wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 08:20 PM JST

PDB ID	:	5ZZN
Title	:	Crystal structure of photosystem II from an SQDG-deficient mutant of Thermosynechococcus elongatus
Authors	:	Nakajima, Y.; Umena, Y.; Nagao, R.; Endo, K.; Kobayashi, K.; Akita, F.; Suga, M.; Wada, H.; Noguchi, T.; Shen, J.R.
Deposited on	:	2018-06-03
Resolution	:	2.10 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:

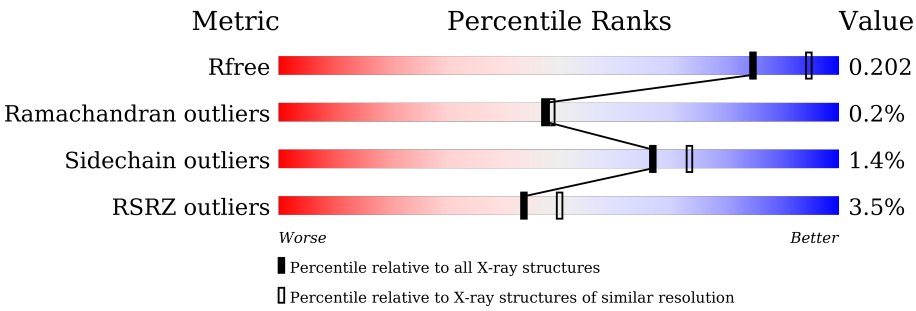
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	98%
2	B	505	99%
2	b	505	97%
3	C	455	97%
3	c	455	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	%, 98%
4	d	342	2%, 99%
5	E	81	9%, 95%
5	e	81	11%, 98%
6	F	34	12%, 94%, 6%
6	f	34	3%, 94%, 6%
7	H	63	3%, 98%
7	h	63	6%, 97%
8	I	37	3%, 92%, 5%
8	i	37	5%, 97%
9	J	40	8%, 92%, 8%
9	j	40	2%, 100%
10	K	37	100%
10	k	37	95%, 5%
11	L	36	8%, 94%, 6%
11	l	36	6%, 94%
12	M	34	3%, 94%
12	m	34	6%, 94%, 6%
13	O	243	4%, 98%
13	o	243	8%, 97%
14	T	30	3%, 90%, 10%
14	t	30	3%, 93%, 7%
15	U	97	2%, 96%
15	u	97	%, 96%
16	V	137	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	137	4% 100%
17	Y	29	10% 93% 7%
17	y	29	17% 93% 7%
18	X	39	10% 97%
18	x	39	10% 95%
19	Z	62	15% 97%
19	z	62	19% 97%

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	404	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	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	-	-	-
22	CLA	C	501	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	D	403	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	D	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	409	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	-
22	CLA	b	620	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
28	LMT	C	520	X	-	-	-
28	LMT	z	101	X	-	-	-
32	HTG	B	624	-	-	-	X
32	HTG	U	203	-	-	-	X

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2626	1717	432	462	15	0	2	0
1	a	334	2629	1721	433	460	15	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	4009	2626	671	699	13	0	5	0
2	b	504	3988	2616	661	698	13	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3526	2303	592	617	14	0	5	0
3	c	455	3531	2311	591	615	14	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	2746	1818	449	467	12	0	3	0
4	d	342	2738	1813	448	464	13	0	2	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	80	665	433	106	126	0	2	0
5	e	81	649	425	105	119	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	274	187	45	41	1	0	0	0
6	f	32	257	175	43	38	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	N	O	S			
7	H	63	509	339	84	84	2	0	1	0
7	h	63	506	337	81	86	2	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	I	35	284	193	44	46	1	0	0	0
8	i	37	294	199	47	47	1	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	37	262	177	41	43	1	0	0	0
9	j	40	279	187	44	47	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	N	O			
10	K	37	296	206	43	47	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	285	199	42	44	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	L	36	292	196	45	51	0	1	0
11	l	35	296	200	45	51	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	264	177	38	48	1	0	1	0
12	m	34	269	180	39	49	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1876	1172	315	385	4	0	4	0
13	o	243	1876	1174	311	385	6	0	6	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	259	181	36	40	2	0	0	0
14	t	30	259	181	36	40	2	0	0	0

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	97	785	497	133	155	0	1	0
15	u	97	783	496	130	157	0	1	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1083	685	183	211	4	0	2	0
16	v	137	1063	672	178	209	4	0	1	0

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Y	29	217	144	35	34	4	0	1	0
17	y	29	209	136	37	33	3	0	0	0

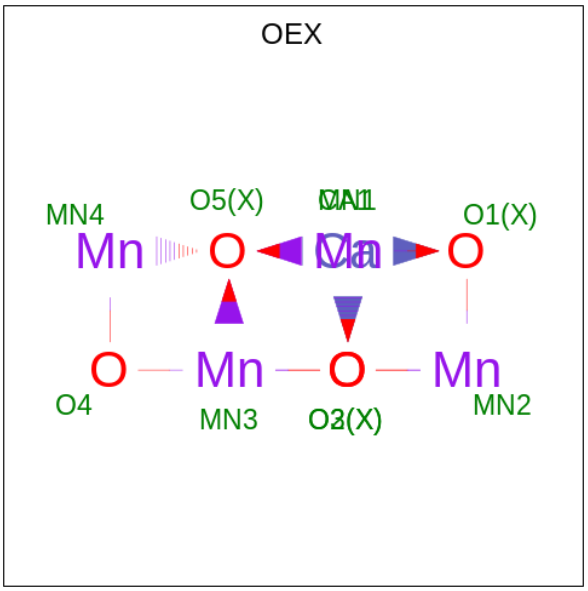
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	X	39	292	196	47	49	0	1	0
18	x	38	289	194	46	49	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Z	62	465	321	67	75	2	0	0	0
19	z	62	459	318	67	72	2	0	0	0

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

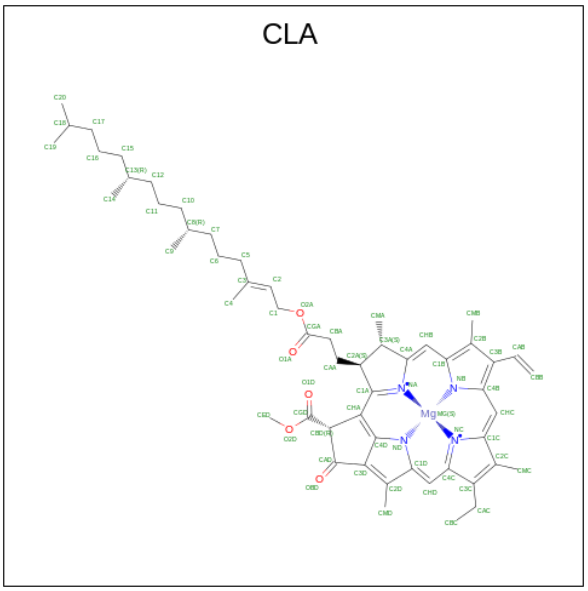


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
20	A	1	10	1	4	5	0	0
20	a	1	10	1	4	5	0	0

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
21	A	2	2	2	0	0
21	a	2	2	2	0	0
21	v	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	Mg	N	O		
22	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	D	1	65	55	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
22	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0

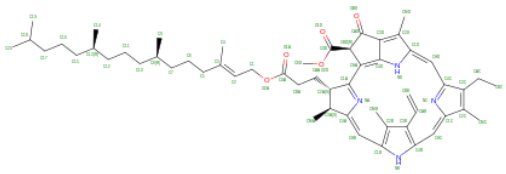
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	d	1	65	55	1	4	5	0	0

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

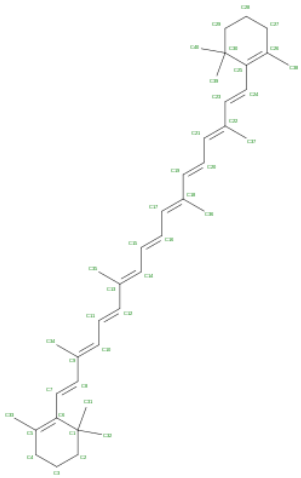
PHO



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	A	1	64	55	4	5	0	0
23	D	1	64	55	4	5	0	0
23	a	1	64	55	4	5	0	0
23	d	1	64	55	4	5	0	0

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

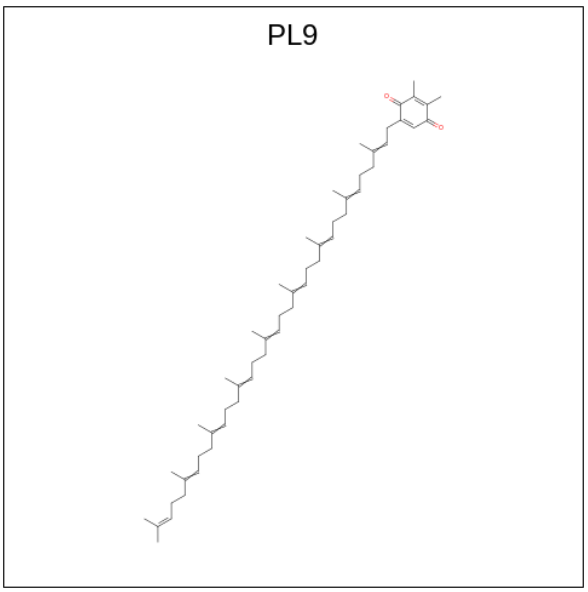
BCR



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
24	A	1	40	40	0	0
24	B	1	40	40	0	0
24	B	1	40	40	0	0
24	B	1	40	40	0	0
24	C	1	40	40	0	0
24	D	1	40	40	0	0
24	K	1	40	40	0	0
24	K	1	40	40	0	0
24	T	1	40	40	0	0
24	Y	1	40	40	0	0
24	a	1	40	40	0	0
24	b	1	40	40	0	0
24	b	1	40	40	0	0
24	b	1	40	40	0	0
24	c	1	40	40	0	0
24	c	1	40	40	0	0
24	d	1	40	40	0	0
24	k	1	40	40	0	0
24	t	1	40	40	0	0
24	y	1	40	40	0	0

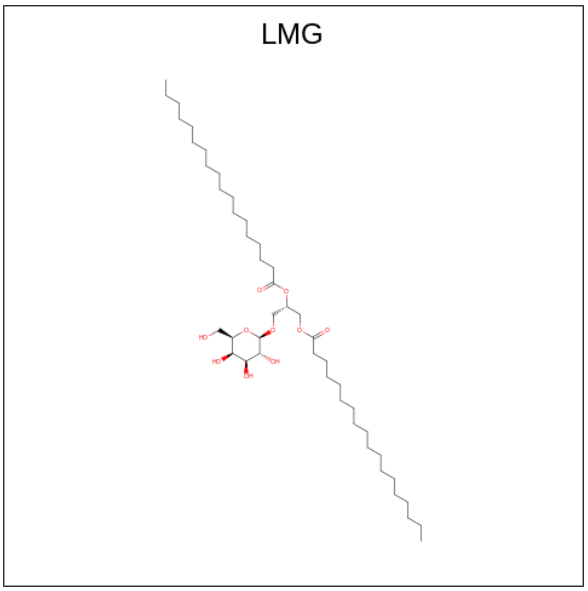
- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

$C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	A	1	55	53	2	0	0
25	D	1	55	53	2	0	0
25	a	1	55	53	2	0	0
25	d	1	55	53	2	0	0

- Molecule 26 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	O		
26	A	1	51	41	10	0	0
26	B	1	51	41	10	0	0
26	C	1	49	39	10	0	0
26	C	1	48	38	10	0	0
26	D	1	47	37	10	0	0
26	a	1	51	41	10	0	0
26	b	1	49	39	10	0	0
26	c	1	38	28	10	0	0
26	c	1	51	41	10	0	0
26	d	1	47	37	10	0	0

- Molecule 27 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	5	119	104	15	0	0
27	B	5	127	117	10	0	0

Continued on next page...

Continued from previous page...

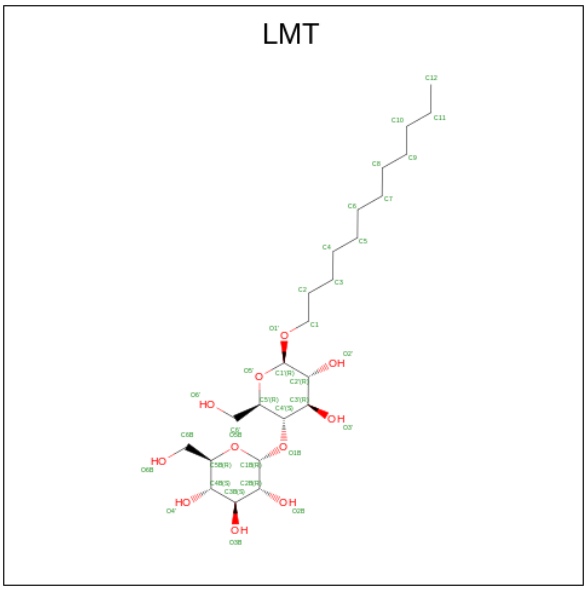
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	2	Total C O 35 30 5	0	0
27	D	1	Total C 16 16	0	0
27	E	2	Total C 29 29	0	0
27	H	2	Total C 14 14	0	0
27	I	4	Total C 59 59	0	0
27	J	1	Total C 16 16	0	0
27	K	1	Total C 10 10	0	0
27	T	1	Total C 13 13	0	0
27	U	1	Total C 14 14	0	0
27	X	1	Total C 16 16	0	0
27	Z	1	Total C 6 6	0	0
27	a	4	Total C O 96 86 10	0	0
27	b	4	Total C O 108 98 10	0	0
27	c	3	Total C O 53 48 5	0	0
27	d	2	Total C O 52 47 5	0	0
27	e	2	Total C 19 19	0	0
27	h	1	Total C 8 8	0	0
27	i	4	Total C 60 60	0	0
27	j	2	Total C O 49 44 5	0	0
27	t	1	Total C 16 16	0	0
27	u	1	Total C 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
27	x	1	16	16	0	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



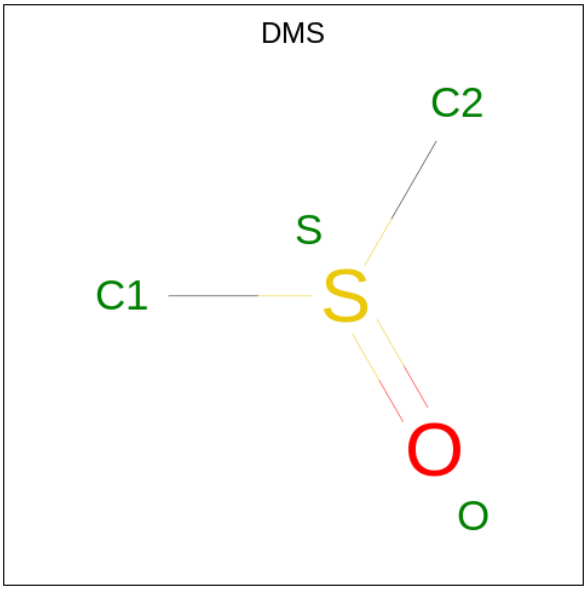
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	A	1	35	24	11	0	0
			Total	C	O		
28	B	1	35	24	11	0	0
			Total	C	O		
28	C	1	35	24	11	0	0
			Total	C	O		
28	F	1	24	18	6	0	0
			Total	C	O		
28	J	1	24	18	6	0	0
			Total	C	O		
28	M	1	35	24	11	0	0
			Total	C	O		
28	M	1	24	18	6	0	0
			Total	C	O		
28	T	1	24	18	6	0	0
			Total	C	O		
28	Z	1	35	24	11	0	0
			Total	C	O		
28	a	1	35	24	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
28	b	1	25	19	6		0	0
			Total	C	O			
28	c	1	35	24	11		0	0
			Total	C	O			
28	j	1	23	18	5		0	0
			Total	C	O			
28	l	1	24	18	6		0	0
			Total	C	O			
28	m	1	35	24	11		0	0
			Total	C	O			
28	m	1	25	18	7		0	0
			Total	C	O			
28	m	1	23	18	5		0	0
			Total	C	O			
28	t	1	24	18	6		0	0
			Total	C	O			
28	z	1	32	21	11		0	0

- Molecule 29 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	A	1	4	2	1	1	0	0
			Total	C	O	S		
29	A	1	4	2	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	A	1	4	2	1	1	0	0
			Total	C	O	S		
29	A	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	E	1	4	2	1	1	0	0
			Total	C	O	S		
29	I	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	U	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	d	1	4	2	1	1	0	0
			Total	C	O	S		
29	d	1	4	2	1	1	0	0
			Total	C	O	S		
29	e	1	4	2	1	1	0	0
			Total	C	O	S		
29	h	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0

Continued on next page...

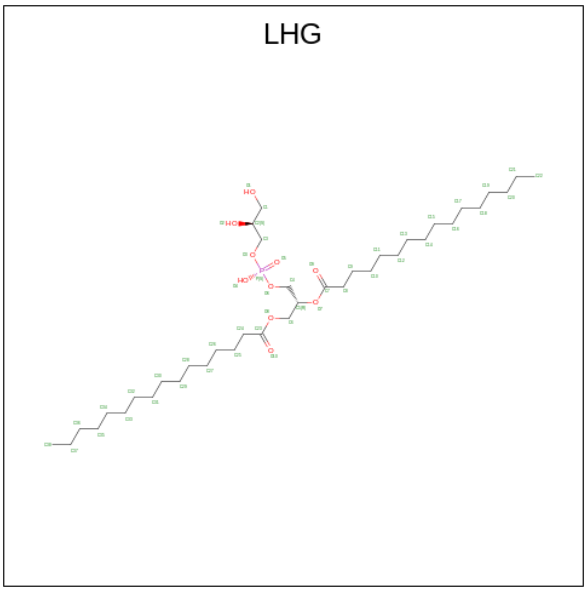
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
29	u	1	4	2	1	1	0	0
29	u	1	4	2	1	1	0	0
29	u	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
30	B	1	1	1	0	0
30	O	1	1	1	0	0
30	V	1	1	1	0	0
30	b	1	1	1	0	0
30	c	1	1	1	0	0
30	o	1	1	1	0	0
30	v	1	1	1	0	0

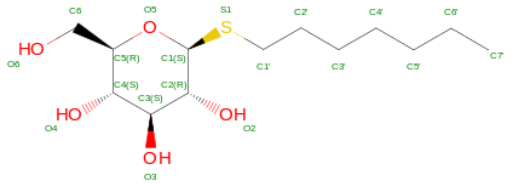
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
31	B	1	49	38	10	1	0	0
31	D	1	49	38	10	1	0	0
31	D	1	49	38	10	1	0	0
31	D	1	44	33	10	1	0	0
31	E	1	49	38	10	1	0	0
31	F	1	38	27	10	1	0	0
31	b	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0
31	d	1	44	33	10	1	0	0
31	e	1	38	29	8	1	0	0
31	f	1	46	35	10	1	0	0

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).

HTG



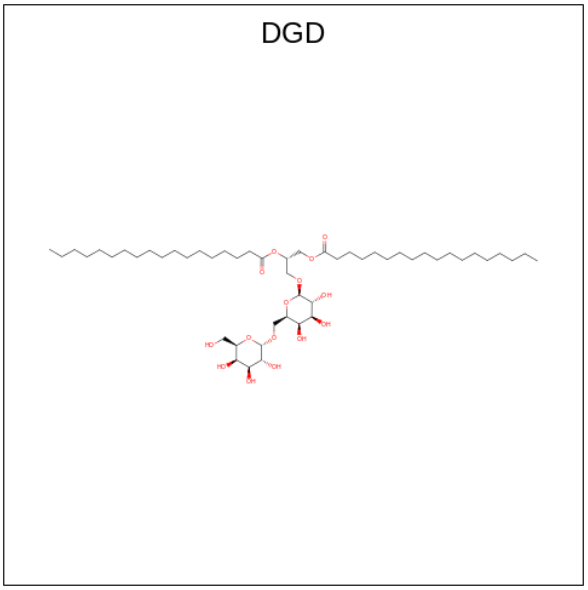
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 18 12 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C S 9 8 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	D	1	Total C O S 16 10 5 1	0	0
32	O	1	Total C O S 19 13 5 1	0	0
32	U	1	Total C O S 14 8 5 1	0	0
32	V	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 17 11 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C S 9 8 1	0	0
32	c	1	Total C O S 15 9 5 1	0	0
32	d	1	Total C O S 16 10 5 1	0	0
32	o	1	Total C O S 19 13 5 1	0	0
32	v	1	Total C O S 16 10 5 1	0	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



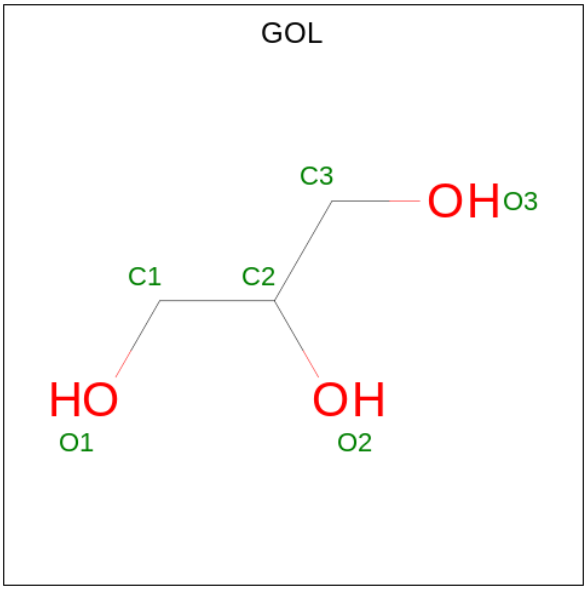
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	D	1	45	36	9	0	0
			Total	C	O		
33	H	1	62	47	15	0	0
			Total	C	O		
33	c	1	62	47	15	0	0
			Total	C	O		
33	c	1	56	41	15	0	0
			Total	C	O		
33	c	1	62	47	15	0	0
			Total	C	O		
33	d	1	48	39	9	0	0
			Total	C	O		
33	h	1	62	47	15	0	0

- Molecule 34 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	C	1	6	3	3	0	0
			Total	C	O		
34	D	1	6	3	3	0	0
			Total	C	O		
34	b	1	6	3	3	0	0
			Total	C	O		
34	c	1	6	3	3	0	0

Continued on next page...

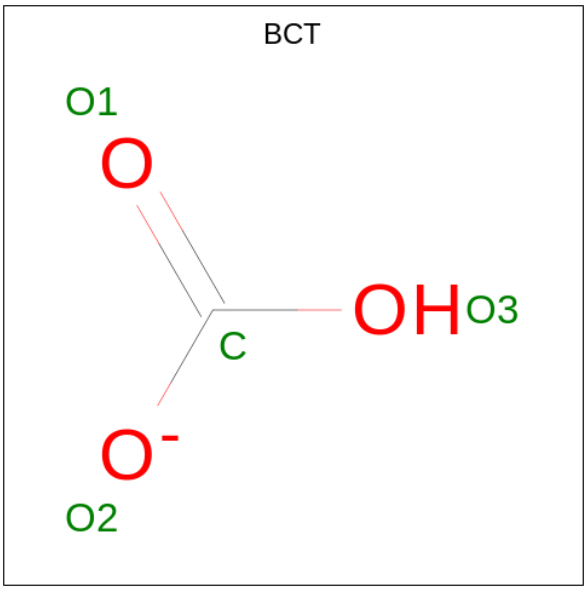
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	e	1	6	3	3	0	0

- Molecule 35 is FE (II) ION (three-letter code: FE2) (formula: Fe).

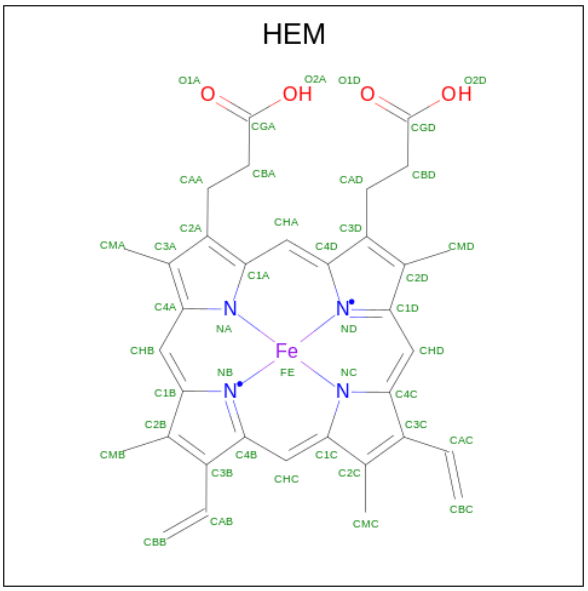
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
35	D	1	1	1	0	0
35	a	1	Total	Fe	0	0
			1	1		

- Molecule 36 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



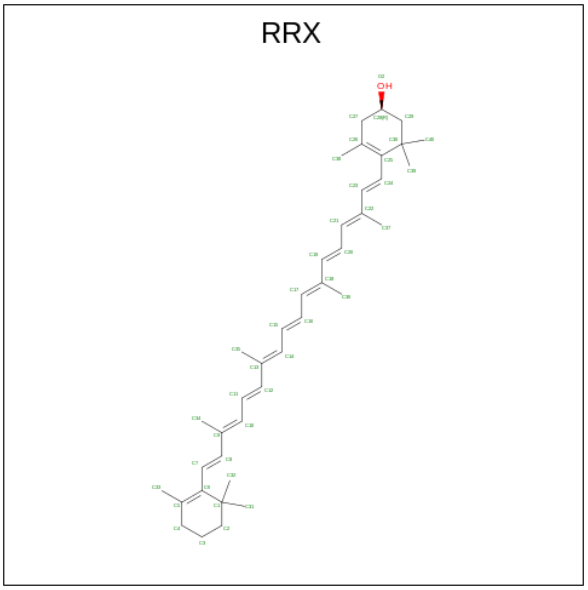
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	D	1	8	2	6	0	1
36	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
37	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
37	f	1	43	34	1	4	4	0	0

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

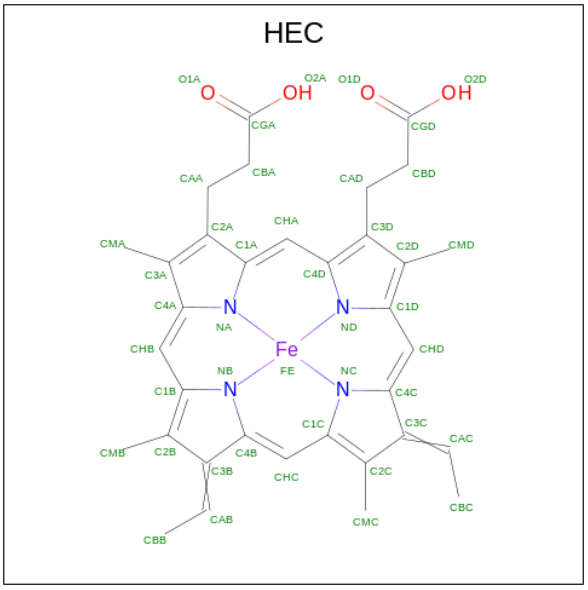


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
38	H	1	41	40	1	0	0
			Total	C	O		
38	h	1	41	40	1	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	K	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0
39	k	1	Total Mg 1 1	0	0

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	V	1	Total C Fe N O 43 34 1 4 4	0	0
40	v	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	139	Total O 141 141	0	2
41	B	260	Total O 263 263	0	3
41	C	216	Total O 216 216	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	D	126	130	130	0	4
			Total	O		
41	E	20	21	21	0	1
			Total	O		
41	F	6	6	6	0	0
			Total	O		
41	H	43	44	44	0	1
			Total	O		
41	I	6	6	6	0	0
			Total	O		
41	J	11	11	11	0	0
			Total	O		
41	K	8	8	8	0	0
			Total	O		
41	L	11	11	11	0	0
			Total	O		
41	M	10	11	11	0	1
			Total	O		
41	O	148	152	152	0	4
			Total	O		
41	T	13	13	13	0	0
			Total	O		
41	U	71	71	71	0	0
			Total	O		
41	V	102	103	103	0	1
			Total	O		
41	Y	4	5	5	0	1
			Total	O		
41	X	12	12	12	0	0
			Total	O		
41	Z	3	3	3	0	0
			Total	O		
41	a	125	126	126	0	1
			Total	O		
41	b	255	260	260	0	5
			Total	O		
41	c	201	203	203	0	2
			Total	O		
41	d	133	135	135	0	2
			Total	O		
41	e	19	20	20	0	1

Continued on next page...

Continued from previous page...

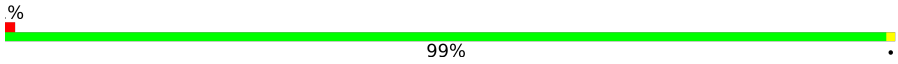
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	f	11	Total O 11 11	0	0
41	h	34	Total O 35 35	0	1
41	i	6	Total O 6 6	0	0
41	j	12	Total O 12 12	0	0
41	k	5	Total O 5 5	0	0
41	l	9	Total O 9 9	0	0
41	m	8	Total O 8 8	0	0
41	o	126	Total O 129 129	0	3
41	t	9	Total O 10 10	0	1
41	u	72	Total O 72 72	0	0
41	v	75	Total O 75 75	0	0
41	y	4	Total O 4 4	0	0
41	x	7	Total O 7 7	0	0
41	z	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

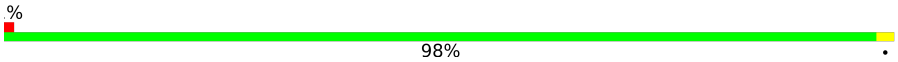
• Molecule 1: Photosystem II protein D1 1

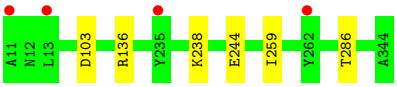
Chain A:



• Molecule 1: Photosystem II protein D1 1

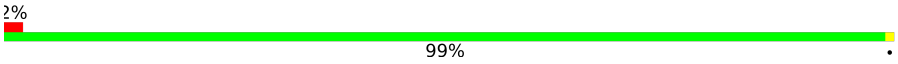
Chain a:

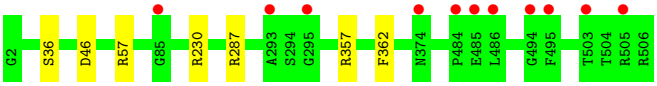




• Molecule 2: Photosystem II CP47 reaction center protein

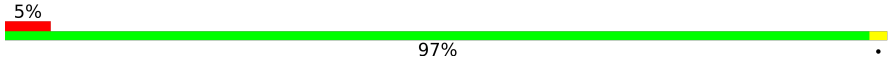
Chain B:

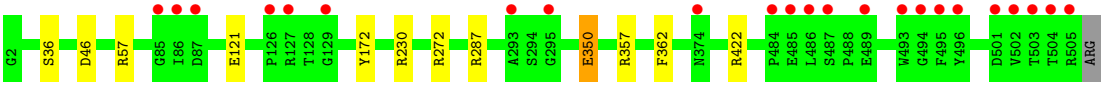




• Molecule 2: Photosystem II CP47 reaction center protein

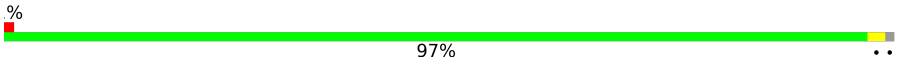
Chain b:

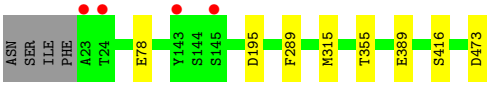




• Molecule 3: Photosystem II CP43 reaction center protein

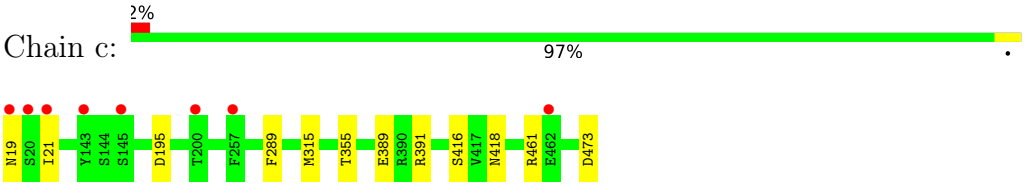
Chain C:





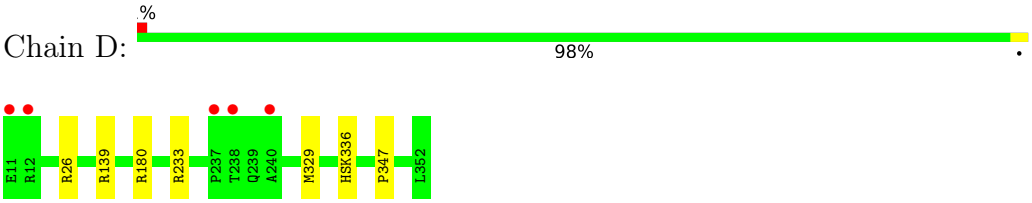
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



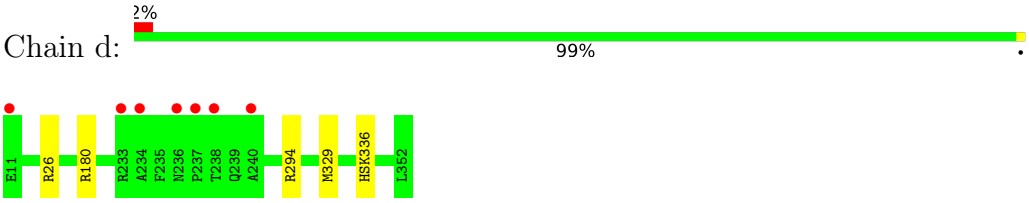
• Molecule 4: Photosystem II D2 protein

Chain D:



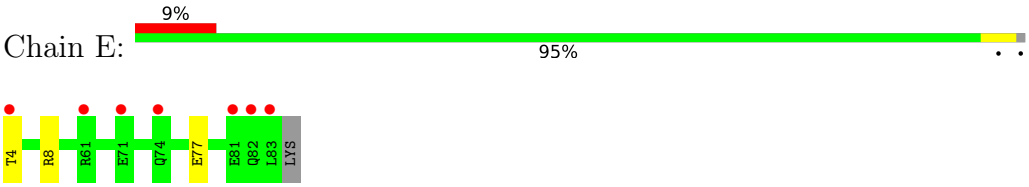
• Molecule 4: Photosystem II D2 protein

Chain d:



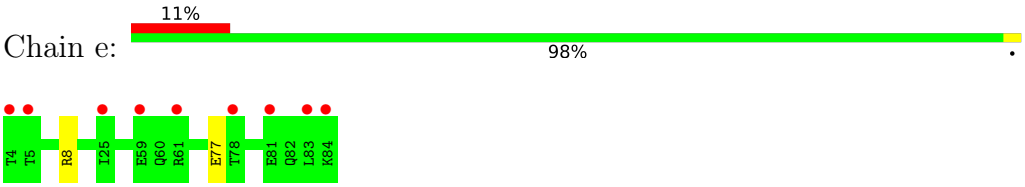
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



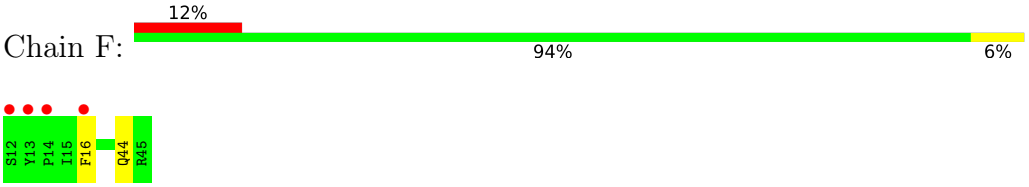
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



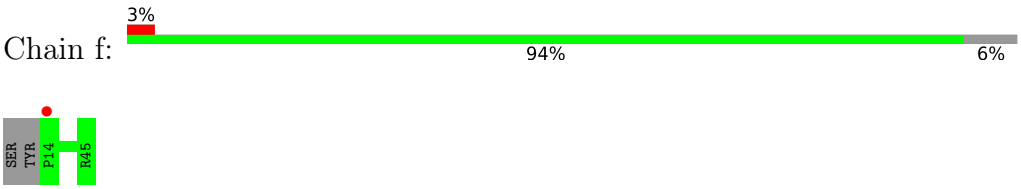
• Molecule 6: Cytochrome b559 subunit beta

Chain F:

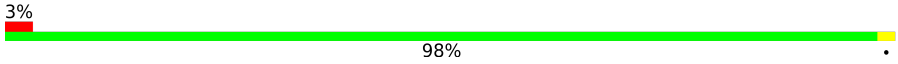


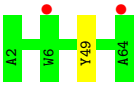
• Molecule 6: Cytochrome b559 subunit beta

Chain f:

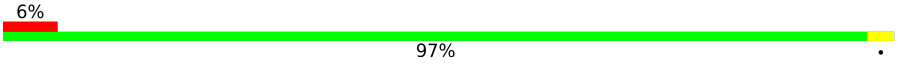


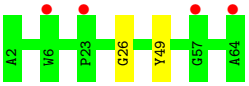
• Molecule 7: Photosystem II reaction center protein H

Chain H: 

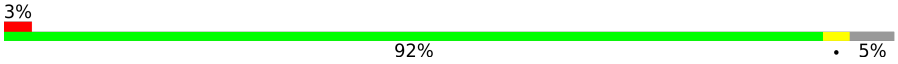


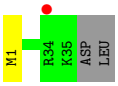
• Molecule 7: Photosystem II reaction center protein H

Chain h: 

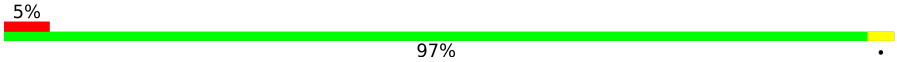


• Molecule 8: Photosystem II reaction center protein I

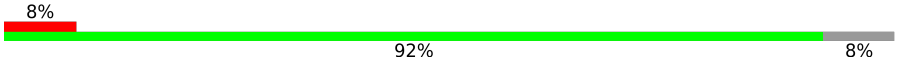
Chain I: 

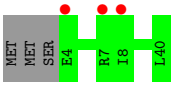


• Molecule 8: Photosystem II reaction center protein I

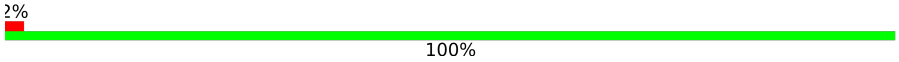
Chain i: 

• Molecule 9: Photosystem II reaction center protein J

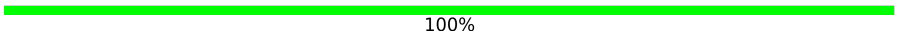
Chain J: 



• Molecule 9: Photosystem II reaction center protein J

Chain j: 

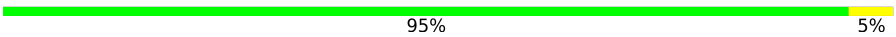
• Molecule 10: Photosystem II reaction center protein K

Chain K: 

There are no outlier residues recorded for this chain.

