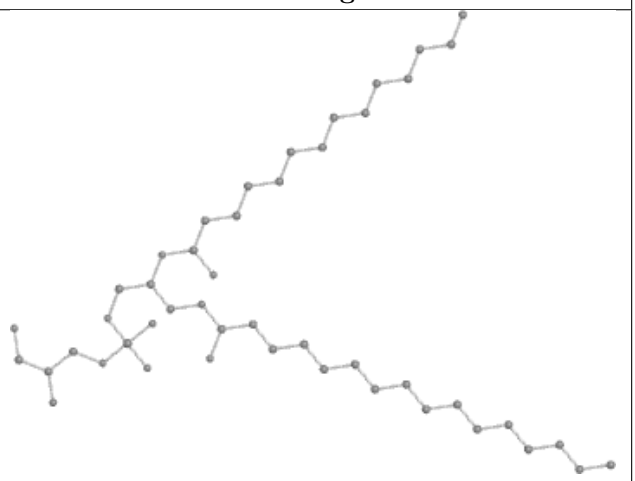
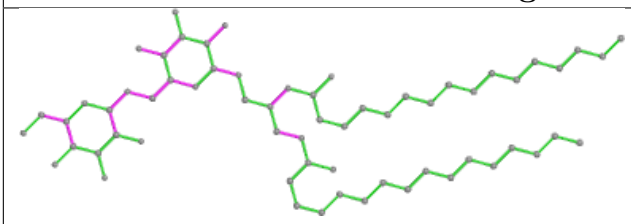


Rings

Ligand DGD H 102



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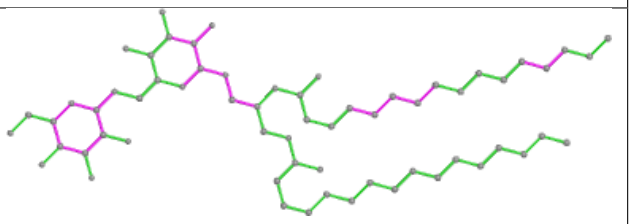
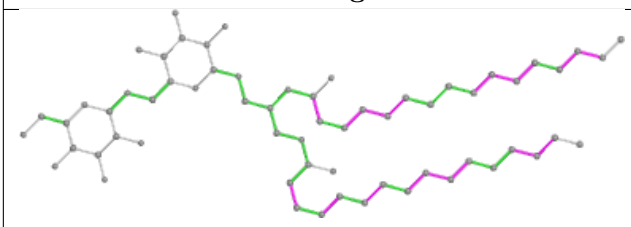


Bond angles



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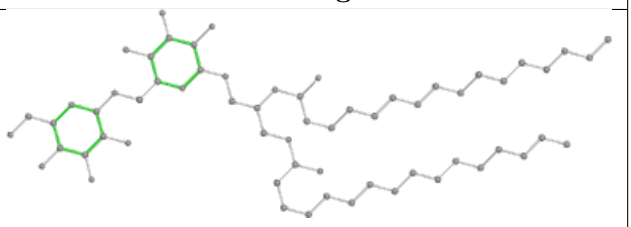
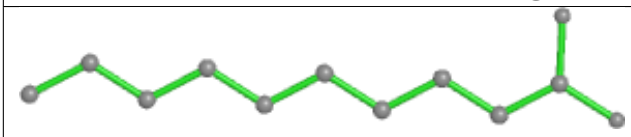
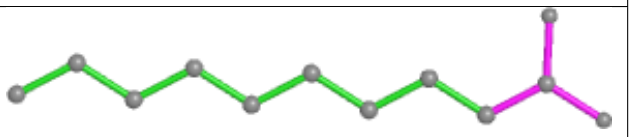


Rings

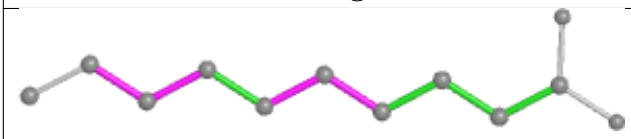
Ligand STE C 520



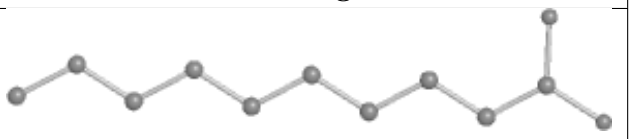
Bond lengths



Bond angles



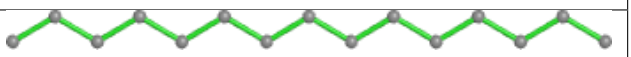
Torsions



Rings

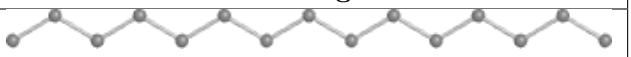
Ligand STE T 102

Bond lengths



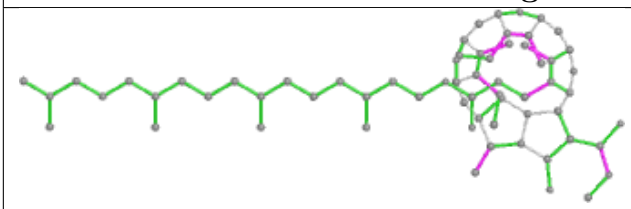
Bond angles

Torsions



Rings

Ligand PHO D 401



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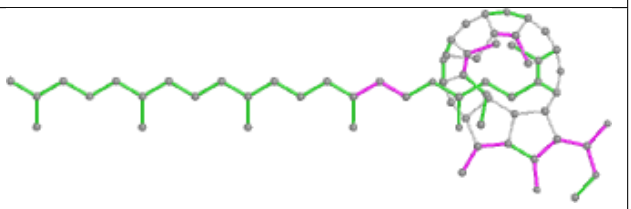
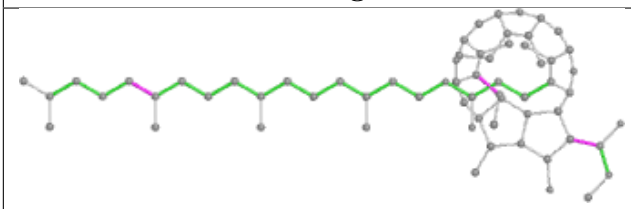


Bond angles



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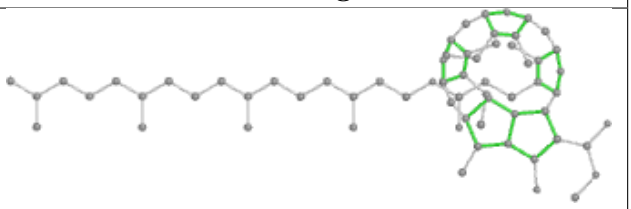
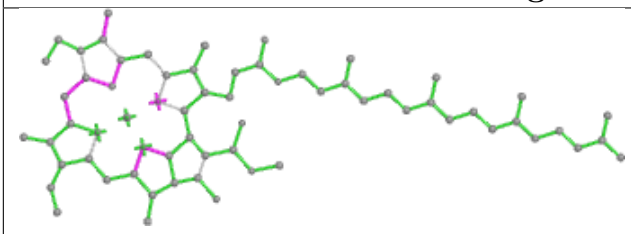


Rings

Ligand CLA b 606



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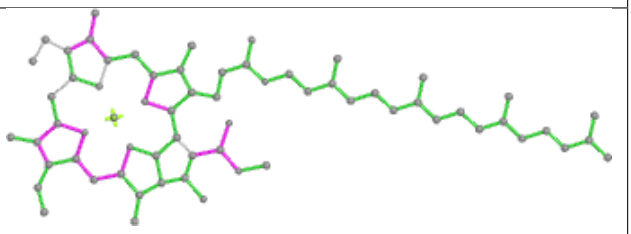
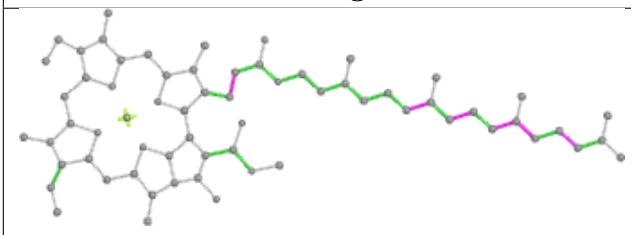


Bond angles



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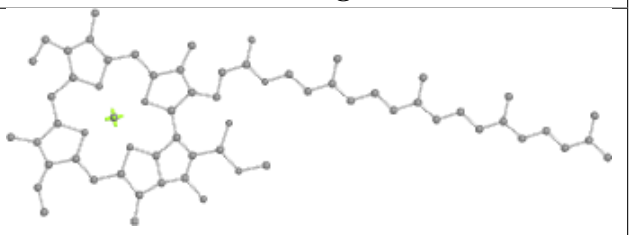
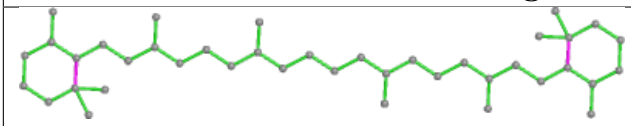
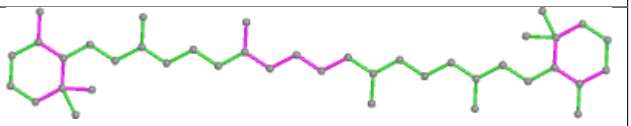


Rings

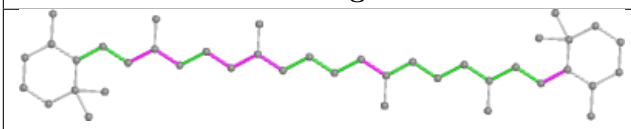
Ligand BCR B 619



Bond lengths



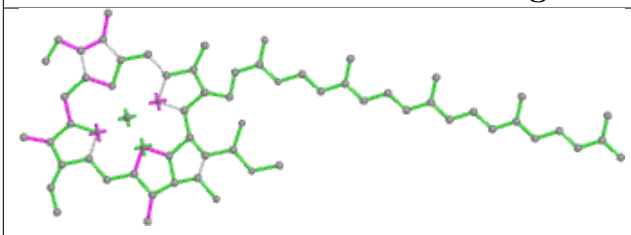
Bond angles



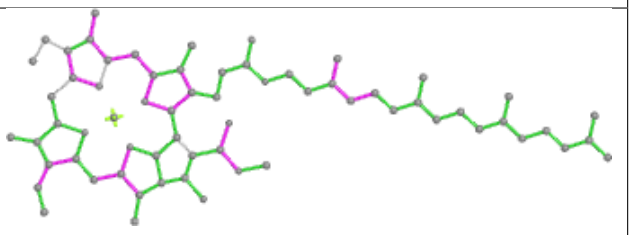
Torsions

Rings

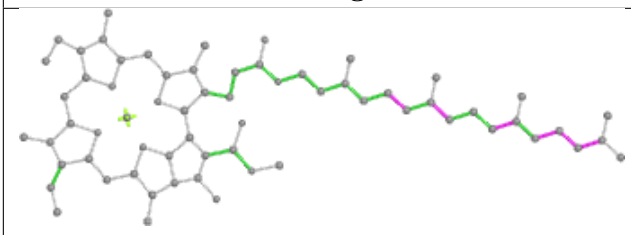
Ligand CLA c 503



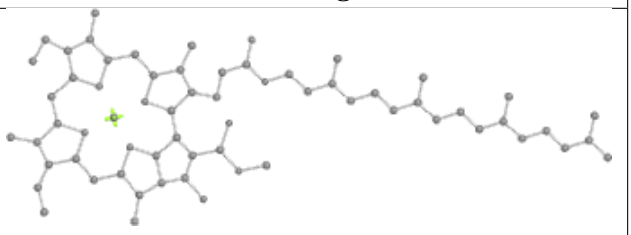
Bond lengths



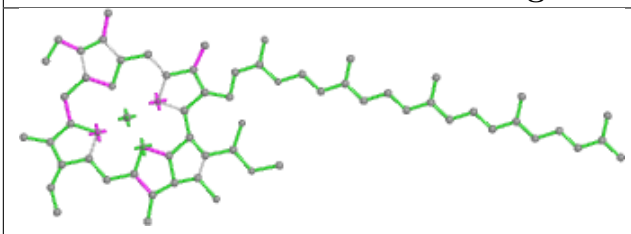
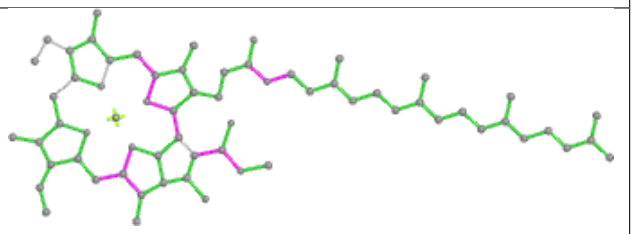
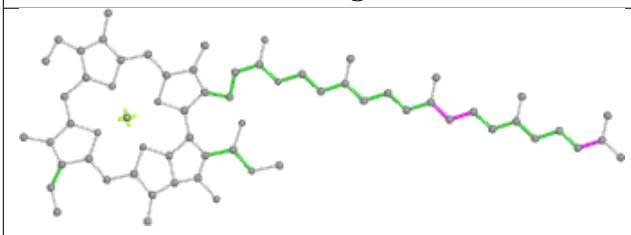
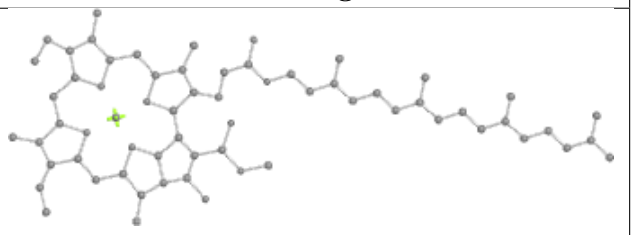
Bond angles

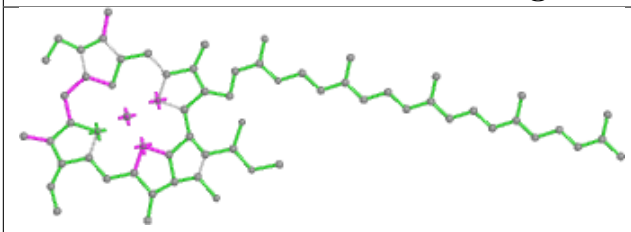
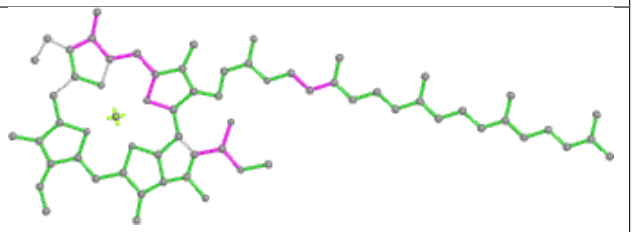
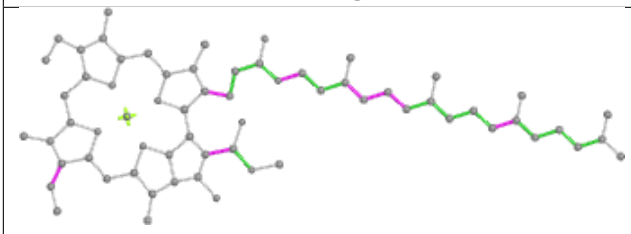
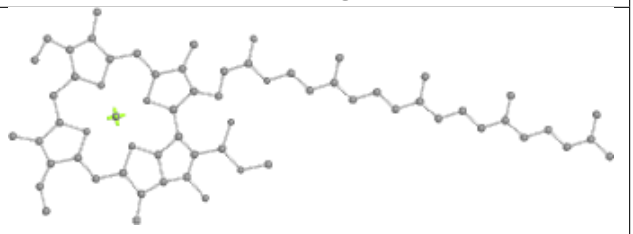


Torsions

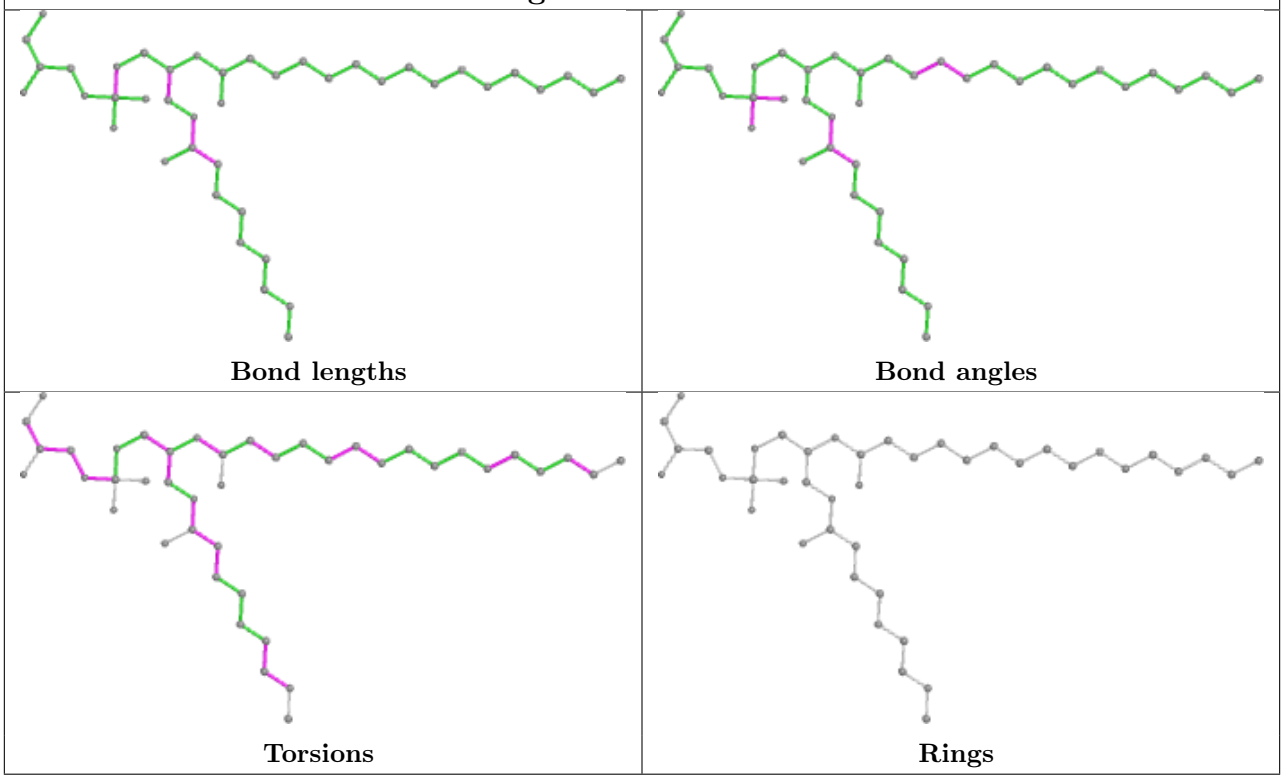


Rings

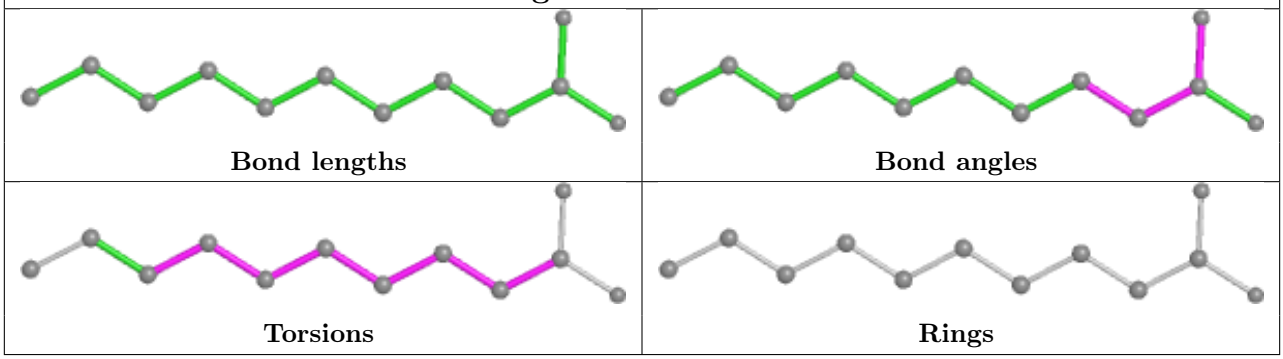
Ligand CLA b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

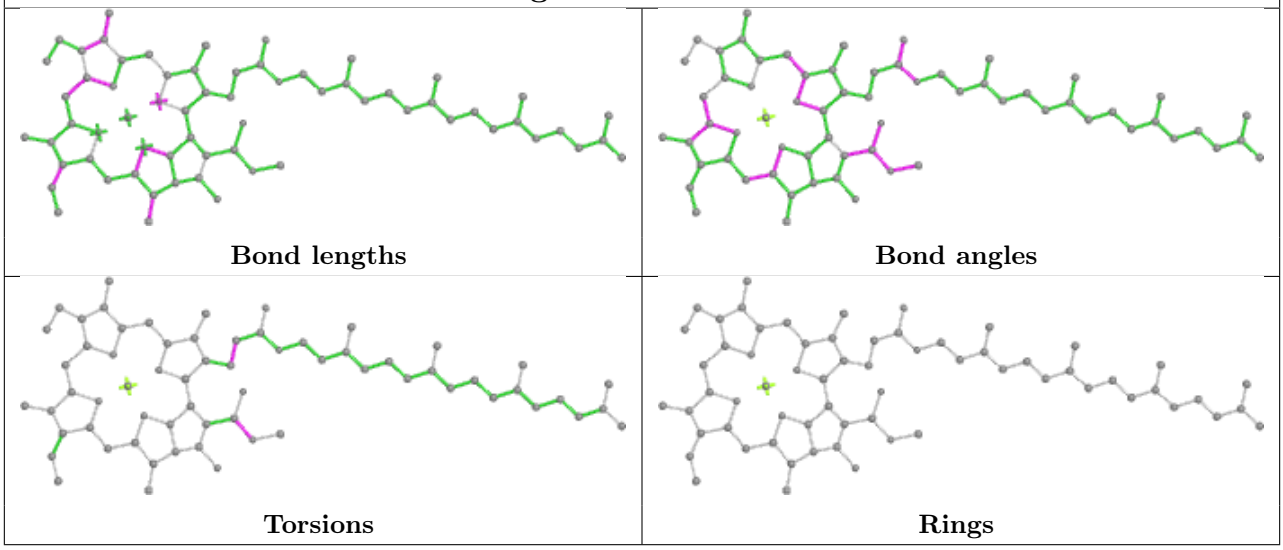
Ligand LHG a 412



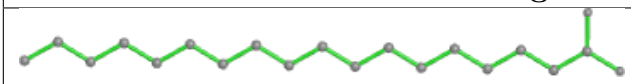
Ligand STE J 101



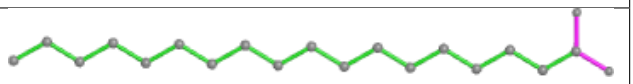
Ligand CLA c 501



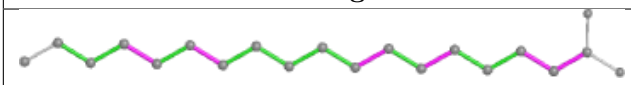
Ligand STE b 624



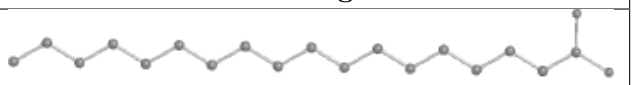
Bond lengths



Bond angles

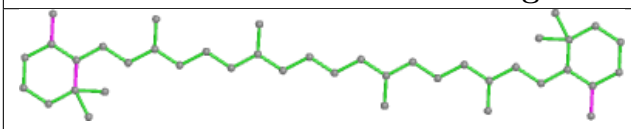


Torsions

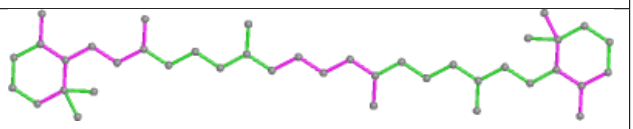


Rings

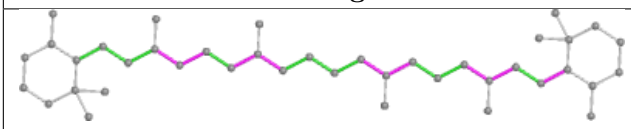
Ligand BCR A 406



Bond lengths



Bond angles



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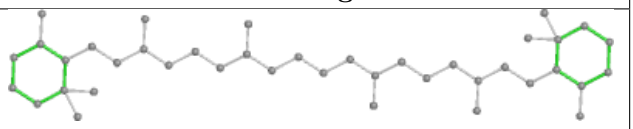
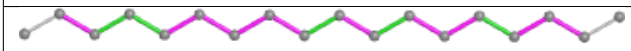


Rings

Ligand STE H 103

Bond lengths

Bond angles



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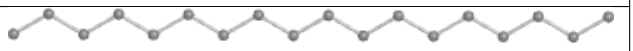
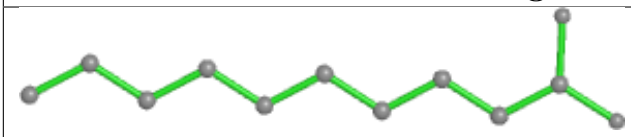
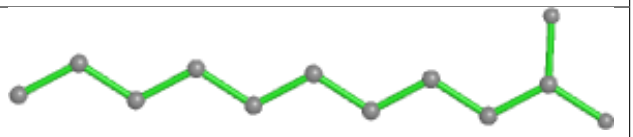


Rings

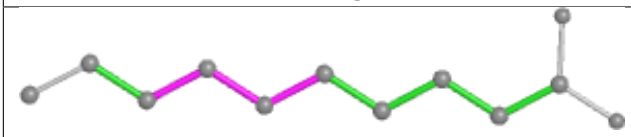
Ligand STE C 522



Bond lengths



Bond angles



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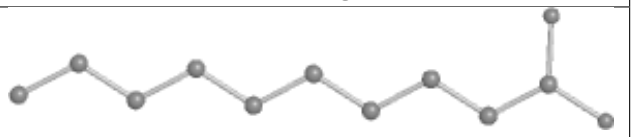
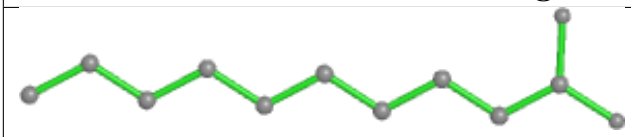
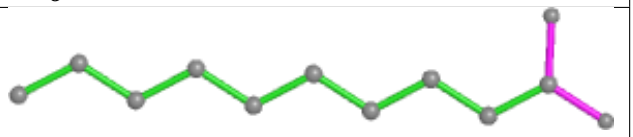


Rings

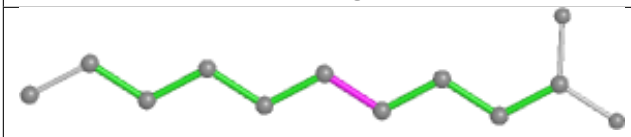
Ligand STE j 101



Bond lengths



Bond angles



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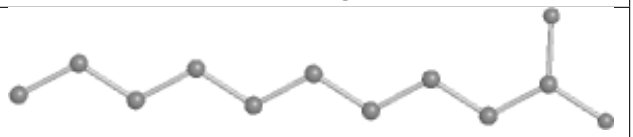
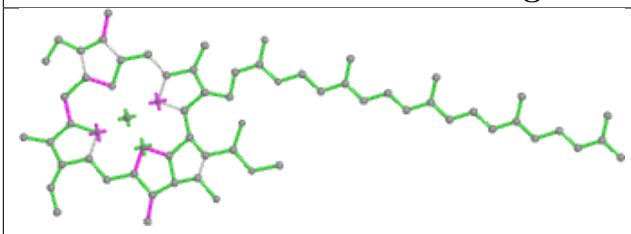
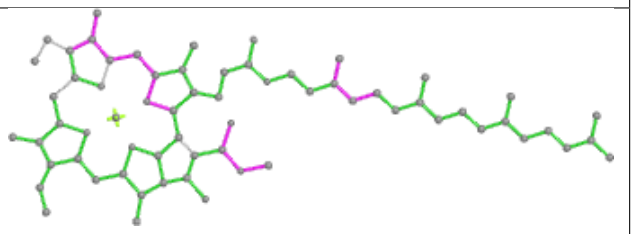
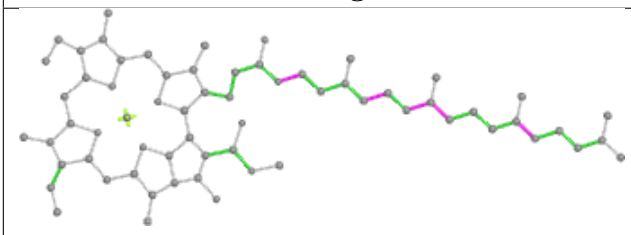
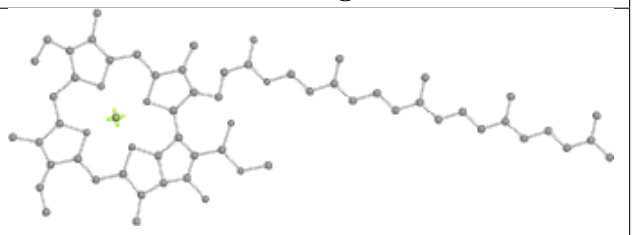
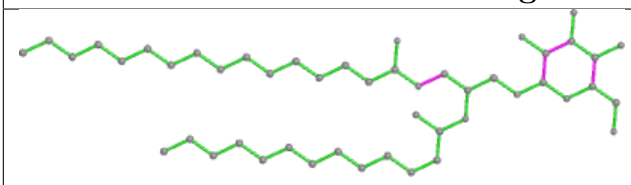
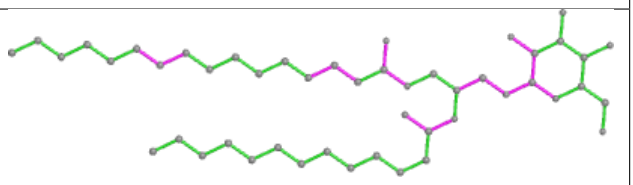
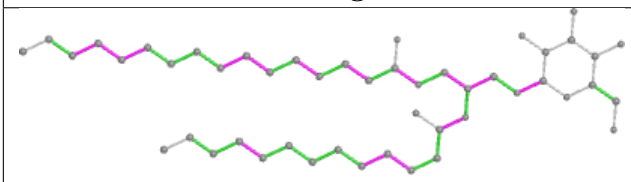
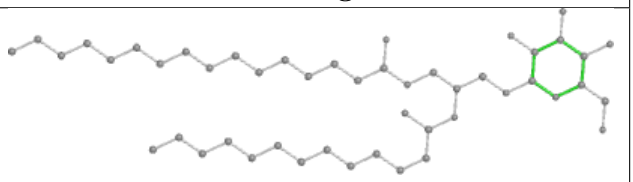
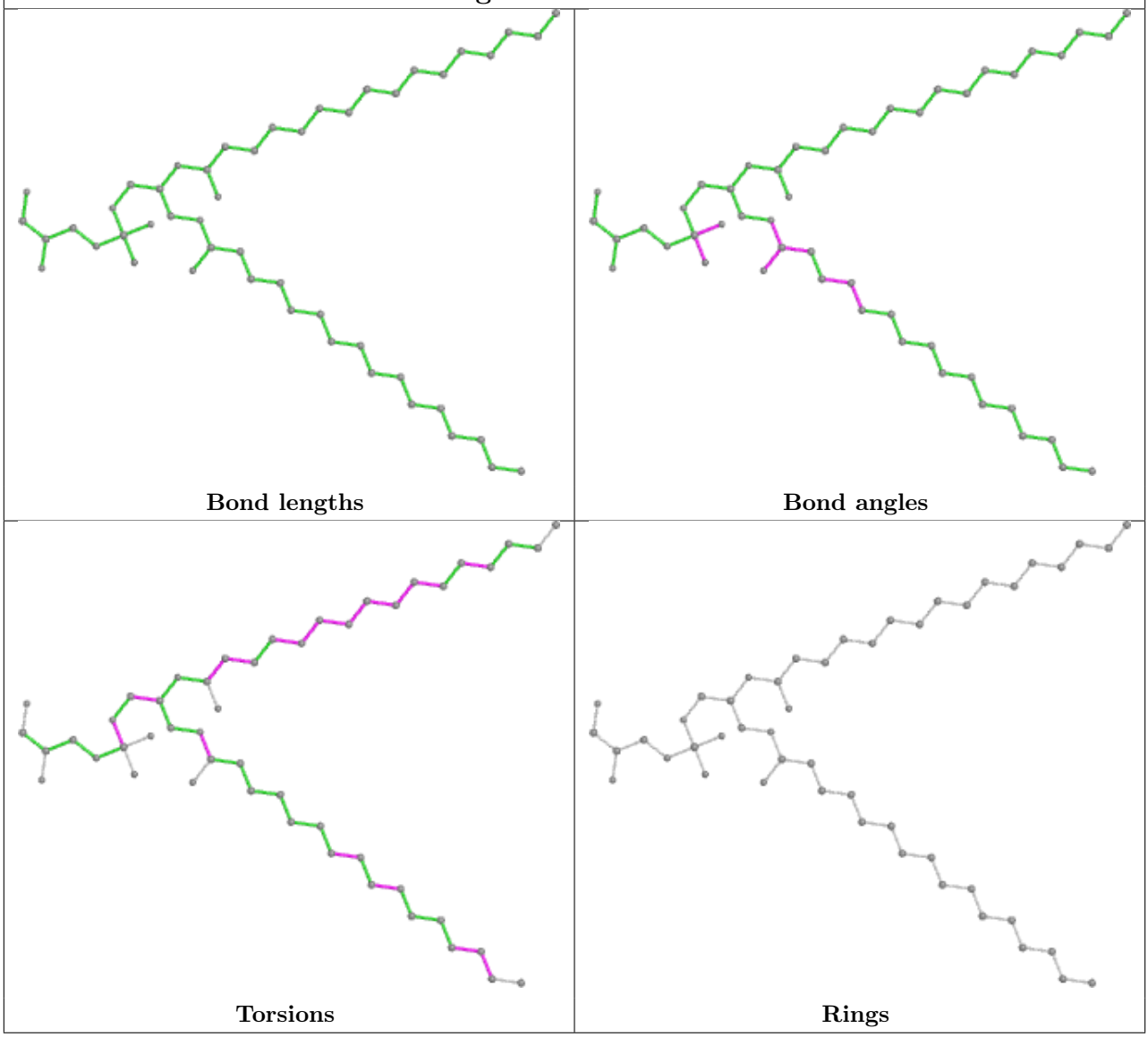


Rings

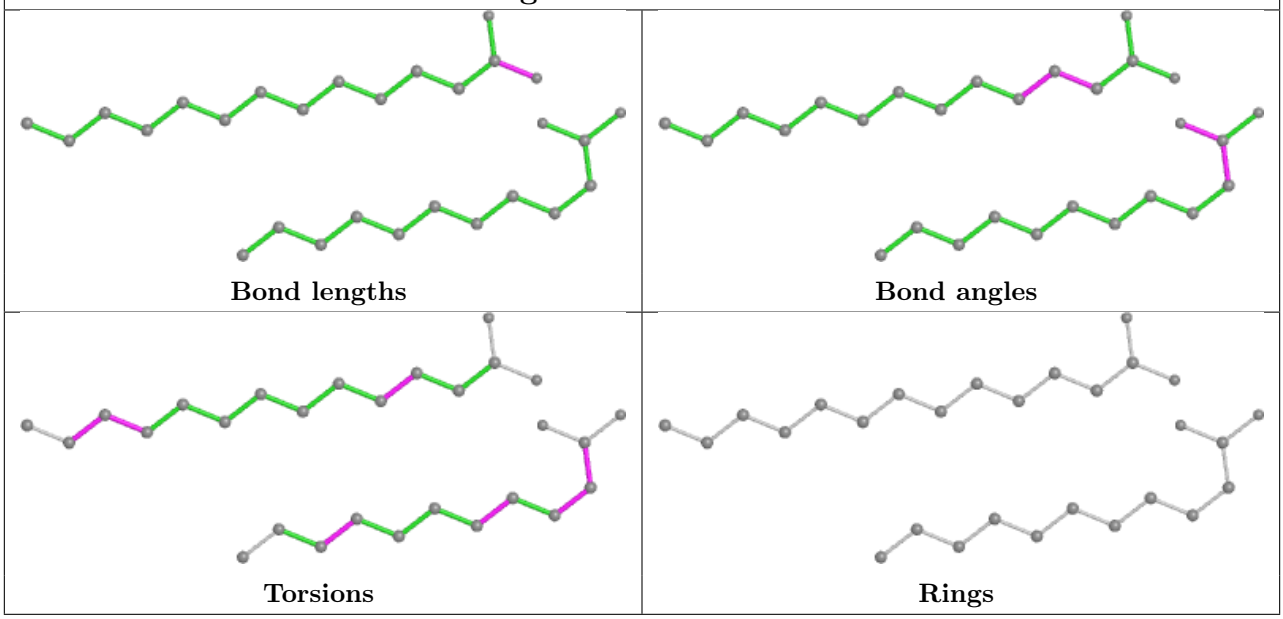
Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

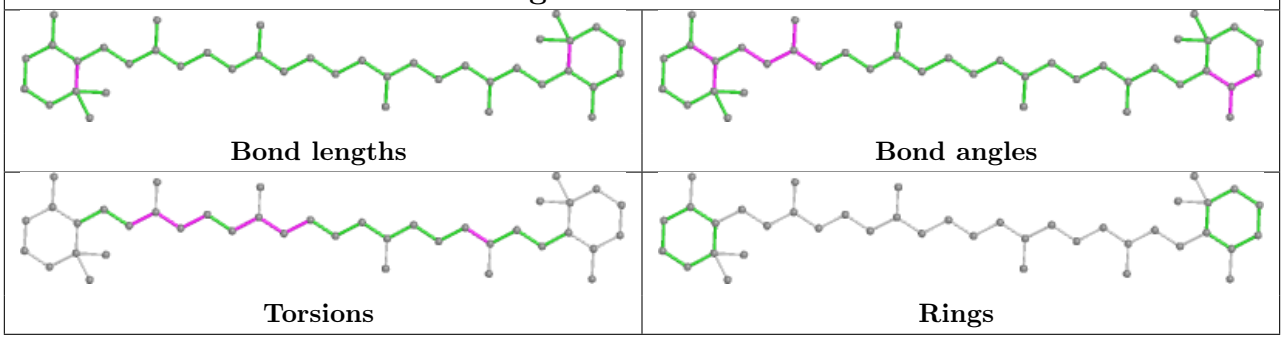
Ligand LHG l 101



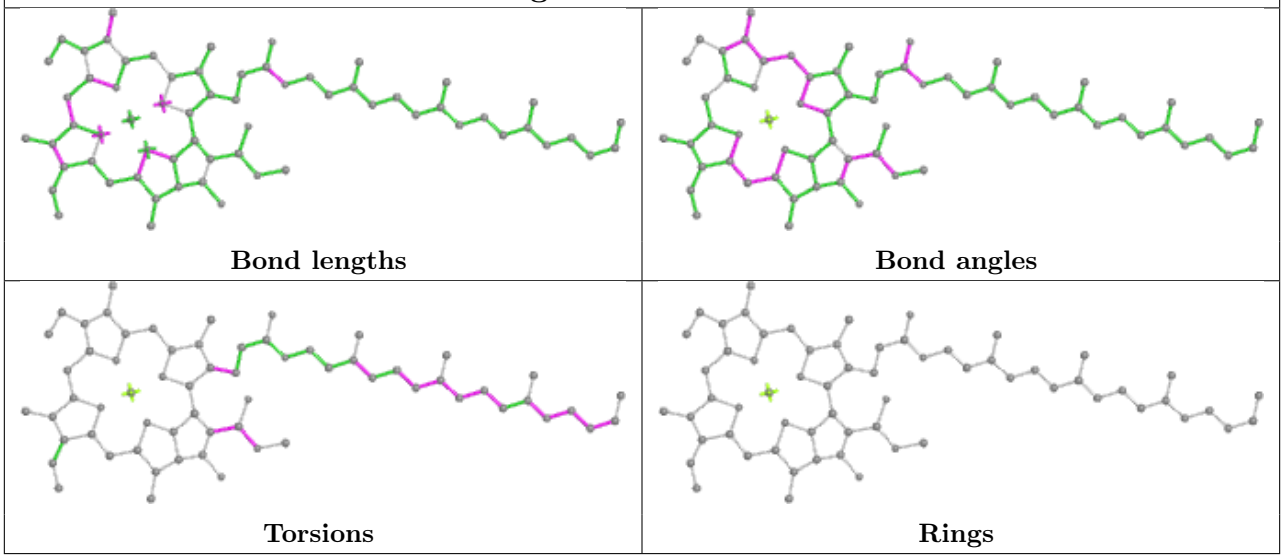
Ligand LMG D 410



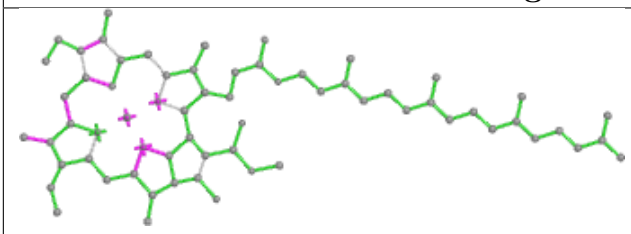
Ligand BCR t 101



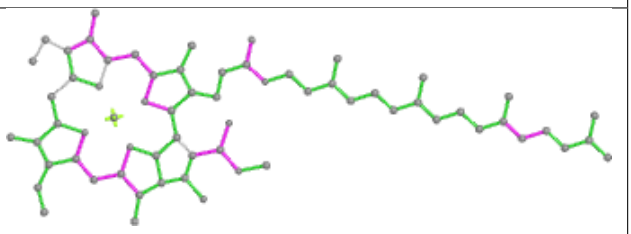
Ligand CLA c 508



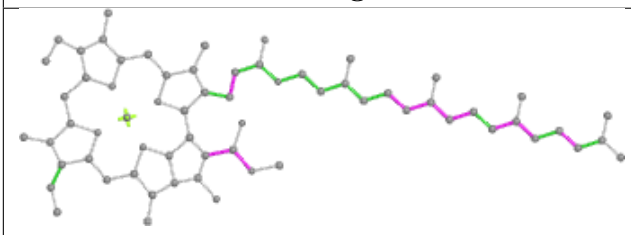
Ligand CLA B 604



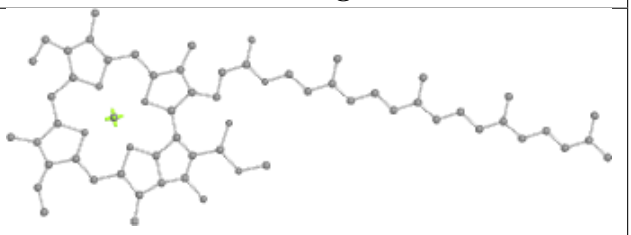
Bond lengths



Bond angles

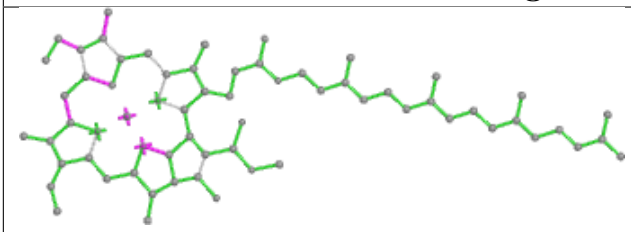


Torsions

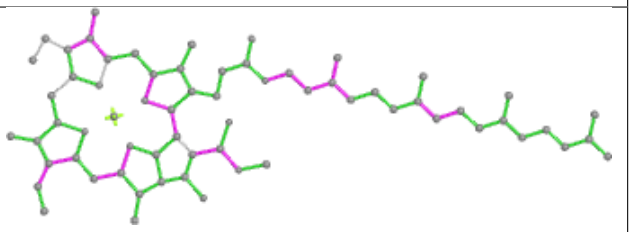


Rings

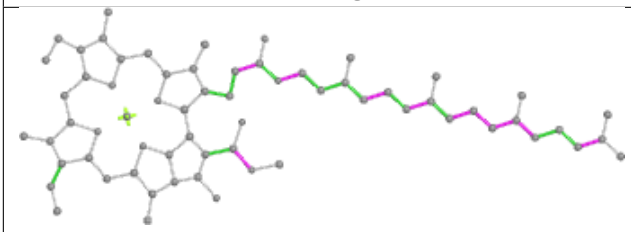
Ligand CLA B 614



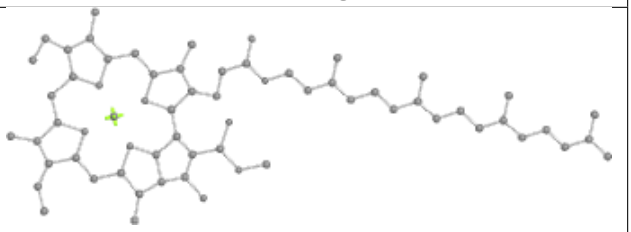
Bond lengths



Bond angles

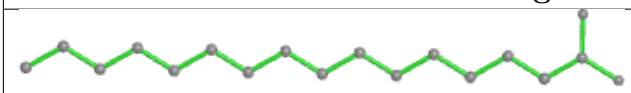


Torsions

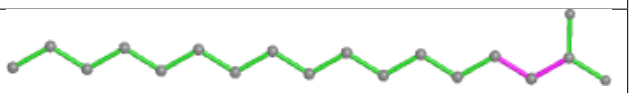


Rings

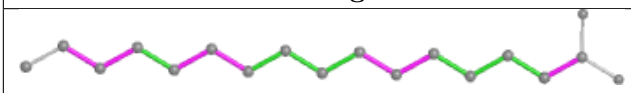
Ligand STE t 104



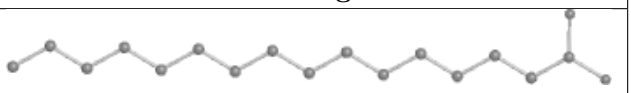
Bond lengths



Bond angles

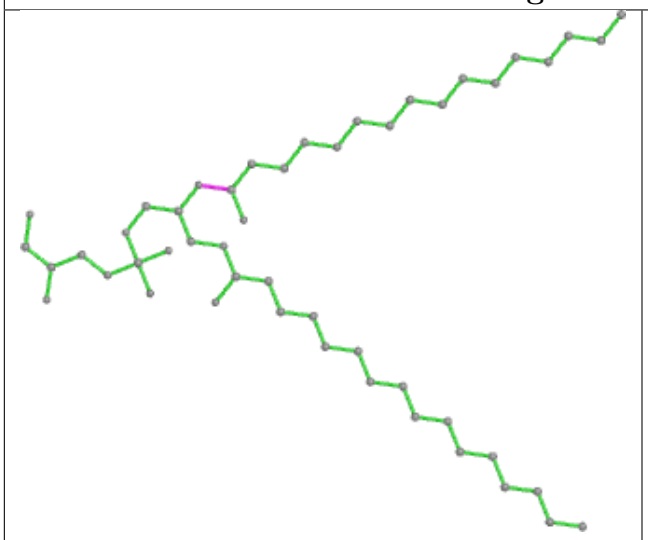


Torsions

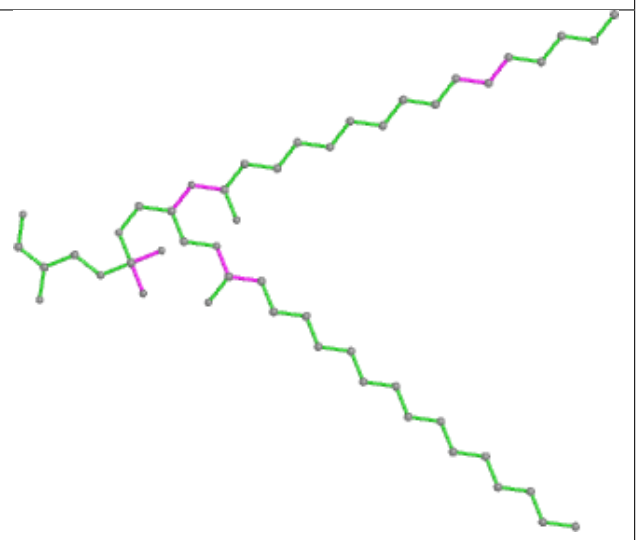


Rings

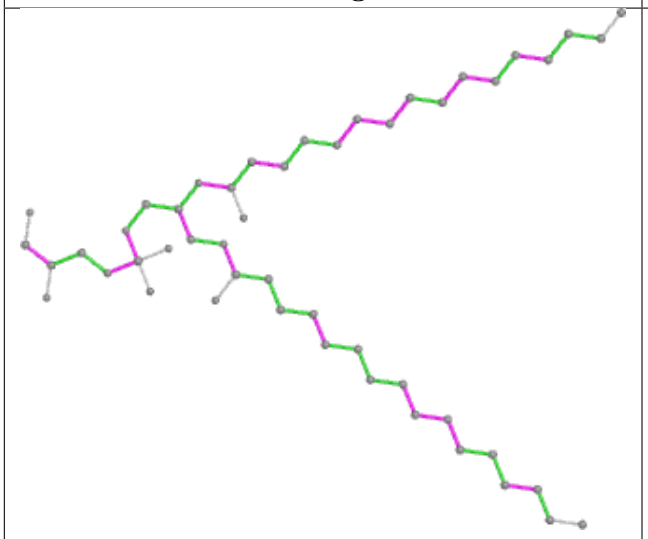
Ligand LHG d 408



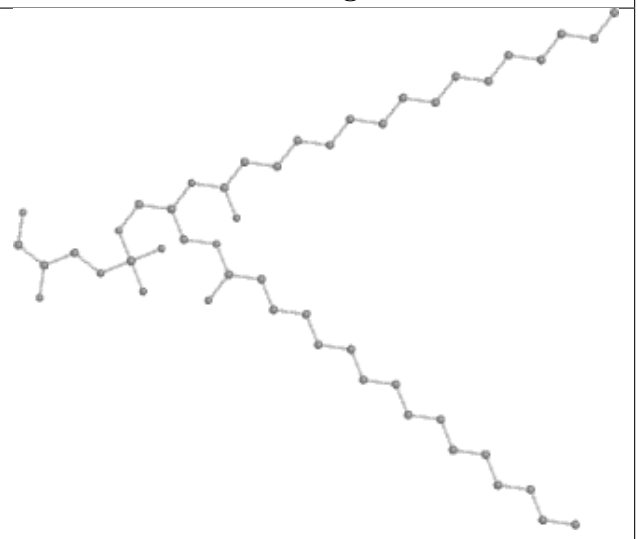
Bond lengths



Bond angles

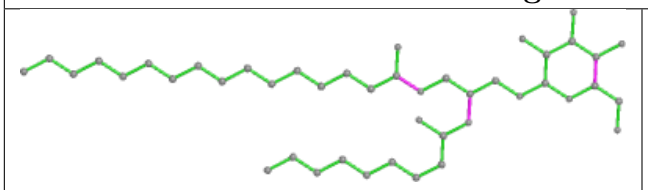


Torsions



Rings

Ligand LMG d 410



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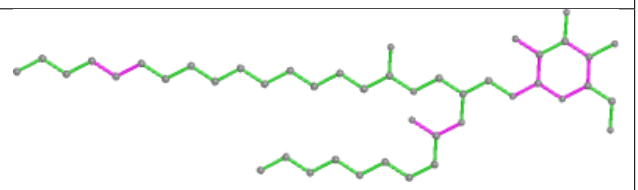
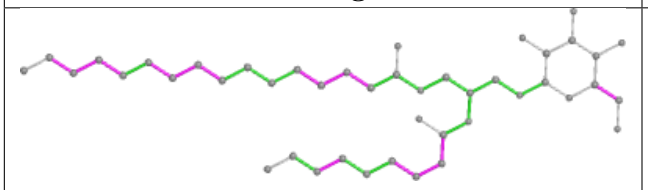
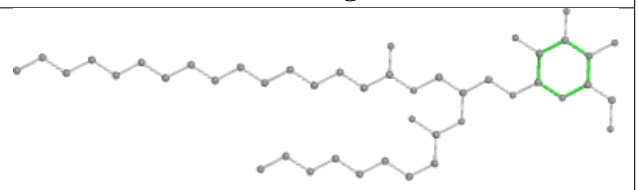


Bond angles

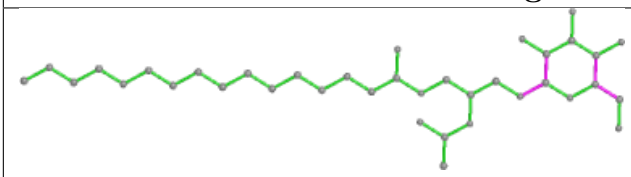


Torsions



Rings

Ligand LMG c 519



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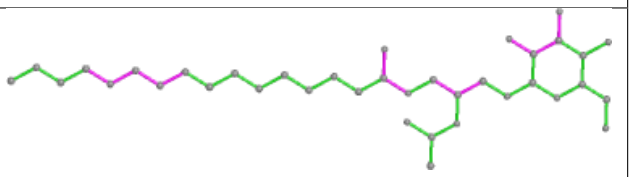
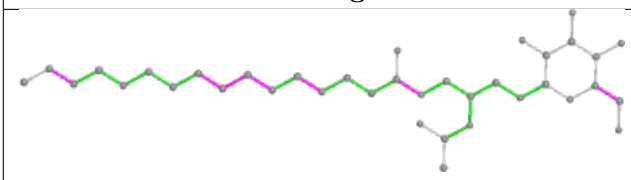
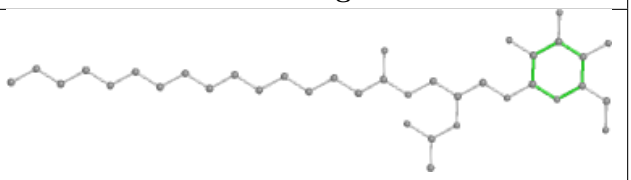


Bond angles

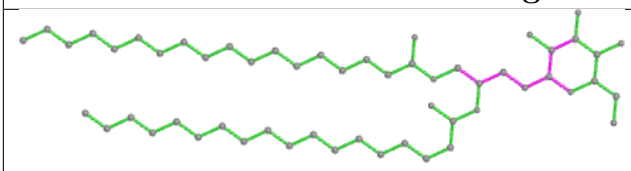


Torsions



Rings

Ligand LMG b 622



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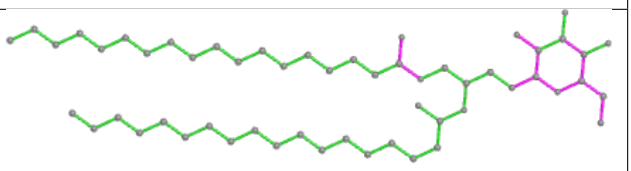
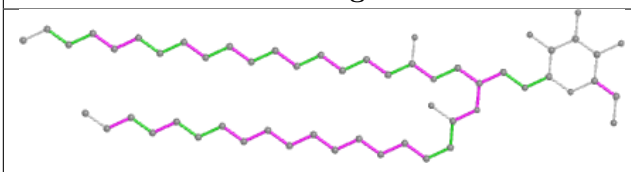
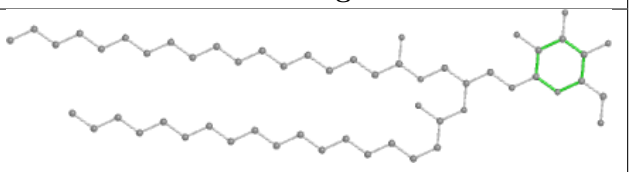


Bond angles

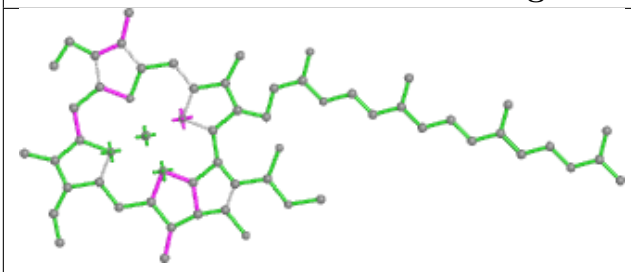


Torsions



Rings

Ligand CLA b 616



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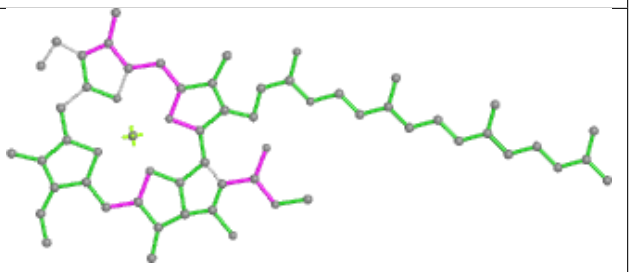
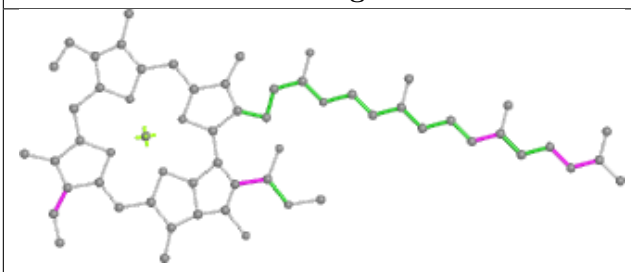


Bond angles



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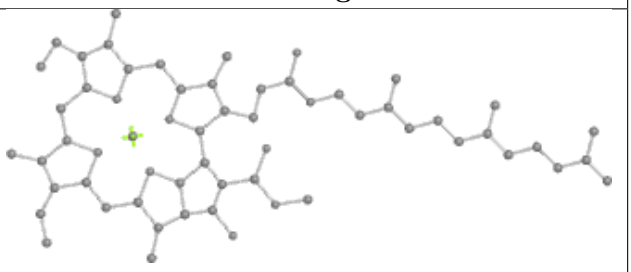

Rings

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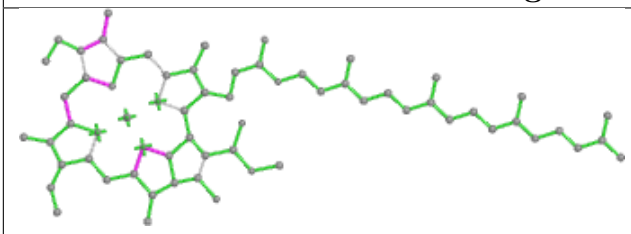

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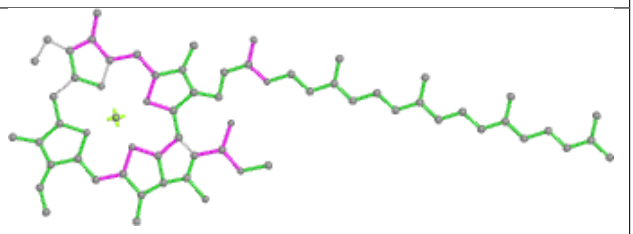
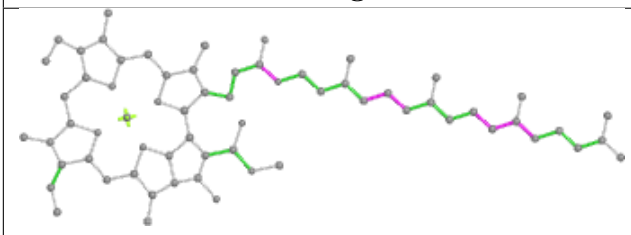


Bond angles



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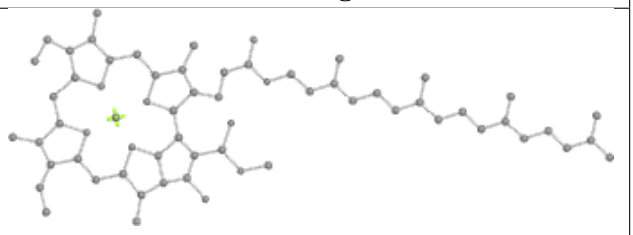
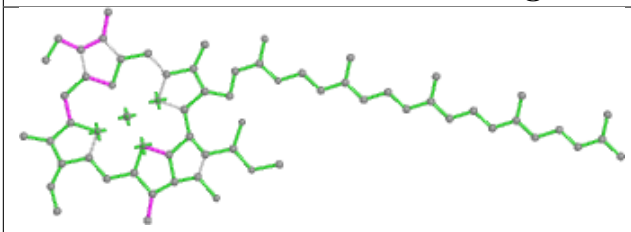


Rings

Ligand CLA C 508



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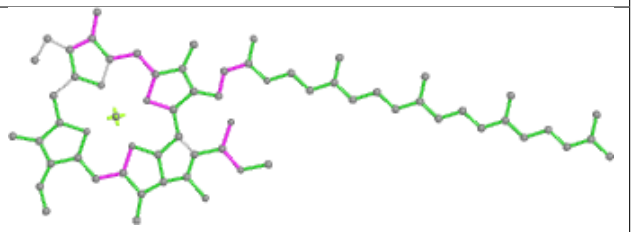
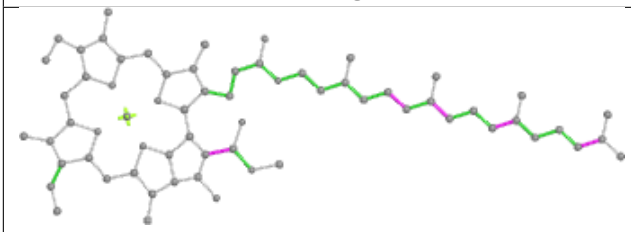


Bond angles



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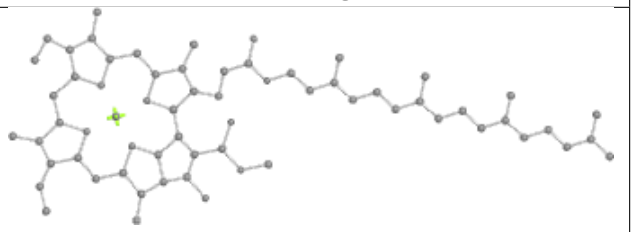
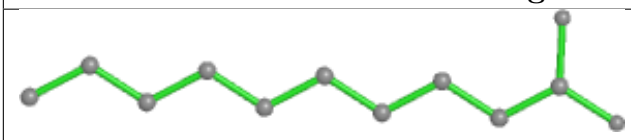


Rings

Ligand STE B 601



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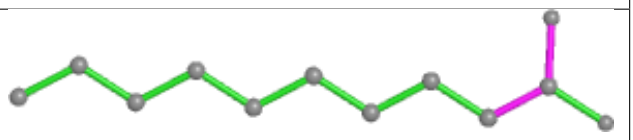
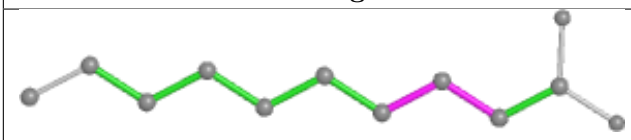


Bond angles



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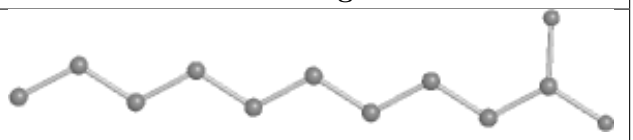
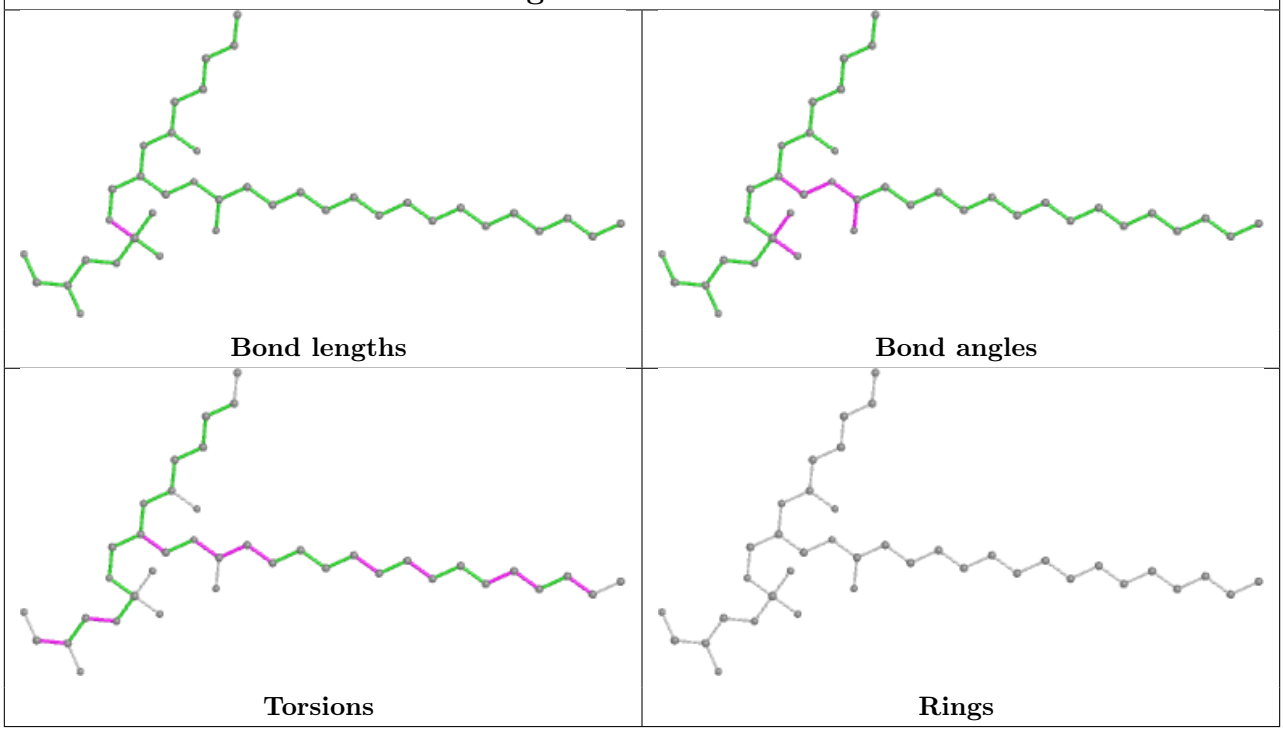
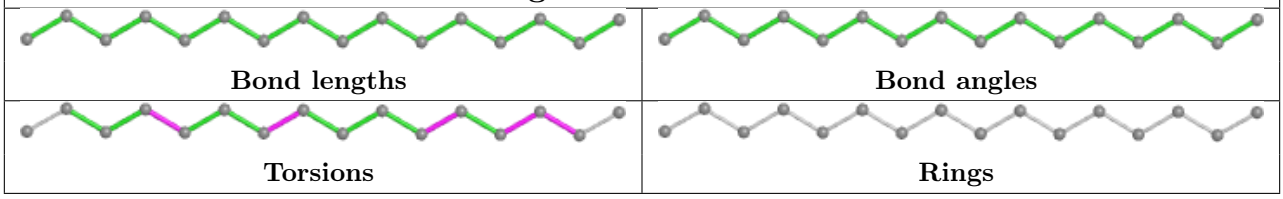


Rings

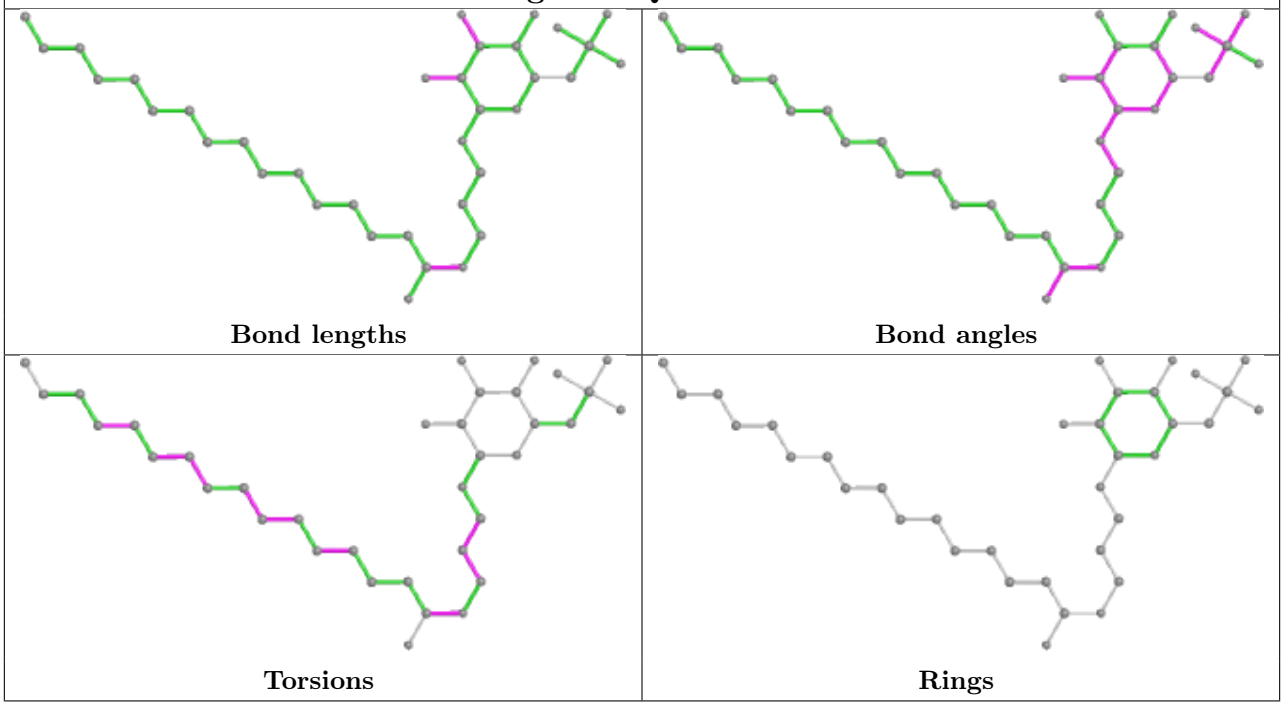
Ligand LHG d 409



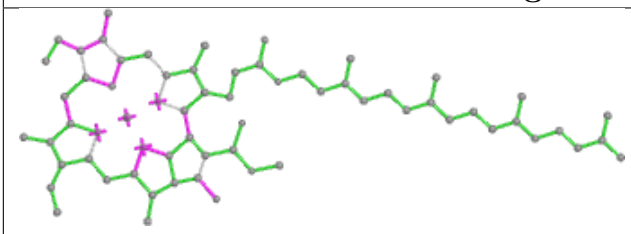
Ligand STE C 521



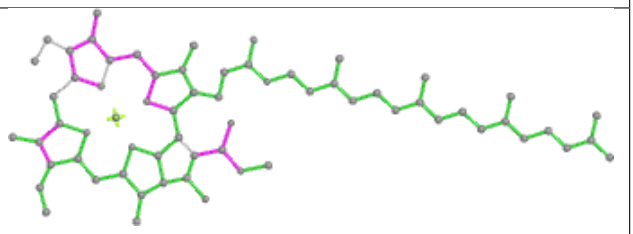
Ligand SQD F 101



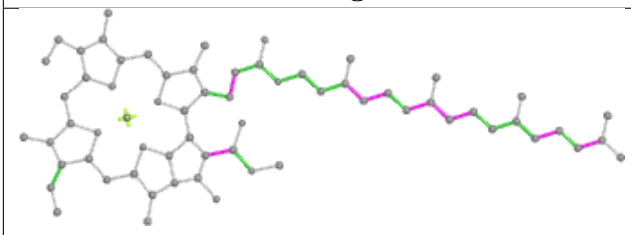
Ligand CLA B 615



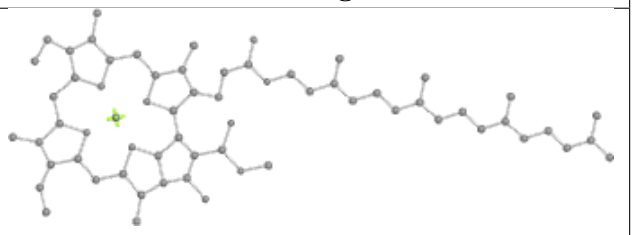
Bond lengths



Bond angles

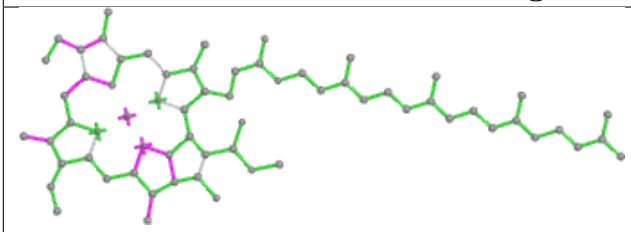


Torsions



Rings

Ligand CLA b 610



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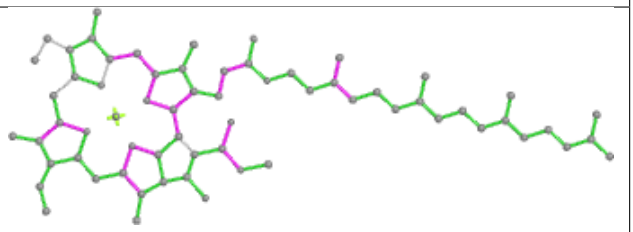

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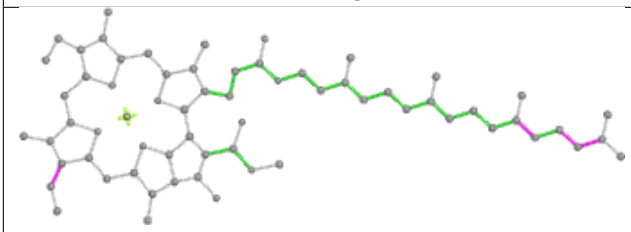

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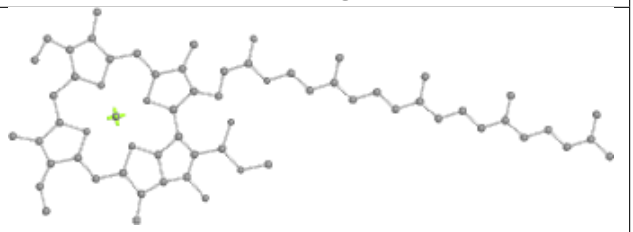
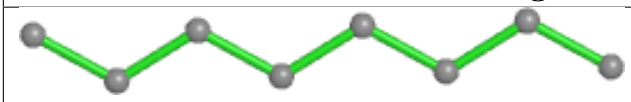