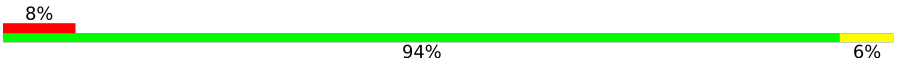
• Molecule 10: Photosystem II reaction center protein K

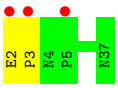
Chain k:



• Molecule 11: Photosystem II reaction center protein L

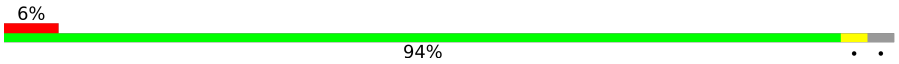
Chain L:

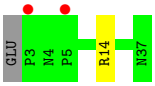




• Molecule 11: Photosystem II reaction center protein L

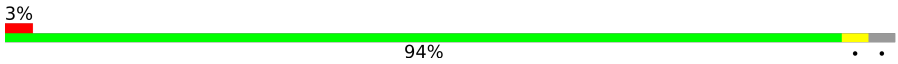
Chain l:





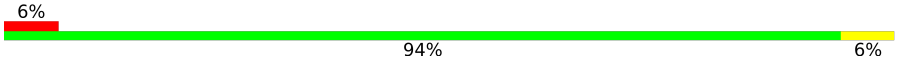
• Molecule 12: Photosystem II reaction center protein M

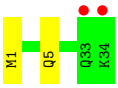
Chain M:



• Molecule 12: Photosystem II reaction center protein M

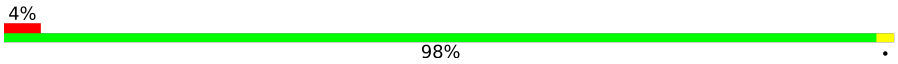
Chain m:

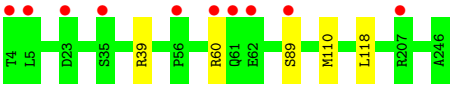




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

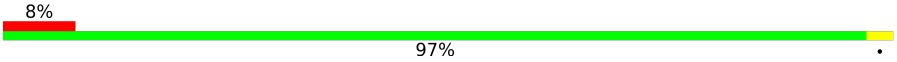
Chain O:

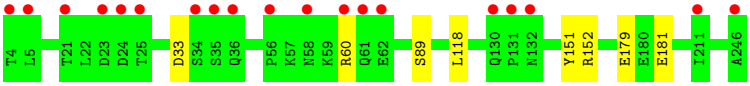




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

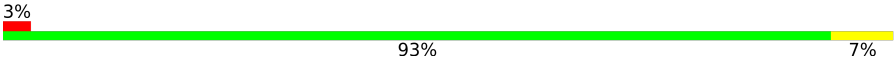




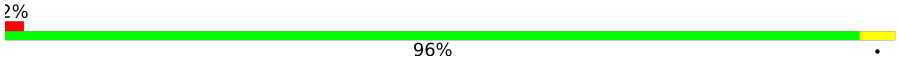
• Molecule 14: Photosystem II reaction center protein T

Chain T:

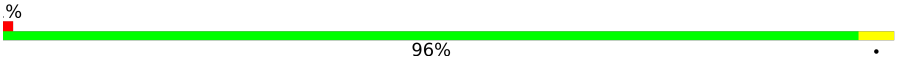
• Molecule 14: Photosystem II reaction center protein T

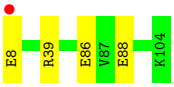
Chain t: 

• Molecule 15: Photosystem II 12 kDa extrinsic protein

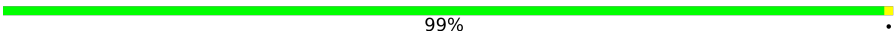
Chain U: 

• Molecule 15: Photosystem II 12 kDa extrinsic protein

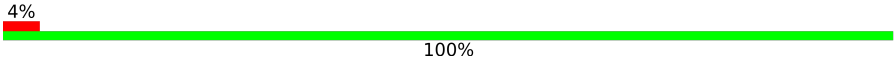
Chain u: 

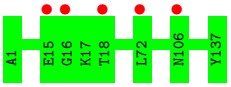


• Molecule 16: Cytochrome c-550

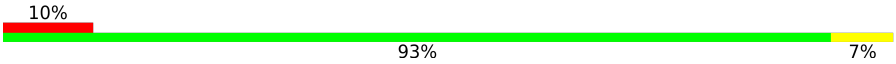
Chain V: 

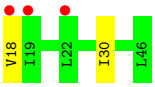
• Molecule 16: Cytochrome c-550

Chain v: 

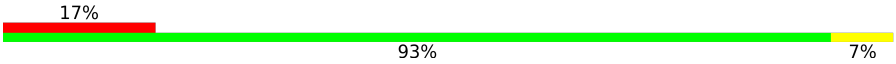


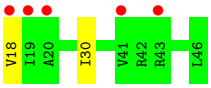
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 

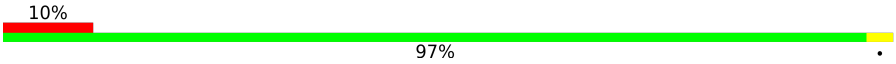


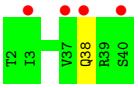
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 

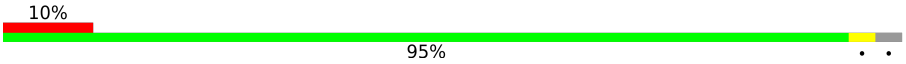


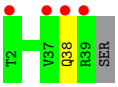
• Molecule 18: Photosystem II reaction center X protein

Chain X: 

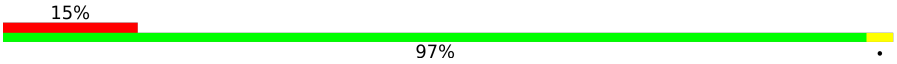


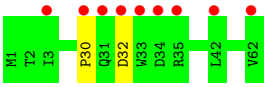
• Molecule 18: Photosystem II reaction center X protein

Chain x: 

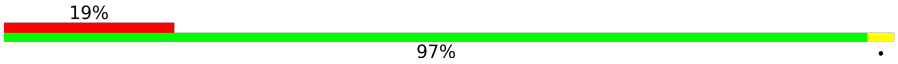


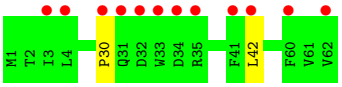
• Molecule 19: Photosystem II reaction center protein Z

Chain Z: 



• Molecule 19: 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	122.25Å 228.43Å 287.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.10) 99.5 (19.93-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.154 , 0.197 0.164 , 0.202	Depositor DCC
R_{free} test set	23043 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53800	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: FME, LHG, PL9, HTG, CA, PHO, CLA, OEX, HEM, BCR, CL, LMT, HEC, LMG, DMS, RRX, DGD, MG, HSK, BCT, FE2, UNL, GOL

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	1.01	0/2711	0.84	2/3699 (0.1%)
1	a	0.97	0/2714	0.83	2/3702 (0.1%)
2	B	0.95	1/4149 (0.0%)	0.84	9/5655 (0.2%)
2	b	0.97	3/4128 (0.1%)	0.86	7/5628 (0.1%)
3	C	0.94	2/3639 (0.1%)	0.82	2/4953 (0.0%)
3	c	0.91	1/3645 (0.0%)	0.81	7/4962 (0.1%)
4	D	0.98	0/2821	0.84	2/3843 (0.1%)
4	d	0.95	0/2813	0.84	1/3831 (0.0%)
5	E	0.87	0/684	0.87	2/935 (0.2%)
5	e	0.86	0/668	0.89	1/913 (0.1%)
6	F	0.94	0/283	0.75	0/386
6	f	0.86	0/265	0.67	0/360
7	H	0.87	0/522	0.77	0/712
7	h	0.90	0/519	0.80	0/708
8	I	0.84	0/281	0.82	0/381
8	i	0.83	0/291	0.79	0/394
9	J	0.87	0/268	0.79	0/363
9	j	0.90	0/285	0.86	0/386
10	K	0.75	0/306	0.77	0/422
10	k	0.72	0/295	0.73	0/407
11	L	1.06	0/298	0.90	1/406 (0.2%)
11	l	1.01	0/303	0.86	1/413 (0.2%)
12	M	0.93	0/257	0.75	0/352
12	m	0.95	0/262	0.86	0/359
13	O	0.89	0/1907	0.91	1/2589 (0.0%)
13	o	0.86	1/1907 (0.1%)	0.88	2/2591 (0.1%)
14	T	1.03	0/258	0.94	1/349 (0.3%)
14	t	0.96	0/258	0.89	0/349
15	U	1.04	1/796 (0.1%)	1.00	2/1078 (0.2%)
15	u	1.05	1/794 (0.1%)	0.93	2/1076 (0.2%)
16	V	0.99	0/1104	0.92	1/1498 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.91	0/1084	0.84	0/1475
17	Y	0.69	0/218	0.81	0/292
17	y	0.63	0/210	0.80	0/281
18	X	0.80	0/295	0.73	0/399
18	x	0.77	0/292	0.74	0/395
19	Z	0.75	0/476	0.71	0/652
19	z	0.65	0/470	0.69	1/645 (0.2%)
All	All	0.94	10/42476 (0.0%)	0.84	47/57839 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	88	GLU	CD-OE2	7.36	1.33	1.25
2	B	36	SER	CB-OG	-6.90	1.33	1.42
3	c	389	GLU	CD-OE2	6.24	1.32	1.25
3	C	389[A]	GLU	CD-OE2	6.18	1.32	1.25
3	C	389[B]	GLU	CD-OE2	6.18	1.32	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	57	ARG	NE-CZ-NH1	7.50	124.05	120.30
13	O	39	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	c	391[A]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
3	c	391[B]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	B	57	ARG	NE-CZ-NH1	6.45	123.52	120.30

There are no chirality outliers.

There are no planarity outliers.

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	334/334 (100%)	328 (98%)	5 (2%)	1 (0%)	41	41
1	a	334/334 (100%)	327 (98%)	6 (2%)	1 (0%)	41	41
2	B	508/505 (101%)	501 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	498 (98%)	8 (2%)	0	100	100
3	C	454/455 (100%)	444 (98%)	9 (2%)	1 (0%)	47	49
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	47	49
4	D	341/342 (100%)	336 (98%)	5 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	80/81 (99%)	78 (98%)	2 (2%)	0	100	100
5	e	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	56 (90%)	6 (10%)	0	100	100
7	h	62/63 (98%)	57 (92%)	4 (6%)	1 (2%)	9	5
8	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
8	i	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
9	J	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/36 (97%)	34 (97%)	0	1 (3%)	4	1
11	l	35/36 (97%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	239 (98%)	5 (2%)	1 (0%)	34	32
13	o	247/243 (102%)	240 (97%)	6 (2%)	1 (0%)	34	32
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
15	u	96/97 (99%)	93 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	28/29 (97%)	27 (96%)	1 (4%)	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	5227/5270 (99%)	5106 (98%)	111 (2%)	10 (0%)	47	49

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	L	3	PRO
3	C	416	SER
3	c	416	SER
13	O	60	ARG
19	Z	30	PRO

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	269/270 (100%)	266 (99%)	3 (1%)	73	79
1	a	270/270 (100%)	267 (99%)	3 (1%)	73	79
2	B	404/403 (100%)	403 (100%)	1 (0%)	93	96
2	b	402/403 (100%)	399 (99%)	3 (1%)	84	88
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	73
3	c	356/356 (100%)	349 (98%)	7 (2%)	55	60
4	D	277/276 (100%)	273 (99%)	4 (1%)	67	73
4	d	276/276 (100%)	273 (99%)	3 (1%)	73	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/72 (100%)	69 (96%)	3 (4%)	30	30
5	e	68/72 (94%)	67 (98%)	1 (2%)	65	71
6	F	27/28 (96%)	25 (93%)	2 (7%)	13	10
6	f	26/28 (93%)	26 (100%)	0	100	100
7	H	54/53 (102%)	53 (98%)	1 (2%)	57	63
7	h	54/53 (102%)	53 (98%)	1 (2%)	57	63
8	I	30/33 (91%)	30 (100%)	0	100	100
8	i	31/33 (94%)	31 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	28/30 (93%)	26 (93%)	2 (7%)	14	11
11	L	32/34 (94%)	32 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	29/30 (97%)	29 (100%)	0	100	100
12	m	29/30 (97%)	28 (97%)	1 (3%)	37	39
13	O	205/206 (100%)	202 (98%)	3 (2%)	65	71
13	o	203/206 (98%)	199 (98%)	4 (2%)	55	60
14	T	26/26 (100%)	25 (96%)	1 (4%)	33	34
14	t	26/26 (100%)	25 (96%)	1 (4%)	33	34
15	U	85/84 (101%)	82 (96%)	3 (4%)	36	38
15	u	85/84 (101%)	83 (98%)	2 (2%)	49	53
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100
17	Y	22/22 (100%)	20 (91%)	2 (9%)	9	6
17	y	20/22 (91%)	18 (90%)	2 (10%)	7	5
18	X	31/32 (97%)	30 (97%)	1 (3%)	39	41
18	x	32/32 (100%)	31 (97%)	1 (3%)	40	43
19	Z	49/52 (94%)	48 (98%)	1 (2%)	55	60
19	z	47/52 (90%)	47 (100%)	0	100	100
All	All	4268/4304 (99%)	4207 (99%)	61 (1%)	67	73

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	X	38	GLN
14	t	25	GLU
2	b	362	PHE
13	o	181	GLU
17	y	30	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	179	GLN
13	o	104	GLN
2	b	289	GLN
16	v	34	GLN
3	c	228	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 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	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	1.32	1 (12%)	7,9,11	1.19	0
8	FME	i	1	8	8,9,10	0.35	0	7,9,11	1.72	2 (28%)
14	FME	T	1	14	8,9,10	0.75	0	7,9,11	1.63	2 (28%)
8	FME	I	1	8	8,9,10	0.72	0	7,9,11	1.81	3 (42%)
12	FME	m	1	12	8,9,10	1.09	1 (12%)	7,9,11	1.01	0
4	HSK	d	336[B]	-	7,11,12	1.34	1 (14%)	3,14,16	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HSK	D	336[B]	-	7,11,12	2.26	1 (14%)	3,14,16	1.56	1 (33%)
4	HSK	d	336[A]	-	7,10,12	1.30	1 (14%)	3,12,16	1.35	0
4	HSK	D	336[A]	-	7,10,12	1.36	1 (14%)	3,12,16	1.89	1 (33%)
14	FME	t	1	14	8,9,10	0.83	0	7,9,11	1.38	1 (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
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	t	1	14	-	3/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	CE1-ND1	-5.83	1.29	1.36
4	D	336[A]	HSK	CE1-ND1	-3.39	1.32	1.36
4	d	336[B]	HSK	CE1-ND1	-3.15	1.32	1.36
4	d	336[A]	HSK	CE1-ND1	-2.72	1.33	1.36
12	M	1	FME	CA-N	2.32	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	3.30	115.69	109.73
8	I	1	FME	C-CA-N	3.12	115.36	109.73
4	D	336[A]	HSK	CD2-NE2-CE1	2.67	109.94	105.78
4	D	336[B]	HSK	CD2-NE2-CE1	2.39	109.50	105.78
8	I	1	FME	O-C-CA	-2.30	118.74	124.78

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE

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 353 ligands modelled in this entry, 18 are monoatomic and 52 are unknown - leaving 283 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	PHO	D	404	-	51,69,69	1.84	9 (17%)	47,99,99	1.25	6 (12%)
29	DMS	B	633	-	3,3,3	2.55	1 (33%)	3,3,3	0.98	0
22	CLA	b	611	41	65,73,73	1.81	15 (23%)	76,113,113	2.29	24 (31%)
22	CLA	b	614	41	65,73,73	1.76	17 (26%)	76,113,113	2.10	24 (31%)
32	HTG	B	629	-	19,19,19	0.97	2 (10%)	23,24,24	1.46	3 (13%)
26	LMG	b	625	-	49,49,55	1.23	3 (6%)	57,57,63	1.18	6 (10%)
37	HEM	F	101	5,6	41,50,50	1.74	7 (17%)	45,82,82	1.92	12 (26%)
36	BCT	d	401[A]	35	2,3,3	0.58	0	2,3,3	1.26	0
22	CLA	c	508	41	65,73,73	2.08	20 (30%)	76,113,113	2.41	22 (28%)
22	CLA	b	608	-	65,73,73	2.05	17 (26%)	76,113,113	2.50	27 (35%)
22	CLA	C	505	-	65,73,73	2.00	19 (29%)	76,113,113	2.20	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	PL9	d	407	-	55,55,55	1.17	9 (16%)	68,69,69	1.47	9 (13%)
22	CLA	c	505	41	65,73,73	2.23	19 (29%)	76,113,113	2.32	27 (35%)
29	DMS	D	420	-	3,3,3	2.61	1 (33%)	3,3,3	0.95	0
29	DMS	b	638	-	3,3,3	3.10	1 (33%)	3,3,3	1.05	0
29	DMS	o	303	-	3,3,3	1.94	1 (33%)	3,3,3	0.78	0
22	CLA	B	613	-	65,73,73	1.89	11 (16%)	76,113,113	2.30	24 (31%)
28	LMT	B	623	-	36,36,36	0.80	1 (2%)	47,47,47	1.68	10 (21%)
32	HTG	c	541	-	15,15,19	1.17	1 (6%)	18,20,24	3.42	6 (33%)
29	DMS	c	530	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
29	DMS	c	532	-	3,3,3	2.72	1 (33%)	3,3,3	0.89	0
22	CLA	B	610	-	65,73,73	1.88	14 (21%)	76,113,113	2.16	21 (27%)
29	DMS	C	530	-	3,3,3	2.06	1 (33%)	3,3,3	0.70	0
22	CLA	B	603	-	65,73,73	2.22	16 (24%)	76,113,113	2.23	24 (31%)
22	CLA	b	606	-	65,73,73	1.99	15 (23%)	76,113,113	2.31	30 (39%)
24	BCR	b	621	-	41,41,41	0.87	1 (2%)	56,56,56	1.47	9 (16%)
24	BCR	B	619	-	41,41,41	1.30	5 (12%)	56,56,56	1.43	7 (12%)
29	DMS	c	540	-	3,3,3	2.84	1 (33%)	3,3,3	0.97	0
29	DMS	u	204	-	3,3,3	2.75	1 (33%)	3,3,3	1.02	0
22	CLA	b	619	-	65,73,73	2.15	17 (26%)	76,113,113	2.45	29 (38%)
32	HTG	D	413	-	16,16,19	1.08	2 (12%)	20,21,24	2.53	6 (30%)
22	CLA	A	408	-	65,73,73	2.07	17 (26%)	76,113,113	2.28	22 (28%)
28	LMT	b	626	-	25,25,36	0.96	1 (4%)	30,30,47	1.57	3 (10%)
29	DMS	c	538	-	3,3,3	3.04	1 (33%)	3,3,3	1.05	0
26	LMG	d	412	39	47,47,55	0.99	3 (6%)	55,55,63	1.30	5 (9%)
32	HTG	O	302	-	19,19,19	1.64	4 (21%)	23,24,24	1.26	3 (13%)
22	CLA	d	405	-	65,73,73	2.12	18 (27%)	76,113,113	2.20	26 (34%)
22	CLA	b	617	-	65,73,73	1.89	14 (21%)	76,113,113	2.00	23 (30%)
29	DMS	o	305	-	3,3,3	2.67	1 (33%)	3,3,3	0.74	0
29	DMS	B	635	-	3,3,3	2.80	1 (33%)	3,3,3	0.64	0
29	DMS	O	304	-	3,3,3	2.65	1 (33%)	3,3,3	0.68	0
34	GOL	c	533	-	5,5,5	0.52	0	5,5,5	0.97	0
24	BCR	y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.71	14 (25%)
23	PHO	d	404	-	51,69,69	1.73	7 (13%)	47,99,99	1.66	5 (10%)
28	LMT	M	101	-	36,36,36	0.66	0	47,47,47	1.37	6 (12%)
29	DMS	D	416	-	3,3,3	2.65	1 (33%)	3,3,3	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	DMS	d	415	-	3,3,3	2.34	1 (33%)	3,3,3	0.81	0
29	DMS	O	307	-	3,3,3	2.72	1 (33%)	3,3,3	0.40	0
29	DMS	o	311	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
22	CLA	C	506	-	65,73,73	2.03	14 (21%)	76,113,113	2.44	20 (26%)
31	LHG	E	101	-	48,48,48	1.04	2 (4%)	51,54,54	0.94	2 (3%)
26	LMG	C	518	-	49,49,55	1.07	2 (4%)	57,57,63	1.25	7 (12%)
29	DMS	b	631	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
29	DMS	B	631	-	3,3,3	2.87	1 (33%)	3,3,3	0.91	0
29	DMS	a	416	-	3,3,3	2.85	1 (33%)	3,3,3	1.15	0
29	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.44	0
22	CLA	c	503	-	65,73,73	2.00	15 (23%)	76,113,113	2.19	26 (34%)
29	DMS	u	202	-	3,3,3	2.76	1 (33%)	3,3,3	1.44	0
29	DMS	o	310	-	3,3,3	2.89	1 (33%)	3,3,3	1.04	0
29	DMS	O	312	-	3,3,3	2.72	1 (33%)	3,3,3	0.68	0
24	BCR	b	623	-	41,41,41	1.17	4 (9%)	56,56,56	1.40	9 (16%)
29	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	1.71	1 (33%)
29	DMS	A	418	-	3,3,3	2.66	1 (33%)	3,3,3	1.18	0
26	LMG	c	520	-	38,38,55	1.29	2 (5%)	46,46,63	1.33	5 (10%)
32	HTG	U	203	-	14,14,19	0.99	1 (7%)	18,19,24	2.78	8 (44%)
22	CLA	c	513	-	65,73,73	2.20	18 (27%)	76,113,113	2.18	24 (31%)
29	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.67	0
22	CLA	C	510	-	65,73,73	2.04	20 (30%)	76,113,113	2.19	18 (23%)
29	DMS	O	305	-	3,3,3	2.90	1 (33%)	3,3,3	1.17	0
20	OEX	A	401	1,3,41	0,15,15	-	-	-		
22	CLA	B	617	-	65,73,73	1.98	17 (26%)	76,113,113	2.39	28 (36%)
29	DMS	B	641	-	3,3,3	2.83	1 (33%)	3,3,3	1.00	0
28	LMT	j	102	-	23,23,36	0.89	0	27,27,47	1.94	6 (22%)
36	BCT	D	402[A]	35	2,3,3	0.45	0	2,3,3	0.63	0
32	HTG	c	524	-	8,8,19	0.55	0	7,7,24	1.33	1 (14%)
29	DMS	O	310	-	3,3,3	2.71	1 (33%)	3,3,3	0.89	0
29	DMS	O	303	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
22	CLA	c	512	3	65,73,73	2.60	18 (27%)	76,113,113	2.20	21 (27%)
29	DMS	v	204	-	3,3,3	2.69	1 (33%)	3,3,3	1.08	0
22	CLA	C	511	3	65,73,73	2.42	16 (24%)	76,113,113	2.49	23 (30%)
29	DMS	A	417	-	3,3,3	2.02	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	LMT	F	102	-	24,24,36	1.31	3 (12%)	29,29,47	1.44	6 (20%)
29	DMS	C	531	-	3,3,3	2.72	1 (33%)	3,3,3	0.72	0
29	DMS	O	309	-	3,3,3	2.76	1 (33%)	3,3,3	0.91	0
29	DMS	c	535	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
29	DMS	c	539	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
29	DMS	o	306	-	3,3,3	2.55	1 (33%)	3,3,3	1.00	0
29	DMS	o	308	-	3,3,3	2.81	1 (33%)	3,3,3	0.41	0
32	HTG	o	301	-	19,19,19	1.94	3 (15%)	23,24,24	1.78	7 (30%)
26	LMG	C	519	-	48,48,55	1.29	3 (6%)	56,56,63	1.79	12 (21%)
29	DMS	C	526	-	3,3,3	2.76	1 (33%)	3,3,3	1.19	0
29	DMS	B	640	-	3,3,3	3.00	1 (33%)	3,3,3	1.33	1 (33%)
32	HTG	b	627	-	19,19,19	0.98	1 (5%)	23,24,24	2.00	4 (17%)
22	CLA	c	510	-	65,73,73	2.13	16 (24%)	76,113,113	2.42	26 (34%)
29	DMS	c	536	-	3,3,3	2.69	1 (33%)	3,3,3	1.07	0
22	CLA	C	513	-	65,73,73	2.74	17 (26%)	76,113,113	2.11	23 (30%)
31	LHG	d	410	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	5 (9%)
22	CLA	B	614	-	65,73,73	2.06	16 (24%)	76,113,113	2.12	20 (26%)
32	HTG	B	642	-	18,18,19	1.11	2 (11%)	22,23,24	2.72	10 (45%)
22	CLA	b	618	-	65,73,73	2.01	19 (29%)	76,113,113	2.50	29 (38%)
26	LMG	c	521	-	51,51,55	1.15	3 (5%)	59,59,63	1.12	7 (11%)
29	DMS	I	105	-	3,3,3	2.69	1 (33%)	3,3,3	1.03	0
29	DMS	B	639	-	3,3,3	2.59	1 (33%)	3,3,3	0.95	0
31	LHG	b	624	-	48,48,48	0.75	2 (4%)	51,54,54	1.10	5 (9%)
29	DMS	h	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
22	CLA	c	507	-	65,73,73	1.90	14 (21%)	76,113,113	2.37	24 (31%)
34	GOL	b	636	-	5,5,5	0.09	0	5,5,5	0.40	0
29	DMS	C	528	-	3,3,3	2.55	1 (33%)	3,3,3	0.52	0
24	BCR	B	620	-	41,41,41	1.24	3 (7%)	56,56,56	1.34	9 (16%)
31	LHG	D	411	-	43,43,48	1.12	3 (6%)	46,49,54	1.08	4 (8%)
22	CLA	b	607	-	65,73,73	1.88	15 (23%)	76,113,113	2.25	22 (28%)
22	CLA	C	507	41	65,73,73	2.30	22 (33%)	76,113,113	2.18	16 (21%)
23	PHO	a	408	-	51,69,69	1.73	9 (17%)	47,99,99	1.10	4 (8%)
24	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.90	18 (32%)
32	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.98	2 (8%)
29	DMS	B	632	-	3,3,3	2.43	1 (33%)	3,3,3	1.58	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	DMS	a	418	-	3,3,3	2.79	1 (33%)	3,3,3	0.71	0
33	DGD	d	408	-	48,48,67	1.37	5 (10%)	56,56,81	1.58	8 (14%)
28	LMT	A	415	-	36,36,36	1.33	4 (11%)	47,47,47	1.97	15 (31%)
22	CLA	B	605	-	65,73,73	1.90	16 (24%)	76,113,113	2.36	30 (39%)
22	CLA	B	607	-	65,73,73	2.19	18 (27%)	76,113,113	2.14	22 (28%)
32	HTG	V	202	-	19,19,19	1.02	2 (10%)	23,24,24	3.35	7 (30%)
28	LMT	a	401	-	36,36,36	1.26	3 (8%)	47,47,47	2.27	16 (34%)
22	CLA	b	613	-	65,73,73	2.17	19 (29%)	76,113,113	2.05	20 (26%)
22	CLA	c	511	-	65,73,73	1.84	15 (23%)	76,113,113	2.50	27 (35%)
29	DMS	e	105	-	3,3,3	2.74	1 (33%)	3,3,3	1.02	0
29	DMS	o	304	-	3,3,3	2.57	1 (33%)	3,3,3	1.49	0
22	CLA	c	509	-	65,73,73	2.33	17 (26%)	76,113,113	2.14	19 (25%)
29	DMS	b	635	-	3,3,3	2.89	1 (33%)	3,3,3	0.94	0
22	CLA	D	403	-	65,73,73	1.94	18 (27%)	76,113,113	2.24	21 (27%)
29	DMS	C	525	-	3,3,3	2.47	1 (33%)	3,3,3	1.10	0
29	DMS	A	419	-	3,3,3	2.96	1 (33%)	3,3,3	0.81	0
24	BCR	K	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.36	10 (17%)
33	DGD	D	408	-	45,45,67	1.49	4 (8%)	53,53,81	1.70	10 (18%)
29	DMS	v	203	-	3,3,3	2.51	1 (33%)	3,3,3	0.76	0
40	HEC	V	201	16	32,50,50	2.02	6 (18%)	24,82,82	1.70	6 (25%)
24	BCR	K	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	3 (5%)
32	HTG	C	536	-	19,19,19	1.22	2 (10%)	23,24,24	1.82	1 (4%)
33	DGD	h	101	-	63,63,67	1.20	4 (6%)	77,77,81	1.43	15 (19%)
34	GOL	e	104	-	5,5,5	0.82	0	5,5,5	1.63	1 (20%)
26	LMG	D	412	39	47,47,55	1.05	3 (6%)	55,55,63	1.14	3 (5%)
29	DMS	o	307	-	3,3,3	2.70	1 (33%)	3,3,3	1.24	0
24	BCR	C	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	4 (7%)
24	BCR	c	516	-	41,41,41	1.11	3 (7%)	56,56,56	1.37	8 (14%)
29	DMS	D	415	-	3,3,3	2.59	1 (33%)	3,3,3	1.23	0
24	BCR	A	409	-	41,41,41	1.44	8 (19%)	56,56,56	1.55	7 (12%)
24	BCR	T	101	-	41,41,41	0.95	0	56,56,56	1.79	14 (25%)
29	DMS	a	420	-	3,3,3	2.81	1 (33%)	3,3,3	1.07	0
29	DMS	b	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.54	0
29	DMS	B	638	-	3,3,3	2.31	1 (33%)	3,3,3	1.19	0
29	DMS	b	632	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	d	402	-	65,73,73	1.82	15 (23%)	76,113,113	2.03	25 (32%)
28	LMT	z	101	-	33,33,36	8.08	2 (6%)	44,44,47	2.76	11 (25%)
29	DMS	c	529	-	3,3,3	2.92	1 (33%)	3,3,3	0.89	0
29	DMS	U	202	-	3,3,3	2.61	1 (33%)	3,3,3	1.60	1 (33%)
29	DMS	v	206	-	3,3,3	2.65	1 (33%)	3,3,3	1.12	0
29	DMS	C	529	-	3,3,3	2.64	1 (33%)	3,3,3	0.81	0
38	RRX	h	102	-	42,42,42	0.98	2 (4%)	57,58,58	1.61	11 (19%)
22	CLA	b	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.60	24 (31%)
34	GOL	D	417	-	5,5,5	0.48	0	5,5,5	0.47	0
29	DMS	D	419	-	3,3,3	2.73	1 (33%)	3,3,3	0.68	0
28	LMT	m	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.03	3 (10%)
28	LMT	c	522	-	36,36,36	0.98	1 (2%)	47,47,47	1.92	10 (21%)
22	CLA	A	406	41	65,73,73	1.65	17 (26%)	76,113,113	2.13	21 (27%)
29	DMS	b	630	-	3,3,3	1.99	1 (33%)	3,3,3	0.40	0
32	HTG	C	535	-	8,8,19	0.55	0	7,7,24	1.05	1 (14%)
29	DMS	B	637	-	3,3,3	2.59	1 (33%)	3,3,3	1.10	0
25	PL9	D	407	-	55,55,55	1.11	6 (10%)	68,69,69	1.47	7 (10%)
31	LHG	d	411	-	43,43,48	1.03	3 (6%)	46,49,54	0.99	5 (10%)
32	HTG	B	628	-	19,19,19	0.49	0	23,24,24	1.76	2 (8%)
22	CLA	B	604	-	65,73,73	1.69	12 (18%)	76,113,113	2.64	28 (36%)
22	CLA	B	608	41	65,73,73	1.77	14 (21%)	76,113,113	2.06	21 (27%)
29	DMS	d	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.95	0
28	LMT	Z	101	-	36,36,36	0.84	2 (5%)	47,47,47	1.46	7 (14%)
22	CLA	a	409	-	65,73,73	1.70	14 (21%)	76,113,113	2.28	20 (26%)
28	LMT	t	102	-	24,24,36	1.12	2 (8%)	29,29,47	1.45	5 (17%)
22	CLA	C	502	-	65,73,73	2.08	15 (23%)	76,113,113	2.40	23 (30%)
29	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	1.60	1 (33%)
22	CLA	A	404	-	65,73,73	1.83	15 (23%)	76,113,113	2.27	23 (30%)
29	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	1.11	0
31	LHG	D	410	-	48,48,48	0.79	3 (6%)	51,54,54	1.07	2 (3%)
20	OEX	a	402	1,3,41	0,15,15	-	-	-		
32	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	2.08	2 (8%)
32	HTG	c	523	-	19,19,19	0.70	0	23,24,24	1.49	3 (13%)
25	PL9	A	410	-	55,55,55	1.15	4 (7%)	68,69,69	2.12	17 (25%)
29	DMS	b	633	-	3,3,3	2.76	1 (33%)	3,3,3	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	LMT	J	102	-	24,24,36	0.80	1 (4%)	29,29,47	1.23	3 (10%)
33	DGD	C	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.17	9 (11%)
29	DMS	V	207	-	3,3,3	2.81	1 (33%)	3,3,3	0.56	0
22	CLA	B	609	-	65,73,73	1.92	15 (23%)	76,113,113	2.38	22 (28%)
22	CLA	c	506	-	65,73,73	1.98	20 (30%)	76,113,113	2.15	25 (32%)
22	CLA	B	612	-	65,73,73	1.94	14 (21%)	76,113,113	2.44	24 (31%)
22	CLA	b	605	41	65,73,73	2.20	16 (24%)	76,113,113	2.48	28 (36%)
22	CLA	c	514	-	65,73,73	2.09	17 (26%)	76,113,113	2.22	26 (34%)
22	CLA	A	405	41	65,73,73	1.99	16 (24%)	76,113,113	2.65	25 (32%)
29	DMS	b	639	-	3,3,3	2.57	1 (33%)	3,3,3	1.52	0
29	DMS	v	207	-	3,3,3	2.99	1 (33%)	3,3,3	1.23	1 (33%)
22	CLA	C	503	-	65,73,73	1.98	16 (24%)	76,113,113	2.09	24 (31%)
22	CLA	b	615	-	65,73,73	1.82	13 (20%)	76,113,113	1.96	22 (28%)
24	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	6 (10%)
29	DMS	C	534	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	0
29	DMS	V	208	-	3,3,3	2.49	1 (33%)	3,3,3	1.17	1 (33%)
29	DMS	V	205	-	3,3,3	2.70	1 (33%)	3,3,3	0.96	0
29	DMS	c	531	-	3,3,3	2.64	1 (33%)	3,3,3	0.66	0
29	DMS	v	205	-	3,3,3	2.46	1 (33%)	3,3,3	0.84	0
32	HTG	d	413	-	16,16,19	0.98	1 (6%)	20,21,24	3.85	6 (30%)
33	DGD	c	519	-	63,63,67	1.04	4 (6%)	77,77,81	1.38	11 (14%)
33	DGD	c	518	-	57,57,67	0.95	4 (7%)	71,71,81	1.09	7 (9%)
29	DMS	E	104	-	3,3,3	2.75	1 (33%)	3,3,3	1.00	0
33	DGD	c	517	-	63,63,67	1.05	3 (4%)	77,77,81	1.06	5 (6%)
23	PHO	A	407	-	51,69,69	1.51	8 (15%)	47,99,99	1.35	9 (19%)
28	LMT	T	102	-	24,24,36	0.57	0	29,29,47	1.55	7 (24%)
36	BCT	D	402[B]	35	2,3,3	0.63	0	2,3,3	0.78	0
24	BCR	a	410	-	41,41,41	1.05	4 (9%)	56,56,56	1.10	5 (8%)
24	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	11 (19%)
22	CLA	c	502	-	65,73,73	2.56	18 (27%)	76,113,113	2.71	23 (30%)
31	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.62	4 (7%)
32	HTG	v	208	-	16,16,19	0.92	1 (6%)	20,21,24	3.35	6 (30%)
28	LMT	m	103	-	23,23,36	0.88	0	27,27,47	1.70	2 (7%)
33	DGD	C	515	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	7 (9%)
22	CLA	B	616	-	65,73,73	2.44	19 (29%)	76,113,113	2.31	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	DMS	D	418	-	3,3,3	2.59	1 (33%)	3,3,3	1.66	0
22	CLA	B	615	-	65,73,73	2.01	13 (20%)	76,113,113	2.54	27 (35%)
28	LMT	M	102	-	24,24,36	0.82	0	29,29,47	1.27	3 (10%)
34	GOL	C	533	-	5,5,5	0.54	0	5,5,5	1.67	1 (20%)
36	BCT	d	401[B]	35	2,3,3	0.78	0	2,3,3	0.66	0
22	CLA	c	504	-	65,73,73	2.55	19 (29%)	76,113,113	2.28	17 (22%)
24	BCR	d	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.61	10 (17%)
22	CLA	B	602	41	65,73,73	2.45	19 (29%)	76,113,113	2.25	28 (36%)
22	CLA	C	512	-	65,73,73	2.26	17 (26%)	76,113,113	2.31	26 (34%)
29	DMS	c	537	-	3,3,3	2.64	1 (33%)	3,3,3	1.13	0
22	CLA	C	508	-	65,73,73	2.14	17 (26%)	76,113,113	2.11	20 (26%)
22	CLA	C	504	41	65,73,73	2.24	16 (24%)	76,113,113	2.21	17 (22%)
24	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.37	8 (14%)
28	LMT	l	101	-	24,24,36	0.83	1 (4%)	29,29,47	0.97	1 (3%)
29	DMS	A	416	-	3,3,3	2.74	1 (33%)	3,3,3	1.01	0
29	DMS	O	306	-	3,3,3	2.80	1 (33%)	3,3,3	1.14	0
32	HTG	b	601	-	19,19,19	1.08	2 (10%)	23,24,24	1.44	4 (17%)
40	HEC	v	202	16	32,50,50	2.15	9 (28%)	24,82,82	1.84	7 (29%)
22	CLA	B	606	-	65,73,73	2.16	16 (24%)	76,113,113	2.46	21 (27%)
22	CLA	b	610	-	65,73,73	2.35	15 (23%)	76,113,113	2.44	23 (30%)
33	DGD	H	101	-	63,63,67	1.22	4 (6%)	77,77,81	1.63	13 (16%)
29	DMS	C	532	-	3,3,3	3.06	1 (33%)	3,3,3	0.95	0
29	DMS	o	309	-	3,3,3	2.65	1 (33%)	3,3,3	1.45	0
22	CLA	b	612	-	65,73,73	1.93	15 (23%)	76,113,113	2.25	25 (32%)
29	DMS	V	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
33	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.00	4 (5%)
22	CLA	b	620	-	65,73,73	2.25	17 (26%)	76,113,113	2.28	26 (34%)
22	CLA	d	403	41	65,73,73	1.94	15 (23%)	76,113,113	2.26	24 (31%)
29	DMS	a	417	-	3,3,3	2.82	1 (33%)	3,3,3	1.16	0
37	HEM	f	101	5,6	41,50,50	2.00	8 (19%)	45,82,82	1.58	9 (20%)
22	CLA	a	407	41	65,73,73	1.93	19 (29%)	76,113,113	2.54	23 (30%)
22	CLA	C	501	-	65,73,73	1.91	15 (23%)	76,113,113	2.79	26 (34%)
26	LMG	B	622	-	51,51,55	1.01	3 (5%)	59,59,63	1.26	7 (11%)
29	DMS	B	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0
22	CLA	a	406	-	65,73,73	1.72	16 (24%)	76,113,113	2.40	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	BCR	b	622	-	41,41,41	1.27	4 (9%)	56,56,56	1.15	4 (7%)
29	DMS	c	528	-	3,3,3	2.31	1 (33%)	3,3,3	1.49	1 (33%)
31	LHG	e	101	-	37,37,48	1.12	2 (5%)	40,42,54	0.95	2 (5%)
26	LMG	a	412	-	51,51,55	1.09	3 (5%)	59,59,63	1.05	3 (5%)
24	BCR	B	618	-	41,41,41	0.91	0	56,56,56	1.34	9 (16%)
28	LMT	C	520	-	36,36,36	0.92	1 (2%)	47,47,47	2.14	10 (21%)
29	DMS	V	204	-	3,3,3	2.63	1 (33%)	3,3,3	1.40	1 (33%)
31	LHG	f	102	-	45,45,48	1.08	2 (4%)	48,51,54	1.07	5 (10%)
32	HTG	C	521	-	19,19,19	0.80	0	23,24,24	1.74	4 (17%)
32	HTG	b	602	-	19,19,19	1.11	2 (10%)	23,24,24	1.64	3 (13%)
25	PL9	a	411	-	55,55,55	0.97	3 (5%)	68,69,69	2.26	20 (29%)
31	LHG	D	409	-	48,48,48	0.90	3 (6%)	51,54,54	1.61	6 (11%)
22	CLA	D	405	-	65,73,73	1.93	17 (26%)	76,113,113	1.93	20 (26%)
22	CLA	C	509	-	65,73,73	1.70	16 (24%)	76,113,113	2.67	30 (39%)
38	RRX	H	102	-	42,42,42	1.09	2 (4%)	57,58,58	1.51	9 (15%)
22	CLA	b	609	-	65,73,73	1.65	10 (15%)	76,113,113	2.47	22 (28%)
31	LHG	B	621	-	48,48,48	0.83	2 (4%)	51,54,54	1.31	6 (11%)
24	BCR	D	406	-	41,41,41	1.40	7 (17%)	56,56,56	1.92	15 (26%)
22	CLA	B	611	41	65,73,73	2.23	18 (27%)	76,113,113	2.15	21 (27%)
29	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.79	0
29	DMS	u	203	-	3,3,3	2.54	1 (33%)	3,3,3	1.25	0
29	DMS	a	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.73	0
29	DMS	B	636	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
32	HTG	b	640	-	17,17,19	2.71	5 (29%)	21,22,24	3.94	12 (57%)
26	LMG	A	411	-	51,51,55	1.04	2 (3%)	59,59,63	1.24	7 (11%)
28	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.53	10 (21%)
31	LHG	F	103	-	37,37,48	1.21	2 (5%)	40,43,54	1.58	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	D	404	-	-	2/37/103/103	0/5/6/6
22	CLA	b	611	41	1/1/15/20	5/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	614	41	1/1/15/20	3/37/115/115	-
32	HTG	B	629	-	-	1/10/30/30	0/1/1/1
26	LMG	b	625	-	-	14/44/64/70	0/1/1/1
37	HEM	F	101	5,6	-	3/12/54/54	-
22	CLA	c	508	41	1/1/15/20	6/37/115/115	-
22	CLA	b	608	-	1/1/15/20	4/37/115/115	-
22	CLA	C	505	-	1/1/15/20	3/37/115/115	-
25	PL9	d	407	-	-	3/53/73/73	0/1/1/1
22	CLA	c	505	41	-	5/37/115/115	-
32	HTG	c	541	-	-	3/6/26/30	0/1/1/1
22	CLA	B	613	-	1/1/15/20	3/37/115/115	-
28	LMT	B	623	-	-	7/21/61/61	0/2/2/2
22	CLA	B	610	-	1/1/15/20	1/37/115/115	-
22	CLA	B	603	-	1/1/15/20	6/37/115/115	-
22	CLA	b	606	-	1/1/15/20	6/37/115/115	-
24	BCR	b	621	-	-	2/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
22	CLA	b	619	-	1/1/15/20	5/37/115/115	-
32	HTG	D	413	-	-	2/7/27/30	0/1/1/1
22	CLA	A	408	-	-	15/37/115/115	-
28	LMT	b	626	-	-	11/17/37/61	0/1/1/2
32	HTG	O	302	-	-	4/10/30/30	0/1/1/1
26	LMG	d	412	39	-	9/42/62/70	0/1/1/1
22	CLA	d	405	-	-	12/37/115/115	-
22	CLA	b	617	-	1/1/15/20	1/37/115/115	-
34	GOL	c	533	-	-	4/4/4/4	-
24	BCR	y	101	-	-	2/29/63/63	0/2/2/2
23	PHO	d	404	-	-	1/37/103/103	0/5/6/6
28	LMT	M	101	-	-	4/21/61/61	0/2/2/2
22	CLA	C	506	-	1/1/15/20	10/37/115/115	-
31	LHG	E	101	-	-	29/53/53/53	-
26	LMG	C	518	-	-	14/44/64/70	0/1/1/1
22	CLA	c	503	-	1/1/15/20	7/37/115/115	-
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
26	LMG	c	520	-	-	9/33/53/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	U	203	-	-	2/5/25/30	0/1/1/1
22	CLA	c	513	-	1/1/15/20	10/37/115/115	-
22	CLA	C	510	-	1/1/15/20	9/37/115/115	-
22	CLA	B	617	-	1/1/15/20	10/37/115/115	-
28	LMT	j	102	-	-	8/15/31/61	0/1/1/2
32	HTG	c	524	-	-	3/6/6/30	-
22	CLA	c	512	3	1/1/15/20	1/37/115/115	-
22	CLA	C	511	3	1/1/15/20	1/37/115/115	-
28	LMT	F	102	-	-	9/15/35/61	0/1/1/2
32	HTG	o	301	-	-	4/10/30/30	0/1/1/1
26	LMG	C	519	-	-	13/43/63/70	0/1/1/1
32	HTG	b	627	-	-	6/10/30/30	0/1/1/1
22	CLA	c	510	-	1/1/15/20	11/37/115/115	-
32	HTG	B	642	-	-	5/9/29/30	0/1/1/1
22	CLA	C	513	-	-	12/37/115/115	-
31	LHG	d	410	-	-	7/53/53/53	-
22	CLA	B	614	-	1/1/15/20	8/37/115/115	-
22	CLA	b	618	-	1/1/15/20	13/37/115/115	-
26	LMG	c	521	-	-	20/46/66/70	0/1/1/1
31	LHG	b	624	-	-	21/53/53/53	-
34	GOL	b	636	-	-	2/4/4/4	-
22	CLA	c	507	-	1/1/15/20	7/37/115/115	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	LHG	D	411	-	-	14/48/48/53	-
22	CLA	b	607	-	1/1/15/20	2/37/115/115	-
22	CLA	C	507	41	1/1/15/20	8/37/115/115	-
23	PHO	a	408	-	-	5/37/103/103	0/5/6/6
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
33	DGD	d	408	-	-	12/42/62/95	0/1/1/2
28	LMT	A	415	-	-	12/21/61/61	0/2/2/2
22	CLA	B	607	-	1/1/15/20	8/37/115/115	-
22	CLA	B	605	-	-	9/37/115/115	-
32	HTG	V	202	-	-	3/10/30/30	0/1/1/1
28	LMT	a	401	-	-	9/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	613	-	-	2/37/115/115	-
22	CLA	c	511	-	1/1/15/20	9/37/115/115	-
22	CLA	c	509	-	-	4/37/115/115	-
22	CLA	D	403	-	1/1/15/20	1/37/115/115	-
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
33	DGD	D	408	-	-	20/39/59/95	0/1/1/2
40	HEC	V	201	16	-	2/10/54/54	-
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
32	HTG	C	536	-	-	3/10/30/30	0/1/1/1
33	DGD	h	101	-	-	15/51/91/95	0/2/2/2
34	GOL	e	104	-	-	1/4/4/4	-
26	LMG	D	412	39	-	12/42/62/70	0/1/1/1
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	BCR	c	516	-	-	0/29/63/63	0/2/2/2
24	BCR	A	409	-	-	1/29/63/63	0/2/2/2
24	BCR	T	101	-	-	4/29/63/63	0/2/2/2
28	LMT	z	101	-	1/1/10/10	6/18/58/61	0/2/2/2
22	CLA	d	402	-	-	4/37/115/115	-
38	RRX	h	102	-	-	0/29/65/65	0/2/2/2
22	CLA	b	616	-	1/1/15/20	4/37/115/115	-
34	GOL	D	417	-	-	3/4/4/4	-
32	HTG	C	535	-	-	3/6/6/30	-
28	LMT	m	102	-	-	8/15/35/61	0/1/1/2
28	LMT	c	522	-	-	6/21/61/61	0/2/2/2
22	CLA	A	406	41	-	4/37/115/115	-
25	PL9	D	407	-	-	1/53/73/73	0/1/1/1
31	LHG	d	411	-	-	11/48/48/53	-
32	HTG	B	628	-	-	3/10/30/30	0/1/1/1
22	CLA	B	604	-	1/1/15/20	4/37/115/115	-
22	CLA	B	608	41	1/1/15/20	6/37/115/115	-
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
22	CLA	a	409	-	1/1/15/20	12/37/115/115	-
28	LMT	t	102	-	-	9/15/35/61	0/1/1/2
22	CLA	C	502	-	-	6/37/115/115	-
22	CLA	A	404	-	1/1/15/20	5/37/115/115	-
32	HTG	B	624	-	-	3/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	D	410	-	-	6/53/53/53	-
32	HTG	c	523	-	-	5/10/30/30	0/1/1/1
25	PL9	A	410	-	-	10/53/73/73	0/1/1/1
28	LMT	J	102	-	-	8/15/35/61	0/1/1/2
33	DGD	C	517	-	-	13/51/91/95	0/2/2/2
22	CLA	c	506	-	1/1/15/20	3/37/115/115	-
22	CLA	B	609	-	-	2/37/115/115	-
22	CLA	B	612	-	-	3/37/115/115	-
22	CLA	b	605	41	1/1/15/20	17/37/115/115	-
22	CLA	c	514	-	-	13/37/115/115	-
22	CLA	A	405	41	-	6/37/115/115	-
22	CLA	C	503	-	-	3/37/115/115	-
22	CLA	b	615	-	-	5/37/115/115	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	DGD	c	519	-	-	11/51/91/95	0/2/2/2
32	HTG	d	413	-	-	2/7/27/30	0/1/1/1
33	DGD	c	518	-	-	15/45/85/95	0/2/2/2
33	DGD	c	517	-	-	14/51/91/95	0/2/2/2
23	PHO	A	407	-	-	2/37/103/103	0/5/6/6
28	LMT	T	102	-	-	6/15/35/61	0/1/1/2
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
24	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
22	CLA	c	502	-	1/1/15/20	6/37/115/115	-
31	LHG	d	409	-	-	11/53/53/53	-
32	HTG	v	208	-	-	3/7/27/30	0/1/1/1
28	LMT	m	103	-	-	6/15/31/61	0/1/1/2
33	DGD	C	515	-	-	16/51/91/95	0/2/2/2
22	CLA	B	616	-	1/1/15/20	9/37/115/115	-
22	CLA	B	615	-	1/1/15/20	11/37/115/115	-
28	LMT	M	102	-	-	6/15/35/61	0/1/1/2
34	GOL	C	533	-	-	2/4/4/4	-
22	CLA	c	504	-	-	2/37/115/115	-
24	BCR	d	406	-	-	2/29/63/63	0/2/2/2
22	CLA	B	602	41	1/1/15/20	14/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	512	-	1/1/15/20	7/37/115/115	-
22	CLA	C	508	-	1/1/15/20	4/37/115/115	-
22	CLA	C	504	41	1/1/15/20	9/37/115/115	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
28	LMT	l	101	-	-	6/15/35/61	0/1/1/2
32	HTG	b	601	-	-	4/10/30/30	0/1/1/1
40	HEC	v	202	16	-	2/10/54/54	-
22	CLA	B	606	-	1/1/15/20	7/37/115/115	-
22	CLA	b	610	-	1/1/15/20	9/37/115/115	-
33	DGD	H	101	-	-	12/51/91/95	0/2/2/2
22	CLA	b	612	-	-	2/37/115/115	-
33	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	b	620	-	1/1/15/20	15/37/115/115	-
22	CLA	d	403	41	-	5/37/115/115	-
37	HEM	f	101	5,6	-	4/12/54/54	-
22	CLA	a	407	41	-	11/37/115/115	-
22	CLA	C	501	-	1/1/15/20	4/37/115/115	-
26	LMG	B	622	-	-	12/46/66/70	0/1/1/1
22	CLA	a	406	-	1/1/15/20	4/37/115/115	-
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
31	LHG	e	101	-	-	18/41/41/53	-
26	LMG	a	412	-	-	14/46/66/70	0/1/1/1
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	LMT	C	520	-	1/1/10/10	13/21/61/61	0/2/2/2
31	LHG	f	102	-	-	16/50/50/53	-
32	HTG	C	521	-	-	3/10/30/30	0/1/1/1
32	HTG	b	602	-	-	1/10/30/30	0/1/1/1
25	PL9	a	411	-	-	10/53/73/73	0/1/1/1
31	LHG	D	409	-	-	10/53/53/53	-
22	CLA	D	405	-	1/1/15/20	7/37/115/115	-
22	CLA	C	509	-	1/1/15/20	8/37/115/115	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
22	CLA	b	609	-	1/1/15/20	2/37/115/115	-
31	LHG	B	621	-	-	14/53/53/53	-
24	BCR	D	406	-	-	2/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	611	41	1/1/15/20	3/37/115/115	-
32	HTG	b	640	-	-	4/8/28/30	0/1/1/1
26	LMG	A	411	-	-	23/46/66/70	0/1/1/1
28	LMT	m	101	-	-	6/21/61/61	0/2/2/2
31	LHG	F	103	-	-	15/42/42/53	-