Rings

Ligand STE Z 102



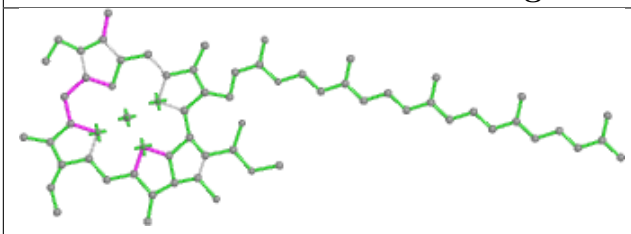
Bond lengths

Bond angles

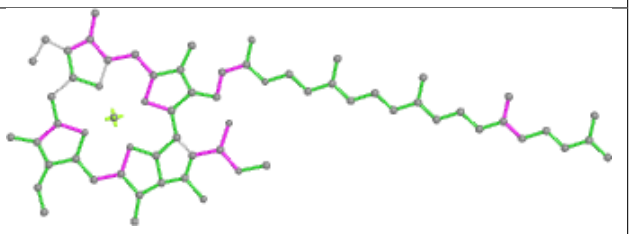
Torsions

Rings

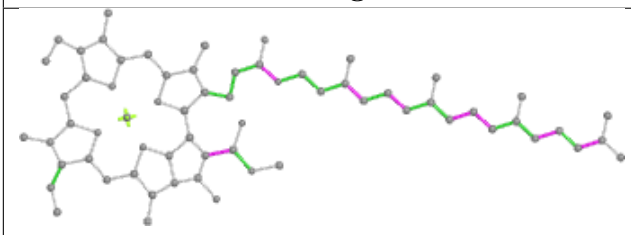
Ligand CLA B 606



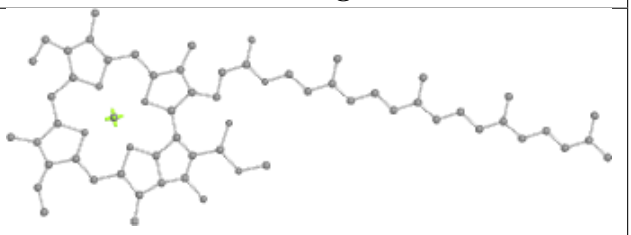
Bond lengths



Bond angles

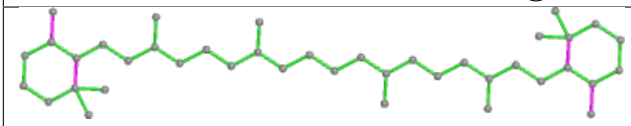


Torsions

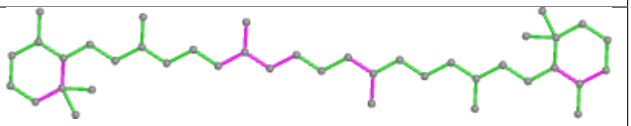


Rings

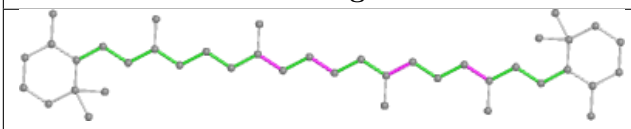
Ligand BCR c 515



Bond lengths



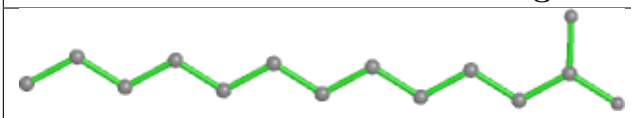
Bond angles



Torsions

Rings

Ligand STE t 102



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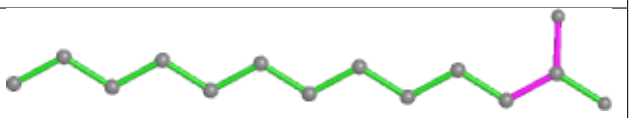
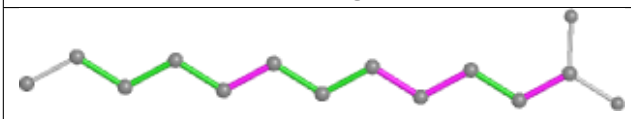
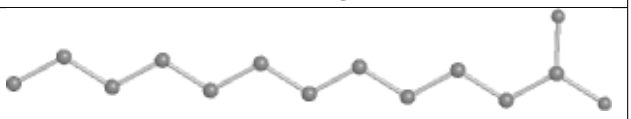


Bond angles

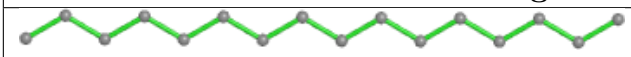


Torsions



Rings

Ligand STE b 620



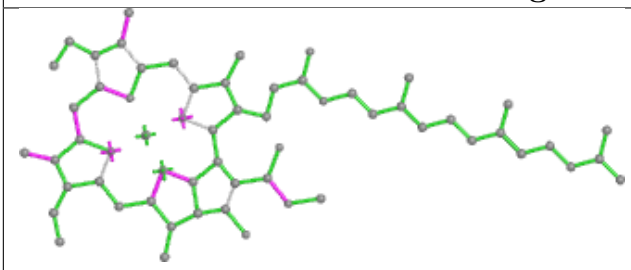
Bond lengths

Bond angles

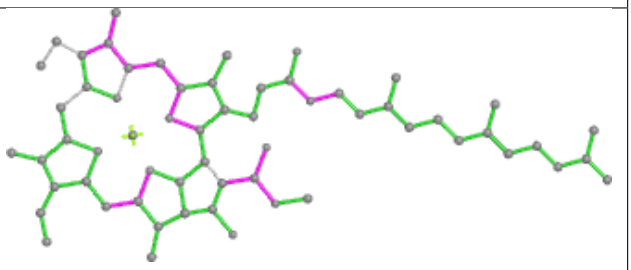
Torsions

Rings

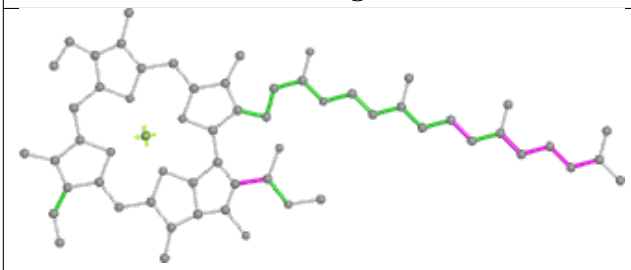
Ligand CLA c 504



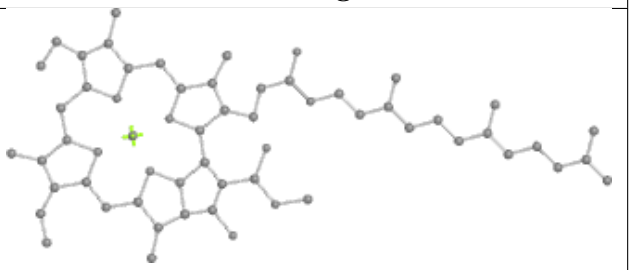
Bond lengths



Bond angles

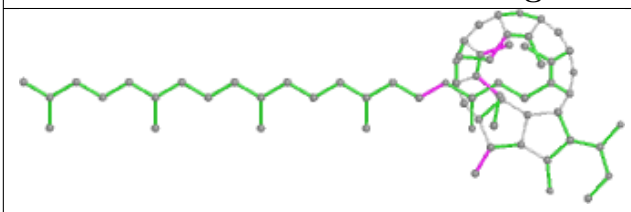


Torsions

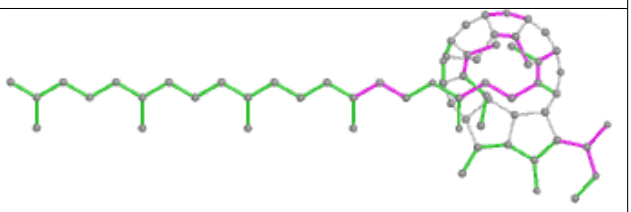


Rings

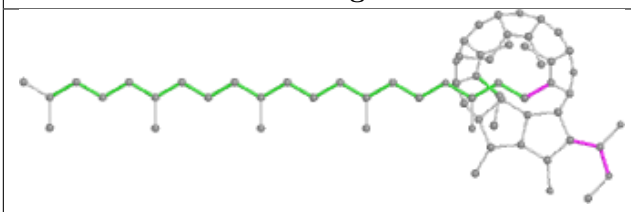
Ligand PHO d 401



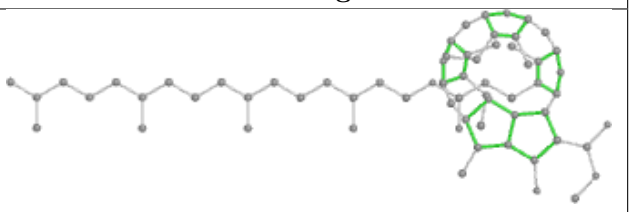
Bond lengths



Bond angles

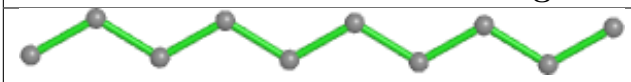


Torsions

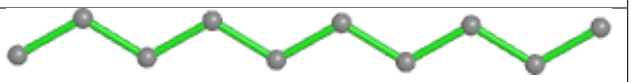


Rings

Ligand STE t 103

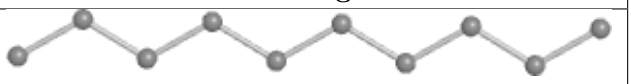


Bond lengths



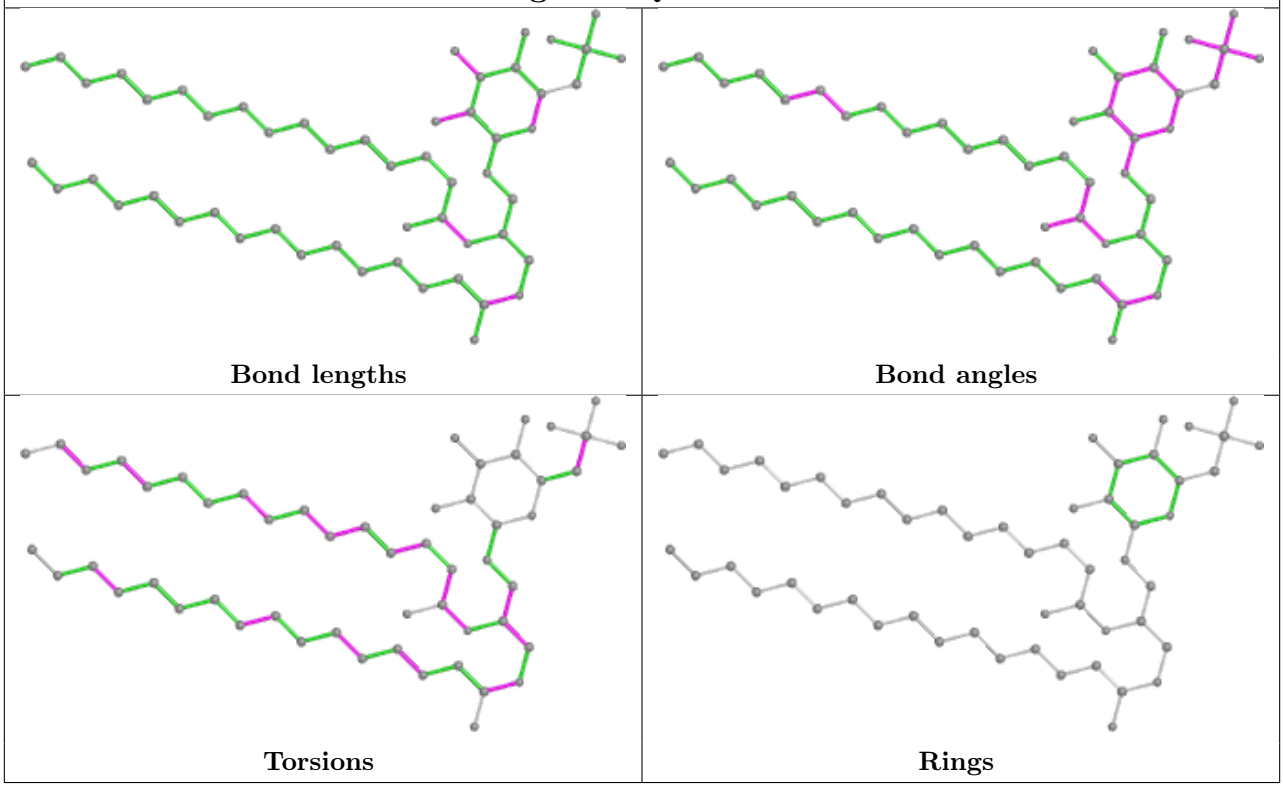
Bond angles

Torsions

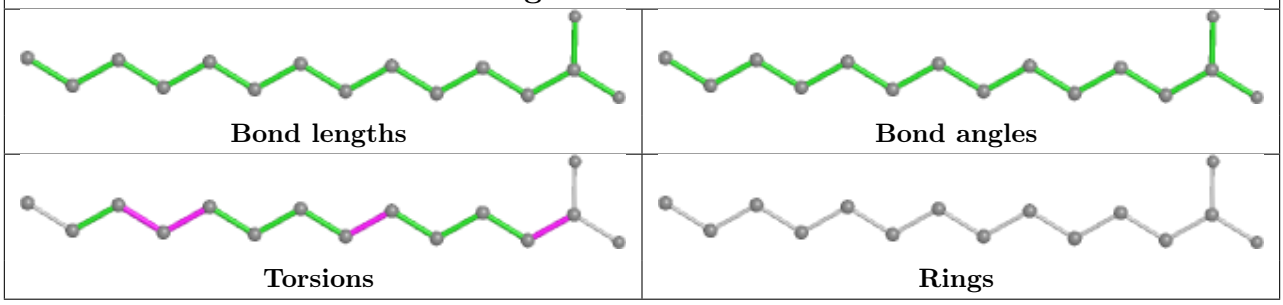


Rings

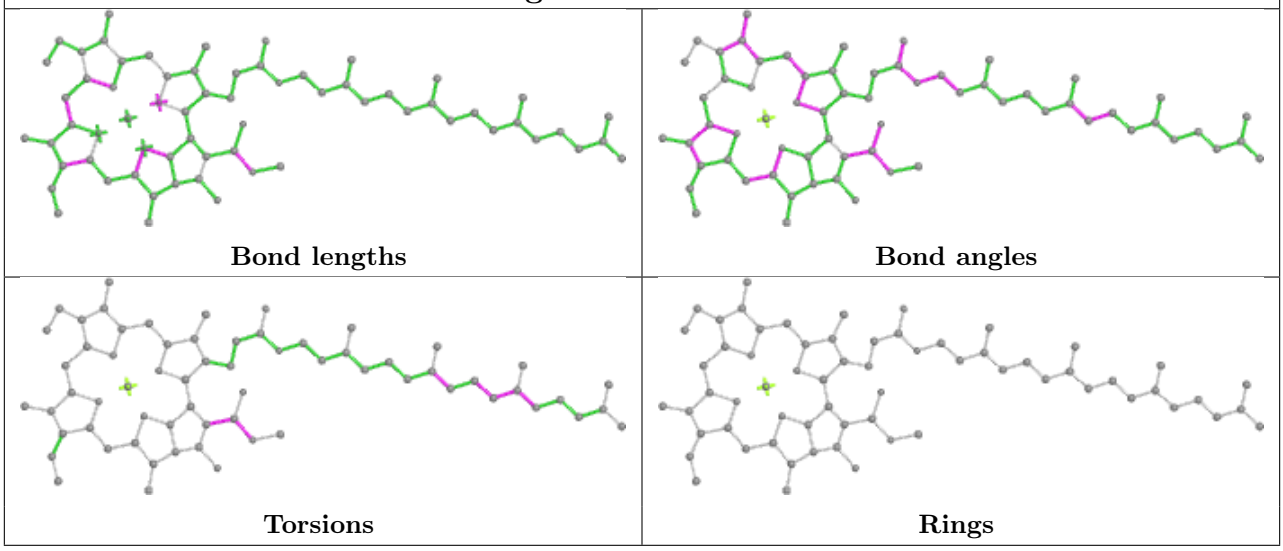
Ligand SQD a 411



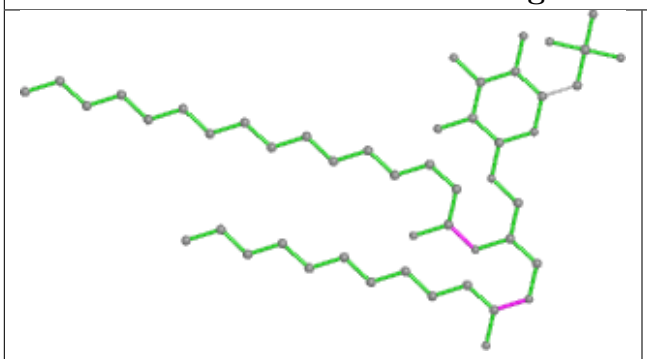
Ligand STE M 102



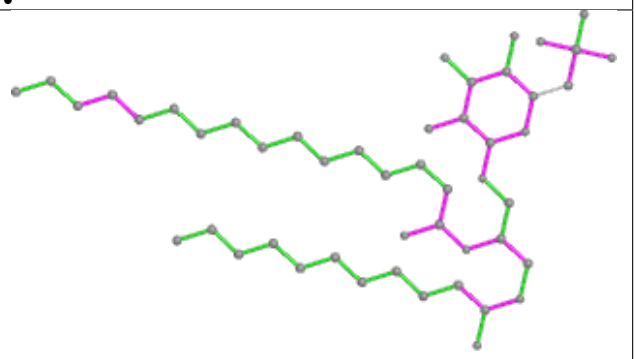
Ligand CLA B 605



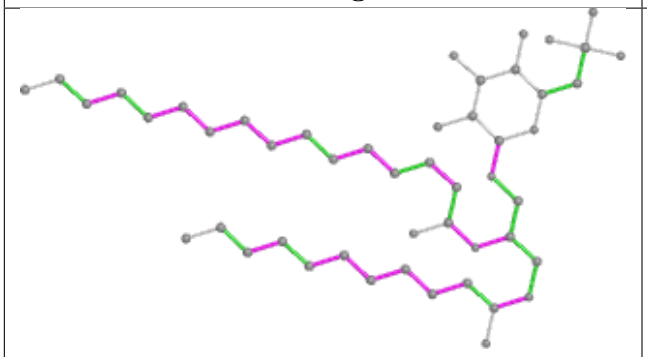
Ligand SQD L 101



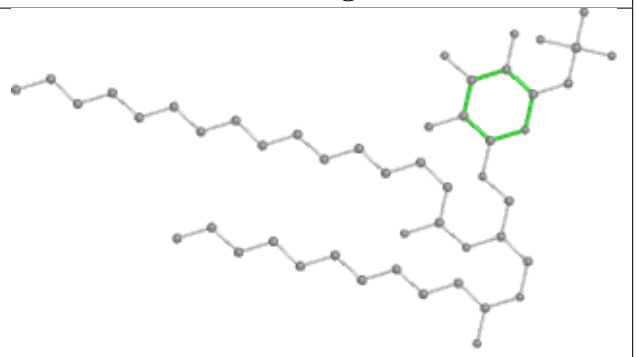
Bond lengths



Bond angles

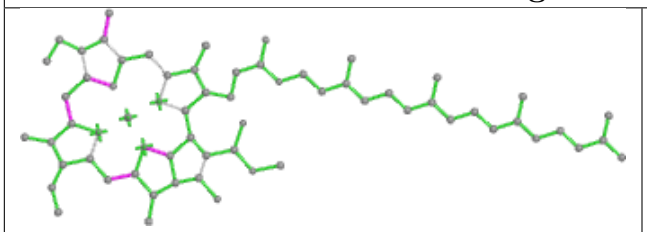


Torsions

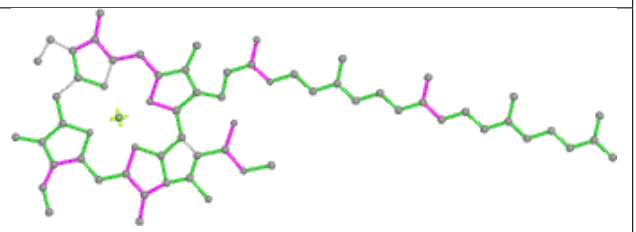


Rings

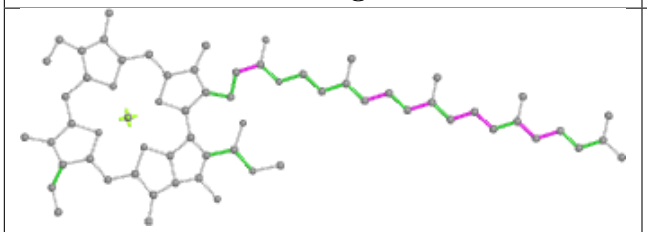
Ligand CLA b 612



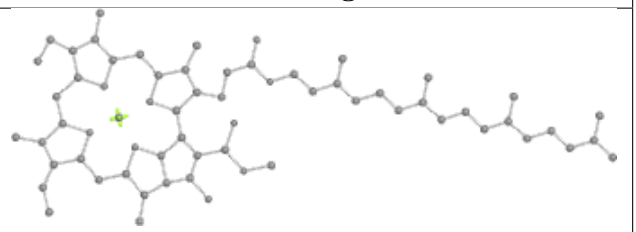
Bond lengths



Bond angles

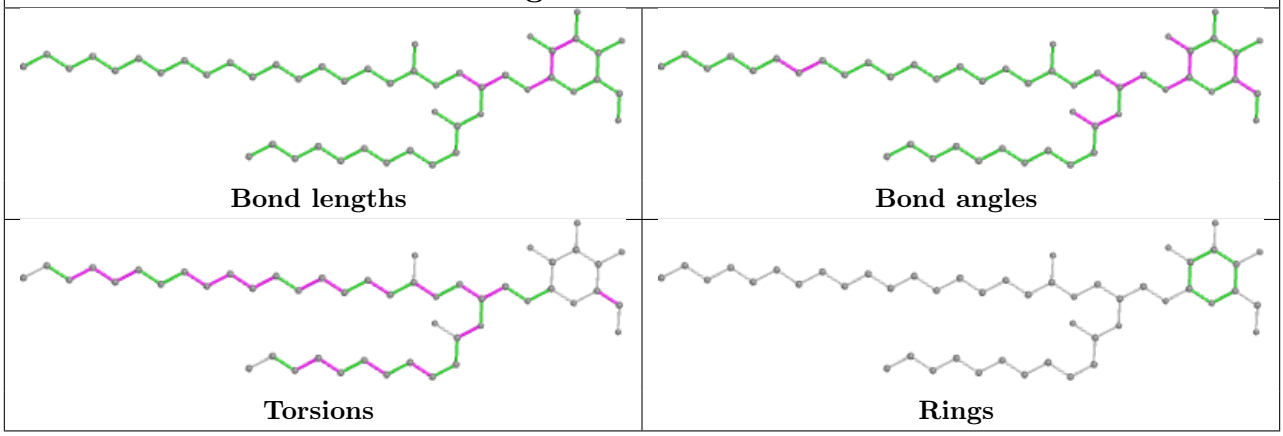


Torsions

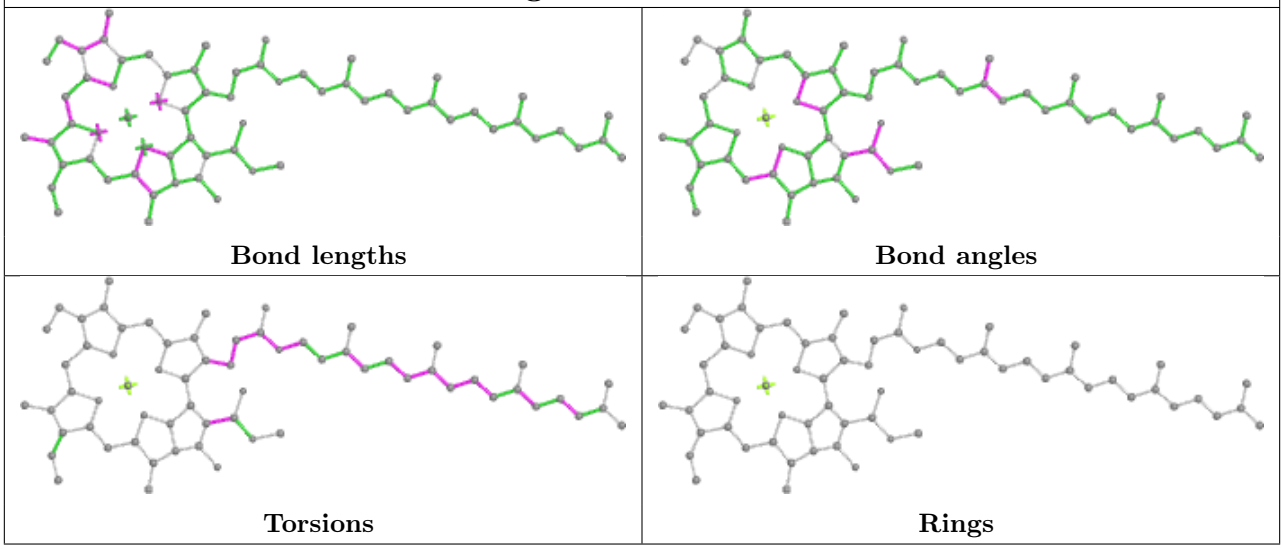


Rings

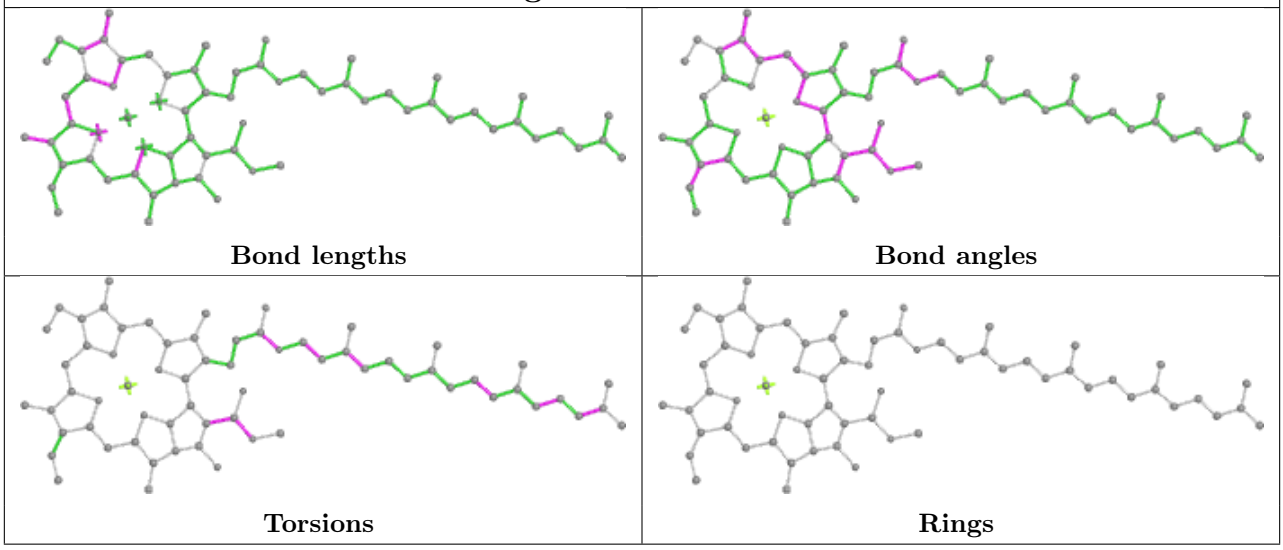
Ligand LMG c 521

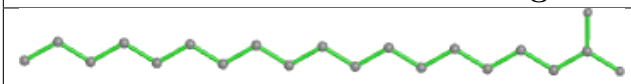
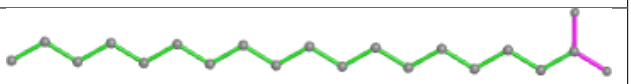
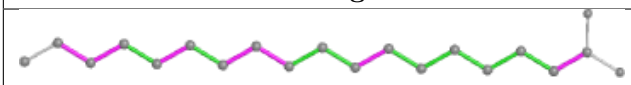
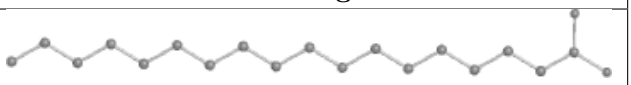


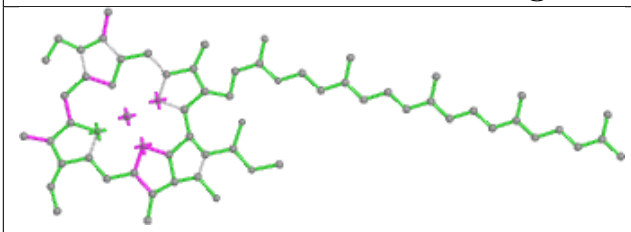
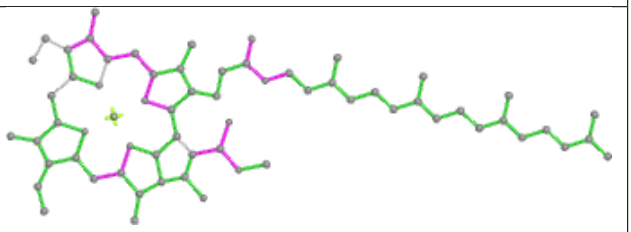
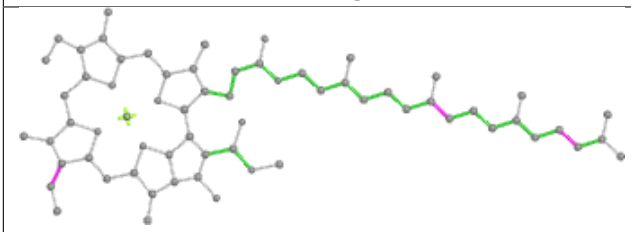
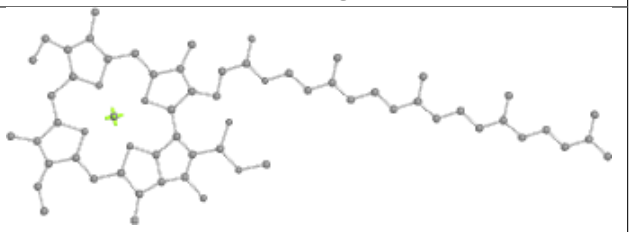
Ligand CLA B 602

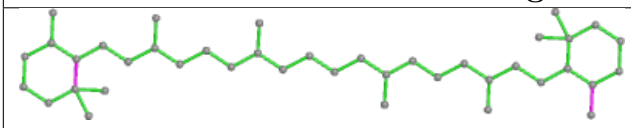
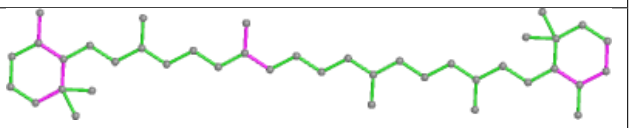
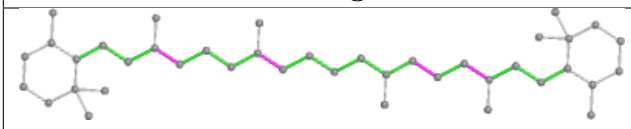
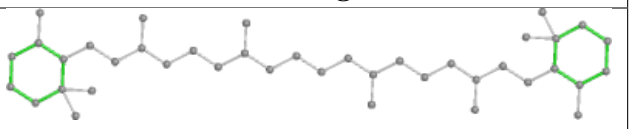


Ligand CLA D 404

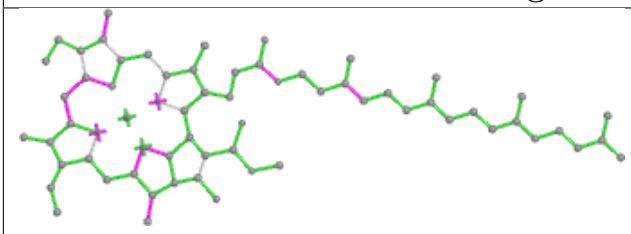


Ligand STE b 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

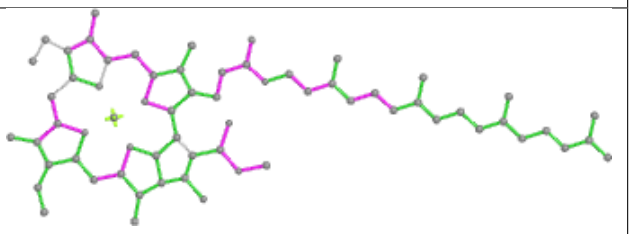
Ligand CLA a 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR a 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

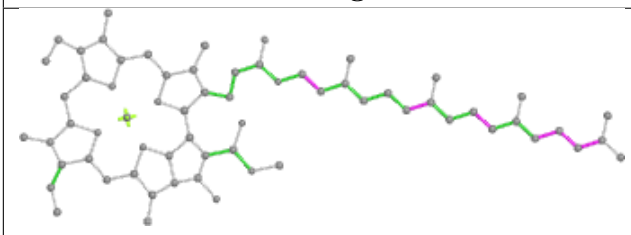
Ligand CLA b 613



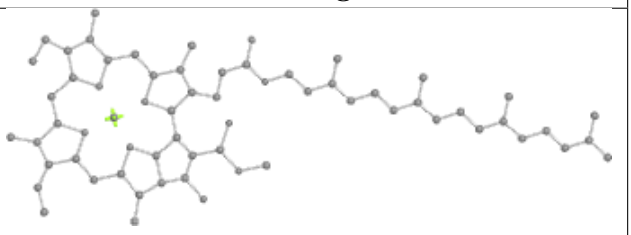
Bond lengths



Bond angles

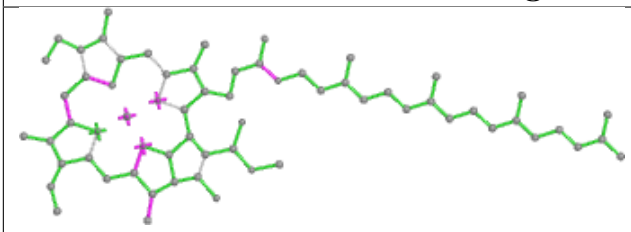


Torsions



Rings

Ligand CLA C 509



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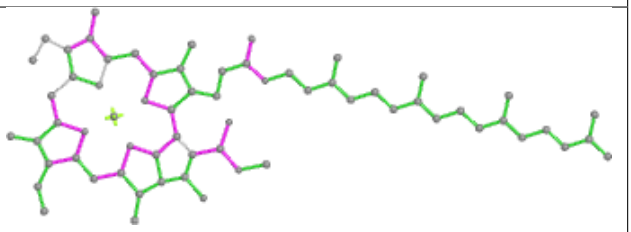
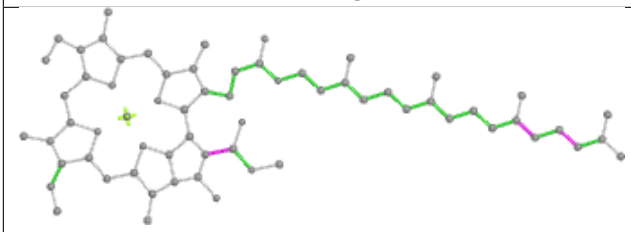
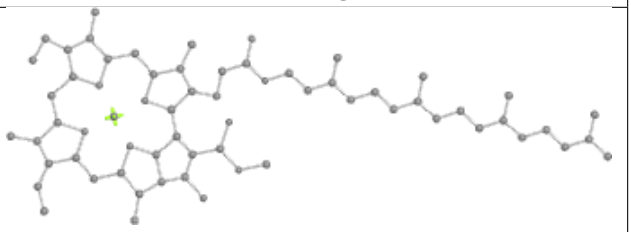


Bond angles

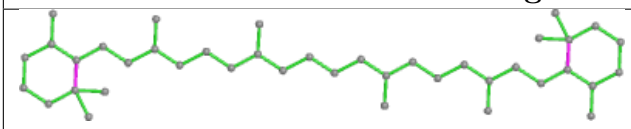


Torsions

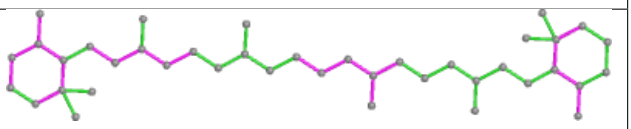


Rings

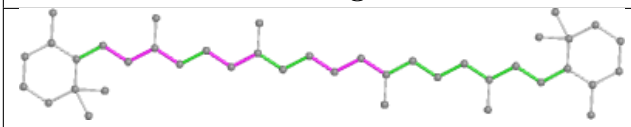
Ligand BCR Z 101



Bond lengths



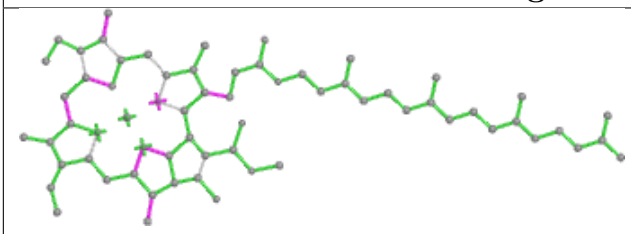
Bond angles



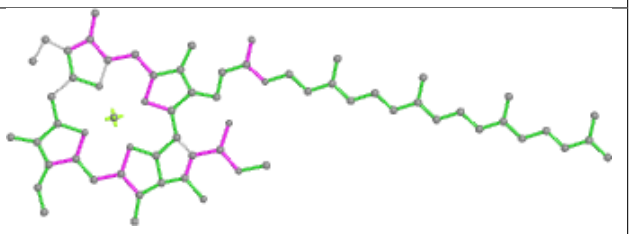
Torsions

Rings

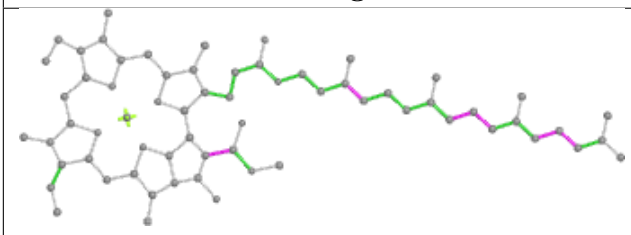
Ligand CLA b 611



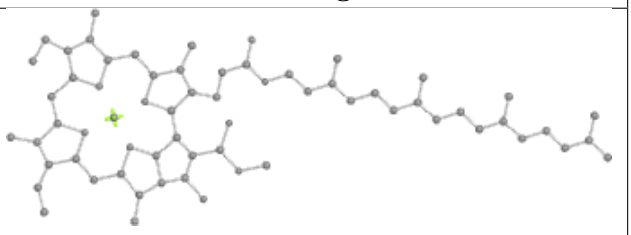
Bond lengths



Bond angles

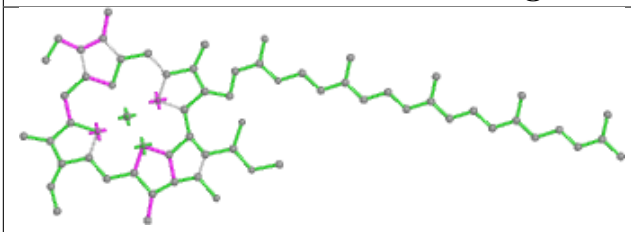


Torsions

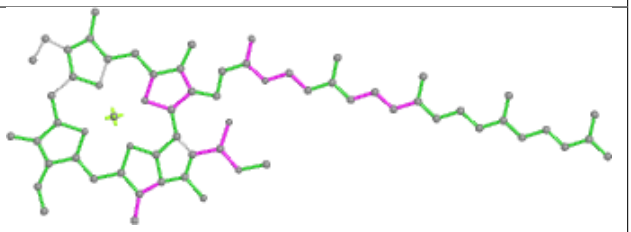


Rings

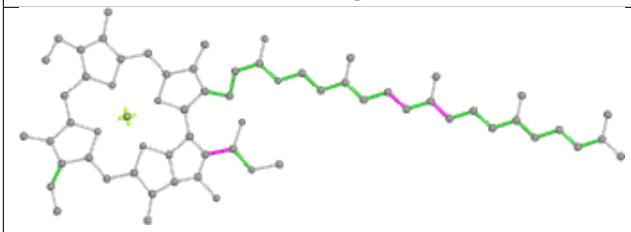
Ligand CLA C 504



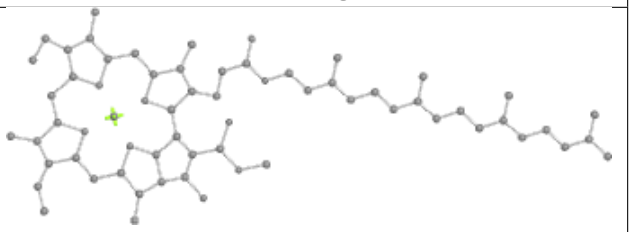
Bond lengths



Bond angles

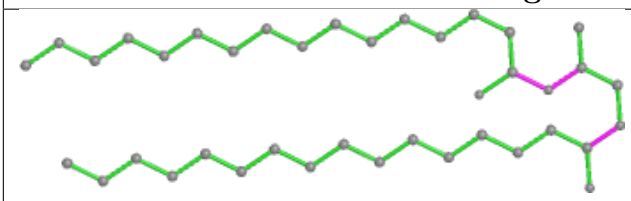


Torsions

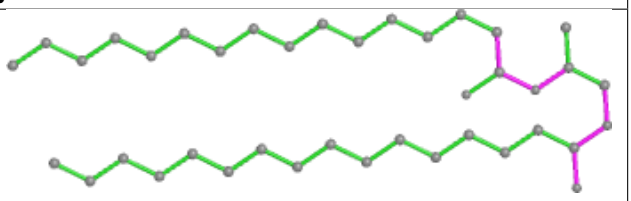


Rings

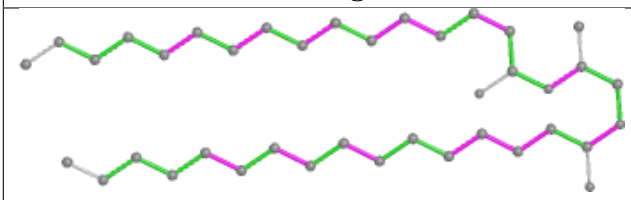
Ligand SQD A 414



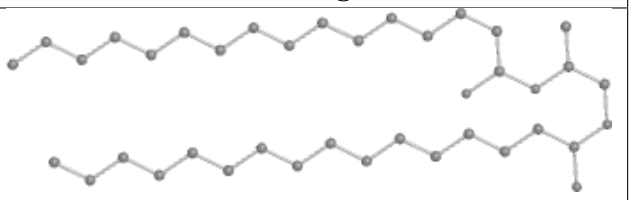
Bond lengths



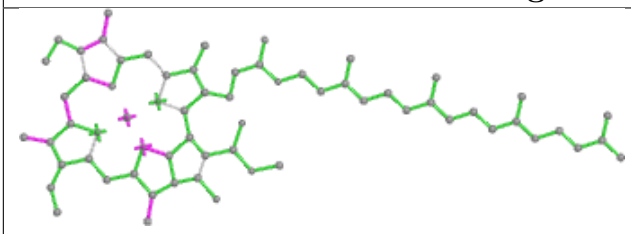
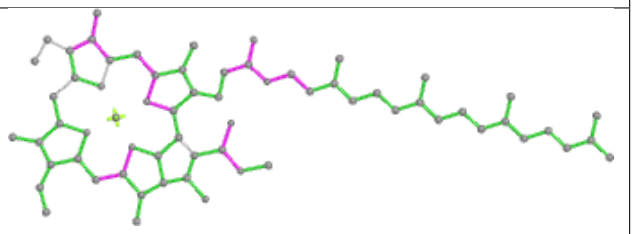
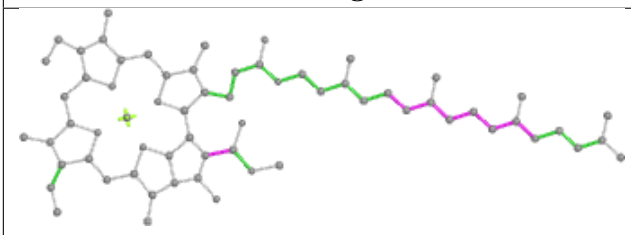
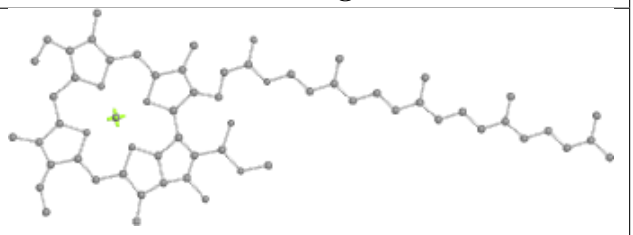
Bond angles

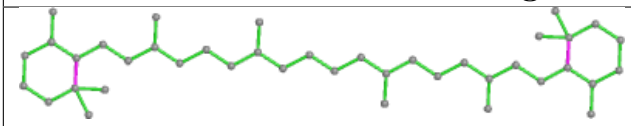
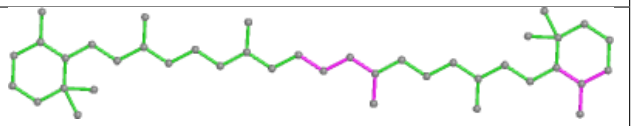
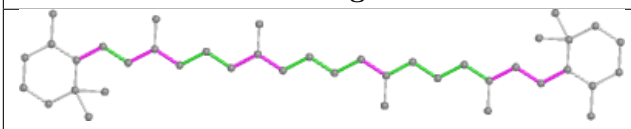
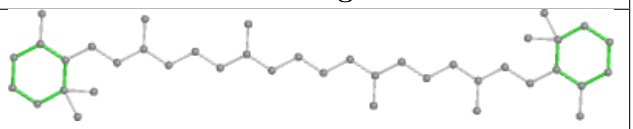


Torsions

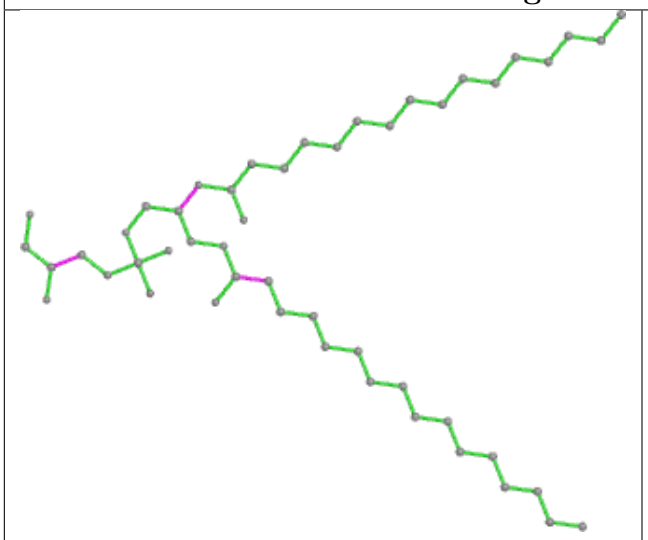


Rings

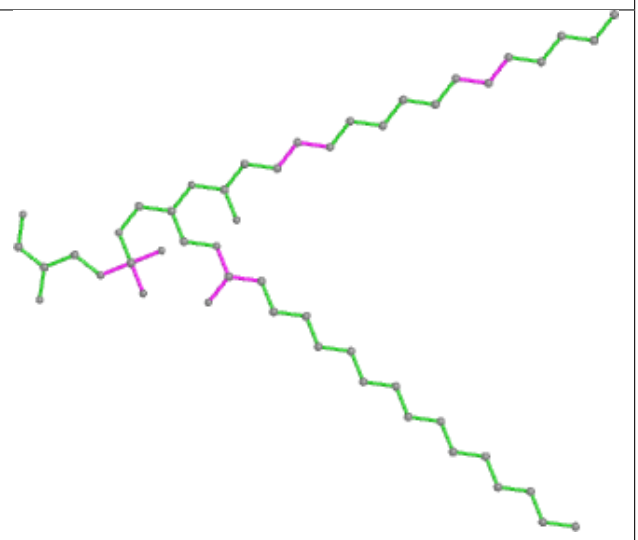
Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

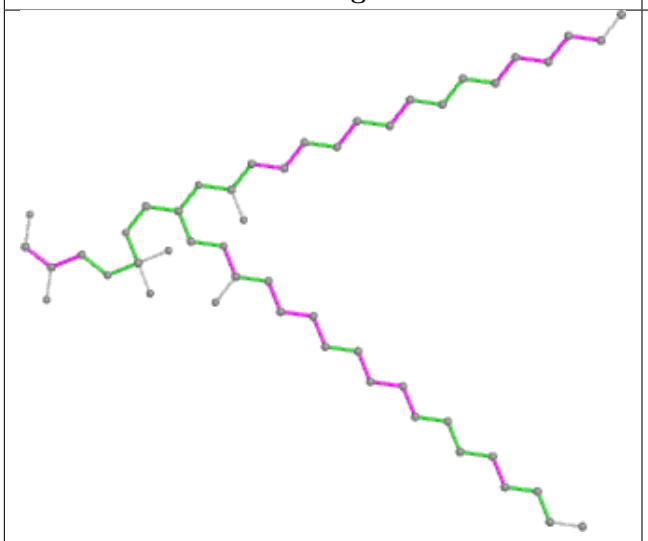
Ligand LHG B 622



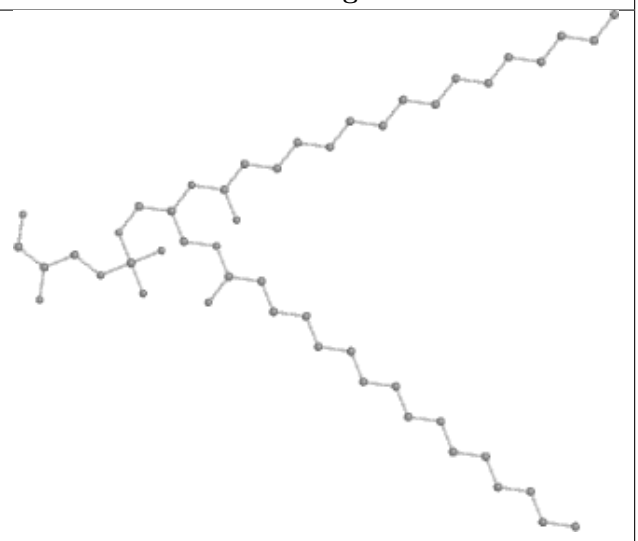
Bond lengths



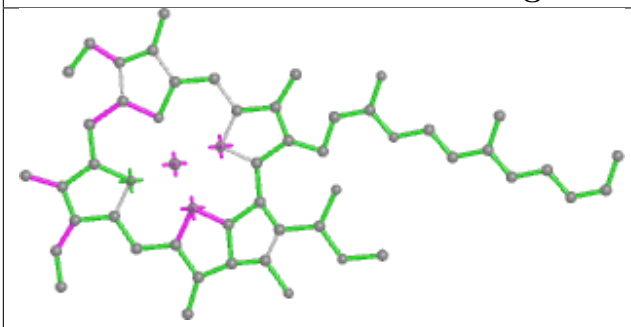
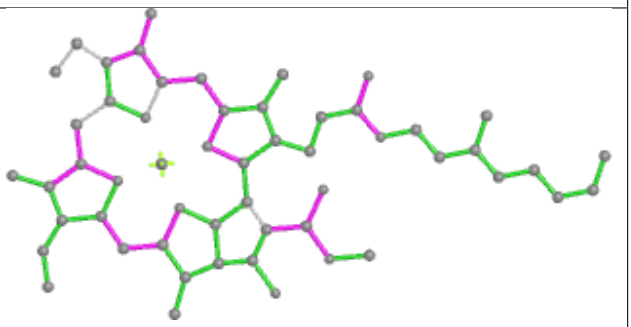
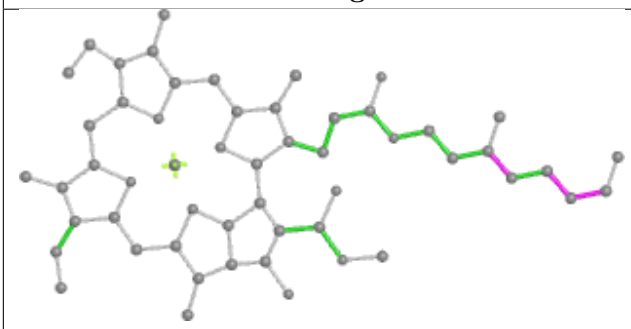
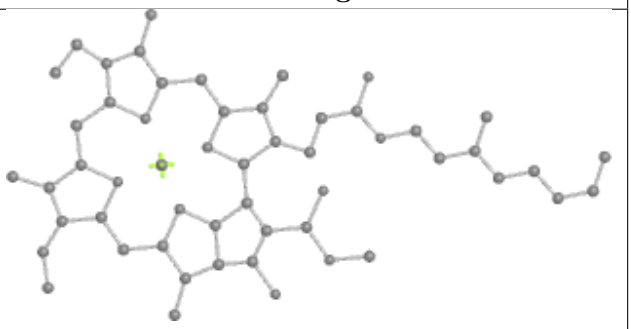
Bond angles

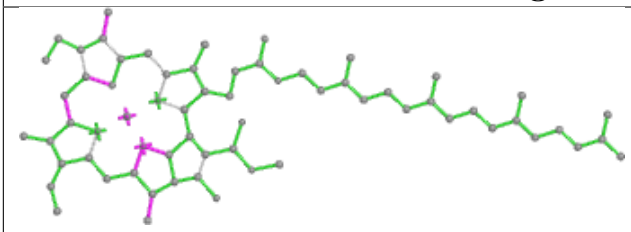
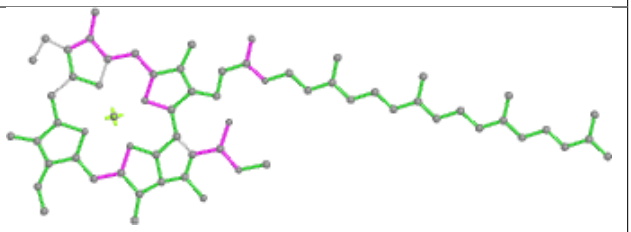
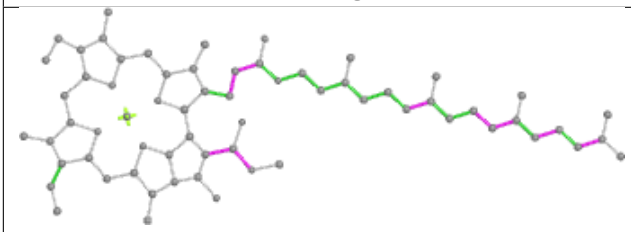
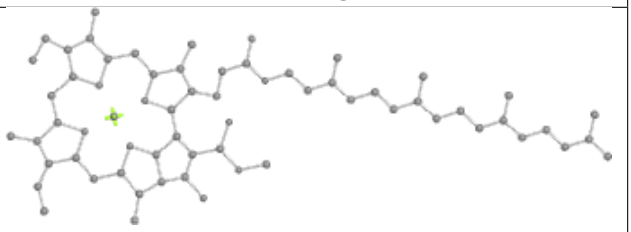


Torsions

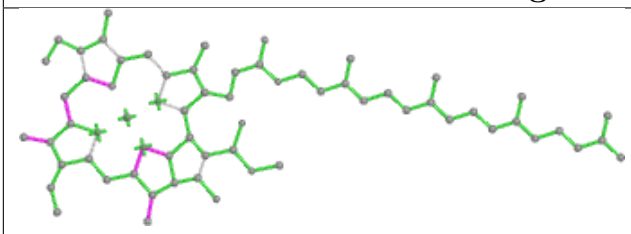


Rings

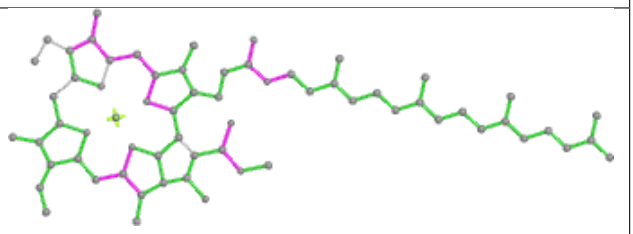
Ligand CLA A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

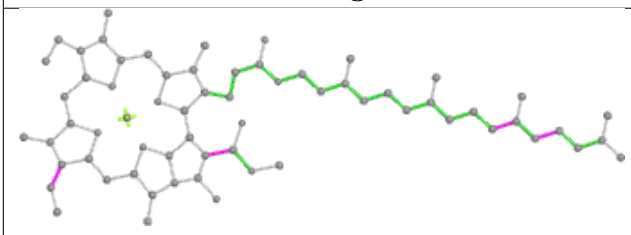
Ligand CLA c 502



Bond lengths



Bond angles



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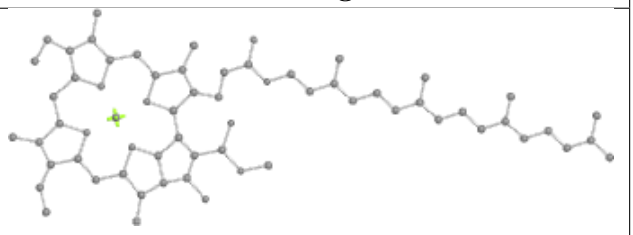
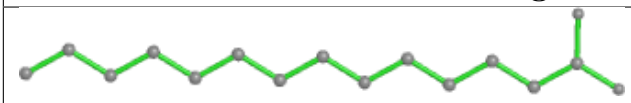


Rings

Ligand STE b 623



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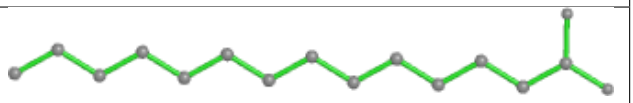
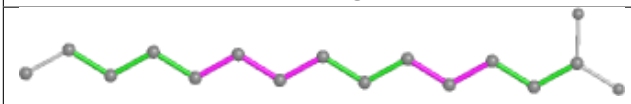


Bond angles



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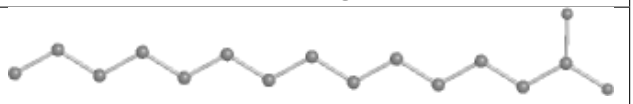
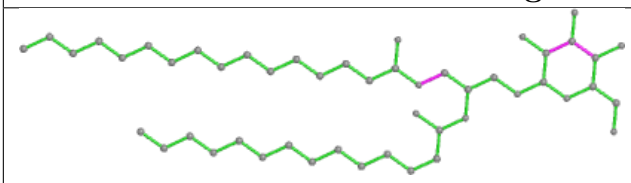
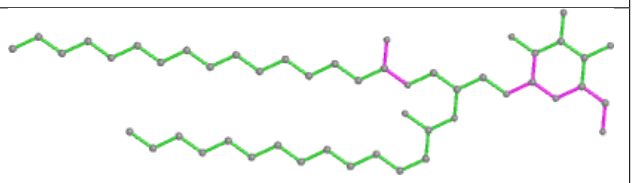


Rings

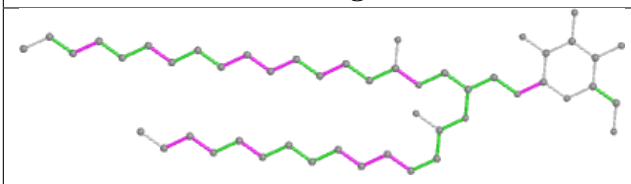
Ligand LMG c 522



Bond lengths



Bond angles



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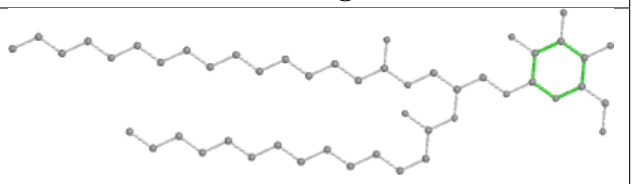
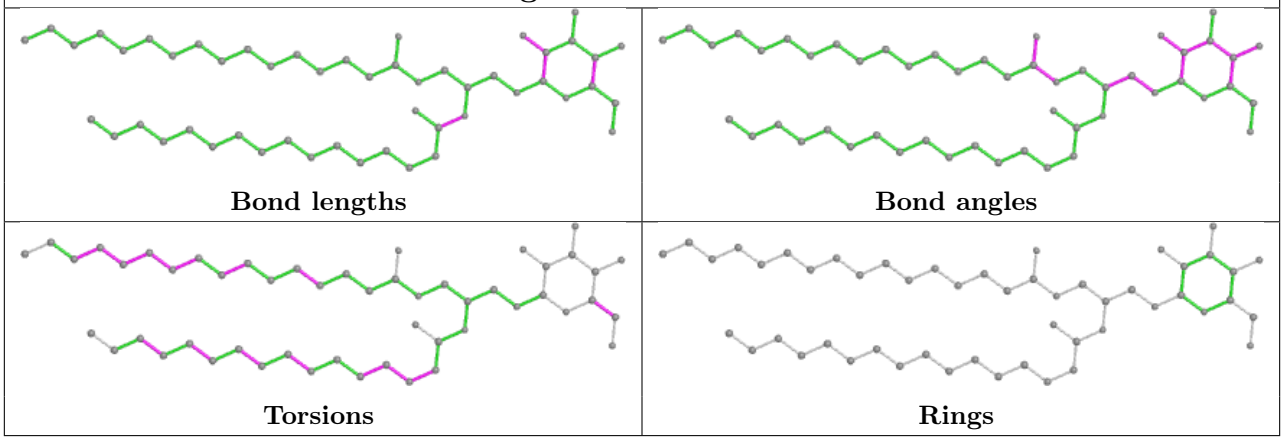
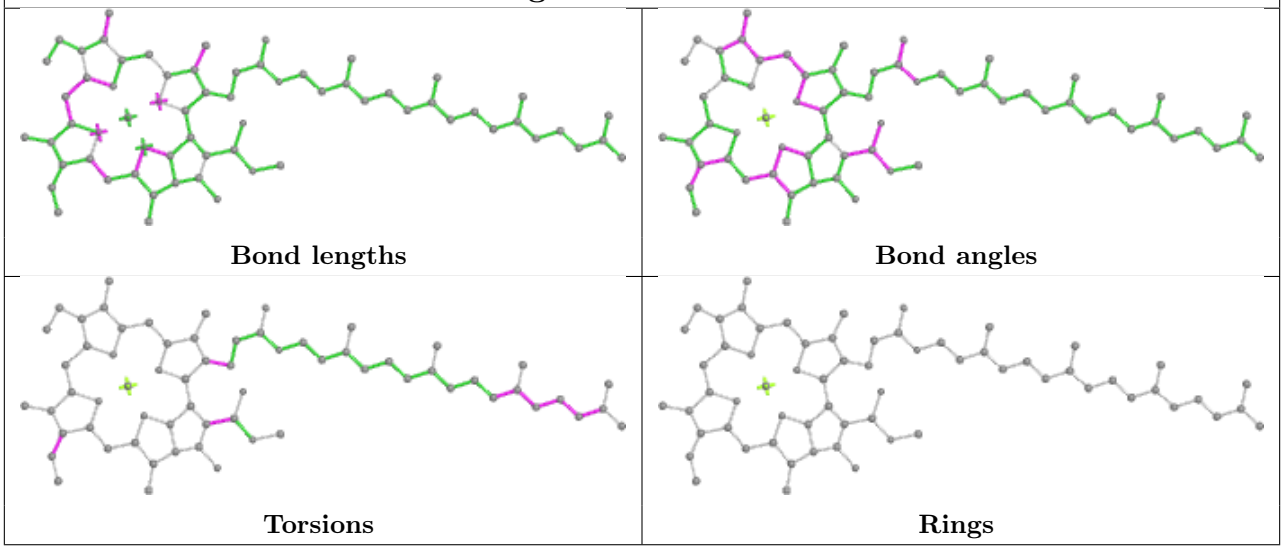


Rings

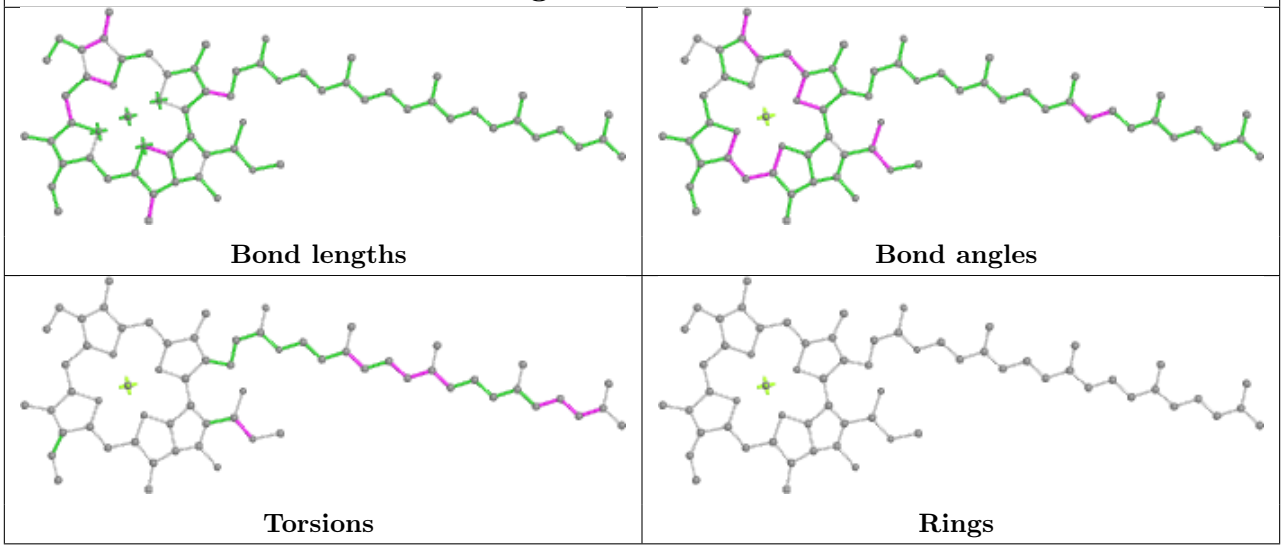
Ligand LMG D 407



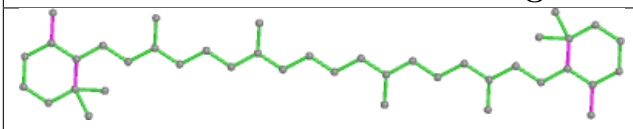
Ligand CLA d 403



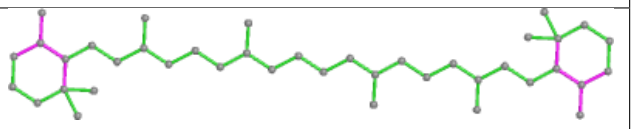
Ligand CLA c 505



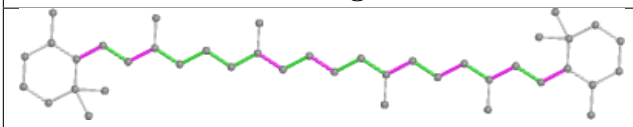
Ligand BCR k 102



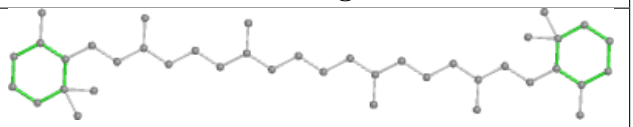
Bond lengths



Bond angles

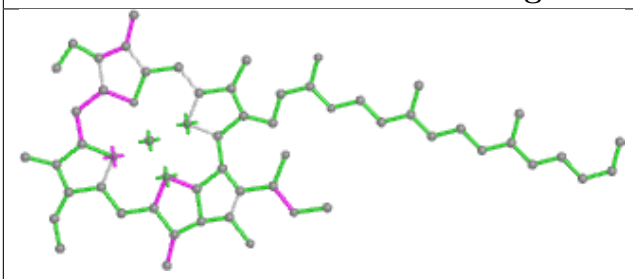


Torsions

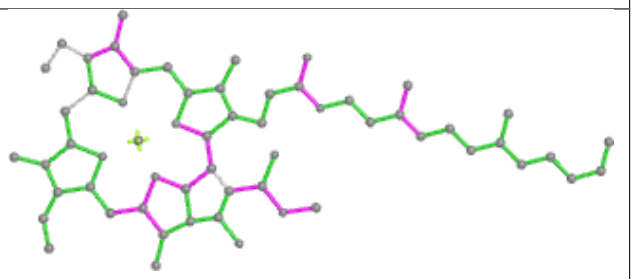


Rings

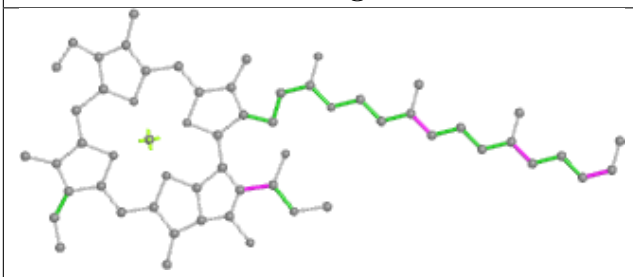
Ligand CLA C 505



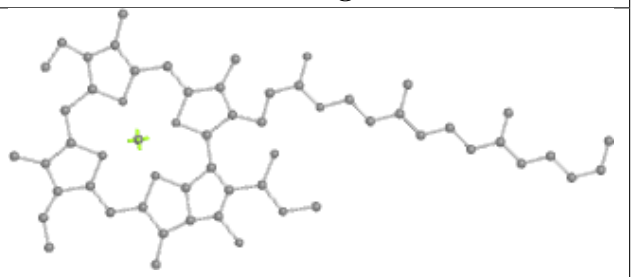
Bond lengths



Bond angles

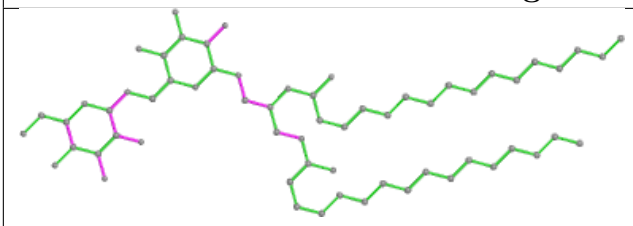


Torsions

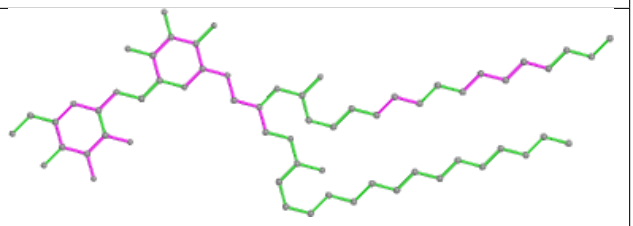


Rings

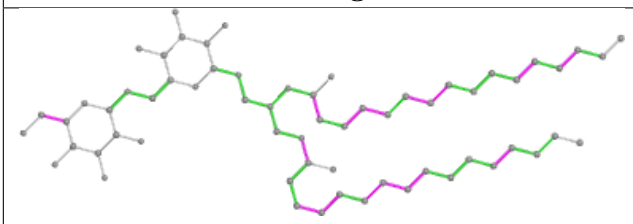
Ligand DGD h 101



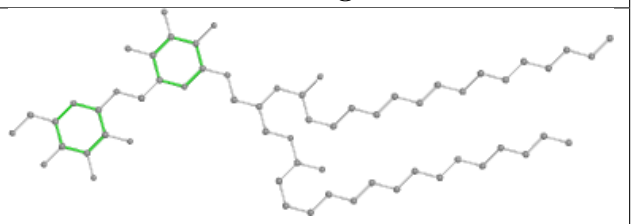
Bond lengths



Bond angles

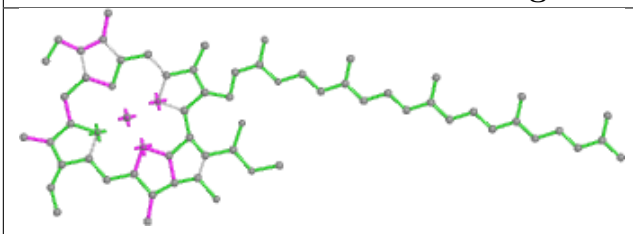


Torsions



Rings

Ligand CLA c 507



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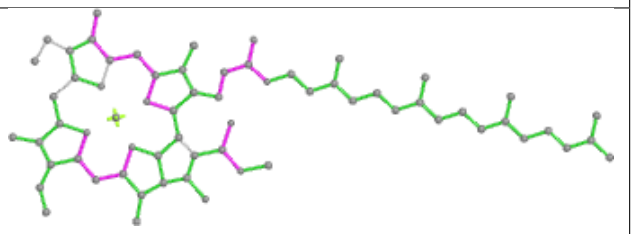
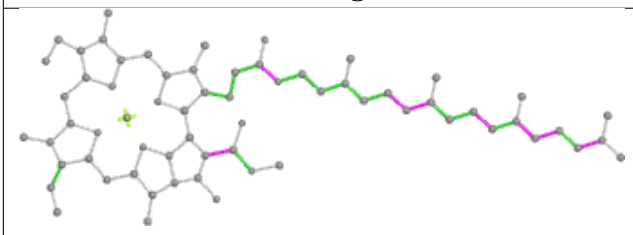
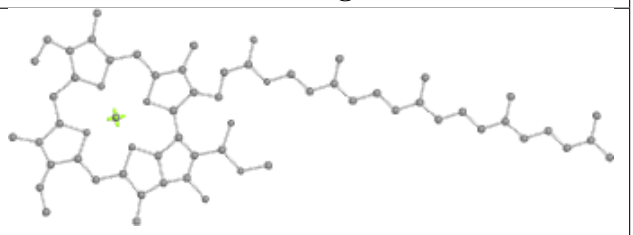