The worst 5 of 1535 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	z	101	LMT	C2-C1	46.12	3.47	1.51
22	C	513	CLA	MG-NA	14.53	2.40	2.06
22	c	512	CLA	MG-NA	13.25	2.37	2.06
22	c	504	CLA	MG-NA	12.94	2.37	2.06
22	C	511	CLA	MG-NA	12.29	2.35	2.06

The worst 5 of 2403 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	413	HTG	C1'-S1-C1	13.68	125.67	100.09
32	c	541	HTG	C1'-S1-C1	12.83	124.08	100.09
22	c	504	CLA	C4A-NA-C1A	11.98	112.09	106.71
22	B	616	CLA	C4A-NA-C1A	11.74	111.99	106.71
32	V	202	HTG	O5-C1-C2	-11.63	95.69	110.31

5 of 52 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	606	CLA	ND

5 of 1209 torsion outliers are listed below:

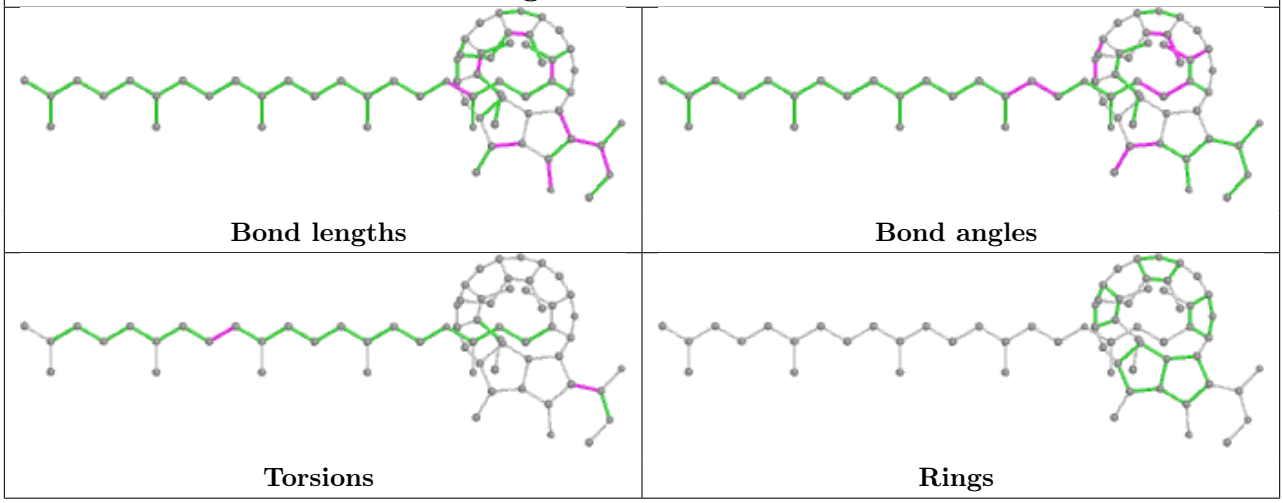
Mol	Chain	Res	Type	Atoms
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	408	CLA	C4-C3-C5-C6
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	C11-C10-C8-C9
22	B	606	CLA	C4-C3-C5-C6

There are no ring outliers.

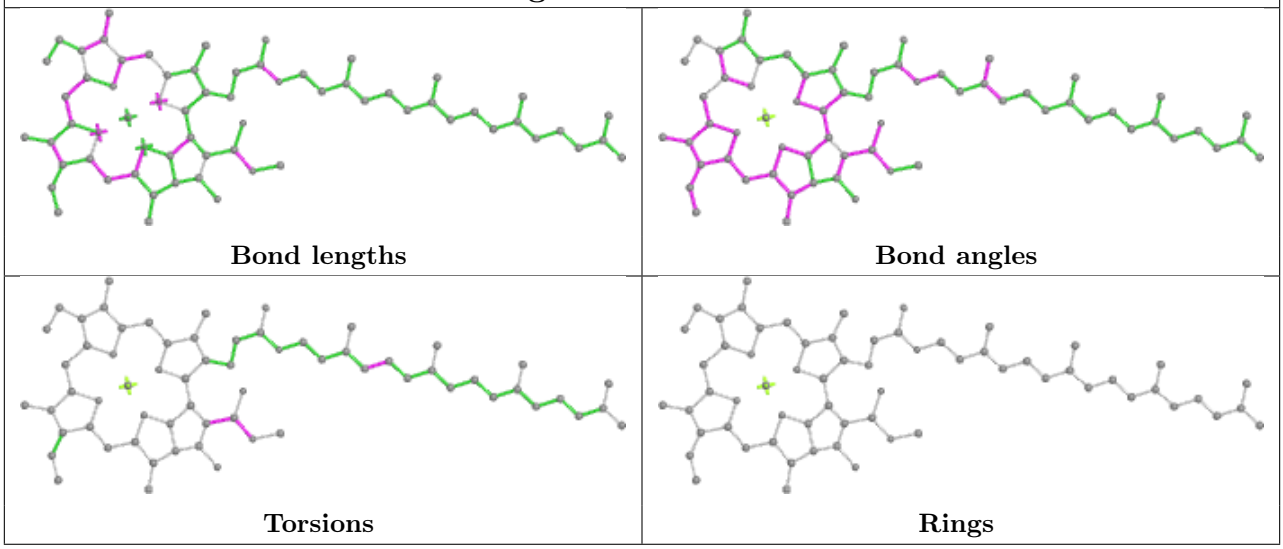
No monomer is involved in short contacts.

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

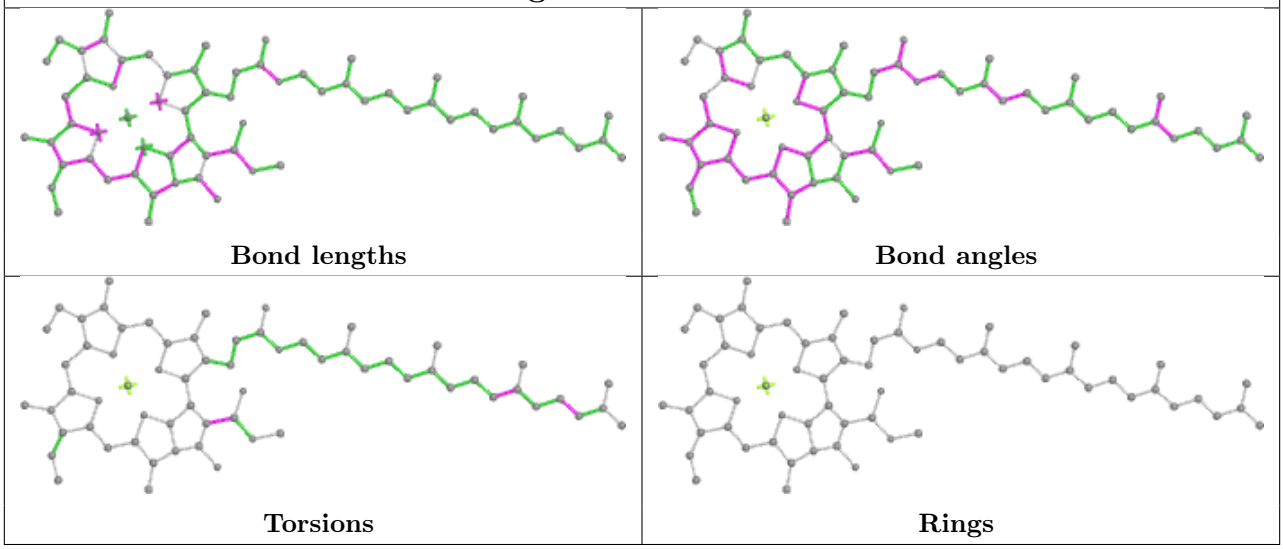
Ligand PHO D 404



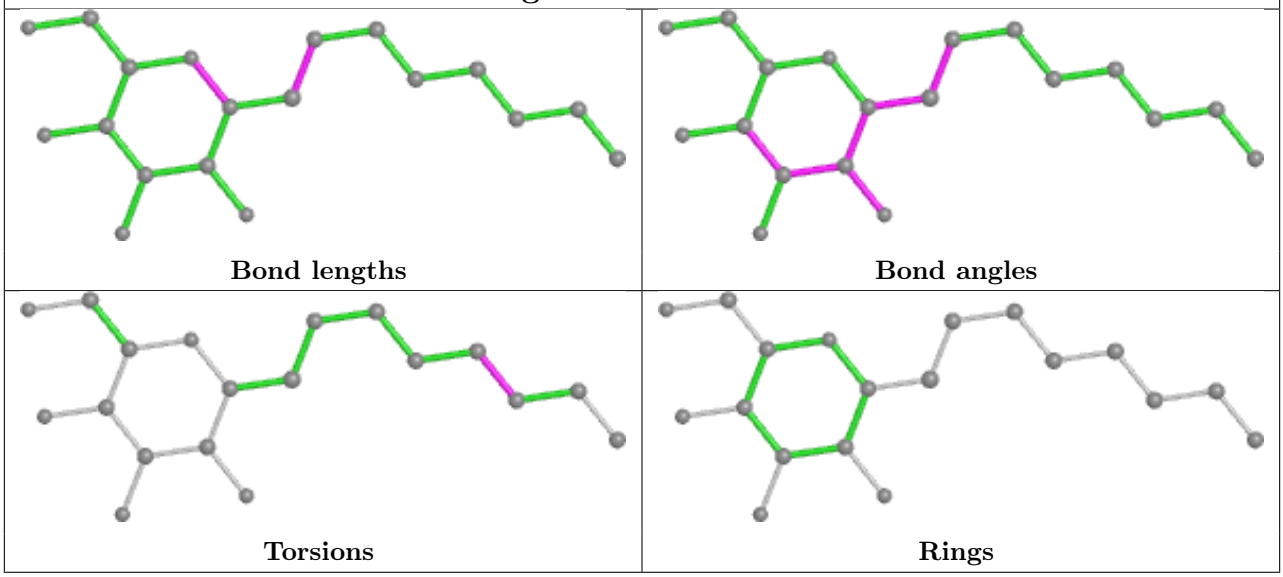
Ligand CLA b 611



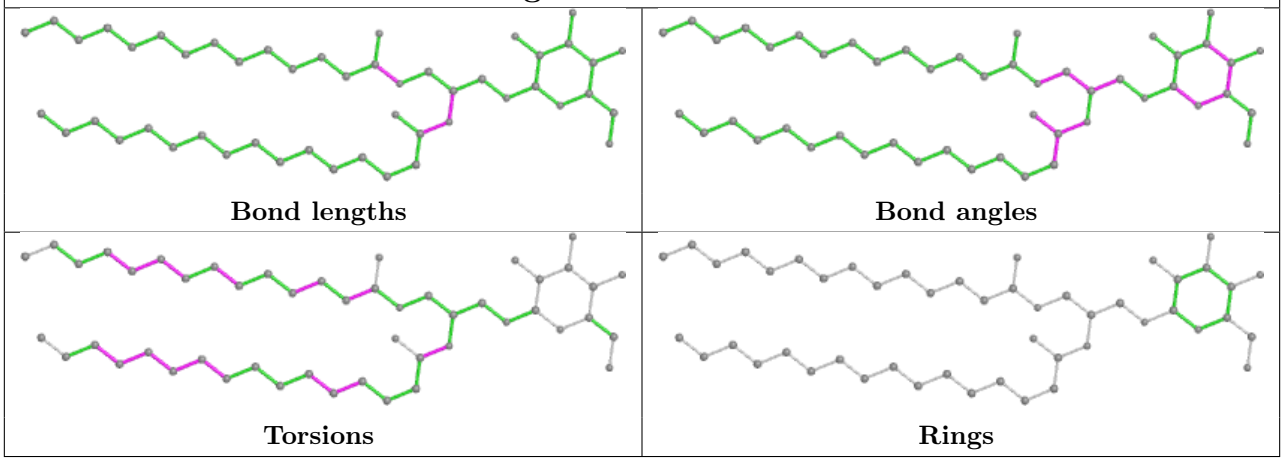
Ligand CLA b 614



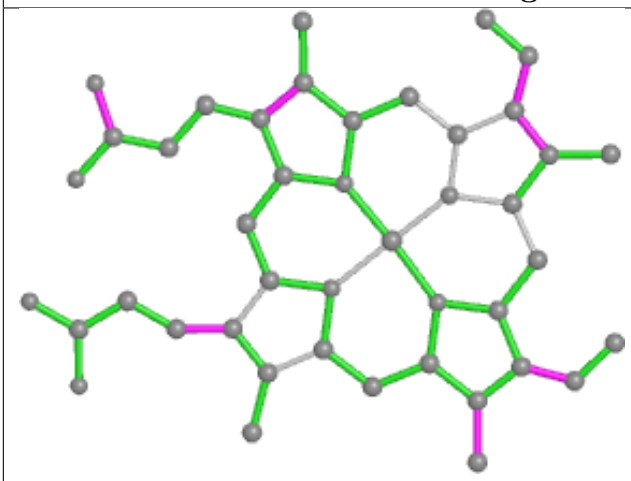
Ligand HTG B 629



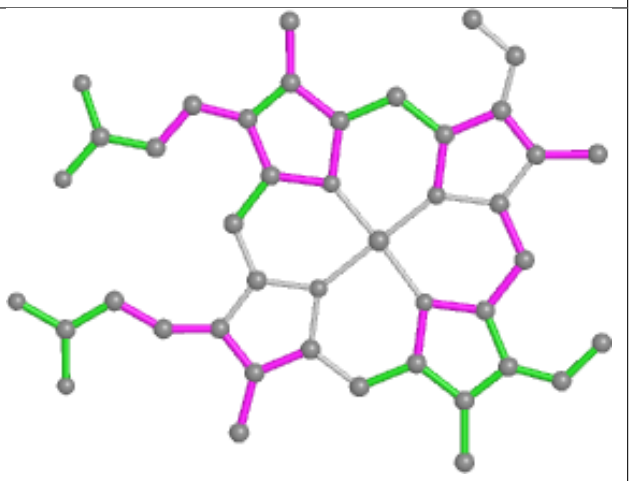
Ligand LMG b 625



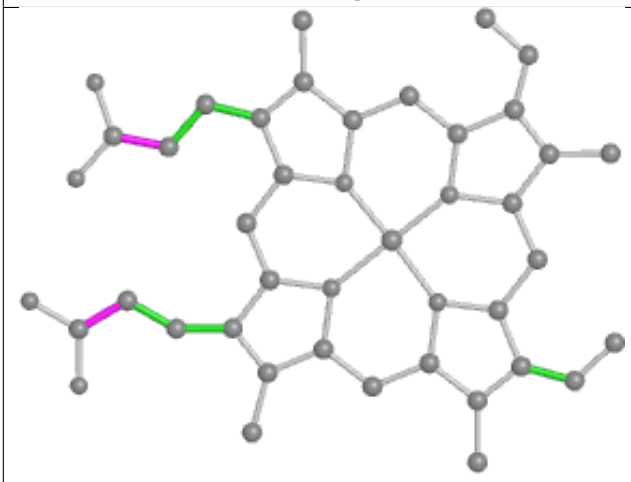
Ligand HEM F 101



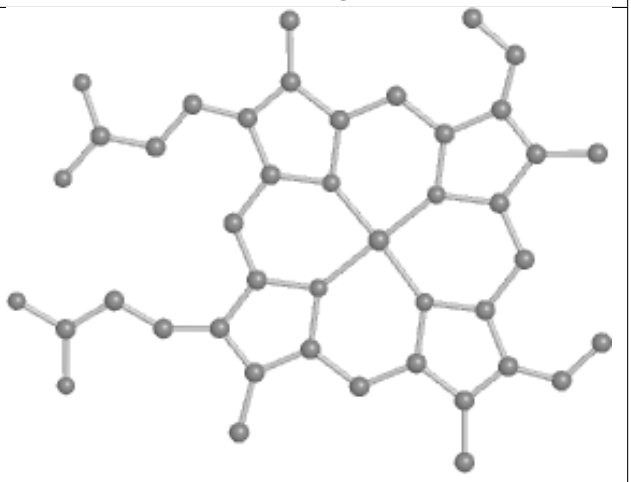
Bond lengths



Bond angles

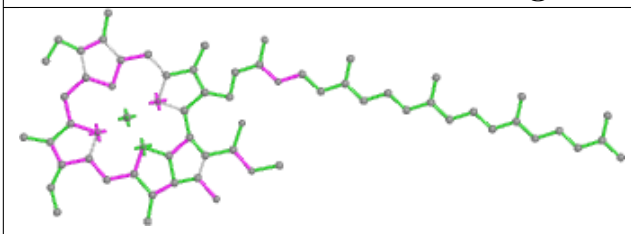


Torsions

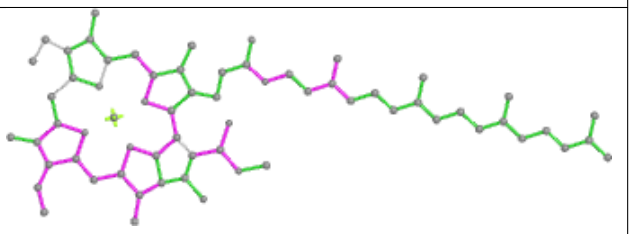


Rings

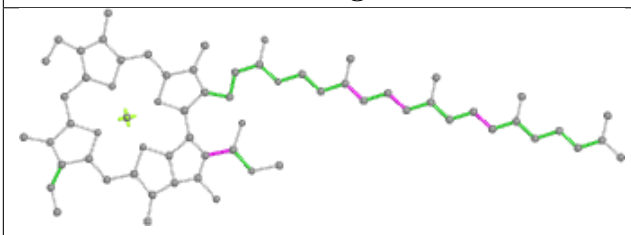
Ligand CLA c 508



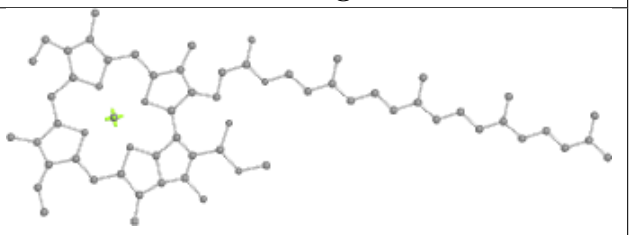
Bond lengths



Bond angles

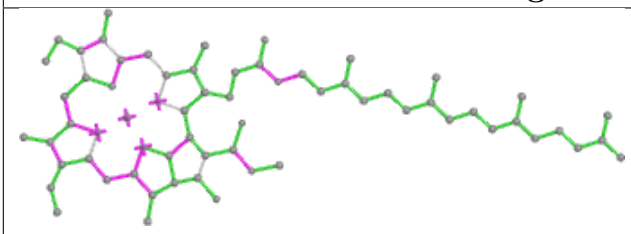


Torsions

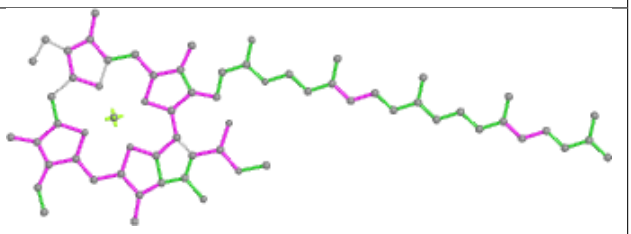


Rings

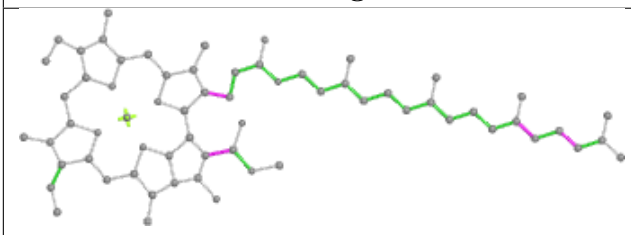
Ligand CLA b 608



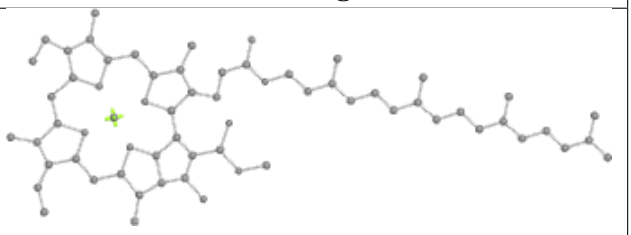
Bond lengths



Bond angles

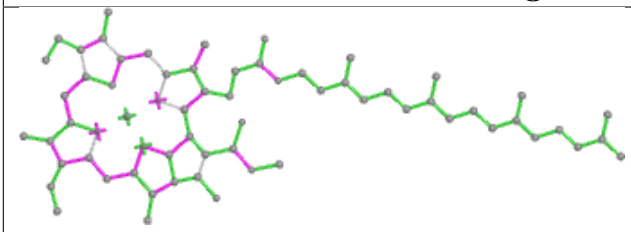


Torsions

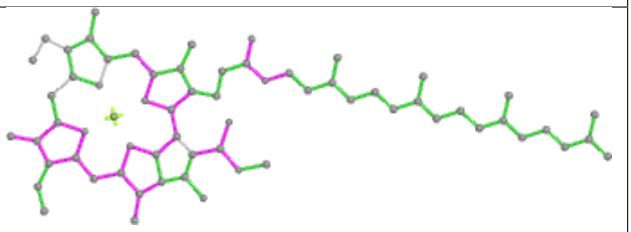


Rings

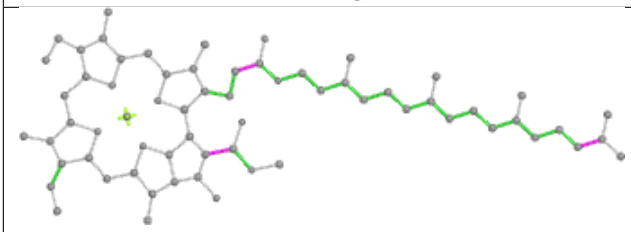
Ligand CLA C 505



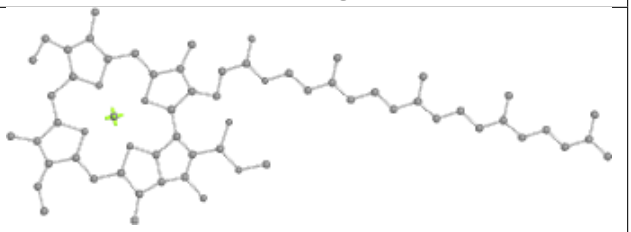
Bond lengths



Bond angles

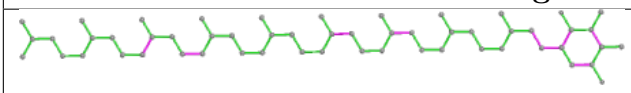


Torsions

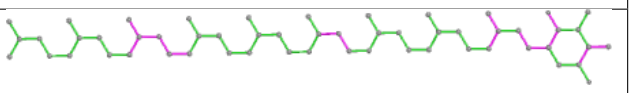


Rings

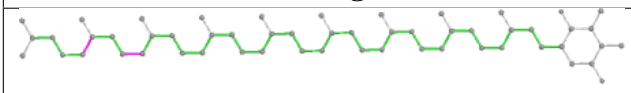
Ligand PL9 d 407



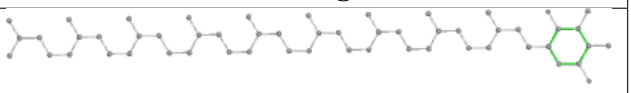
Bond lengths



Bond angles

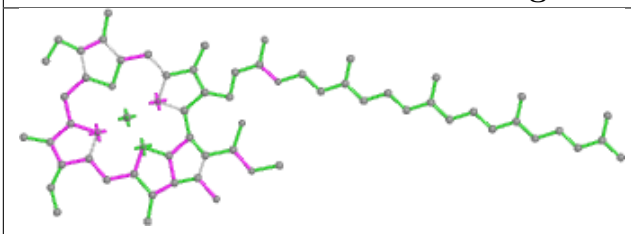


Torsions

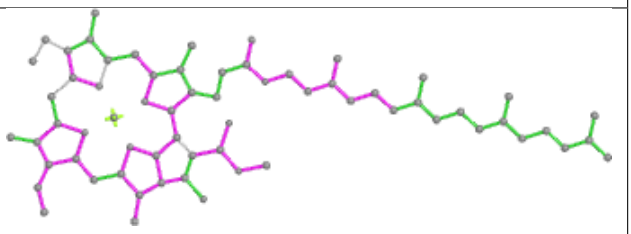


Rings

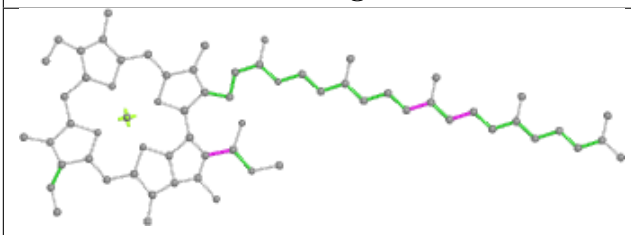
Ligand CLA c 505



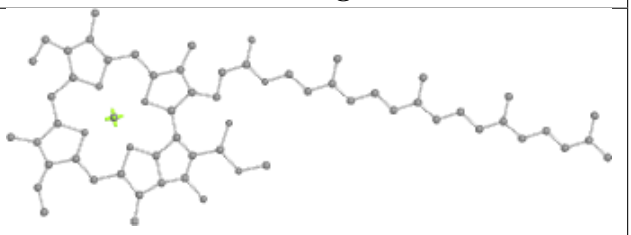
Bond lengths



Bond angles

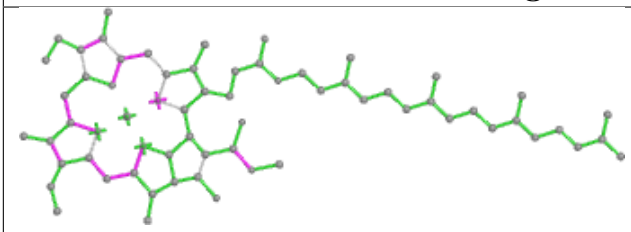


Torsions

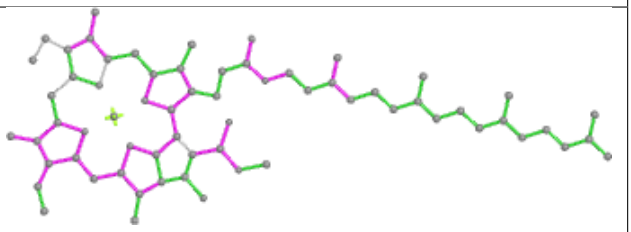


Rings

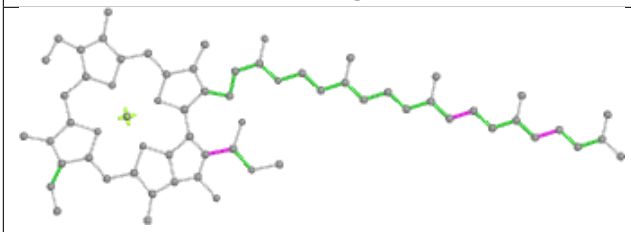
Ligand CLA B 613



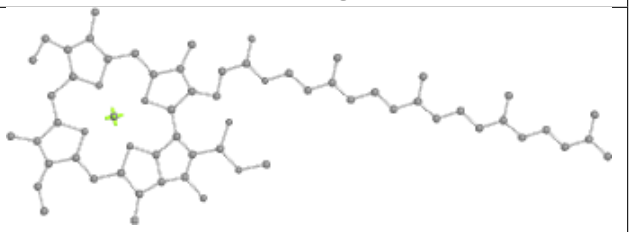
Bond lengths



Bond angles

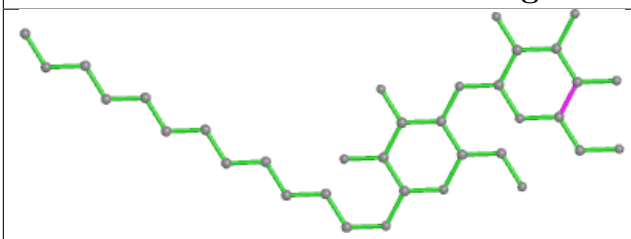


Torsions

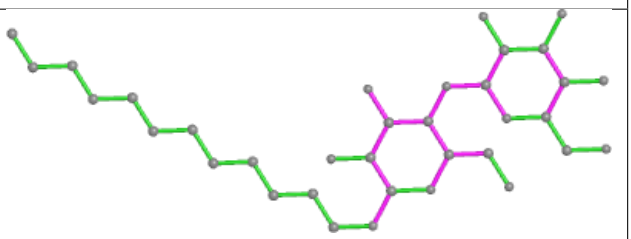


Rings

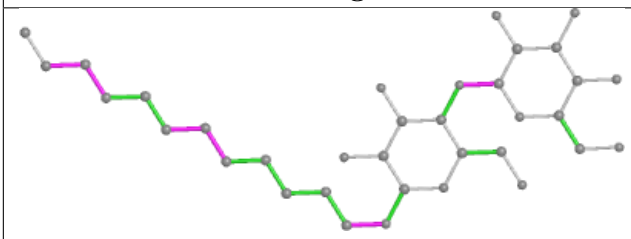
Ligand LMT B 623



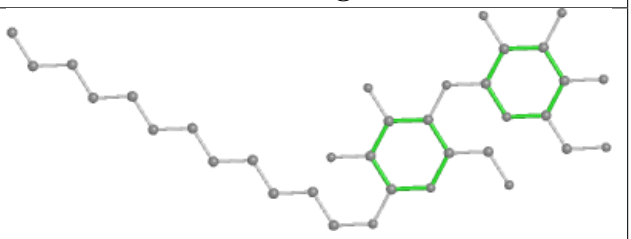
Bond lengths



Bond angles

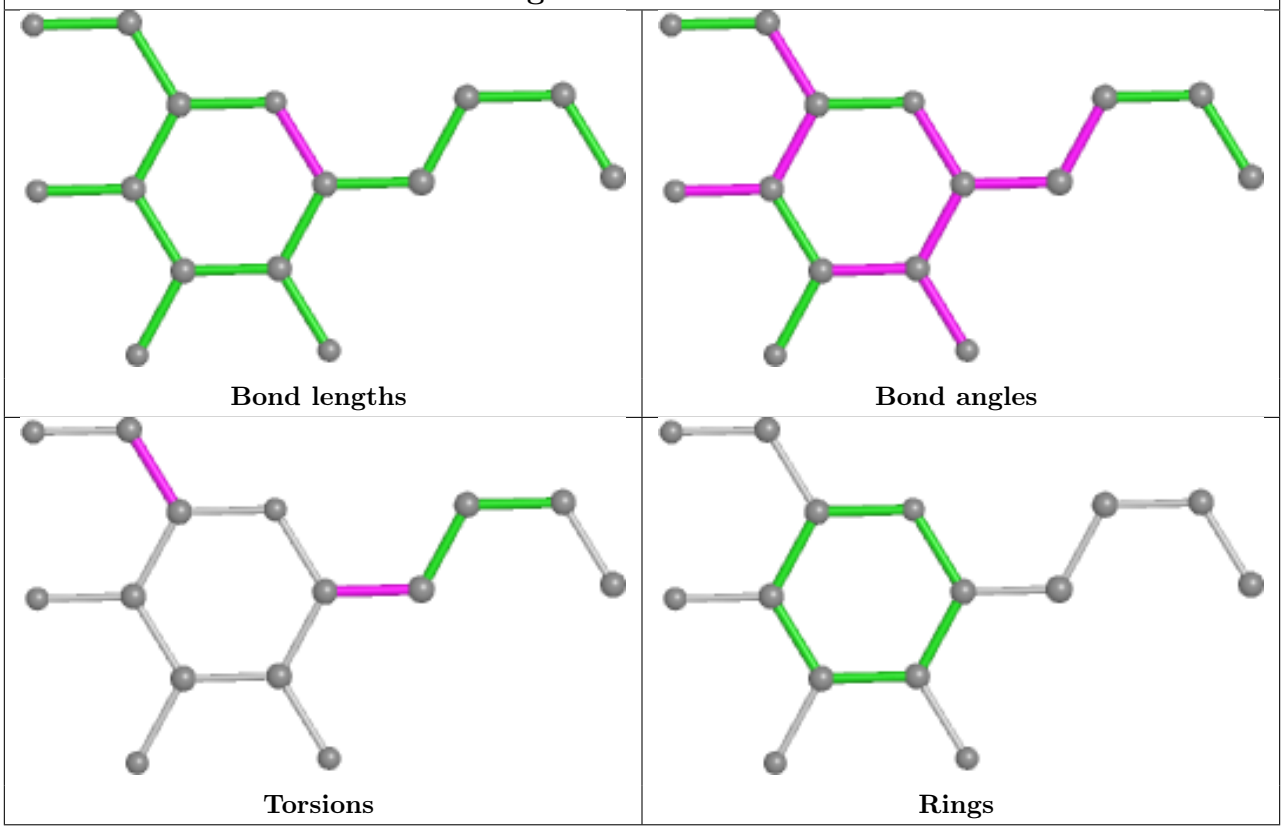


Torsions

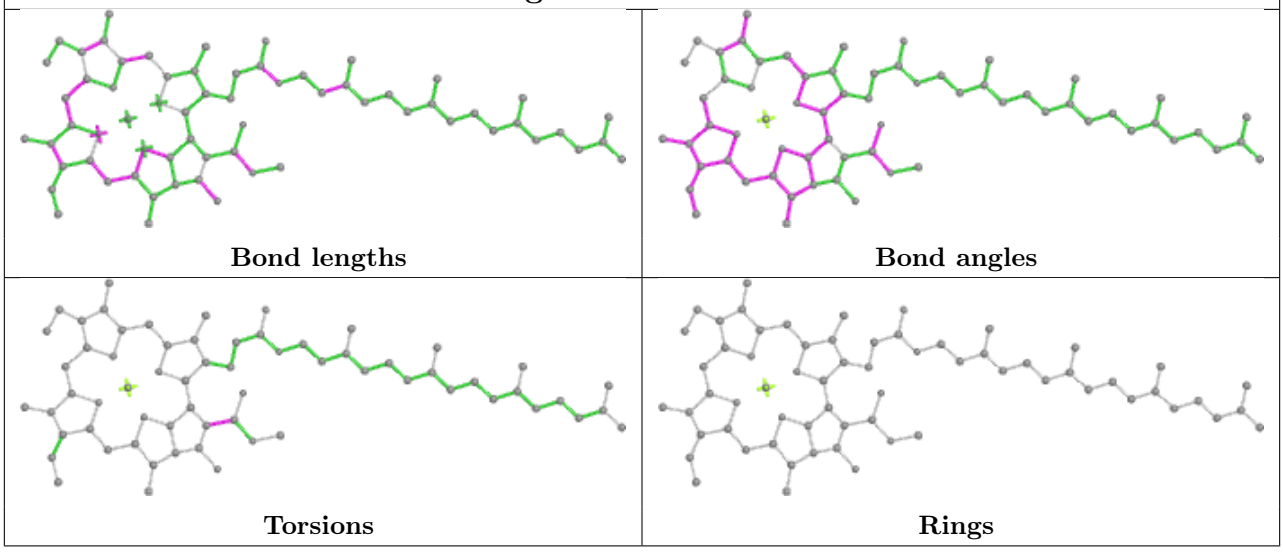


Rings

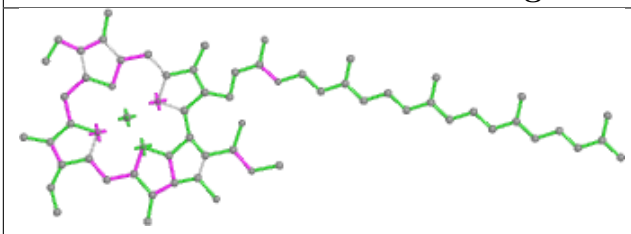
Ligand HTG c 541



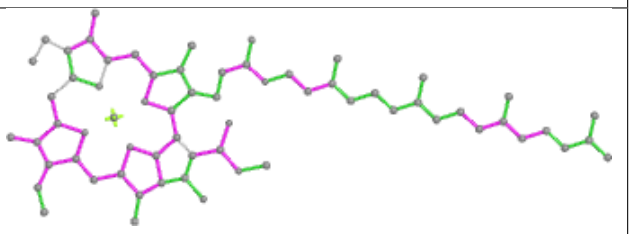
Ligand CLA B 610



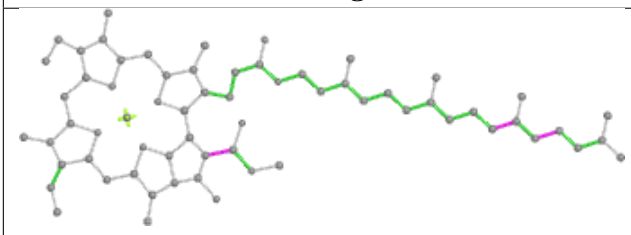
Ligand CLA B 603



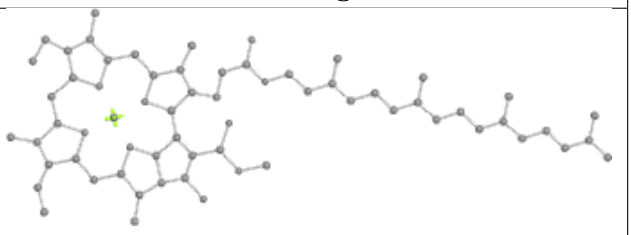
Bond lengths



Bond angles

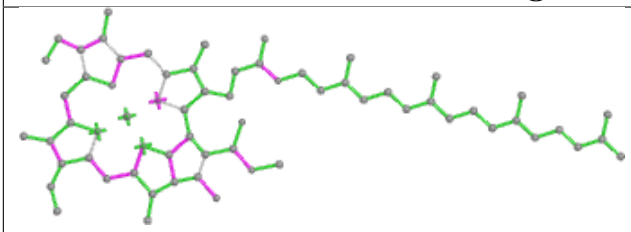


Torsions

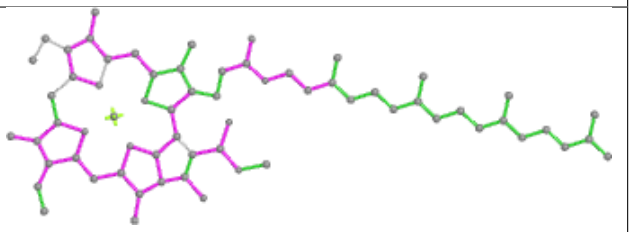


Rings

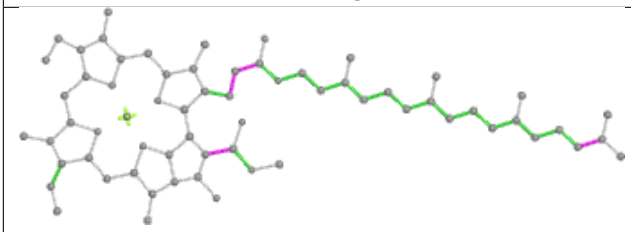
Ligand CLA b 606



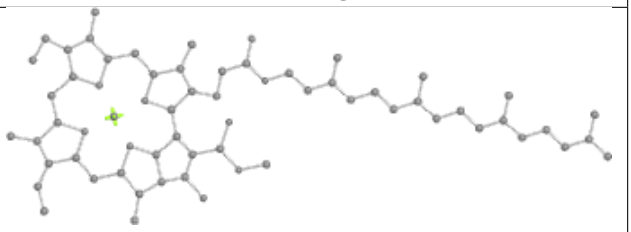
Bond lengths



Bond angles

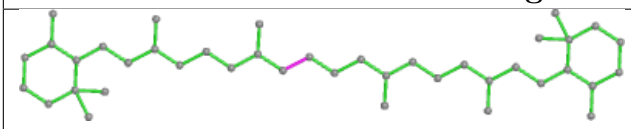