Bond angles

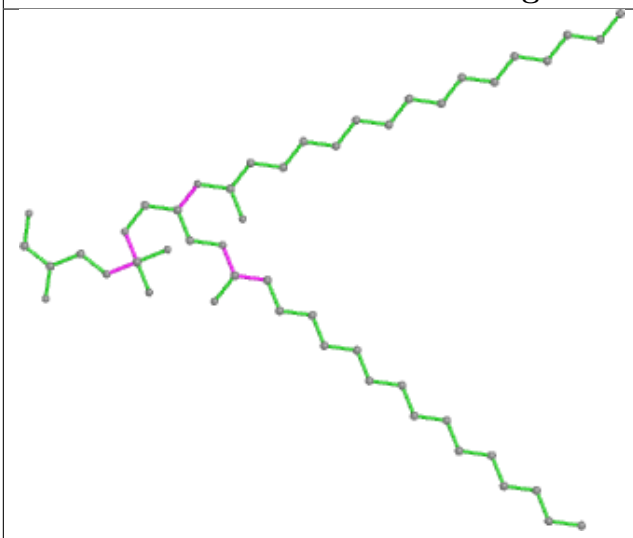


Torsions



Rings

Ligand LHG A 413



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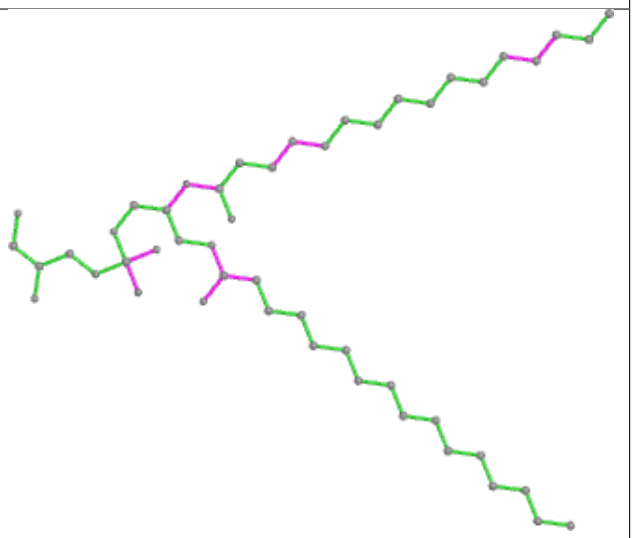
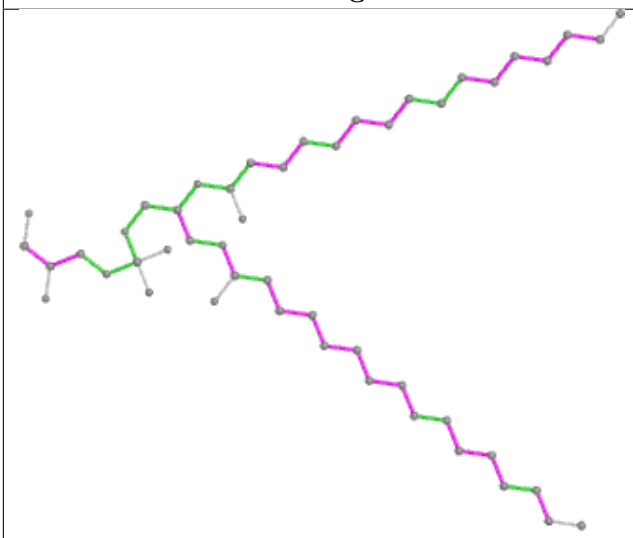
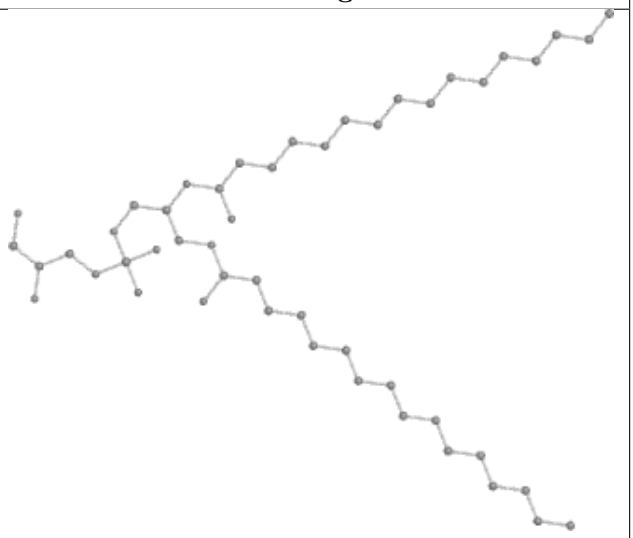


Bond angles

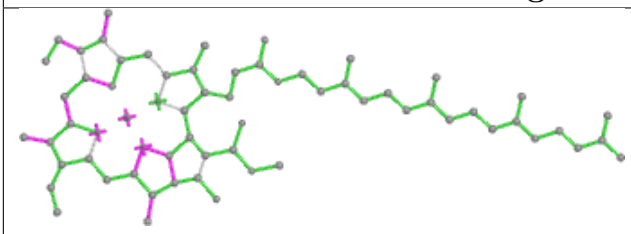


Torsions

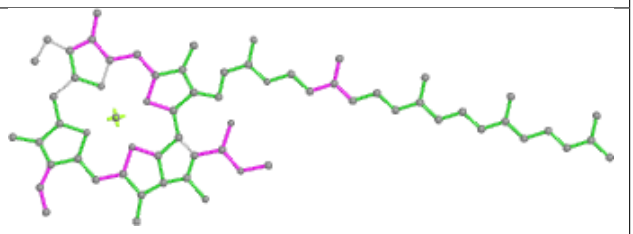


Rings

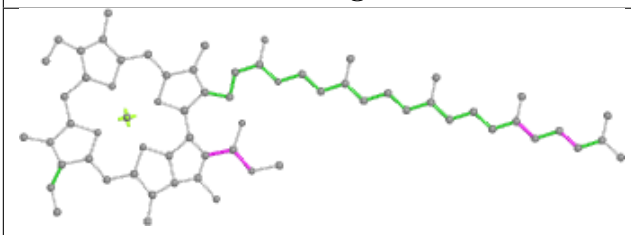
Ligand CLA b 609



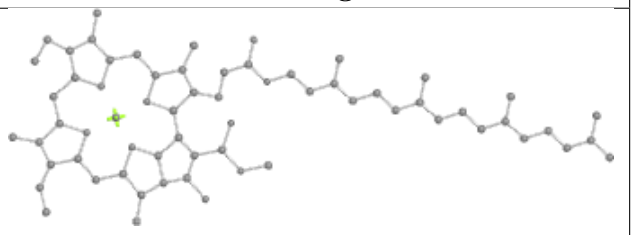
Bond lengths



Bond angles

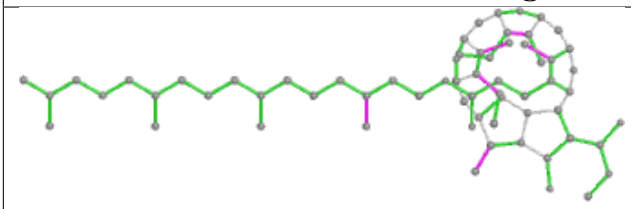


Torsions



Rings

Ligand PHO A 404



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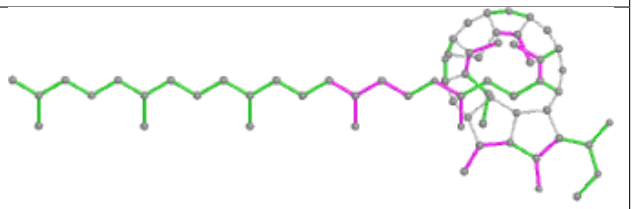
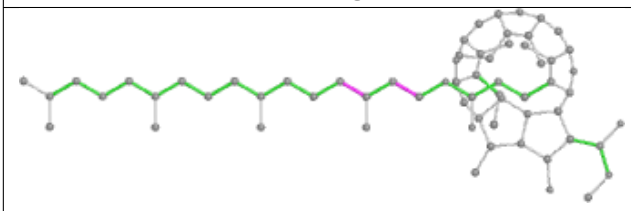
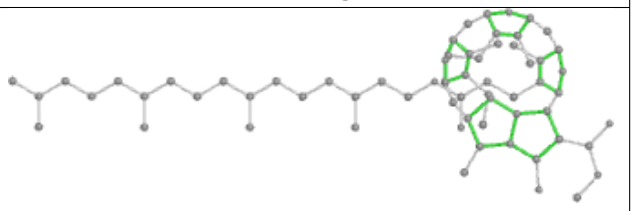


Bond angles

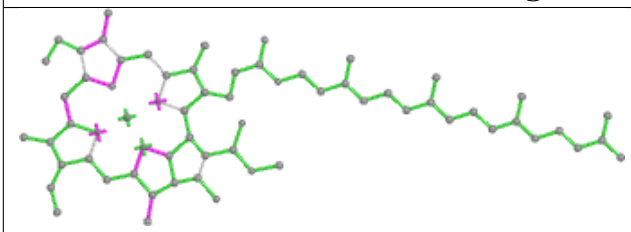


Torsions



Rings

Ligand CLA C 512



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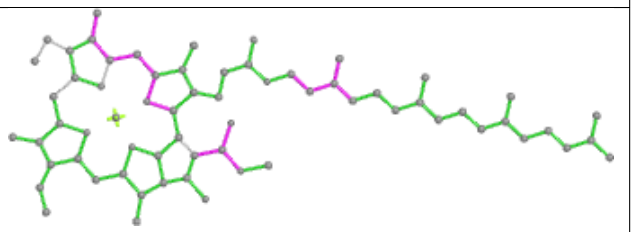
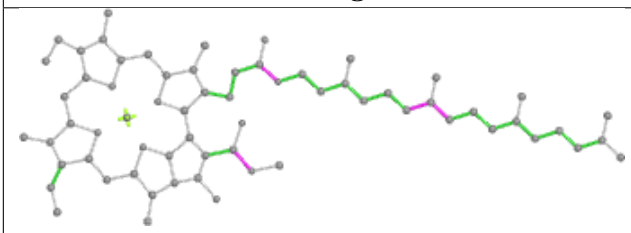
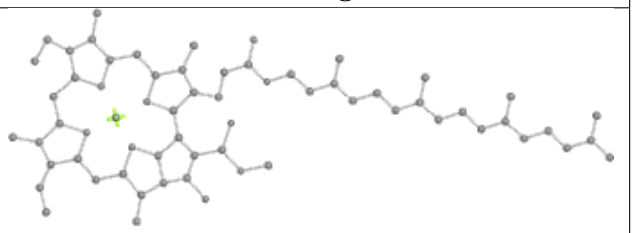


Bond angles

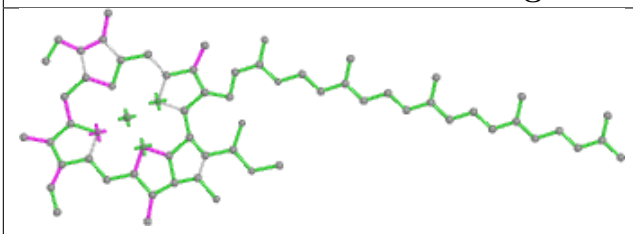


Torsions



Rings

Ligand CLA B 608



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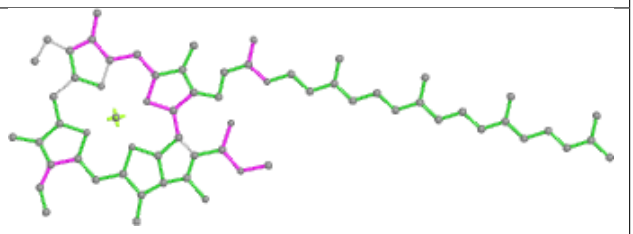
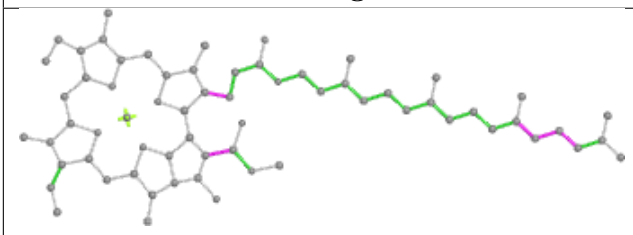


Bond angles



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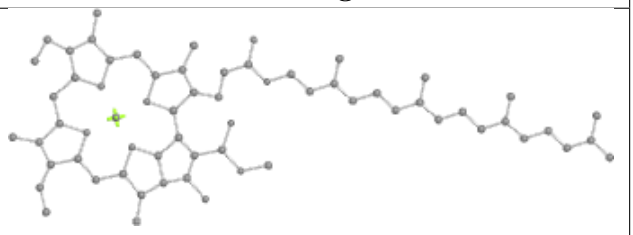
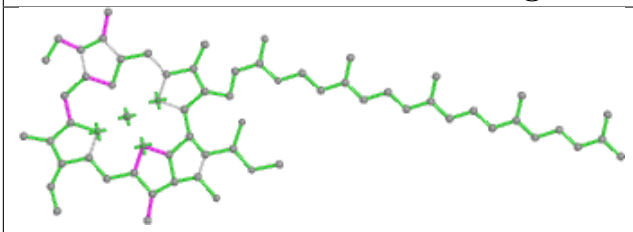


Rings

Ligand CLA D 403



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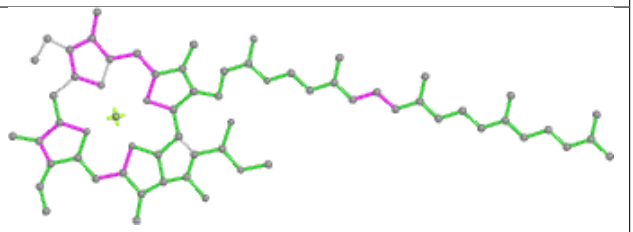
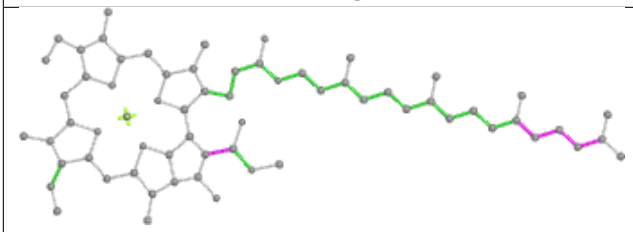


Bond angles



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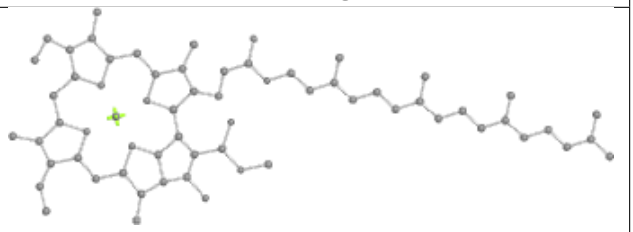
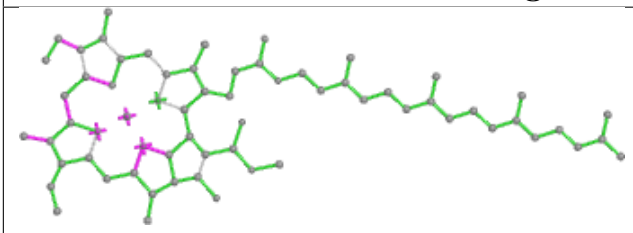
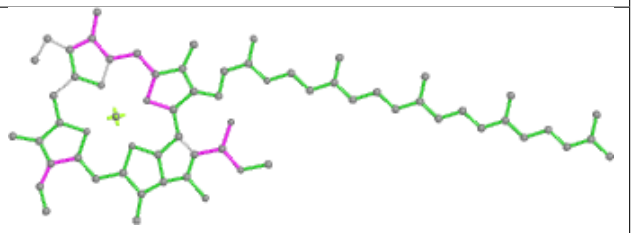


Rings

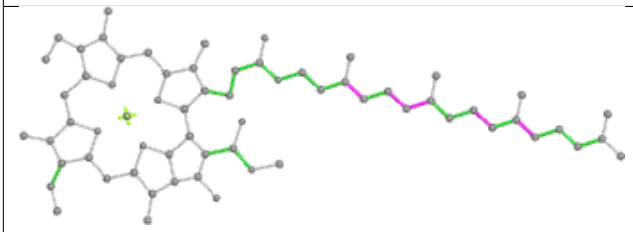
Ligand CLA C 506



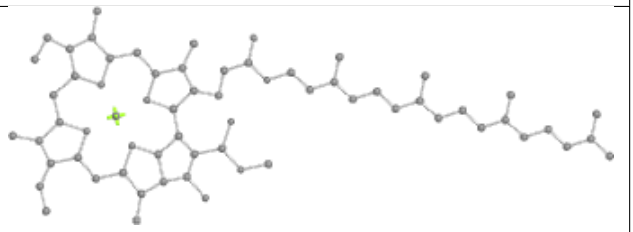
Bond lengths



Bond angles

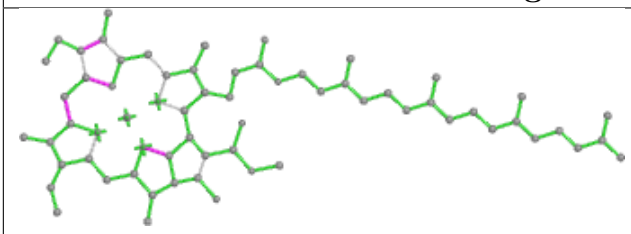


Torsions



Rings

Ligand CLA C 507



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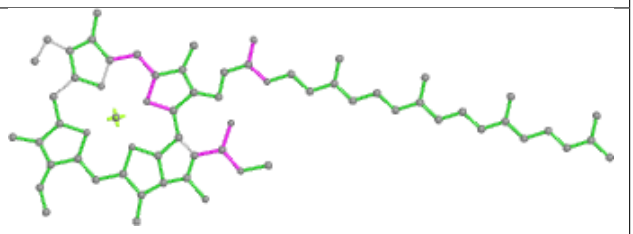
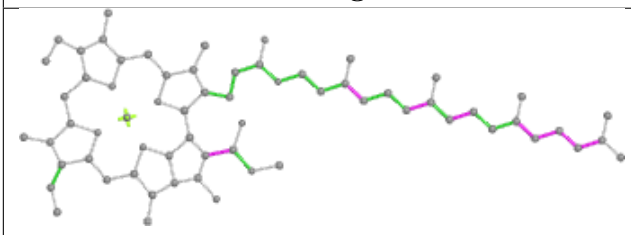
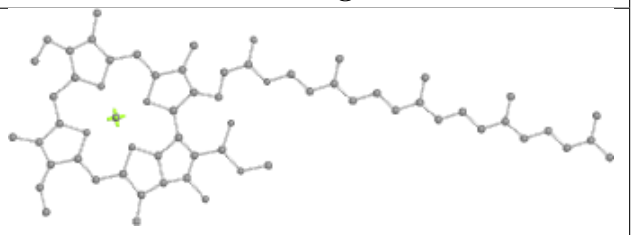


Bond angles

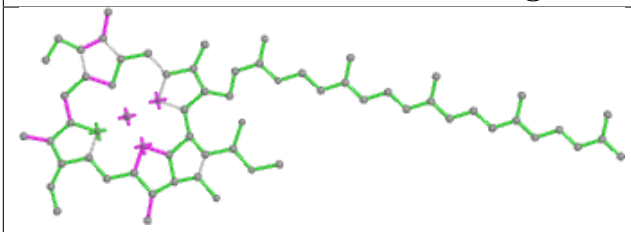


Torsions



Rings

Ligand CLA C 502



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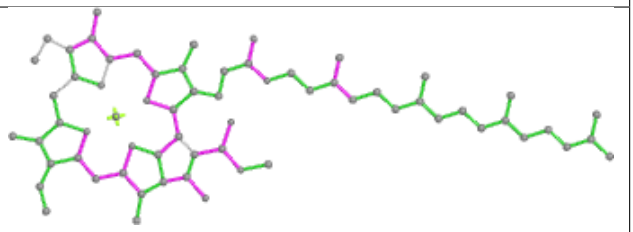
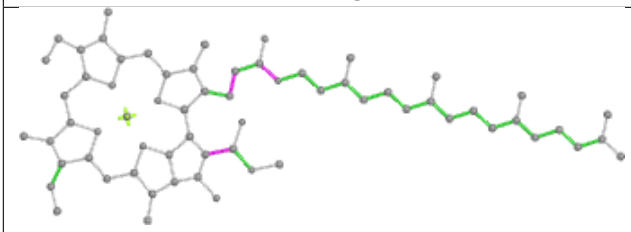
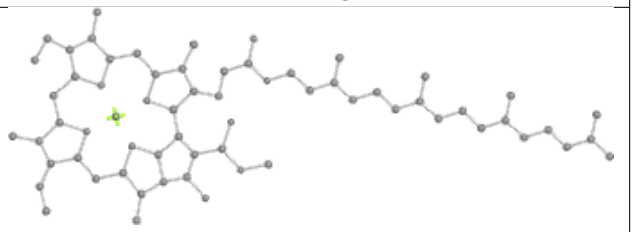


Bond angles

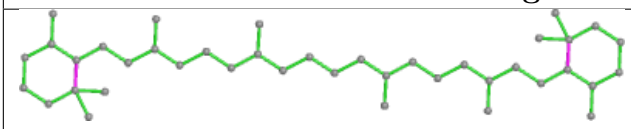


Torsions

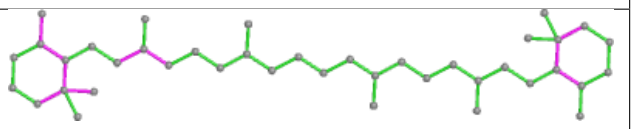


Rings

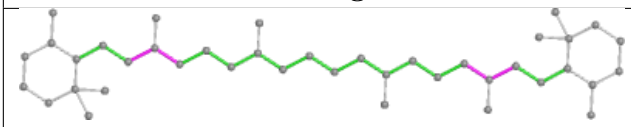
Ligand BCR B 620



Bond lengths



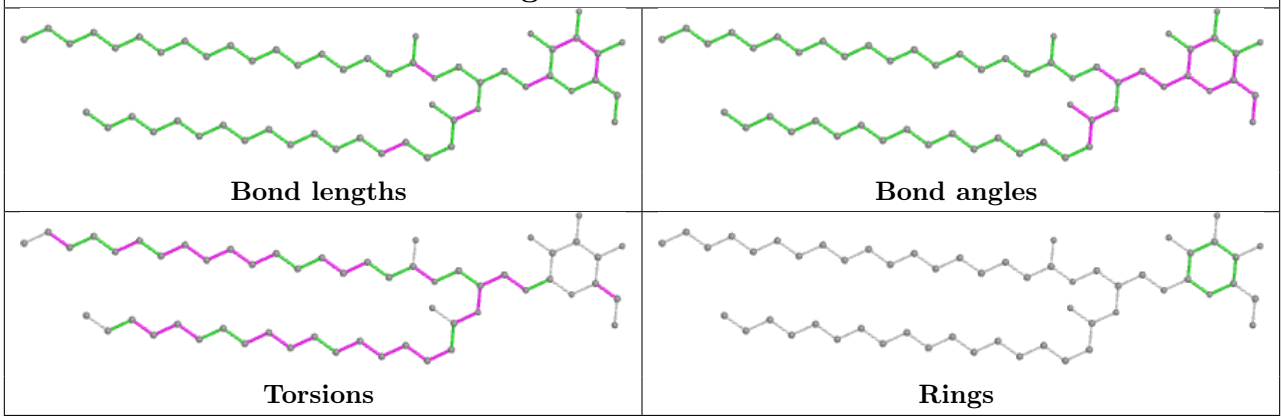
Bond angles



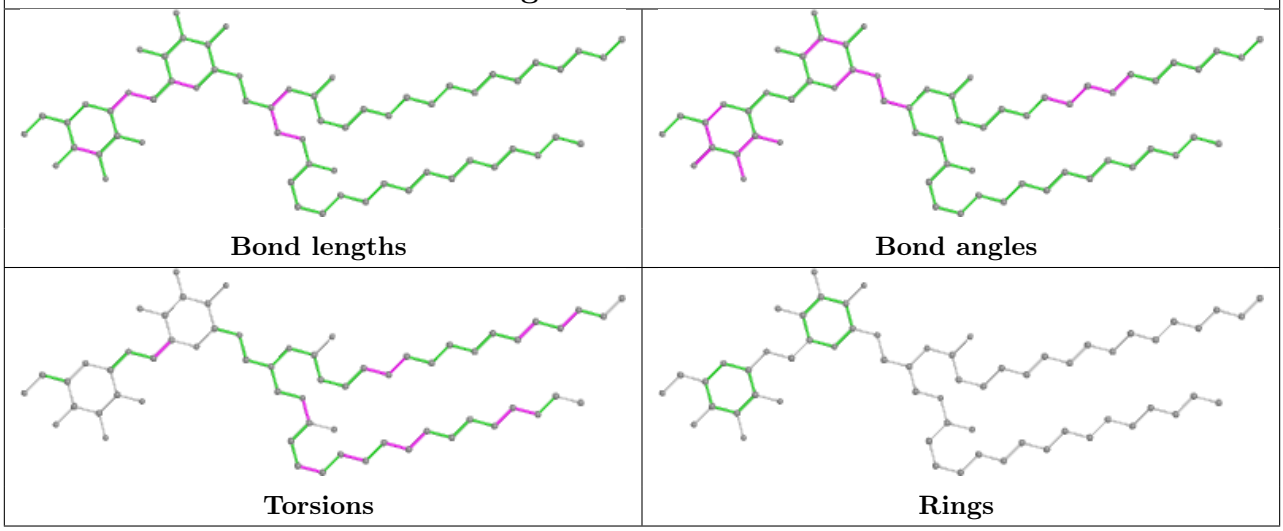
Torsions

Rings

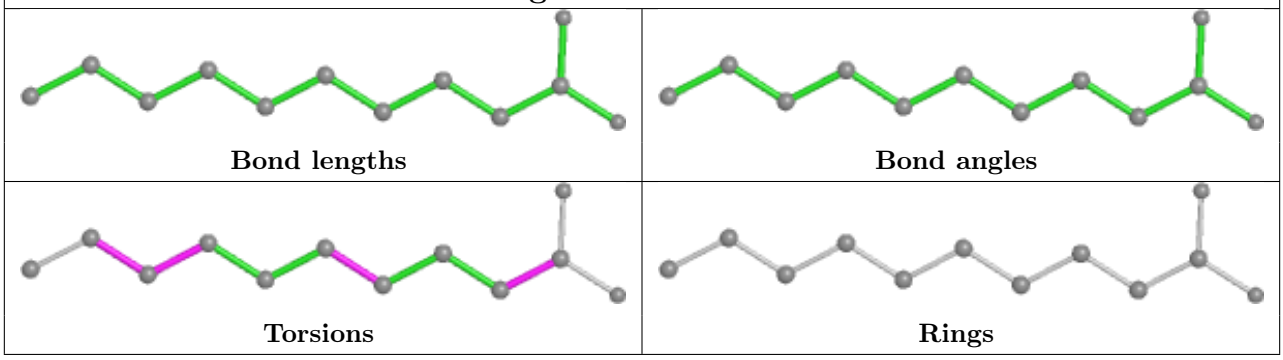
Ligand LMG B 627



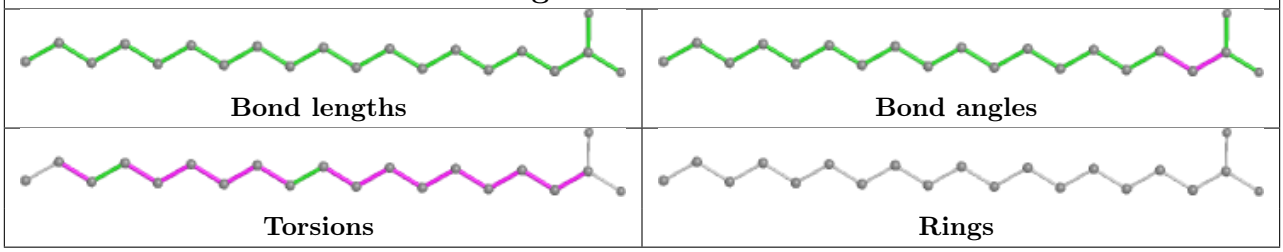
Ligand DGD C 519



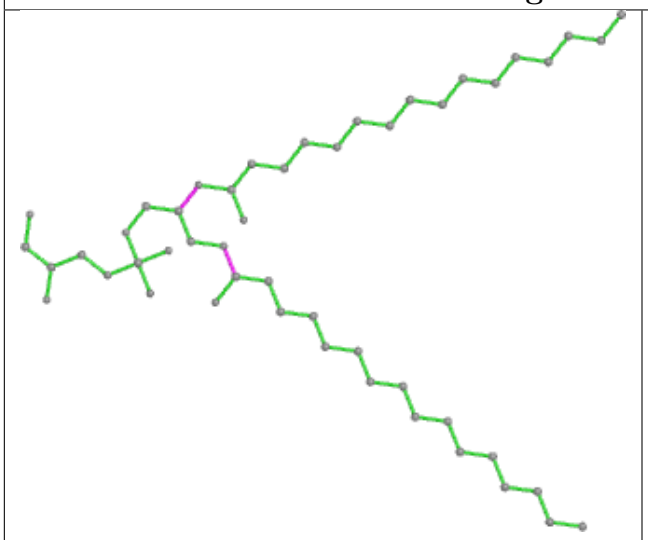
Ligand STE E 102



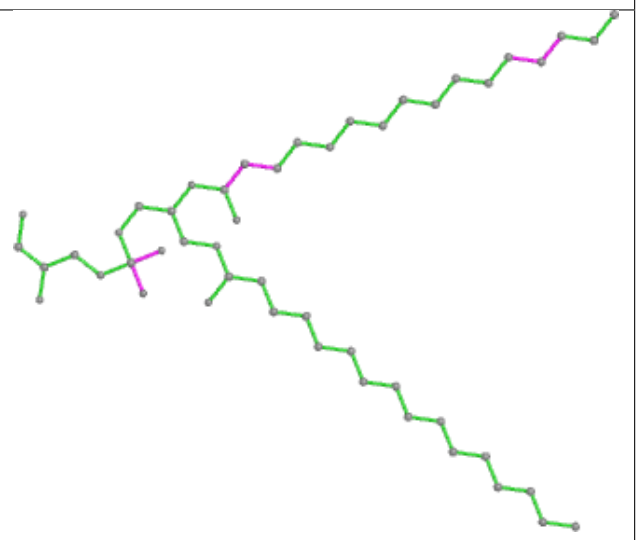
Ligand STE x 102



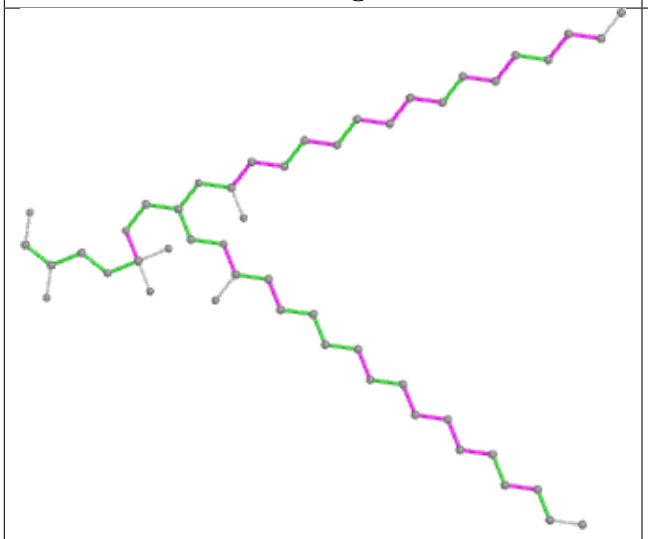
Ligand LHG L 102



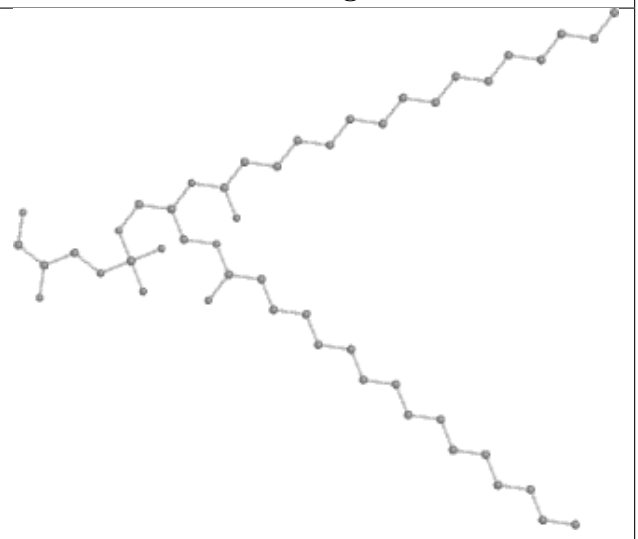
Bond lengths



Bond angles

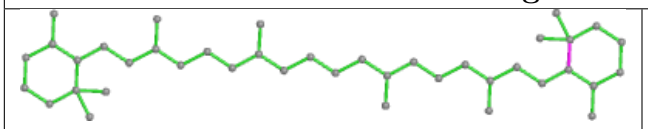


Torsions



Rings

Ligand BCR H 101



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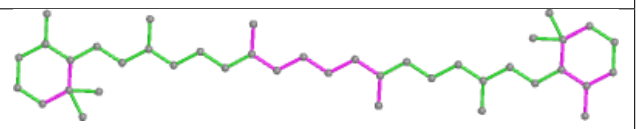
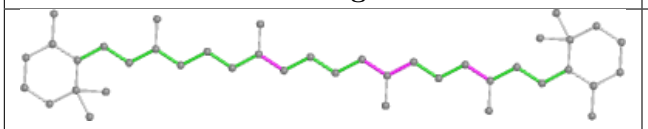


Bond angles



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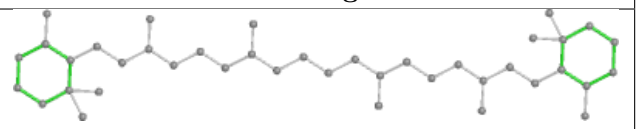
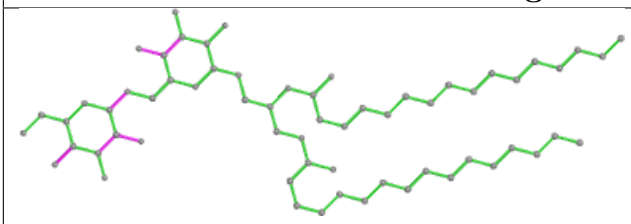


Rings

Ligand DGD c 518



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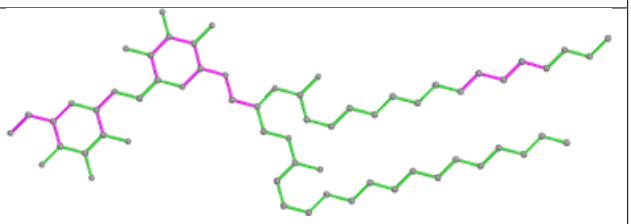
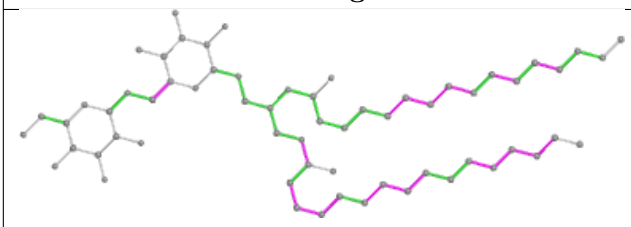


Bond angles



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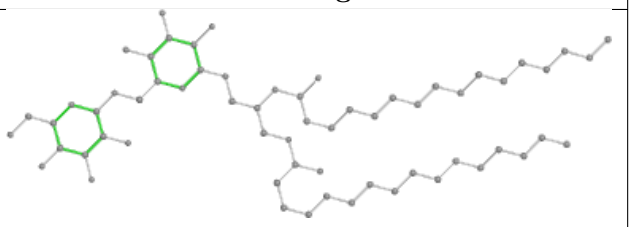
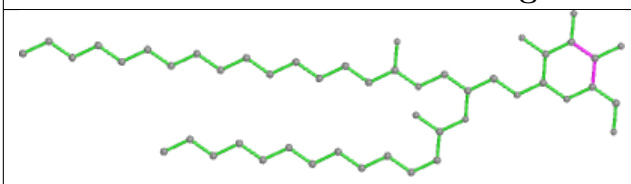


Rings

Ligand LMG C 516



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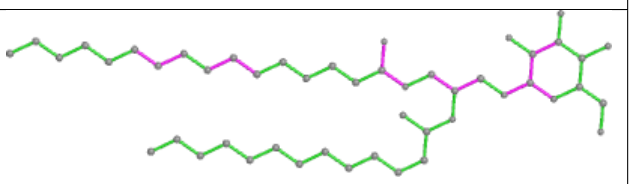
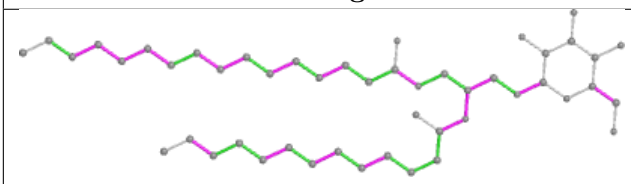


Bond angles



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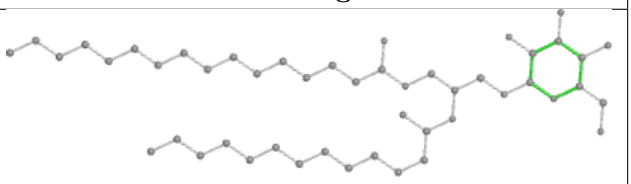
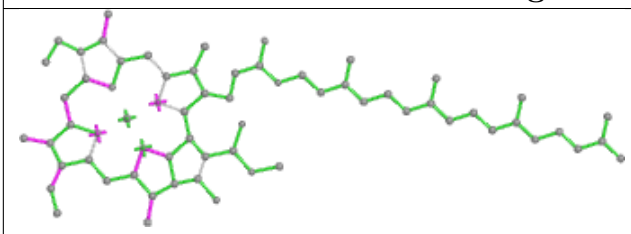
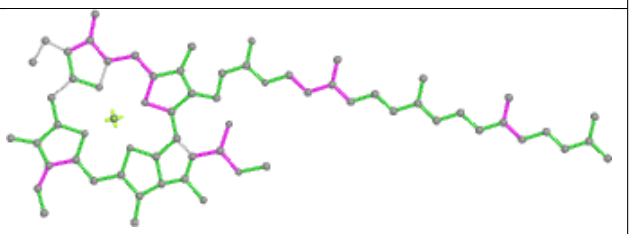


Rings

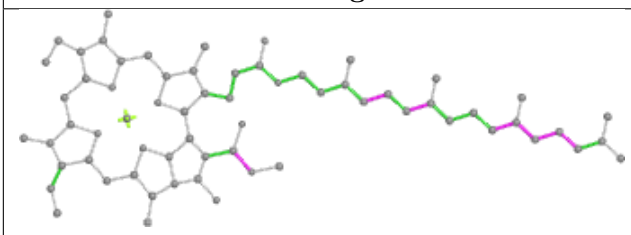
Ligand CLA b 602



Bond lengths



Bond angles



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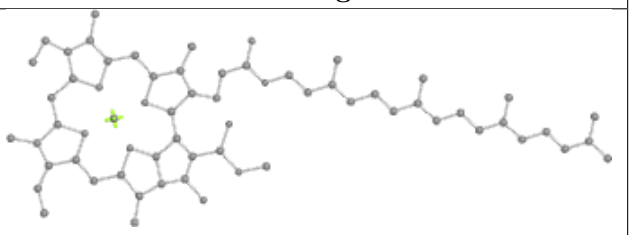
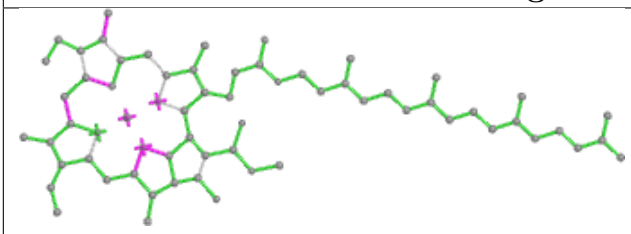


Rings

Ligand CLA d 402



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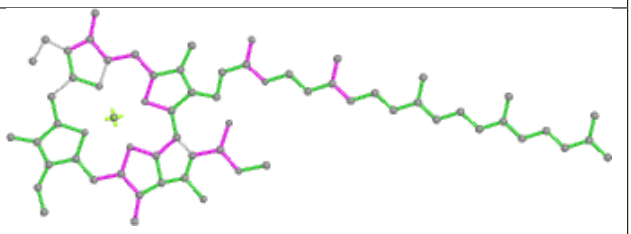
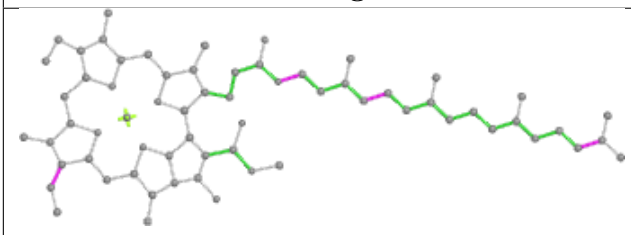


Bond angles



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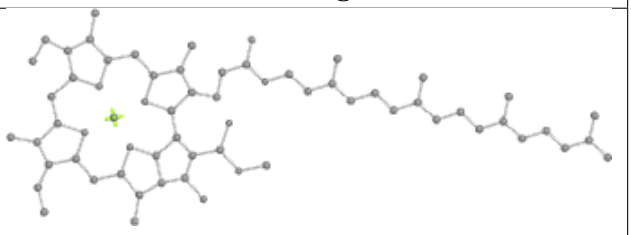
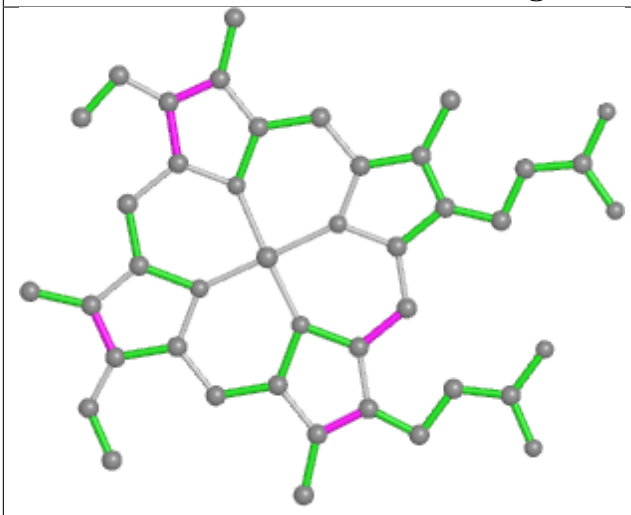
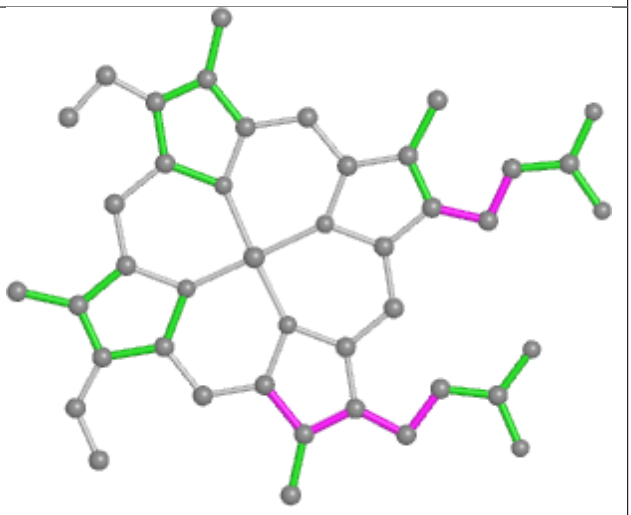


Rings

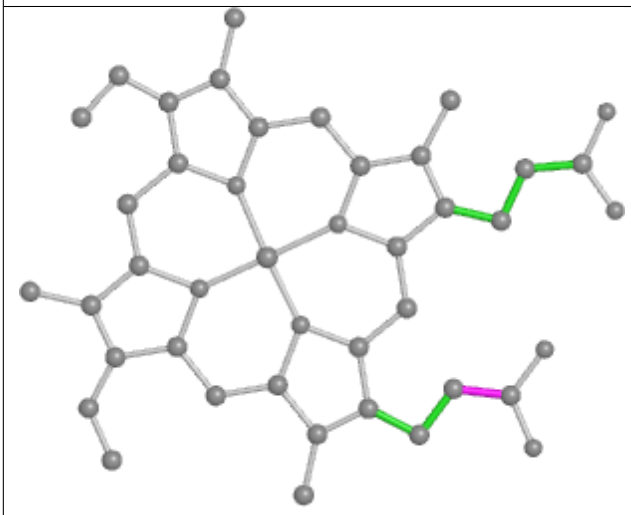
Ligand HEC e 101



Bond lengths



Bond angles



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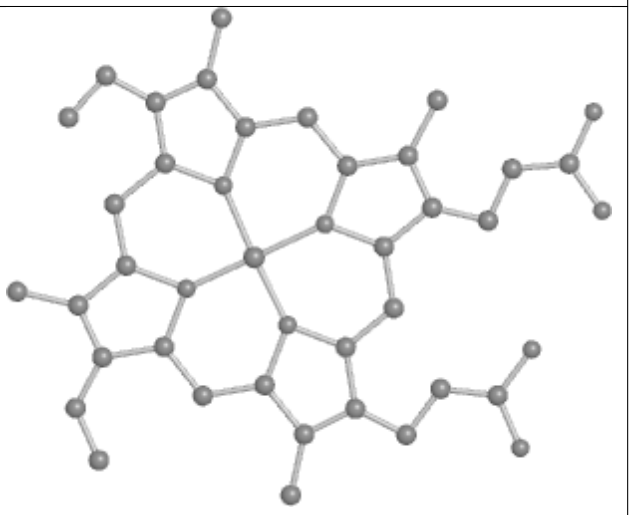
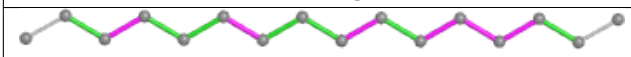


Rings

Ligand STE B 625

Bond lengths

Bond angles



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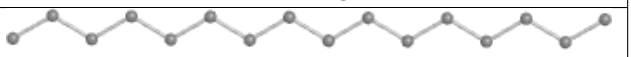
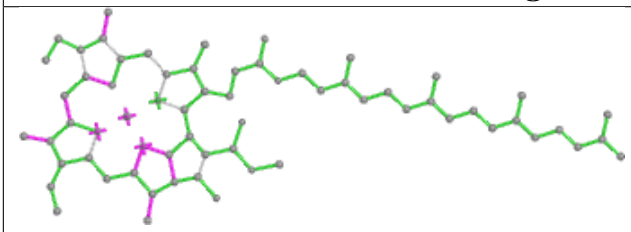


Rings

Ligand CLA C 511



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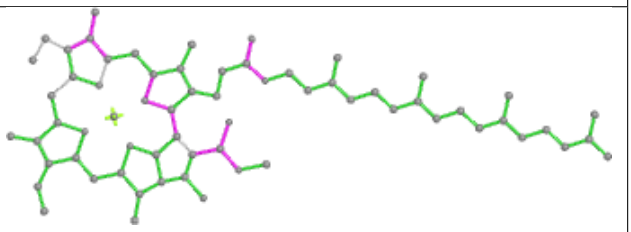
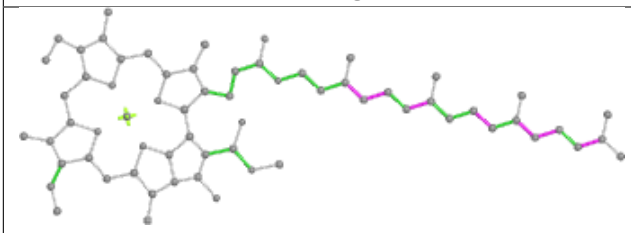


Bond angles



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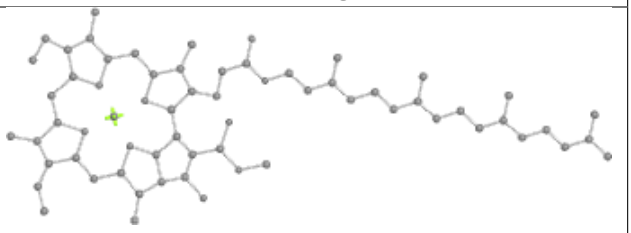
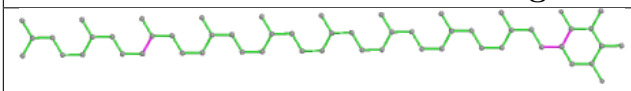


Rings

Ligand PL9 A 410



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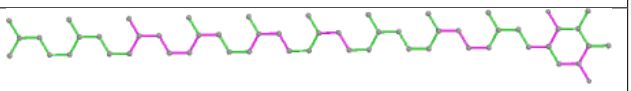
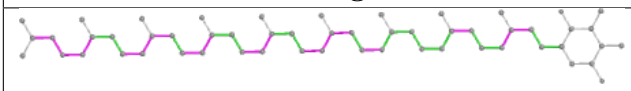
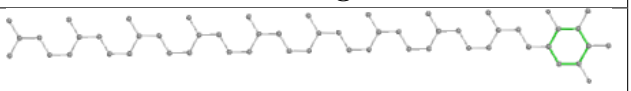


Bond angles

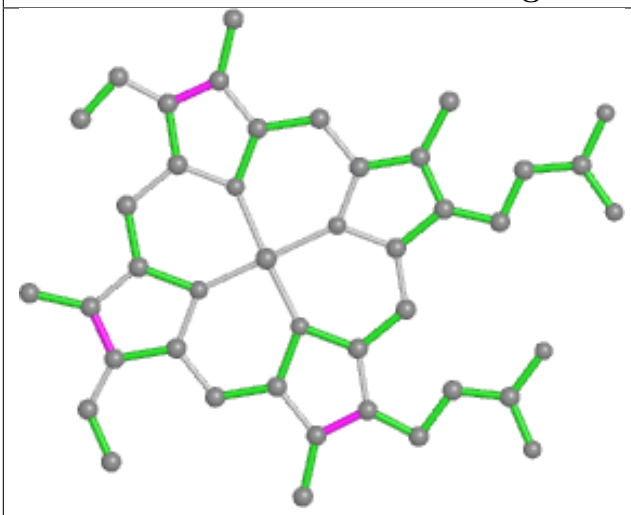


Torsions



Rings

Ligand HEC V 201



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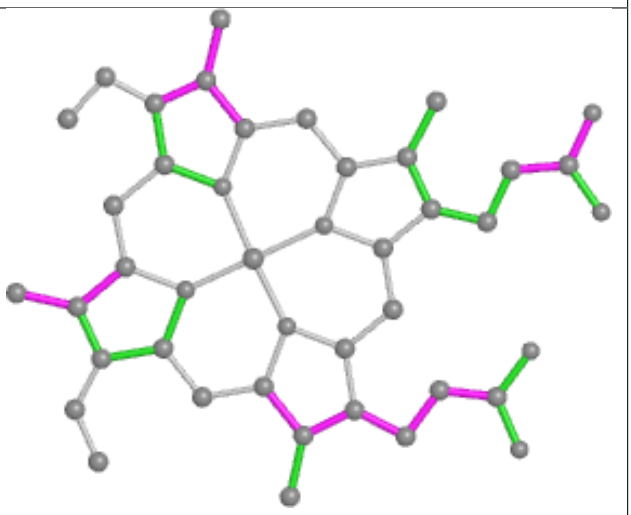
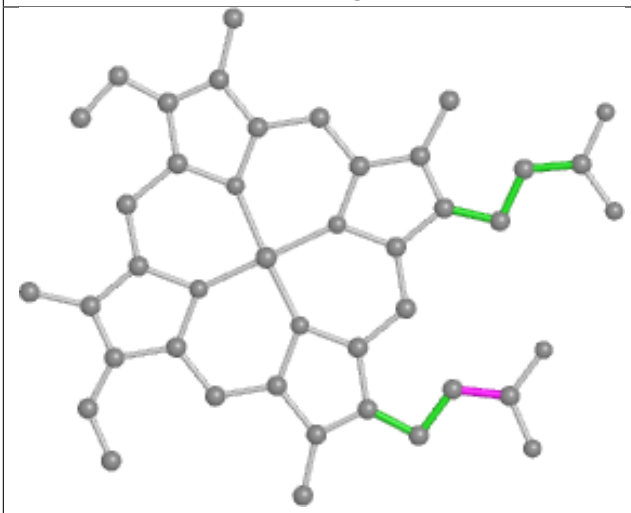


Bond angles



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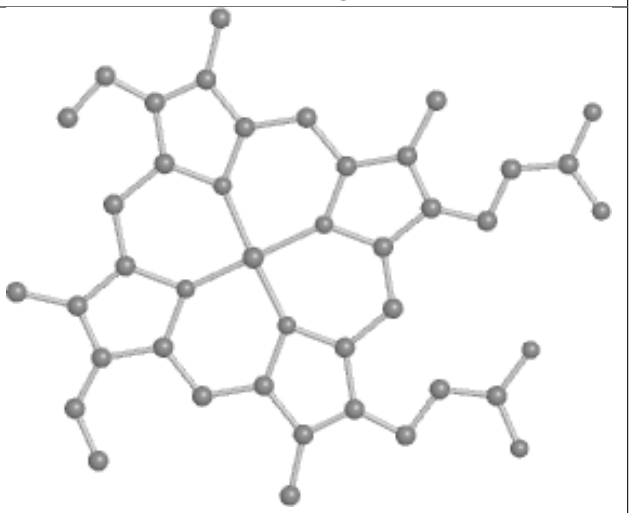
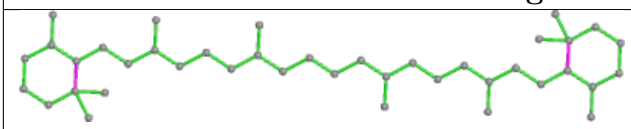


Rings

Ligand BCR k 103



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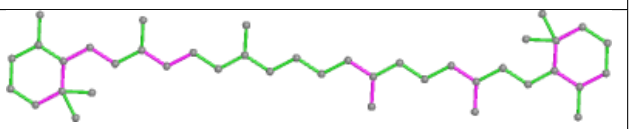
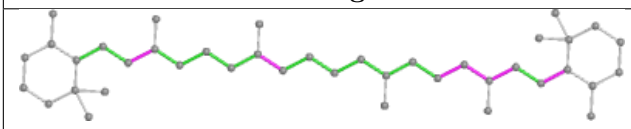
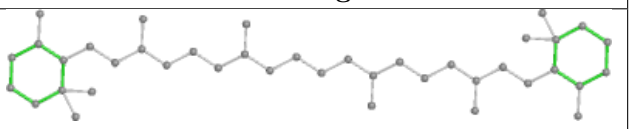


Bond angles

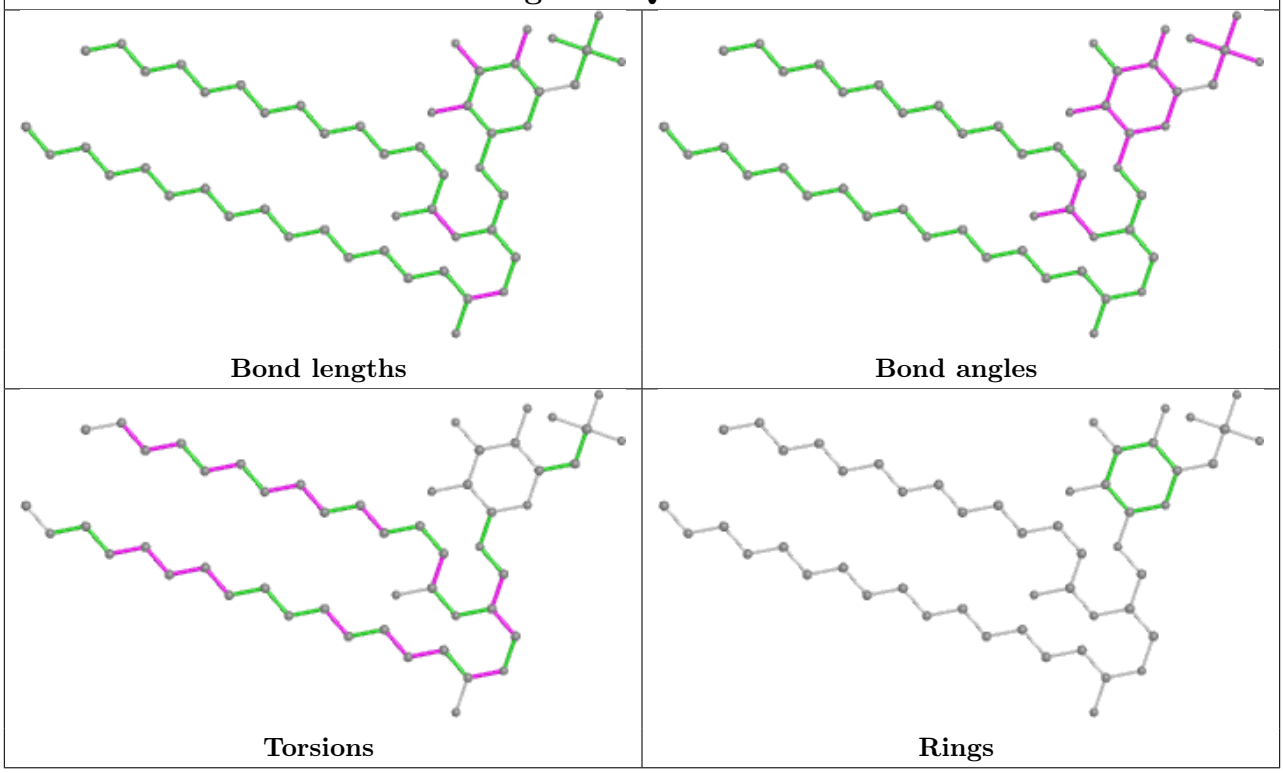


Torsions

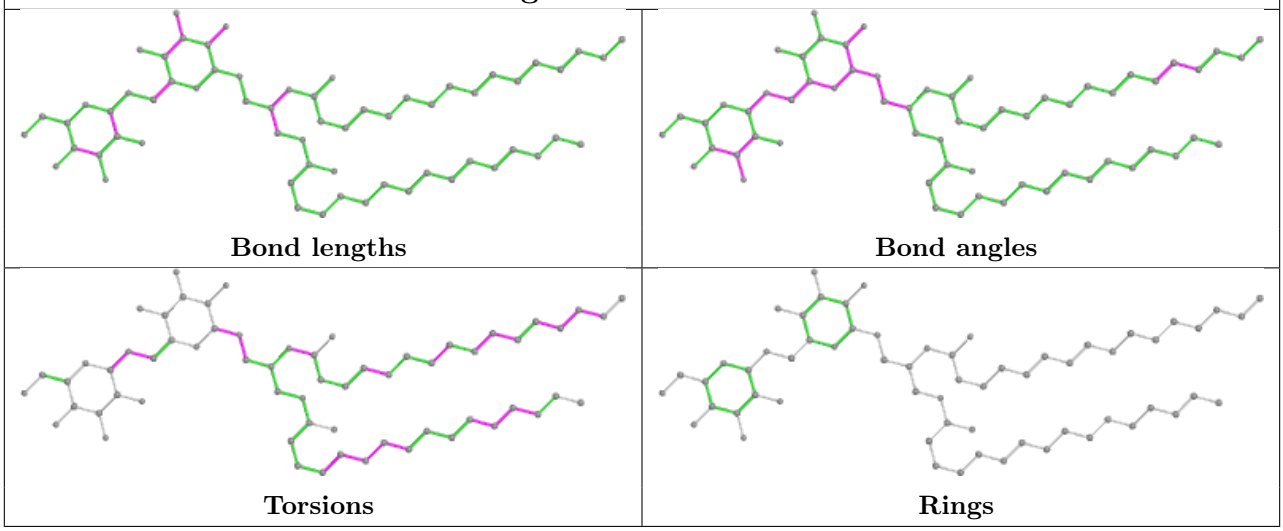


Rings

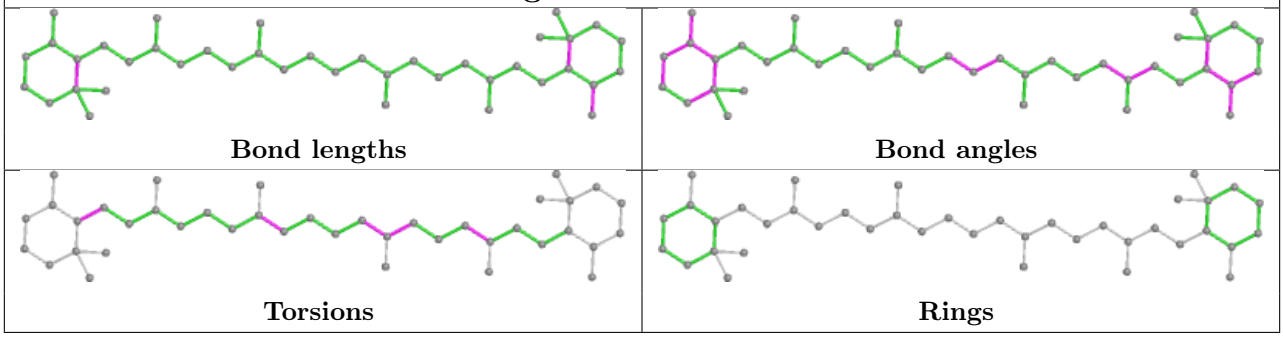
Ligand SQD A 412



Ligand DGD C 518



Ligand BCR B 618



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%)	-0.48	3 (0%)	84	85	25, 31, 49, 74	0
1	a	334/334 (100%)	-0.51	1 (0%)	94	94	24, 33, 58, 85	0
2	B	505/506 (99%)	-0.45	5 (0%)	82	84	25, 35, 62, 85	0
2	b	505/506 (99%)	-0.27	17 (3%)	45	47	27, 38, 71, 104	0
3	C	442/461 (95%)	-0.36	4 (0%)	84	85	27, 38, 54, 78	0
3	c	451/461 (97%)	-0.32	6 (1%)	77	79	27, 41, 61, 93	0
4	D	341/352 (96%)	-0.43	1 (0%)	94	94	24, 32, 48, 82	0
4	d	341/352 (96%)	-0.36	2 (0%)	89	89	26, 36, 59, 85	0
5	E	82/84 (97%)	-0.12	2 (2%)	59	62	34, 52, 69, 83	0
5	e	82/84 (97%)	0.09	5 (6%)	21	23	43, 58, 78, 83	0
6	F	34/45 (75%)	-0.56	1 (2%)	51	55	36, 44, 63, 73	0
6	f	34/45 (75%)	-0.36	1 (2%)	51	55	43, 50, 78, 84	0
7	H	65/66 (98%)	-0.14	1 (1%)	73	75	34, 41, 59, 80	0
7	h	63/66 (95%)	0.20	4 (6%)	20	22	43, 53, 66, 69	0
8	I	35/38 (92%)	-0.32	2 (5%)	23	25	35, 41, 68, 78	0
8	i	35/38 (92%)	-0.02	3 (8%)	10	11	34, 41, 79, 91	0
9	J	36/40 (90%)	0.01	4 (11%)	5	5	36, 49, 73, 87	0
9	j	36/40 (90%)	0.09	4 (11%)	5	5	38, 51, 85, 94	0
10	K	37/46 (80%)	0.07	2 (5%)	25	28	46, 53, 74, 77	0
10	k	37/46 (80%)	-0.13	0	100	100	48, 54, 67, 81	0
11	L	37/37 (100%)	-0.59	0	100	100	26, 33, 63, 79	0
11	l	36/37 (97%)	-0.29	3 (8%)	11	12	28, 33, 69, 81	0
12	M	32/36 (88%)	-0.17	1 (3%)	49	52	29, 36, 60, 71	0
12	m	31/36 (86%)	-0.19	0	100	100	29, 36, 55, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.15	10 (4%) 37 40	27, 44, 78, 124	0
13	o	244/272 (89%)	-0.19	13 (5%) 26 29	28, 42, 76, 118	0
14	R	34/40 (85%)	1.79	11 (32%) 0 0	57, 72, 91, 102	0
14	r	31/40 (77%)	3.41	23 (74%) 0 0	75, 92, 106, 121	0
15	T	29/30 (96%)	-0.59	1 (3%) 45 47	27, 33, 63, 78	0
15	t	29/30 (96%)	-0.34	3 (10%) 6 6	29, 35, 82, 91	0
16	U	97/134 (72%)	-0.34	3 (3%) 49 52	34, 44, 69, 84	0
16	u	97/134 (72%)	-0.53	0 100 100	31, 42, 60, 81	0
17	V	137/163 (84%)	-0.61	0 100 100	32, 42, 57, 77	0
17	v	137/163 (84%)	-0.28	3 (2%) 62 65	34, 47, 68, 81	0
18	X	38/41 (92%)	0.01	3 (7%) 12 14	40, 51, 71, 79	0
18	x	39/41 (95%)	0.44	5 (12%) 3 3	48, 59, 87, 102	0
19	Y	27/46 (58%)	1.23	9 (33%) 0 0	55, 71, 90, 94	0
19	y	30/46 (65%)	0.57	4 (13%) 3 3	58, 73, 85, 96	0
20	Z	62/62 (100%)	0.71	11 (17%) 1 1	52, 65, 108, 123	0
20	z	62/62 (100%)	0.72	11 (17%) 1 1	51, 71, 104, 112	0
All	All	5302/5666 (93%)	-0.26	182 (3%) 45 47	24, 40, 73, 124	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.4
14	r	14	LEU	7.3
2	b	495	PHE	7.1
14	r	9	LEU	6.7
14	r	10	LEU	6.5

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
15	FME	t	1	10/11	0.93	0.09	36,49,70,70	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	0.95	0.10	33,45,71,71	0
12	FME	m	1	10/11	0.95	0.14	36,55,70,84	0
12	FME	M	1	10/11	0.96	0.14	45,54,77,86	0
8	FME	i	1	10/11	0.96	0.17	45,57,75,77	0
8	FME	I	1	10/11	0.97	0.15	42,54,64,72	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
32	STE	H	103	18/20	0.71	0.34	42,77,99,99	0
32	STE	E	102	12/20	0.74	0.27	50,78,89,94	0
32	STE	k	101	12/20	0.76	0.25	49,73,89,92	0
32	STE	b	624	20/20	0.77	0.21	46,70,82,93	0
32	STE	B	625	16/20	0.77	0.24	47,64,74,78	0
32	STE	a	414	12/20	0.80	0.28	45,68,75,81	0
33	LMG	c	521	48/55	0.80	0.26	40,79,111,123	0
32	STE	c	520	20/20	0.81	0.23	42,61,83,84	0
28	LHG	a	412	42/49	0.83	0.25	54,83,108,130	0
22	CLA	C	513	65/65	0.83	0.21	38,56,101,105	0
32	STE	x	102	20/20	0.83	0.19	36,63,81,81	0
28	LHG	A	413	49/49	0.83	0.23	56,78,116,120	0
32	STE	d	411	17/20	0.84	0.18	44,58,70,77	0
29	SQD	a	413	36/54	0.84	0.19	27,65,92,100	0
32	STE	t	104	18/20	0.84	0.17	42,62,76,80	0
32	STE	C	521	16/20	0.84	0.17	43,59,70,71	0
33	LMG	D	409	33/55	0.84	0.17	34,56,86,94	0
32	STE	M	104	18/20	0.84	0.18	37,54,88,89	0
32	STE	j	101	12/20	0.85	0.17	39,61,75,80	0
27	PL9	A	410	55/55	0.85	0.24	37,69,85,95	0
24	BCR	H	101	40/40	0.85	0.16	32,48,64,73	0
32	STE	J	101	12/20	0.85	0.16	48,62,72,84	0
33	LMG	B	627	55/55	0.85	0.16	34,60,84,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	x	101	40/40	0.85	0.16	37,56,74,79	0
33	LMG	b	622	55/55	0.85	0.29	47,74,101,110	0
32	STE	h	102	14/20	0.85	0.24	47,67,84,84	0
32	STE	B	626	15/20	0.86	0.17	42,65,83,83	0
33	LMG	D	410	28/55	0.86	0.16	31,51,69,73	0
30	DGD	A	415	66/66	0.86	0.17	44,65,85,95	0
32	STE	I	101	15/20	0.86	0.13	44,58,80,81	0
22	CLA	c	512	65/65	0.87	0.16	45,61,100,112	0
22	CLA	C	514	65/65	0.87	0.21	44,64,100,106	0
22	CLA	b	601	65/65	0.87	0.18	46,71,90,108	0
32	STE	b	623	16/20	0.87	0.17	49,62,84,86	0
29	SQD	A	414	39/54	0.87	0.18	37,66,87,95	0
32	STE	b	626	20/20	0.87	0.18	46,73,96,101	0
29	SQD	L	101	49/54	0.88	0.14	45,61,96,100	0
32	STE	b	625	10/20	0.88	0.25	44,54,67,68	0
32	STE	B	621	17/20	0.88	0.17	35,53,68,75	0
32	STE	b	621	20/20	0.88	0.23	37,58,76,81	0
27	PL9	a	410	55/55	0.88	0.20	41,70,89,102	0
32	STE	B	601	12/20	0.89	0.44	48,70,94,97	0
29	SQD	B	623	54/54	0.89	0.15	34,65,92,110	0
24	BCR	K	101	40/40	0.89	0.13	40,56,73,77	0
24	BCR	d	405	40/40	0.89	0.15	31,52,87,102	0
33	LMG	Y	101	48/55	0.89	0.17	43,75,97,104	0
24	BCR	k	102	40/40	0.89	0.14	46,63,80,82	0
32	STE	Z	102	8/20	0.89	0.15	43,60,72,72	0
33	LMG	c	522	49/55	0.89	0.14	32,58,90,114	0
22	CLA	B	602	65/65	0.90	0.14	34,60,89,98	0
32	STE	T	102	15/20	0.90	0.16	42,58,81,89	0
32	STE	C	522	12/20	0.90	0.10	33,45,57,61	0
24	BCR	k	103	40/40	0.90	0.18	39,55,69,76	0
33	LMG	M	101	51/55	0.90	0.12	33,52,76,86	0
32	STE	b	620	16/20	0.90	0.17	33,55,75,78	0
22	CLA	a	405	65/65	0.90	0.15	22,42,90,105	0
22	CLA	c	513	65/65	0.90	0.20	44,68,109,121	0
32	STE	C	520	12/20	0.90	0.15	37,53,65,75	0
32	STE	D	411	20/20	0.91	0.14	35,55,70,74	0
32	STE	L	103	12/20	0.91	0.20	52,64,88,89	0
32	STE	t	102	14/20	0.91	0.13	35,53,60,65	0
32	STE	B	624	12/20	0.91	0.10	35,53,67,74	0
29	SQD	f	101	41/54	0.91	0.19	60,81,107,111	0
22	CLA	D	404	65/65	0.91	0.14	24,46,105,117	0
33	LMG	C	516	48/55	0.91	0.13	36,58,77,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	503	65/65	0.92	0.14	32,45,65,79	0
22	CLA	B	616	65/65	0.92	0.14	27,40,69,86	0
32	STE	M	102	15/20	0.92	0.14	36,49,63,72	0
33	LMG	D	407	51/55	0.92	0.17	31,58,97,101	0
22	CLA	d	404	65/65	0.92	0.15	32,52,97,105	0
22	CLA	b	616	60/65	0.92	0.14	29,48,91,98	0
22	CLA	c	502	65/65	0.92	0.16	32,47,64,70	0
30	DGD	C	518	62/66	0.92	0.15	34,53,108,130	0
24	BCR	Z	101	40/40	0.92	0.16	38,60,75,77	0
24	BCR	c	514	40/40	0.92	0.19	45,58,79,80	0
22	CLA	c	508	64/65	0.92	0.15	32,46,83,100	0
30	DGD	c	517	62/66	0.93	0.13	33,55,98,104	0
24	BCR	C	501	40/40	0.93	0.18	40,53,72,81	0
24	BCR	D	405	40/40	0.93	0.13	28,47,85,101	0
22	CLA	c	510	65/65	0.93	0.15	33,51,65,73	0
22	CLA	C	508	65/65	0.93	0.15	26,45,61,66	0
22	CLA	B	617	60/65	0.93	0.15	26,43,92,113	0
22	CLA	b	615	65/65	0.93	0.14	28,43,64,70	0
32	STE	t	103	10/20	0.93	0.17	41,58,70,73	0
33	LMG	c	519	37/55	0.93	0.15	43,67,84,87	0
24	BCR	B	620	40/40	0.93	0.12	24,47,67,76	0
32	STE	M	103	10/20	0.93	0.15	35,45,55,66	0
33	LMG	m	101	51/55	0.93	0.12	34,54,73,90	0
24	BCR	b	617	40/40	0.94	0.12	27,45,60,60	0
30	DGD	c	518	62/66	0.94	0.14	28,56,95,100	0
30	DGD	h	101	62/66	0.94	0.13	33,51,67,72	0
24	BCR	b	619	40/40	0.94	0.10	33,50,65,70	0
22	CLA	A	405	54/65	0.94	0.13	20,36,63,73	0
22	CLA	c	509	65/65	0.94	0.19	33,51,70,75	0
22	CLA	C	512	65/65	0.94	0.14	35,55,72,85	0
22	CLA	c	511	65/65	0.94	0.13	38,56,77,82	0
22	CLA	b	602	65/65	0.94	0.15	24,46,67,75	0
22	CLA	b	606	65/65	0.94	0.12	28,43,79,93	0
27	PL9	D	406	55/55	0.94	0.12	23,37,53,55	0
22	CLA	B	605	65/65	0.94	0.14	23,36,74,84	0
24	BCR	B	618	40/40	0.94	0.12	26,43,64,65	0
24	BCR	B	619	40/40	0.94	0.11	23,39,54,57	0
22	CLA	B	607	65/65	0.94	0.11	22,38,76,83	0
22	CLA	C	507	65/65	0.94	0.13	27,48,95,114	0
29	SQD	F	101	36/54	0.94	0.17	46,73,94,100	0
24	BCR	C	515	40/40	0.94	0.12	27,45,58,67	0
29	SQD	a	411	54/54	0.94	0.15	41,67,95,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	c	503	65/65	0.94	0.16	35,48,61,67	0
22	CLA	c	505	65/65	0.94	0.17	30,45,72,77	0
22	CLA	c	506	65/65	0.94	0.14	30,54,101,105	0
22	CLA	c	507	65/65	0.94	0.15	28,48,63,65	0
30	DGD	C	519	62/66	0.94	0.12	28,54,75,83	0
33	LMG	d	410	44/55	0.94	0.15	36,55,89,104	0
30	DGD	H	102	62/66	0.94	0.11	29,47,62,66	0
22	CLA	B	611	65/65	0.95	0.15	21,34,48,55	0
29	SQD	A	412	52/54	0.95	0.15	36,61,94,98	0
22	CLA	C	505	59/65	0.95	0.12	28,45,82,99	0
22	CLA	c	504	60/65	0.95	0.11	33,48,83,88	0
22	CLA	C	506	65/65	0.95	0.14	23,41,72,82	0
22	CLA	a	403	65/65	0.95	0.14	25,43,98,116	0
24	BCR	T	101	40/40	0.95	0.09	28,44,60,68	0
22	CLA	B	615	65/65	0.95	0.15	26,41,84,94	0
22	CLA	A	403	65/65	0.95	0.14	22,37,87,101	0
22	CLA	C	509	65/65	0.95	0.12	34,46,105,121	0
30	DGD	C	517	62/66	0.95	0.13	22,43,84,95	0
22	CLA	b	604	65/65	0.95	0.14	23,40,82,97	0
24	BCR	c	515	40/40	0.95	0.10	30,44,65,69	0
22	CLA	C	510	65/65	0.95	0.18	28,48,68,74	0
30	DGD	c	516	62/66	0.95	0.13	23,45,81,92	0
22	CLA	b	608	65/65	0.95	0.14	27,44,70,75	0
22	CLA	b	609	65/65	0.95	0.14	27,47,81,86	0
22	CLA	b	613	65/65	0.95	0.14	23,37,82,87	0
23	PHO	a	404	64/64	0.95	0.13	21,33,41,46	0
22	CLA	b	614	65/65	0.95	0.14	23,42,80,89	0
22	CLA	C	511	65/65	0.95	0.14	29,48,70,77	0
22	CLA	B	603	65/65	0.95	0.17	23,41,59,61	0
22	CLA	C	504	65/65	0.96	0.14	33,47,56,61	0
22	CLA	d	402	65/65	0.96	0.12	21,37,65,68	0
22	CLA	d	403	65/65	0.96	0.12	20,34,52,56	0
22	CLA	B	614	65/65	0.96	0.15	22,36,73,83	0
23	PHO	A	404	64/64	0.96	0.11	21,30,42,45	0
22	CLA	c	501	65/65	0.96	0.13	28,44,56,68	0
24	BCR	t	101	40/40	0.96	0.09	29,42,56,57	0
23	PHO	d	401	64/64	0.96	0.11	26,42,52,62	0
24	BCR	A	406	40/40	0.96	0.09	24,38,47,56	0
22	CLA	b	603	65/65	0.96	0.15	24,40,71,82	0
22	CLA	B	608	65/65	0.96	0.11	20,36,65,71	0
27	PL9	d	406	55/55	0.96	0.11	19,37,48,56	0
28	LHG	A	411	47/49	0.96	0.13	31,52,79,95	0