Torsions

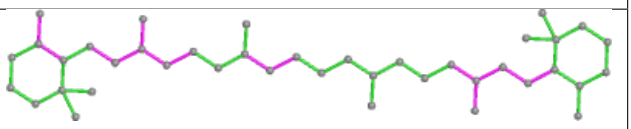


Rings

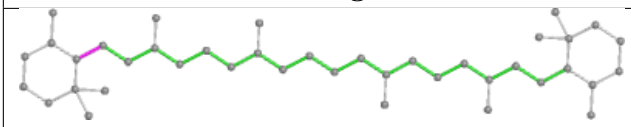
Ligand BCR b 621



Bond lengths



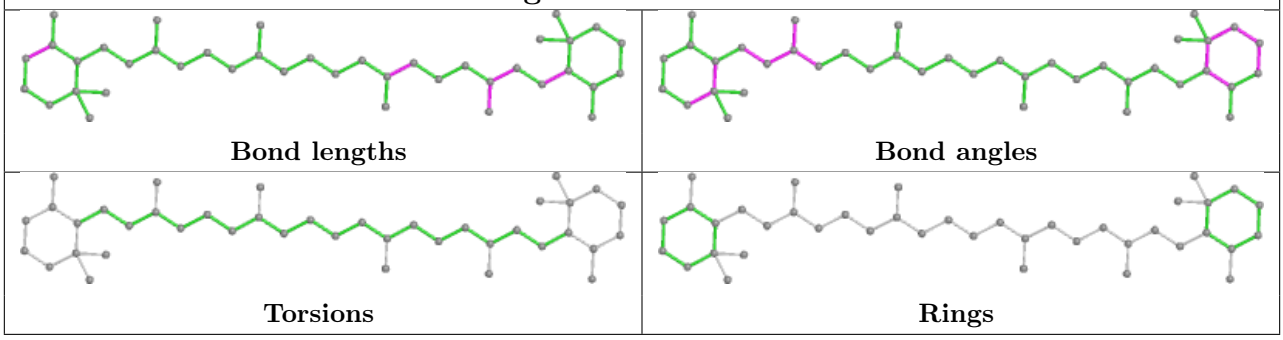
Bond angles



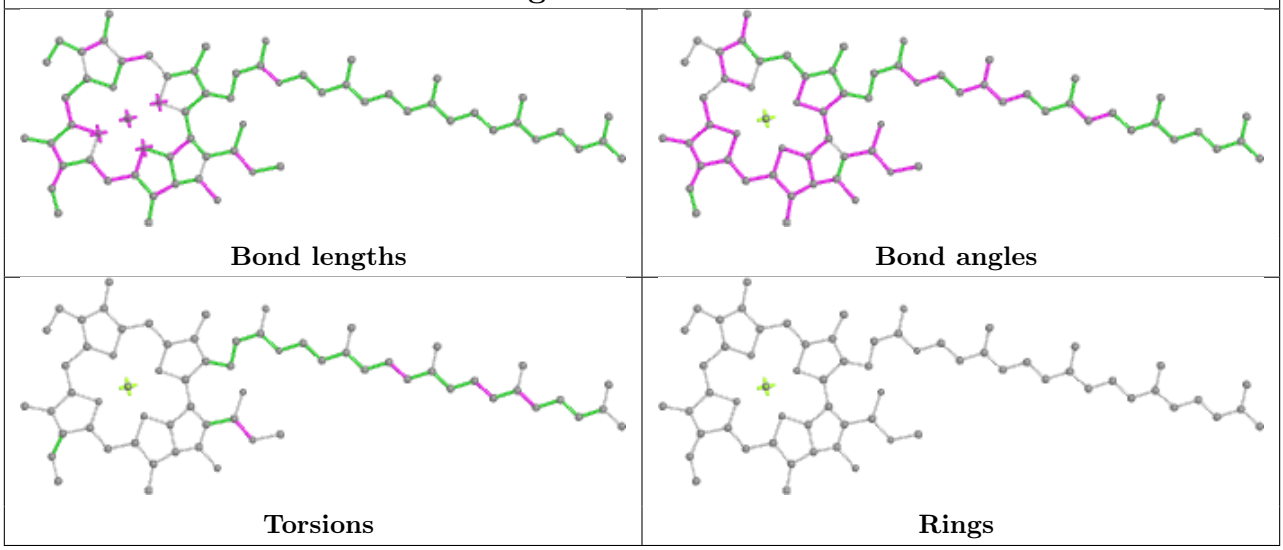
Torsions

Rings

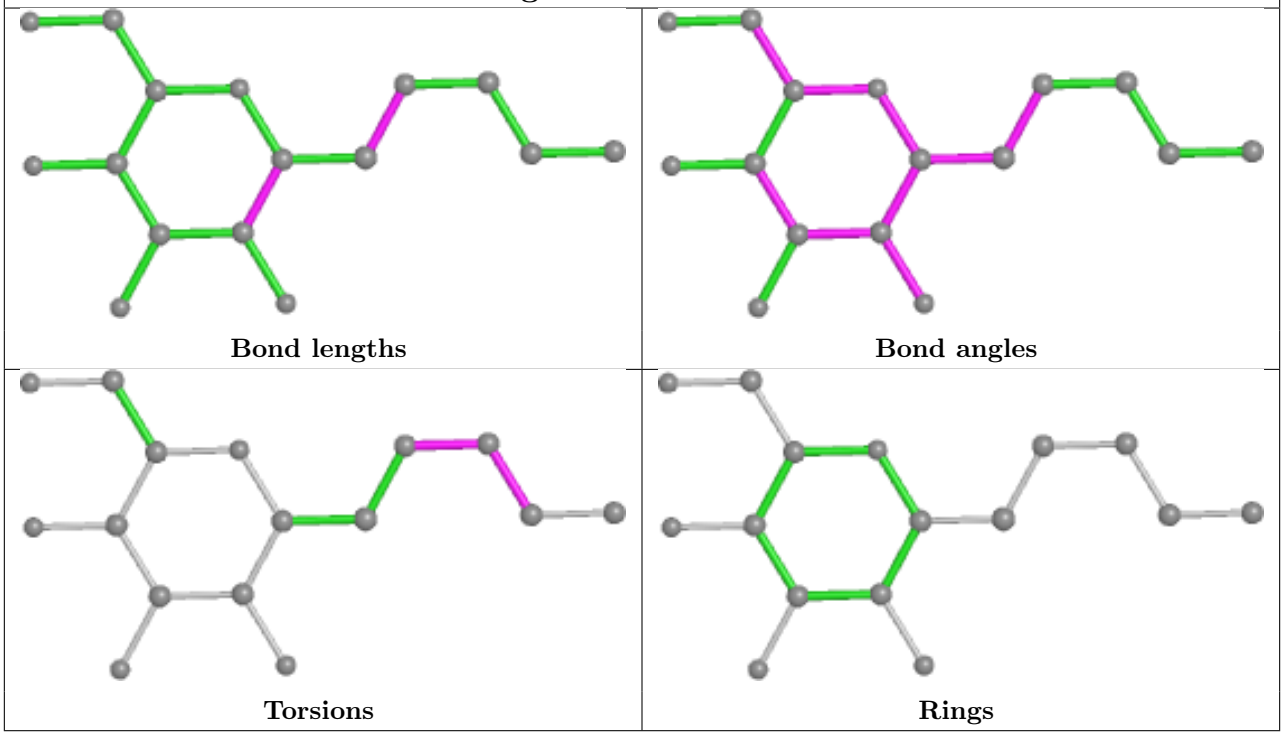
Ligand BCR B 619



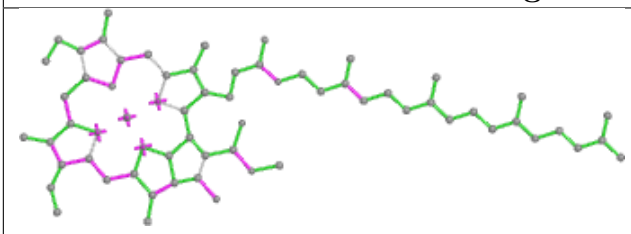
Ligand CLA b 619



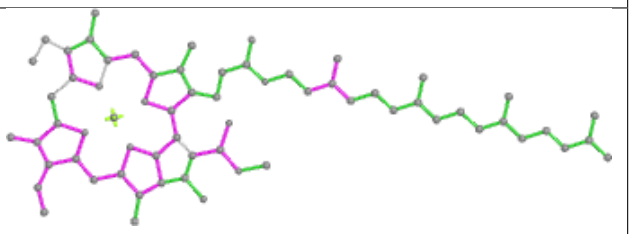
Ligand HTG D 413



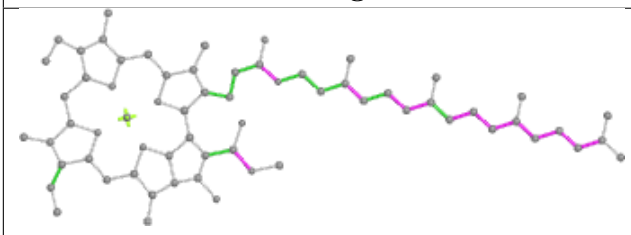
Ligand CLA A 408



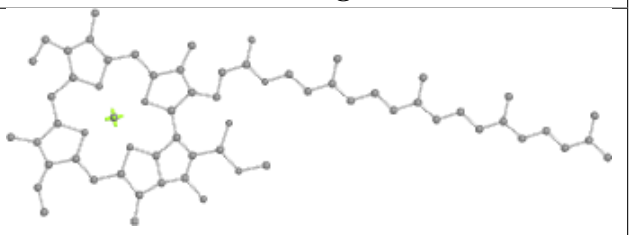
Bond lengths



Bond angles

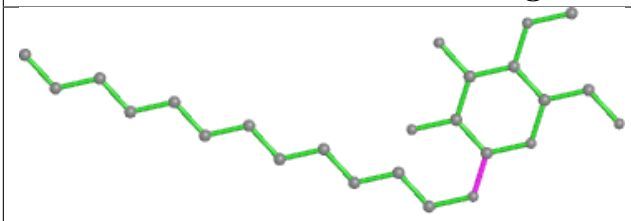


Torsions

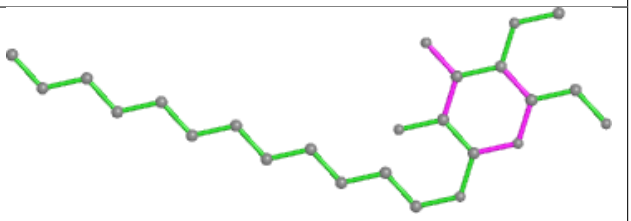


Rings

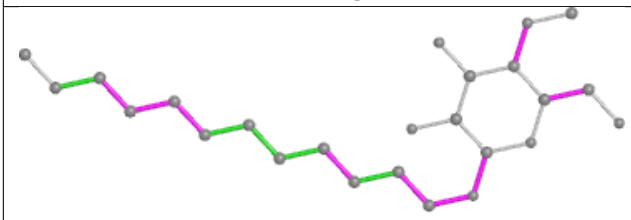
Ligand LMT b 626



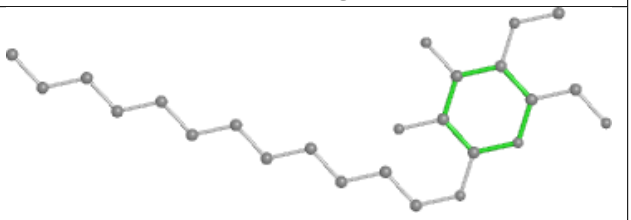
Bond lengths



Bond angles

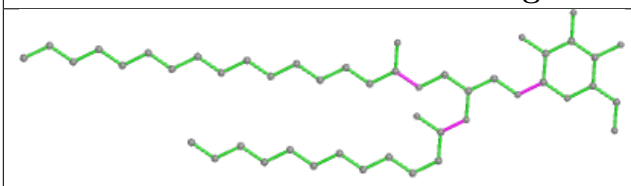


Torsions

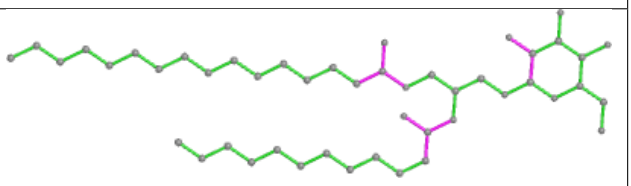


Rings

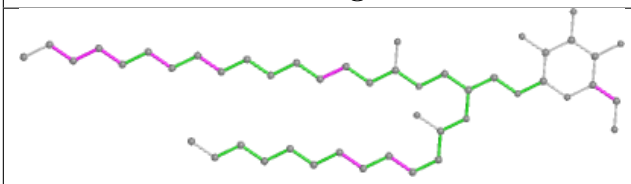
Ligand LMG d 412



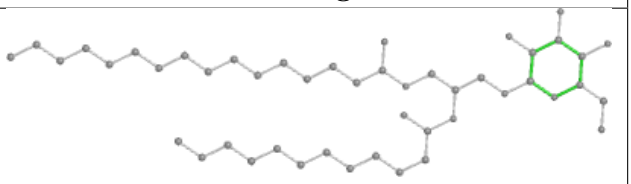
Bond lengths



Bond angles

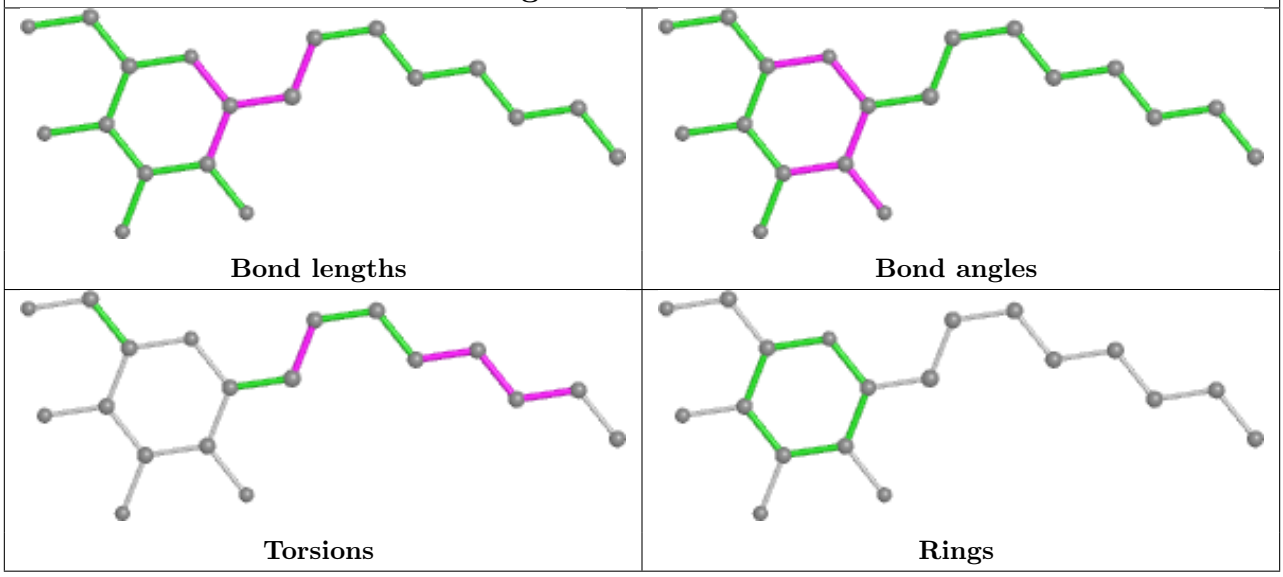


Torsions

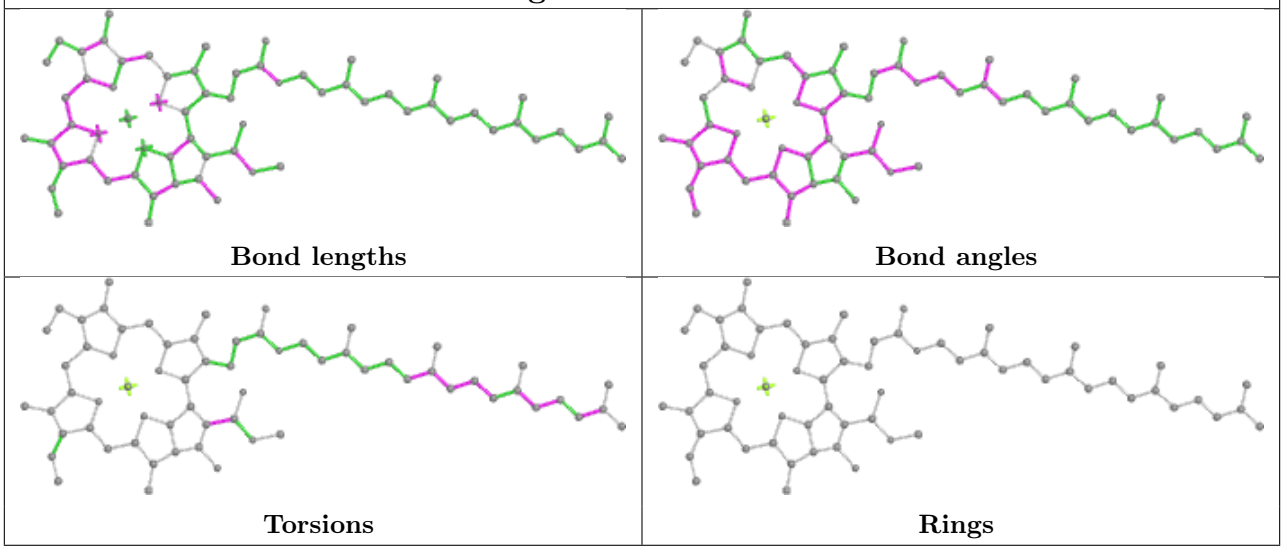


Rings

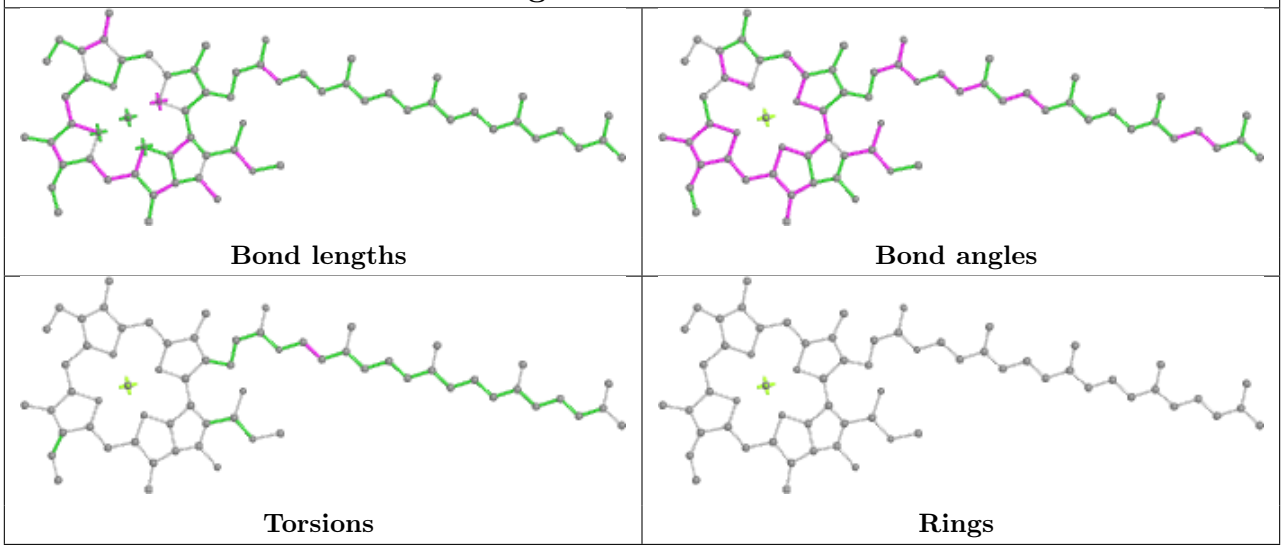
Ligand HTG O 302



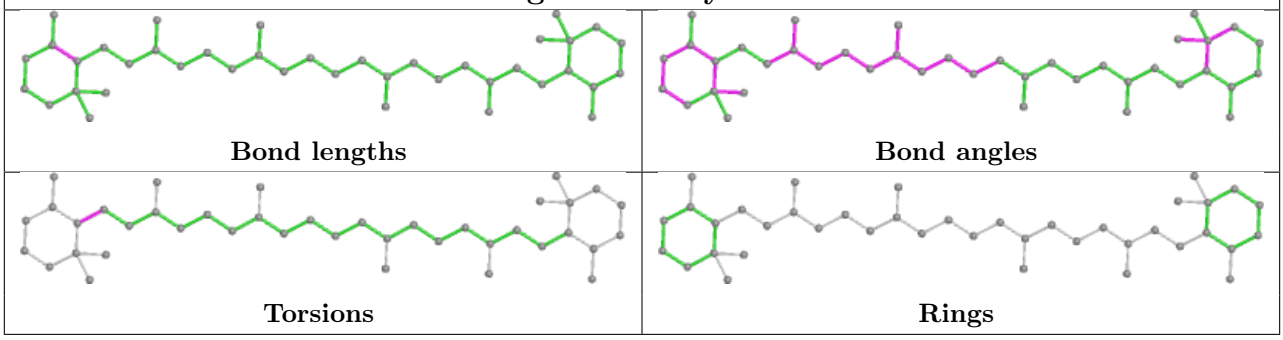
Ligand CLA d 405



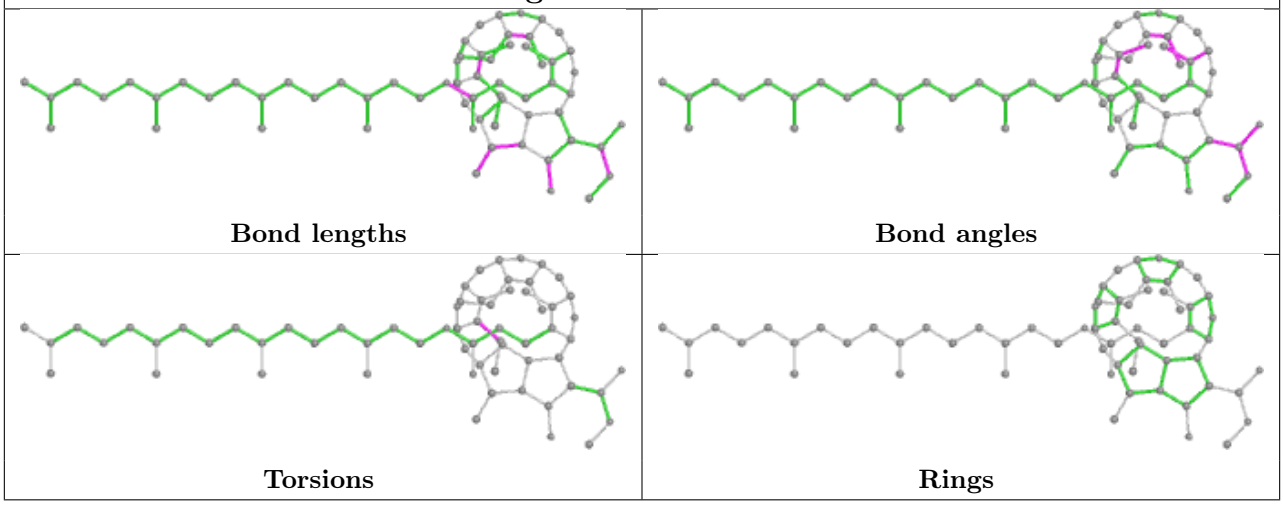
Ligand CLA b 617



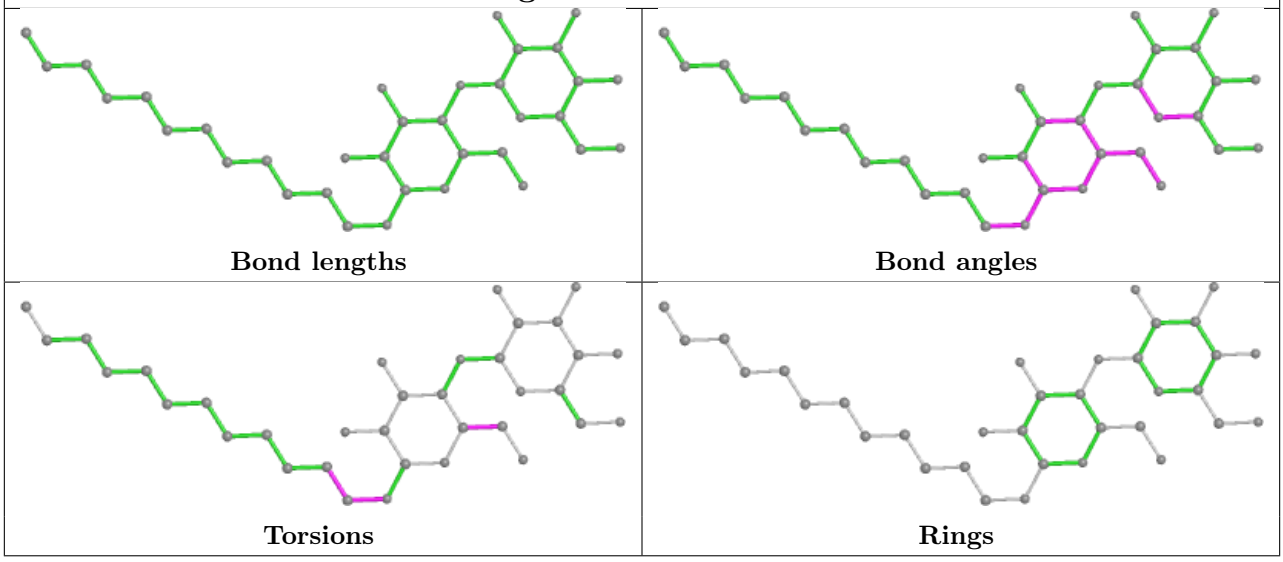
Ligand BCR y 101



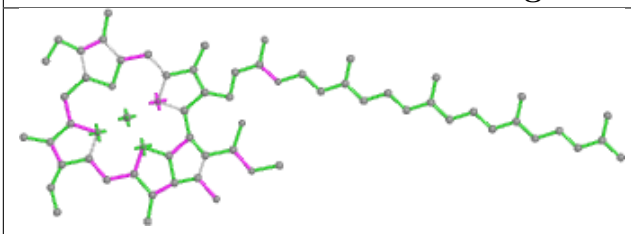
Ligand PHO d 404



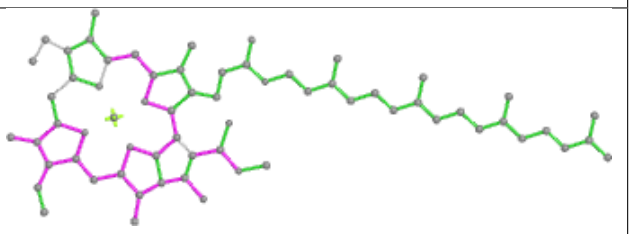
Ligand LMT M 101



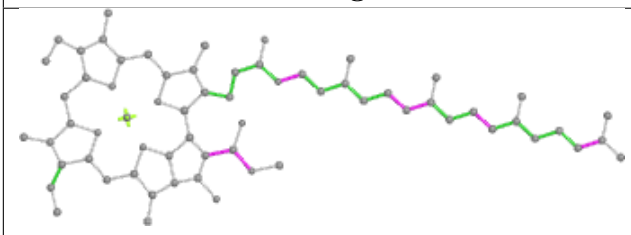
Ligand CLA C 506



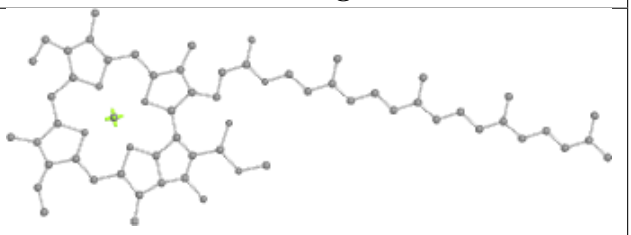
Bond lengths



Bond angles

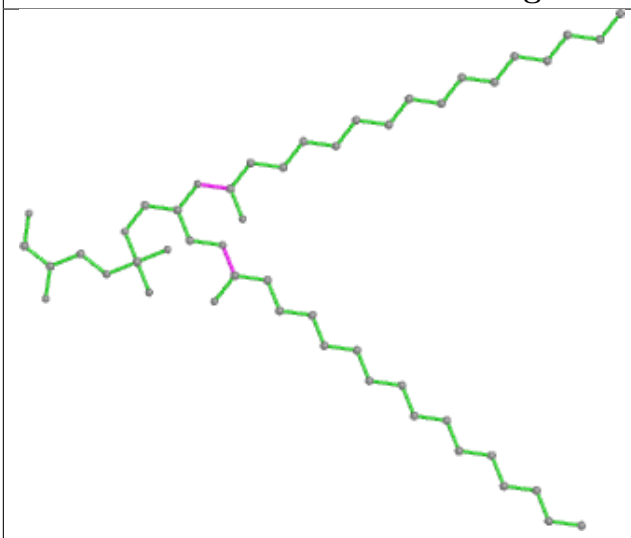


Torsions

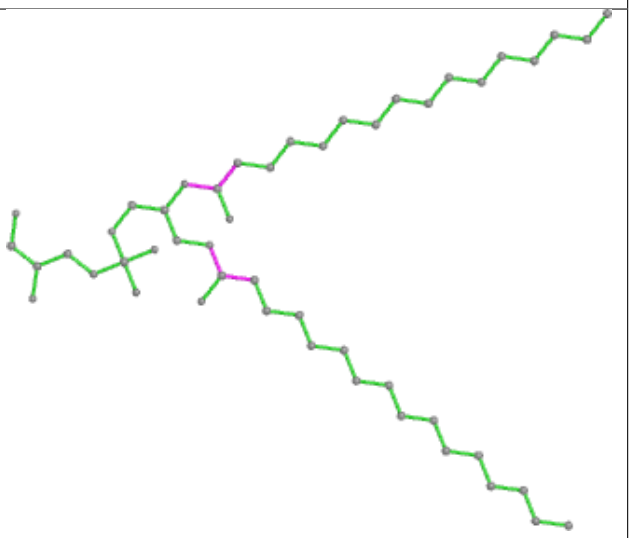


Rings

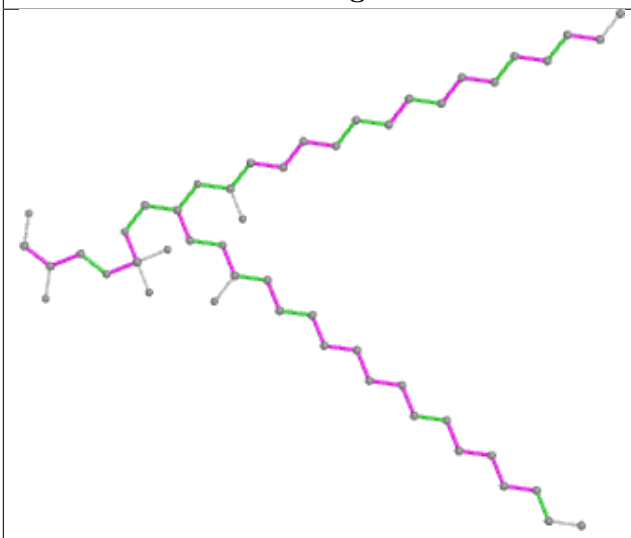
Ligand LHG E 101



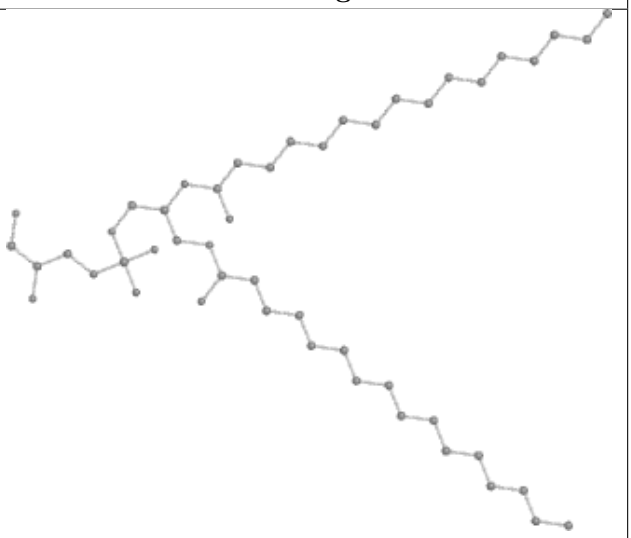
Bond lengths



Bond angles

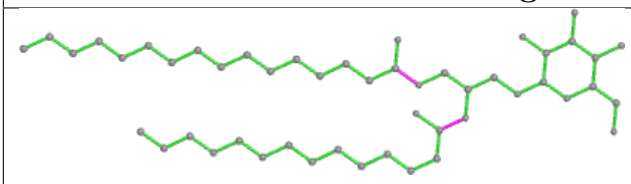


Torsions

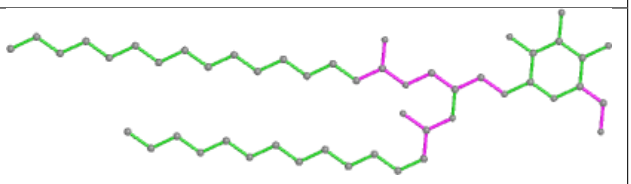


Rings

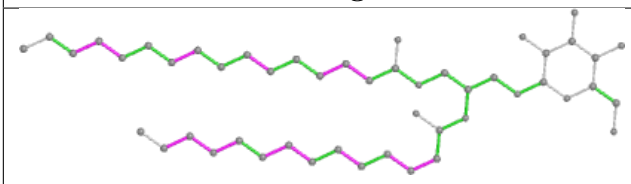
Ligand LMG C 518



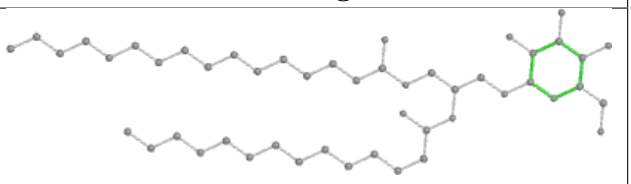
Bond lengths



Bond angles

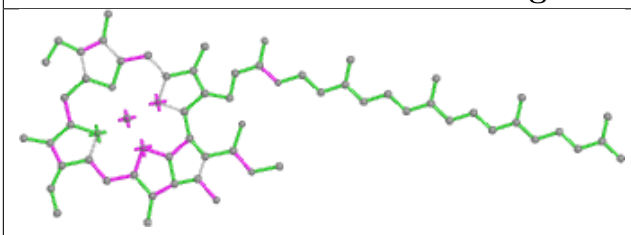


Torsions

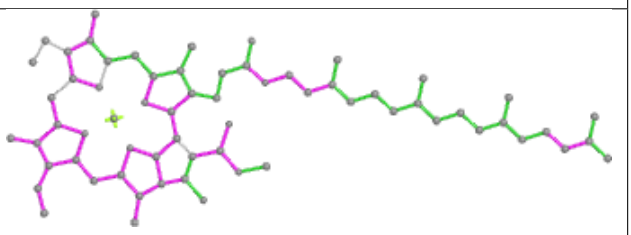


Rings

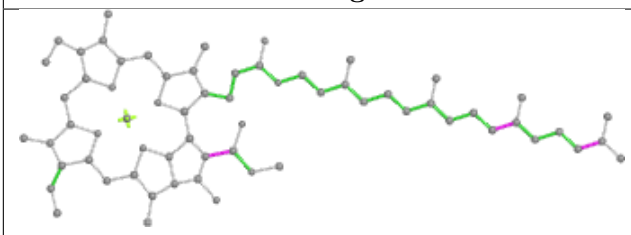
Ligand CLA c 503



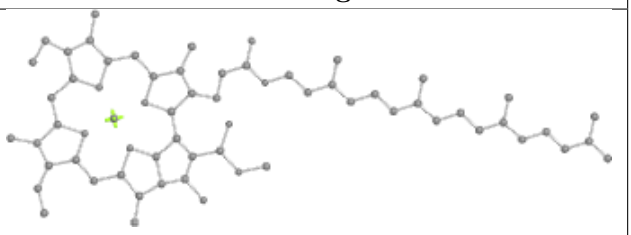
Bond lengths



Bond angles

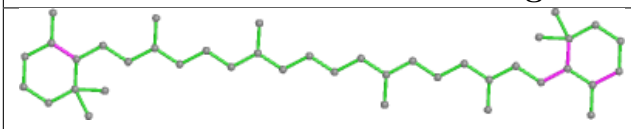


Torsions

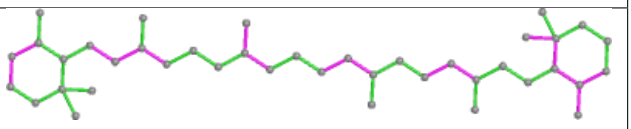


Rings

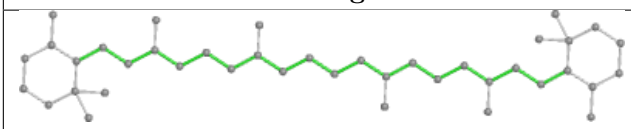
Ligand BCR b 623



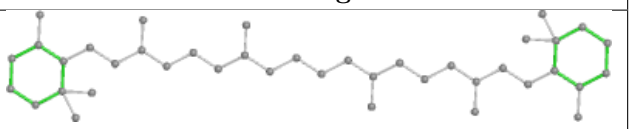
Bond lengths



Bond angles

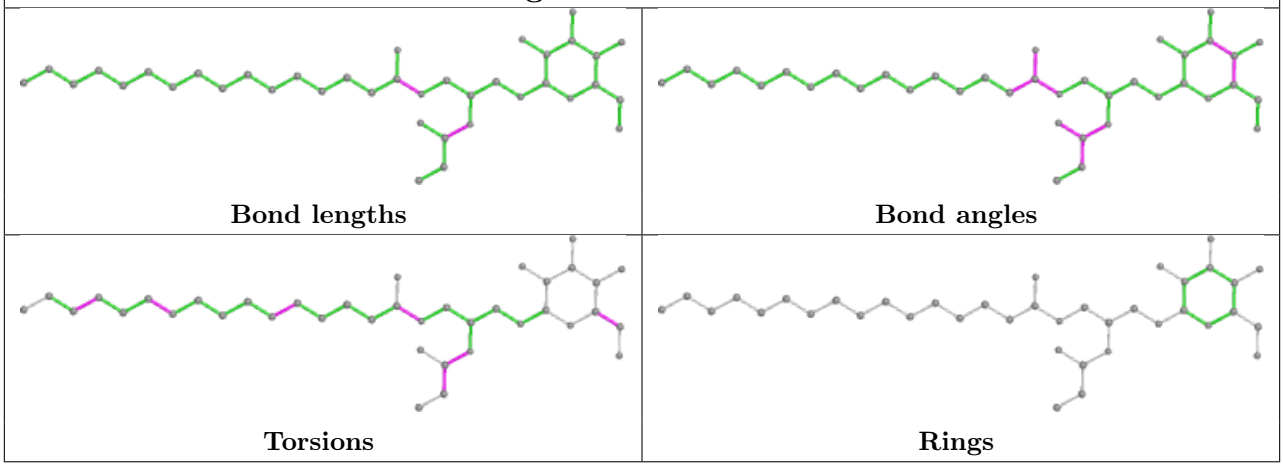


Torsions

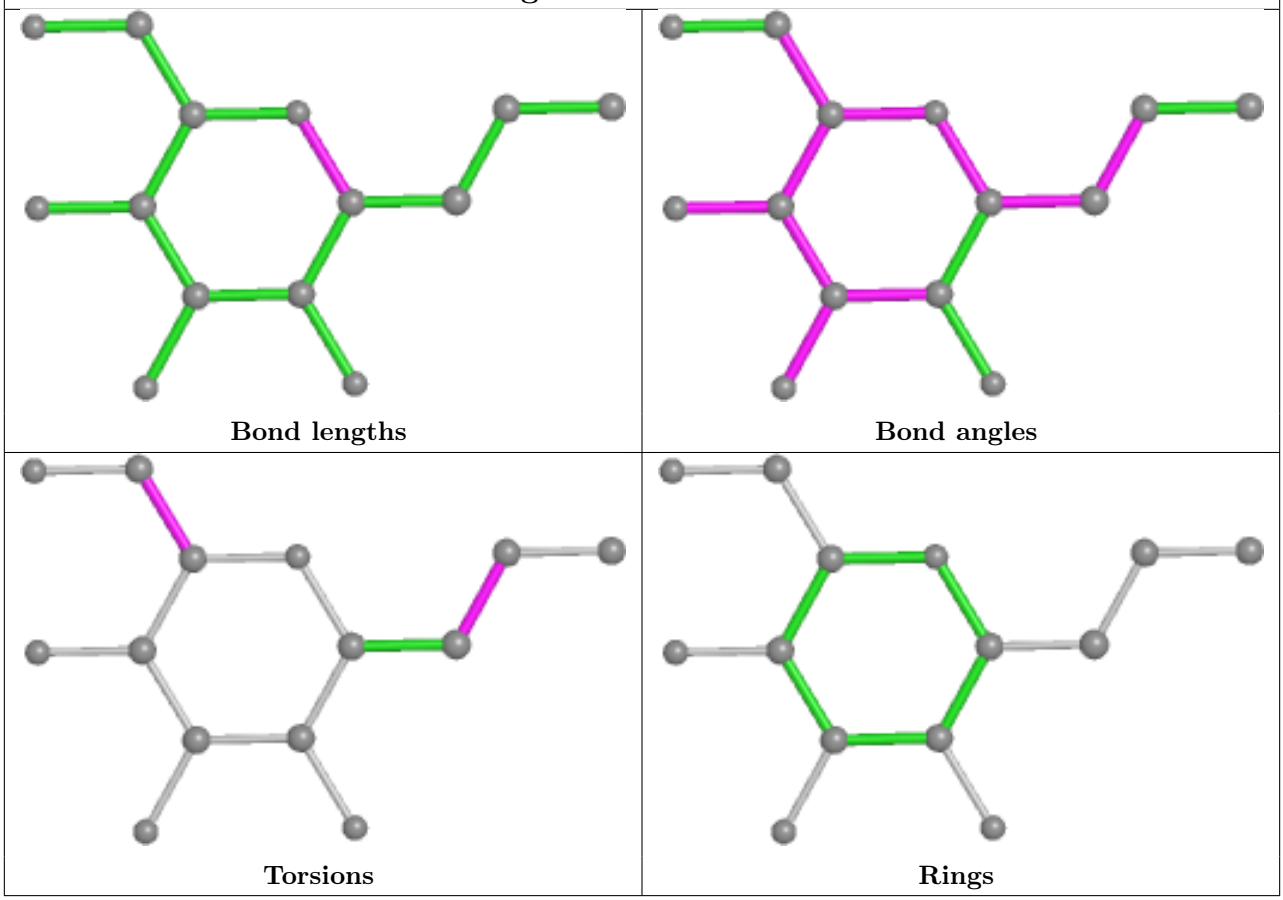


Rings

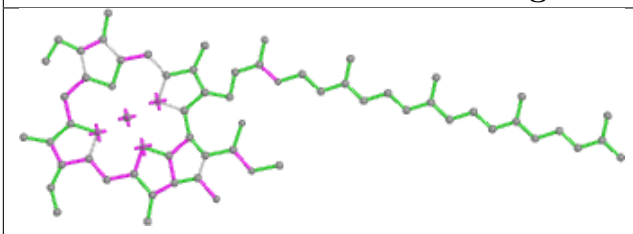
Ligand LMG c 520



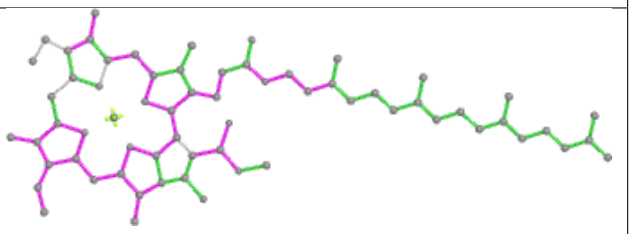
Ligand HTG U 203



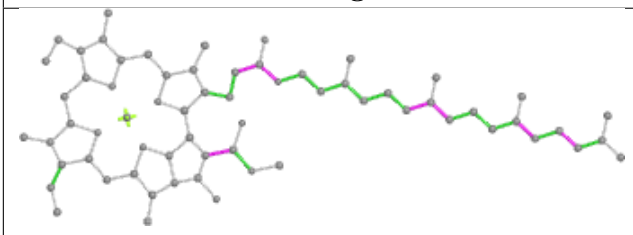
Ligand CLA c 513



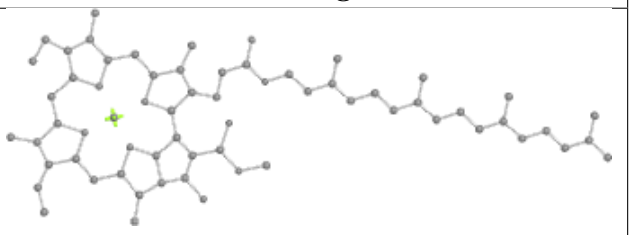
Bond lengths



Bond angles

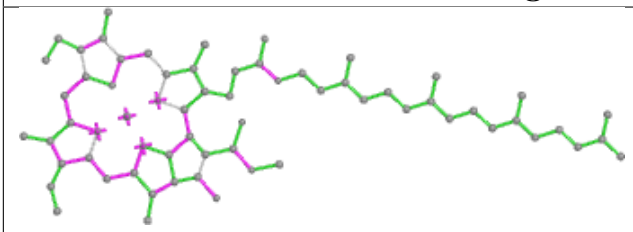


Torsions

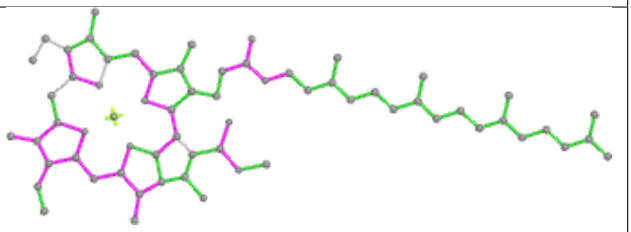


Rings

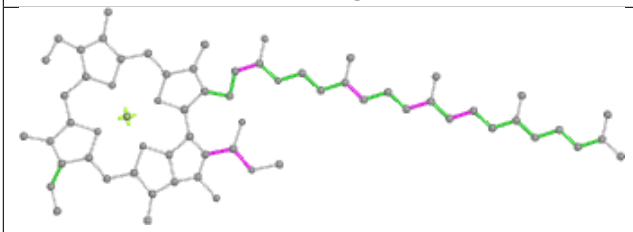
Ligand CLA C 510



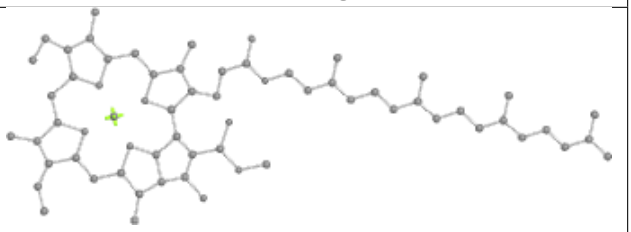
Bond lengths



Bond angles

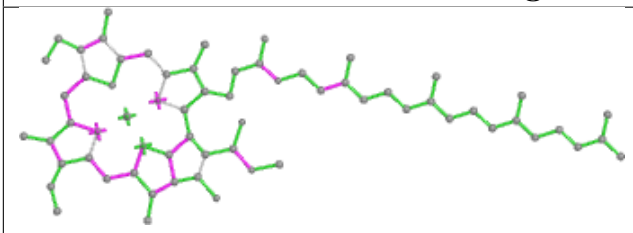


Torsions

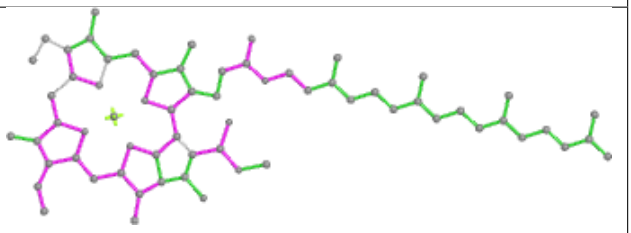


Rings

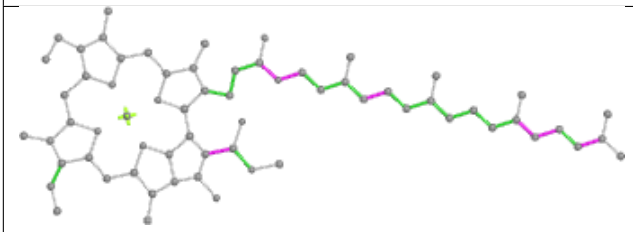
Ligand CLA B 617



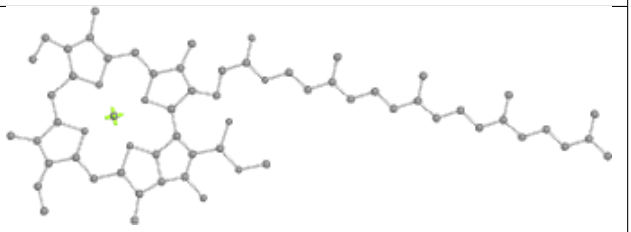
Bond lengths



Bond angles

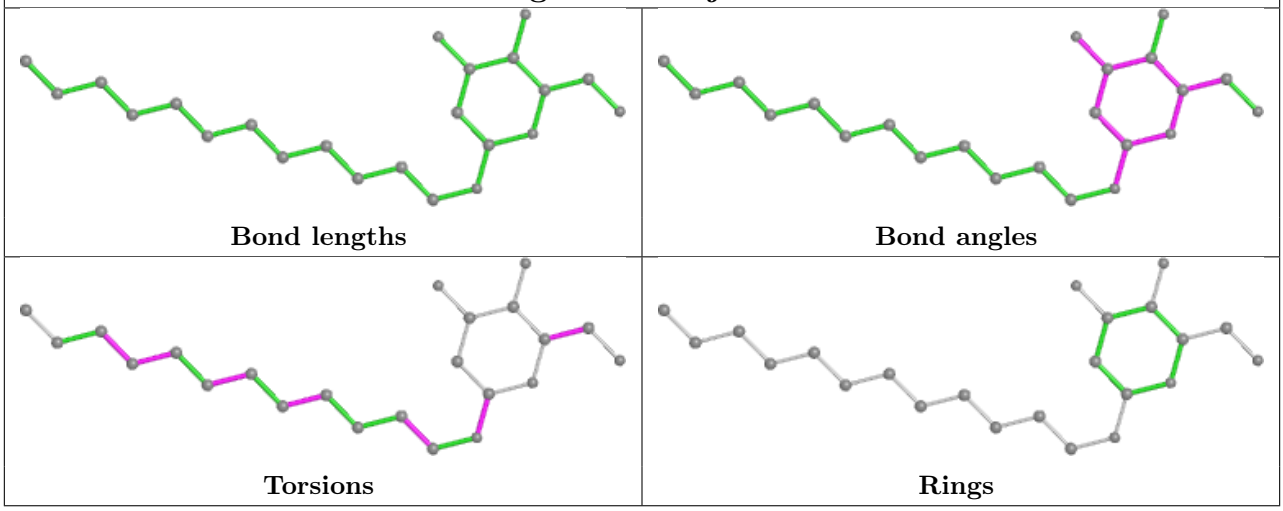


Torsions

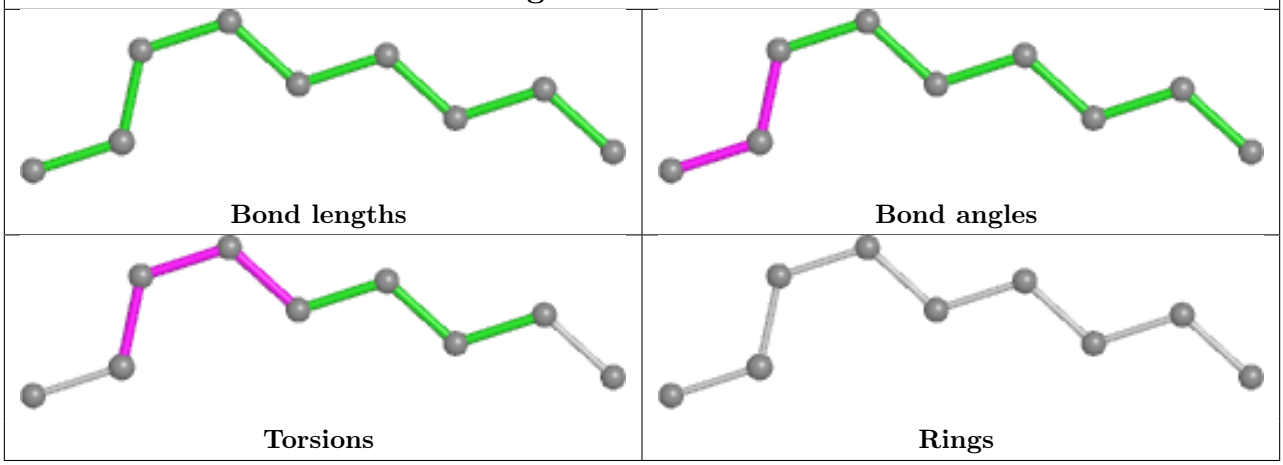


Rings

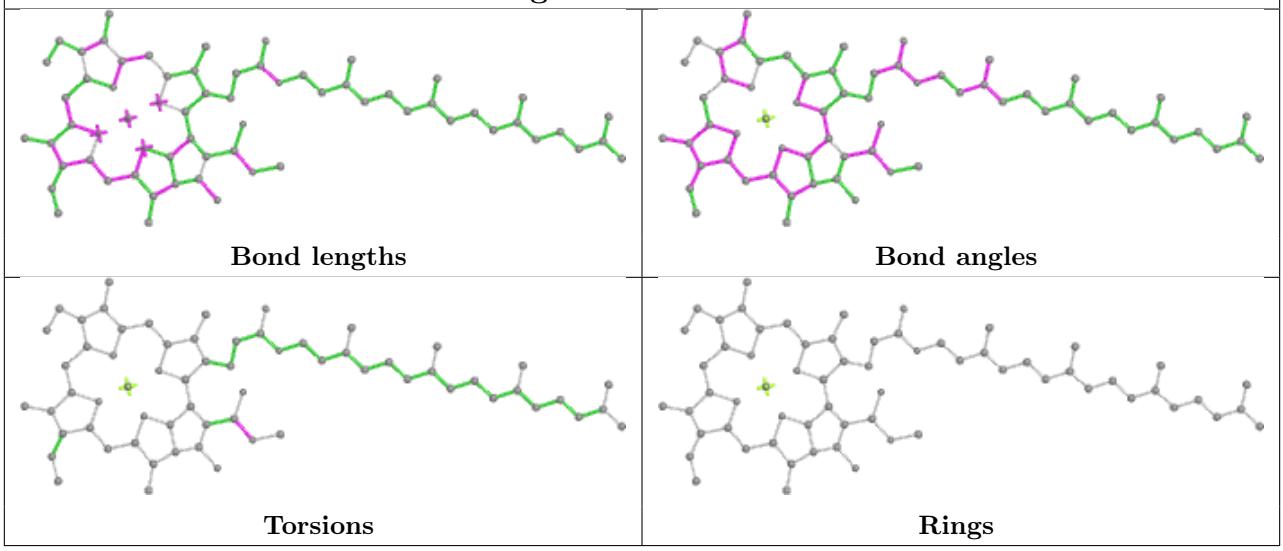
Ligand LMT j 102



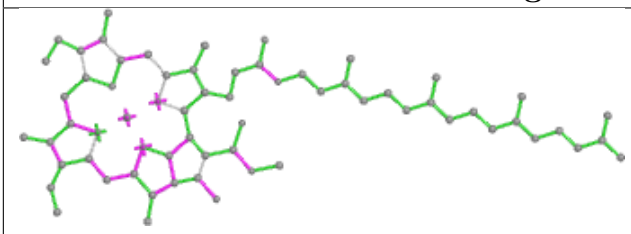
Ligand HTG c 524



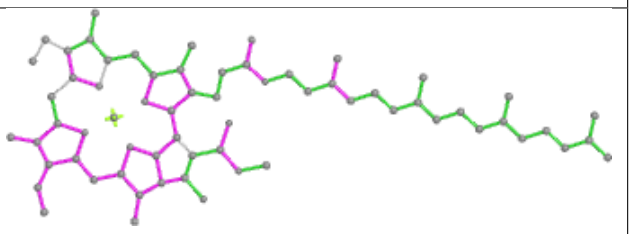
Ligand CLA c 512



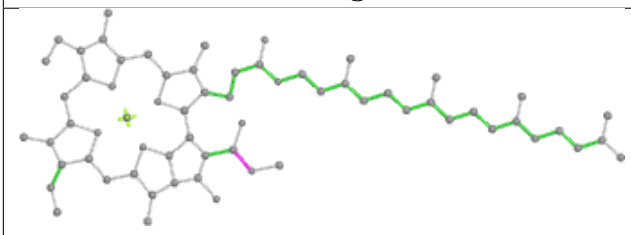
Ligand CLA C 511



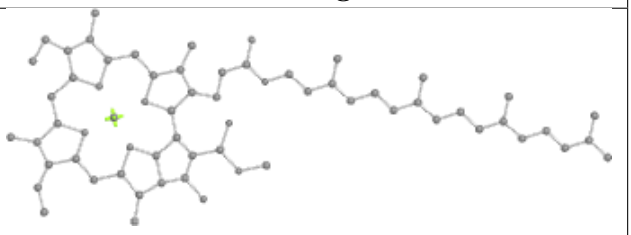
Bond lengths



Bond angles

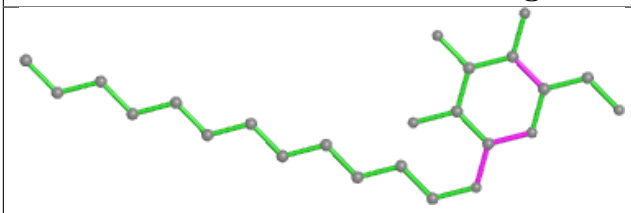


Torsions

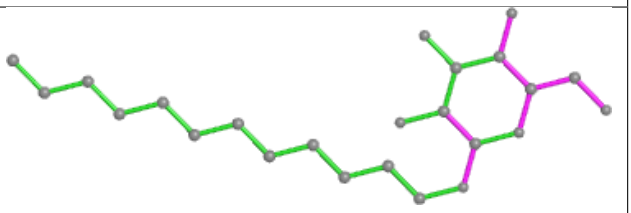


Rings

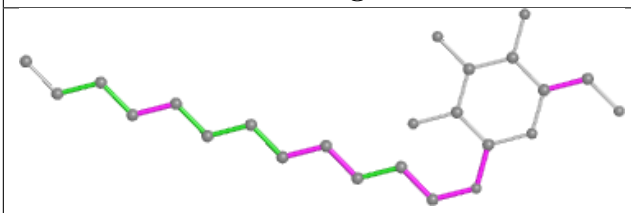
Ligand LMT F 102



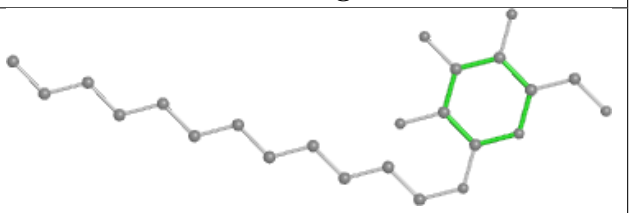
Bond lengths



Bond angles

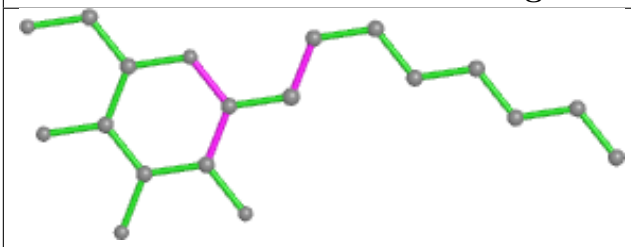


Torsions

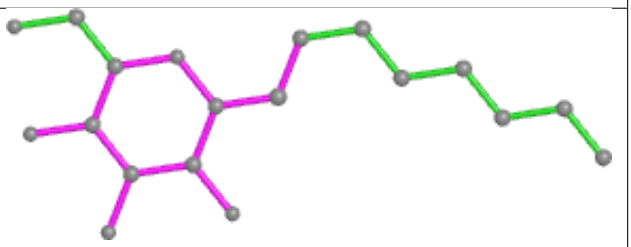


Rings

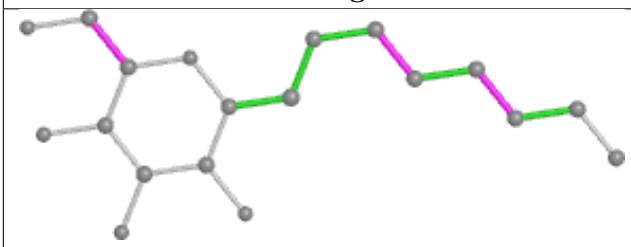
Ligand HTG o 301



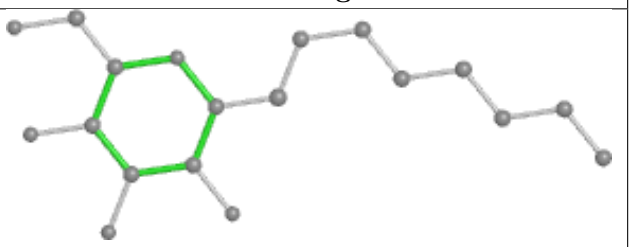
Bond lengths



Bond angles

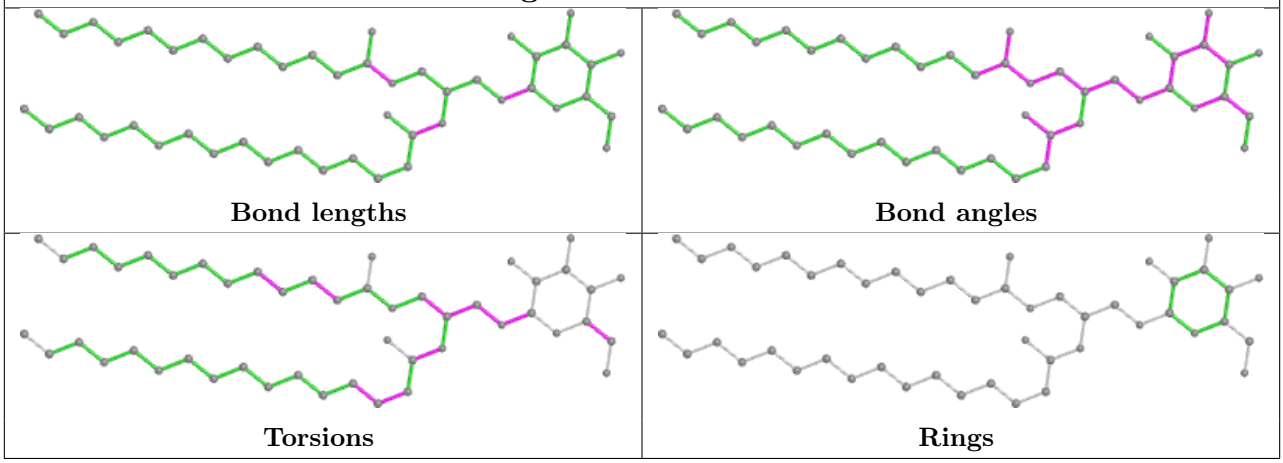


Torsions

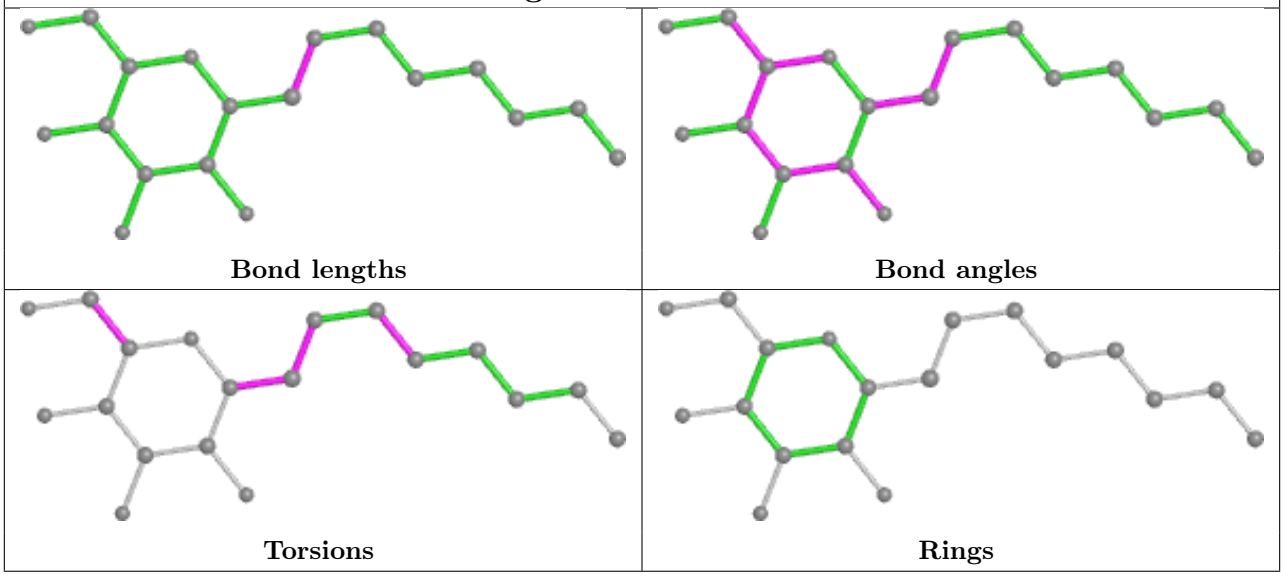


Rings

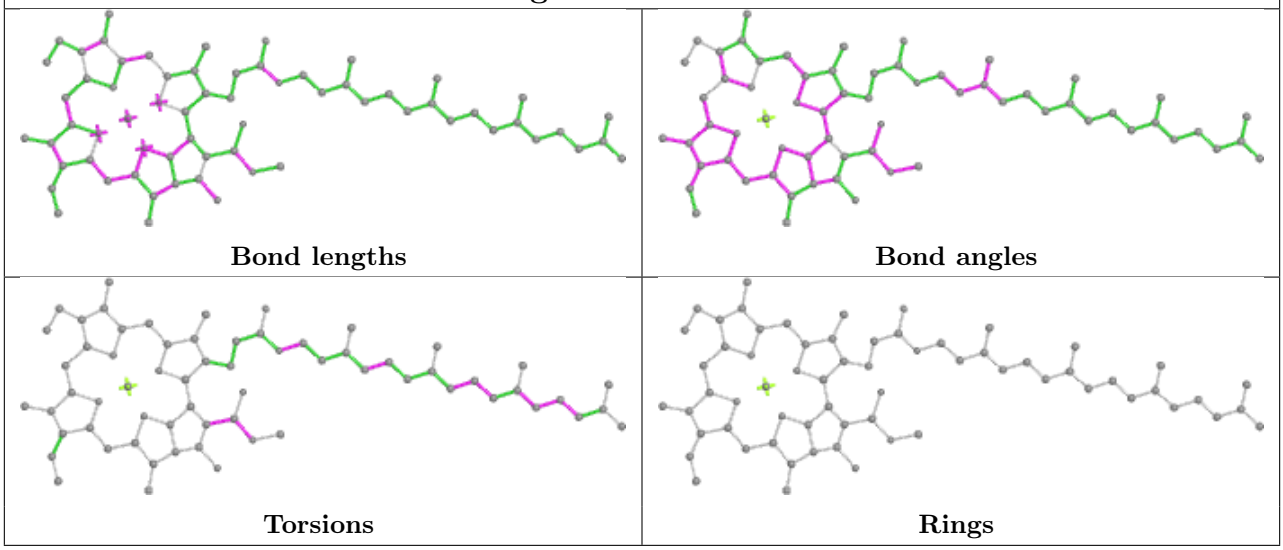
Ligand LMG C 519



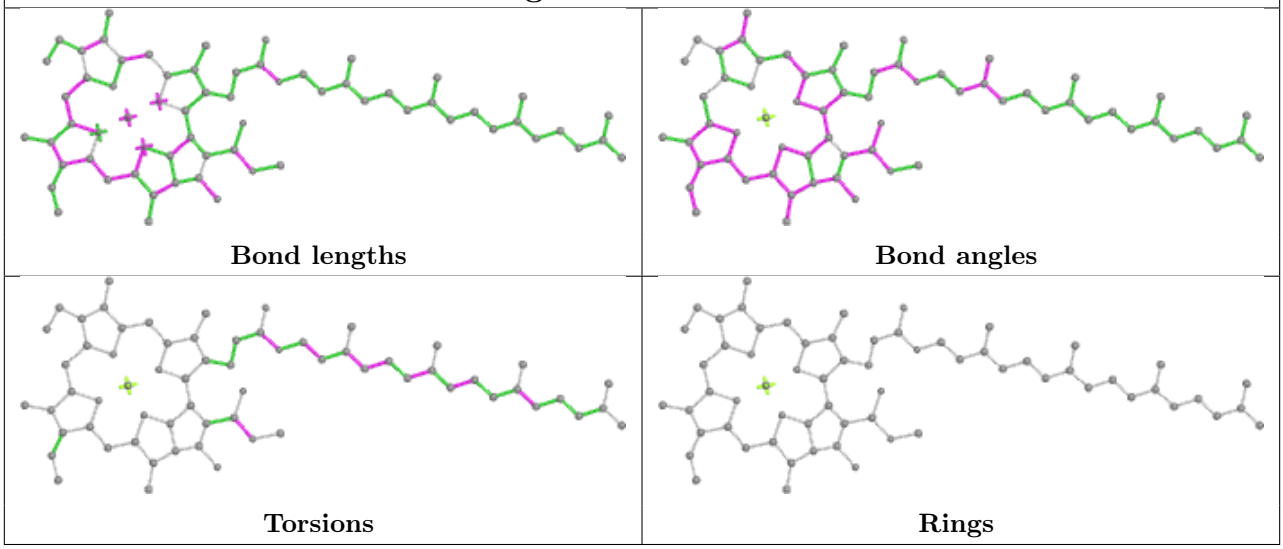
Ligand HTG b 627



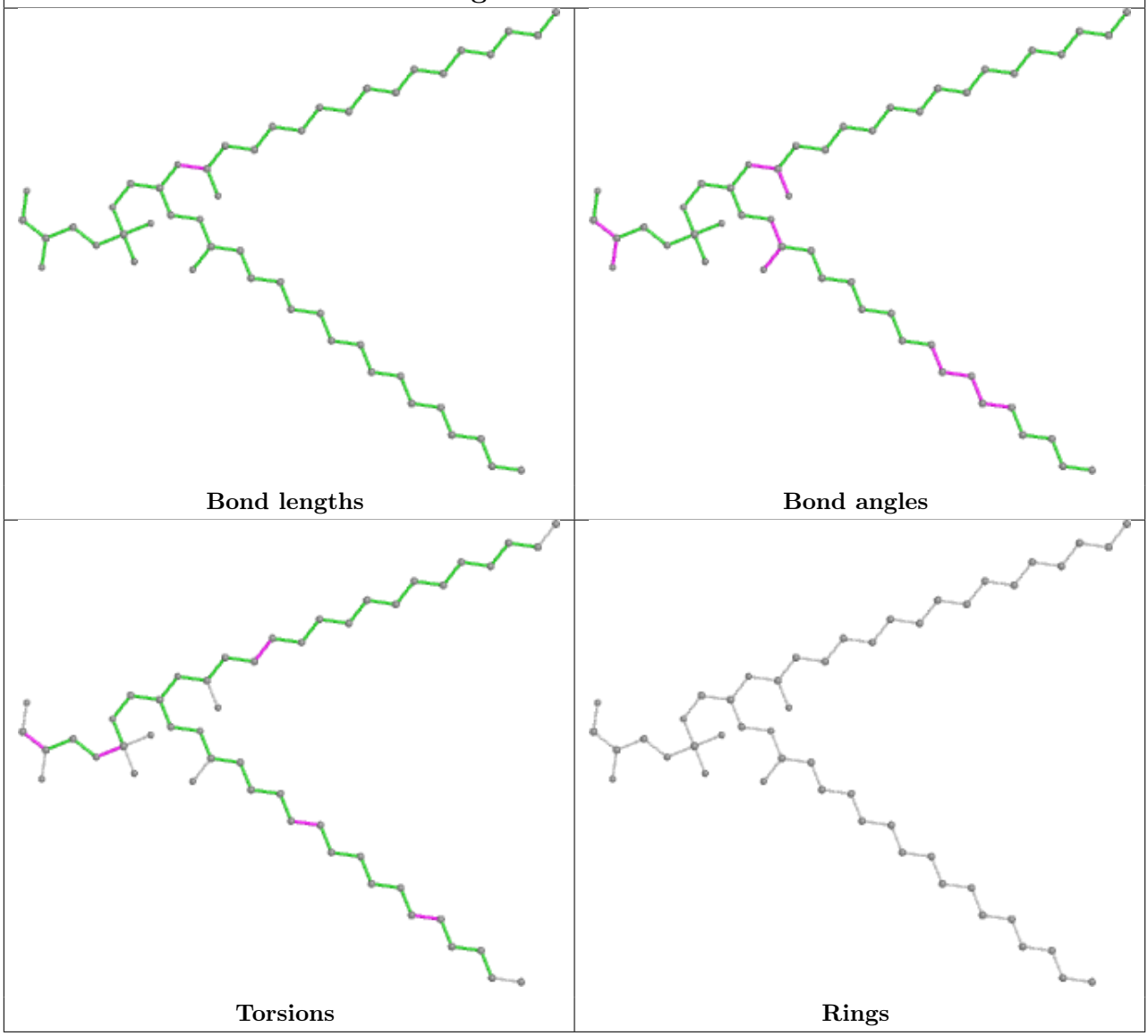
Ligand CLA c 510

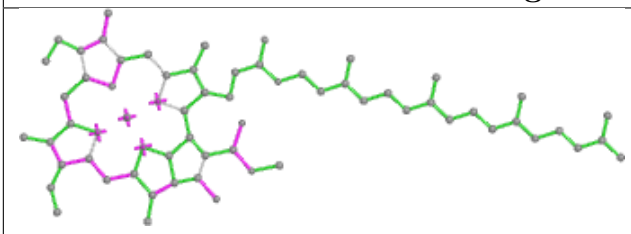
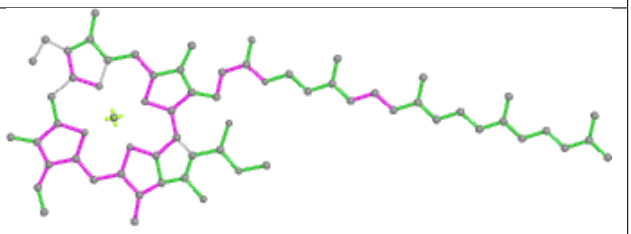
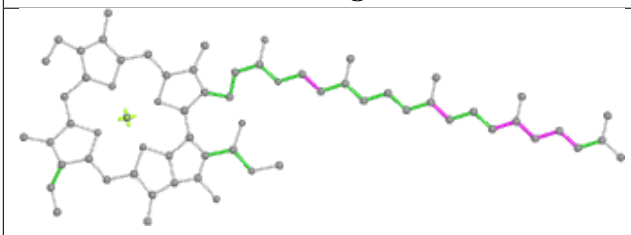
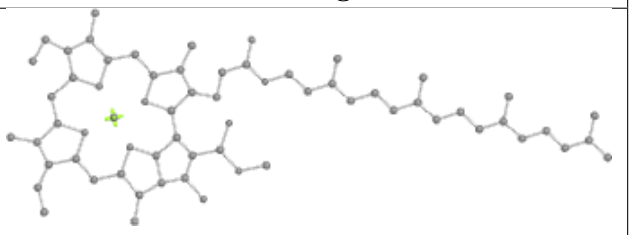


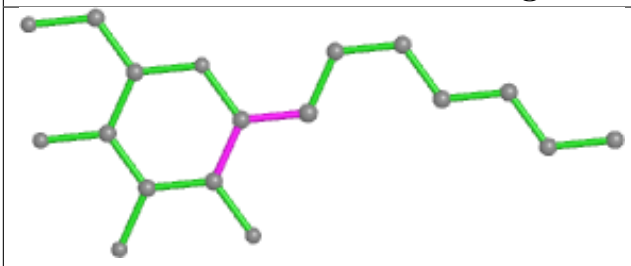
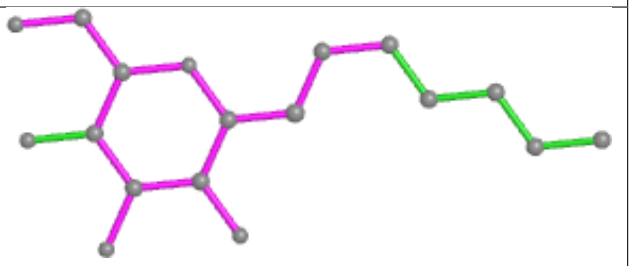
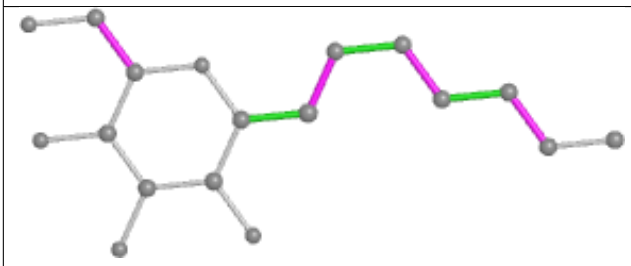
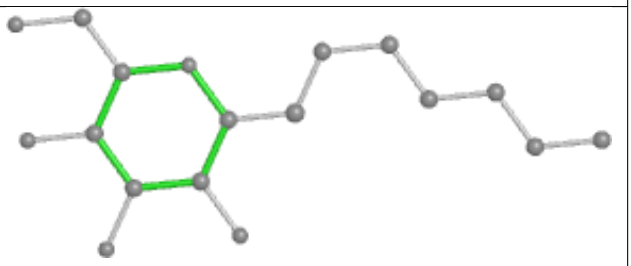
Ligand CLA C 513

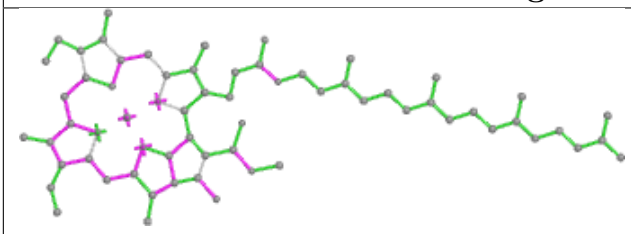
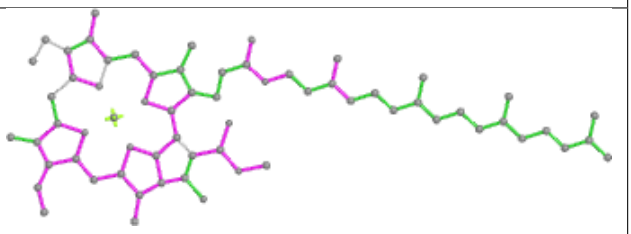
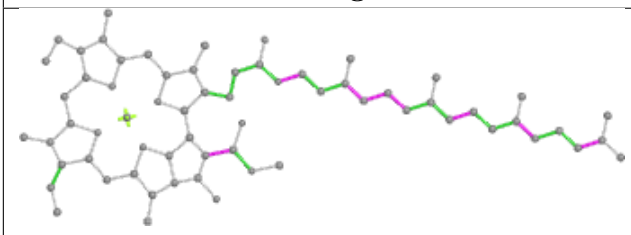
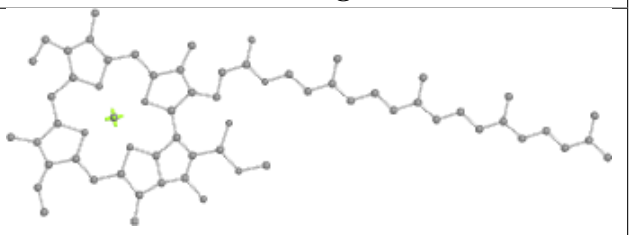


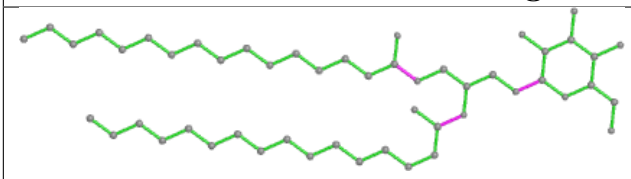
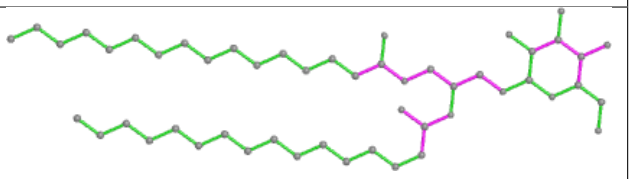
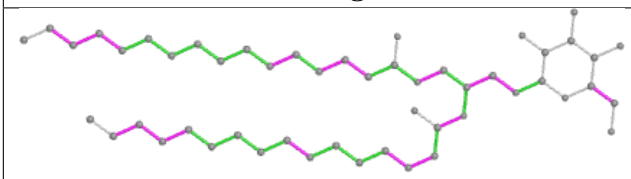
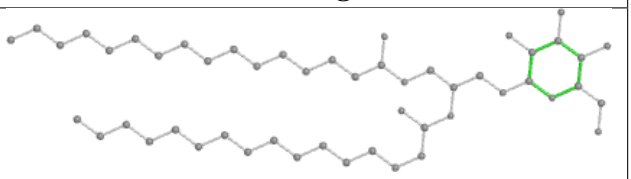
Ligand LHG d 410



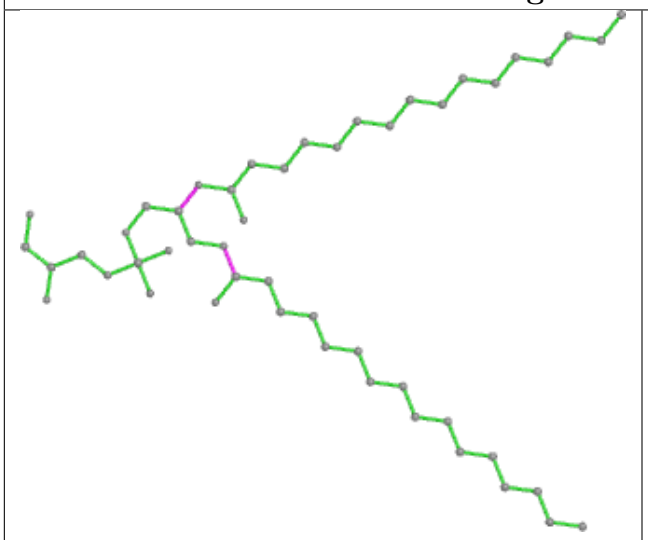
Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG B 642	
 Bond lengths	 Bond angles
 Torsions	 Rings

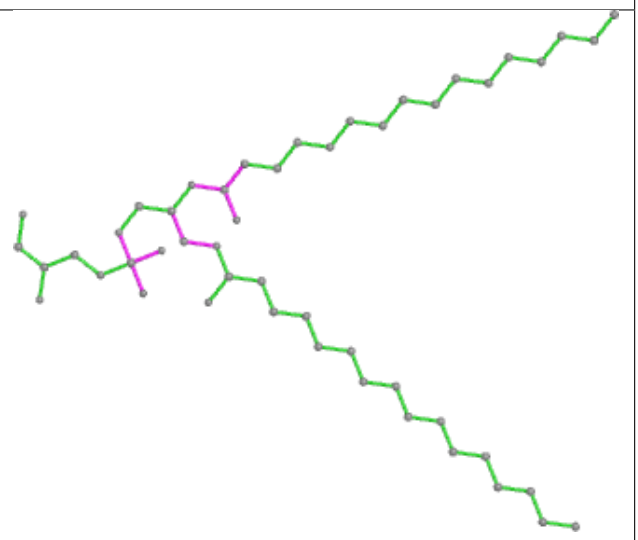
Ligand CLA b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