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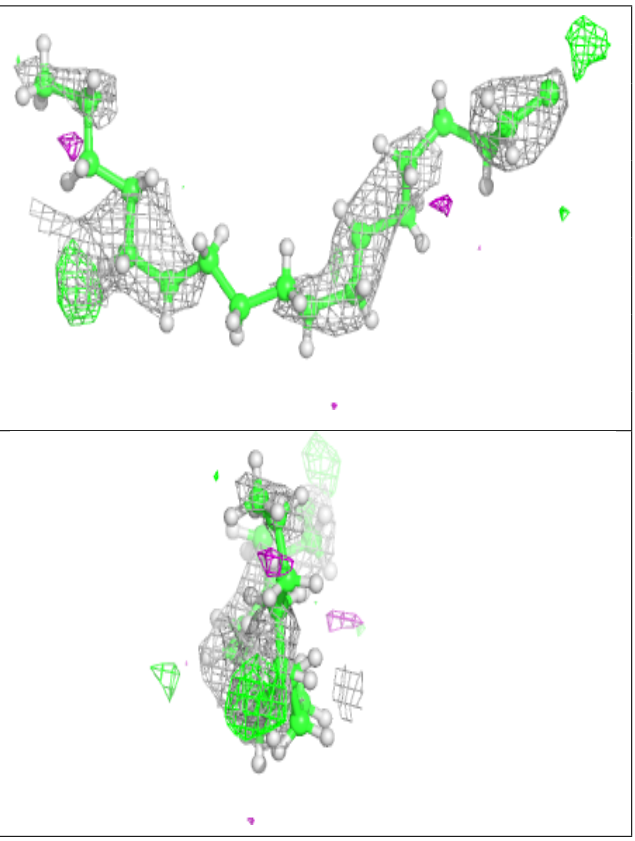
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	605	65/65	0.96	0.13	23,38,53,61	0
28	LHG	B	622	49/49	0.96	0.11	31,47,68,81	0
22	CLA	B	610	65/65	0.96	0.11	26,38,61,72	0
28	LHG	d	407	49/49	0.96	0.13	34,52,74,84	0
28	LHG	d	409	39/49	0.96	0.11	32,51,66,69	0
28	LHG	l	101	49/49	0.96	0.11	25,48,61,78	0
22	CLA	D	403	65/65	0.96	0.11	20,33,54,61	0
22	CLA	B	604	65/65	0.96	0.16	23,36,64,67	0
22	CLA	b	610	65/65	0.96	0.18	27,40,52,62	0
22	CLA	b	611	65/65	0.96	0.13	21,36,56,68	0
22	CLA	b	612	65/65	0.96	0.17	22,36,52,56	0
22	CLA	C	502	65/65	0.96	0.12	25,37,54,57	0
24	BCR	a	406	40/40	0.96	0.09	23,38,49,54	0
22	CLA	B	613	65/65	0.96	0.14	20,34,53,58	0
24	BCR	b	618	40/40	0.96	0.09	27,42,54,58	0
34	HEC	E	101	43/43	0.96	0.12	36,50,69,75	0
34	HEC	e	101	43/43	0.96	0.12	44,61,79,83	0
22	CLA	B	612	65/65	0.97	0.13	22,34,50,54	0
22	CLA	a	402	65/65	0.97	0.10	19,33,47,55	0
22	CLA	B	609	65/65	0.97	0.12	23,36,56,62	0
28	LHG	D	408	49/49	0.97	0.10	24,41,54,60	0
28	LHG	L	102	49/49	0.97	0.10	27,42,59,71	0
23	PHO	D	401	64/64	0.97	0.11	22,35,45,50	0
22	CLA	A	402	65/65	0.97	0.10	21,29,43,61	0
28	LHG	d	408	49/49	0.97	0.10	27,43,59,66	0
22	CLA	b	607	65/65	0.97	0.12	21,39,70,81	0
22	CLA	D	402	65/65	0.97	0.11	17,32,59,66	0
34	HEC	V	201	43/43	0.97	0.13	25,37,45,53	0
22	CLA	B	606	65/65	0.97	0.13	22,36,52,56	0
26	BCT	A	409	4/4	0.98	0.16	26,33,35,42	0
34	HEC	v	201	43/43	0.98	0.13	32,39,52,59	0
31	OEX	A	416	10/10	0.99	0.13	25,31,33,37	0
31	OEX	a	415	10/10	0.99	0.12	22,30,32,33	0
25	CL	a	407	1/1	0.99	0.05	32,32,32,32	0
25	CL	a	408	1/1	0.99	0.07	32,32,32,32	0
21	FE2	A	401	1/1	0.99	0.09	30,30,30,30	0
26	BCT	a	409	4/4	0.99	0.22	31,31,44,52	0
21	FE2	a	401	1/1	0.99	0.10	38,38,38,38	0
25	CL	A	407	1/1	0.99	0.07	32,32,32,32	0
25	CL	A	408	1/1	0.99	0.06	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

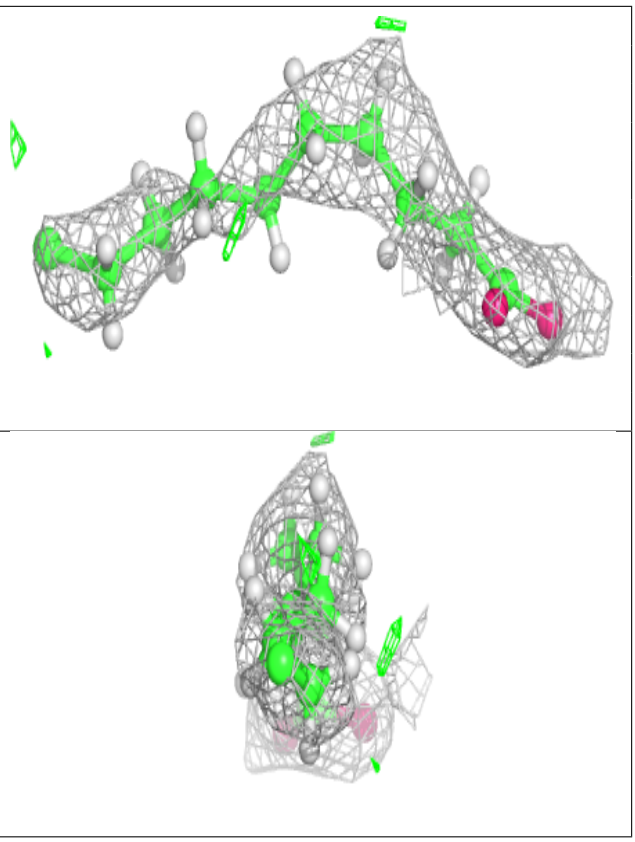
Electron density around STE H 103:

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



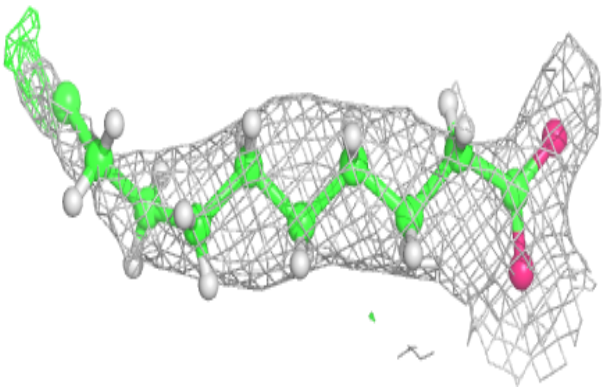
Electron density around STE E 102:

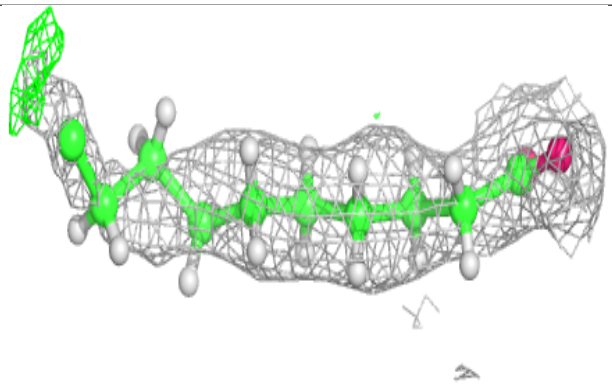
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

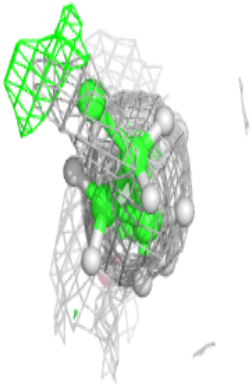


Electron density around STE k 101:

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

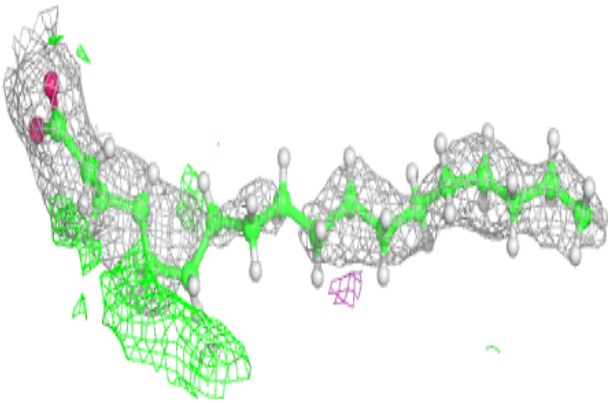


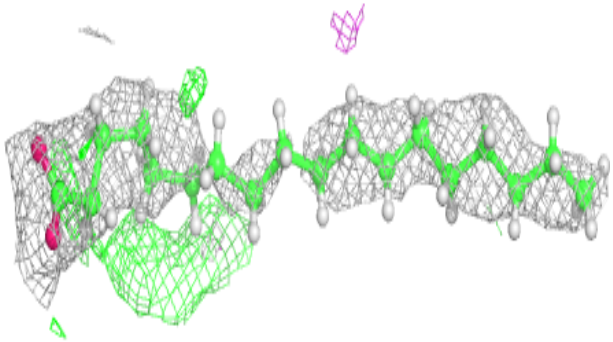


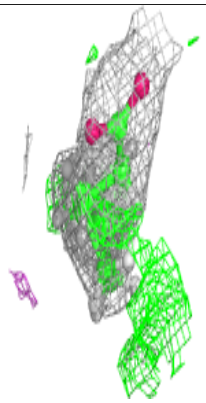


Electron density around STE b 624:

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

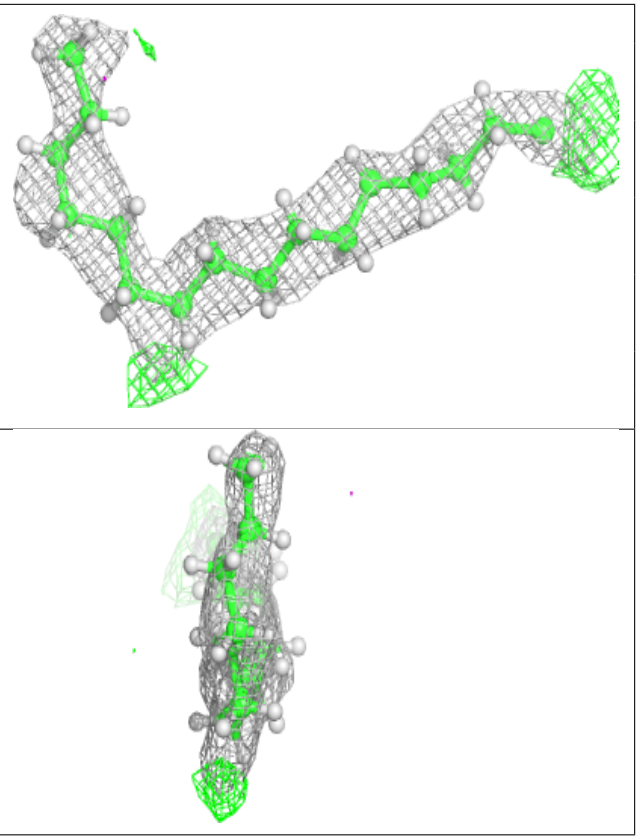


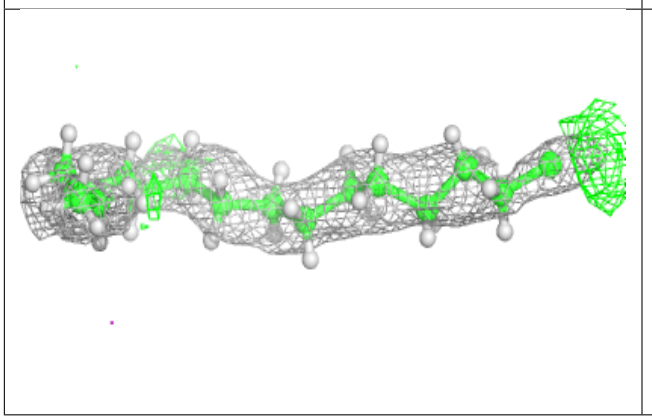




Electron density around STE B 625:

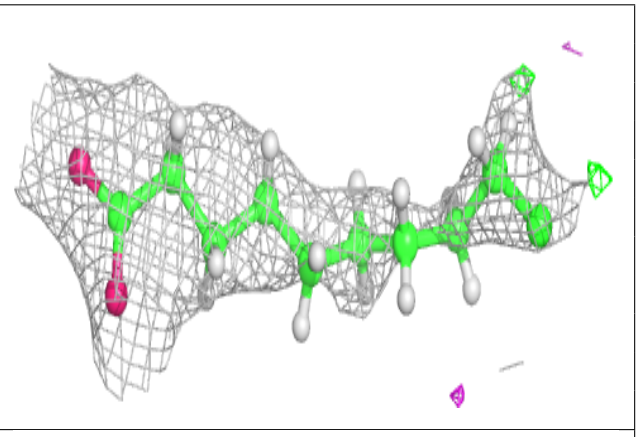
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

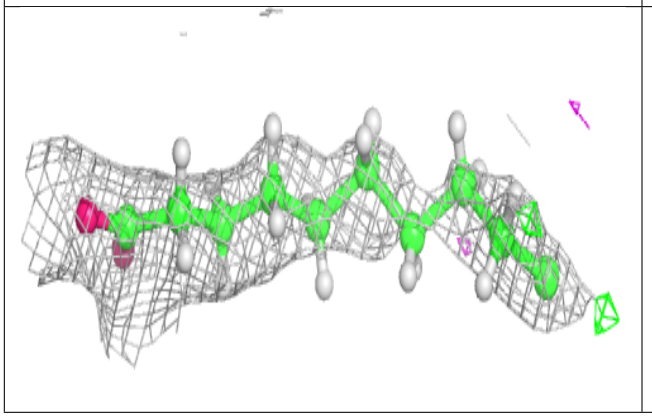


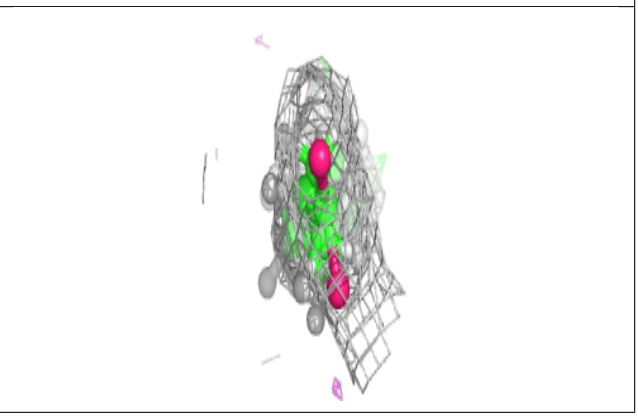


Electron density around STE a 414:

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

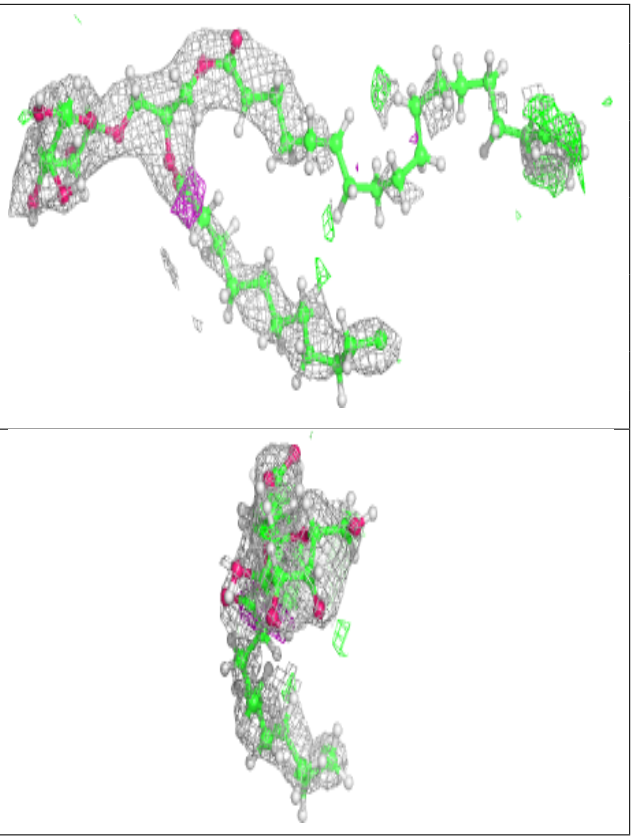






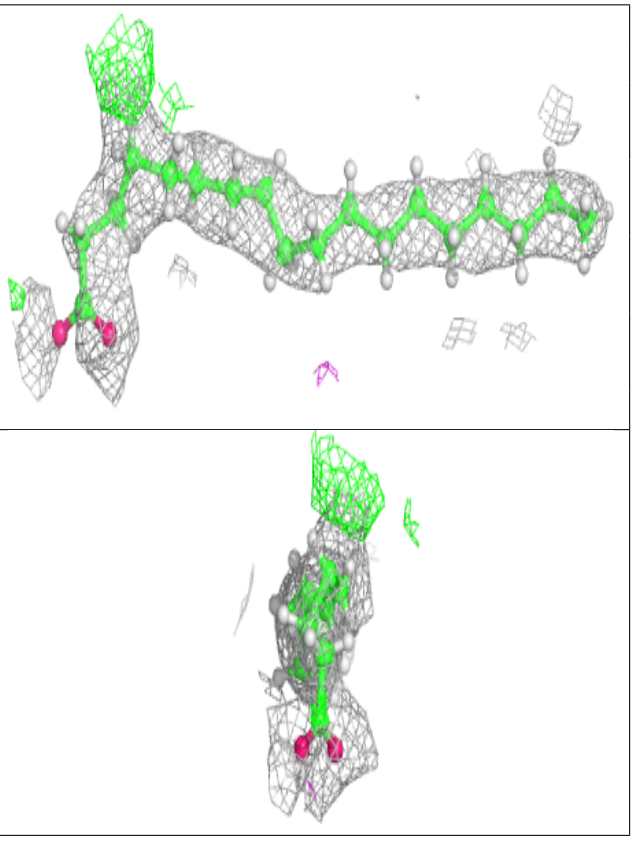
Electron density around LMG c 521:

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



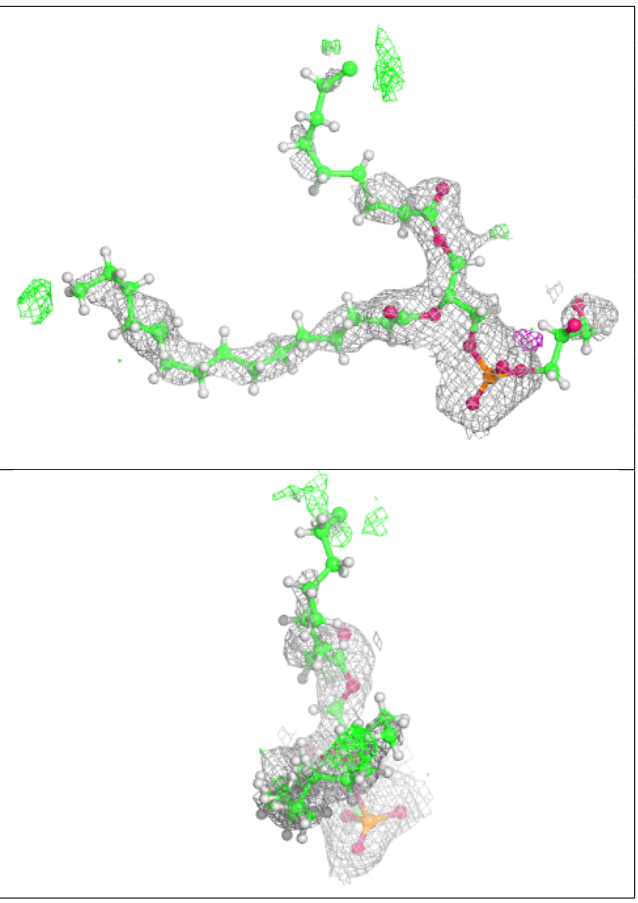
Electron density around STE c 520:

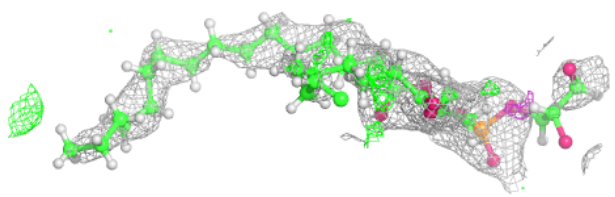
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG a 412:

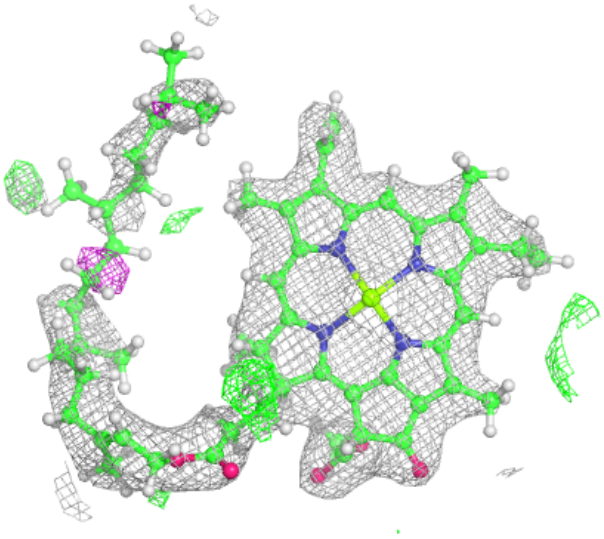
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

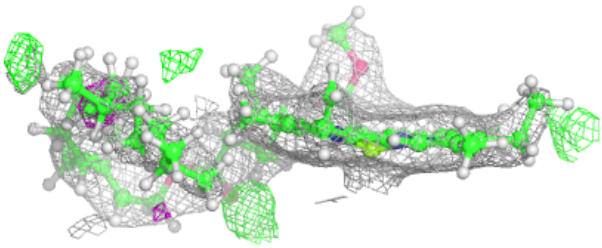




Electron density around CLA C 513:

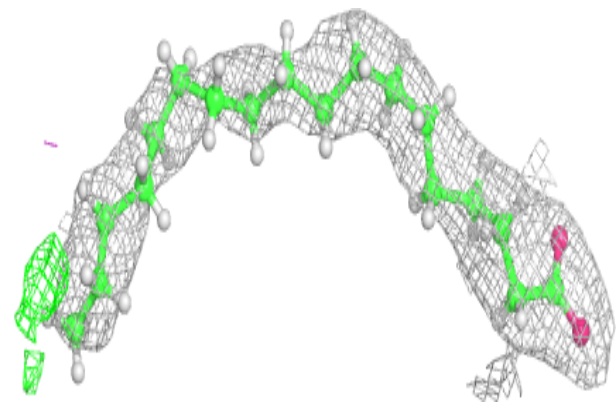
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

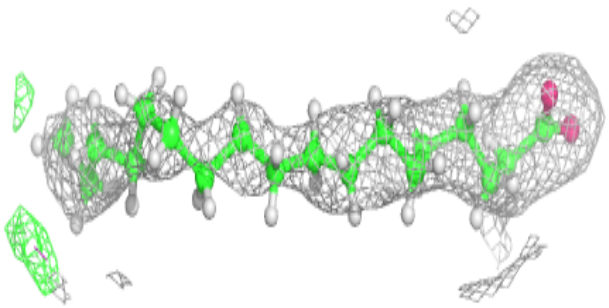


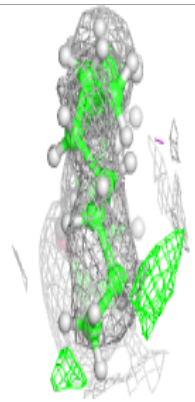


Electron density around STE x 102:

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

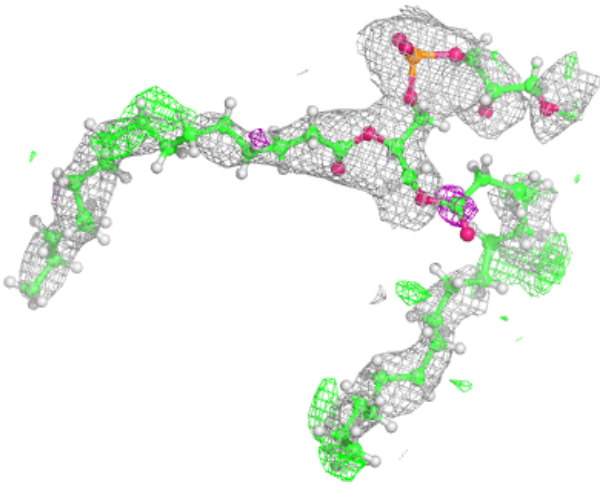


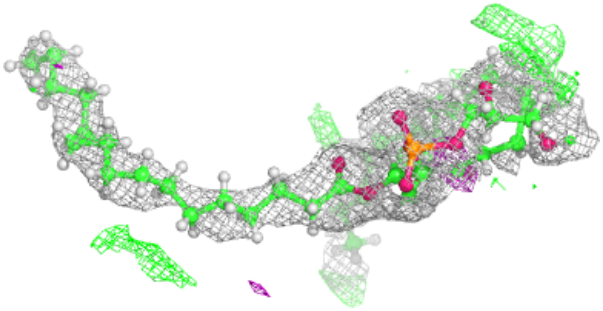


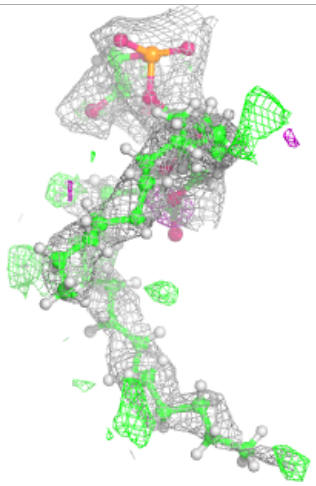


Electron density around LHG A 413:

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

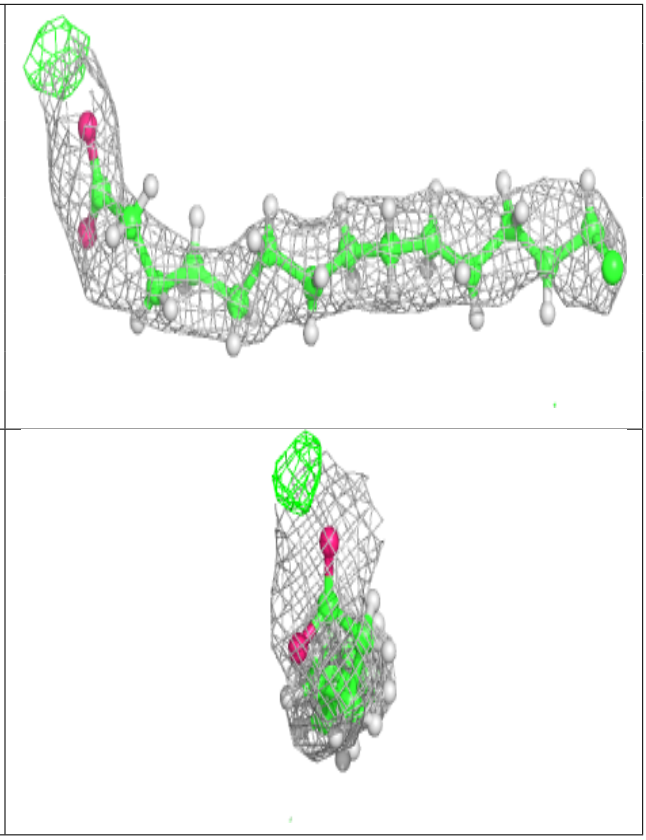


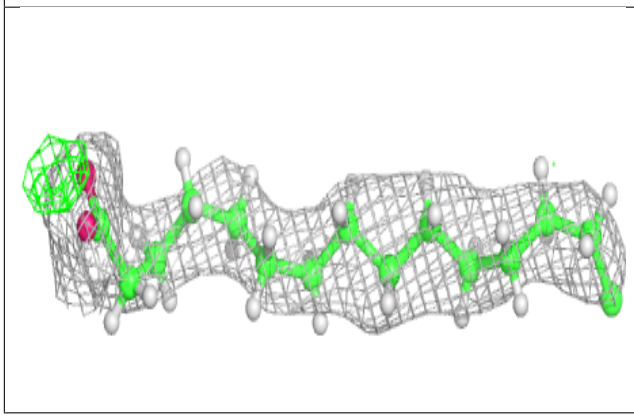




Electron density around STE d 411:

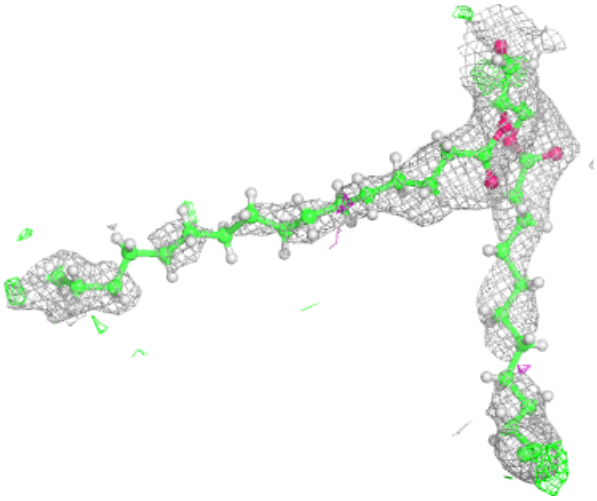
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

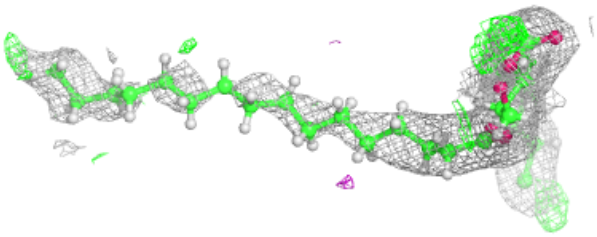


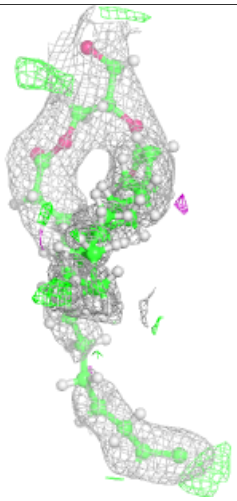


Electron density around SQD a 413:

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

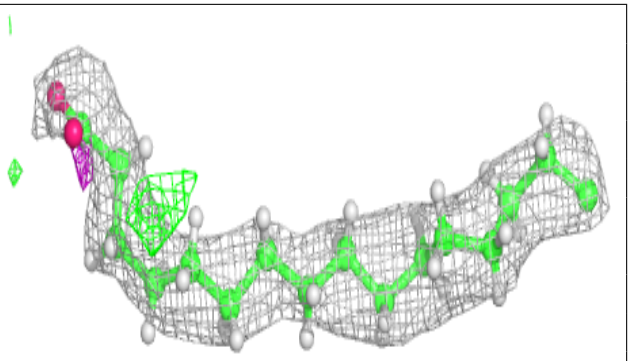


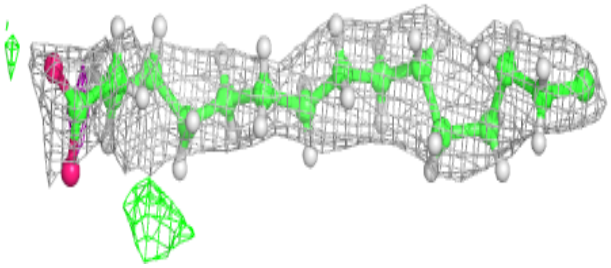


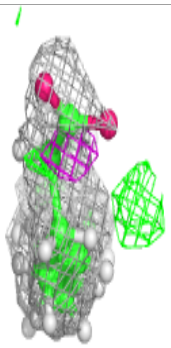


Electron density around STE t 104:

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

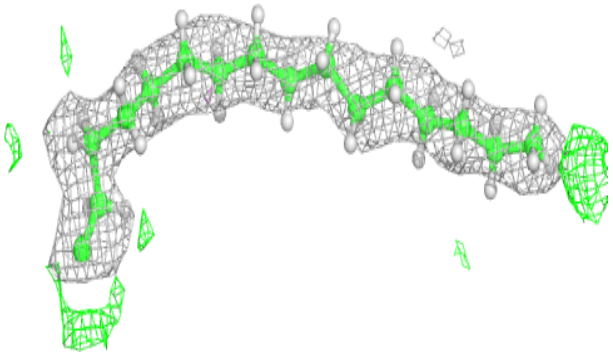


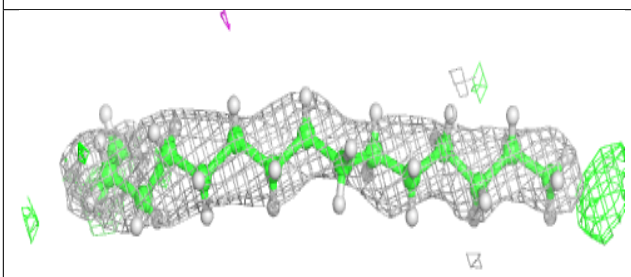


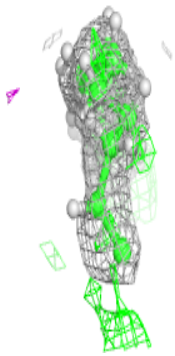


Electron density around STE C 521:

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

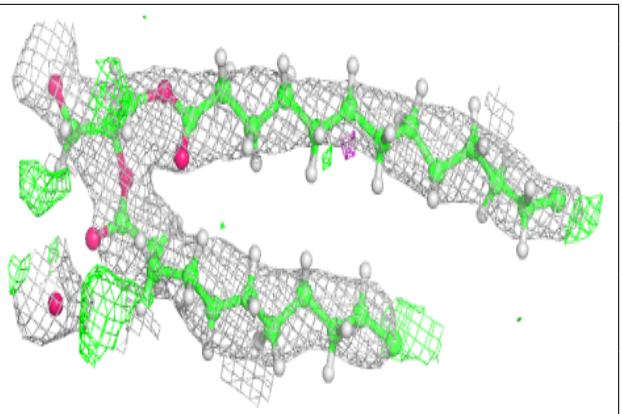


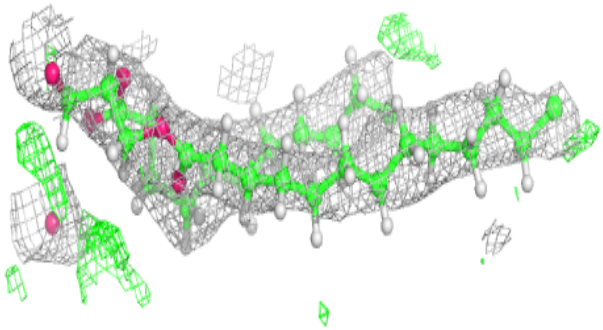


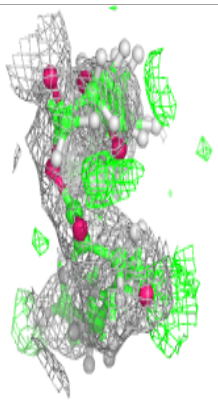


Electron density around LMG D 409:

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

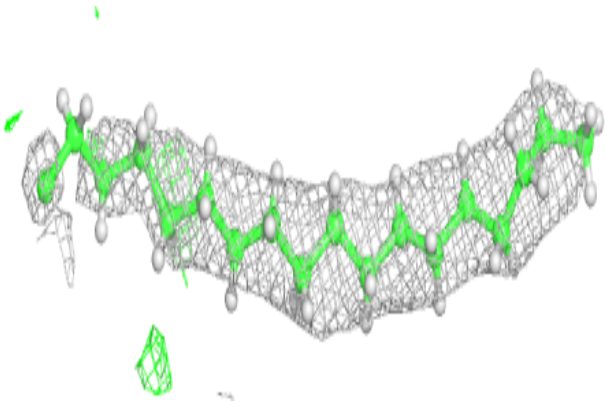


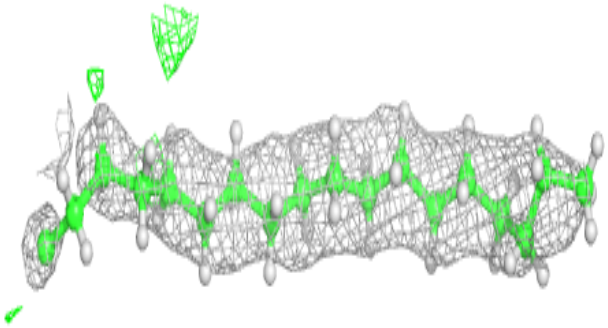


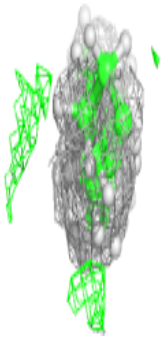


Electron density around STE M 104:

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

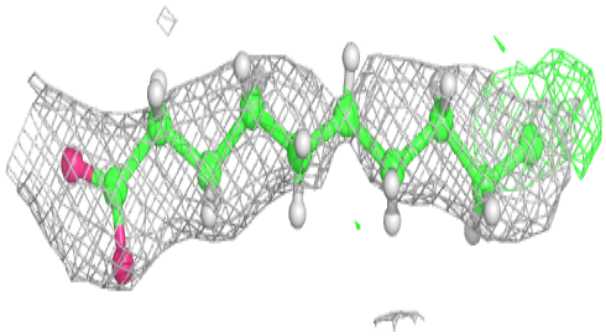


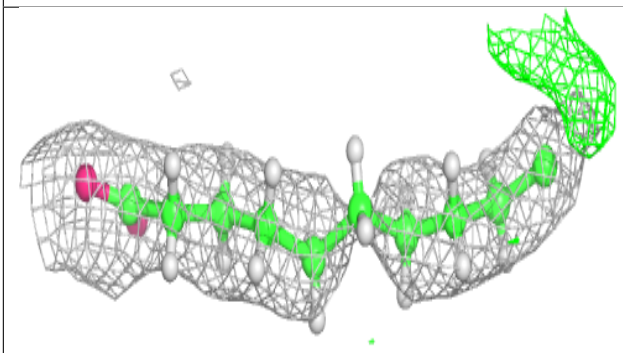


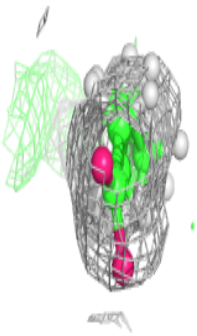


Electron density around STE j 101:

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

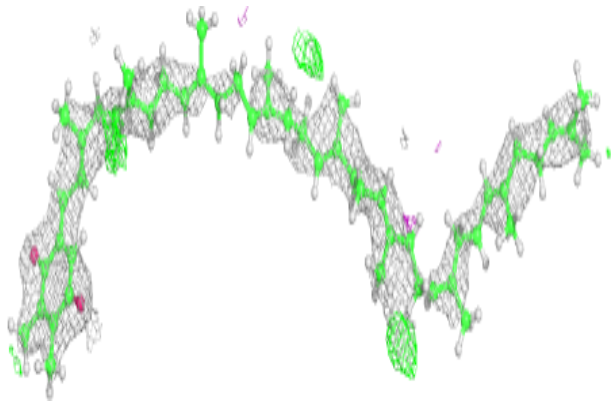


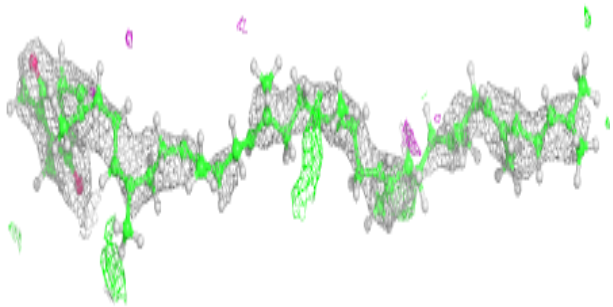


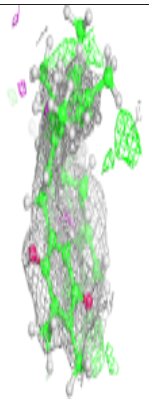


Electron density around PL9 A 410:

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

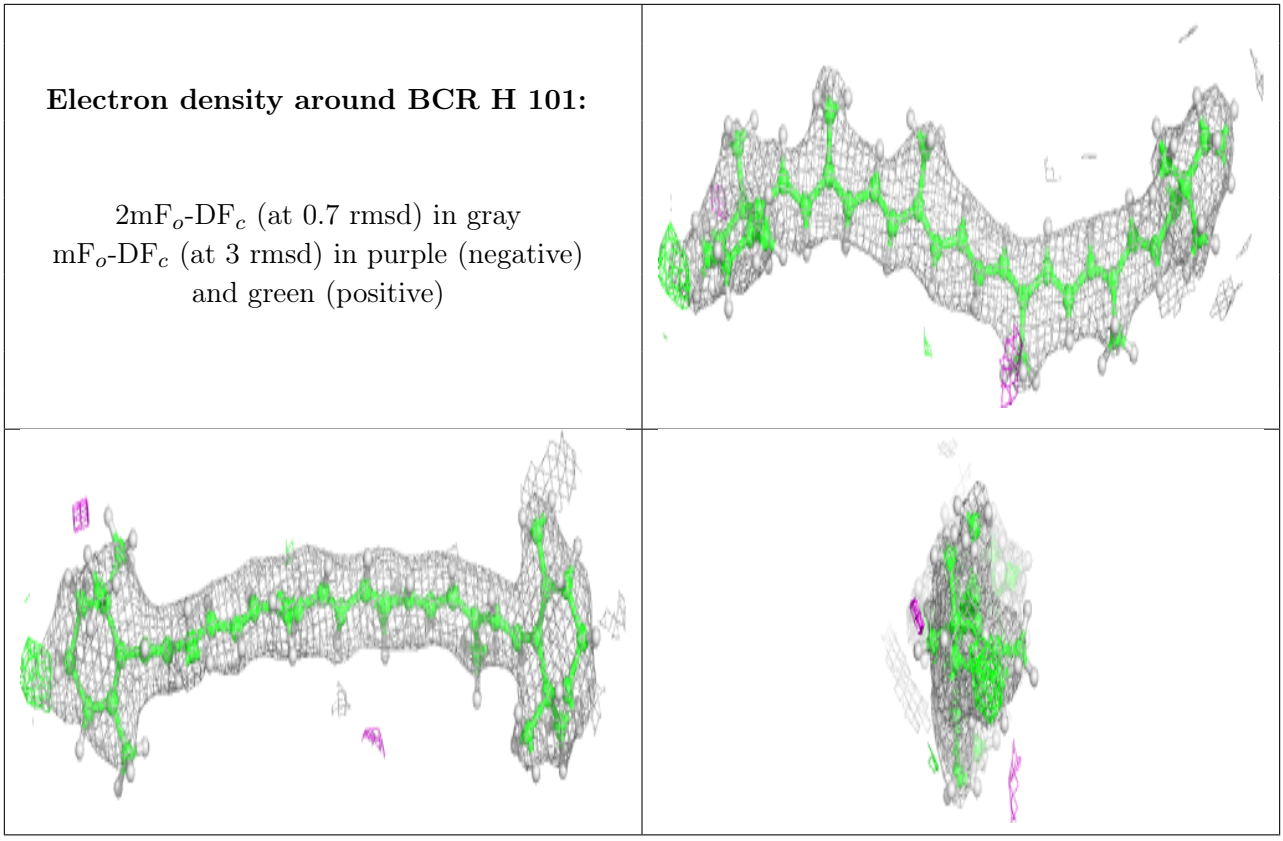






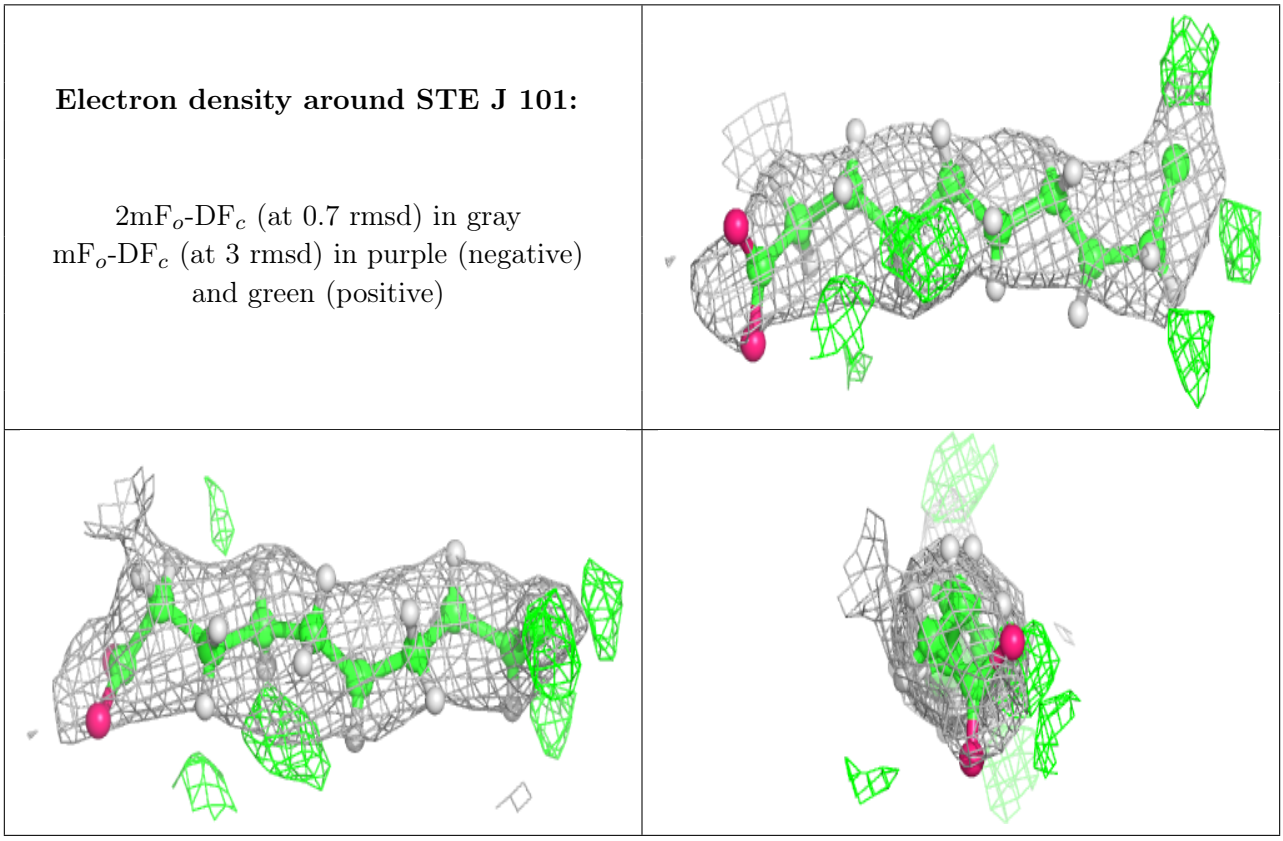
Electron density around BCR H 101:

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



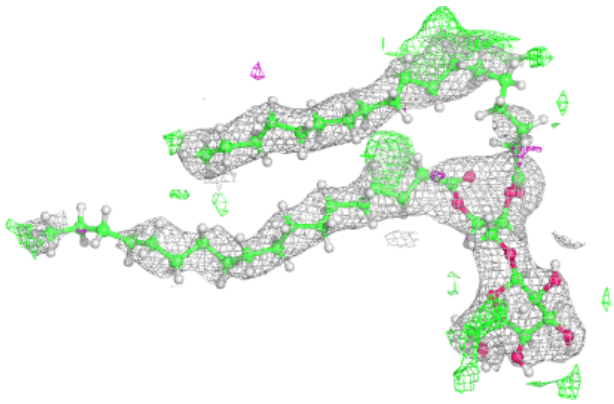
Electron density around STE J 101:

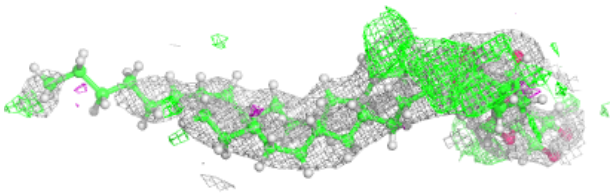
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

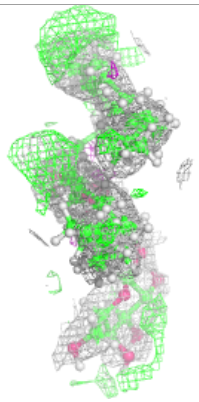


Electron density around LMG B 627:

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

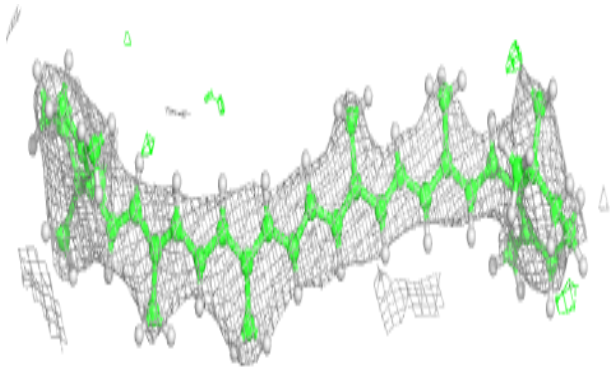


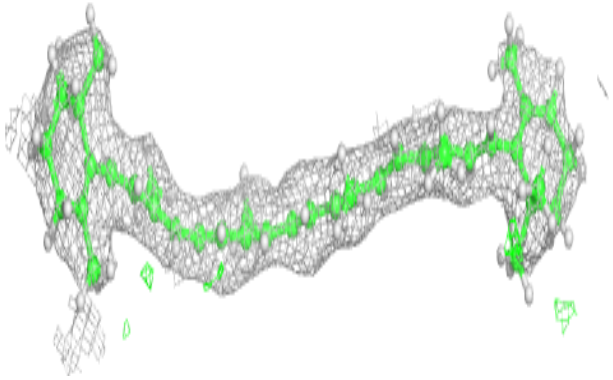


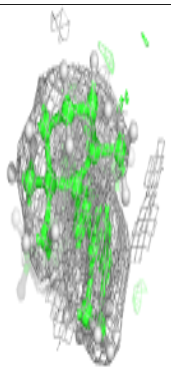


Electron density around BCR x 101:

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

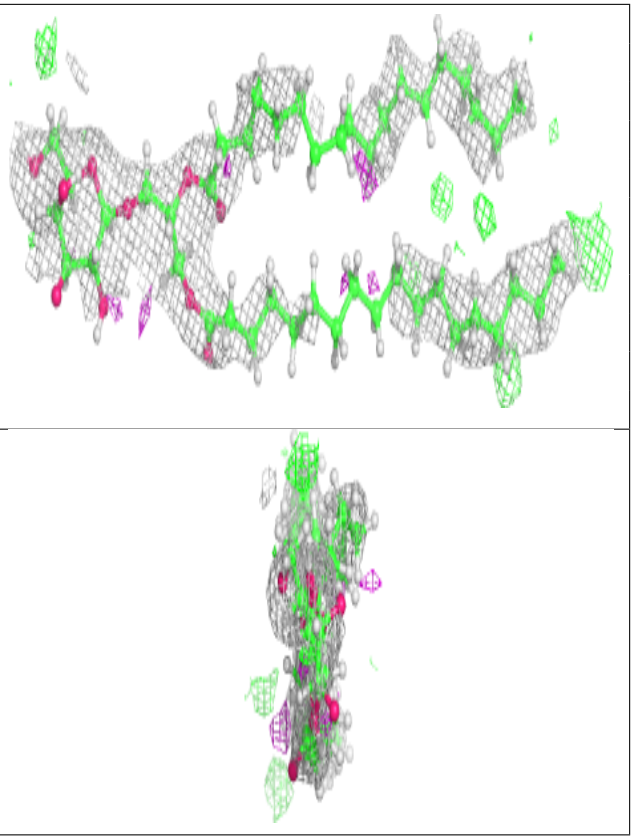


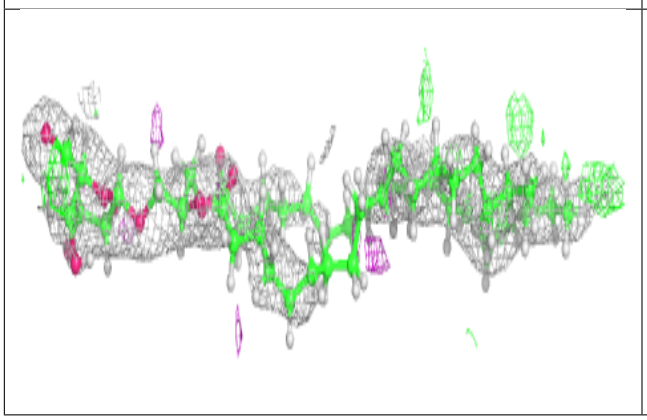




Electron density around LMG b 622:

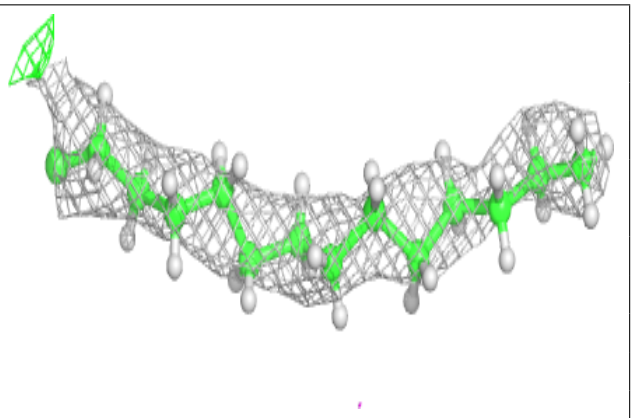
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

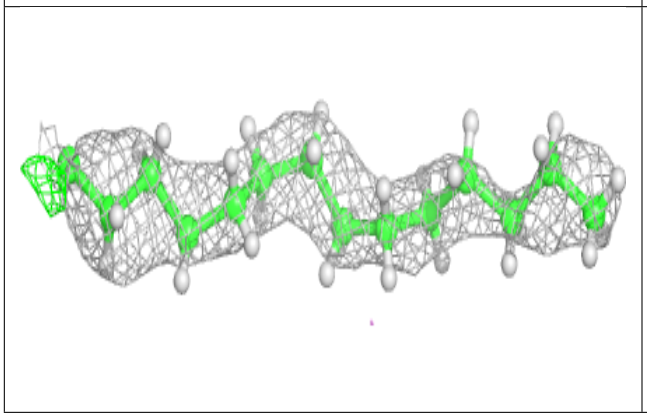


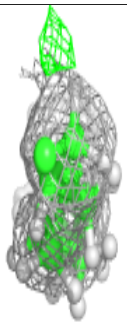


Electron density around STE h 102:

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

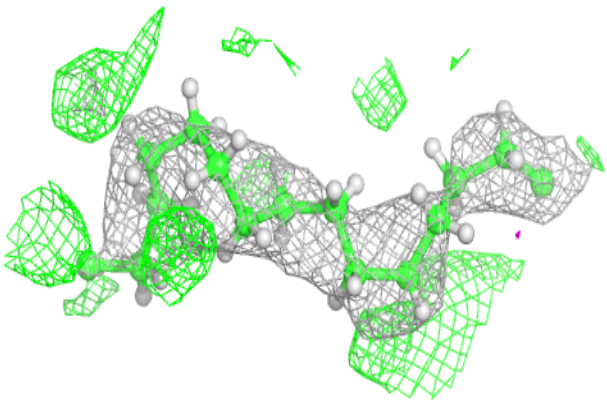


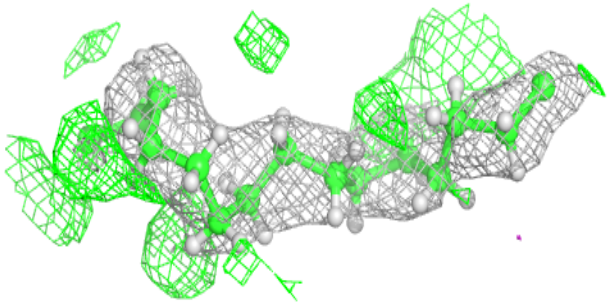


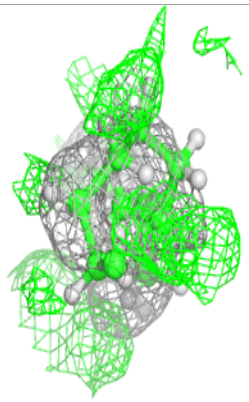


Electron density around STE B 626:

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

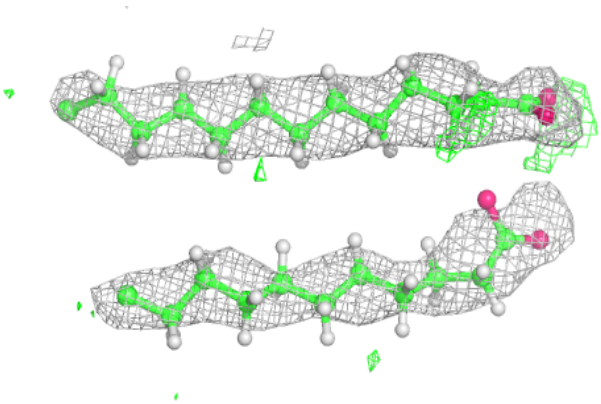


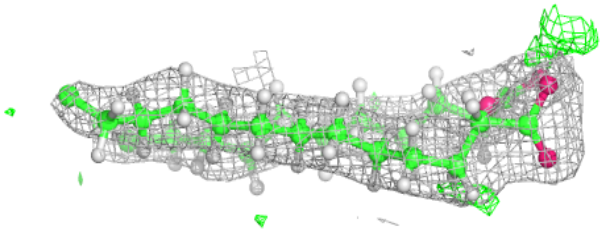


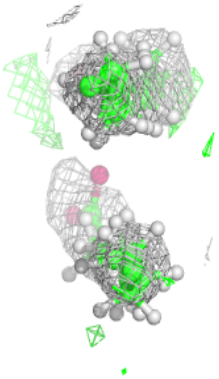


Electron density around LMG D 410:

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

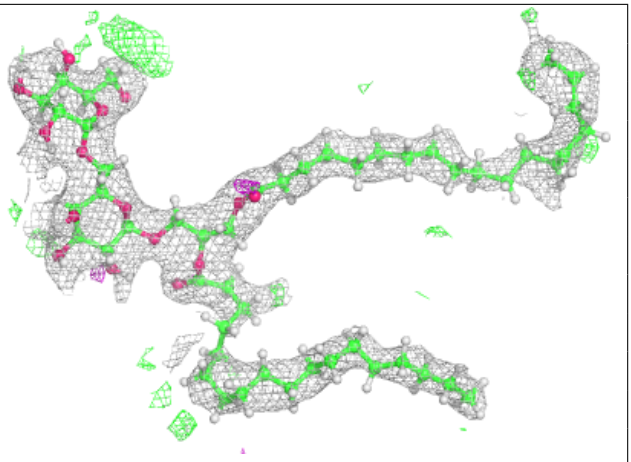


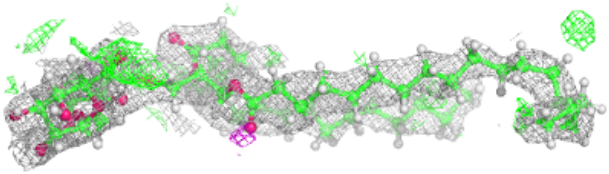


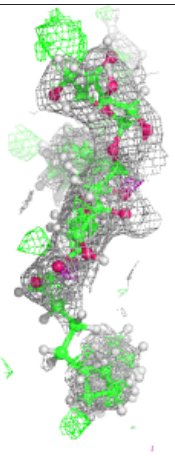


Electron density around DGD A 415:

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

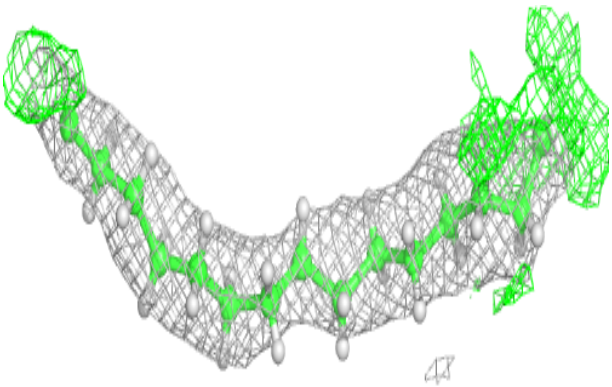


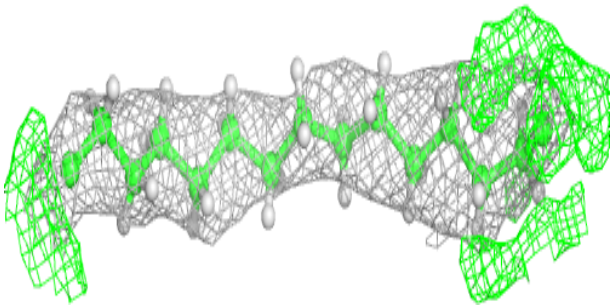


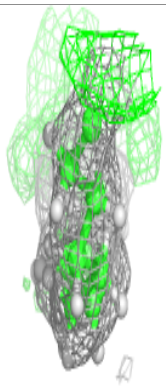


Electron density around STE I 101:

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

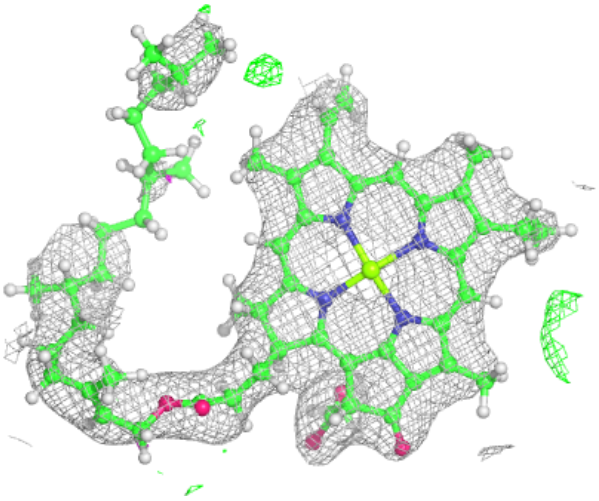


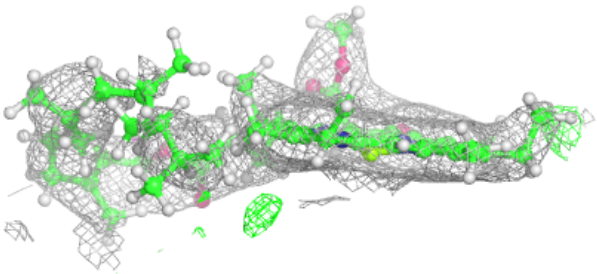


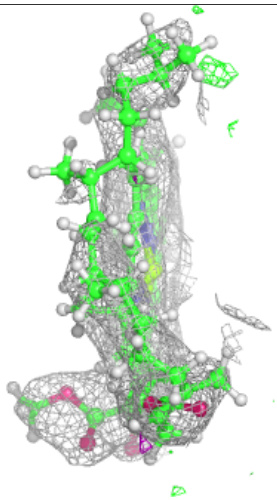


Electron density around CLA c 512:

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

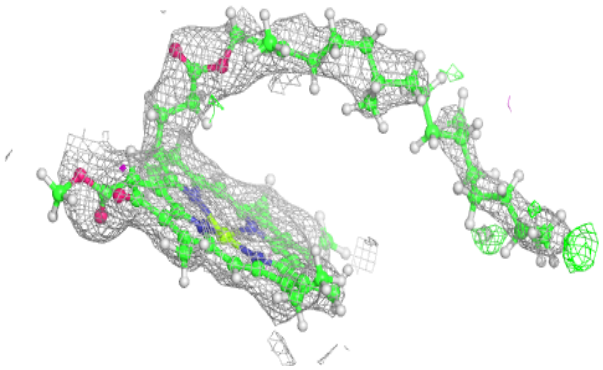


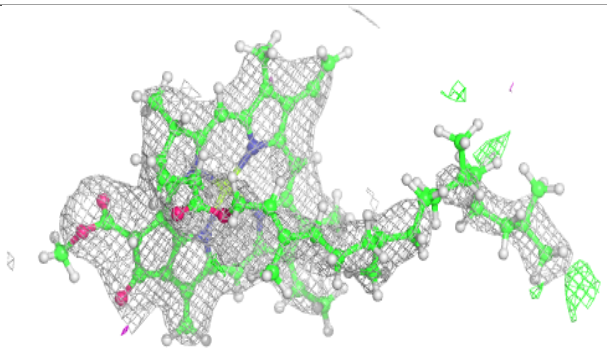


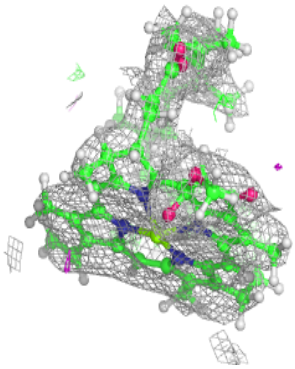


Electron density around CLA C 514:

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

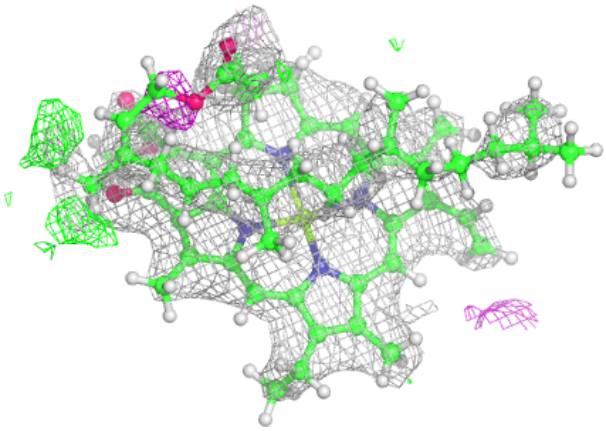


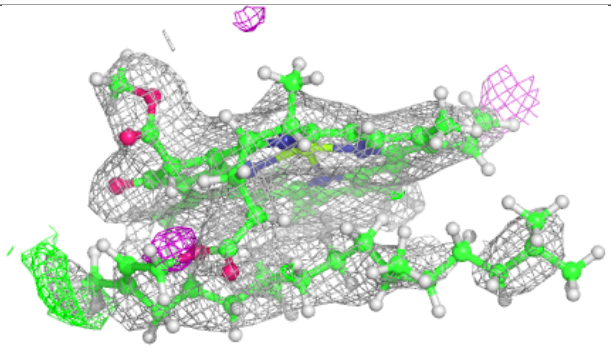


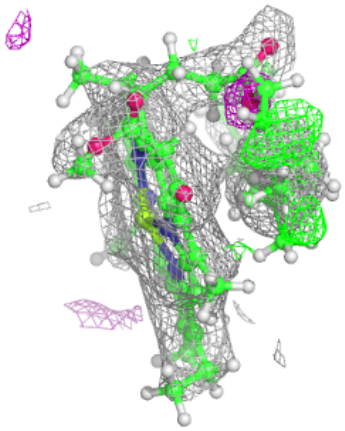


Electron density around CLA b 601:

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

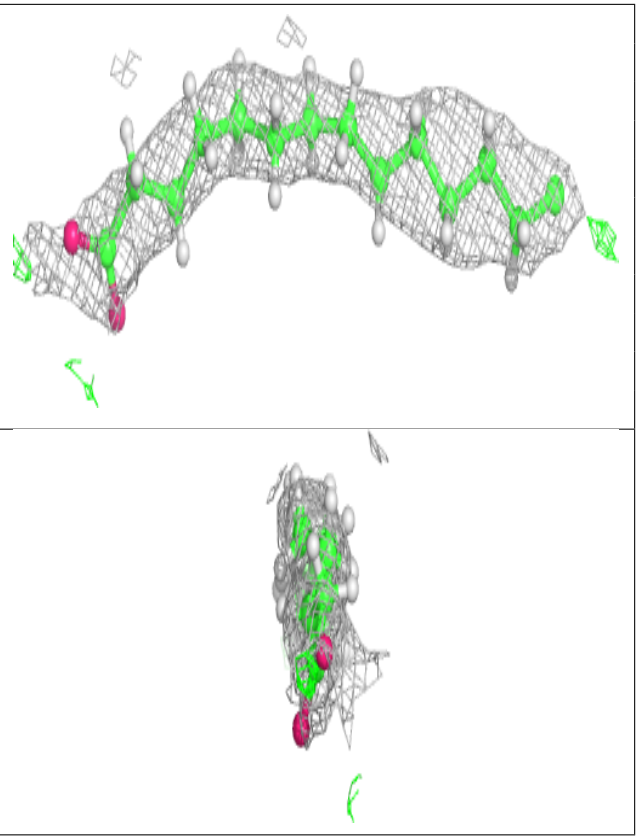


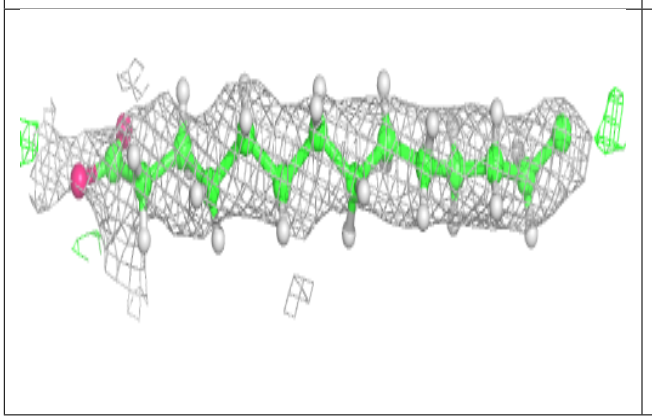




Electron density around STE b 623:

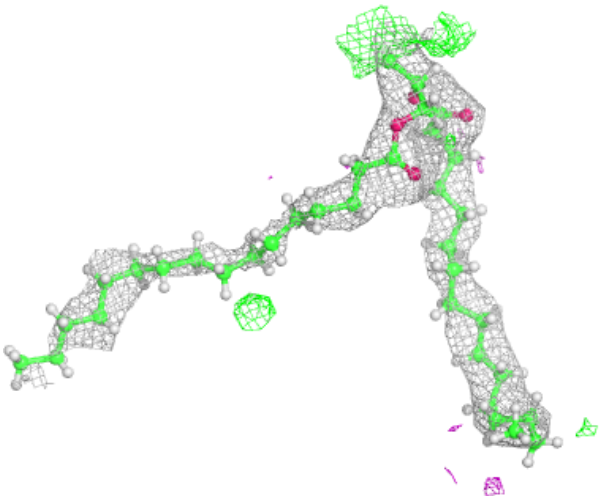
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

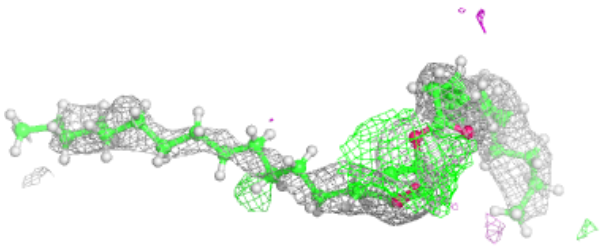


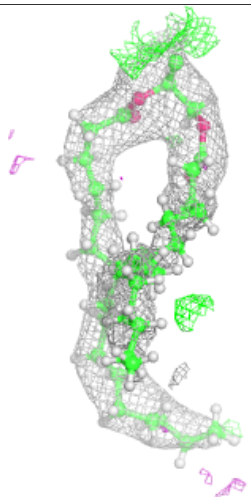


Electron density around SQD A 414:

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

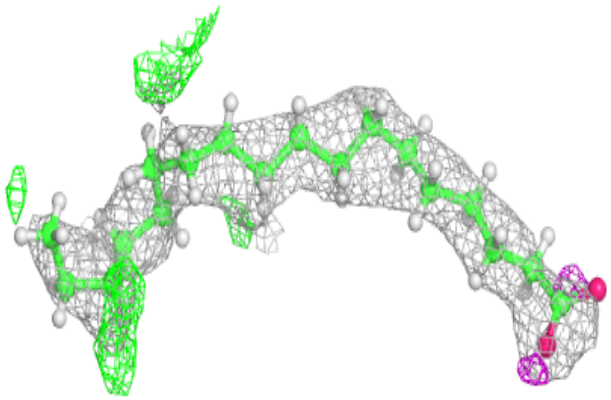


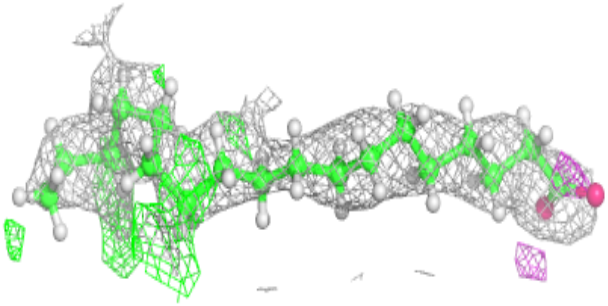


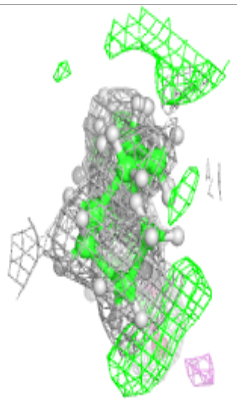


Electron density around STE b 626:

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

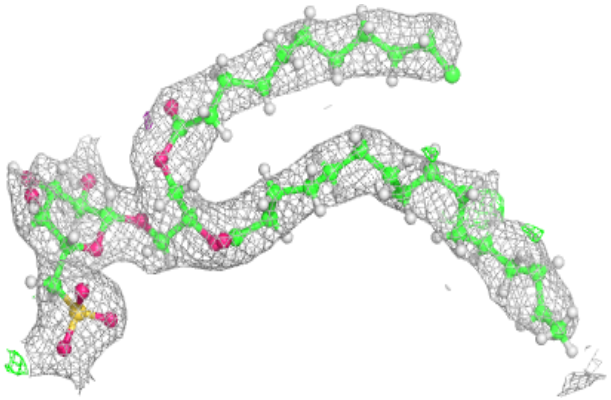


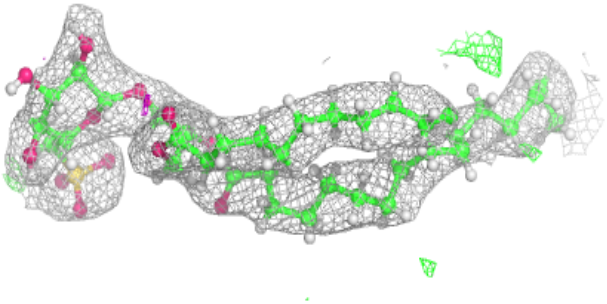




Electron density around SQD L 101:

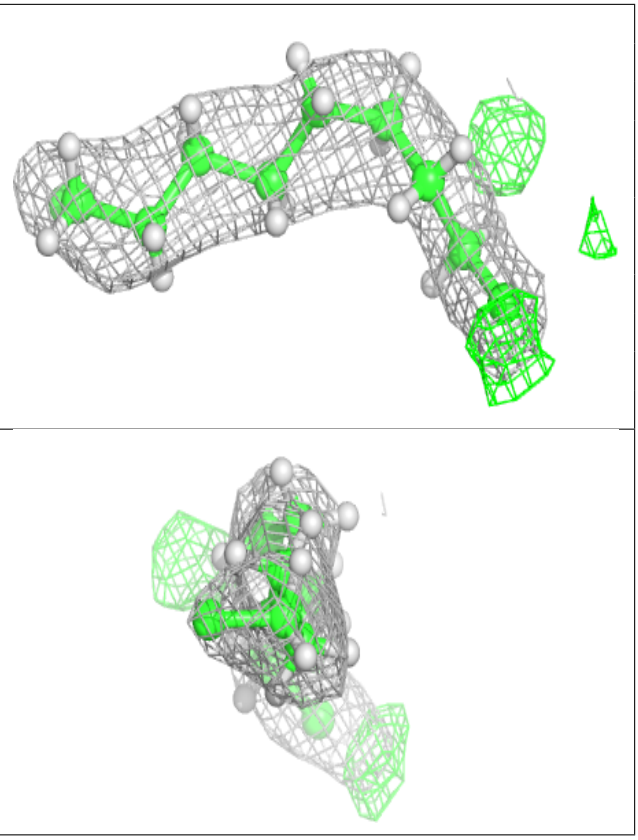
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





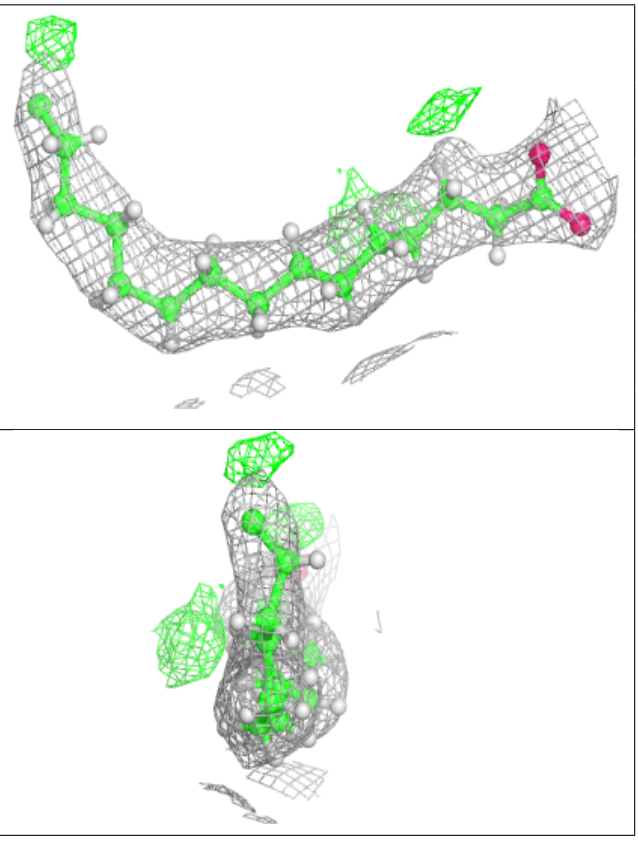
Electron density around STE b 625:

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



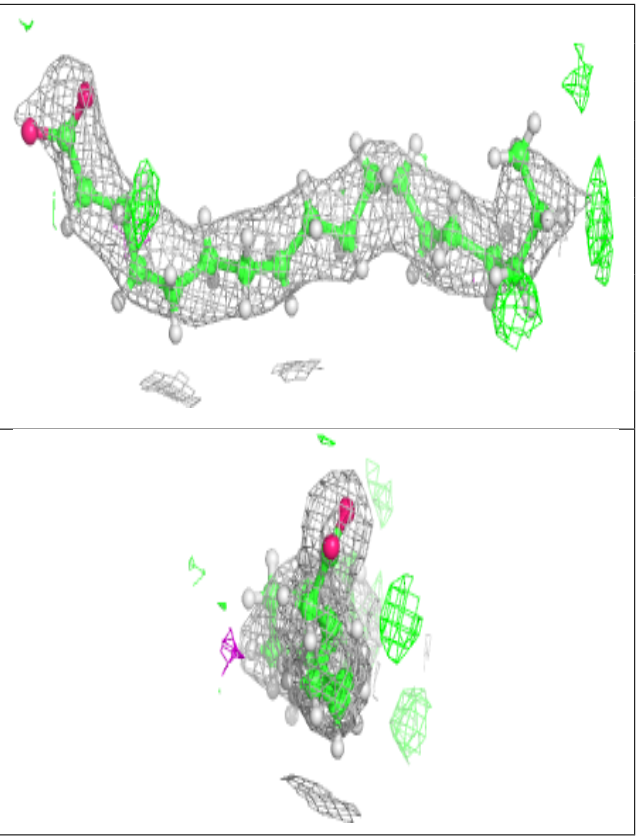
Electron density around STE B 621:

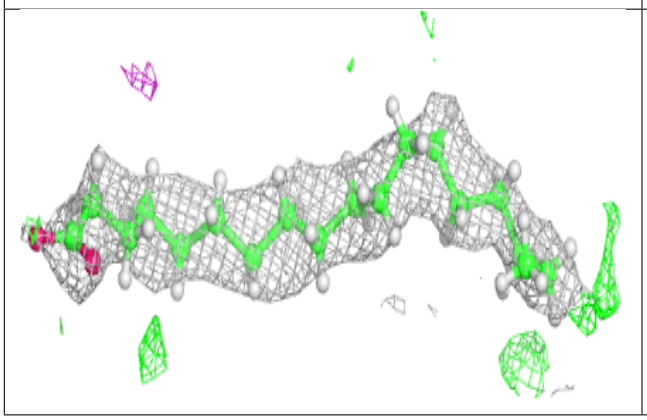
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around STE b 621:

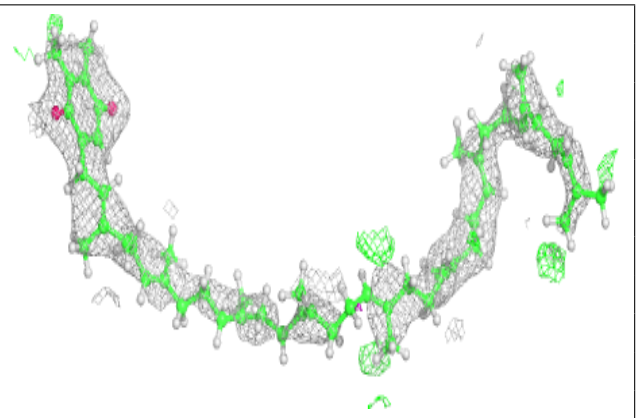
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

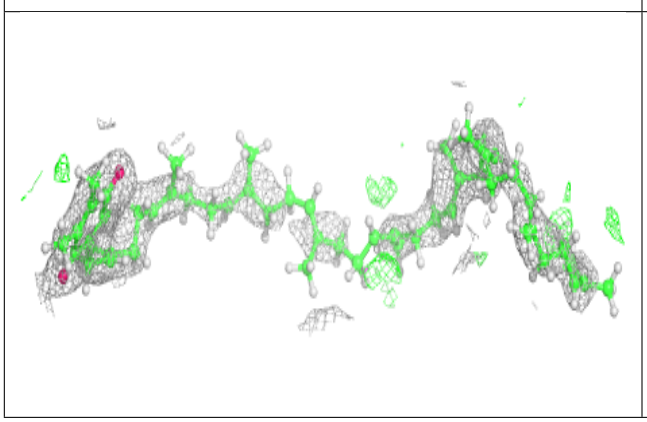


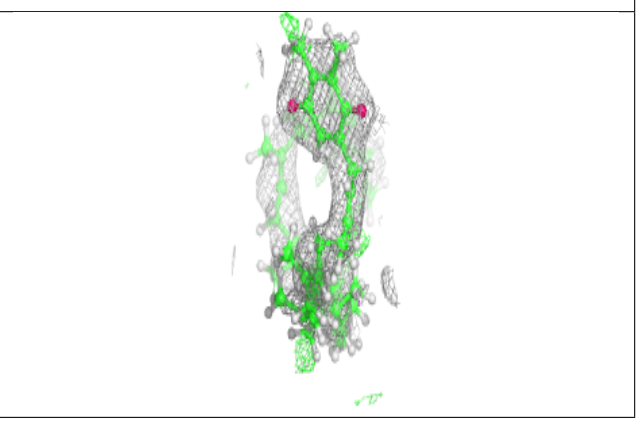


Electron density around PL9 a 410:

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

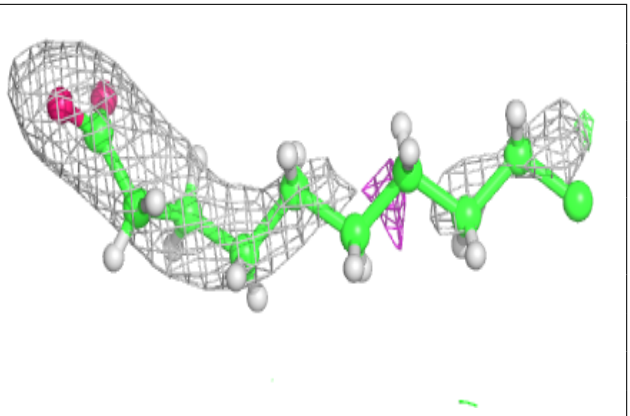


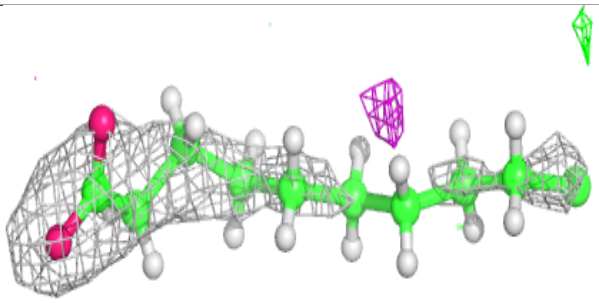


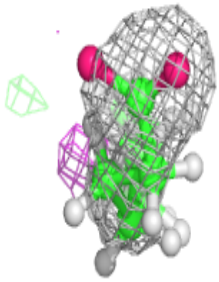


Electron density around STE B 601:

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

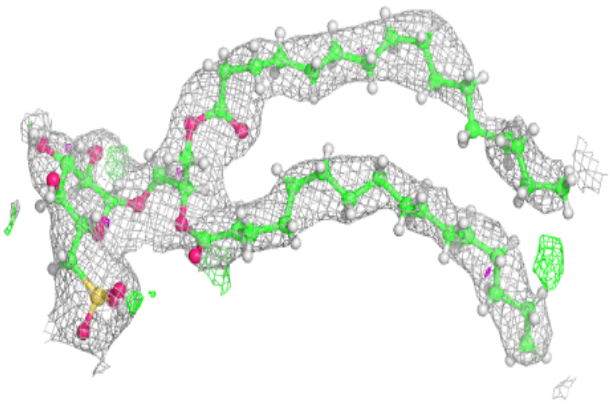


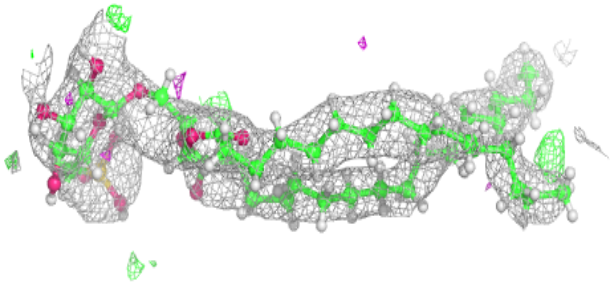


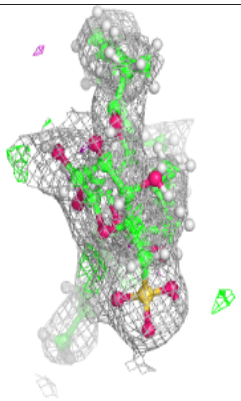


Electron density around SQD B 623:

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

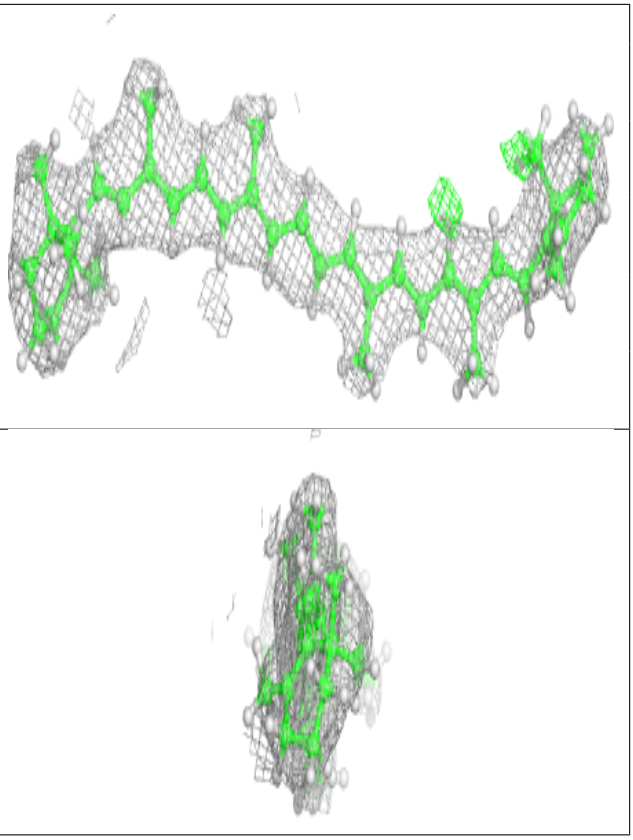






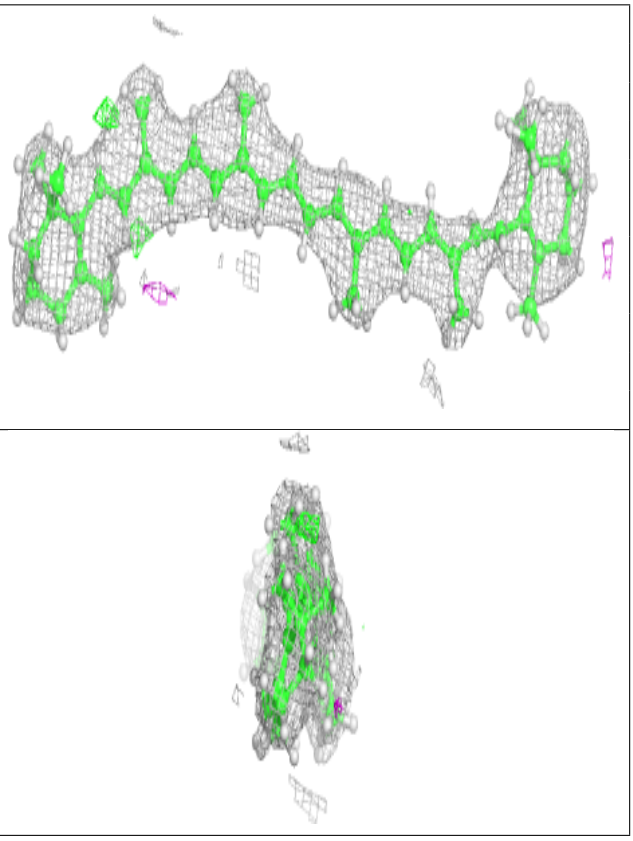
Electron density around BCR K 101:

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



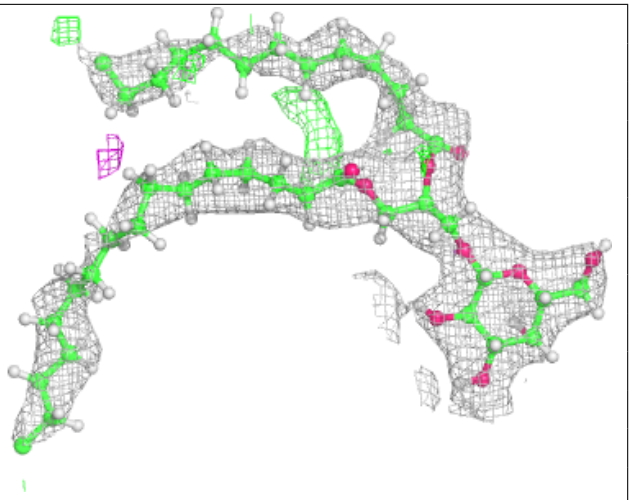
Electron density around BCR d 405:

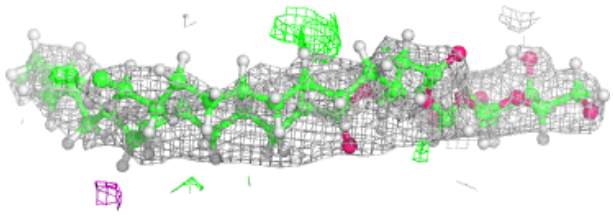
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

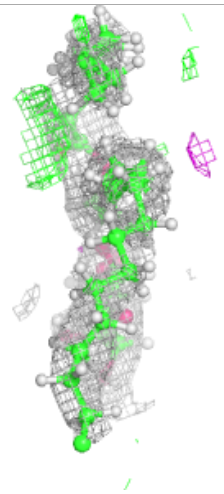


Electron density around LMG Y 101:

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

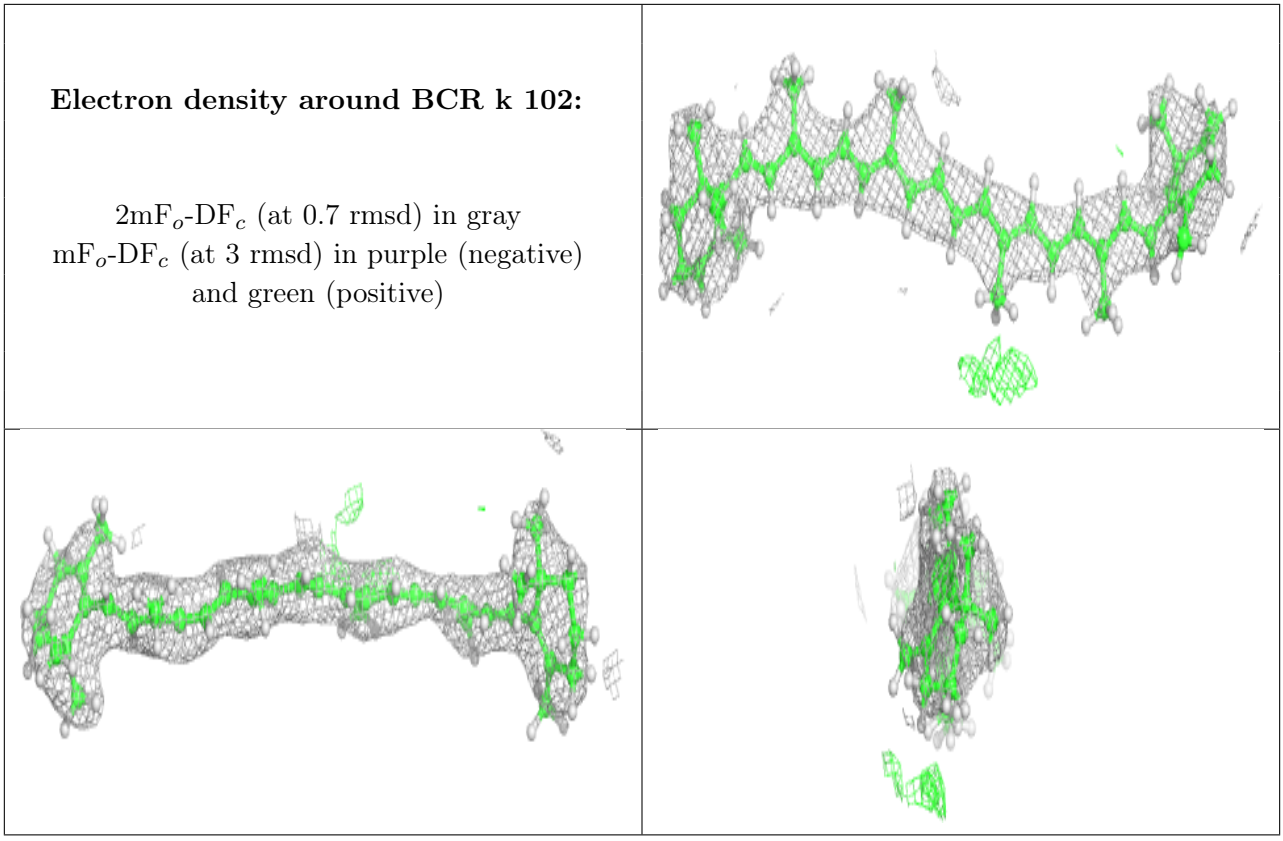






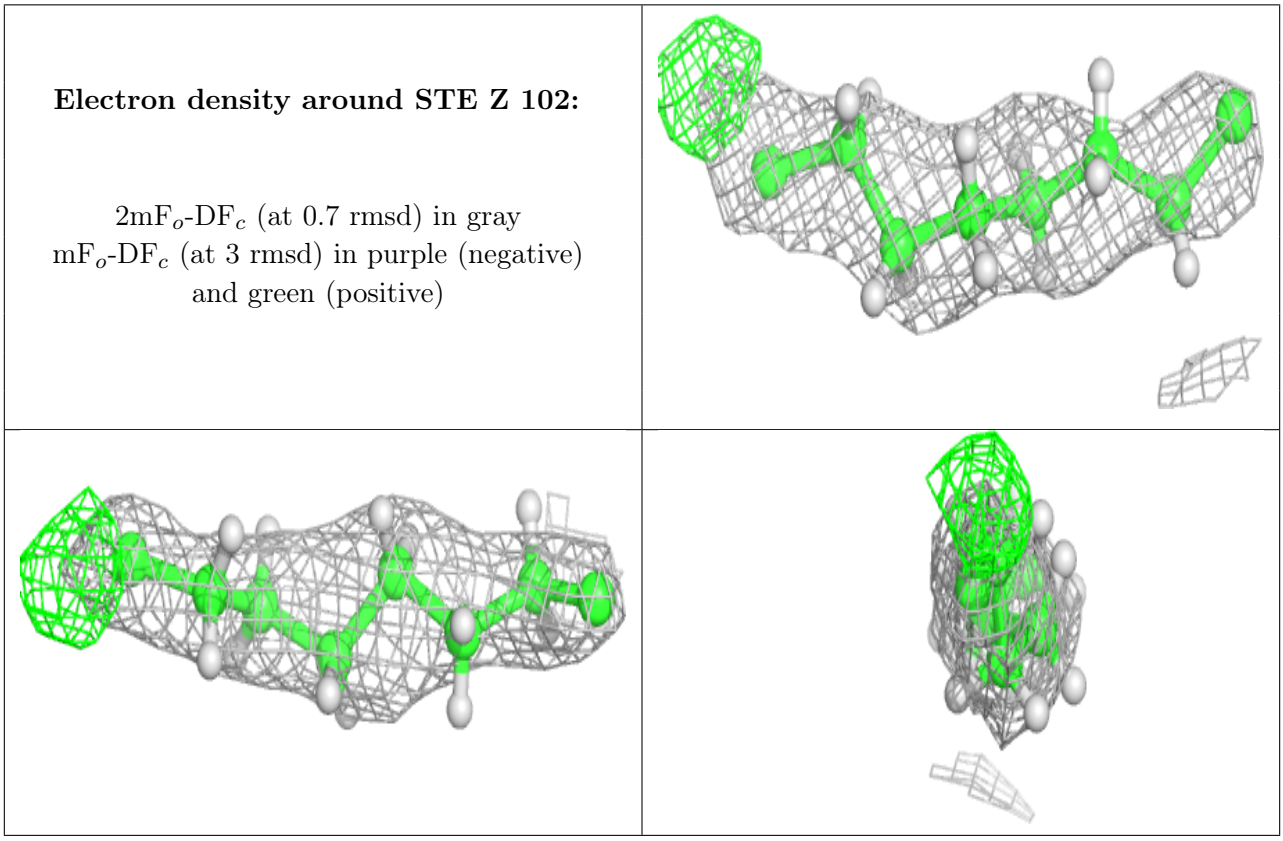
Electron density around BCR k 102:

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



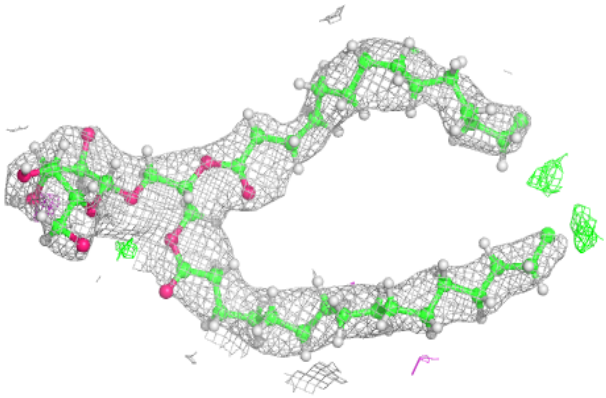
Electron density around STE Z 102:

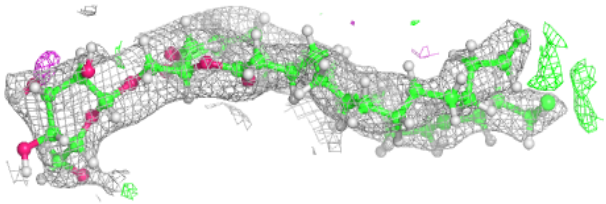
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

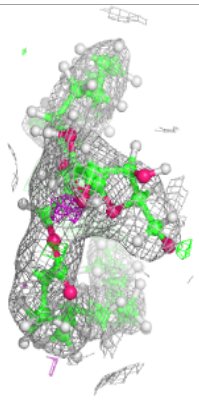


Electron density around LMG c 522:

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

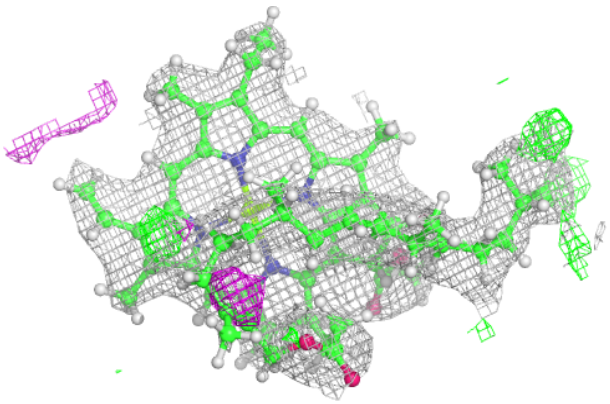


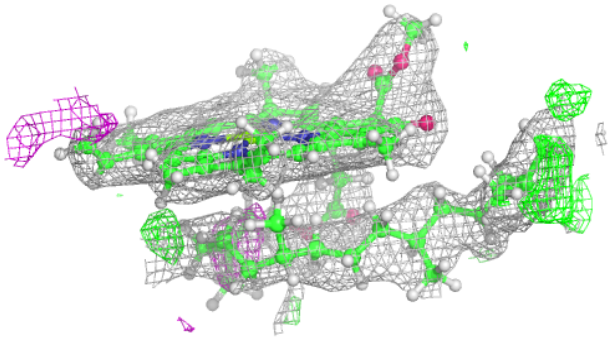


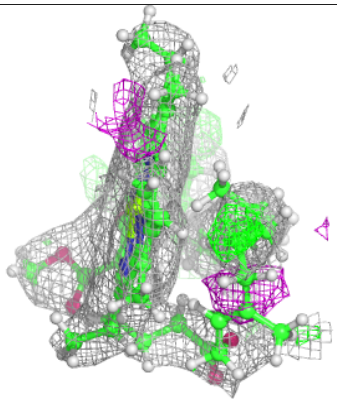


Electron density around CLA B 602:

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

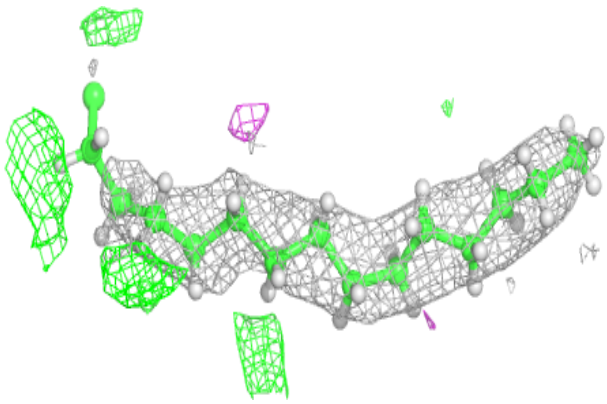


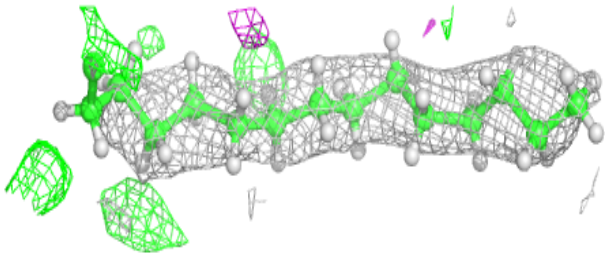


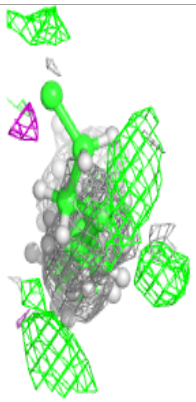


Electron density around STE T 102:

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

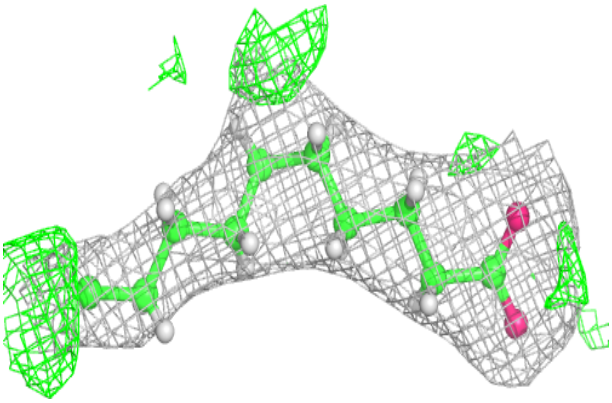


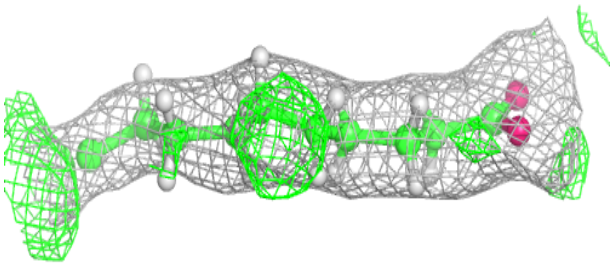


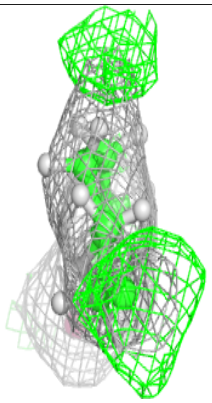


Electron density around STE C 522:

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

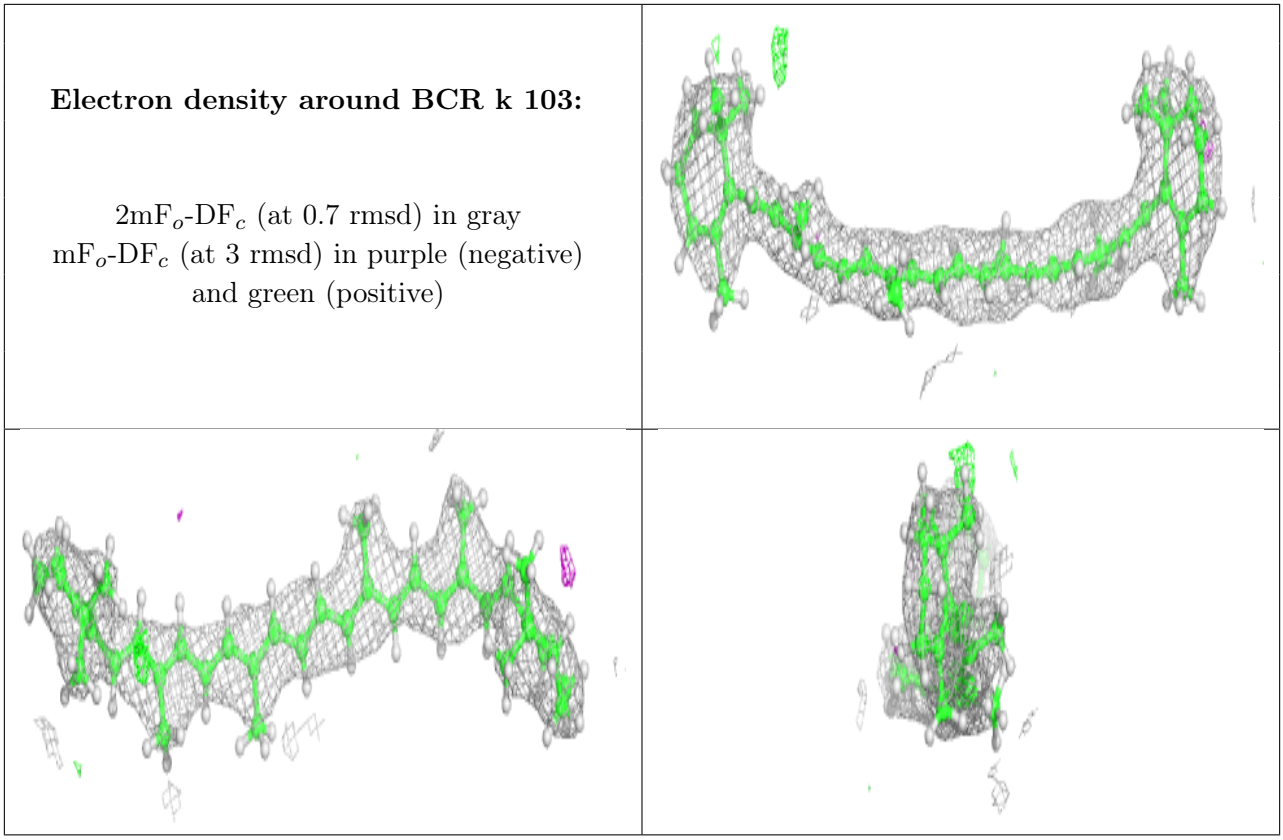






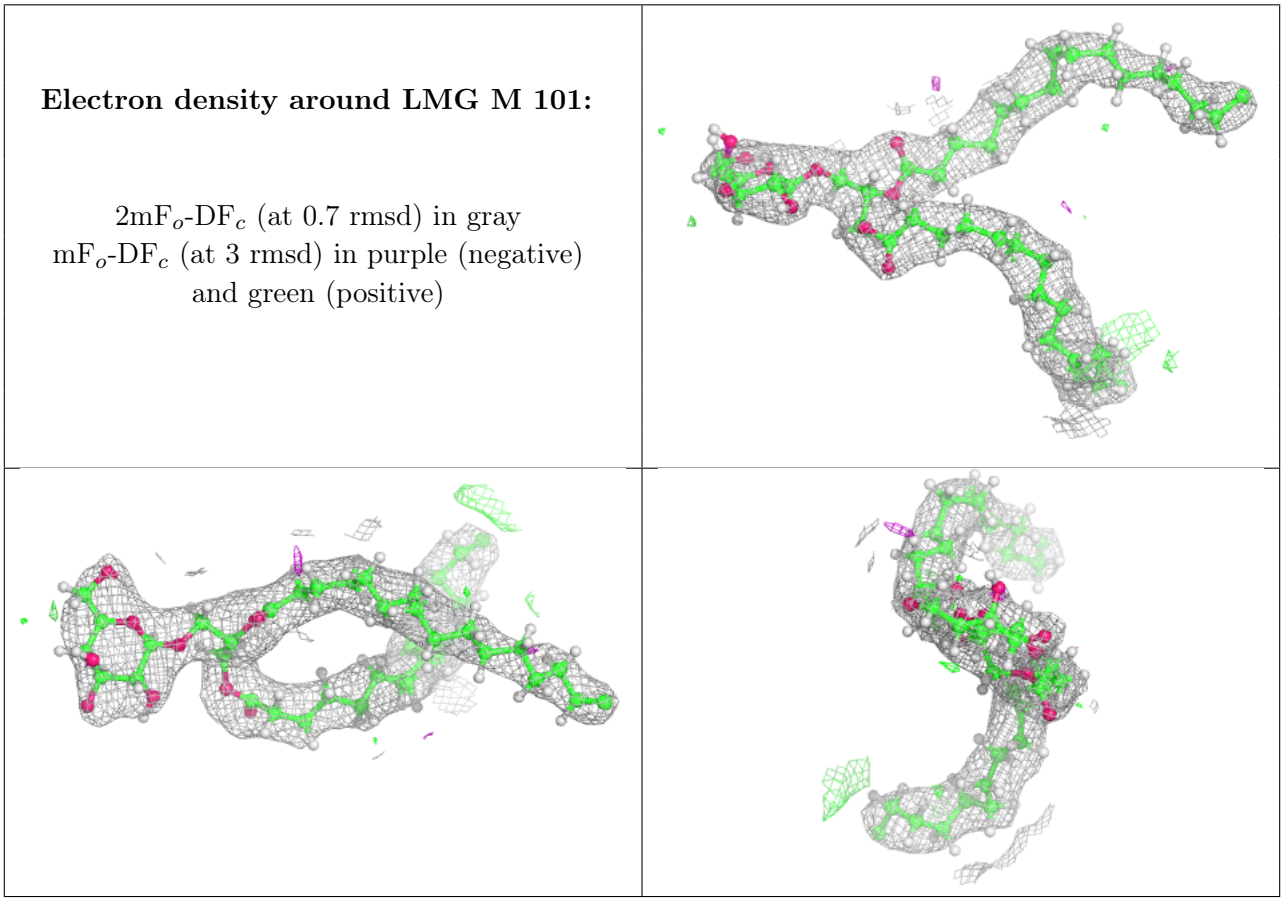
Electron density around BCR k 103:

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



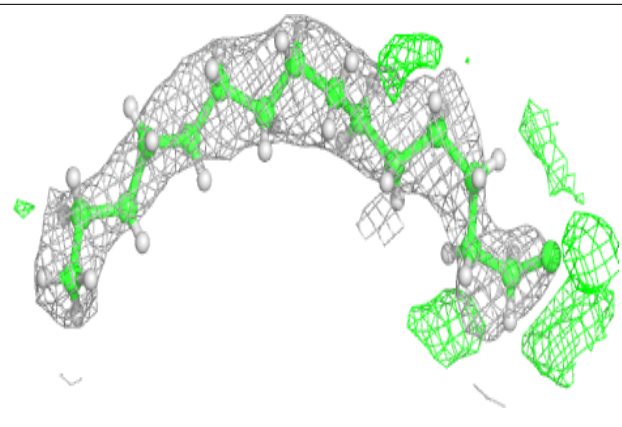
Electron density around LMG M 101:

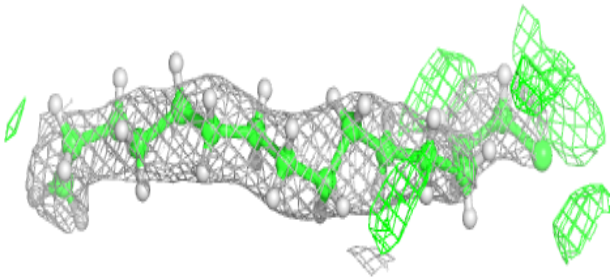
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

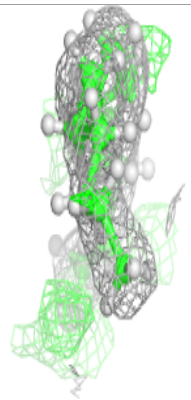


Electron density around STE b 620:

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

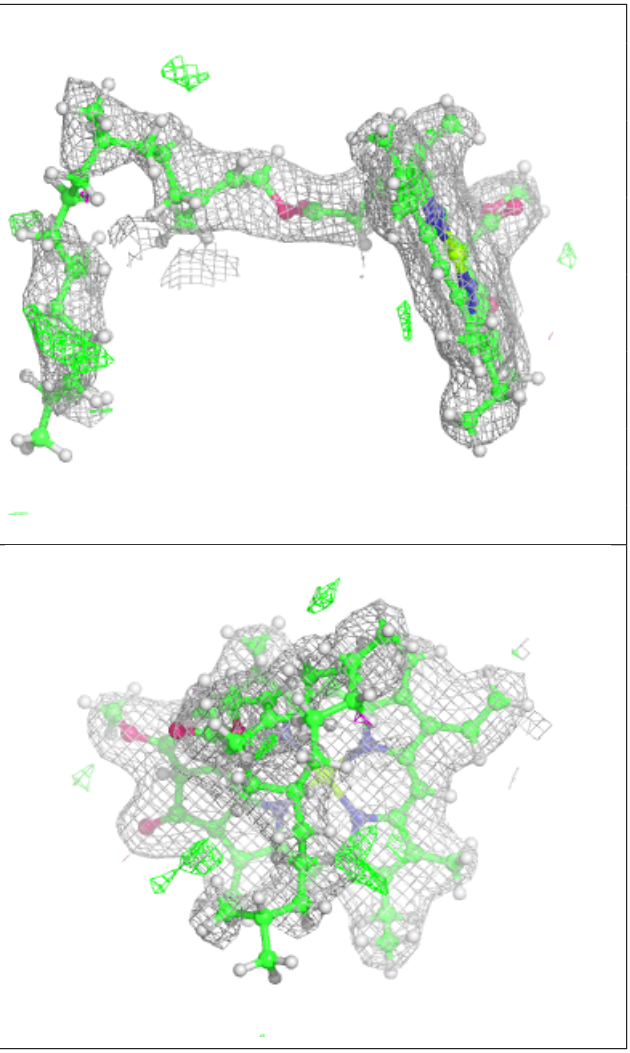






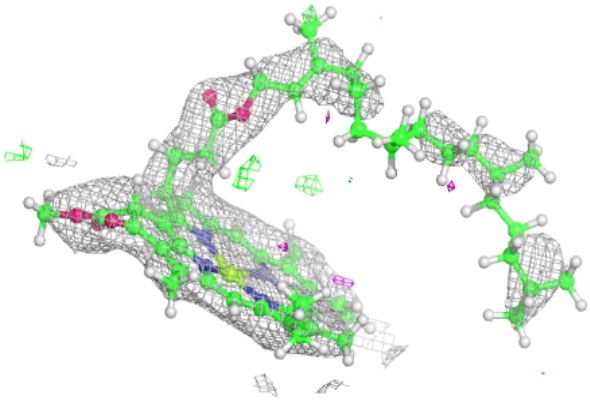
Electron density around CLA a 405:

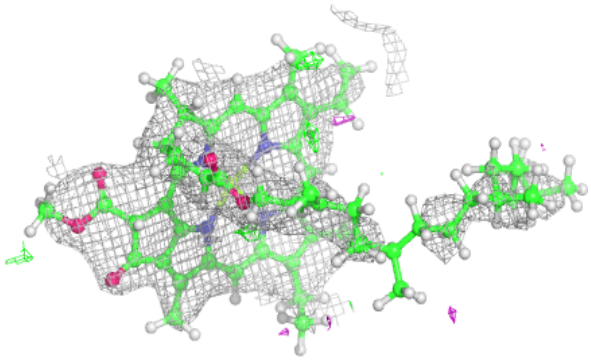
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

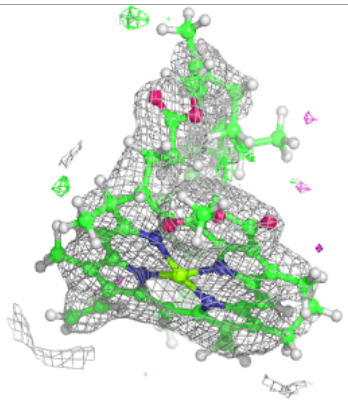


Electron density around CLA c 513:

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

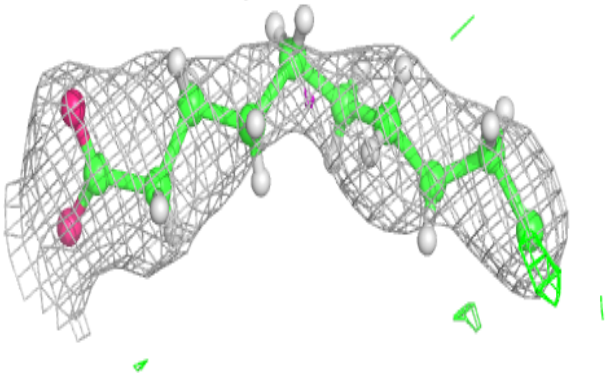


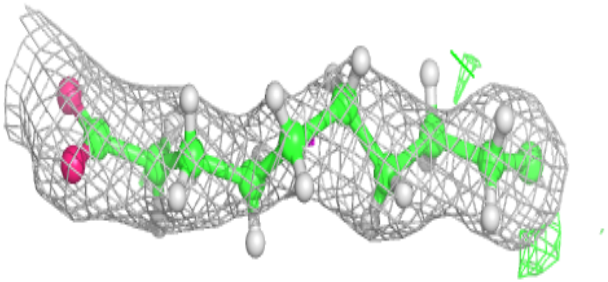


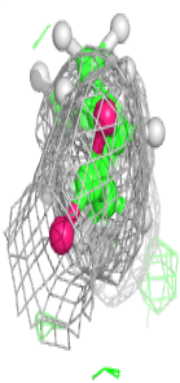


Electron density around STE C 520:

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

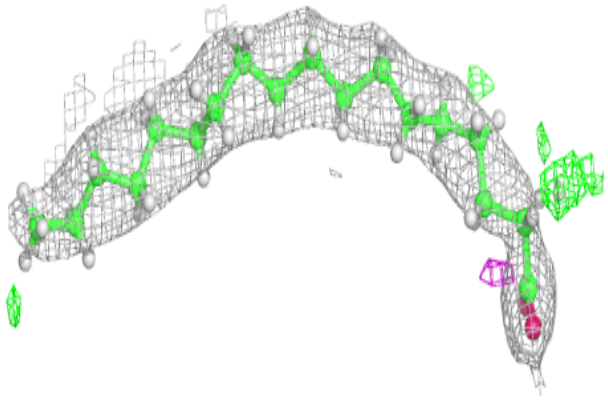


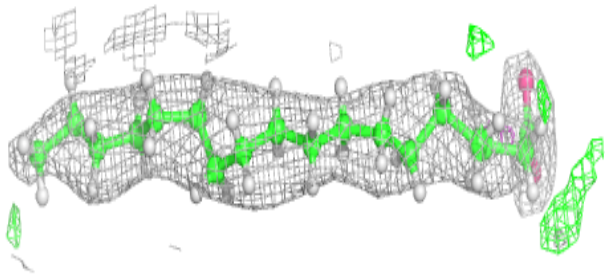


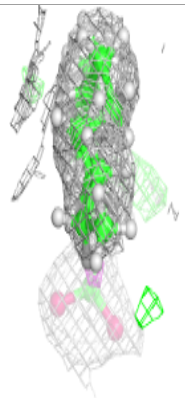


Electron density around STE D 411:

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

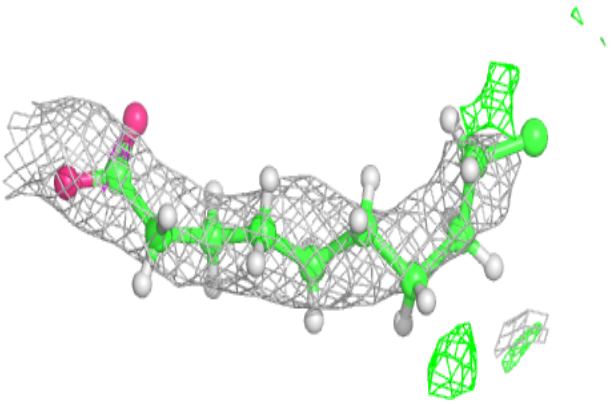


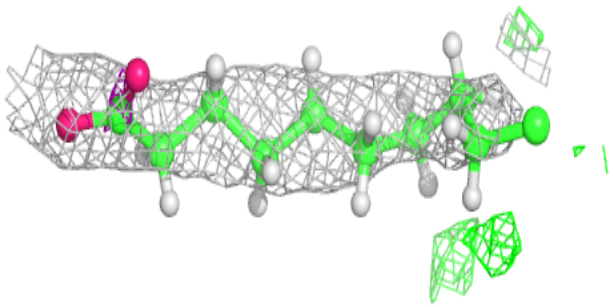


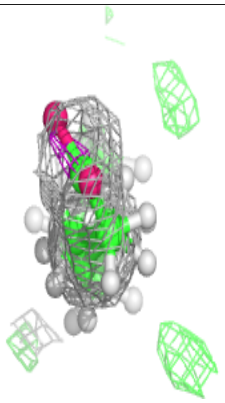


Electron density around STE L 103:

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

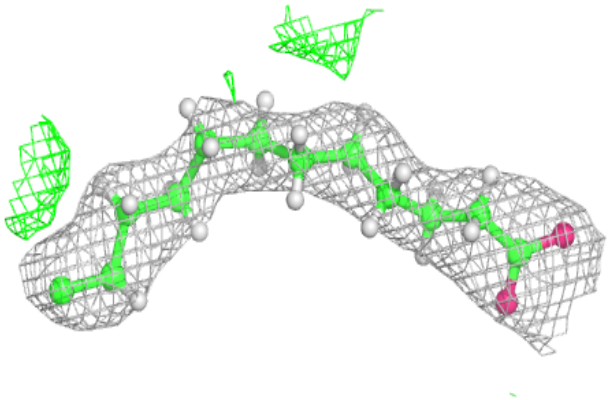


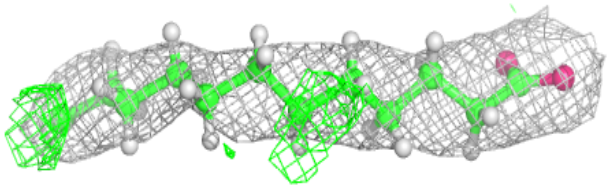


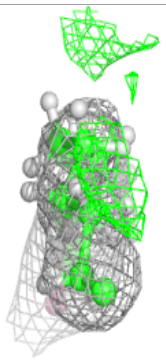


Electron density around STE t 102:

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

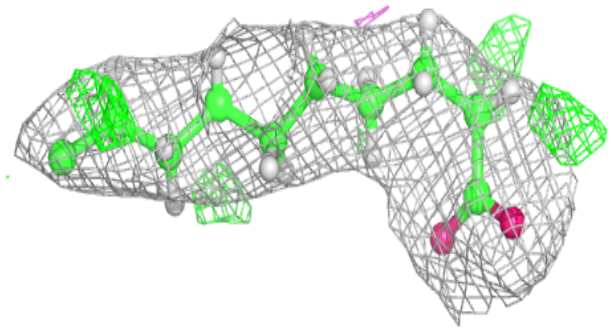


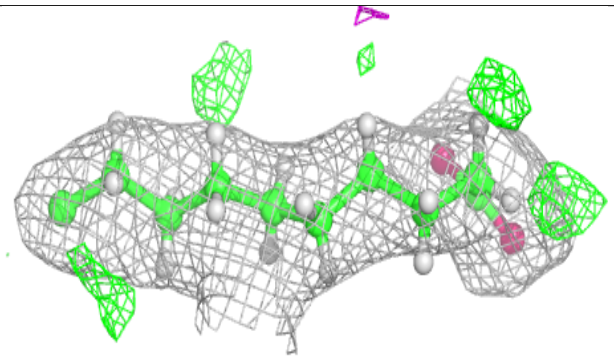


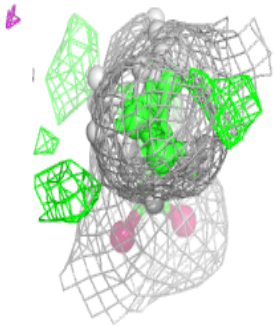


Electron density around STE B 624:

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

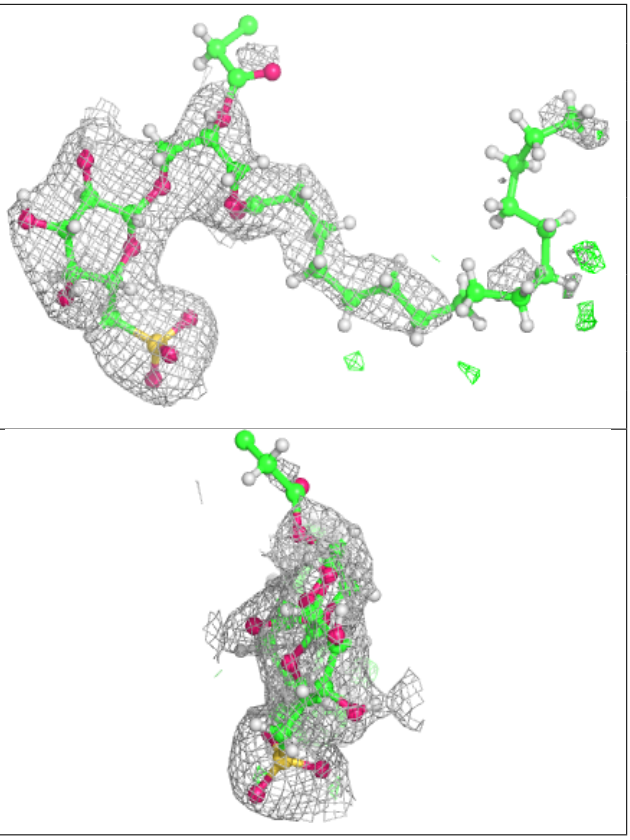


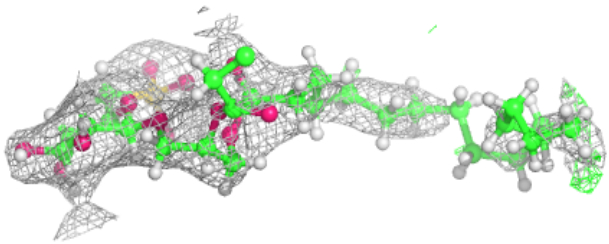




Electron density around SQD f 101:

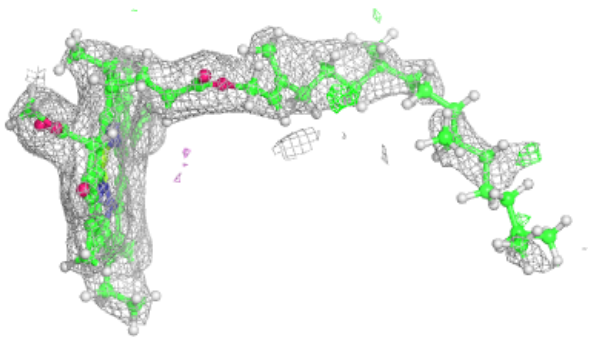
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

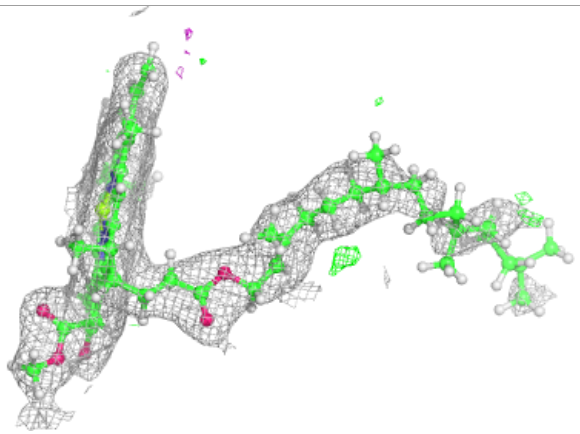


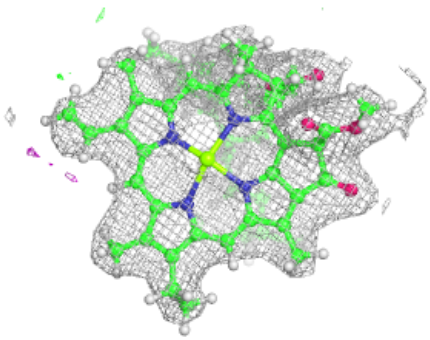


Electron density around CLA D 404:

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

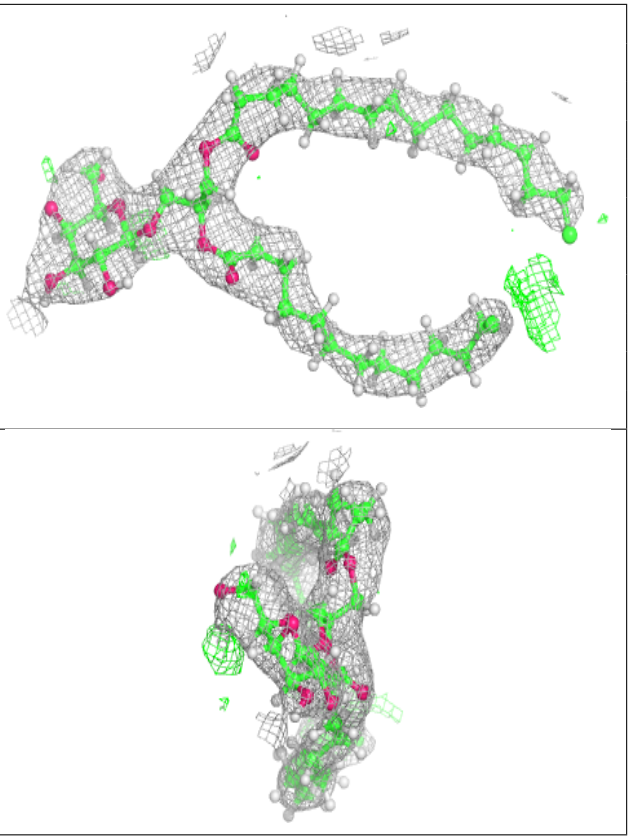






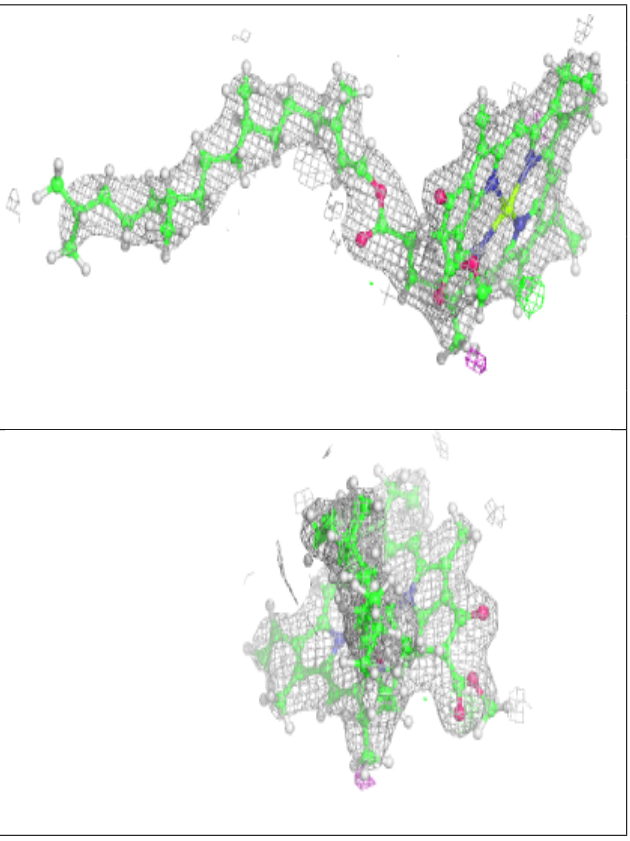
Electron density around LMG C 516:

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



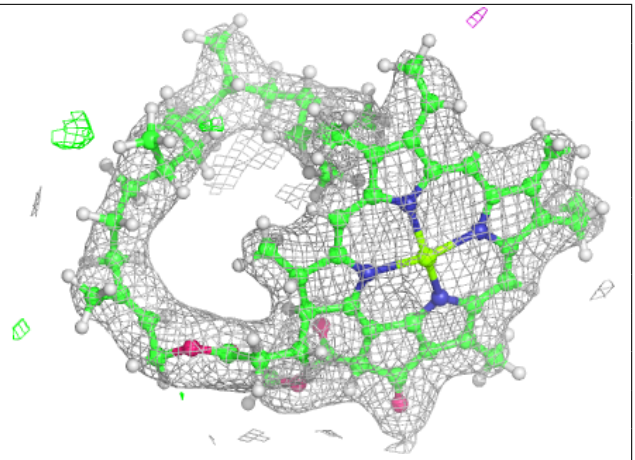
Electron density around CLA C 503:

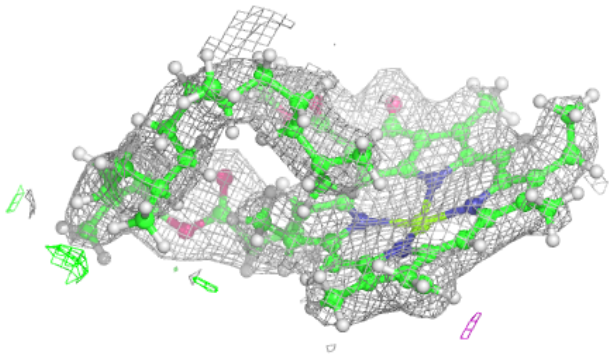
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

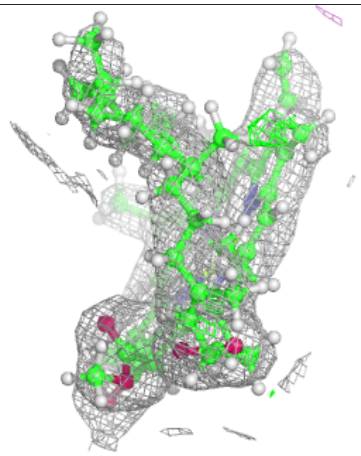


Electron density around CLA B 616:

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

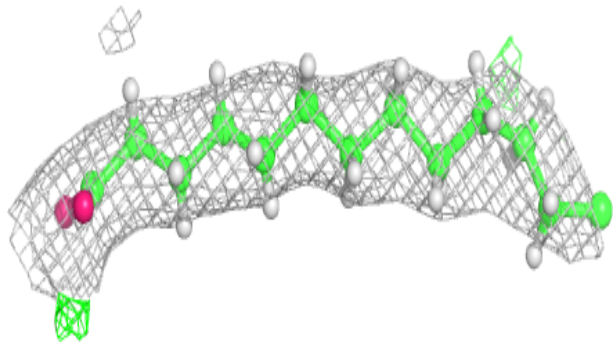


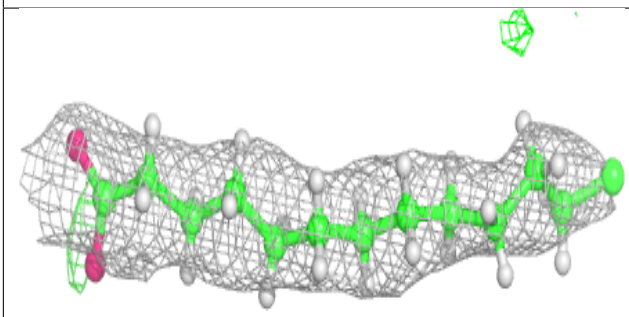


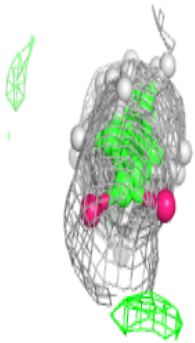


Electron density around STE M 102:

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

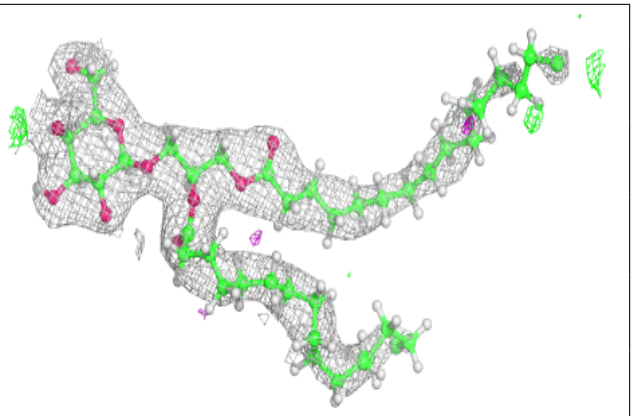


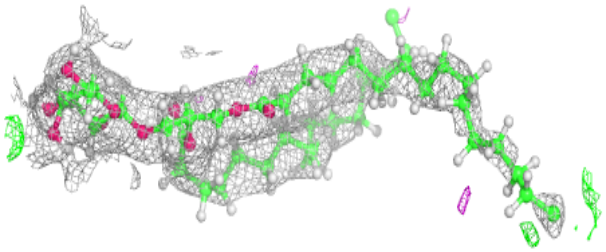


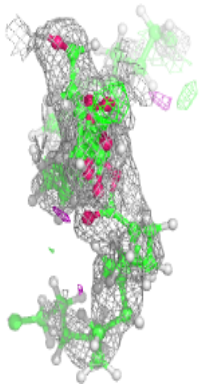


Electron density around LMG D 407:

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

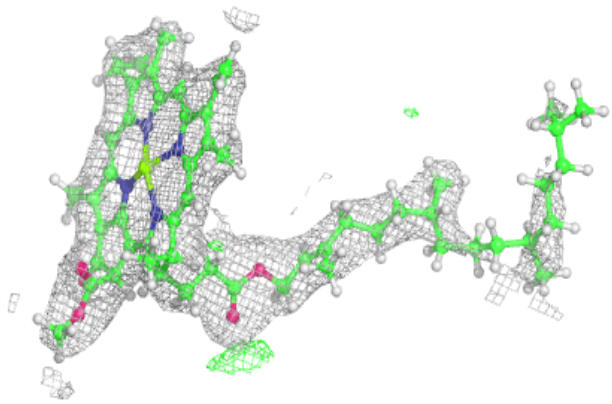


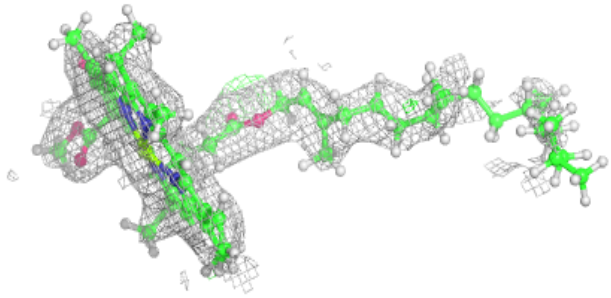


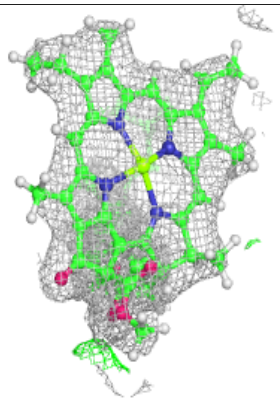


Electron density around CLA d 404:

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

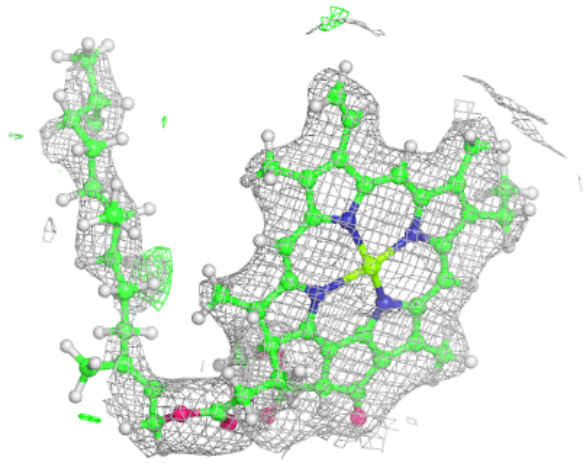


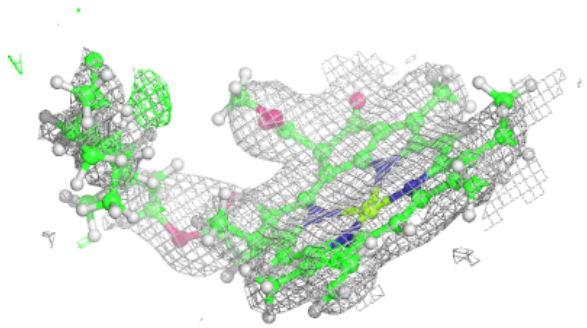


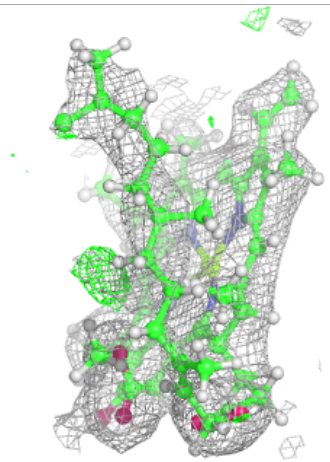


Electron density around CLA b 616:

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

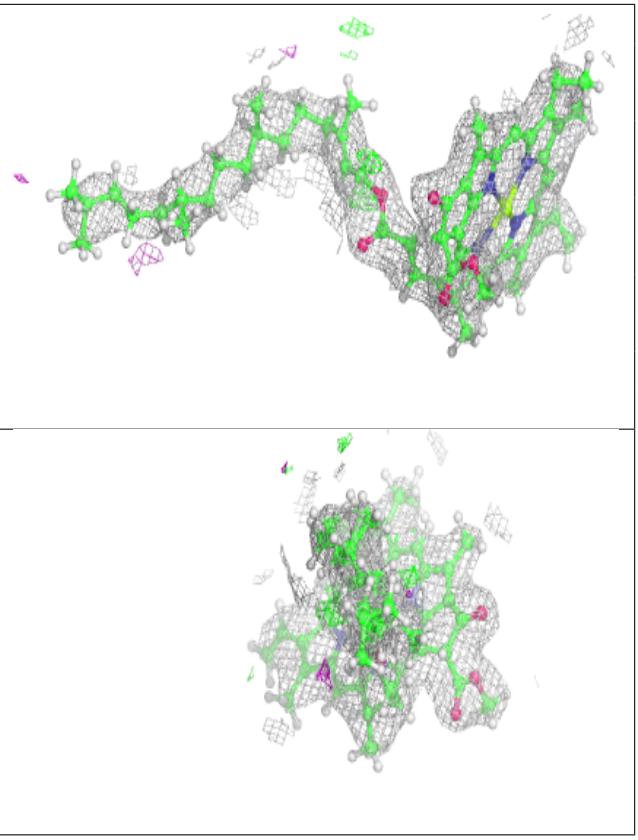






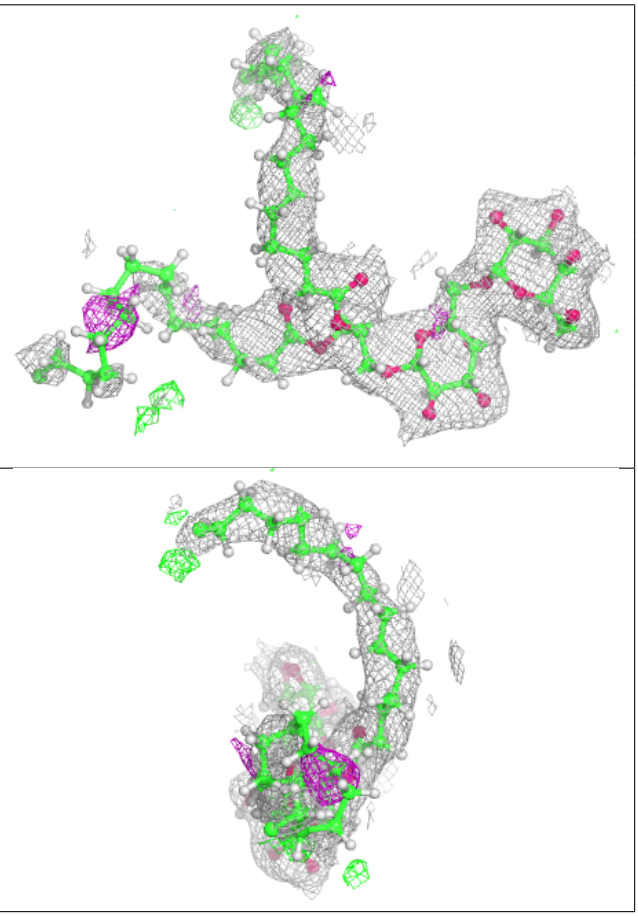
Electron density around CLA c 502:

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



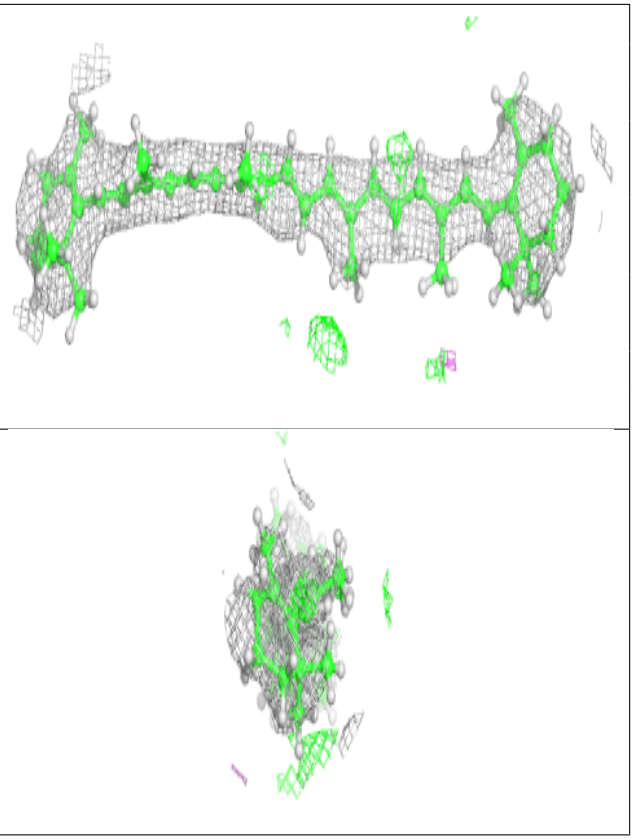
Electron density around DGD C 518:

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



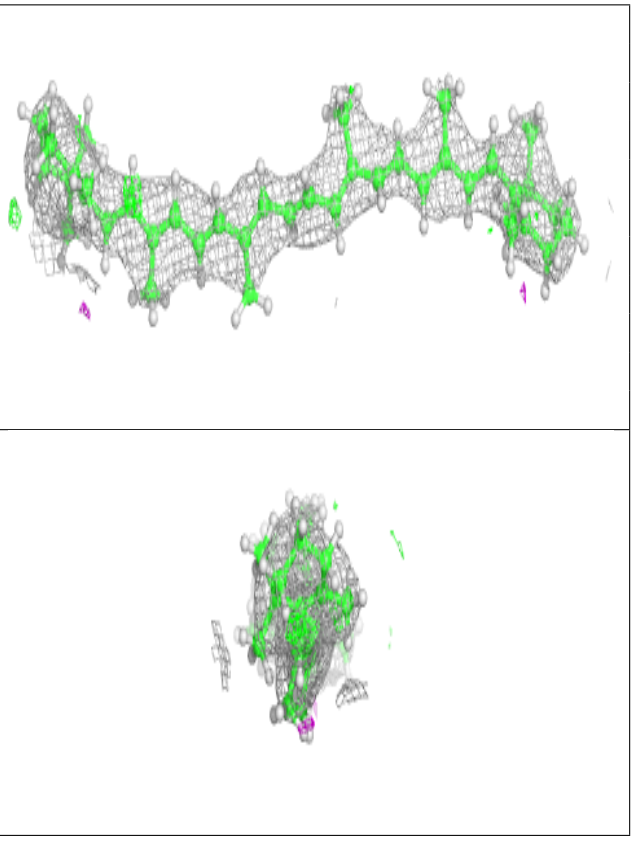
Electron density around BCR Z 101:

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



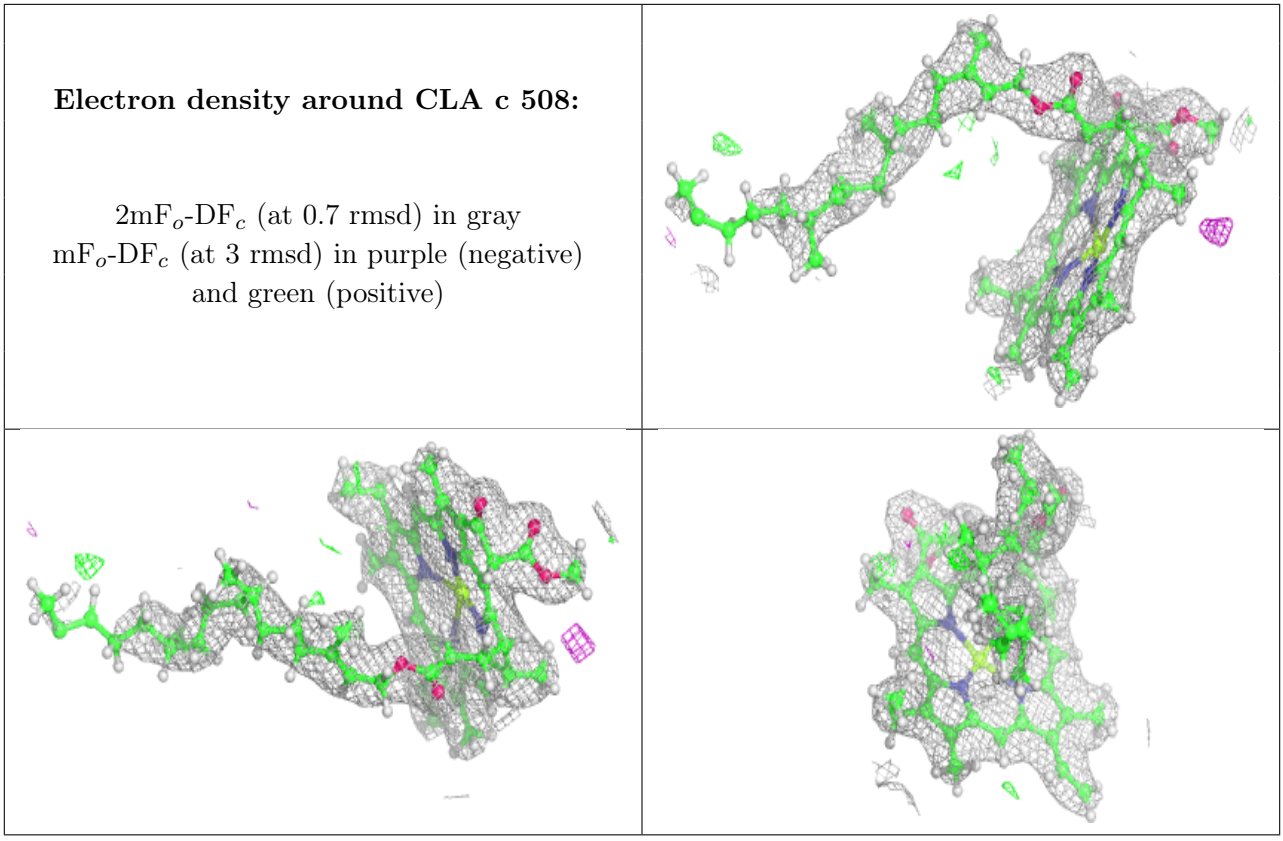
Electron density around BCR c 514:

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



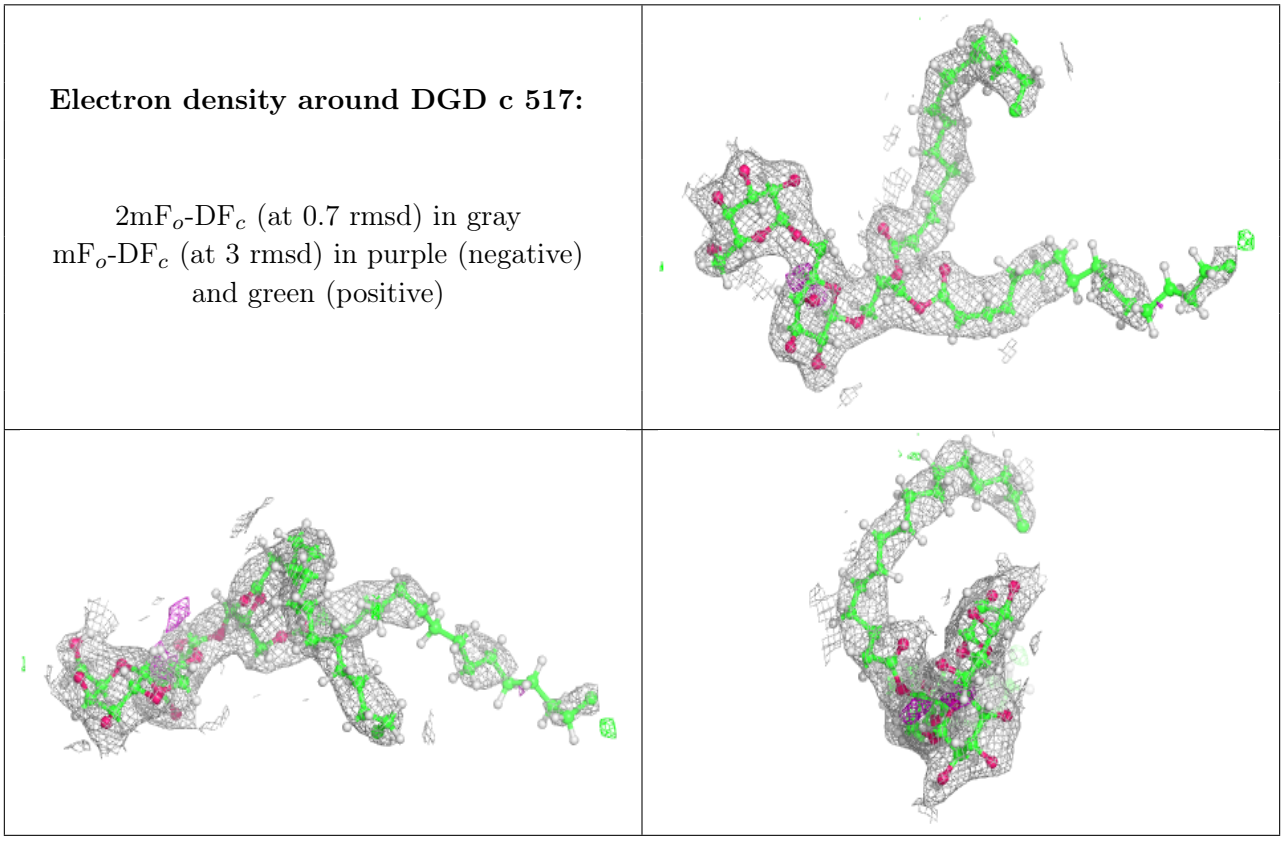
Electron density around CLA c 508:

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



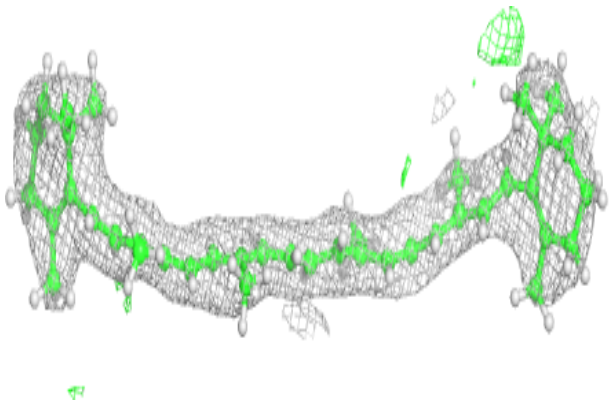
Electron density around DGD c 517:

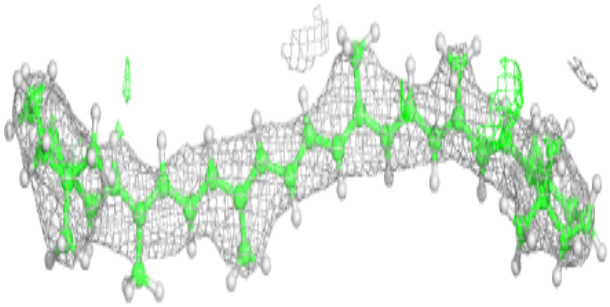
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

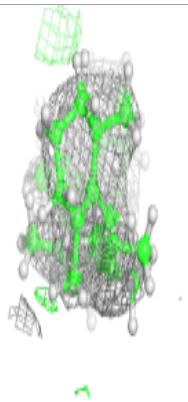


Electron density around BCR C 501:

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

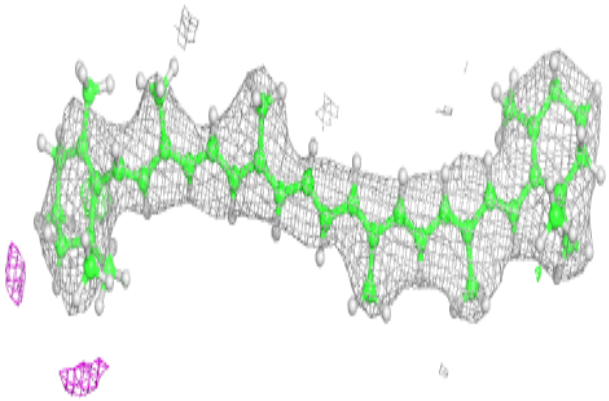


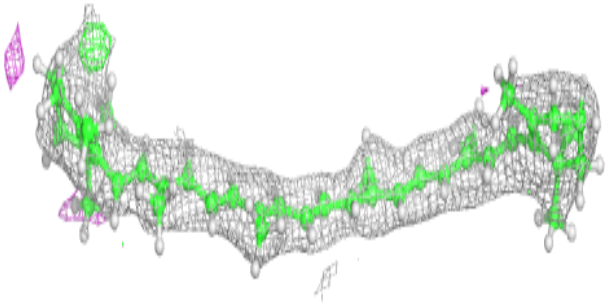


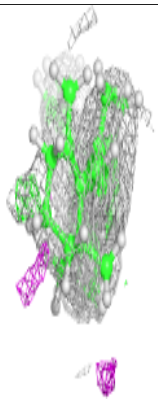


Electron density around BCR D 405:

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

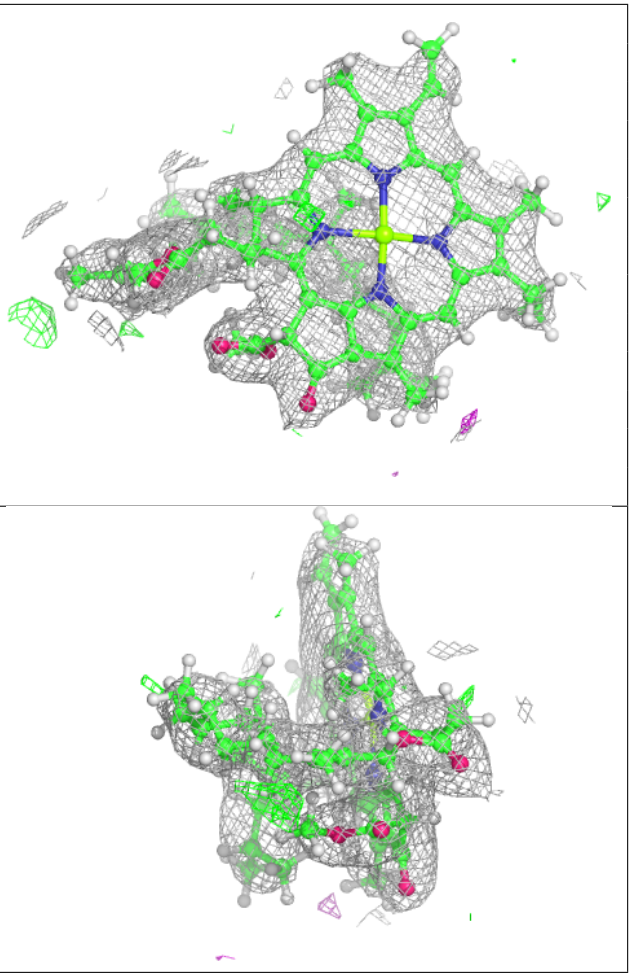






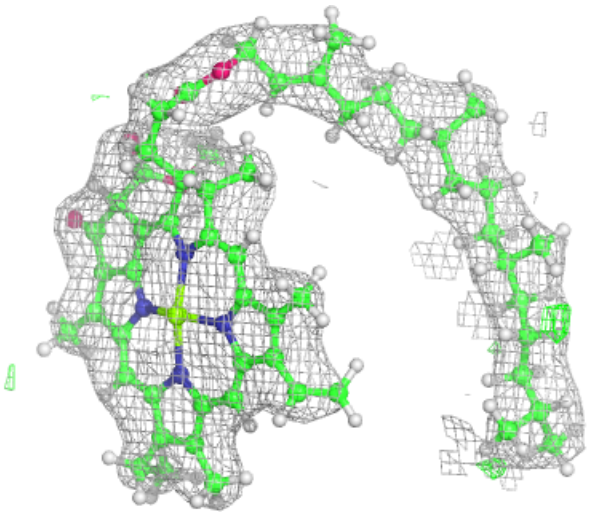
Electron density around CLA c 510:

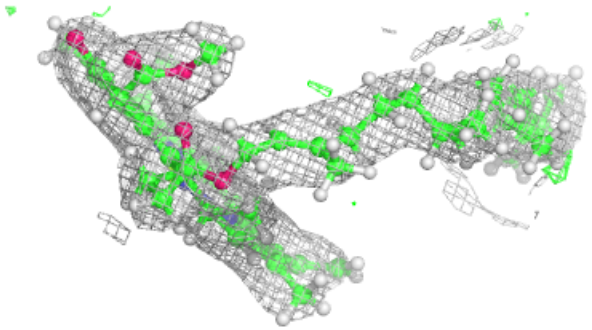
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

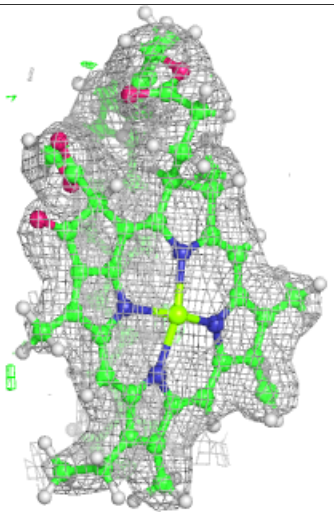


Electron density around CLA C 508:

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

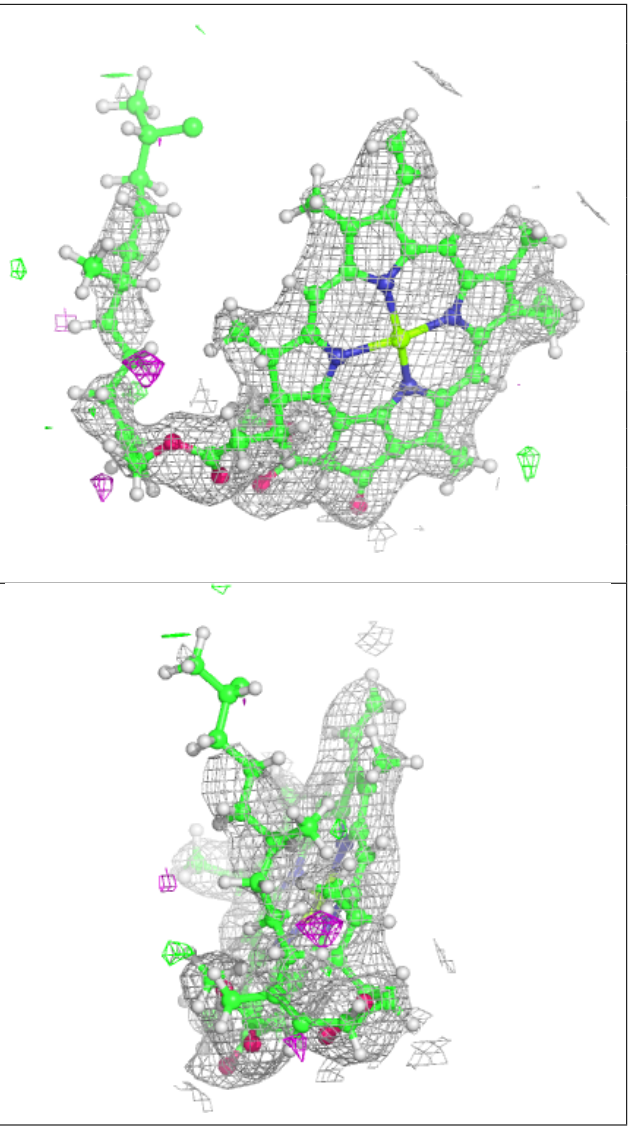






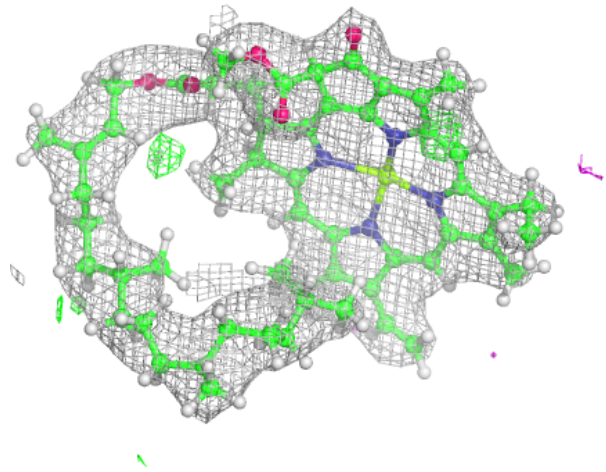
Electron density around CLA B 617:

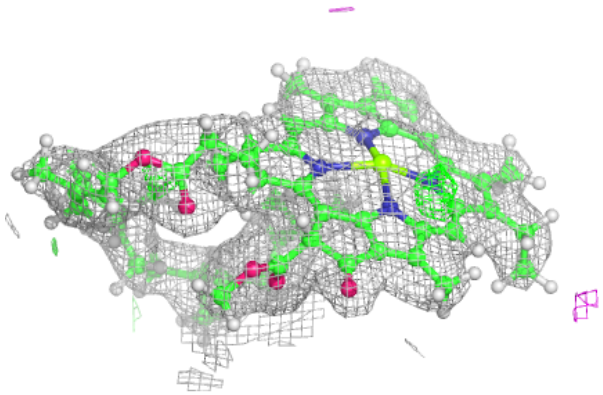
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

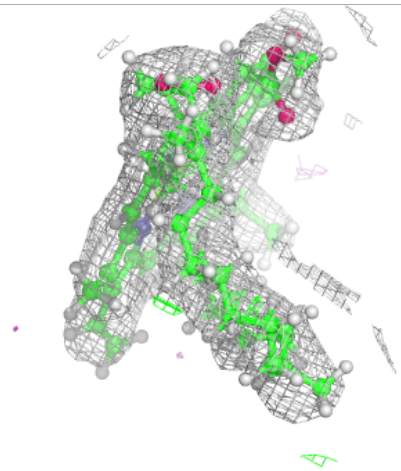


Electron density around CLA b 615:

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

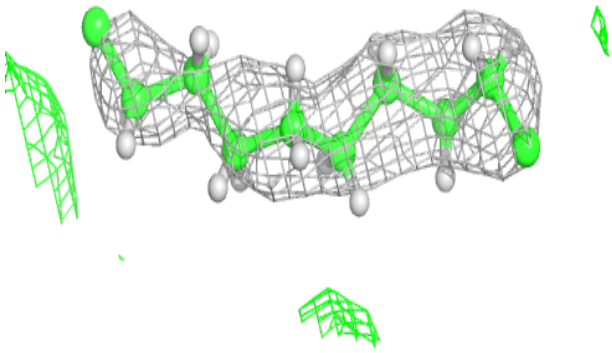


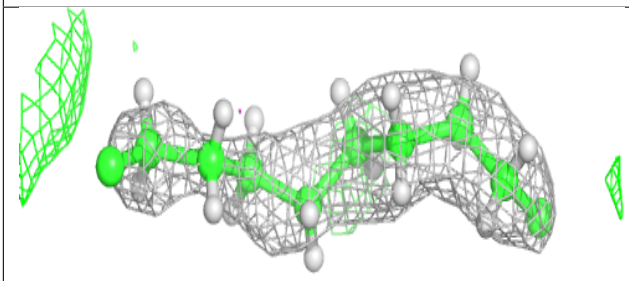


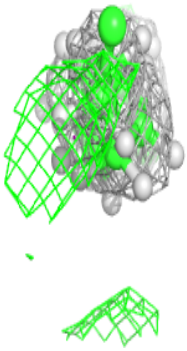


Electron density around STE t 103:

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

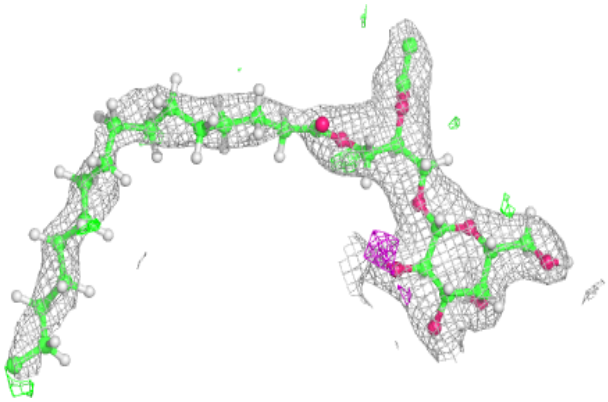


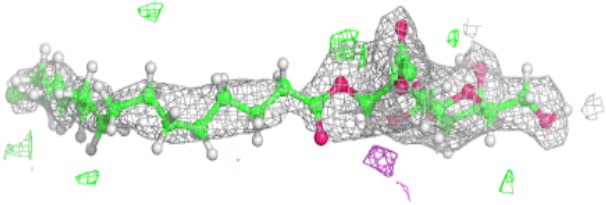


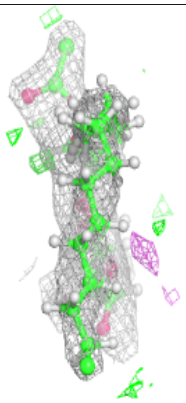


Electron density around LMG c 519:

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

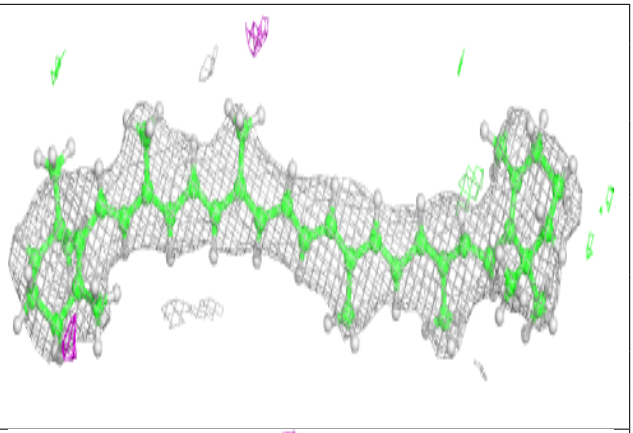


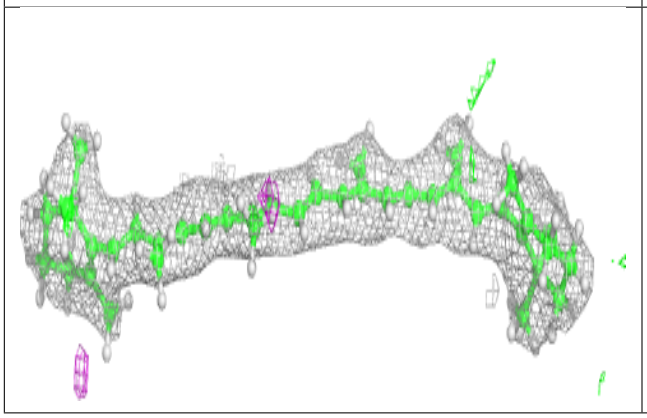


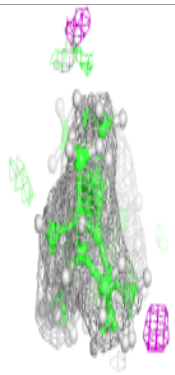


Electron density around BCR B 620:

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

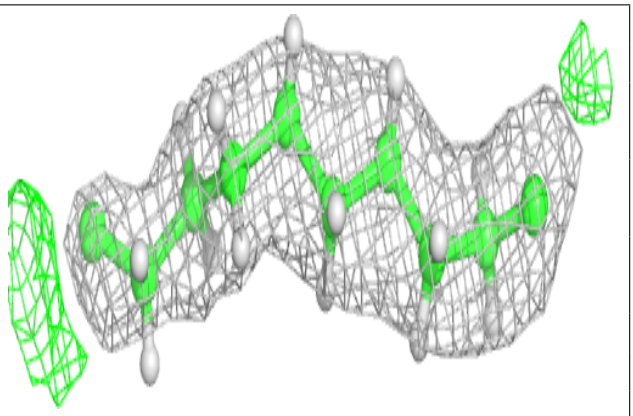


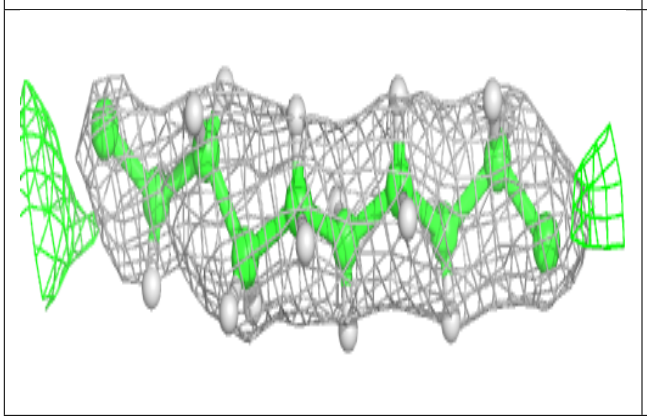


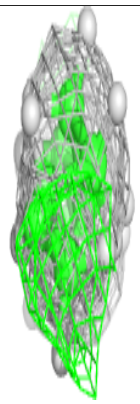


Electron density around STE M 103:

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

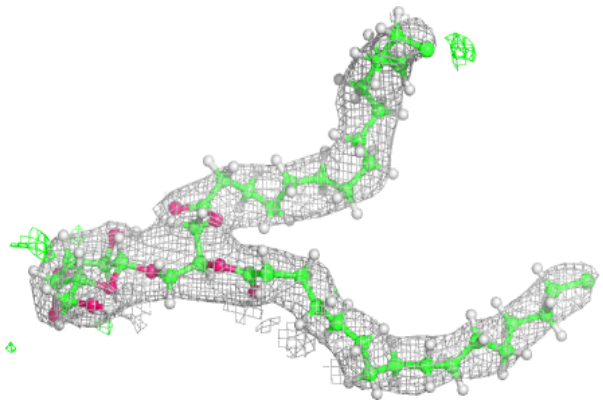


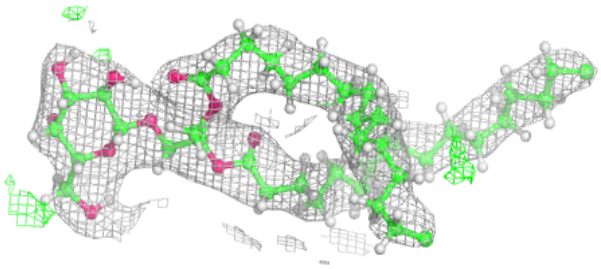


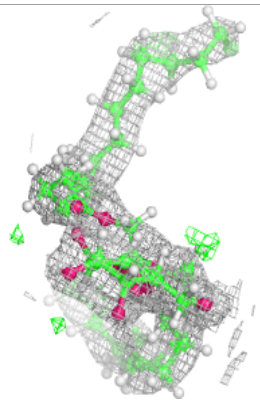


Electron density around LMG m 101:

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

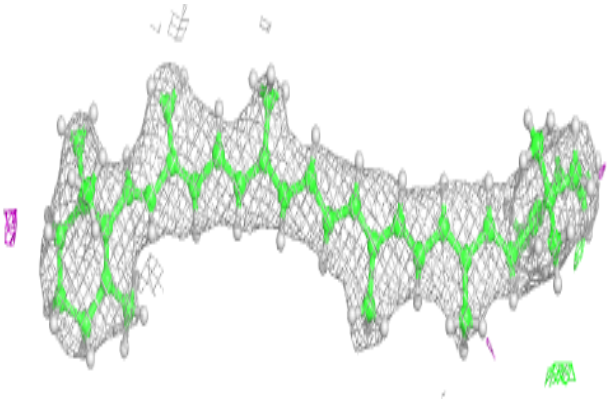


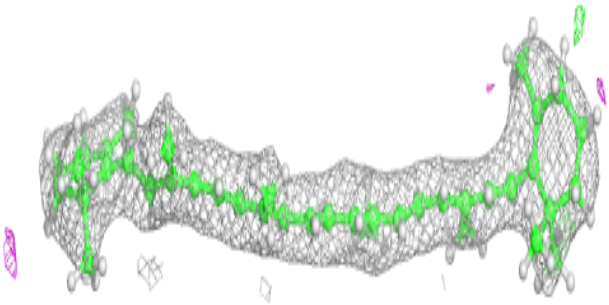


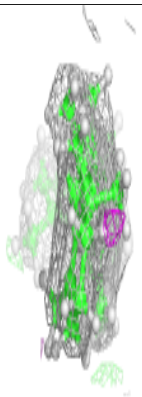


Electron density around BCR b 617:

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

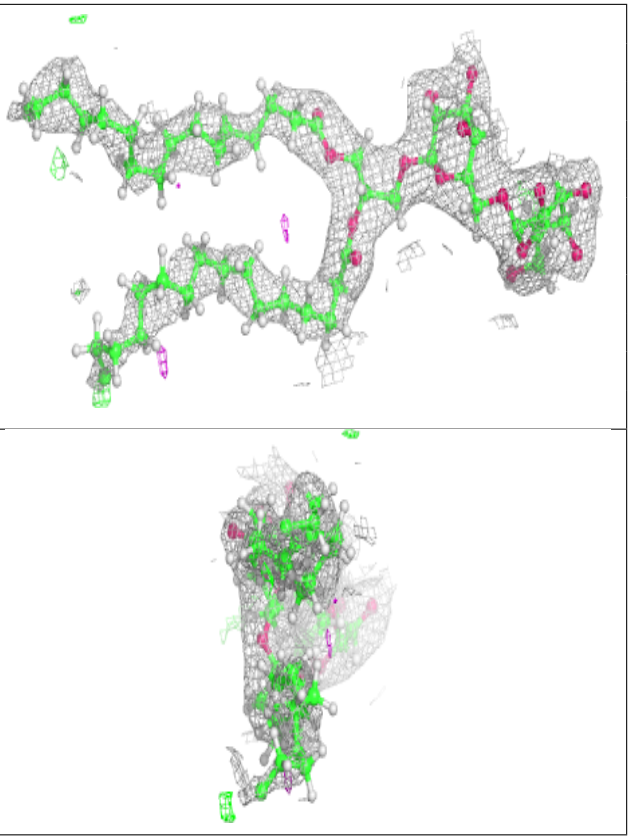






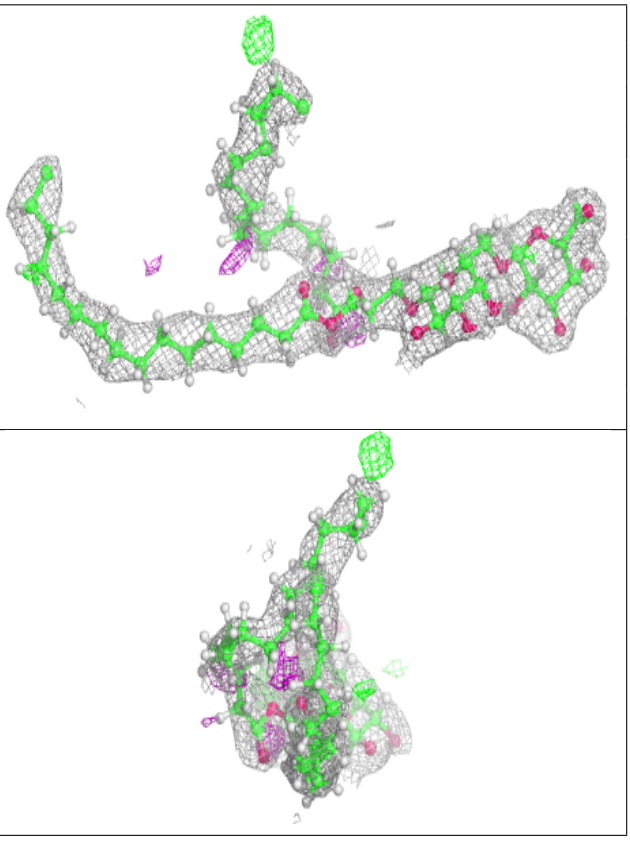
Electron density around DGD c 518:

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



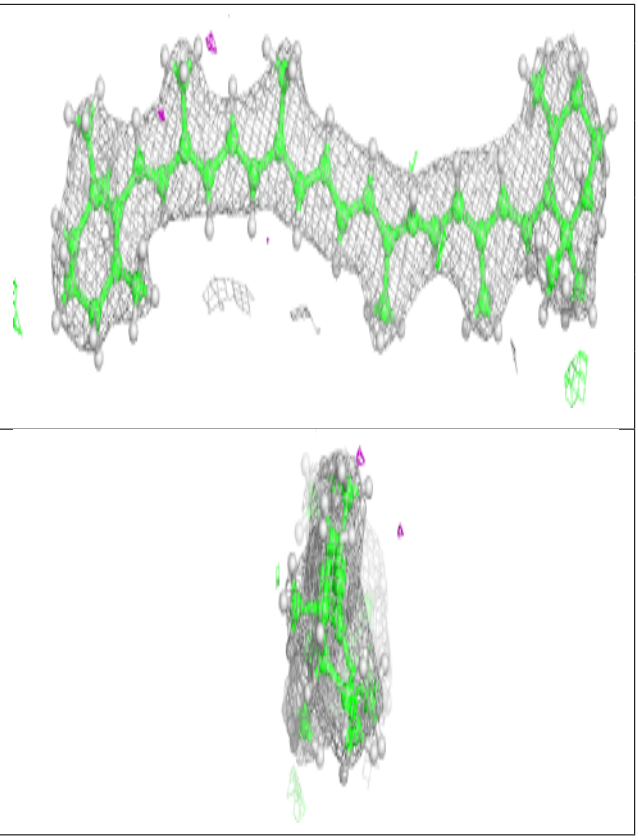
Electron density around DGD h 101:

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



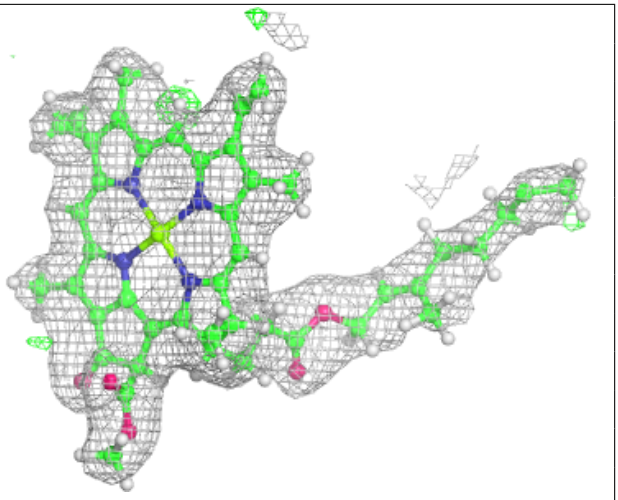
Electron density around BCR b 619:

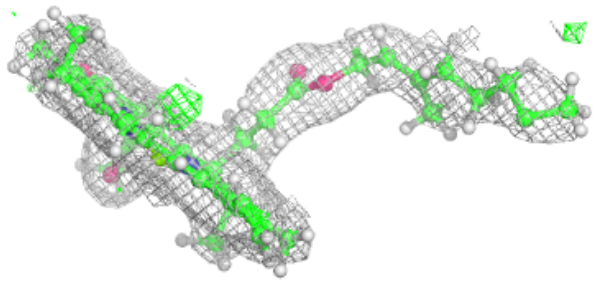
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

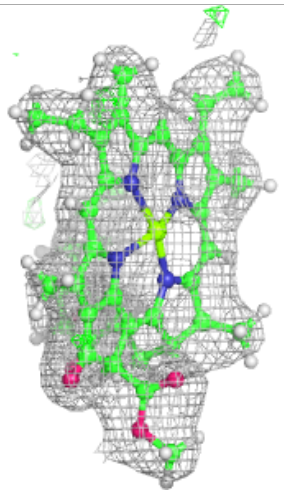


Electron density around CLA A 405:

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

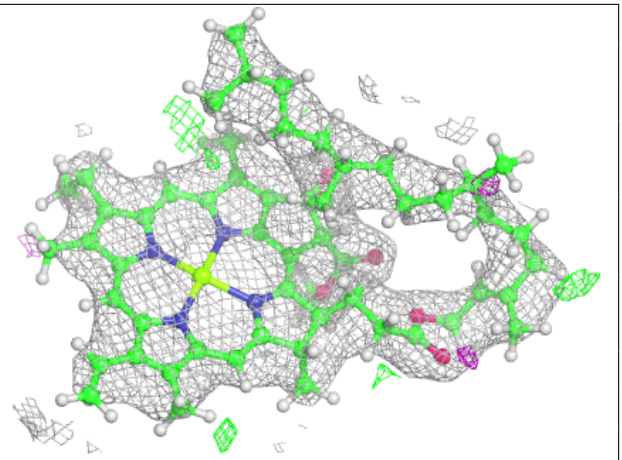


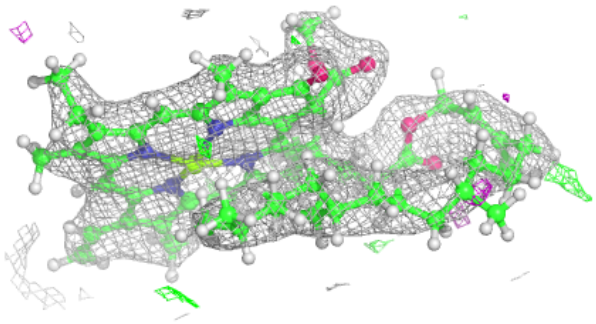


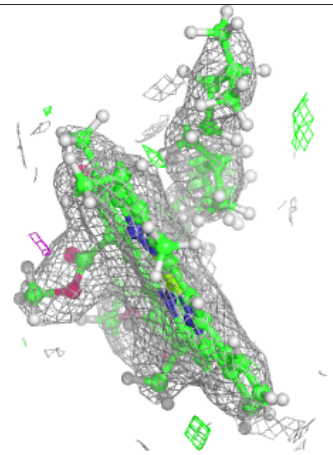


Electron density around CLA c 509:

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

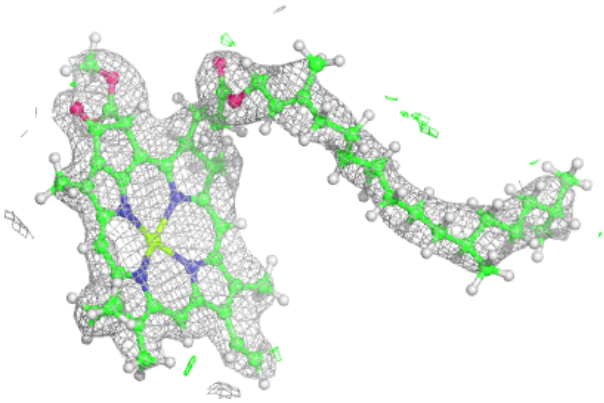


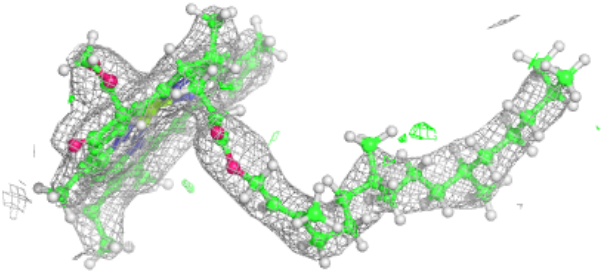


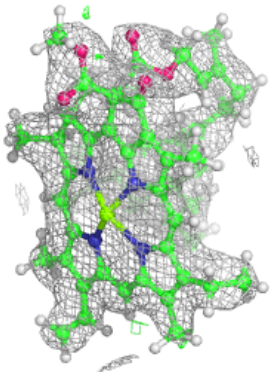


Electron density around CLA C 512:

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

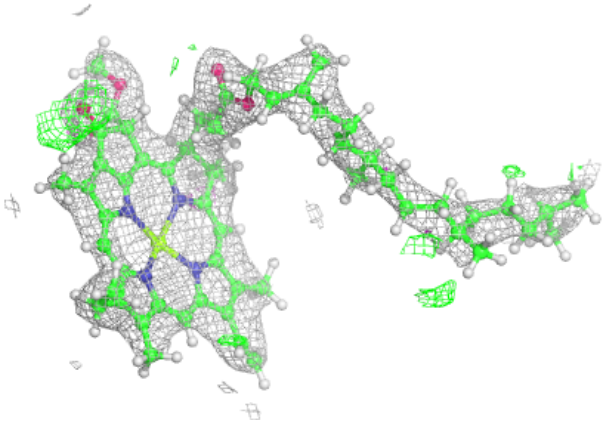


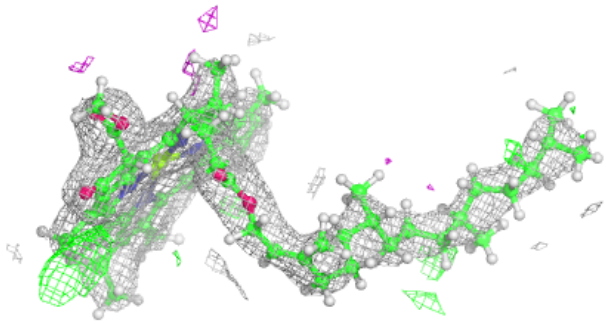


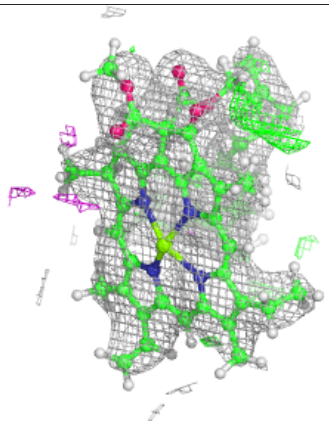


Electron density around CLA c 511:

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

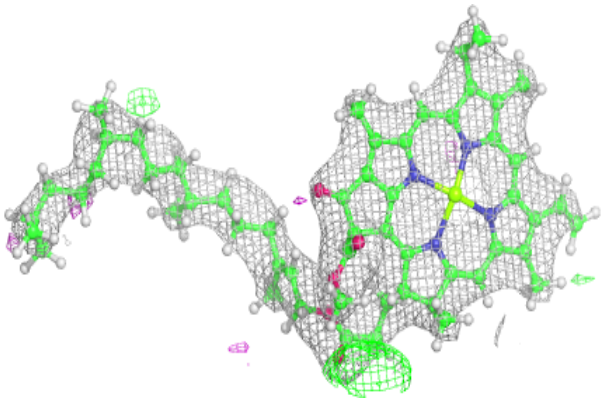


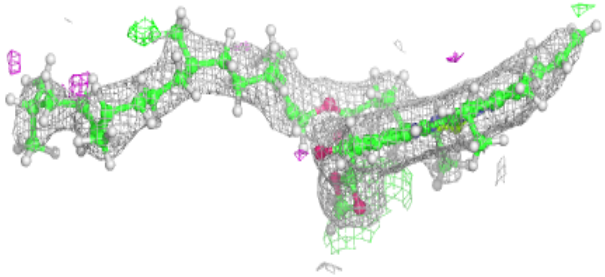


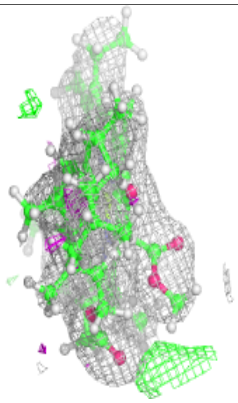


Electron density around CLA b 602:

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

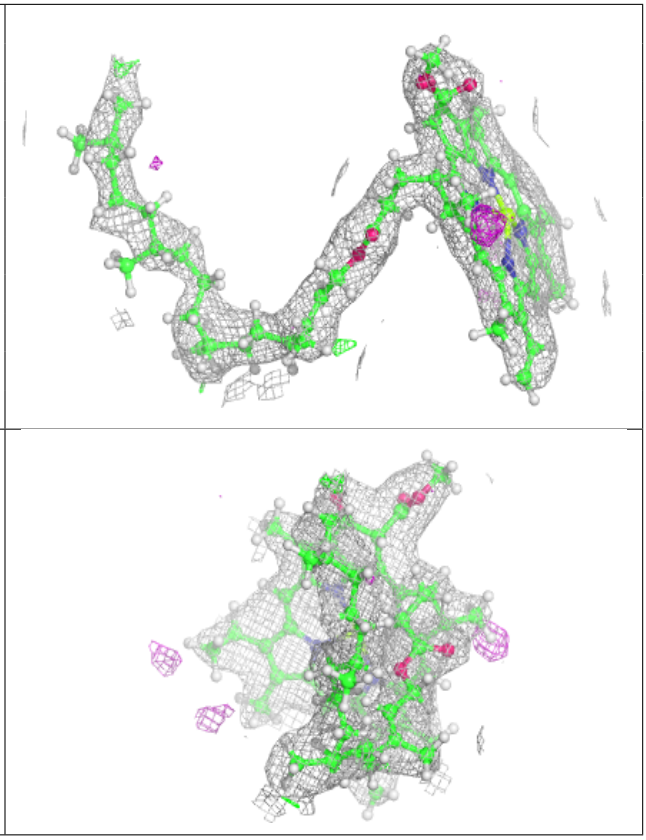






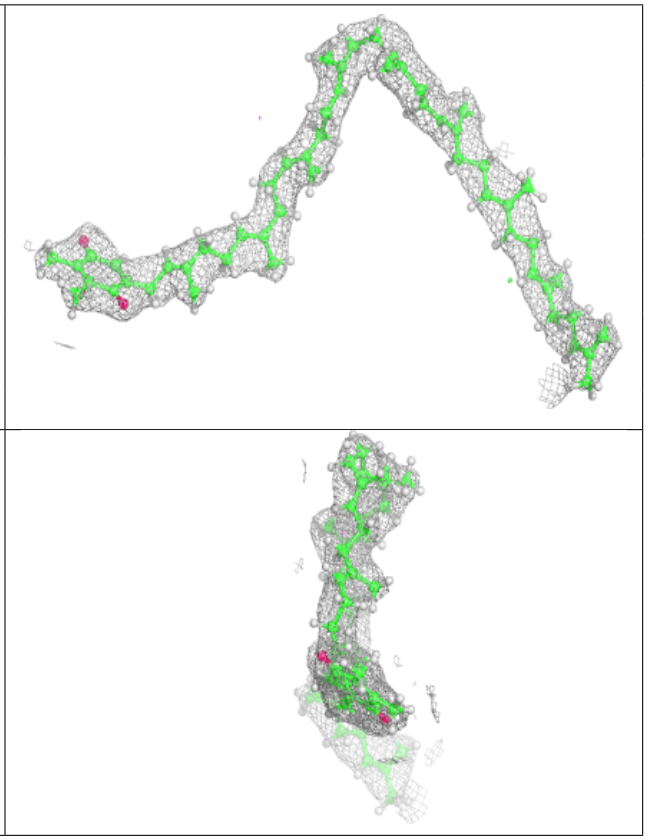
Electron density around CLA b 606:

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



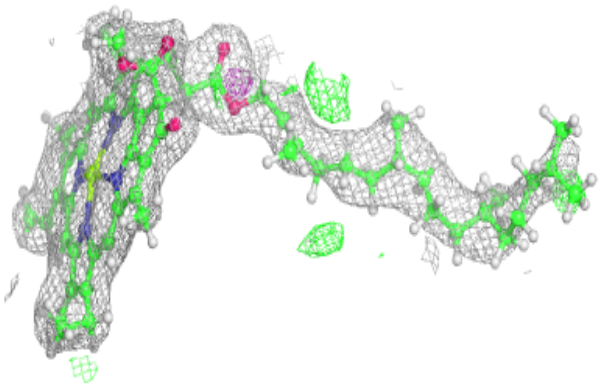
Electron density around PL9 D 406:

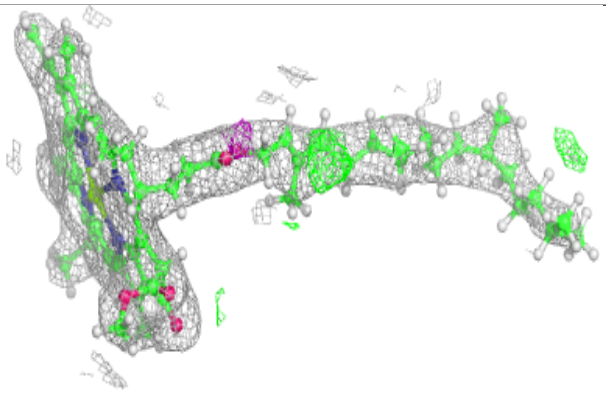
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

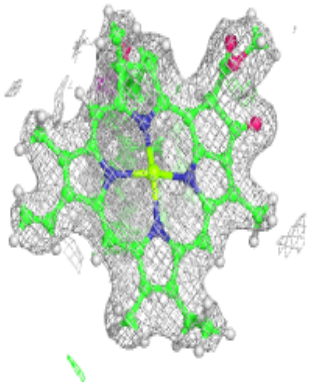


Electron density around CLA B 605:

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

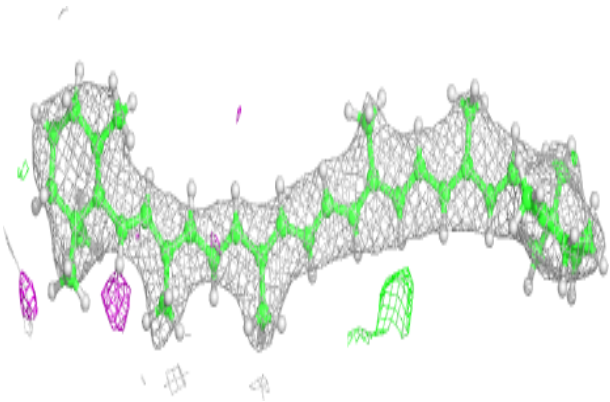


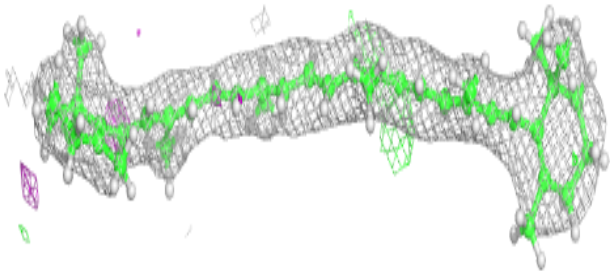


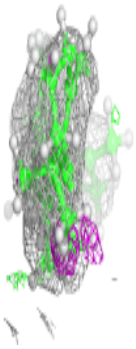


Electron density around BCR B 618:

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

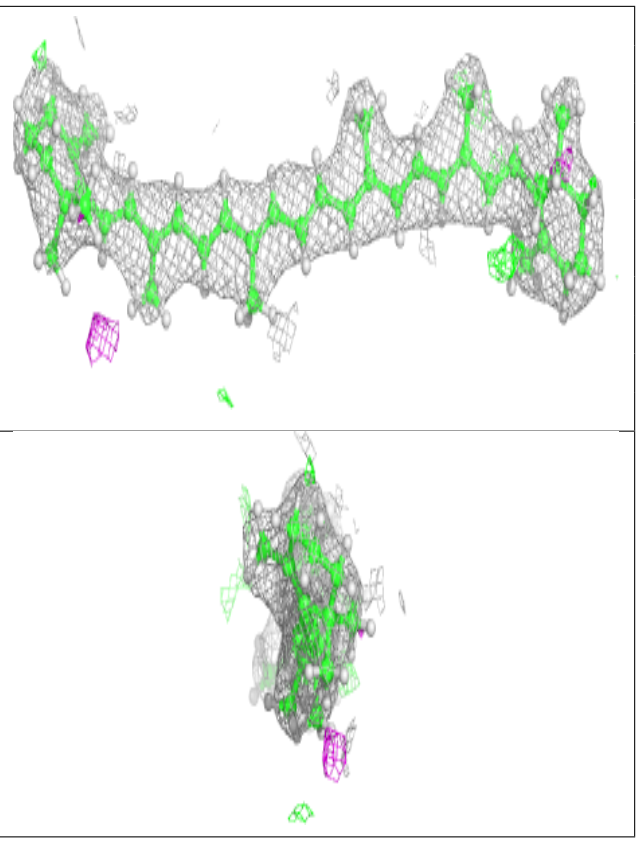






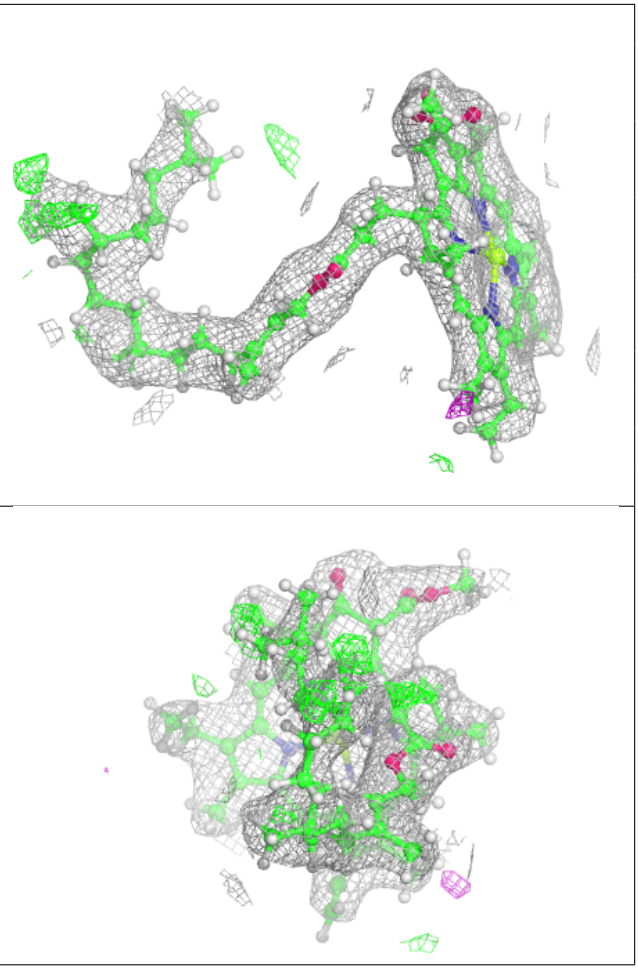
Electron density around BCR B 619:

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



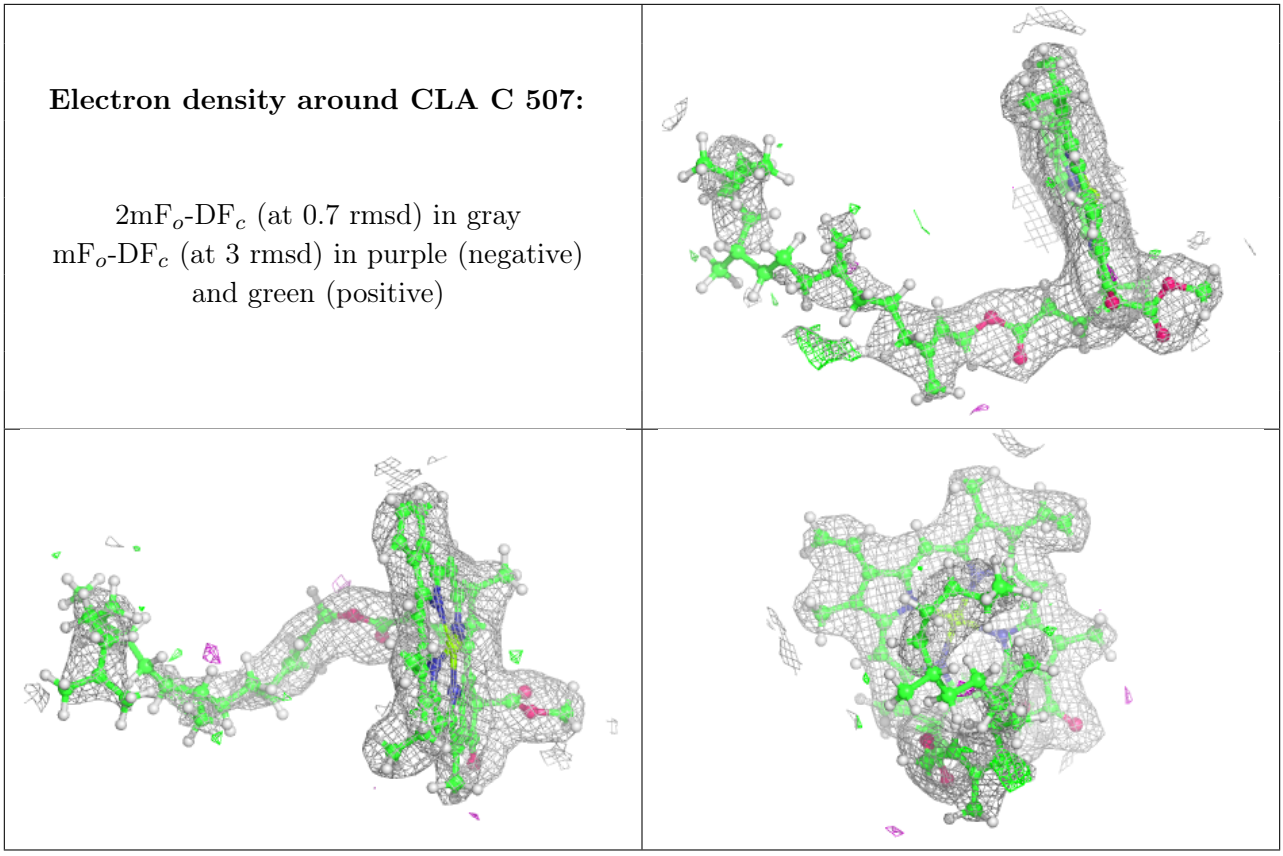
Electron density around CLA B 607:

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



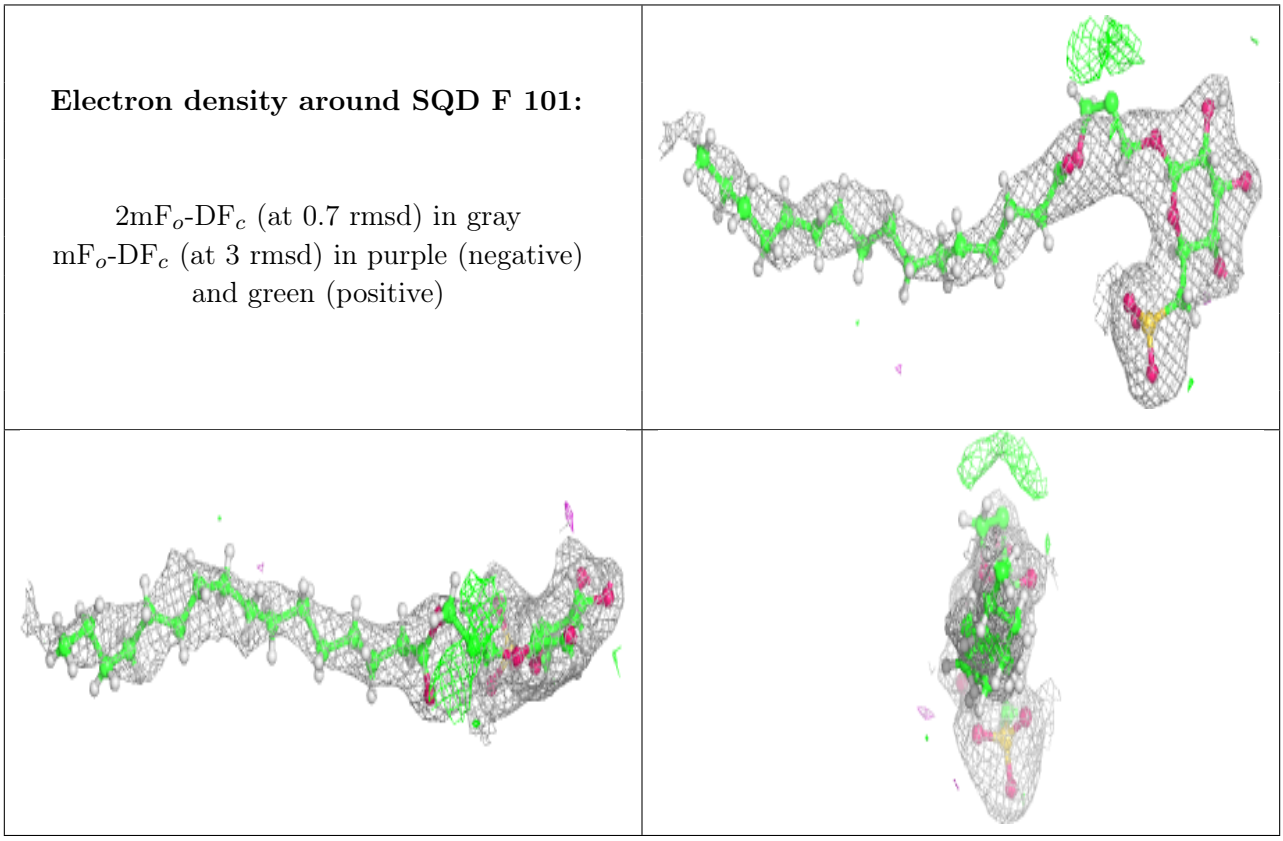
Electron density around CLA C 507:

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



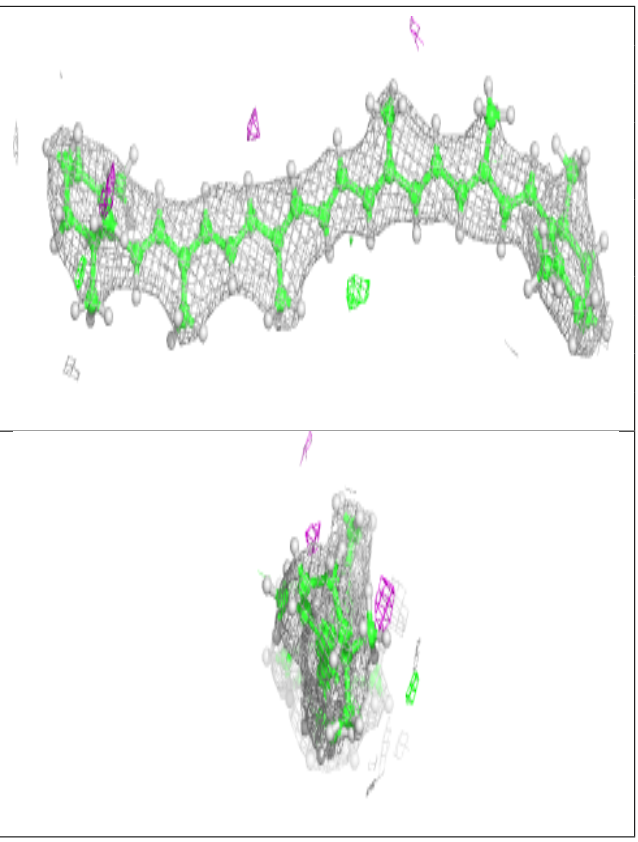
Electron density around SQD F 101:

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



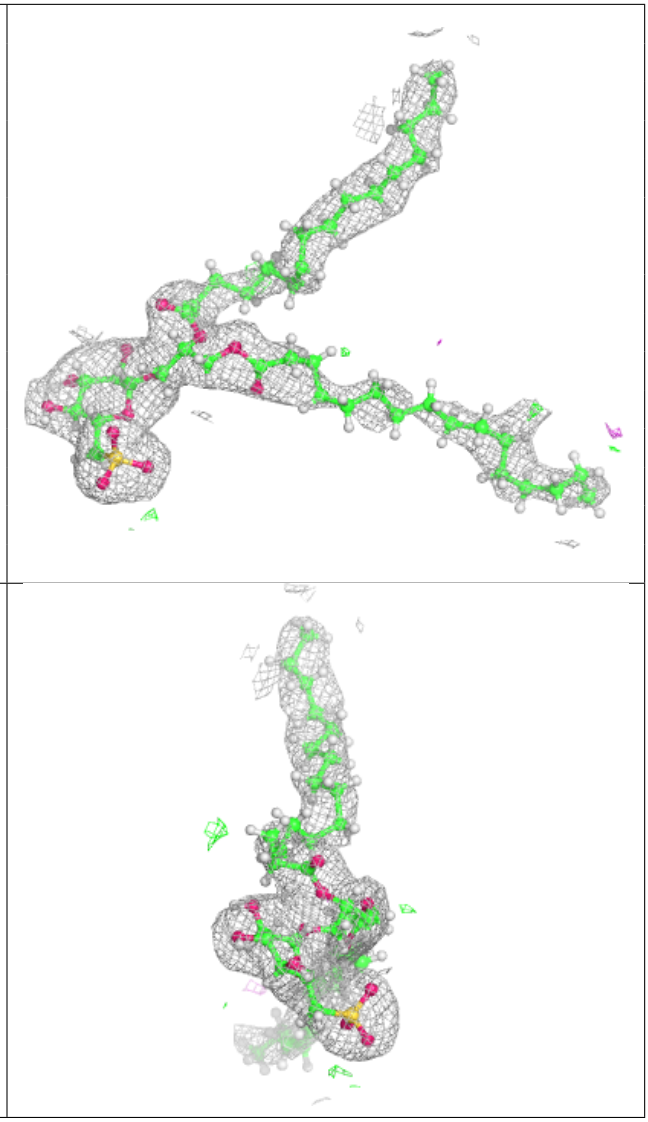
Electron density around BCR C 515:

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



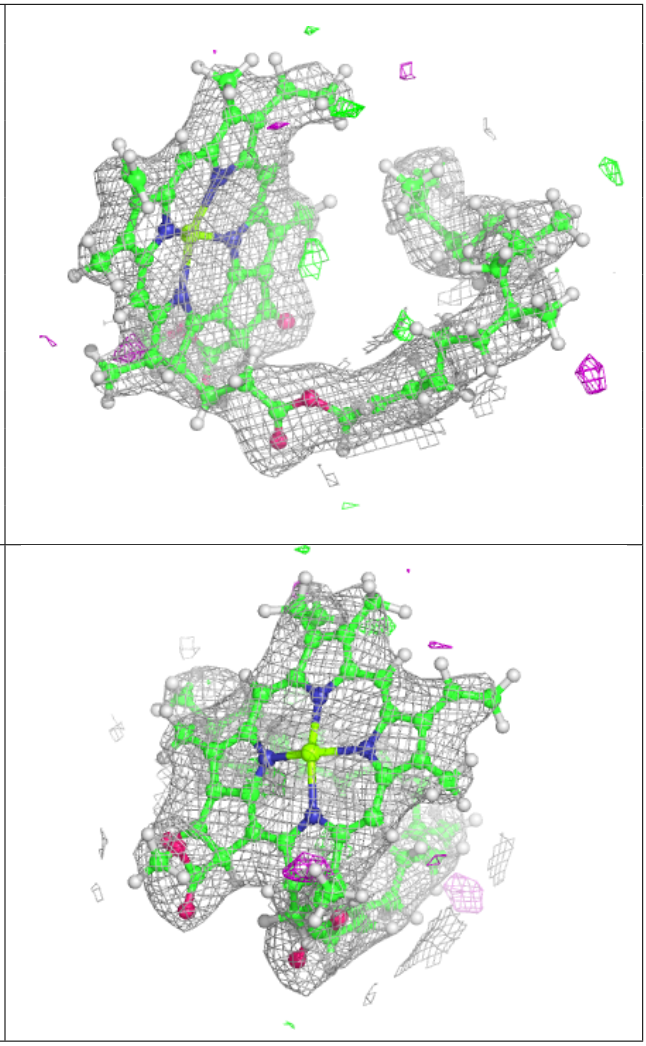
Electron density around SQD a 411:

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



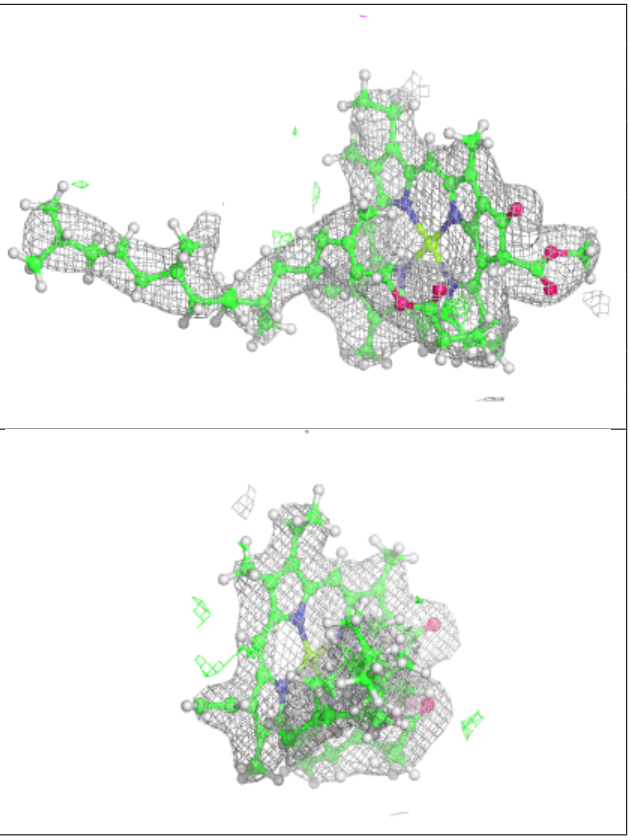
Electron density around CLA c 503:

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



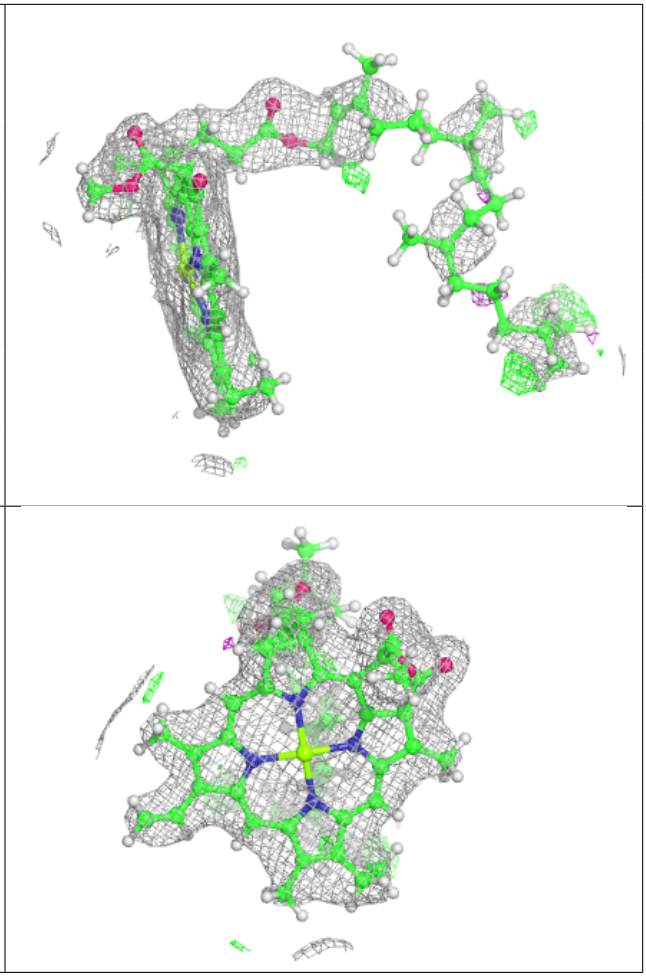
Electron density around CLA c 505:

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



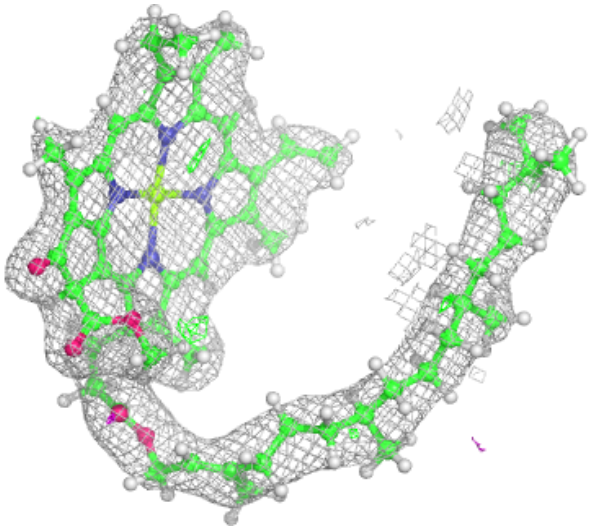
Electron density around CLA c 506:

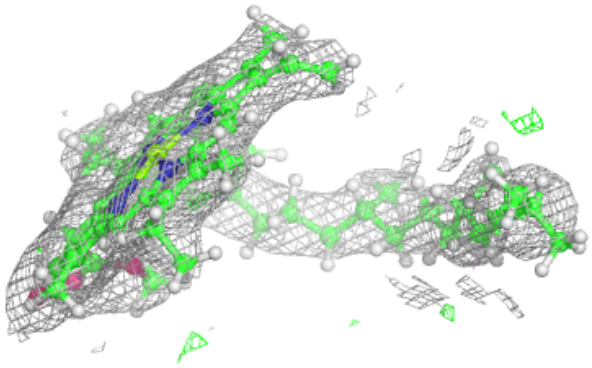
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

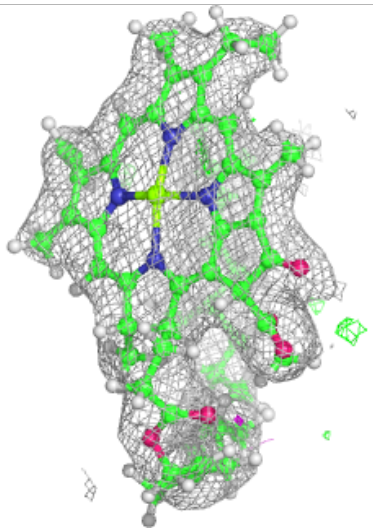


Electron density around CLA c 507:

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

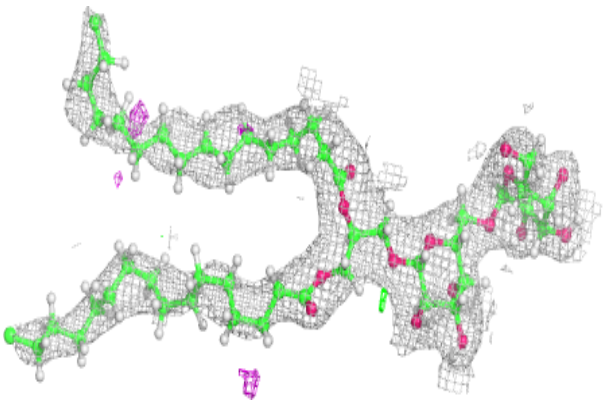


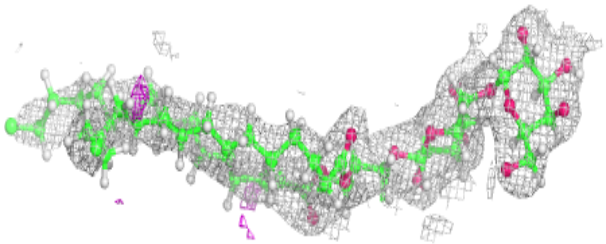




Electron density around DGD C 519:

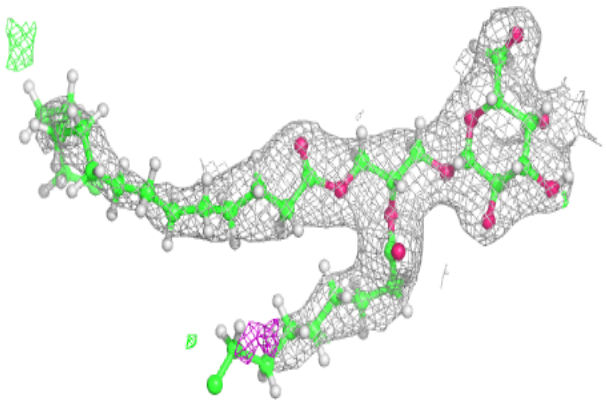
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

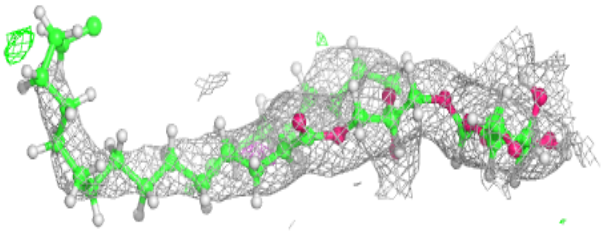


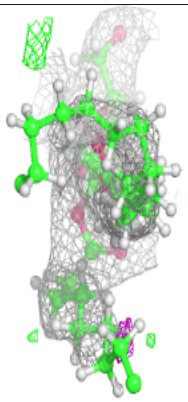


Electron density around LMG d 410:

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

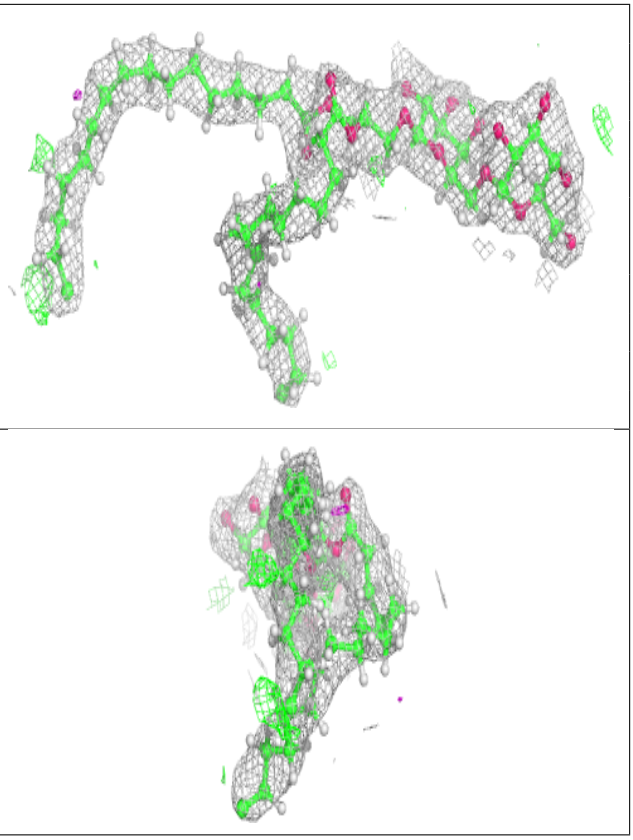






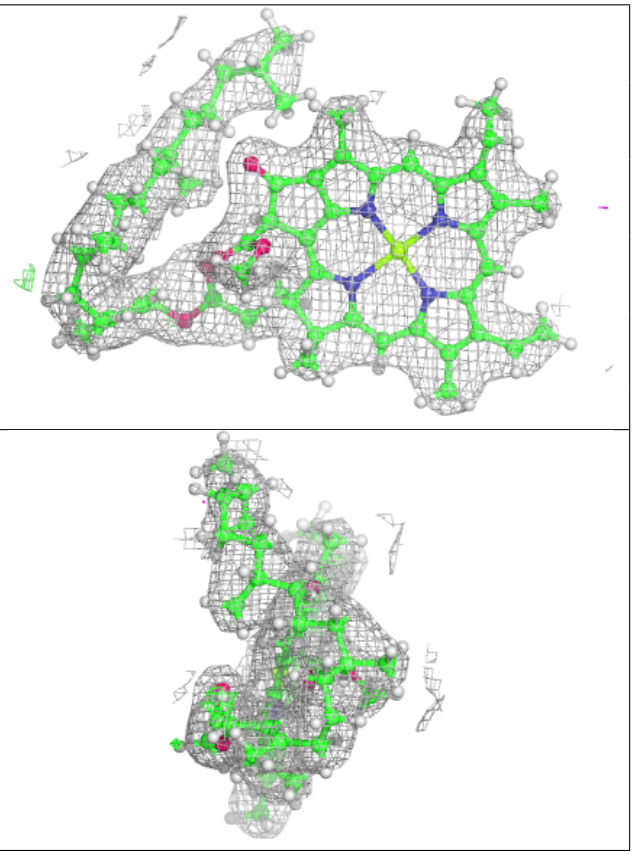
Electron density around DGD H 102:

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



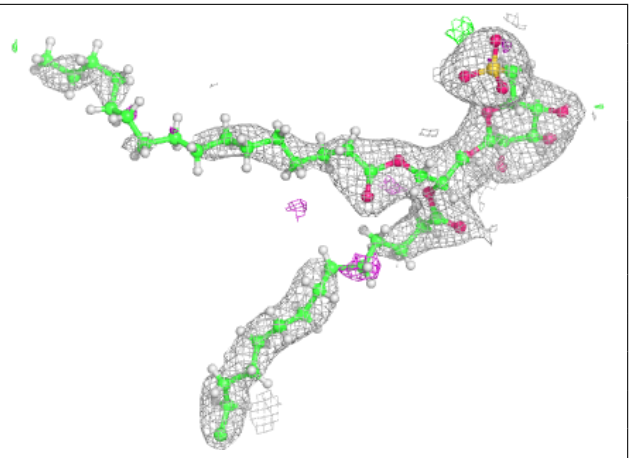
Electron density around CLA B 611:

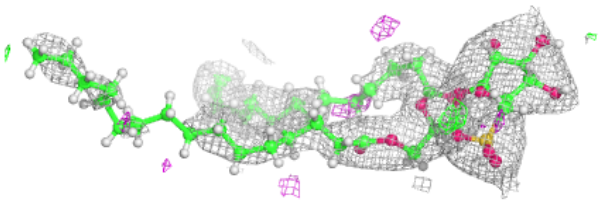
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

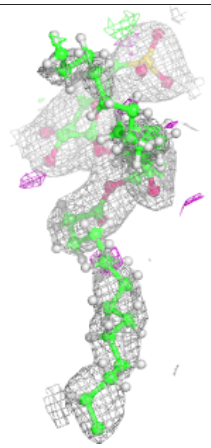


Electron density around SQD A 412:

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

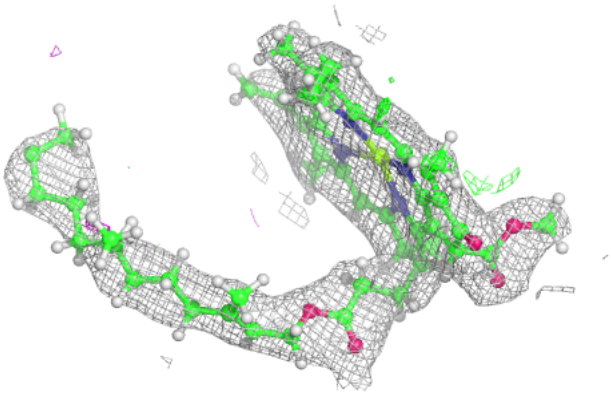


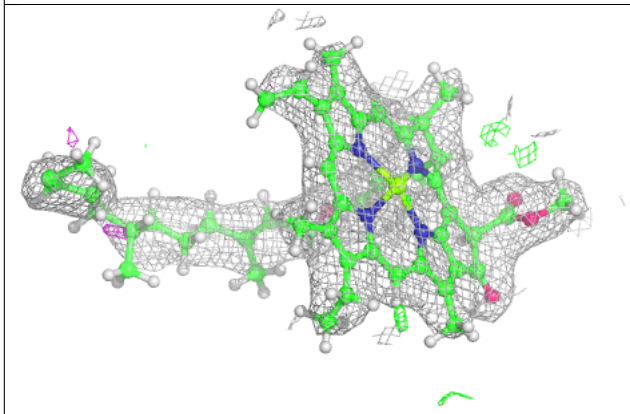


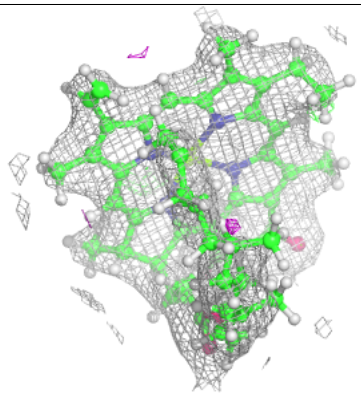


Electron density around CLA C 505:

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

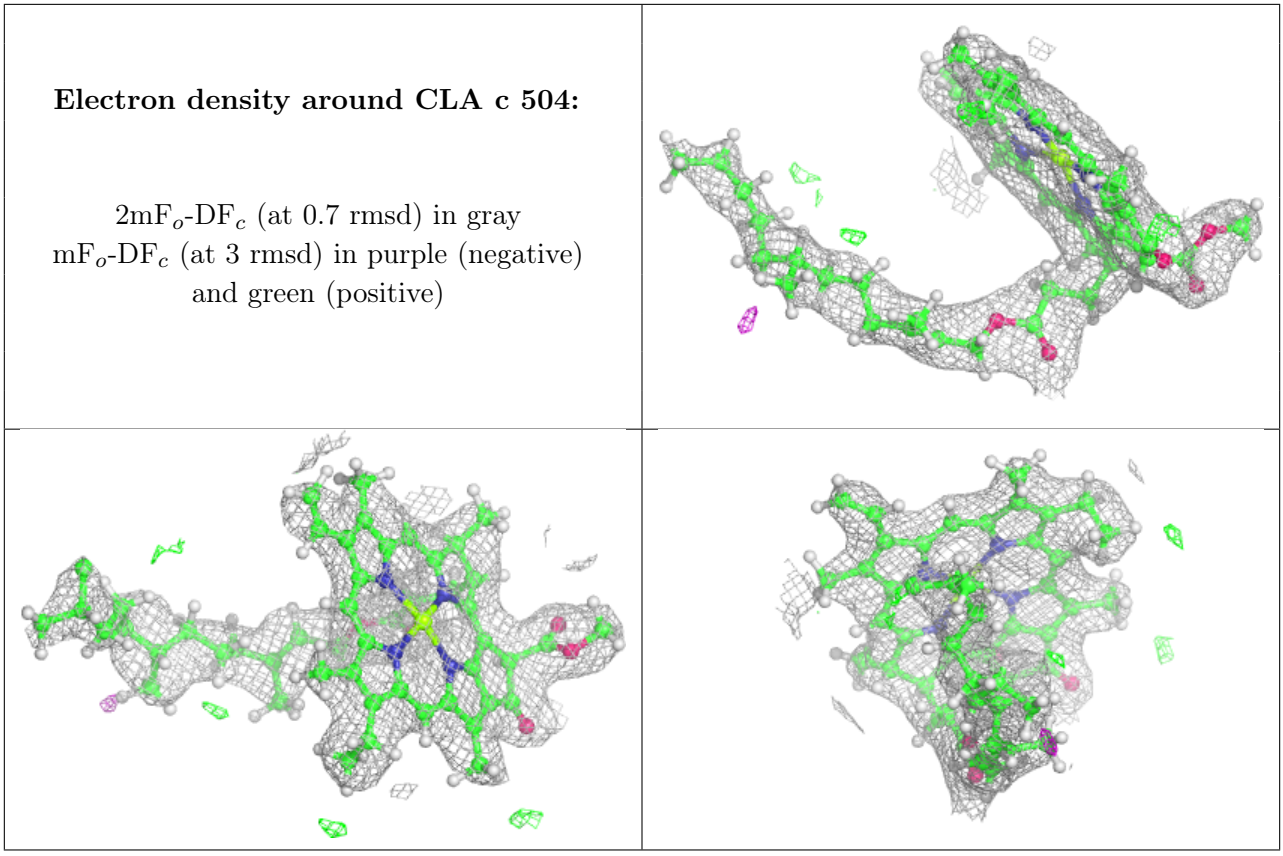






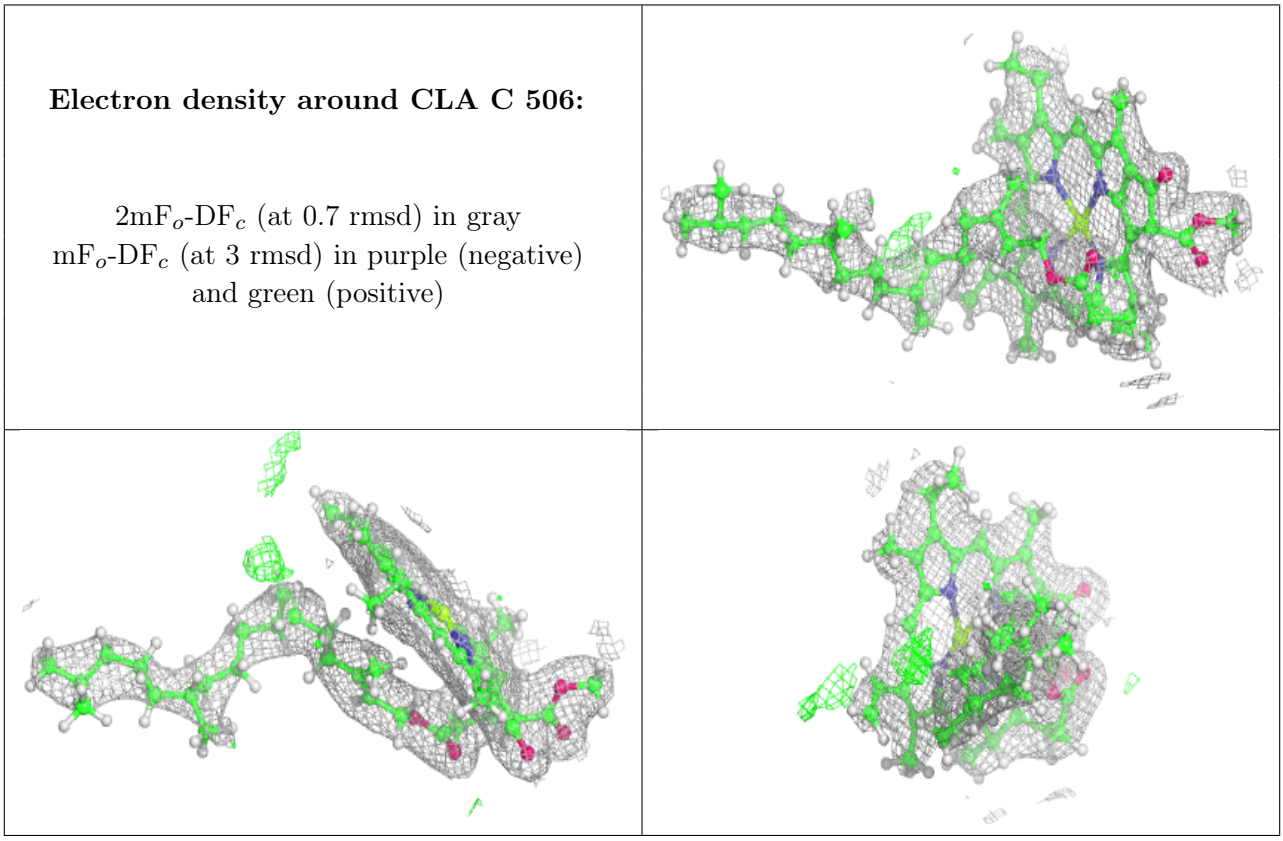
Electron density around CLA c 504:

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



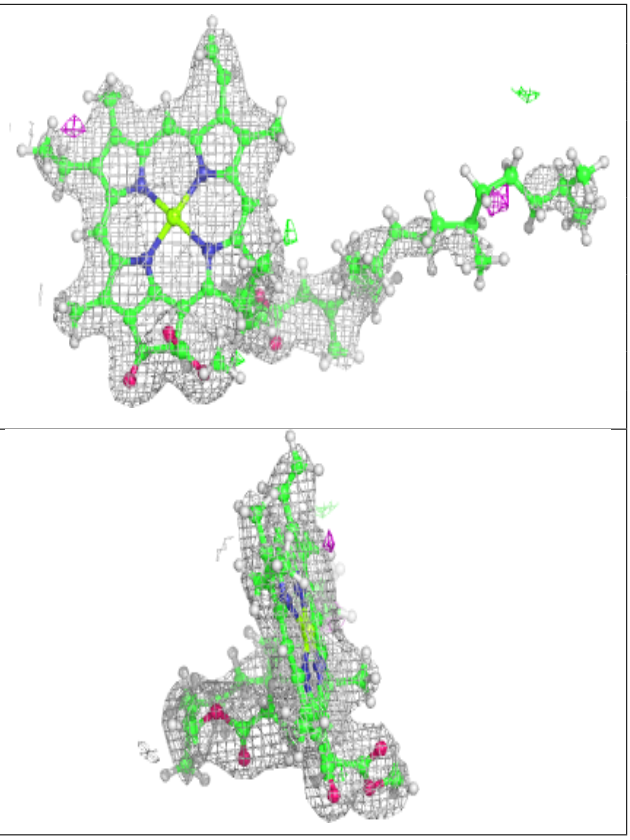
Electron density around CLA C 506:

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



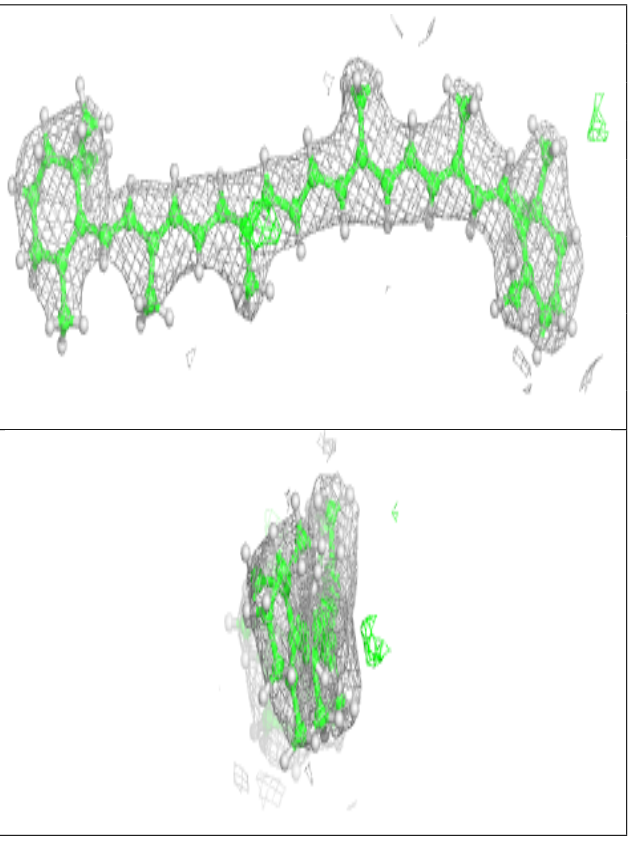
Electron density around CLA a 403:

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



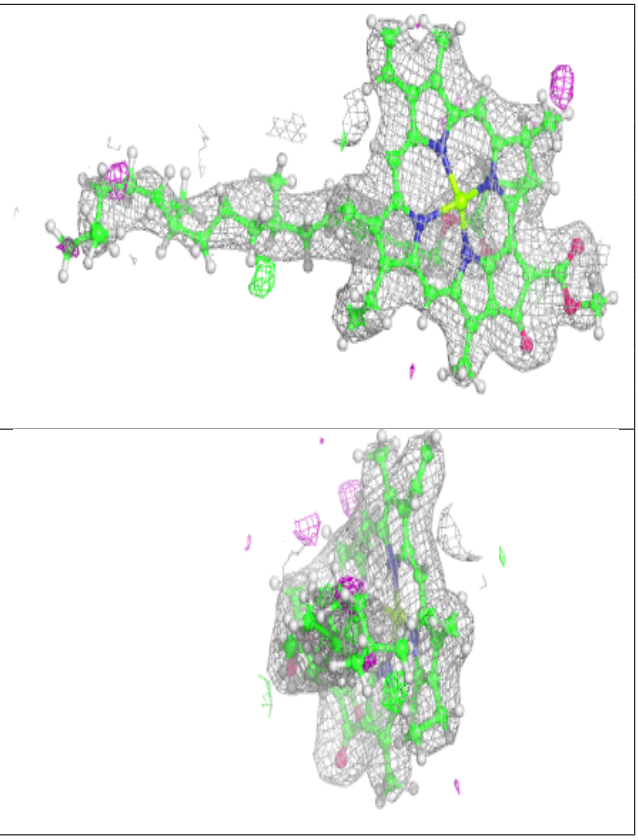
Electron density around BCR T 101:

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



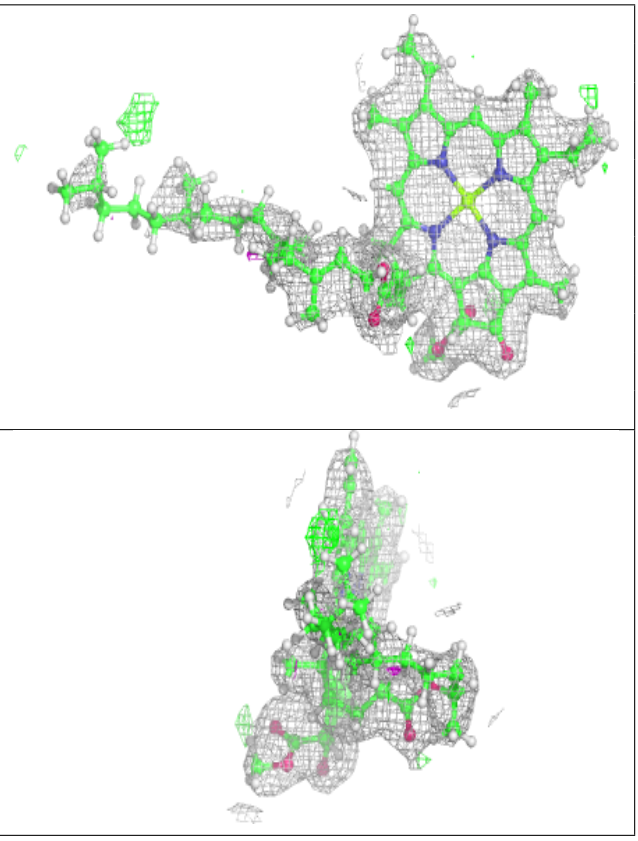
Electron density around CLA B 615:

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



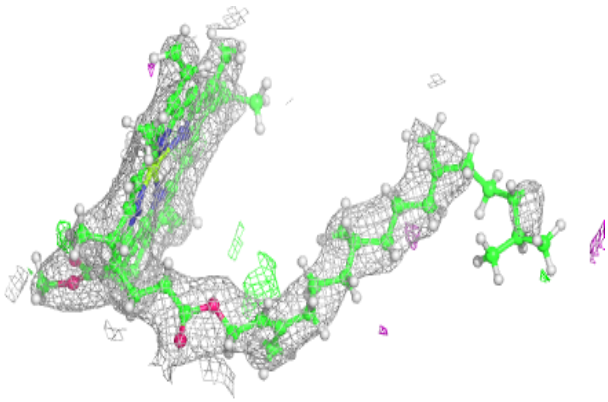
Electron density around CLA A 403:

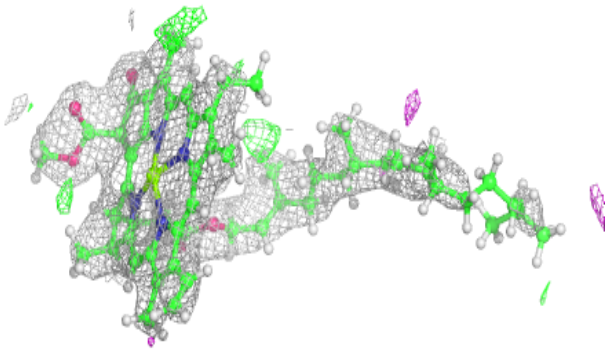
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

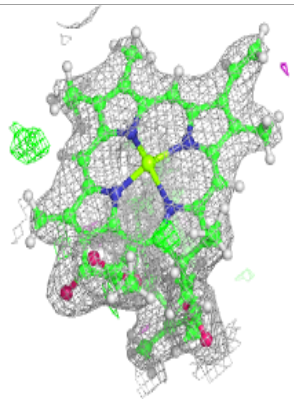


Electron density around CLA C 509:

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

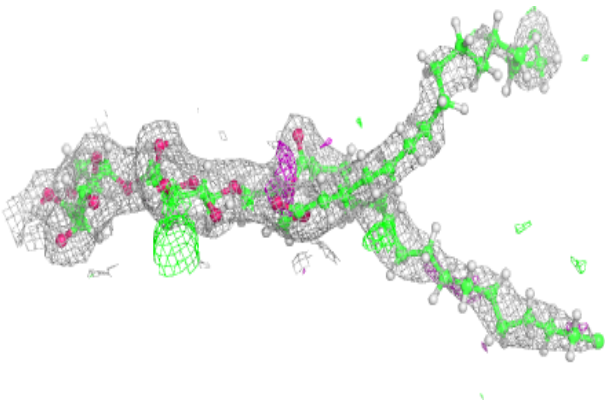


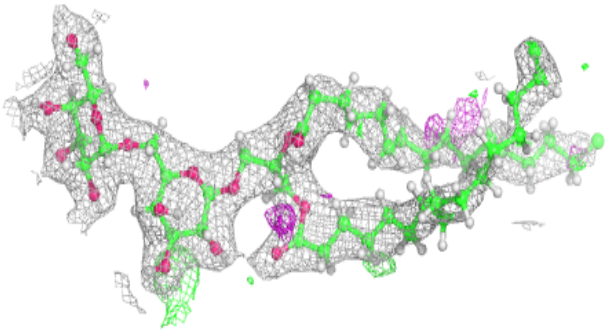


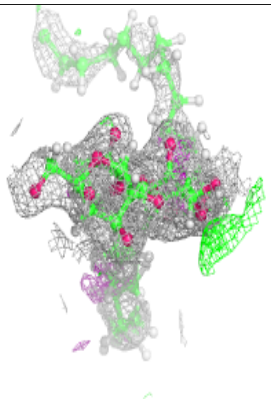


Electron density around DGD C 517:

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

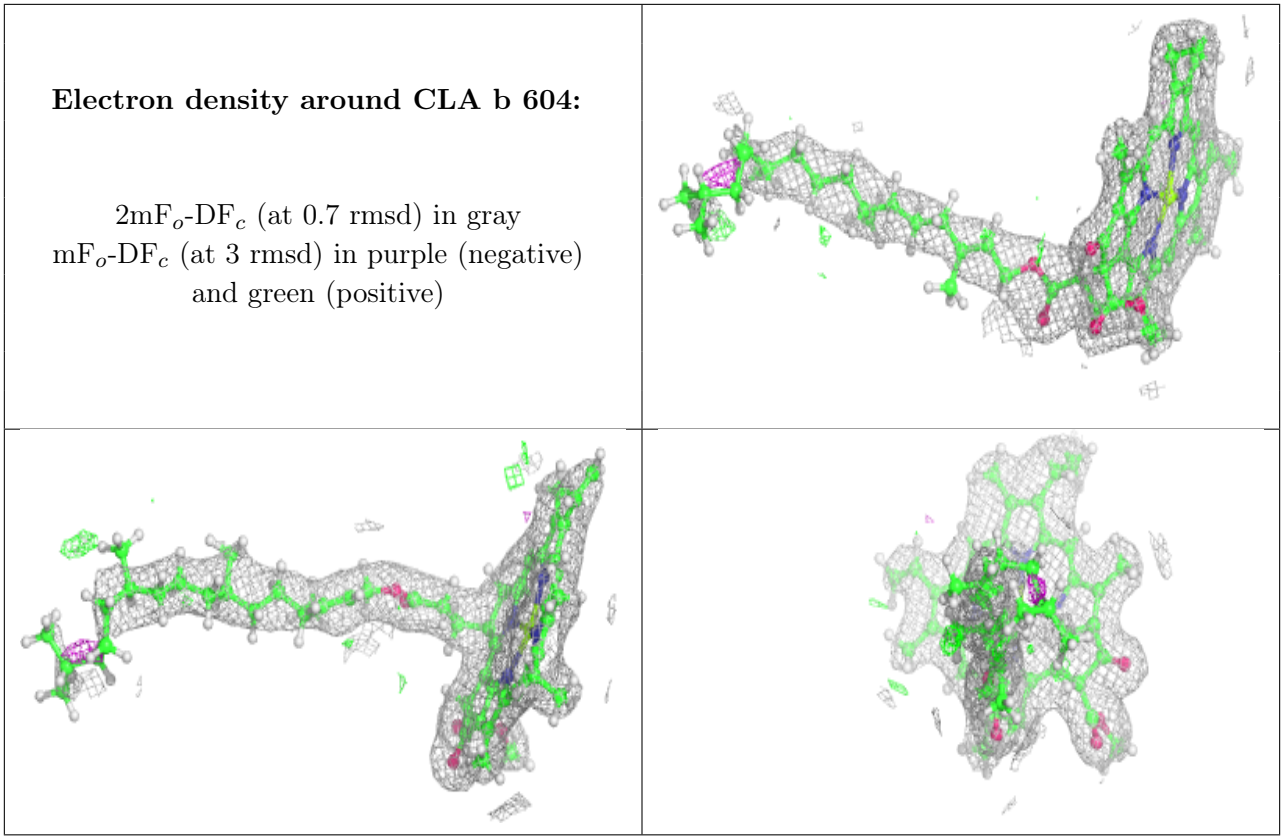






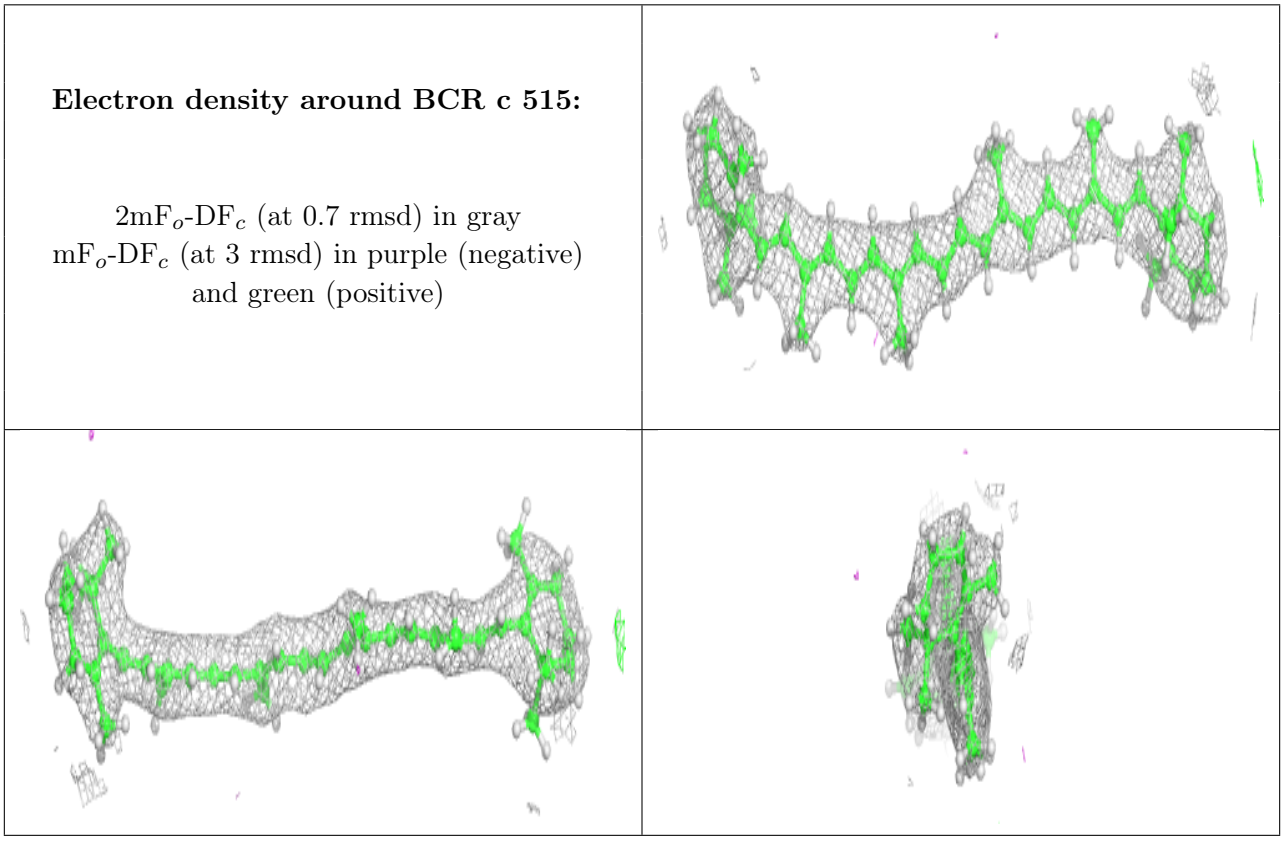
Electron density around CLA b 604:

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



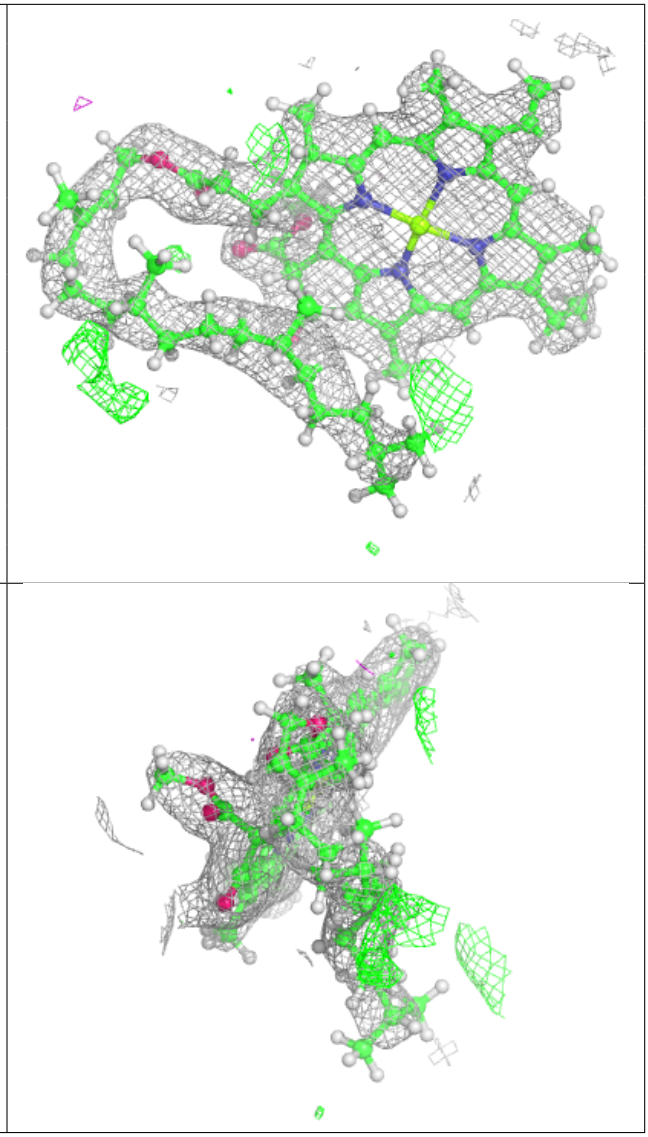
Electron density around BCR c 515:

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



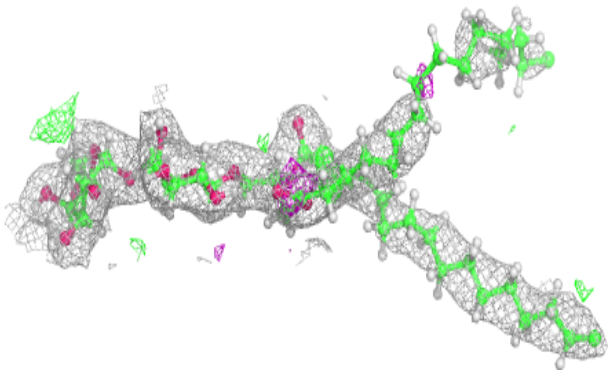
Electron density around CLA C 510:

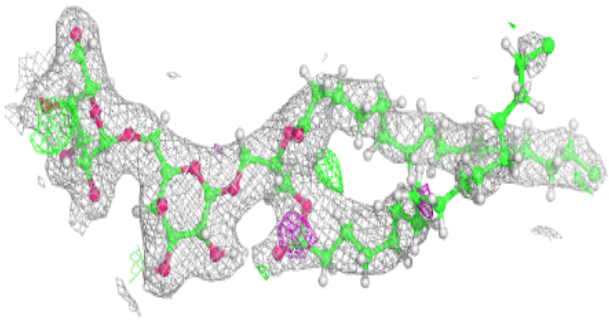
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

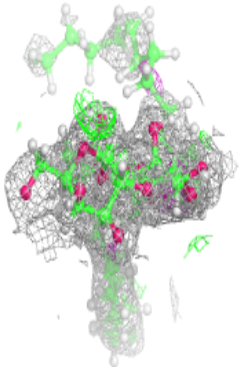


Electron density around DGD c 516:

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

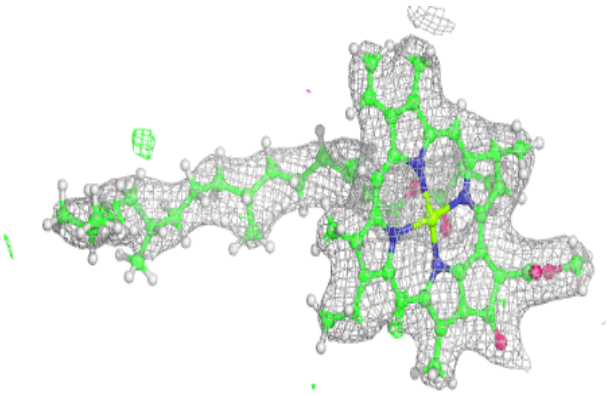


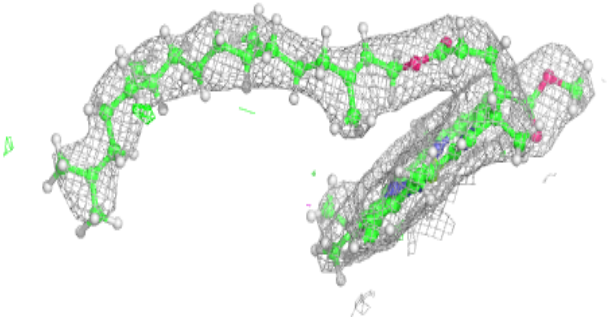


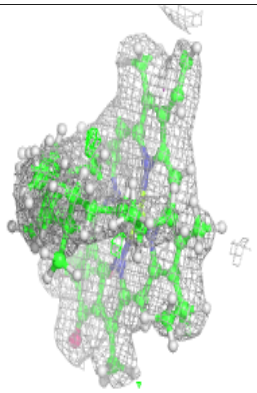


Electron density around CLA b 608:

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

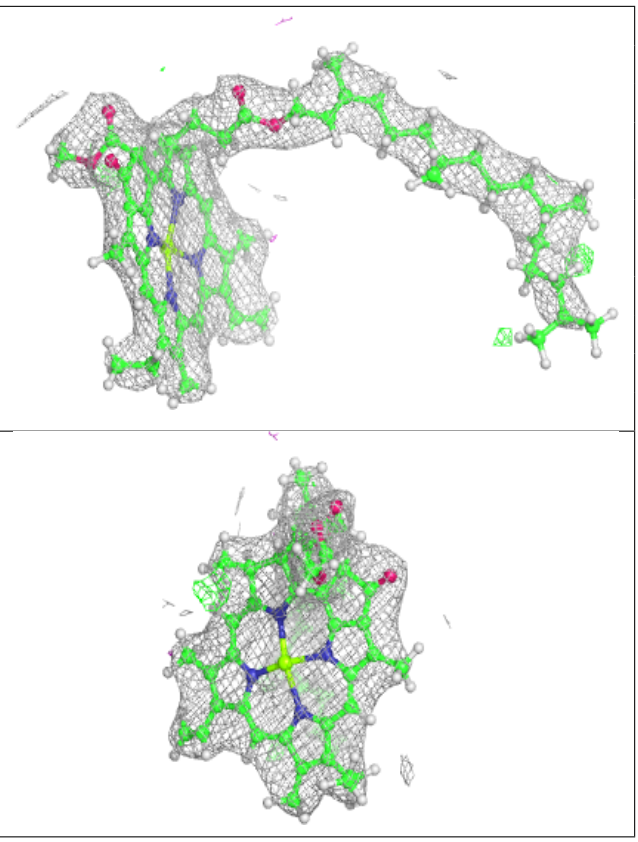






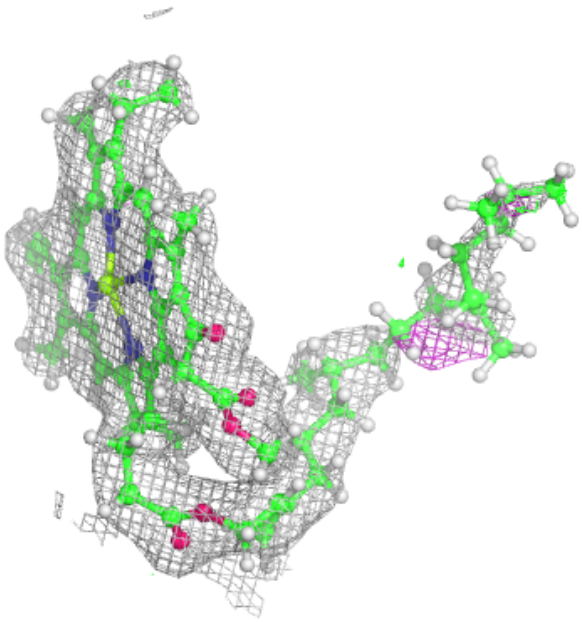
Electron density around CLA b 609:

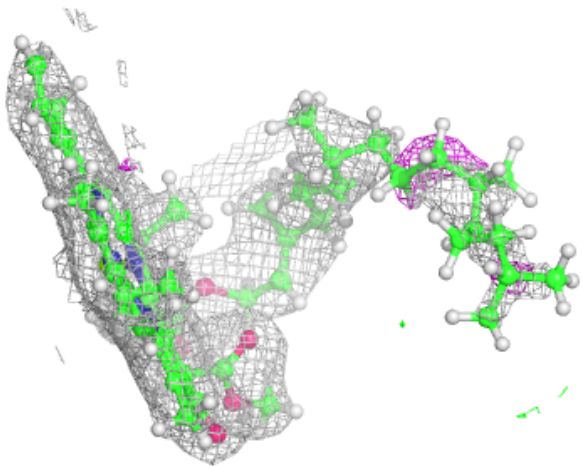
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

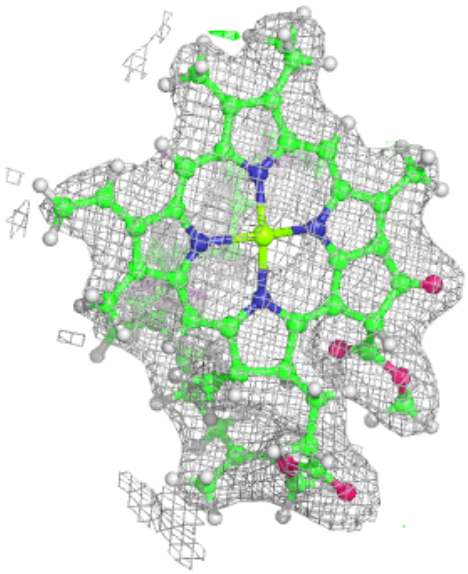


Electron density around CLA b 613:

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

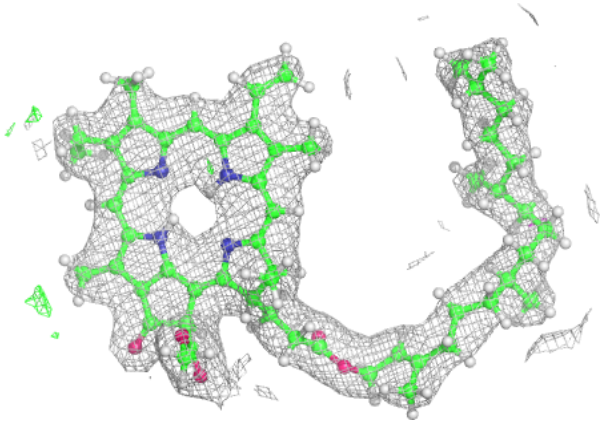


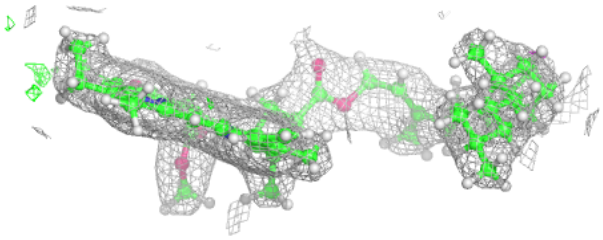


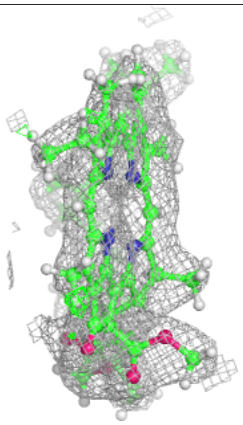


Electron density around PHO a 404:

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

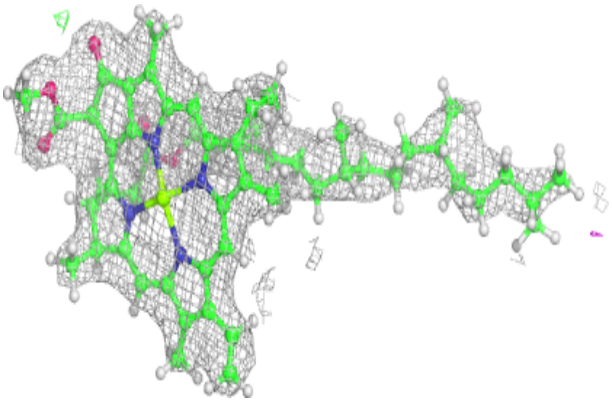


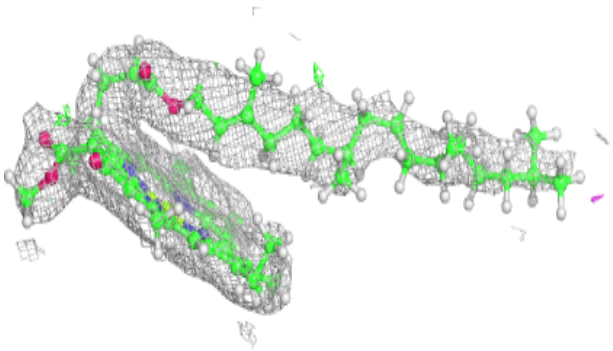


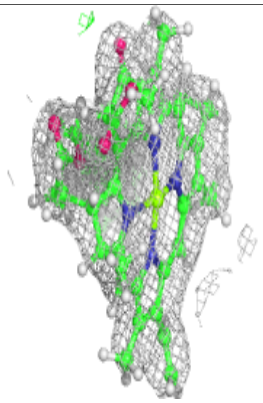


Electron density around CLA b 614:

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

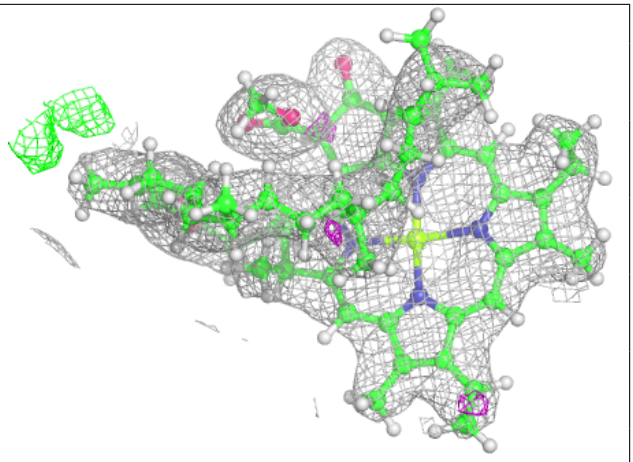


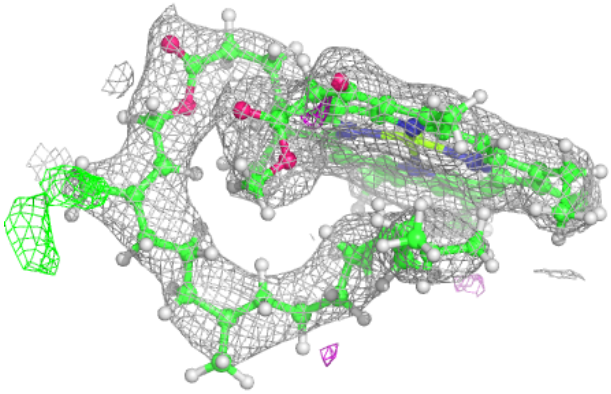


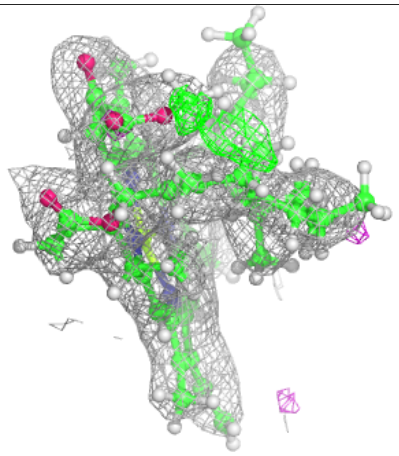


Electron density around CLA C 511:

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

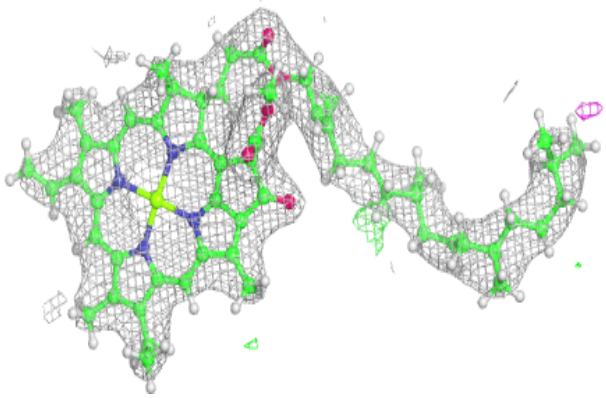


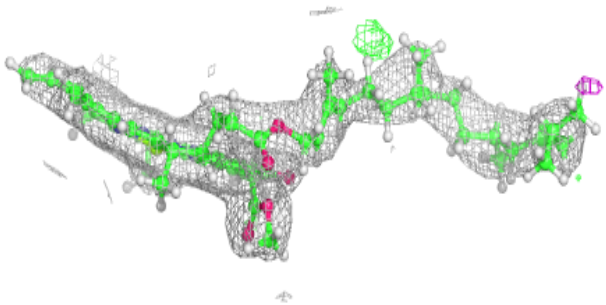


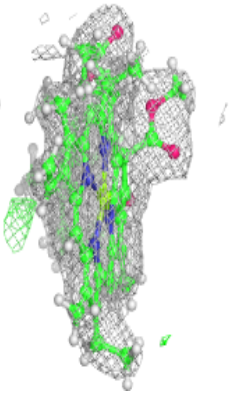


Electron density around CLA B 603:

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

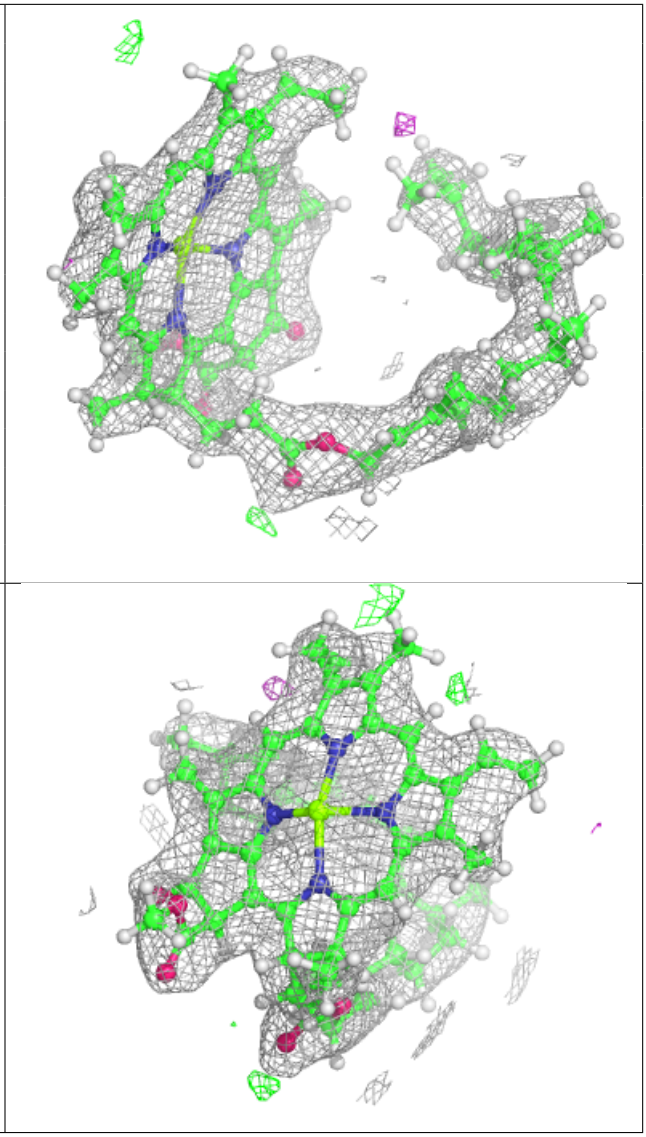






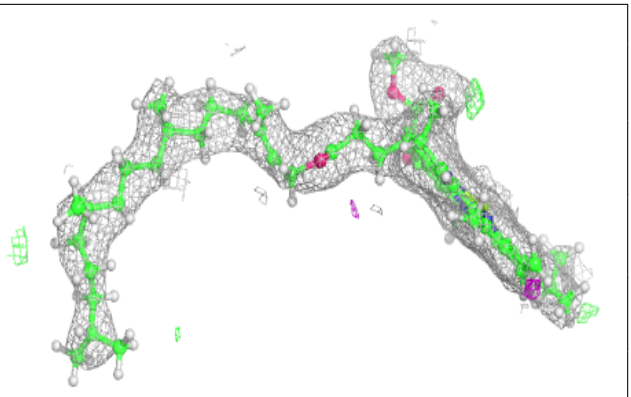
Electron density around CLA C 504:

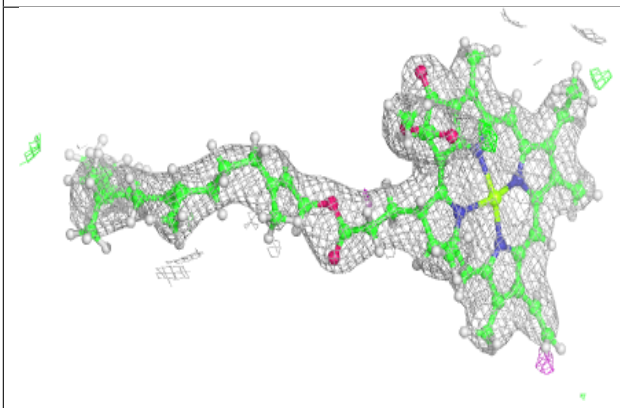
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

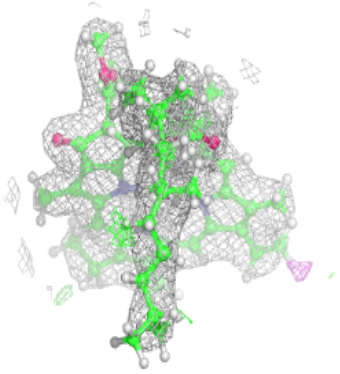


Electron density around CLA d 402:

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

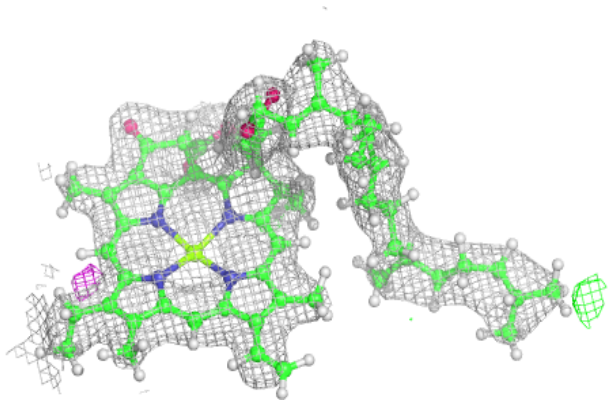


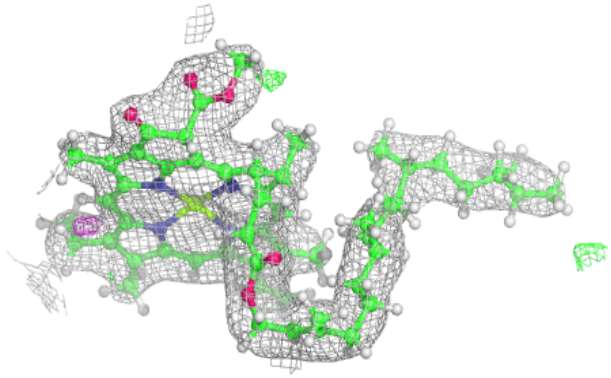


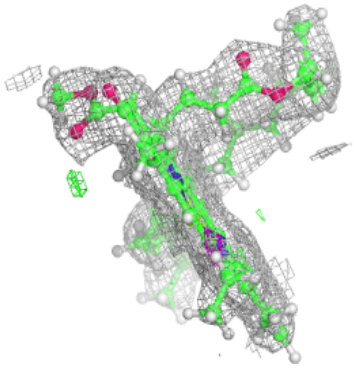


Electron density around CLA d 403:

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

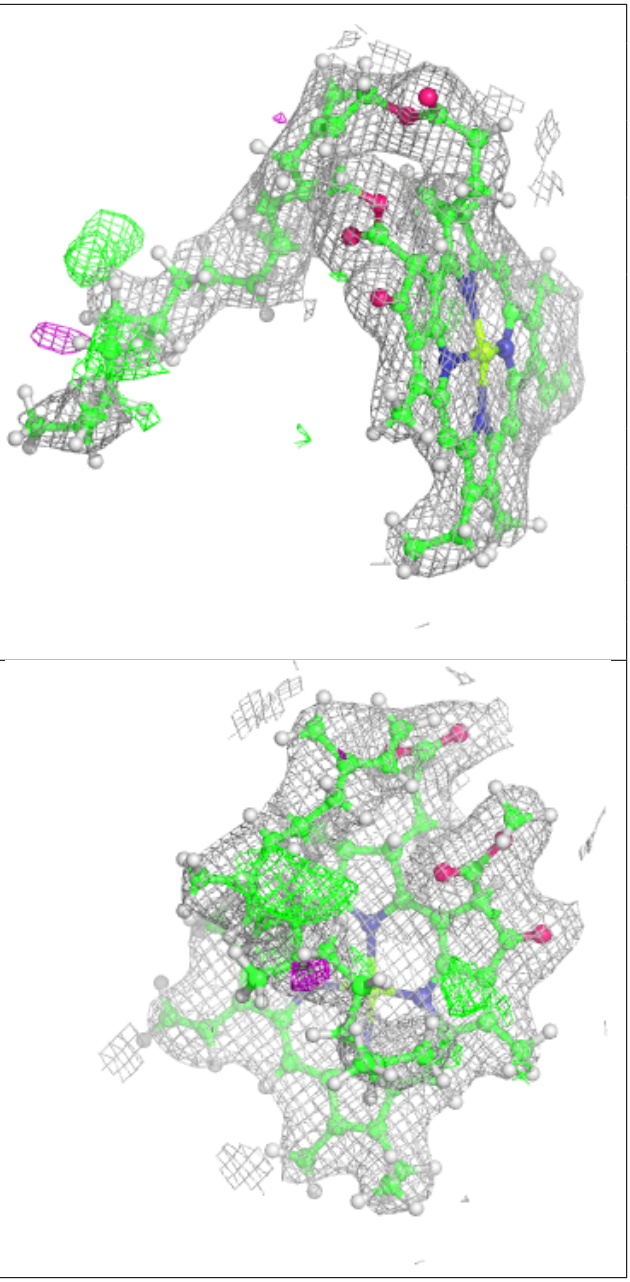






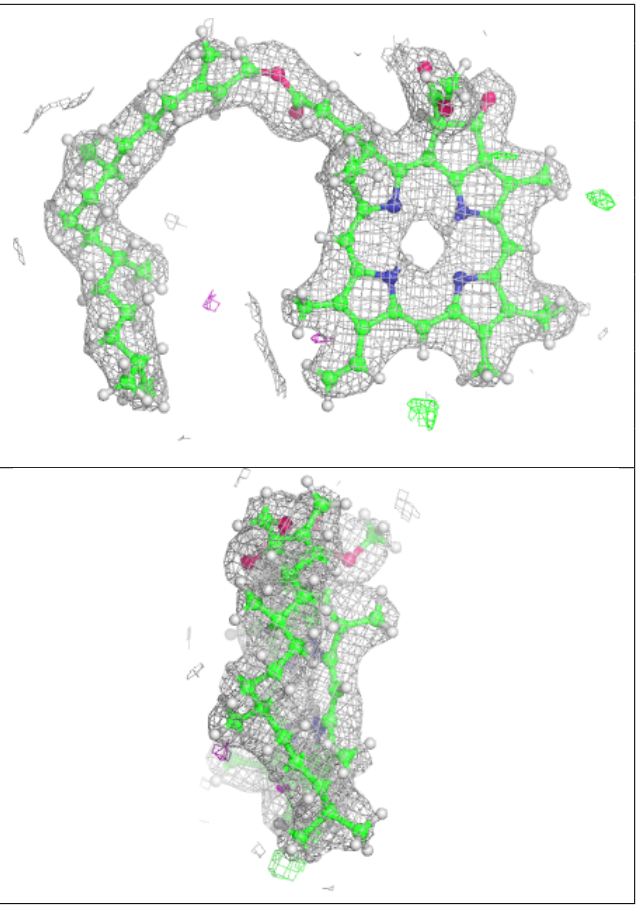
Electron density around CLA B 614:

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



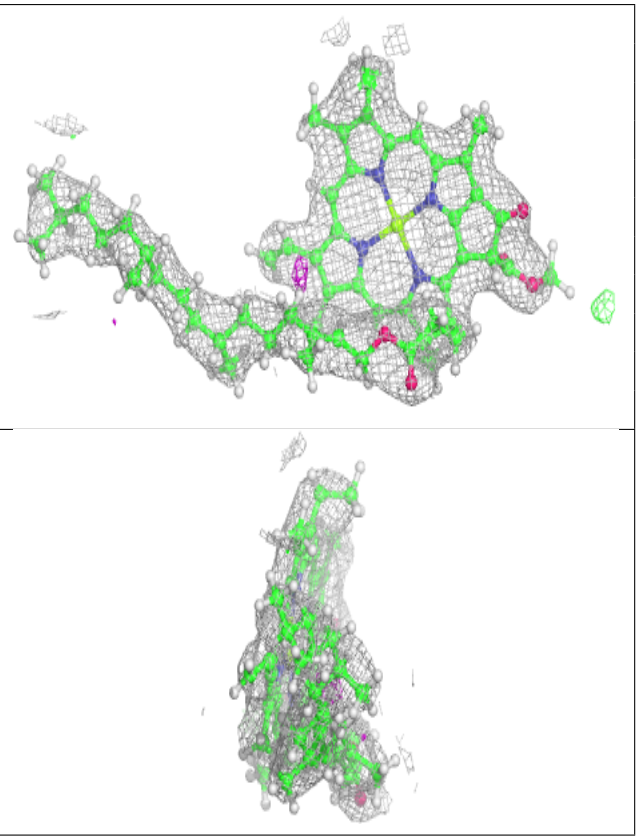
Electron density around PHO A 404:

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



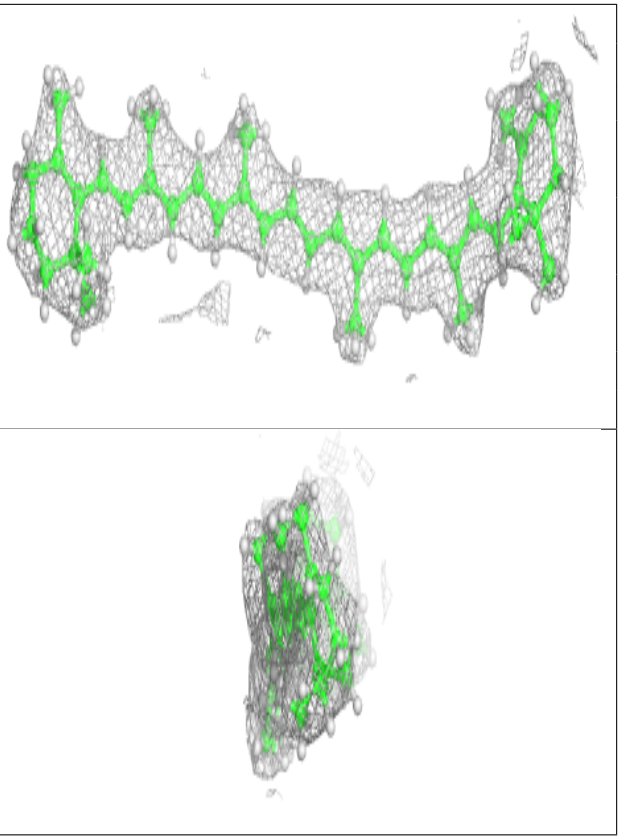
Electron density around CLA c 501:

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



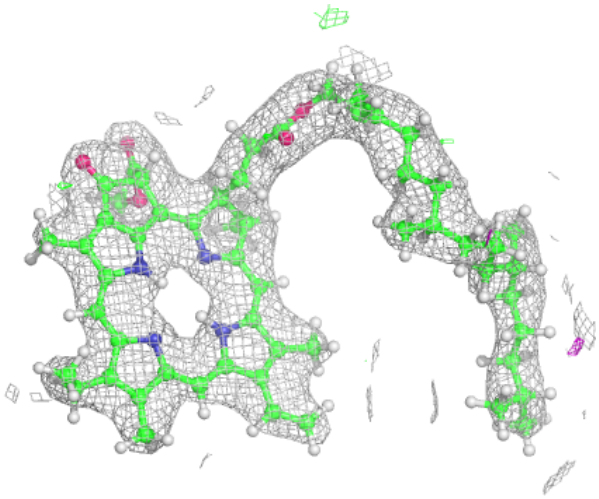
Electron density around BCR t 101:

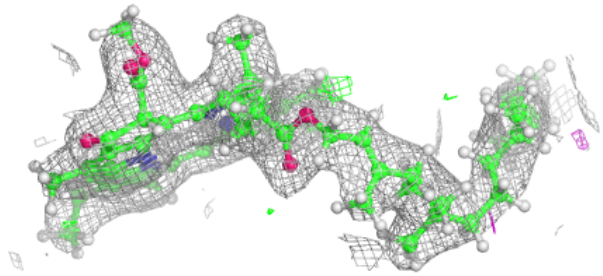
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

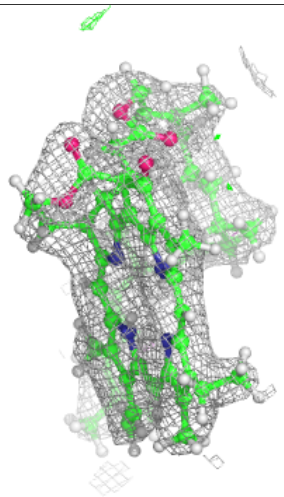


Electron density around PHO d 401:

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

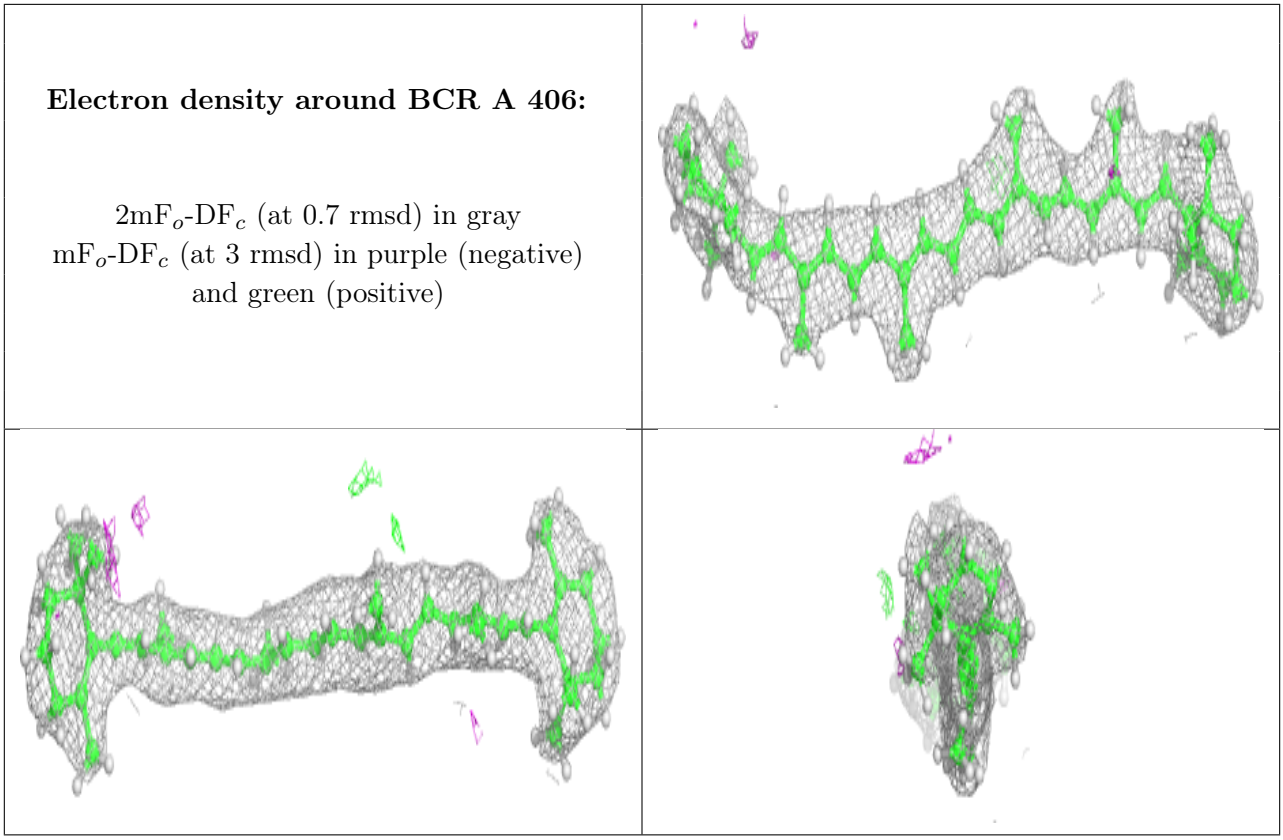






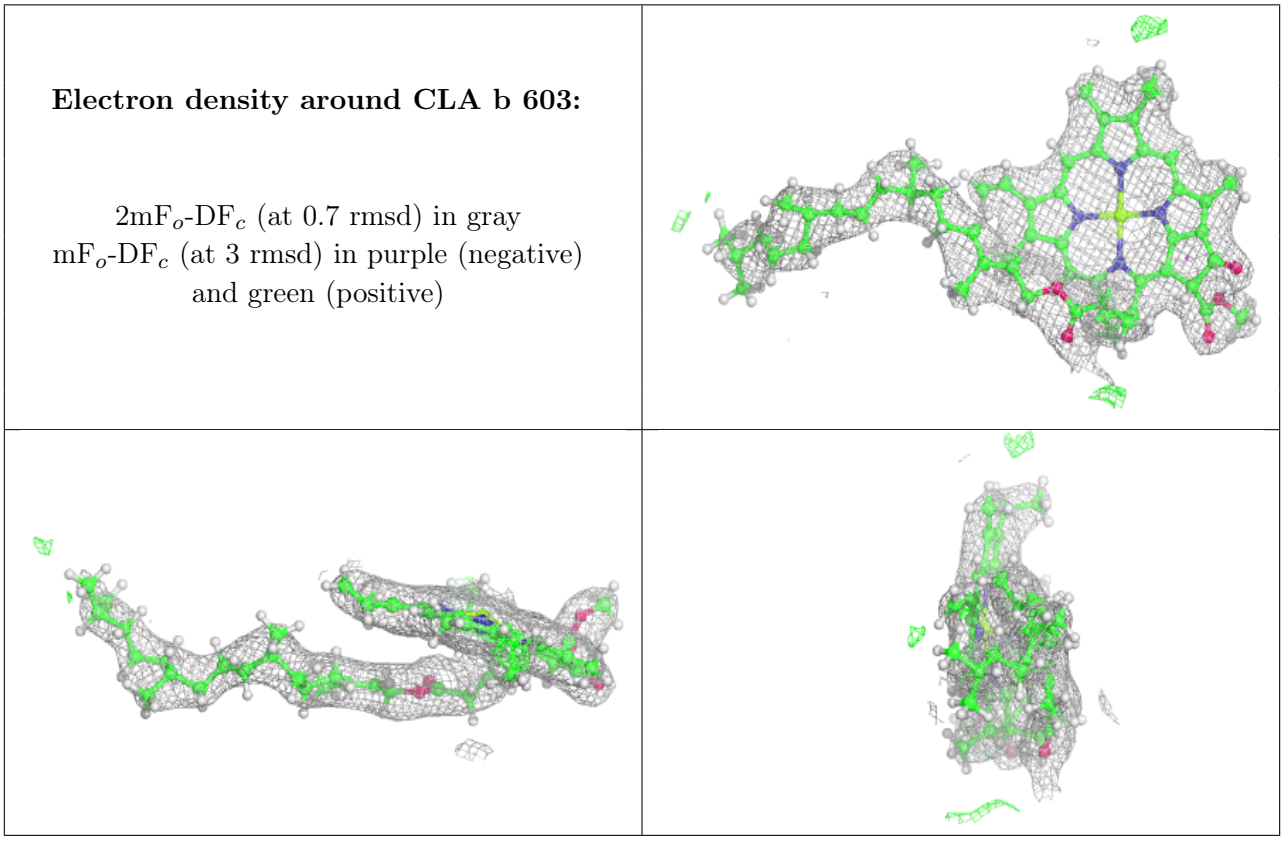
Electron density around BCR A 406:

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



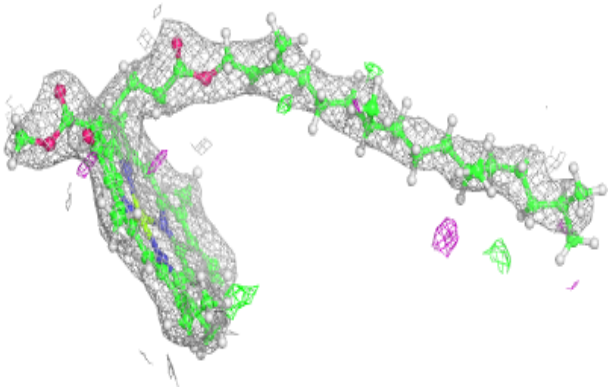
Electron density around CLA b 603:

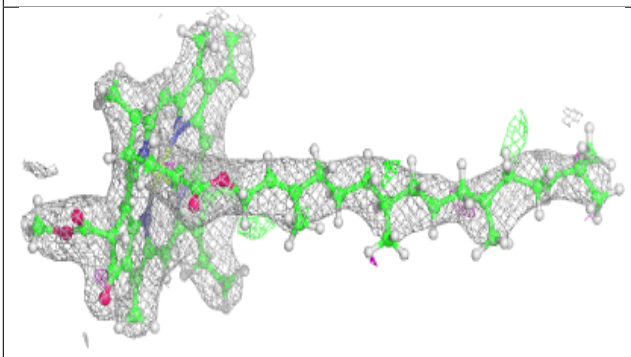
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

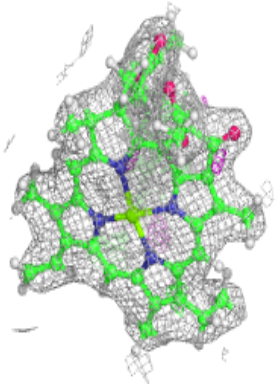


Electron density around CLA B 608:

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

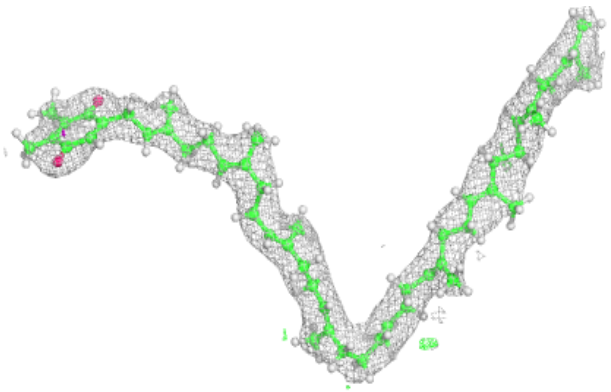


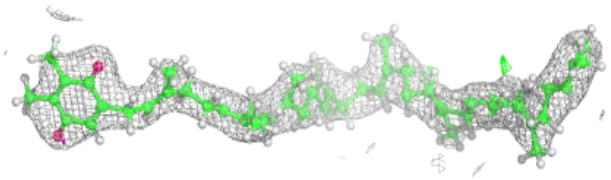


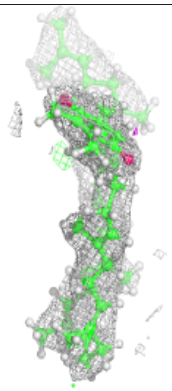


Electron density around PL9 d 406:

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

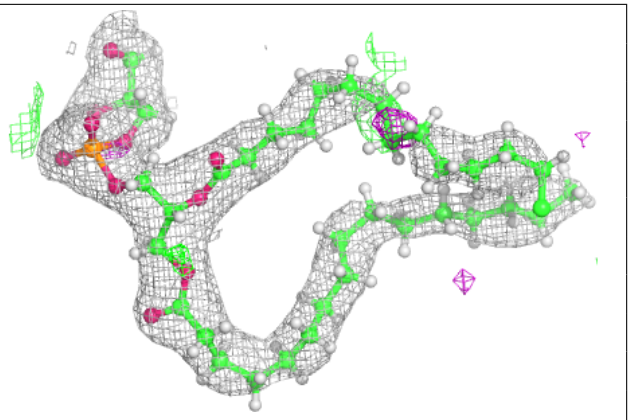


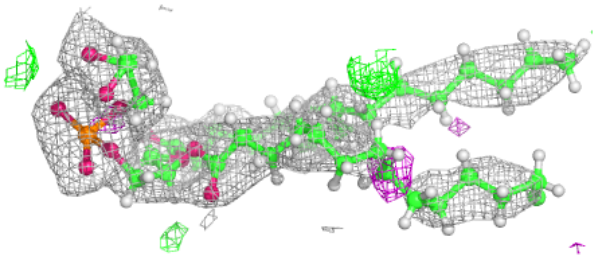


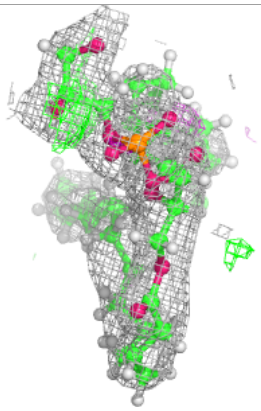


Electron density around LHG A 411:

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

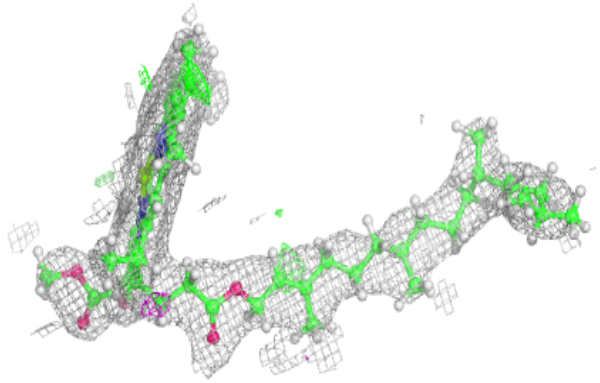


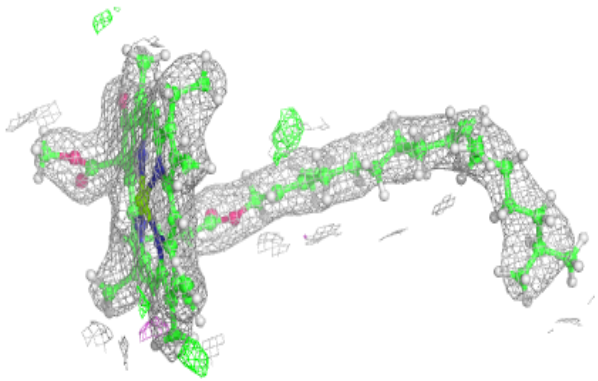


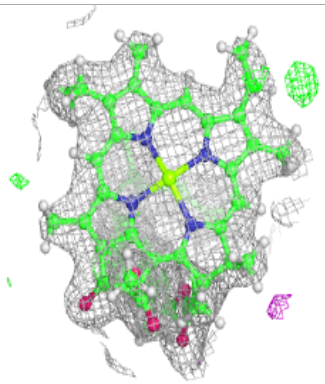


Electron density around CLA b 605:

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

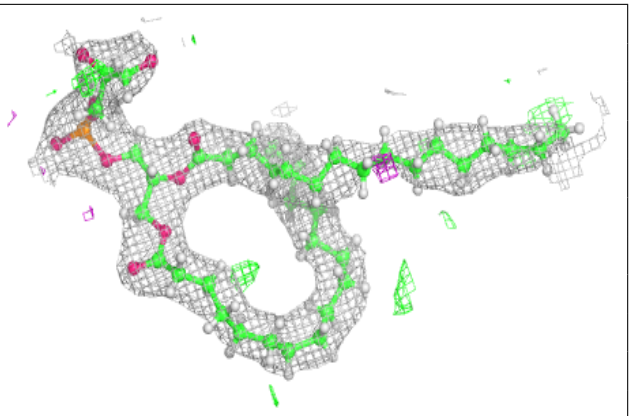


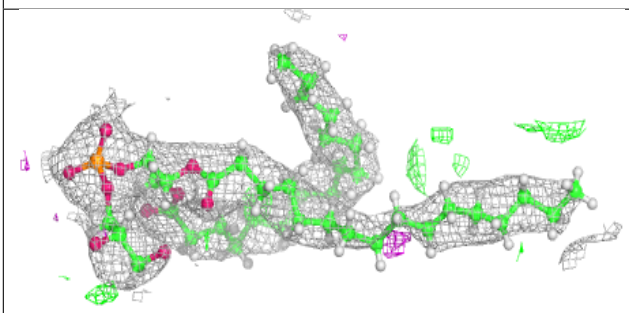


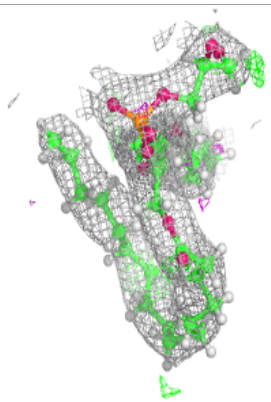


Electron density around LHG B 622:

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

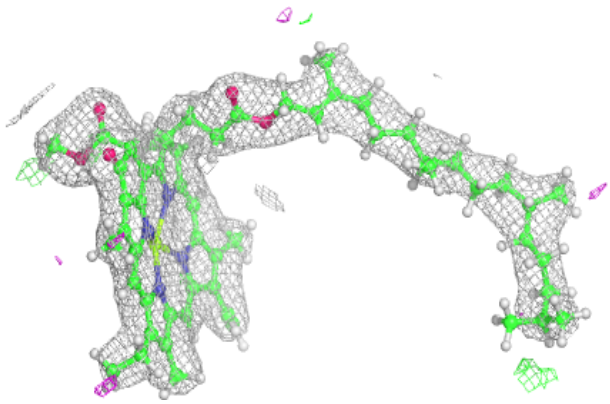


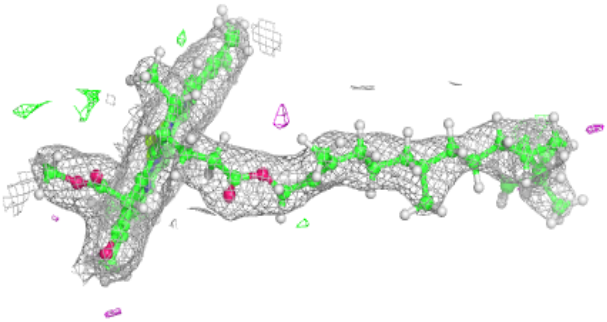


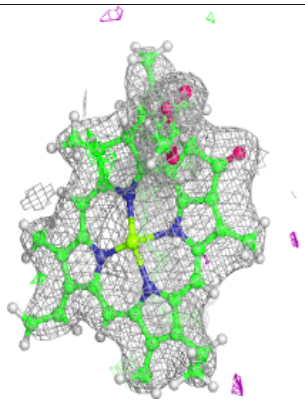


Electron density around CLA B 610:

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

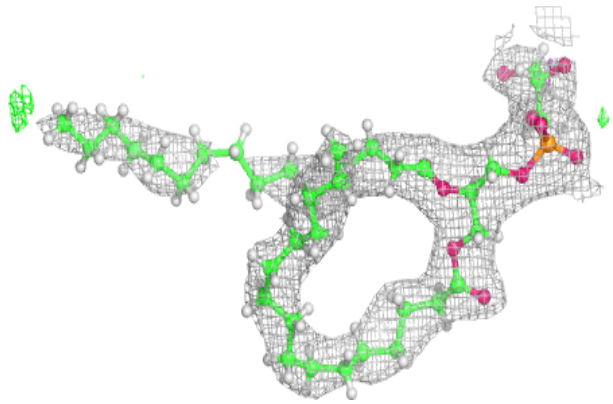


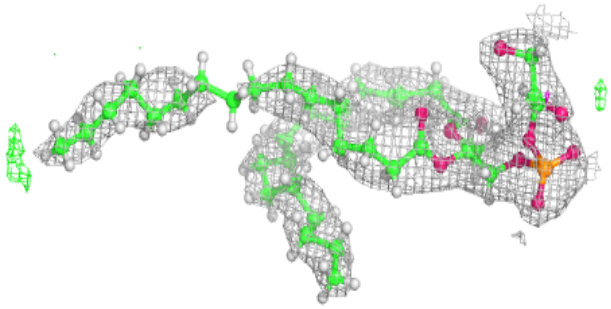


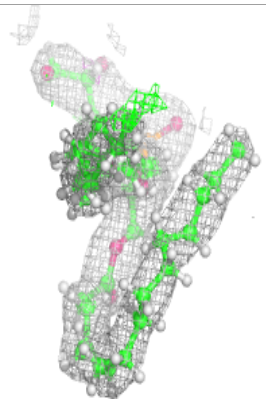


Electron density around LHG d 407:

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

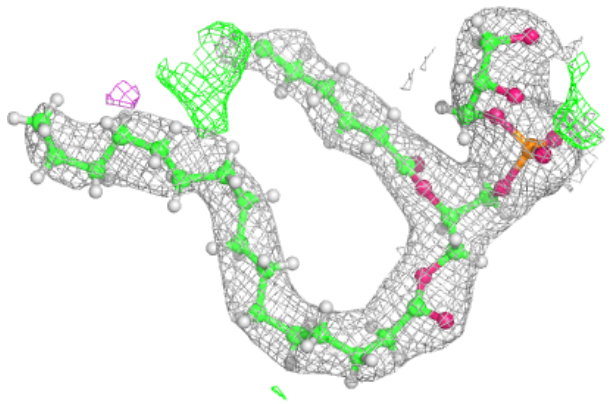


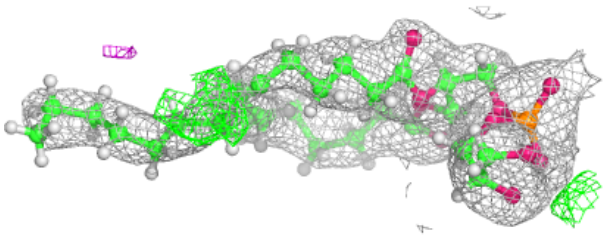


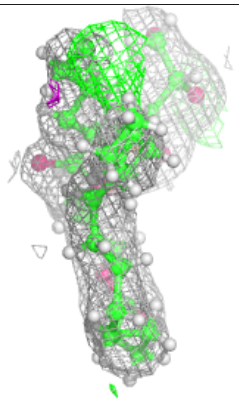


Electron density around LHG d 409:

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

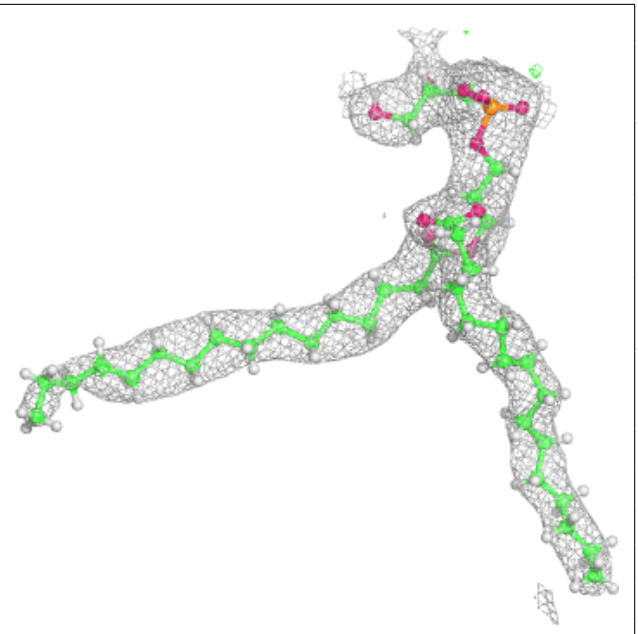


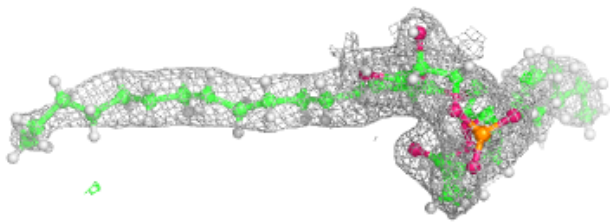


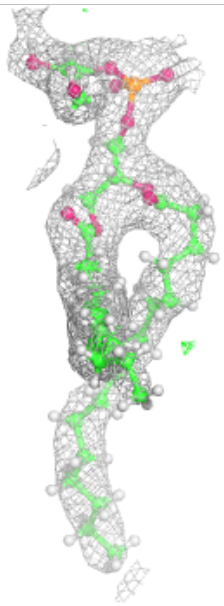


Electron density around LHG l 101:

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

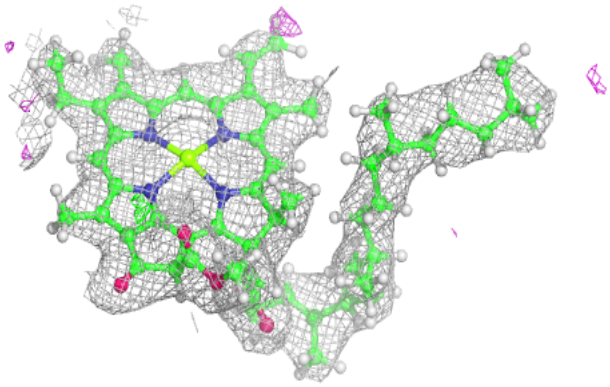


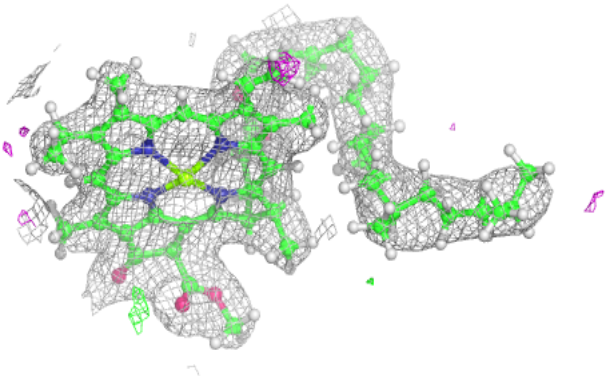


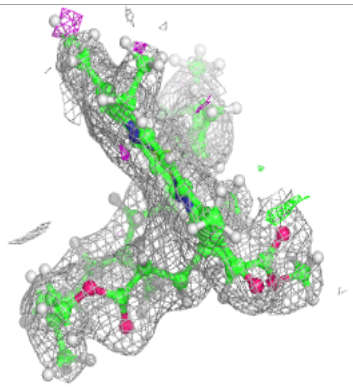


Electron density around CLA D 403:

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

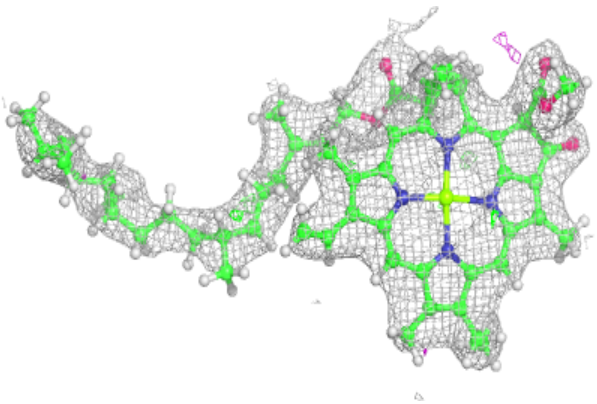


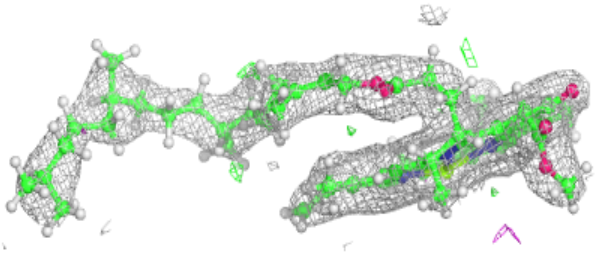


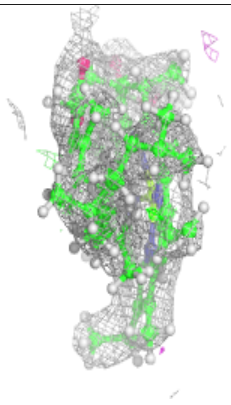


Electron density around CLA B 604:

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

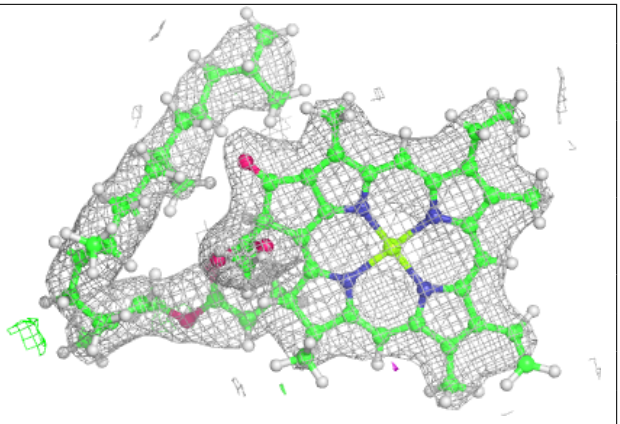


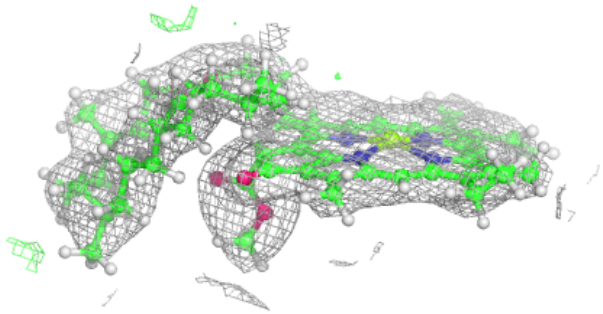


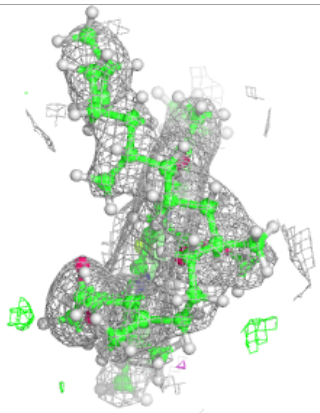


Electron density around CLA b 610:

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

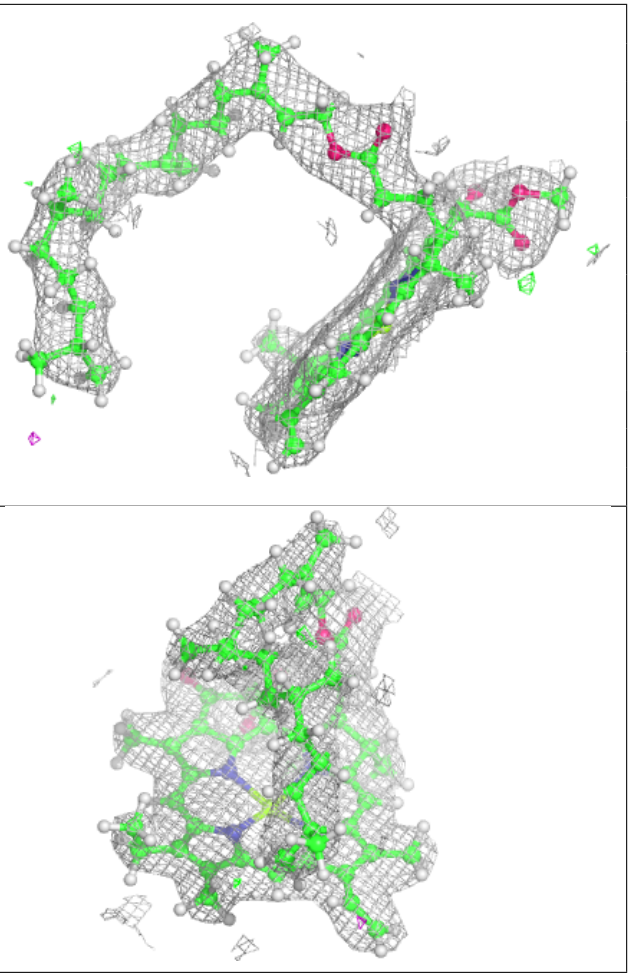






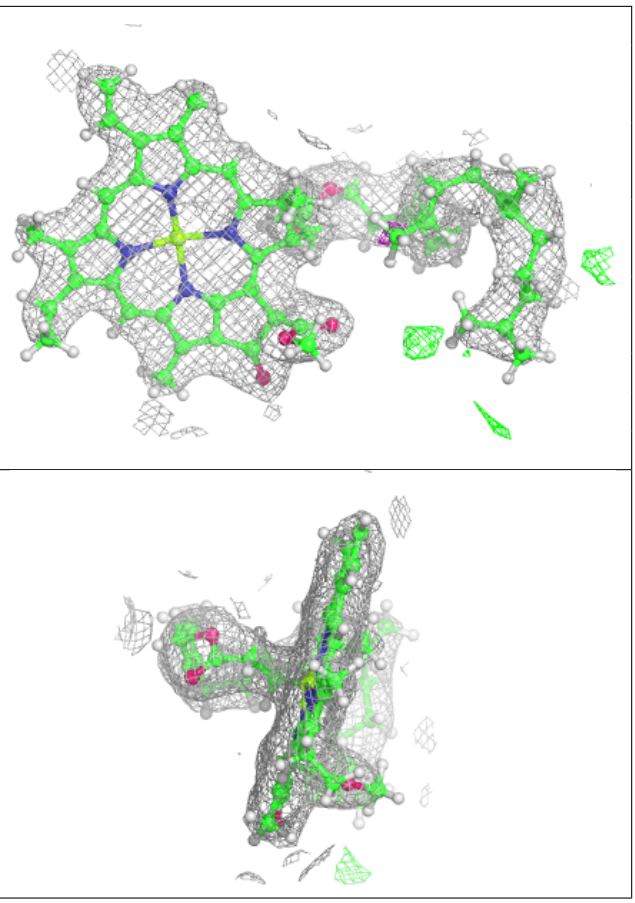
Electron density around CLA b 611:

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



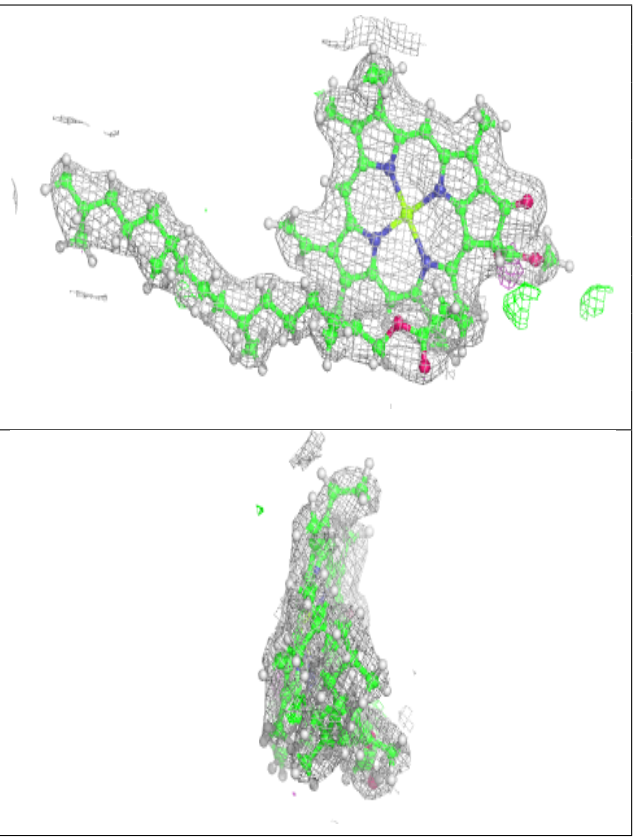
Electron density around CLA b 612:

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



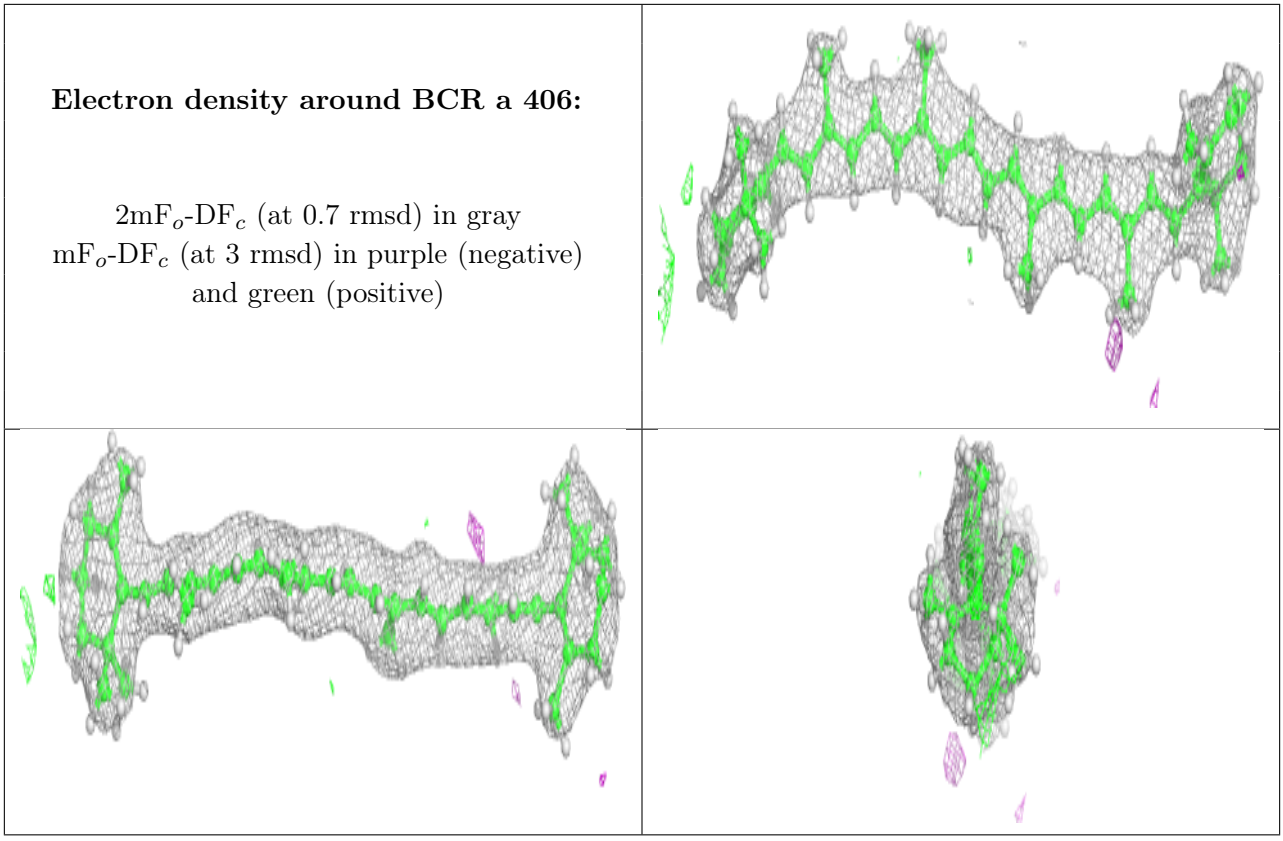
Electron density around CLA C 502:

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



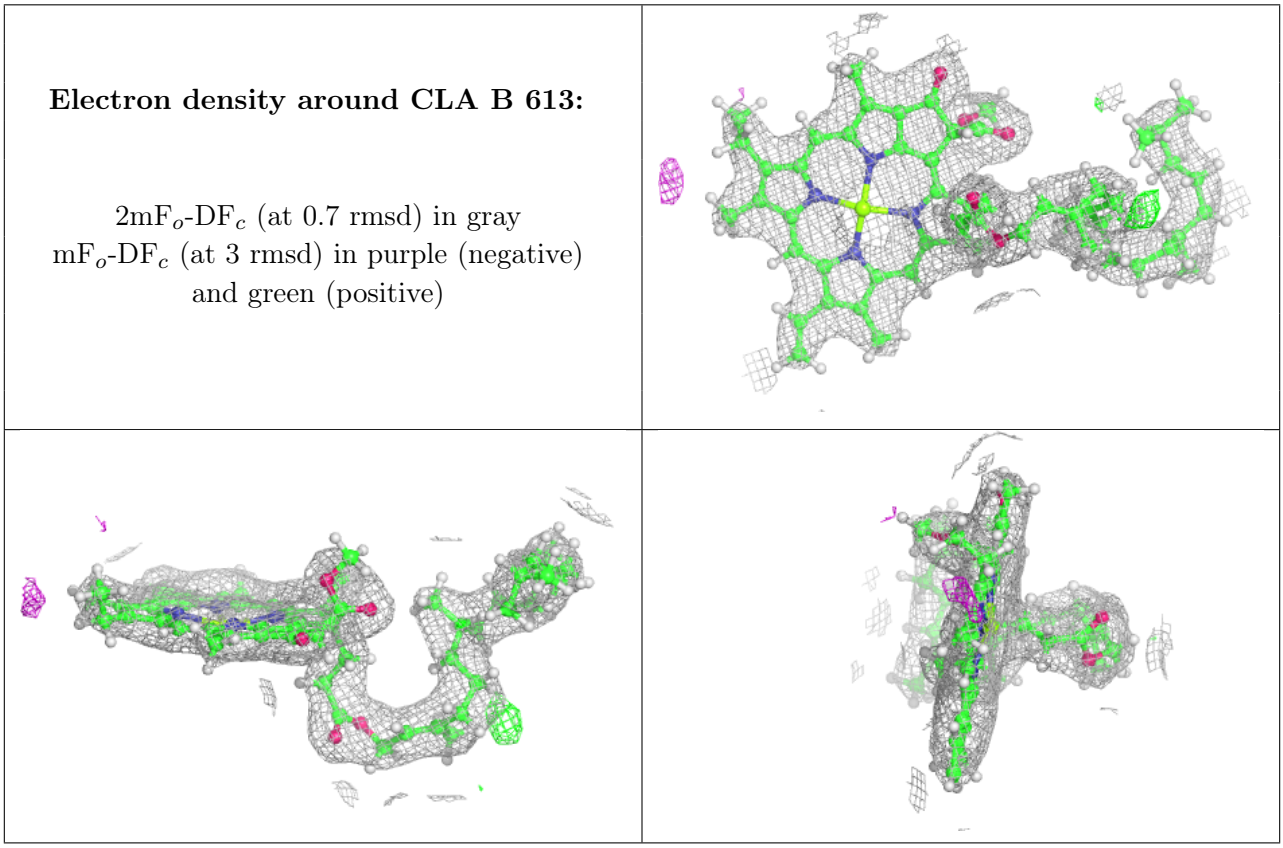
Electron density around BCR a 406:

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



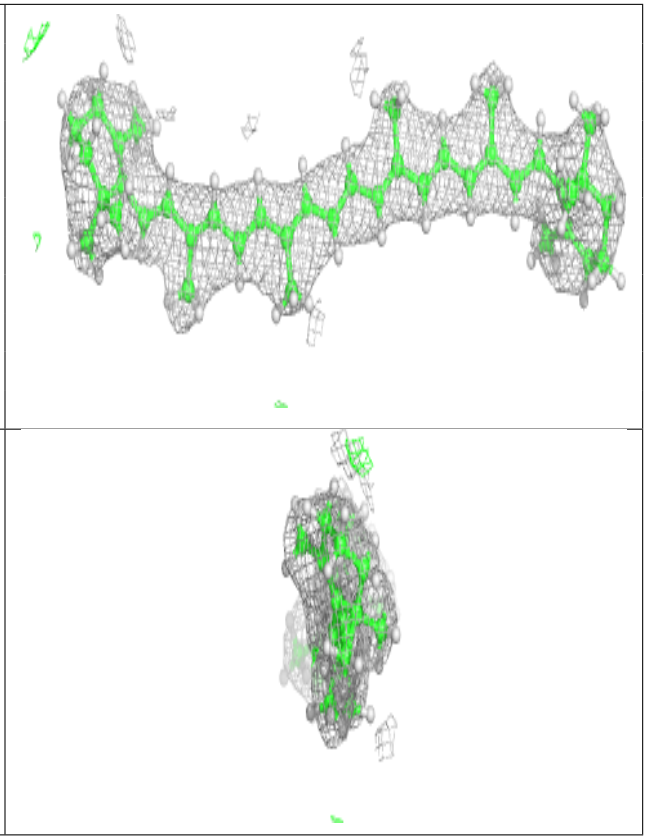
Electron density around CLA B 613:

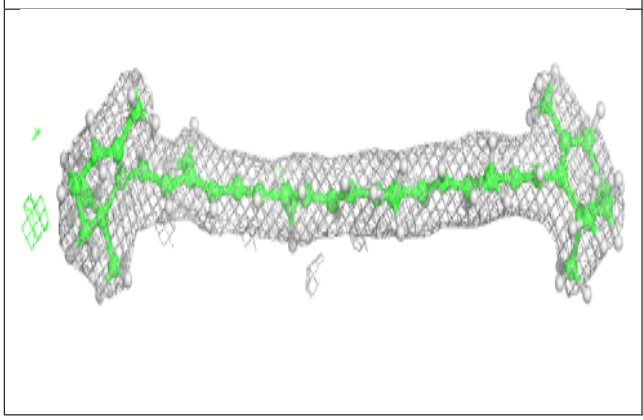
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCR b 618:

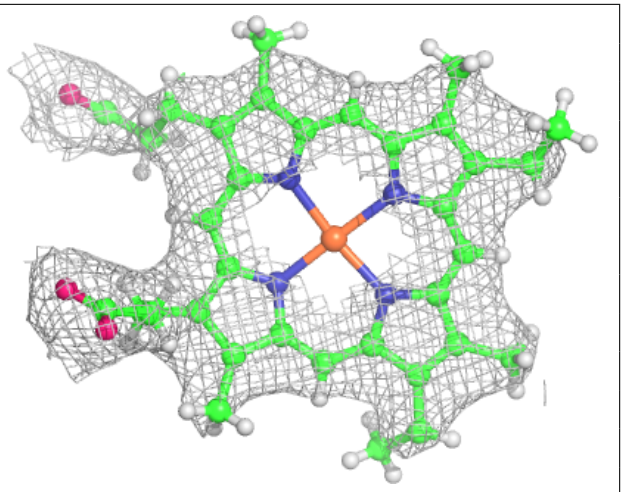
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

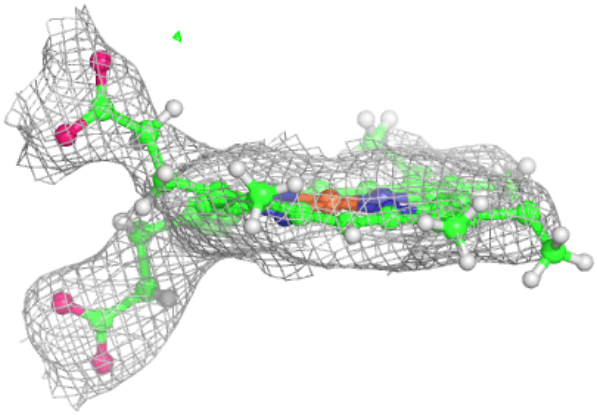


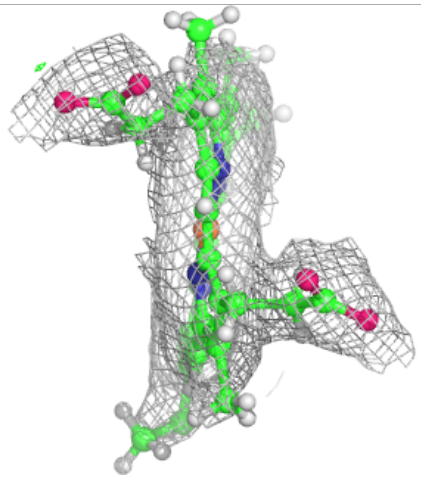


Electron density around HEC E 101:

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

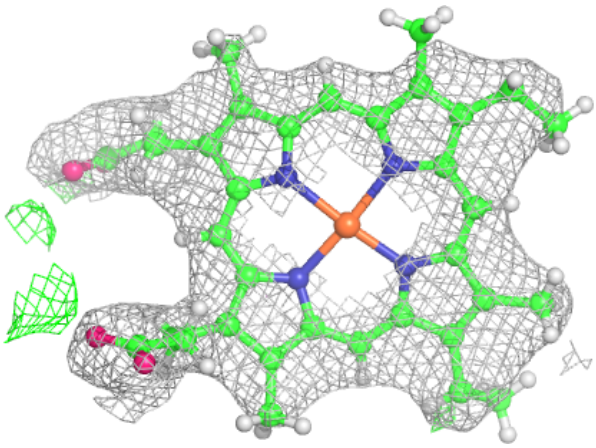


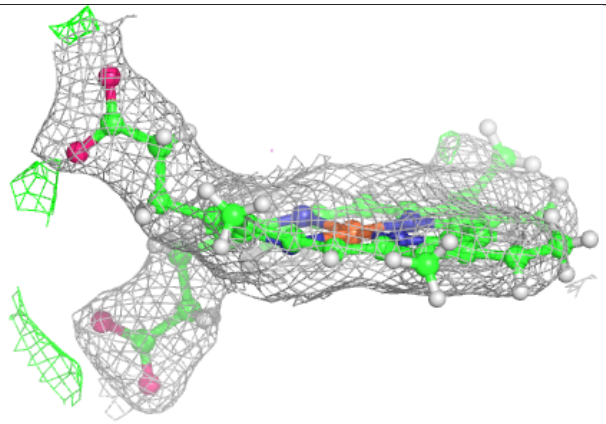


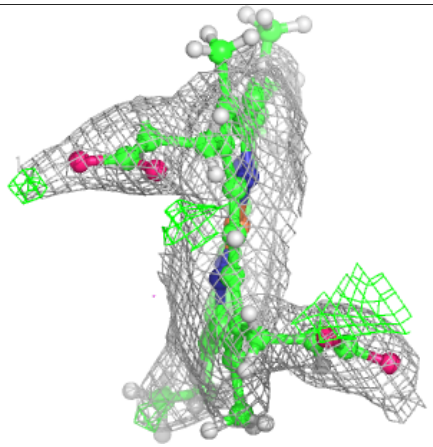


Electron density around HEC e 101:

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

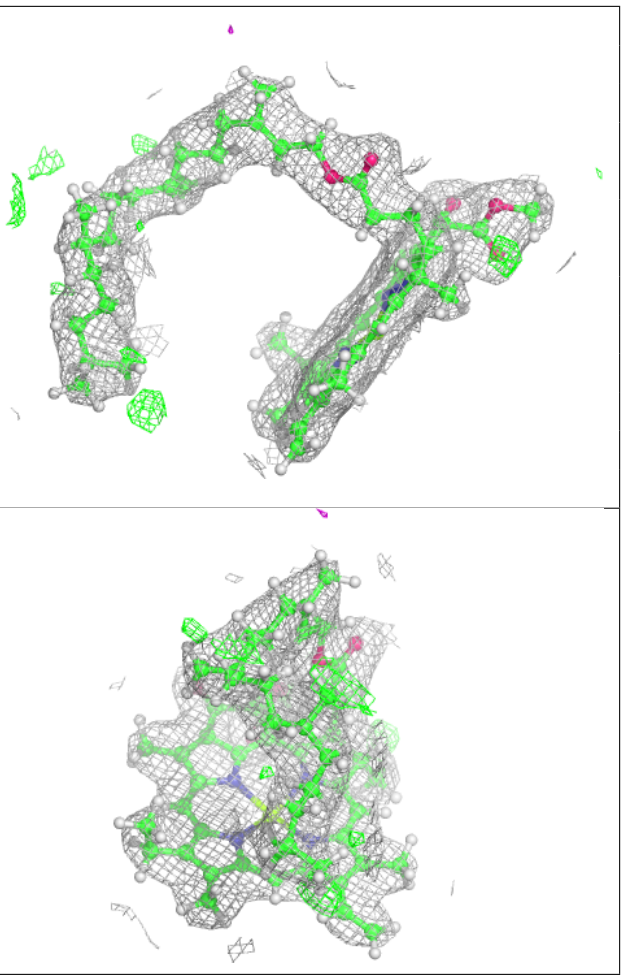






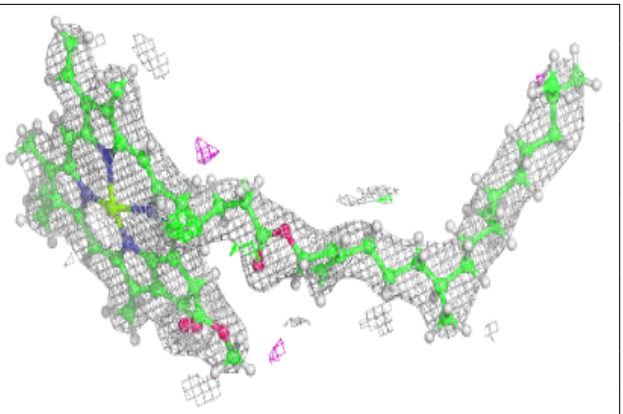
Electron density around CLA B 612:

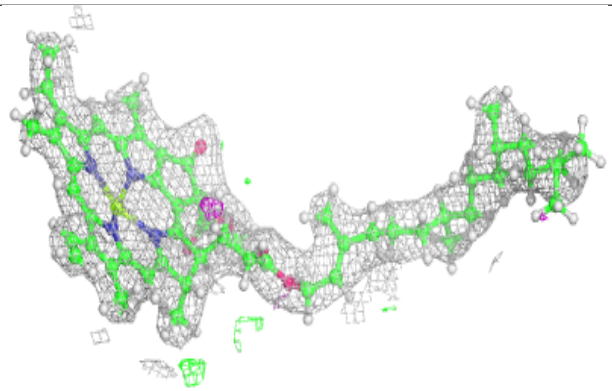
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

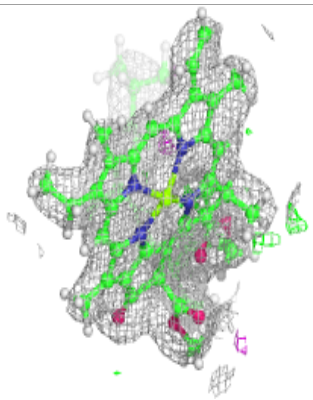


Electron density around CLA a 402:

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

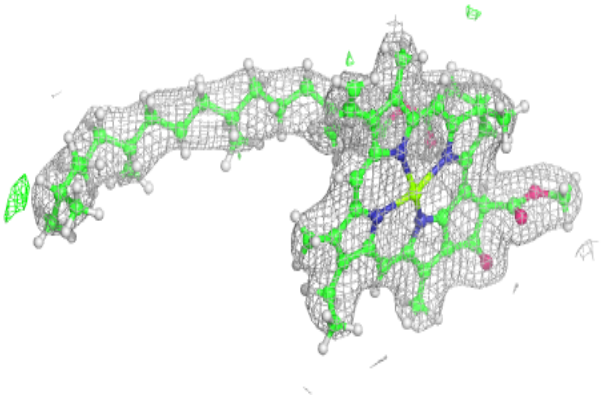


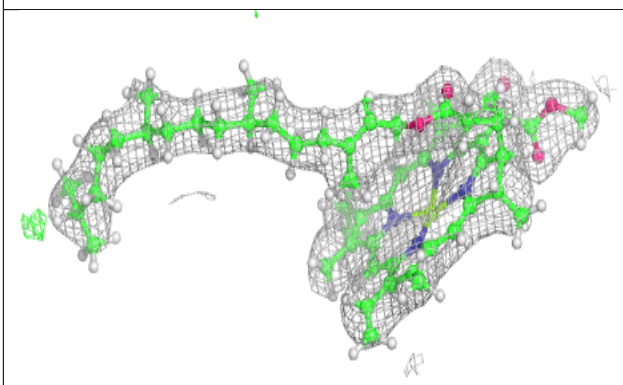


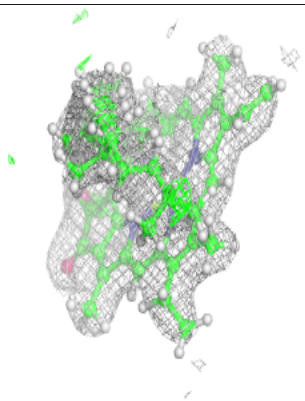


Electron density around CLA B 609:

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

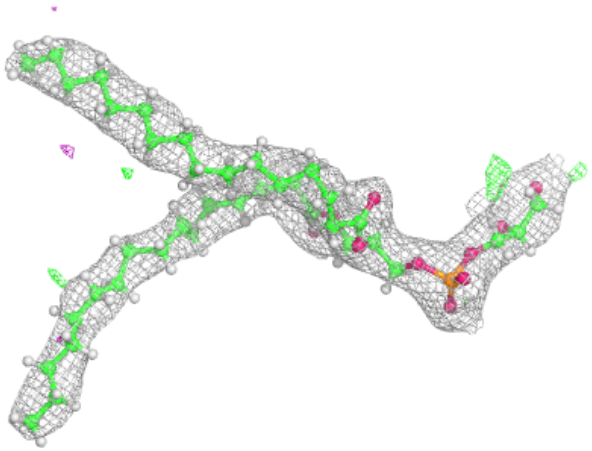


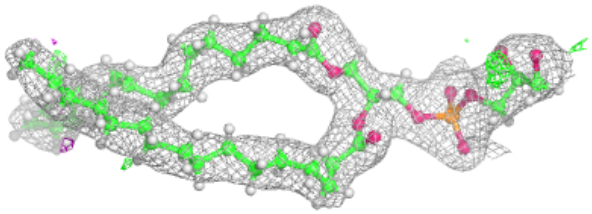


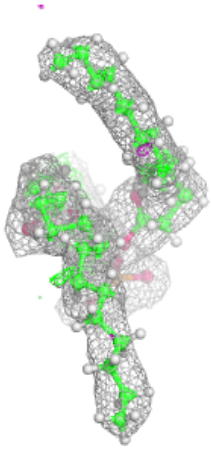


Electron density around LHG D 408:

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

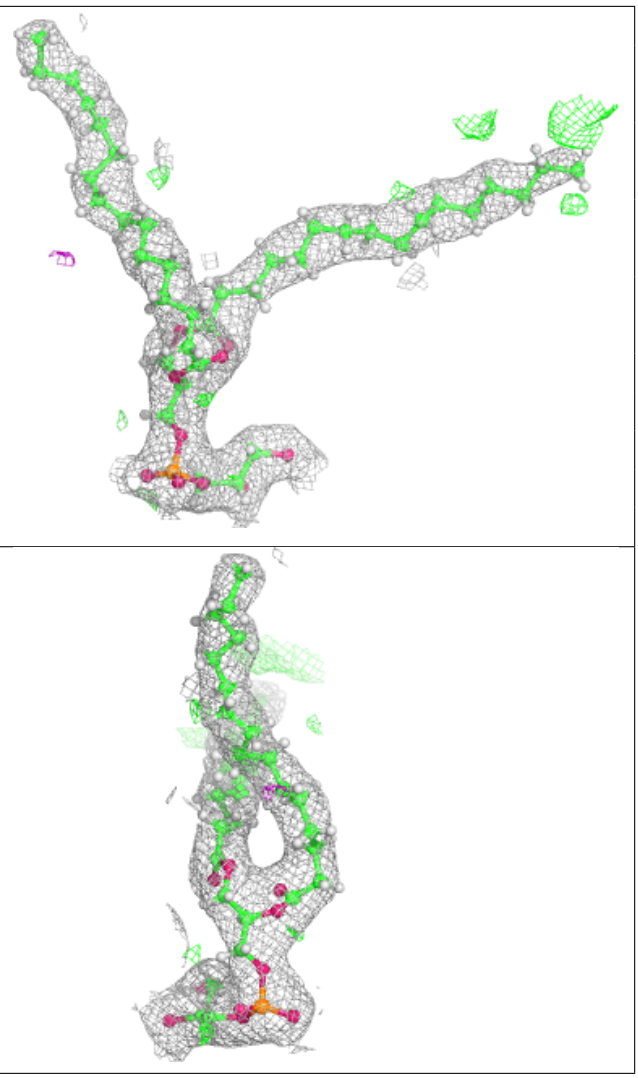






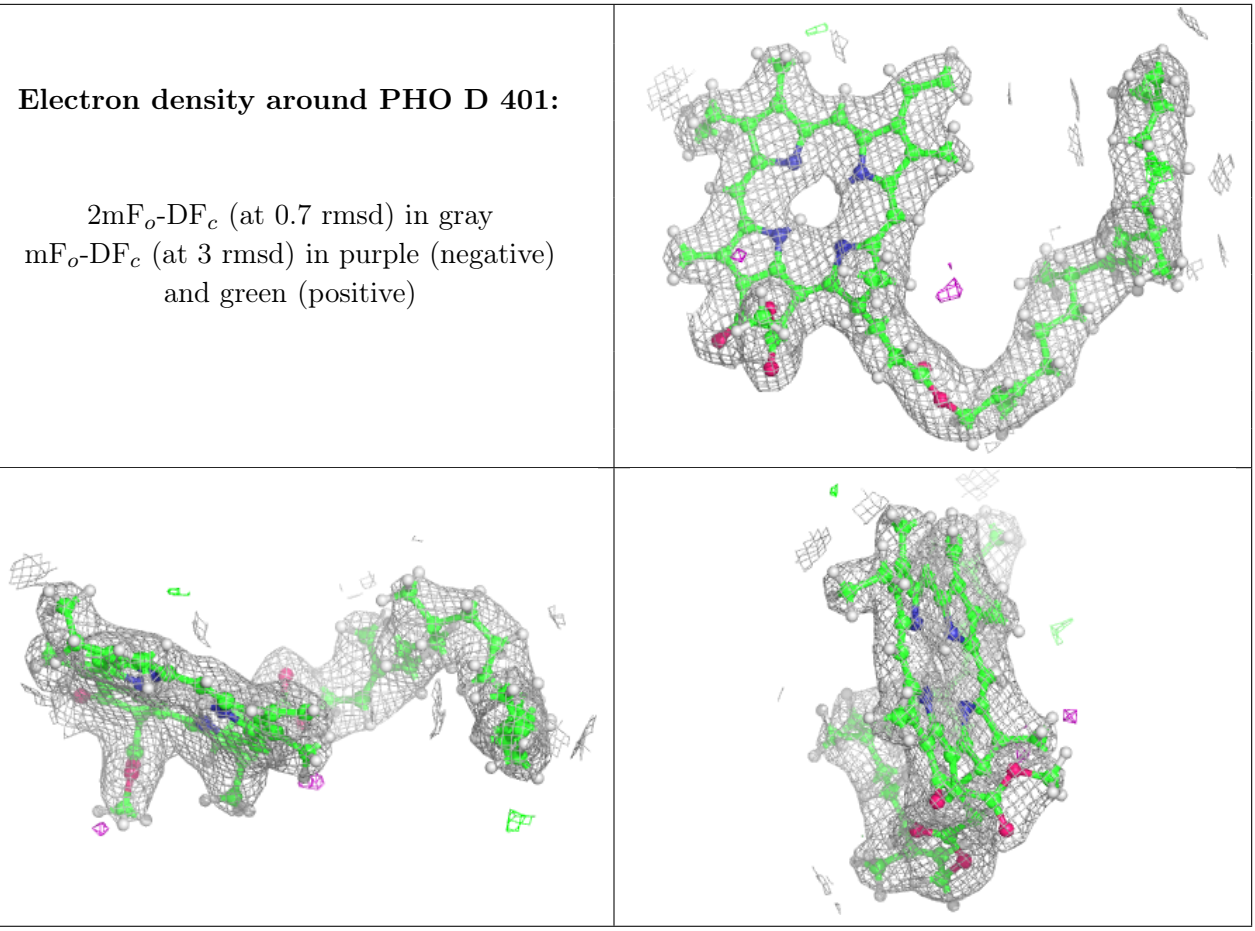
Electron density around LHG L 102:

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



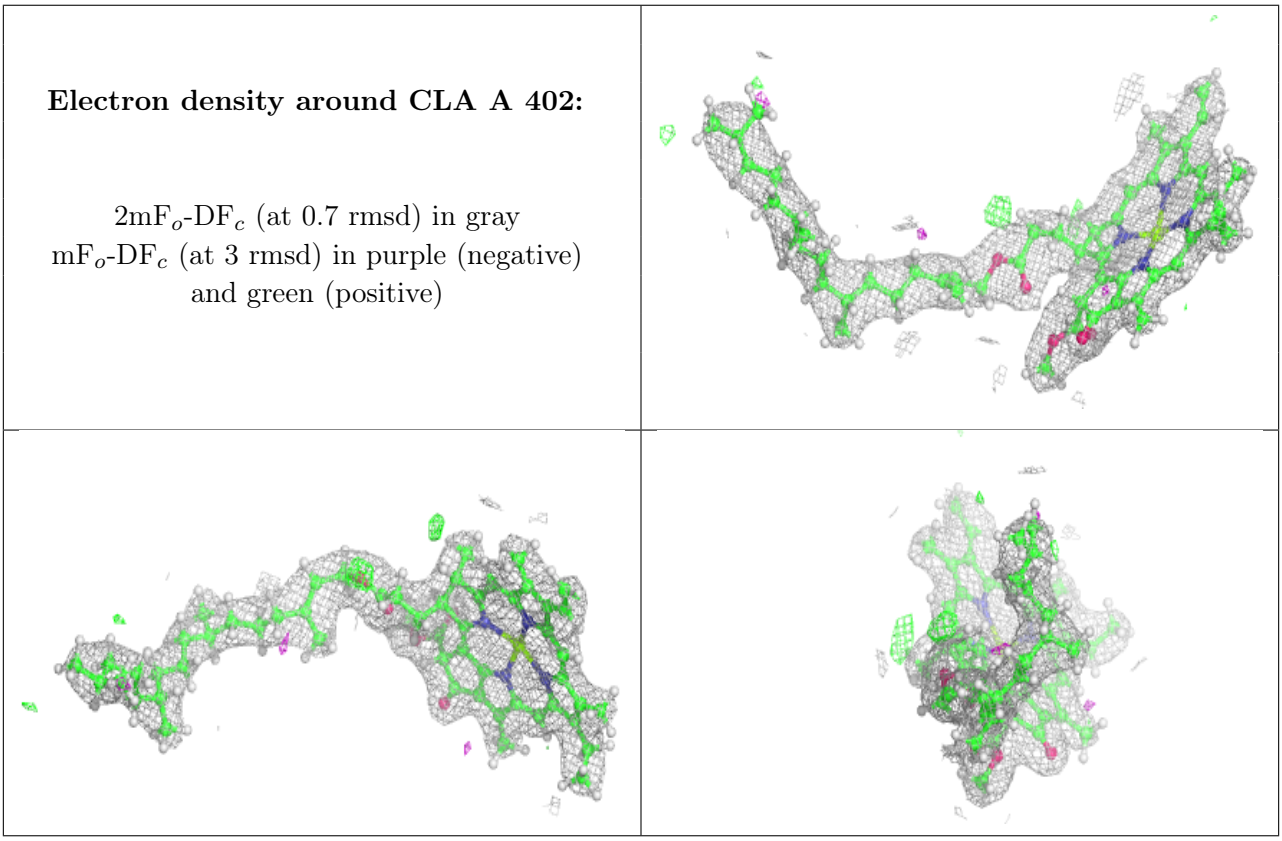
Electron density around PHO D 401:

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



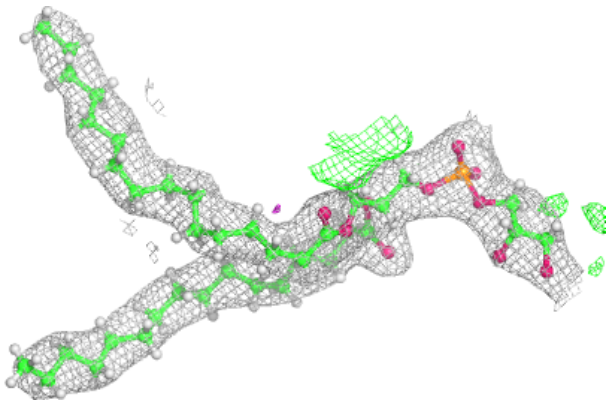
Electron density around CLA A 402:

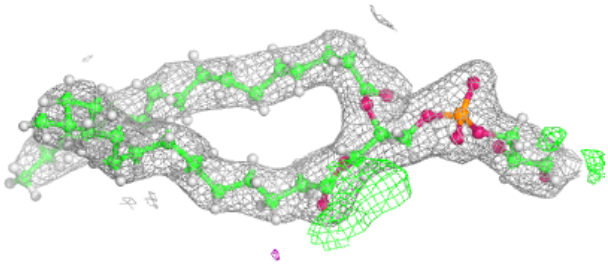
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

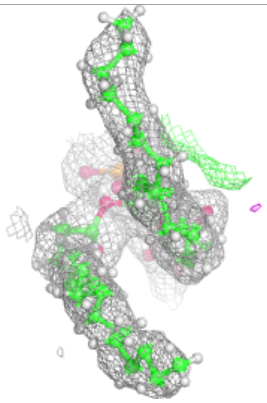


Electron density around LHG d 408:

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

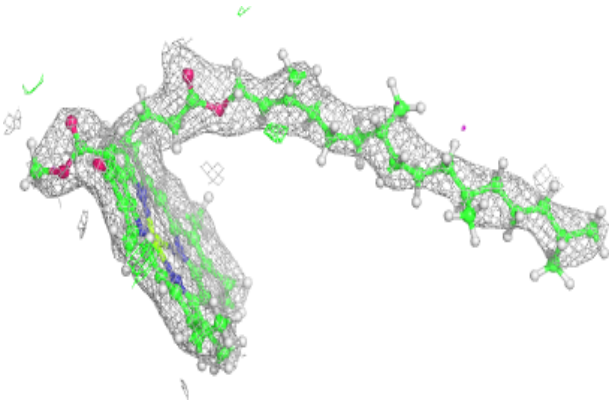


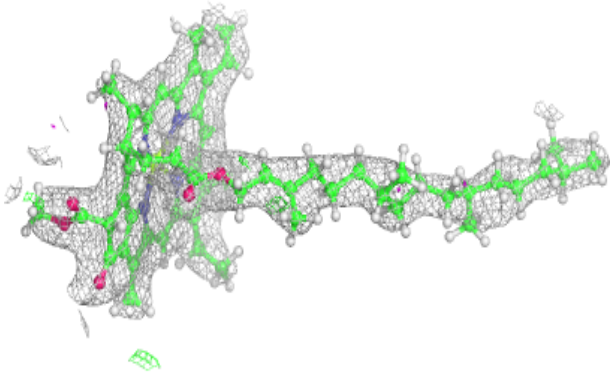


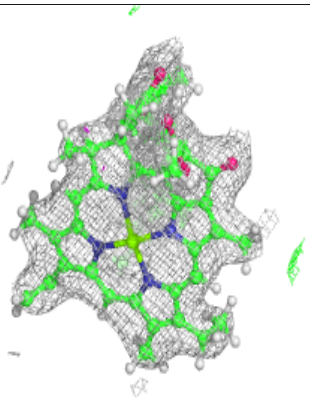


Electron density around CLA b 607:

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

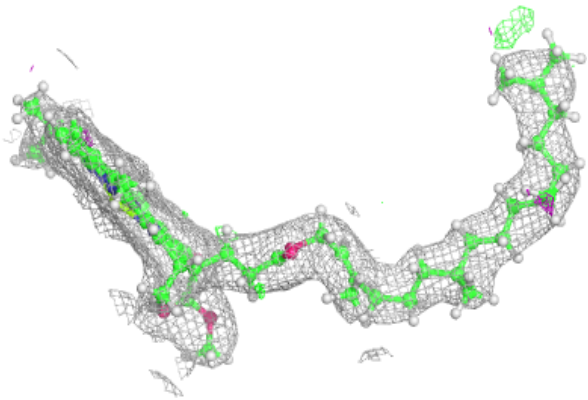


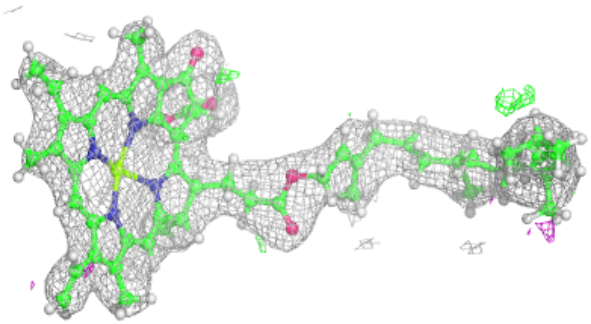


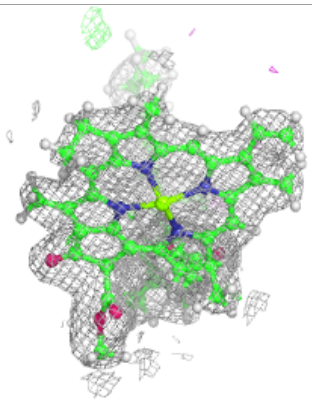


Electron density around CLA D 402:

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

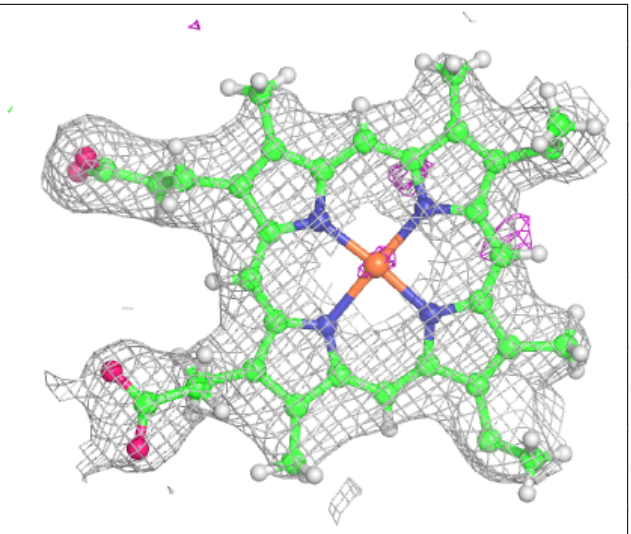


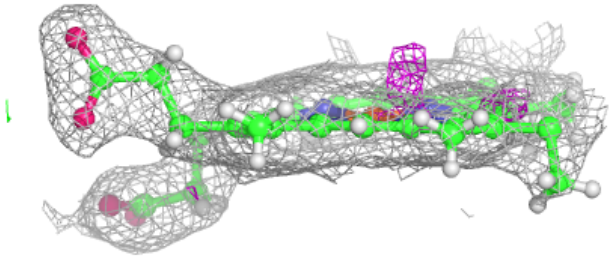


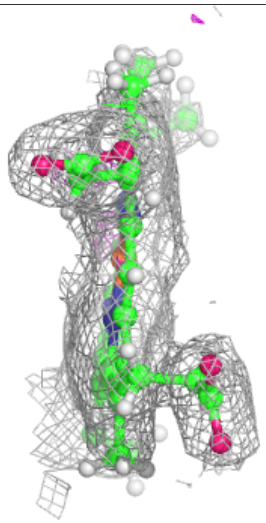


Electron density around HEC V 201:

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

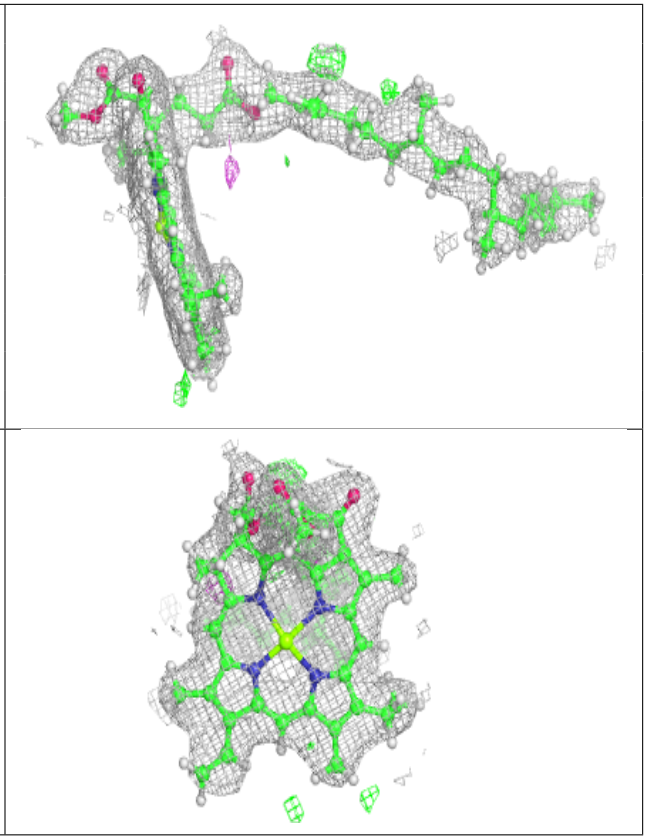


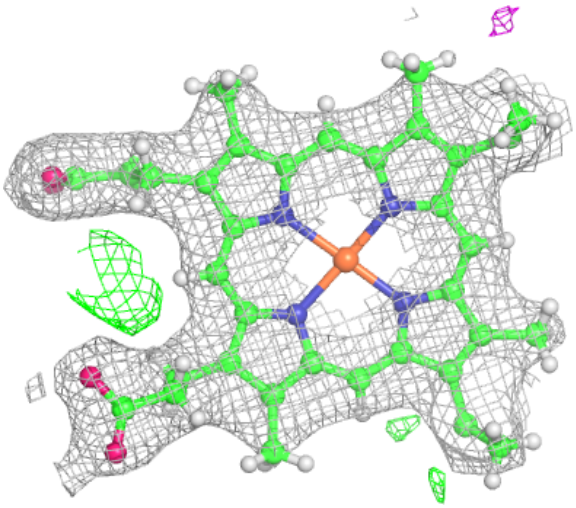
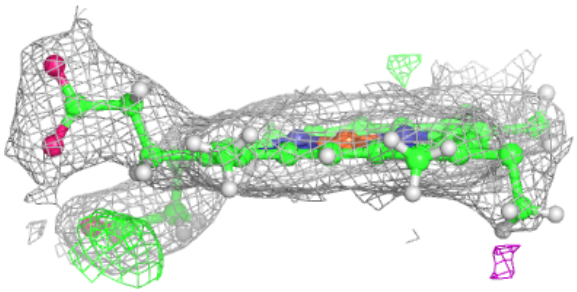
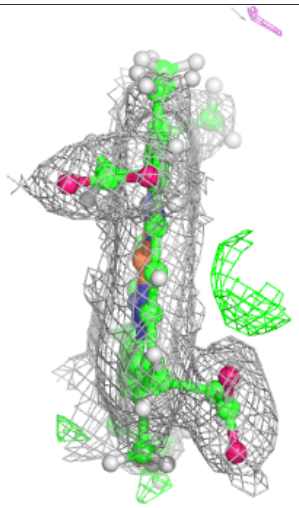




Electron density around CLA B 606:

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



Electron density around 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.