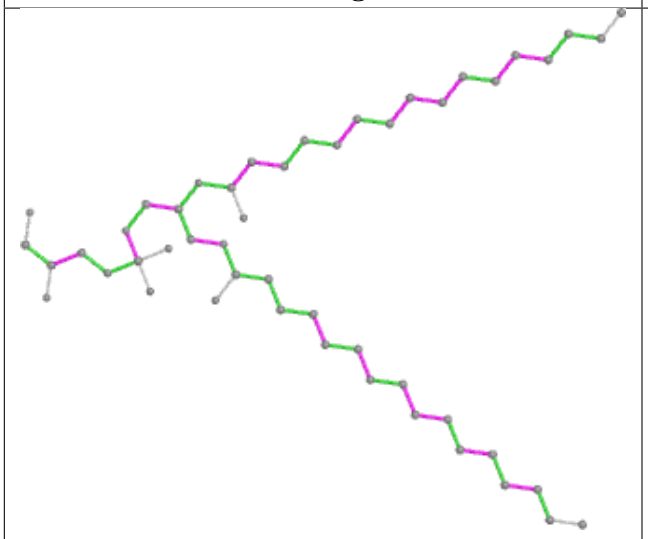
Ligand LHG b 624



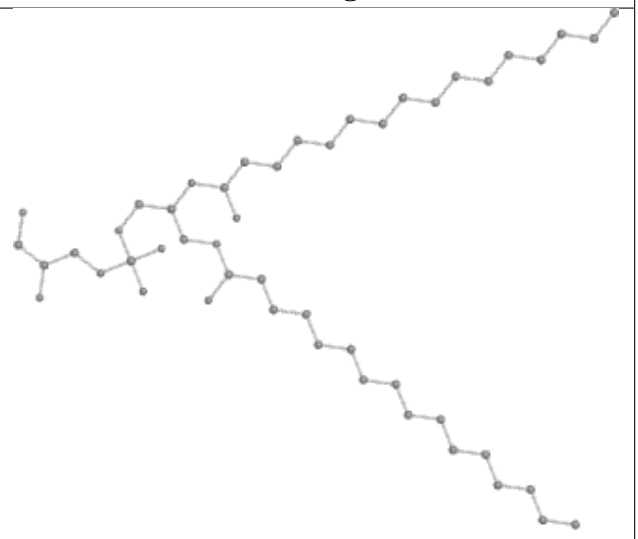
Bond lengths



Bond angles

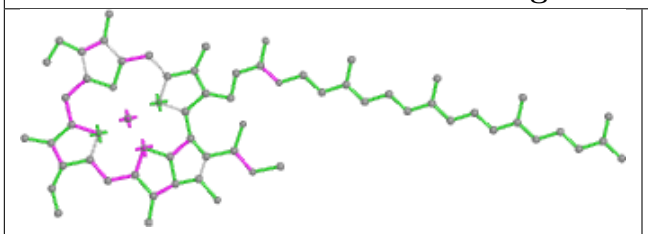


Torsions

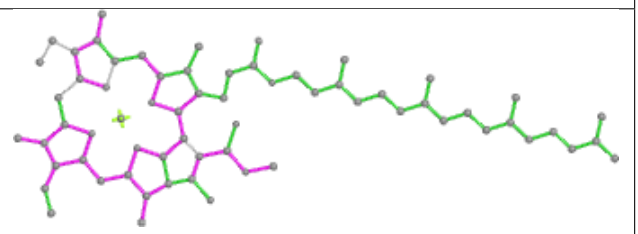


Rings

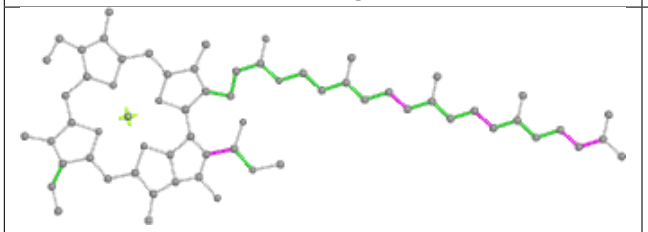
Ligand CLA c 507



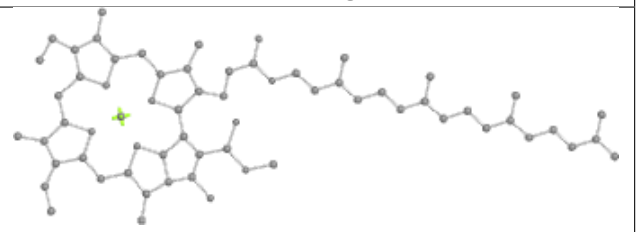
Bond lengths



Bond angles

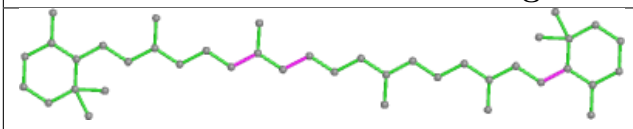


Torsions

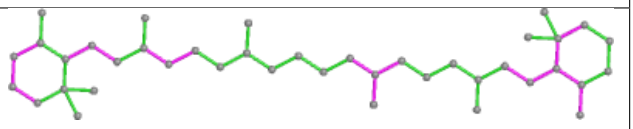


Rings

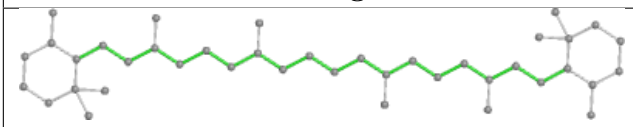
Ligand BCR B 620



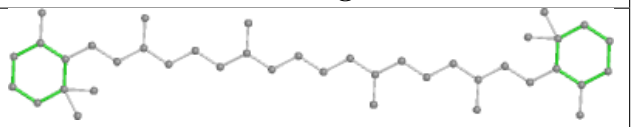
Bond lengths



Bond angles

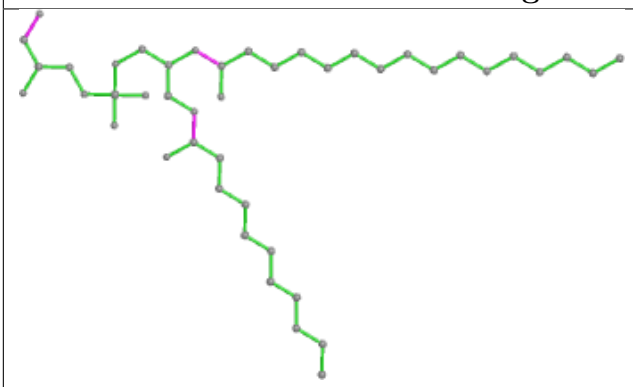


Torsions

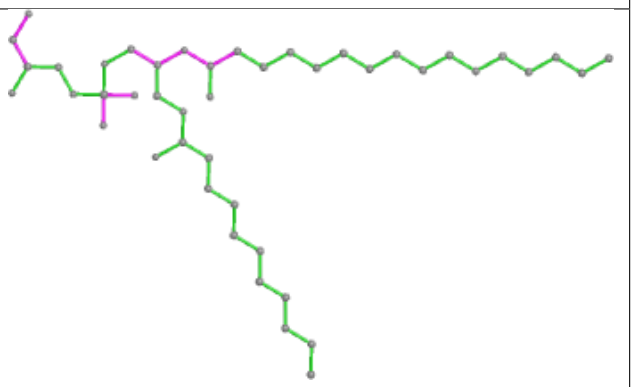


Rings

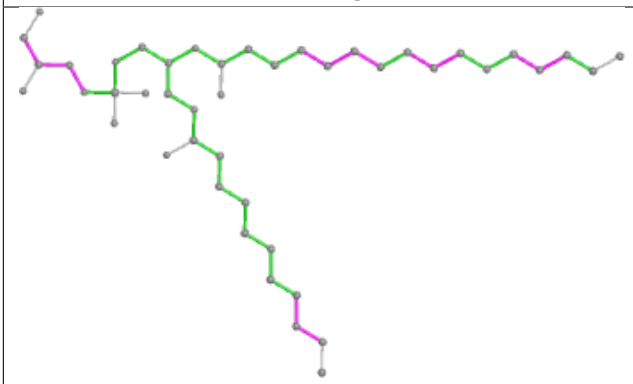
Ligand LHG D 411



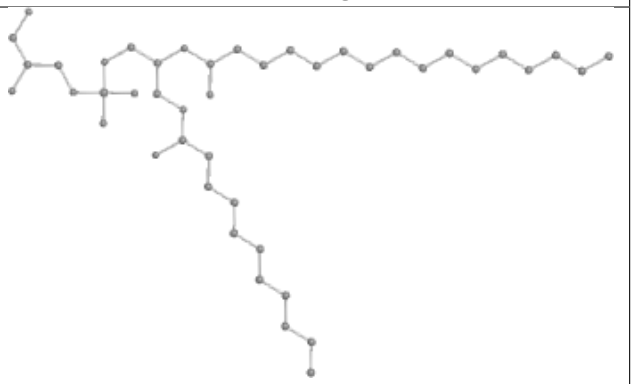
Bond lengths



Bond angles

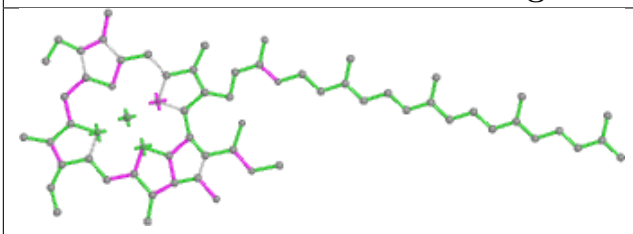


Torsions

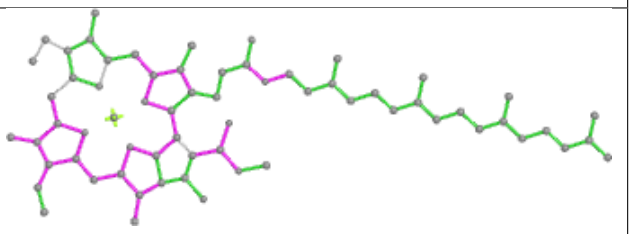


Rings

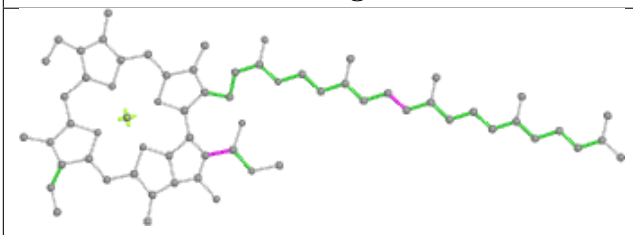
Ligand CLA b 607



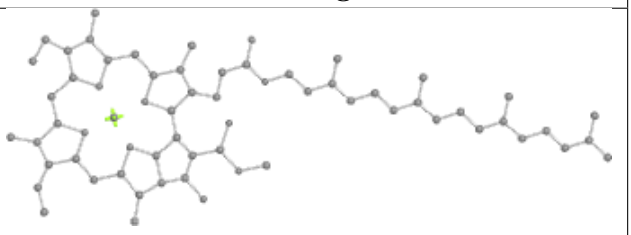
Bond lengths



Bond angles

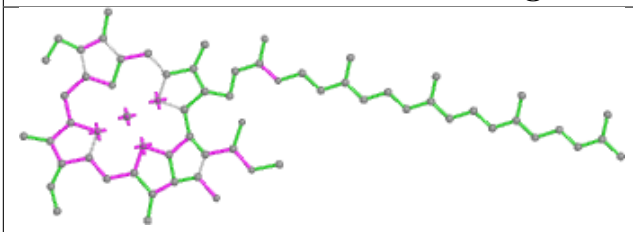


Torsions

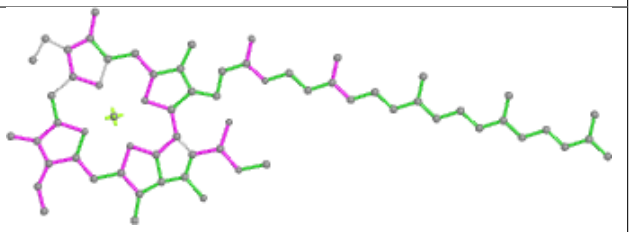


Rings

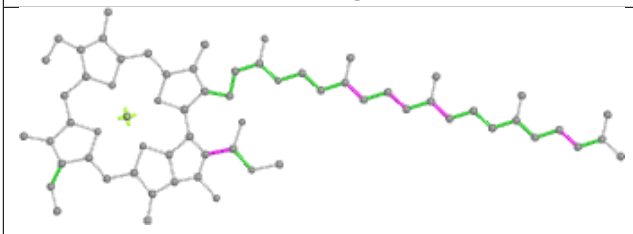
Ligand CLA C 507



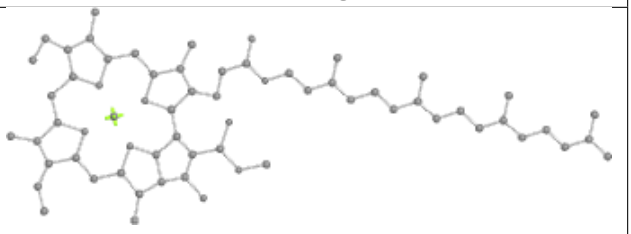
Bond lengths



Bond angles

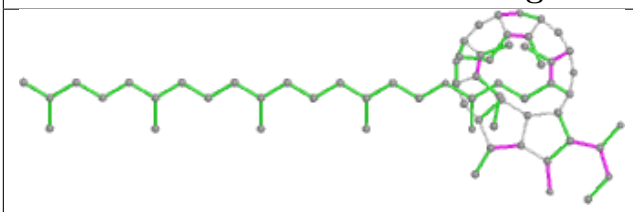


Torsions

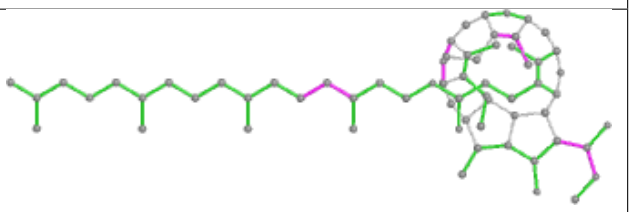


Rings

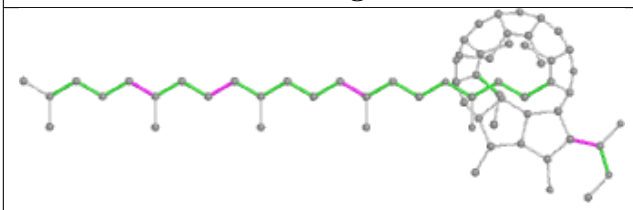
Ligand PHO a 408



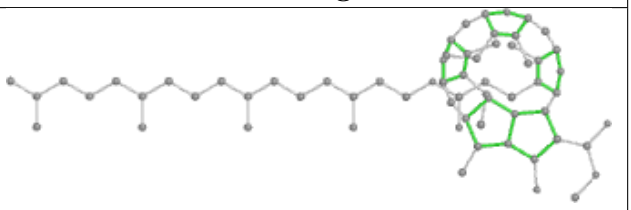
Bond lengths



Bond angles

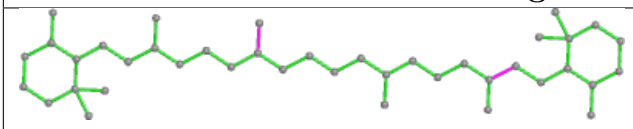


Torsions

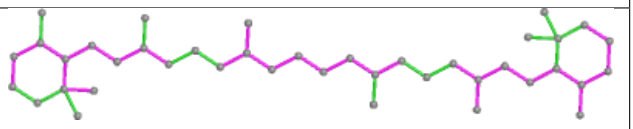


Rings

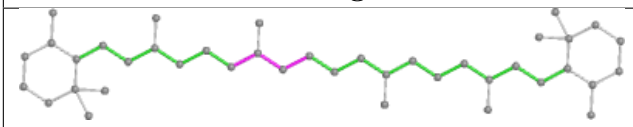
Ligand BCR t 101



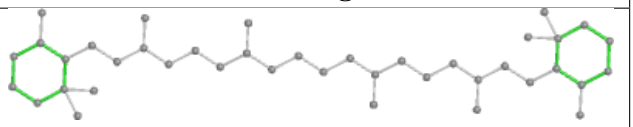
Bond lengths



Bond angles

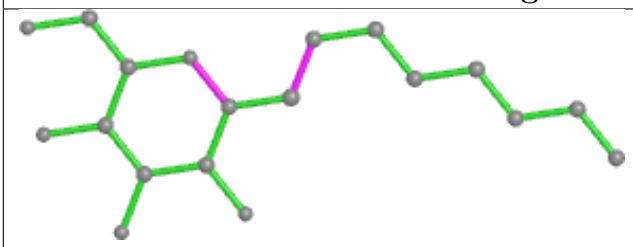


Torsions

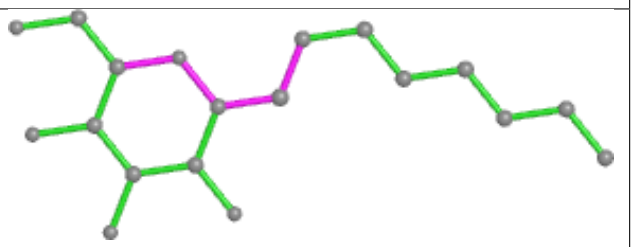


Rings

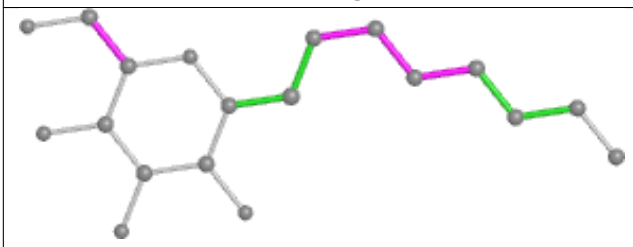
Ligand HTG C 522



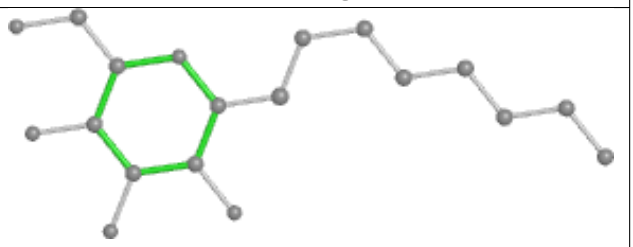
Bond lengths



Bond angles

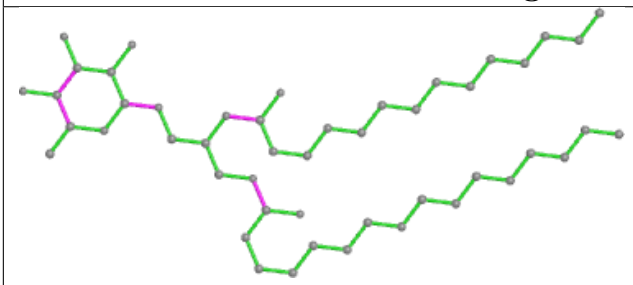


Torsions

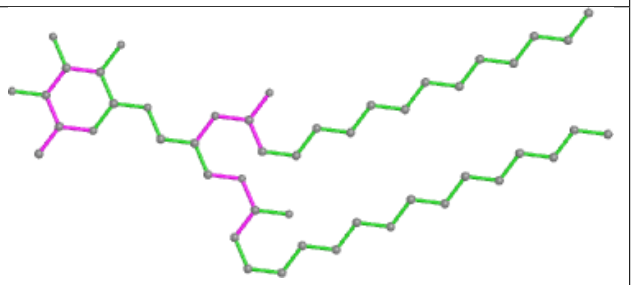


Rings

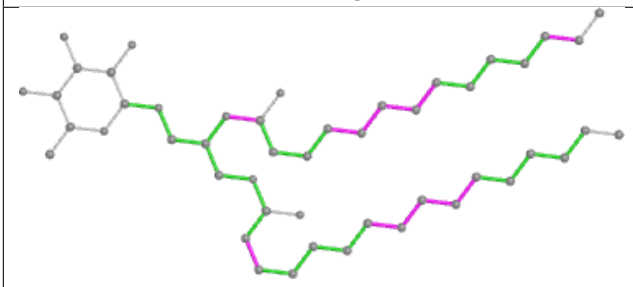
Ligand DGD d 408



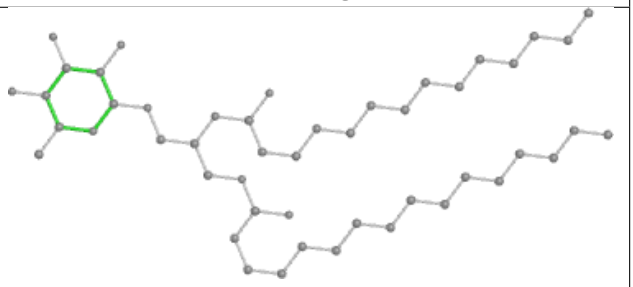
Bond lengths



Bond angles

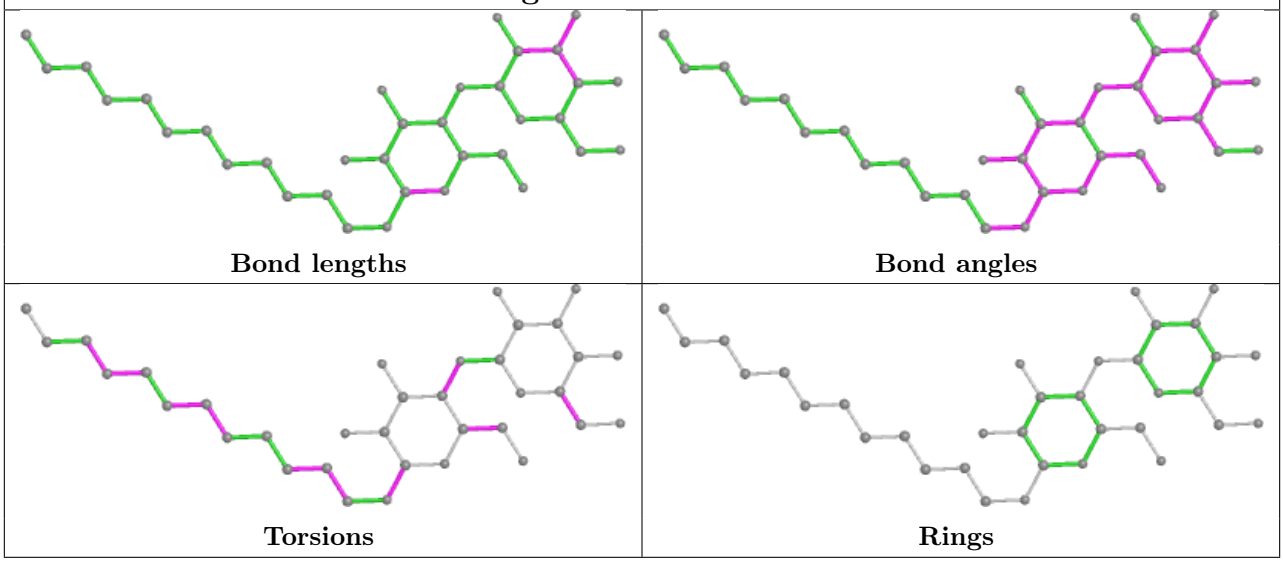


Torsions

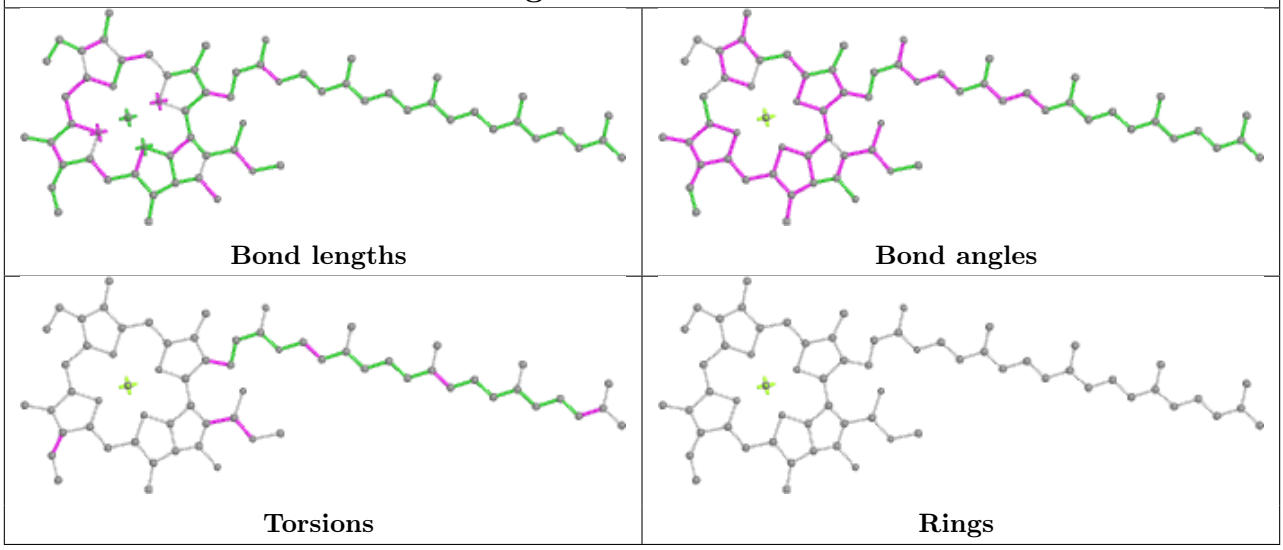


Rings

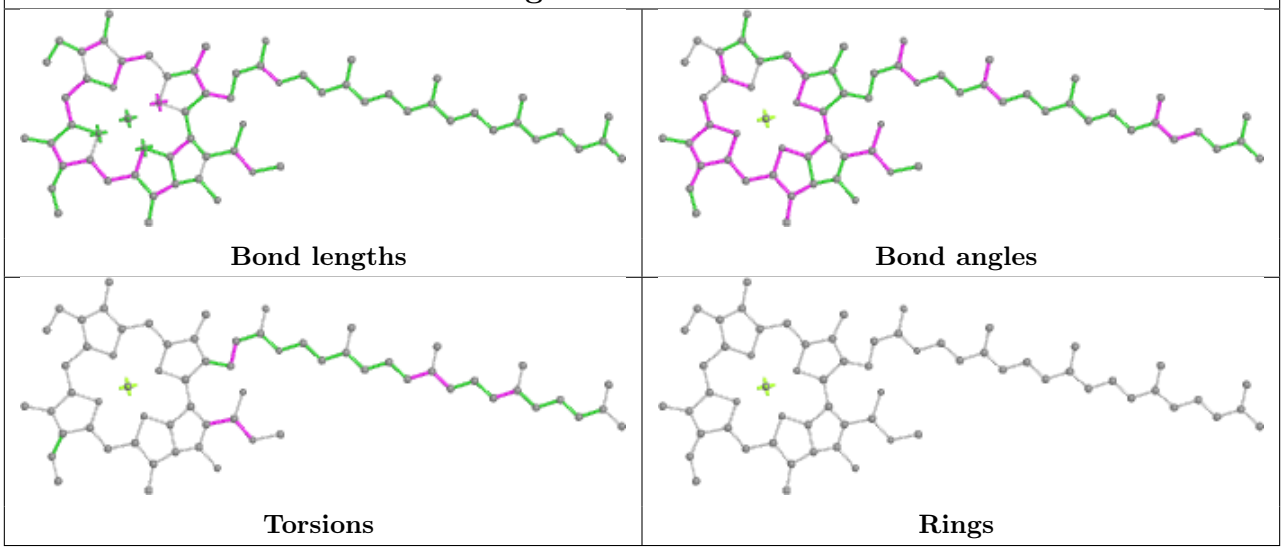
Ligand LMT A 415



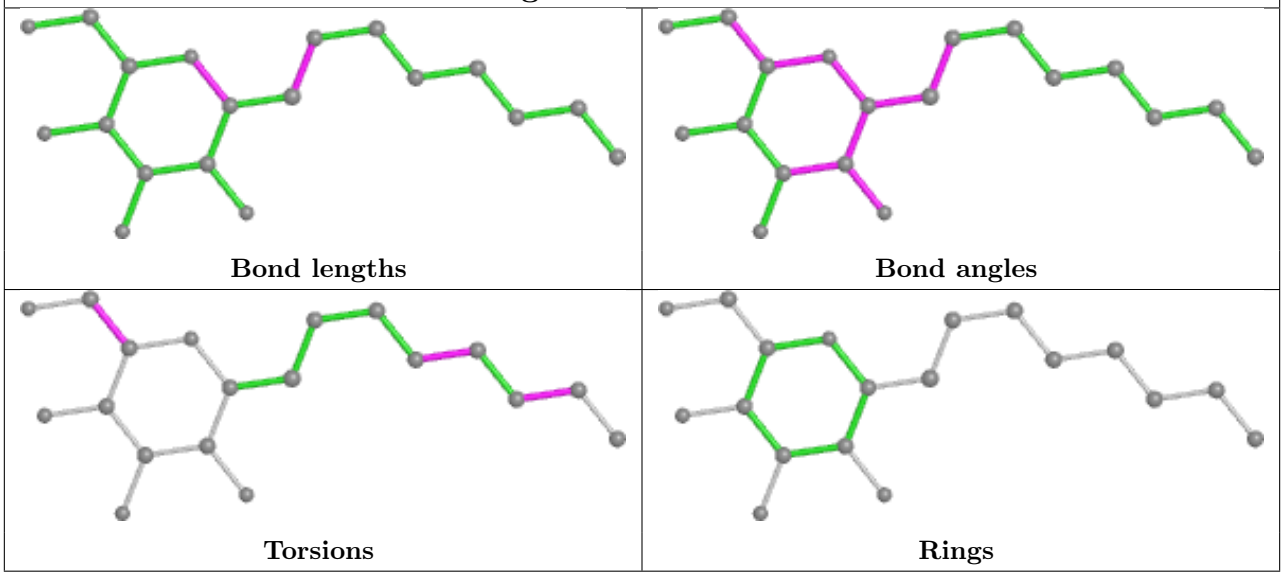
Ligand CLA B 605



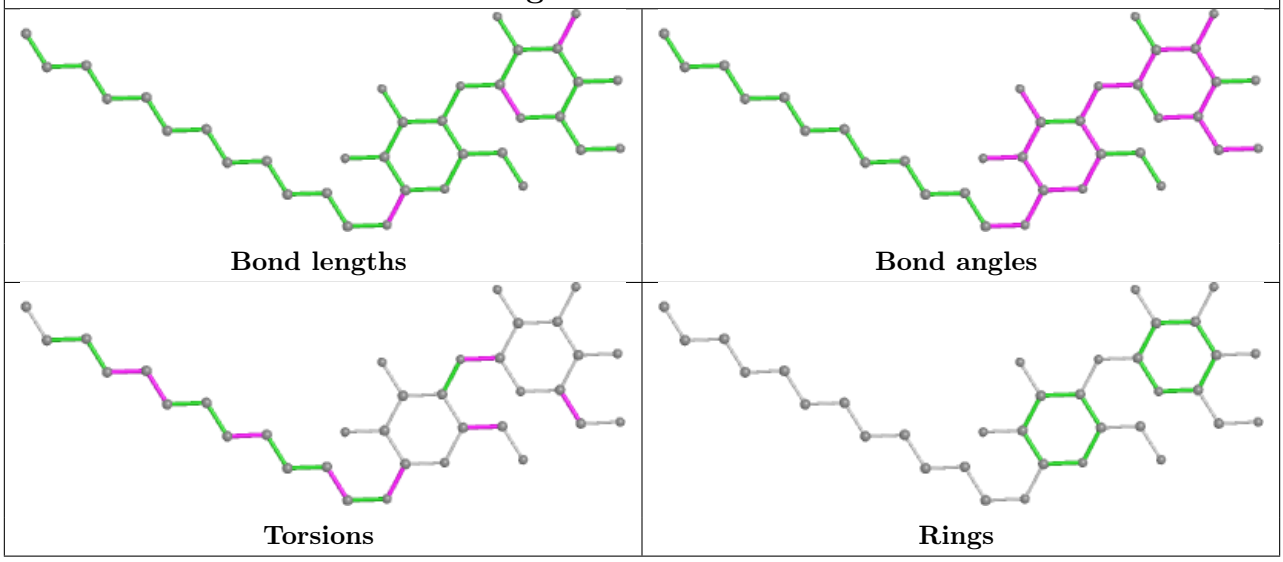
Ligand CLA B 607



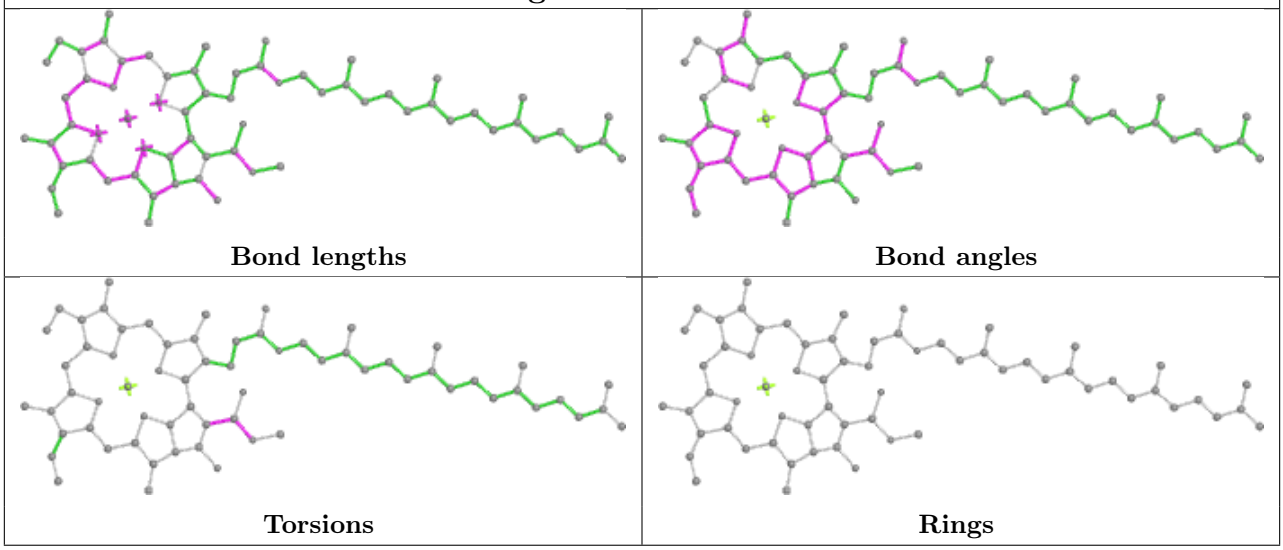
Ligand HTG V 202



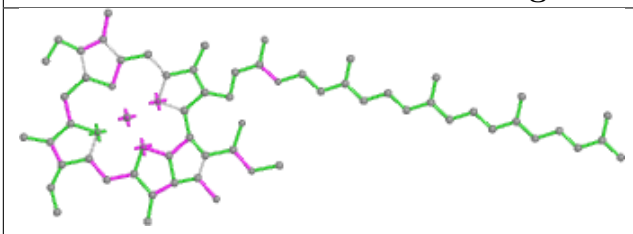
Ligand LMT a 401



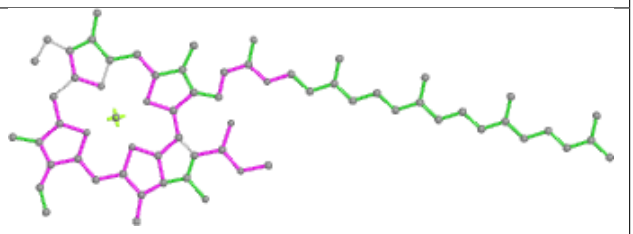
Ligand CLA b 613



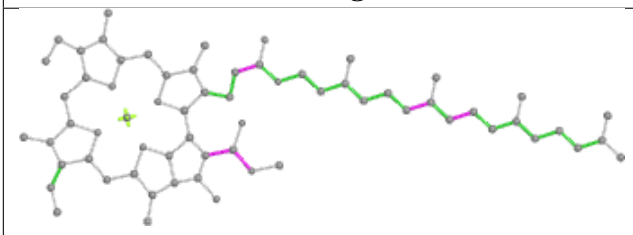
Ligand CLA c 511



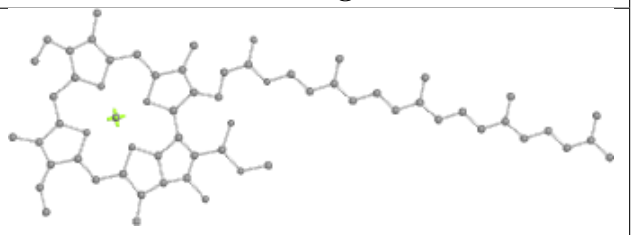
Bond lengths



Bond angles

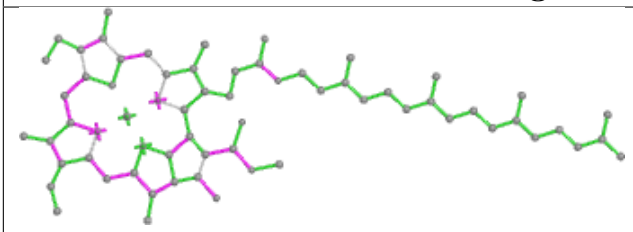


Torsions

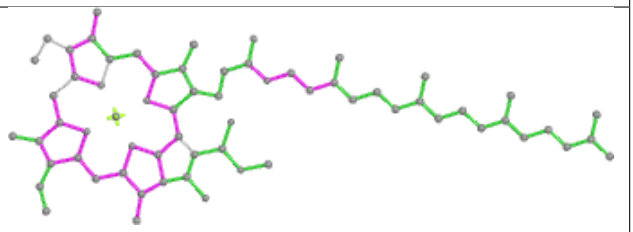


Rings

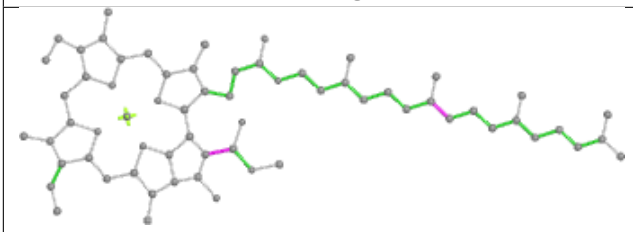
Ligand CLA c 509



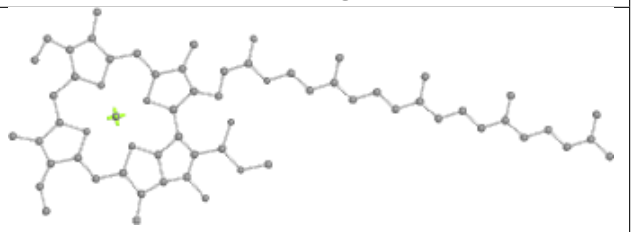
Bond lengths



Bond angles

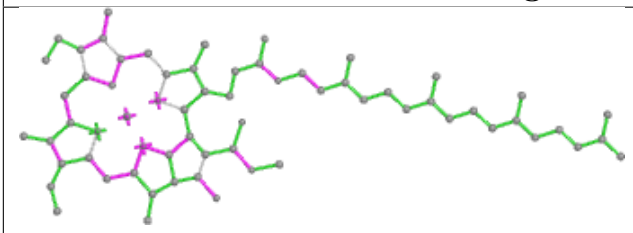


Torsions

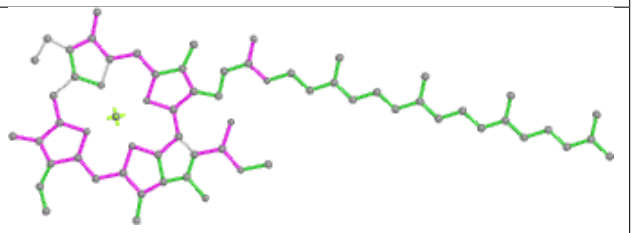


Rings

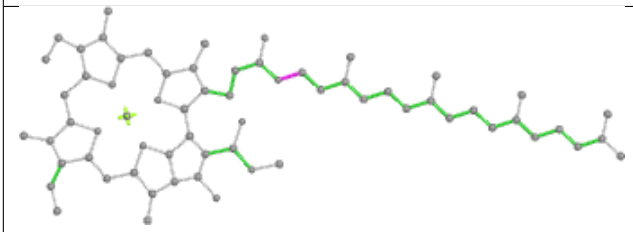
Ligand CLA D 403



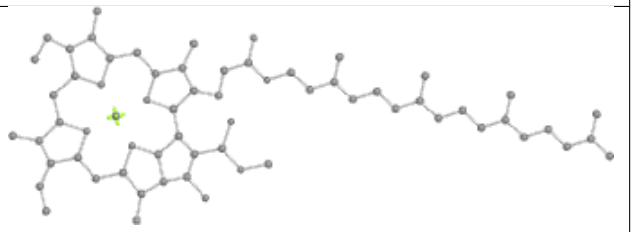
Bond lengths



Bond angles

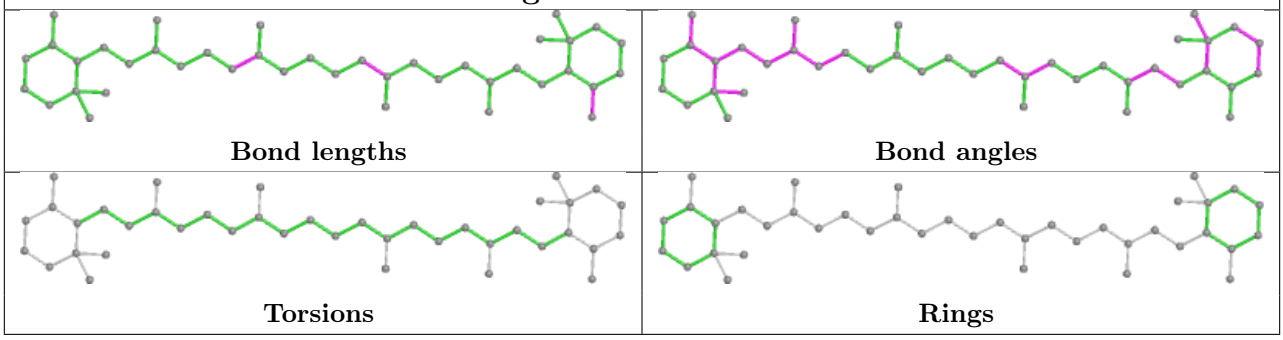


Torsions

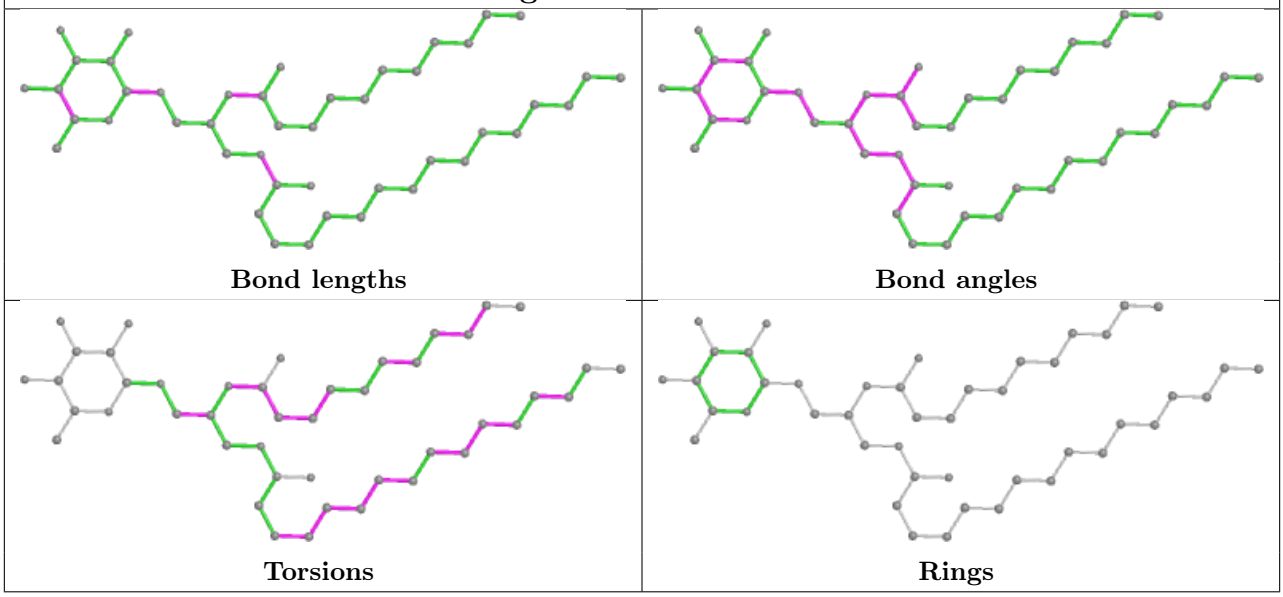


Rings

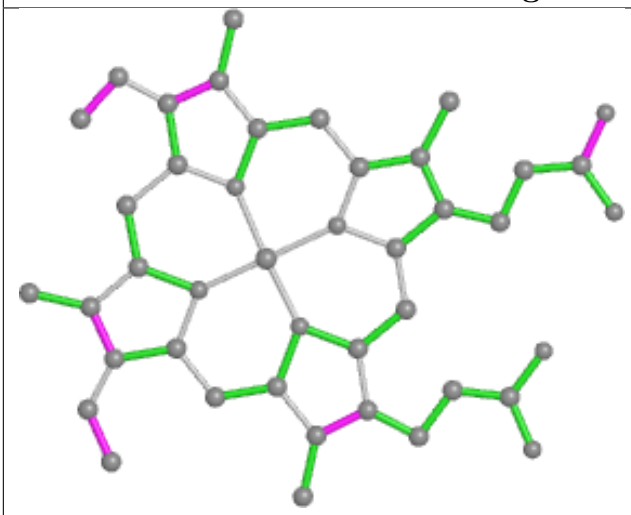
Ligand BCR K 101



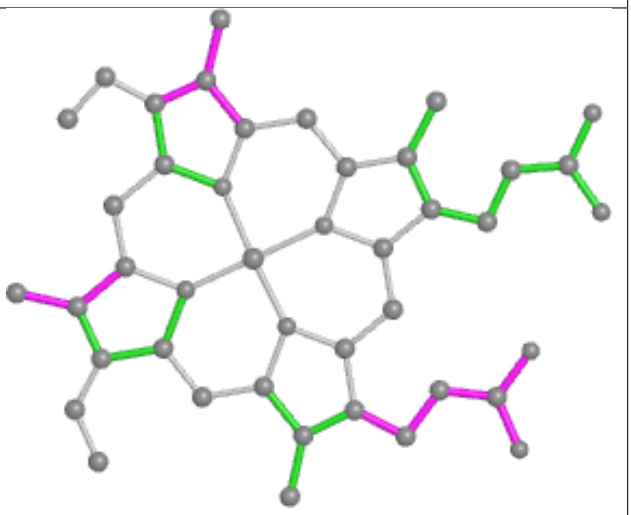
Ligand DGD D 408



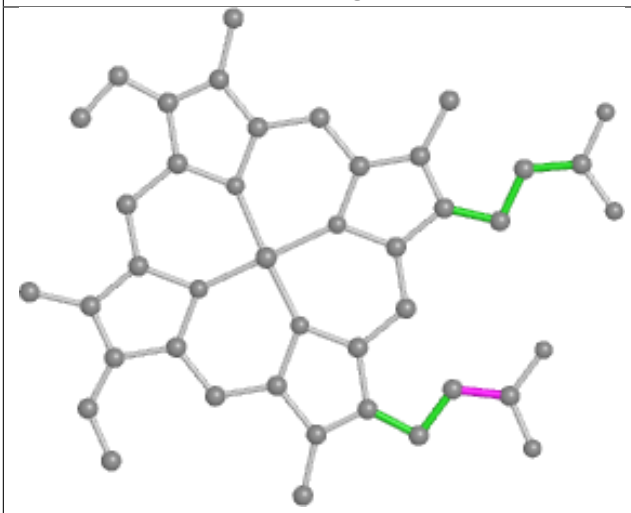
Ligand HEC V 201



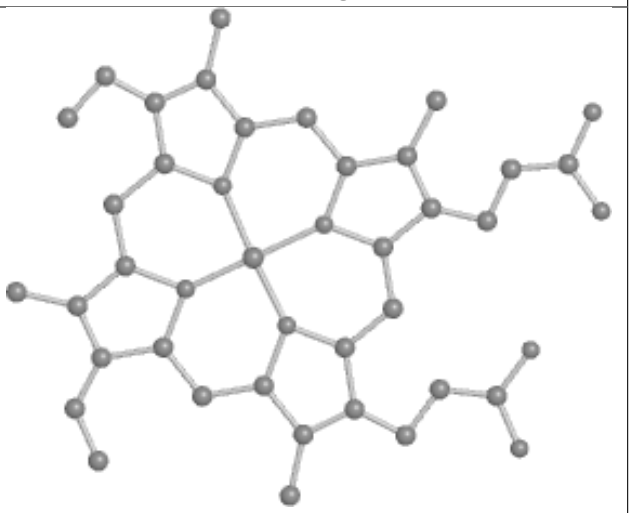
Bond lengths



Bond angles

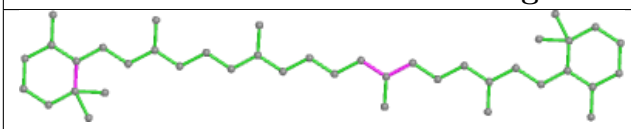


Torsions

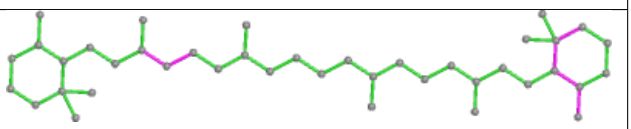


Rings

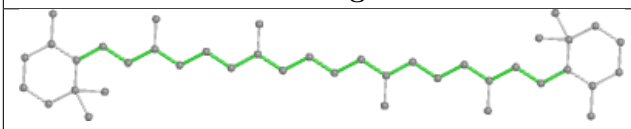
Ligand BCR K 102



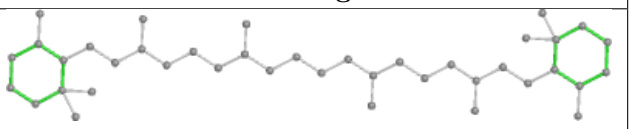
Bond lengths



Bond angles

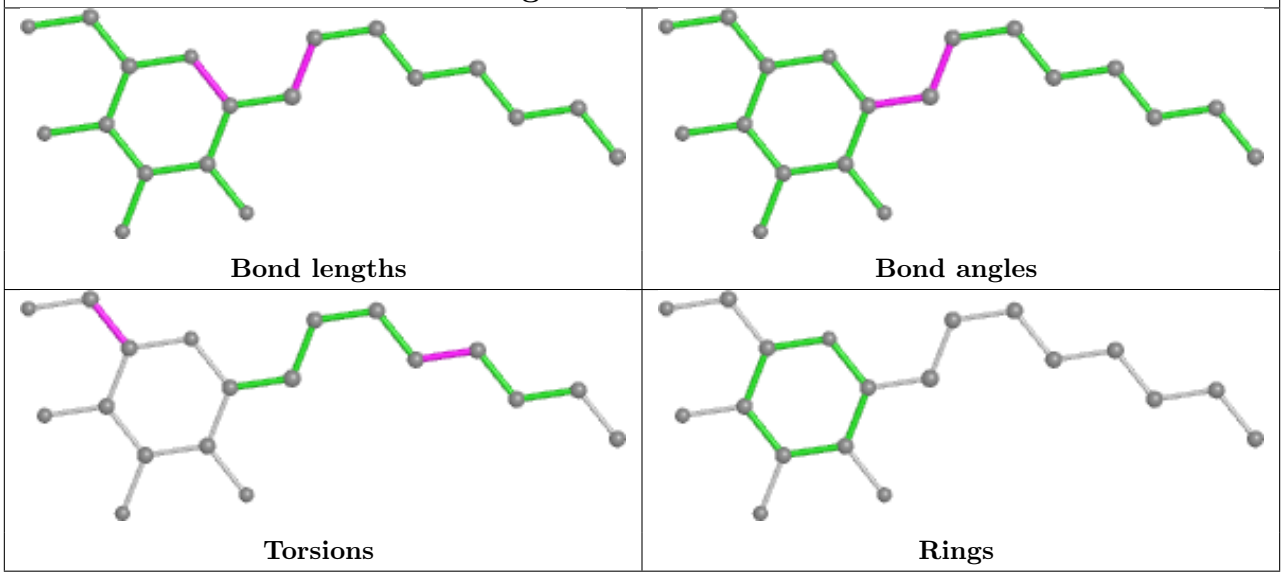


Torsions

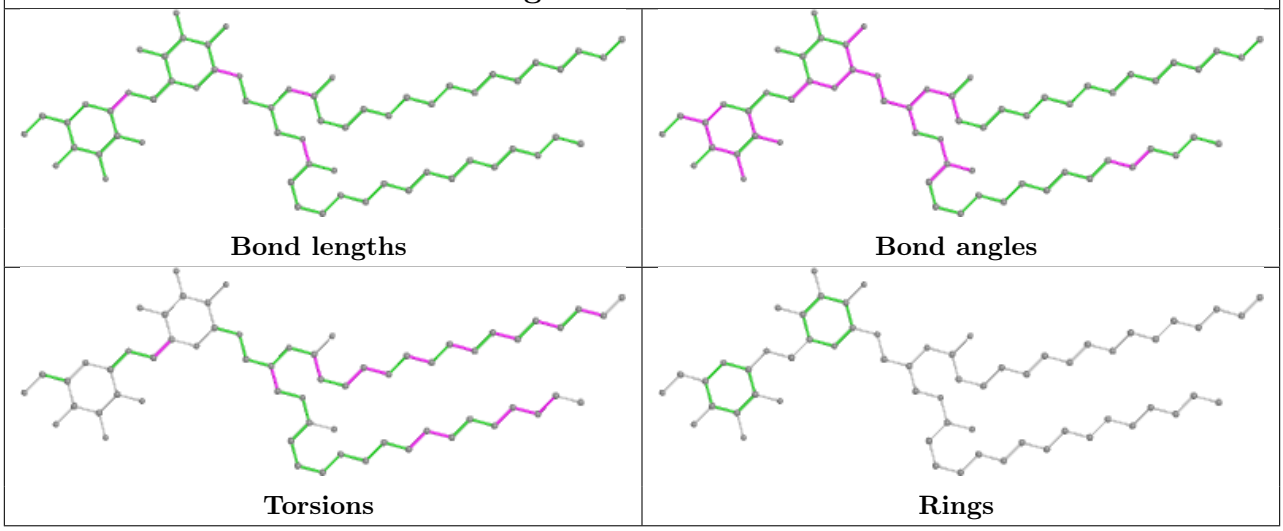


Rings

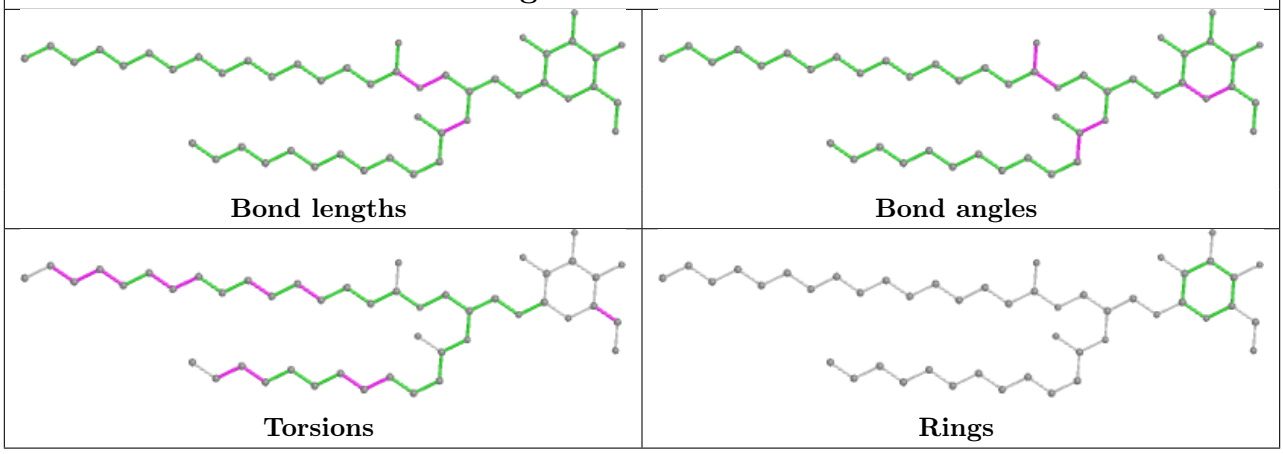
Ligand HTG C 536



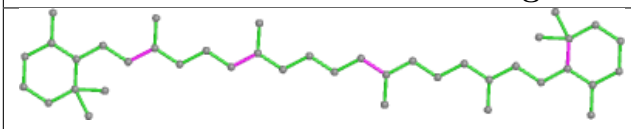
Ligand DGD h 101



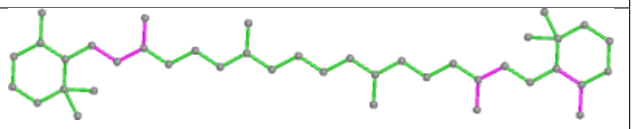
Ligand LMG D 412



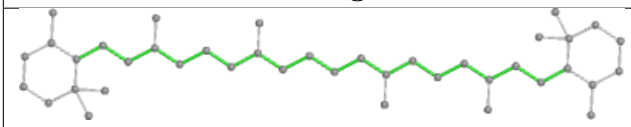
Ligand BCR C 514



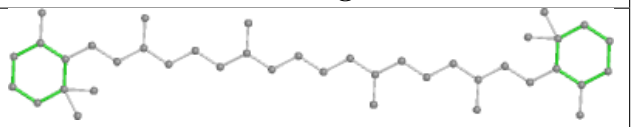
Bond lengths



Bond angles

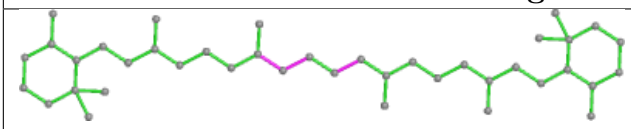


Torsions

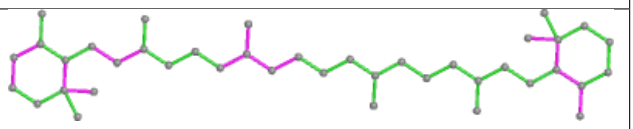


Rings

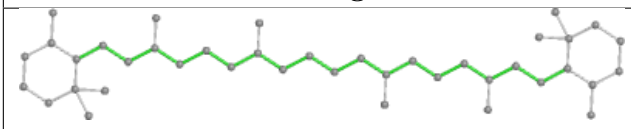
Ligand BCR c 516



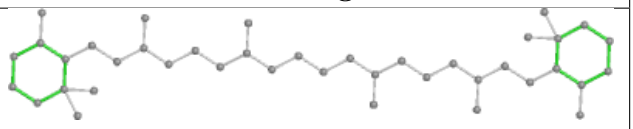
Bond lengths



Bond angles

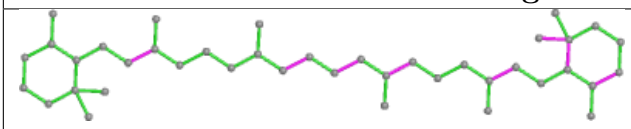


Torsions

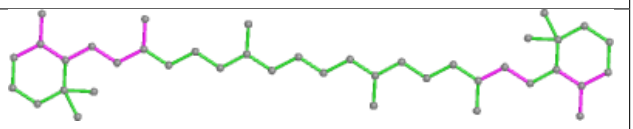


Rings

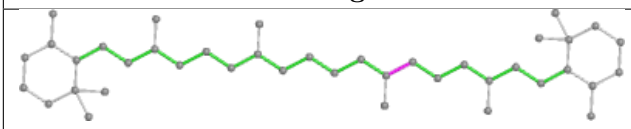
Ligand BCR A 409



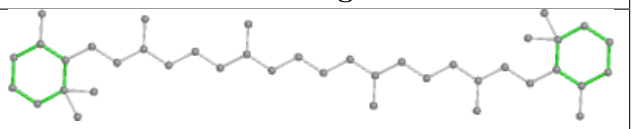
Bond lengths



Bond angles

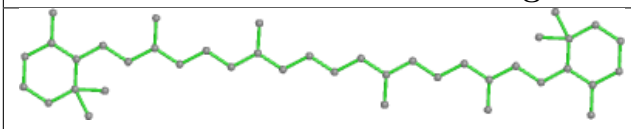


Torsions

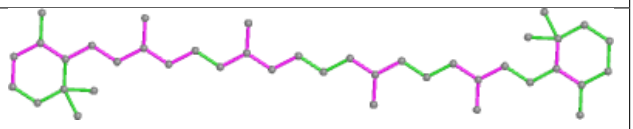


Rings

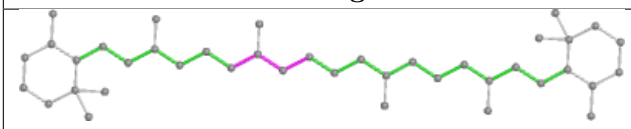
Ligand BCR T 101



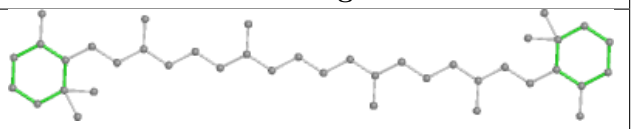
Bond lengths



Bond angles

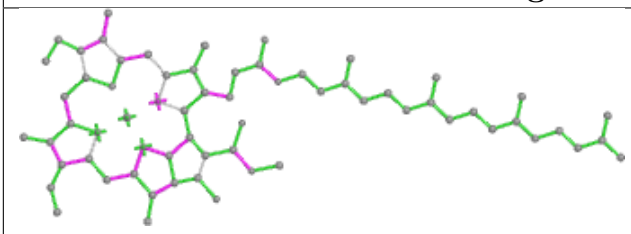


Torsions

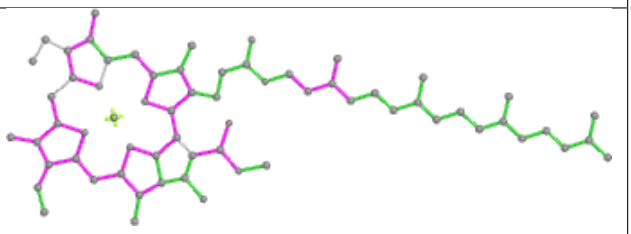


Rings

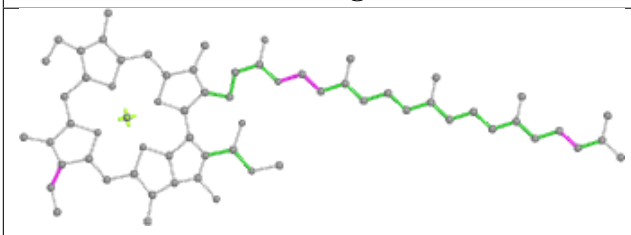
Ligand CLA d 402



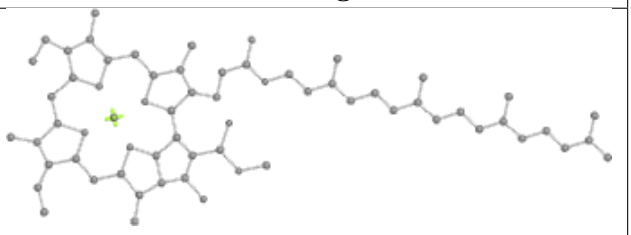
Bond lengths



Bond angles

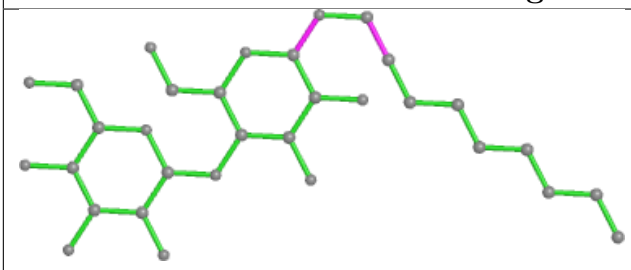


Torsions

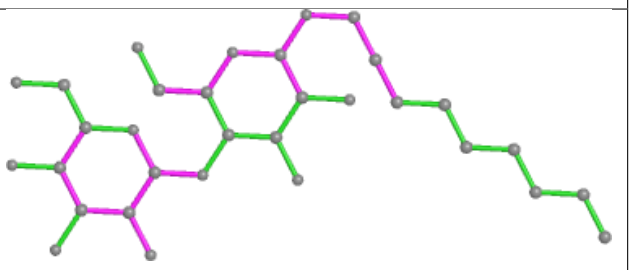


Rings

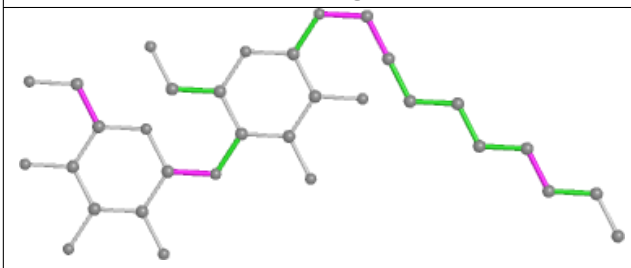
Ligand LMT z 101



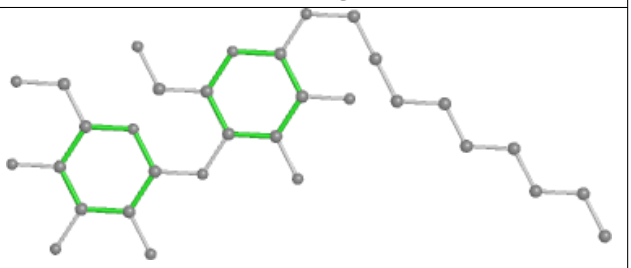
Bond lengths



Bond angles

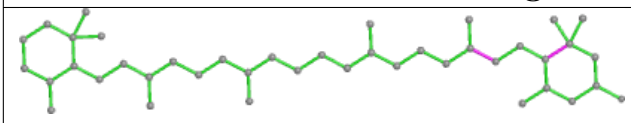


Torsions

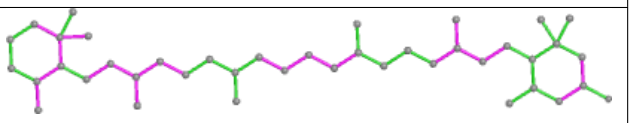


Rings

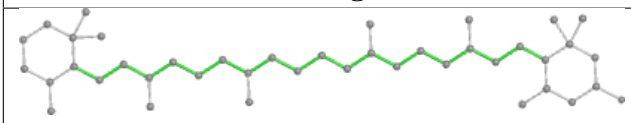
Ligand RRX h 102



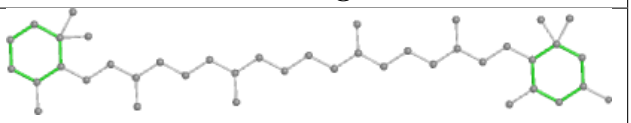
Bond lengths



Bond angles

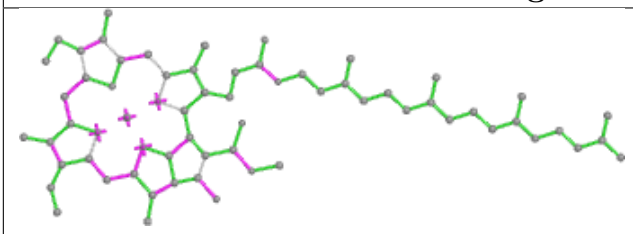


Torsions

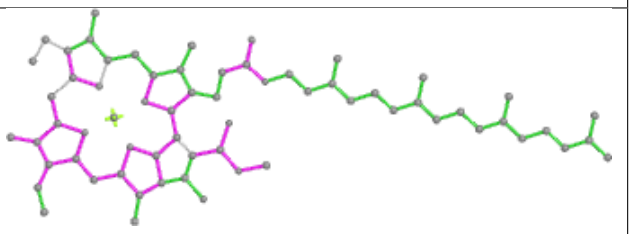


Rings

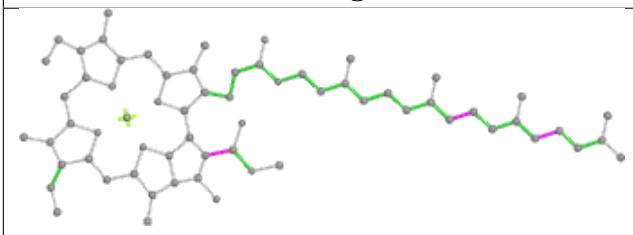
Ligand CLA b 616



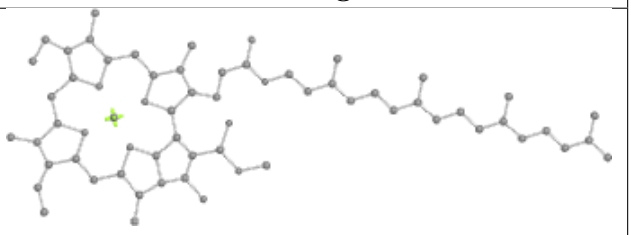
Bond lengths



Bond angles

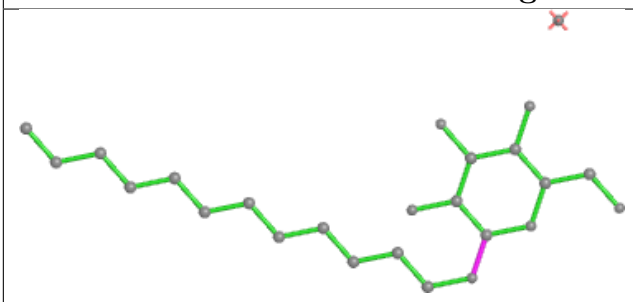


Torsions

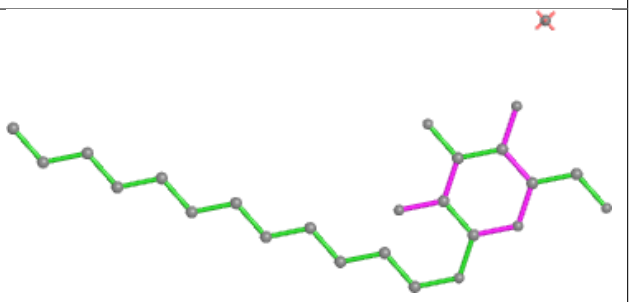


Rings

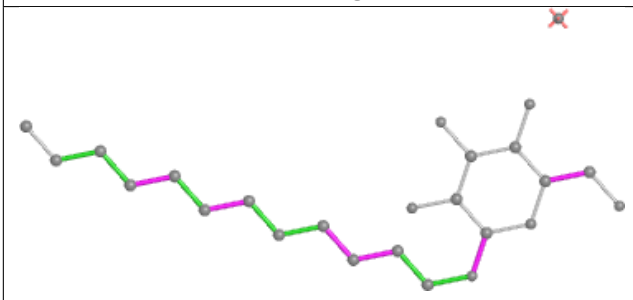
Ligand LMT m 102



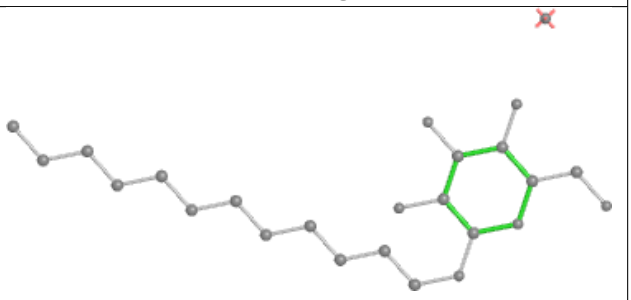
Bond lengths



Bond angles

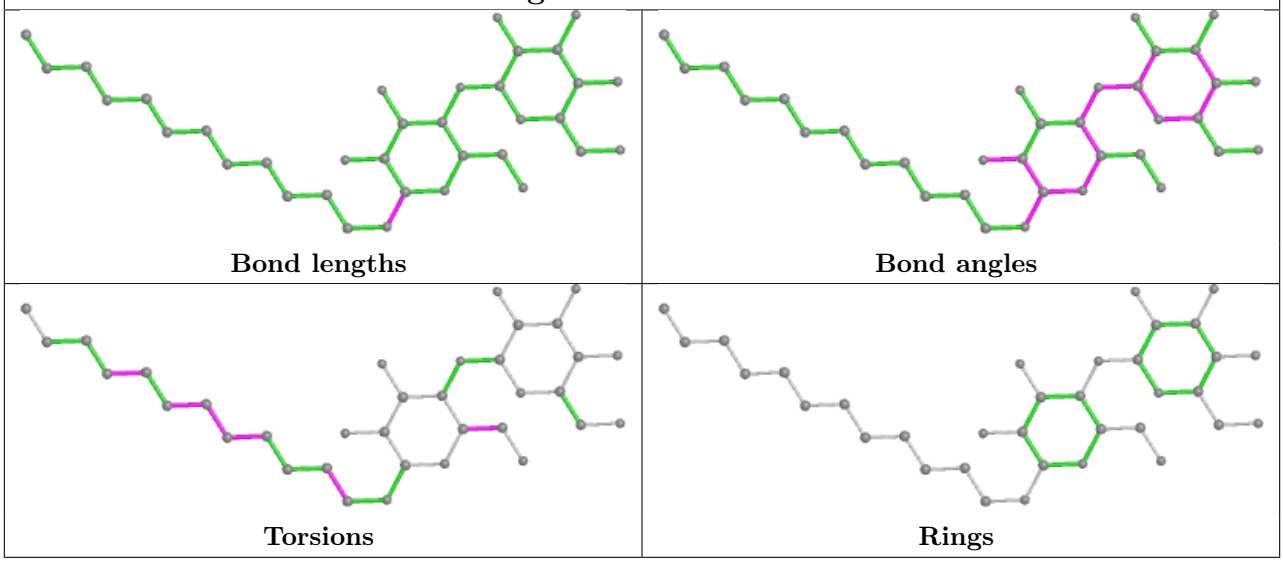


Torsions

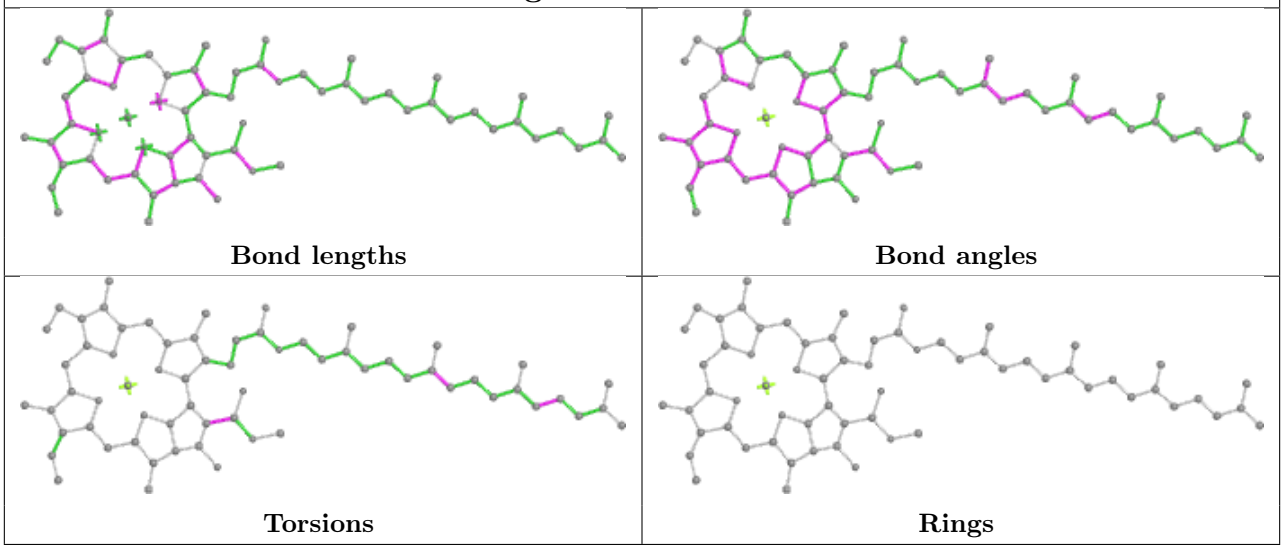


Rings

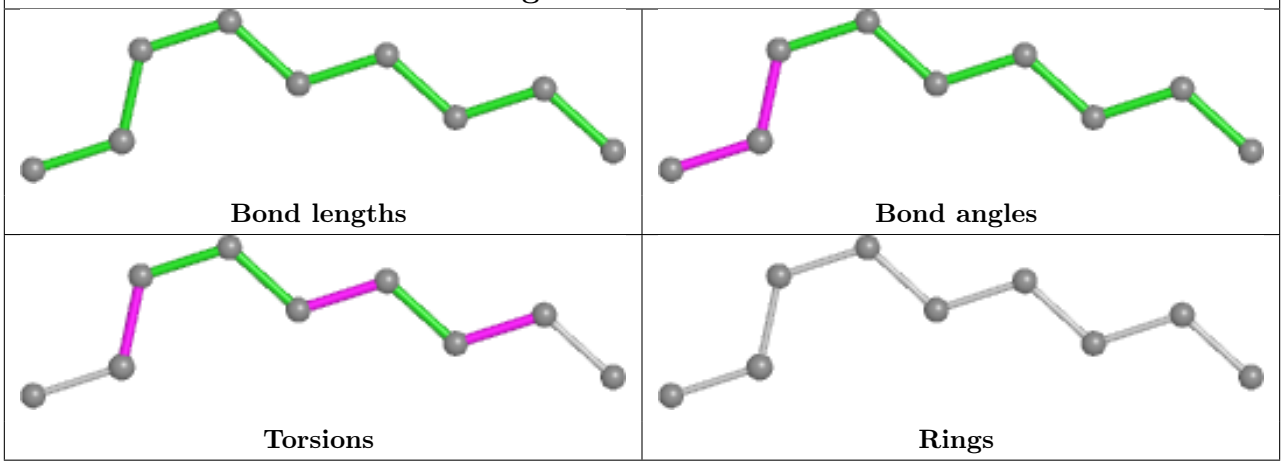
Ligand LMT c 522

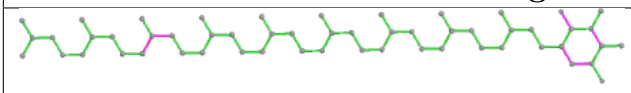
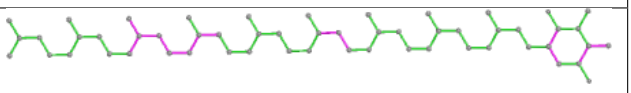
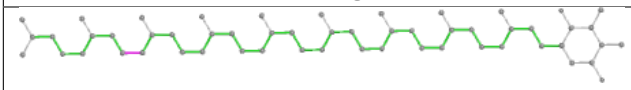
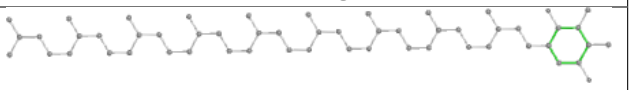


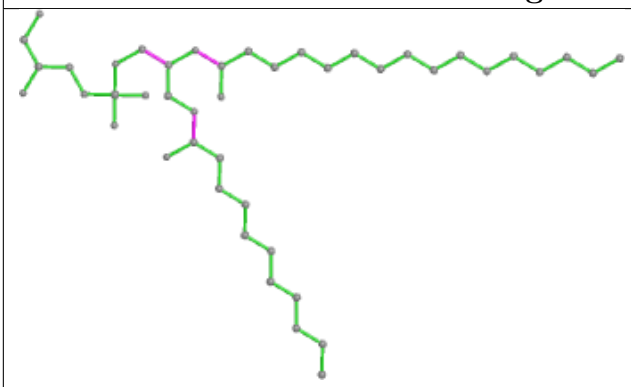
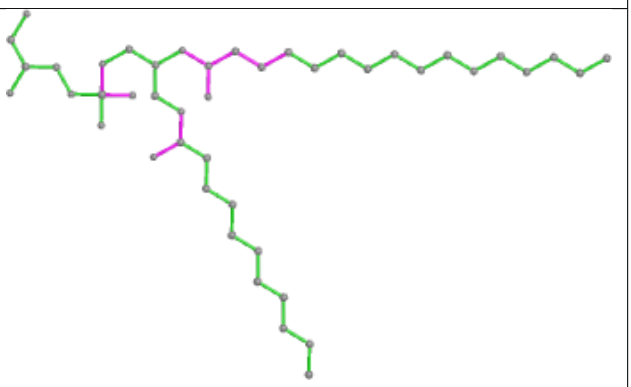
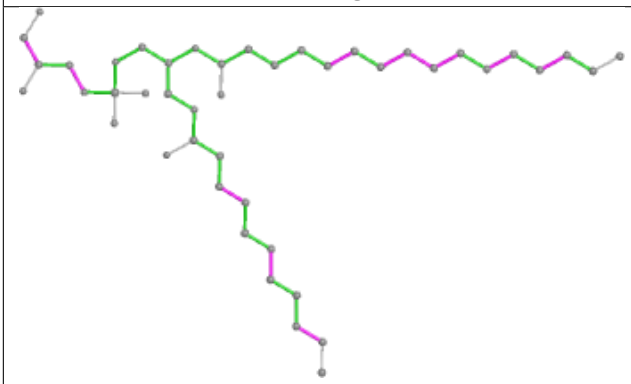
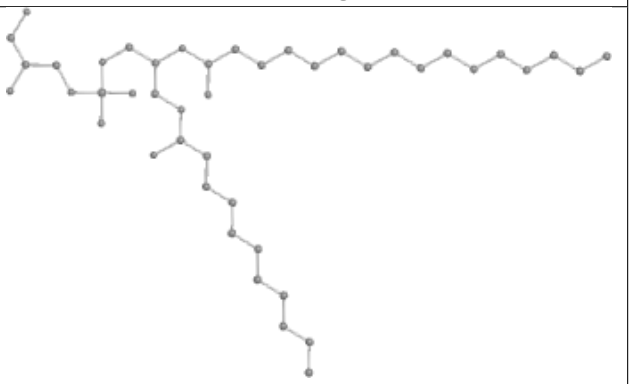
Ligand CLA A 406



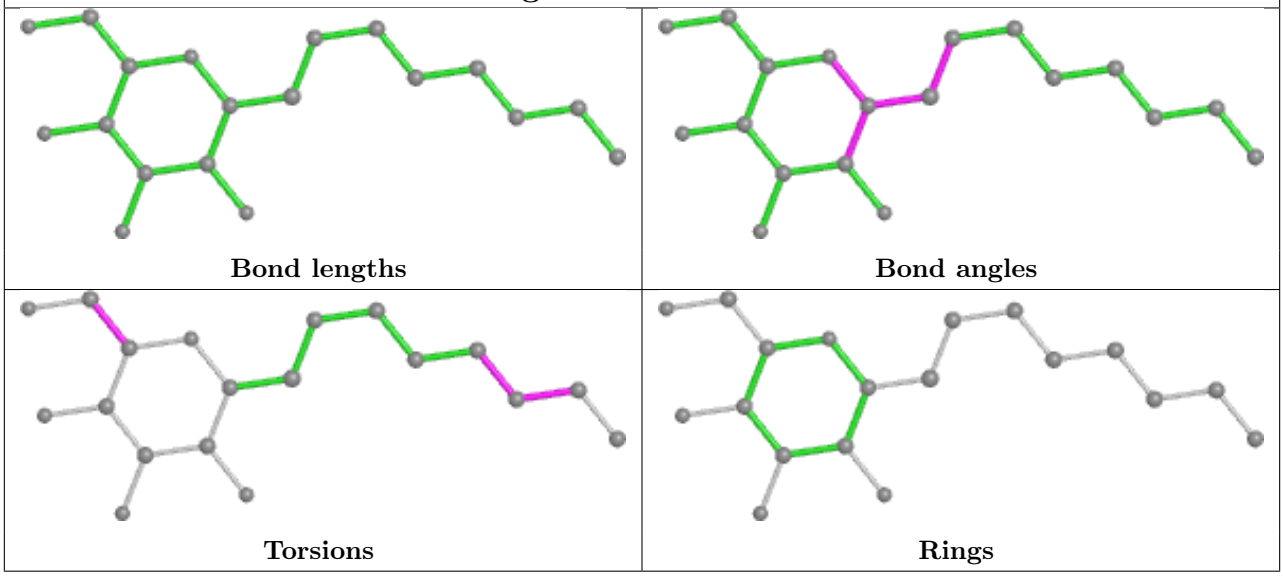
Ligand HTG C 535



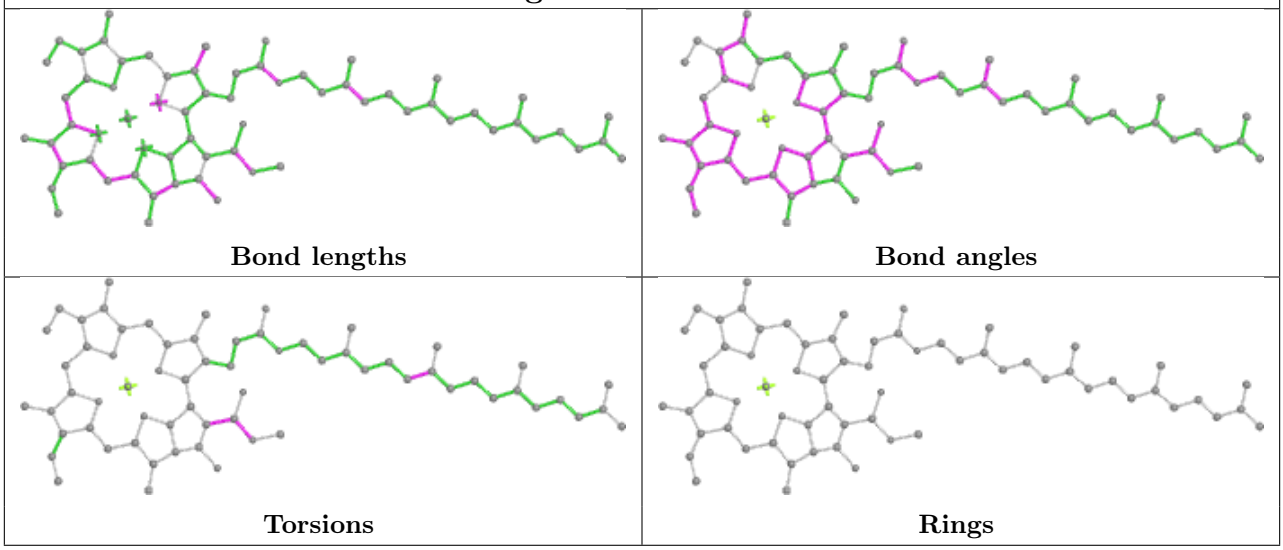
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

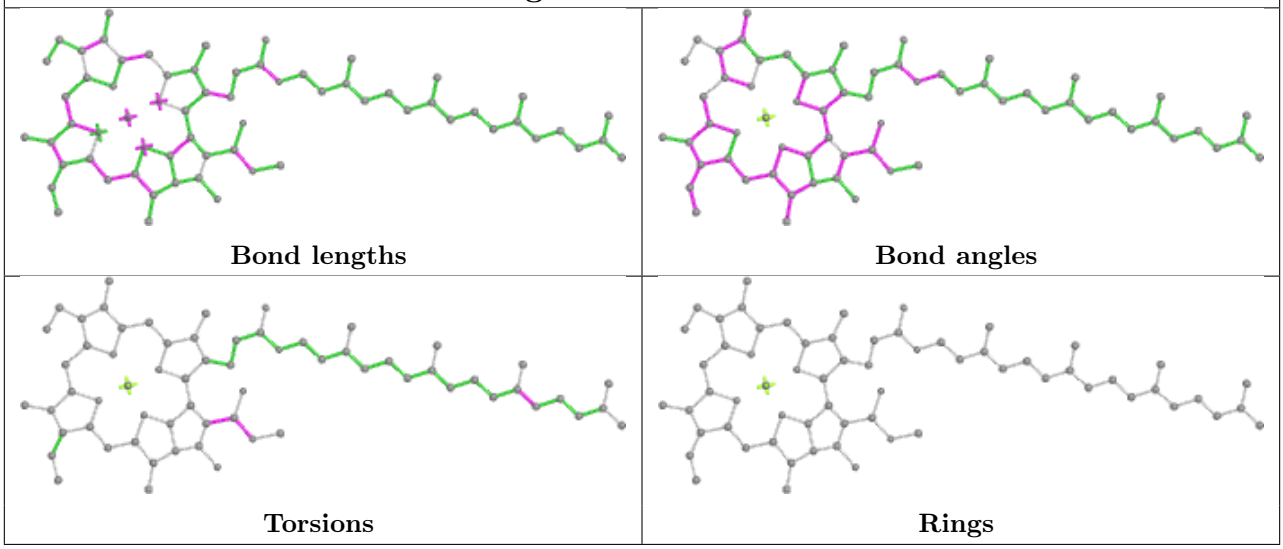
Ligand HTG B 628



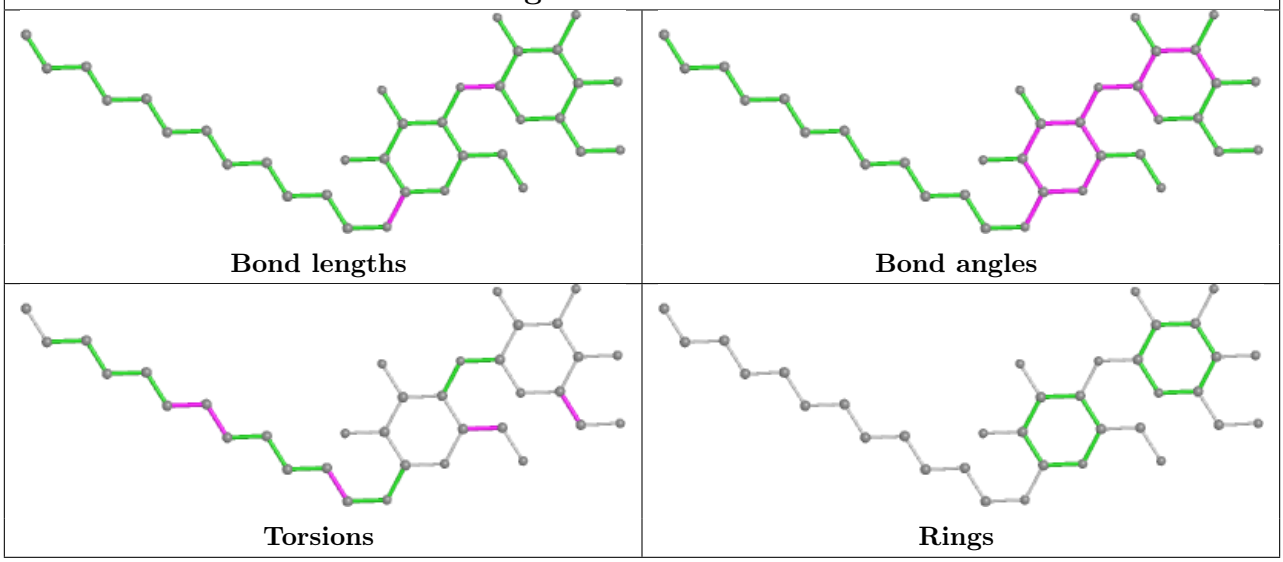
Ligand CLA B 604



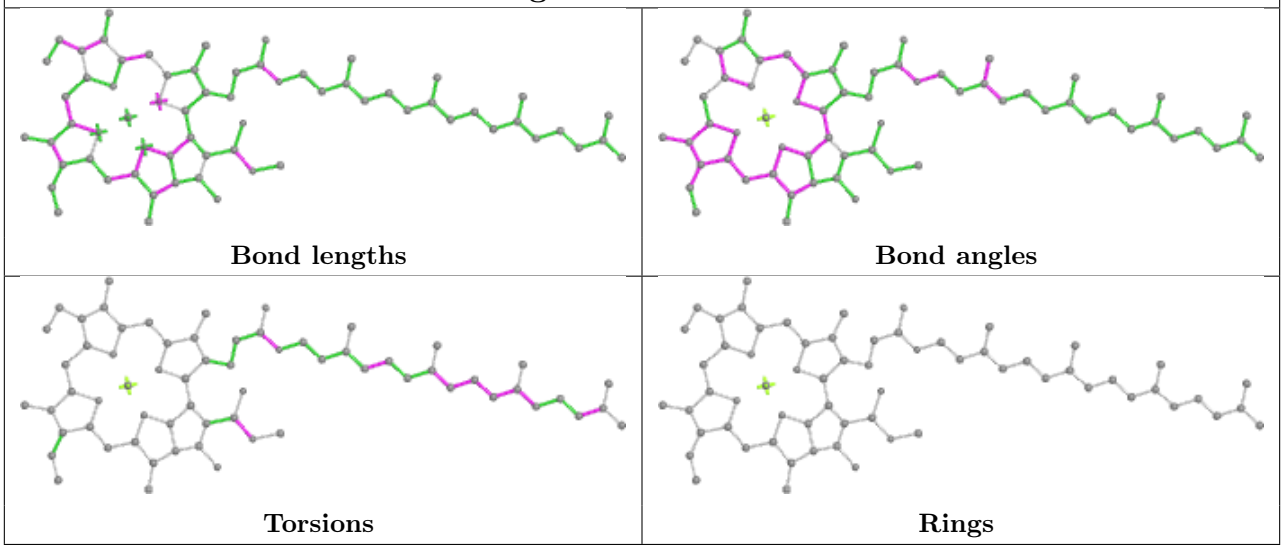
Ligand CLA B 608



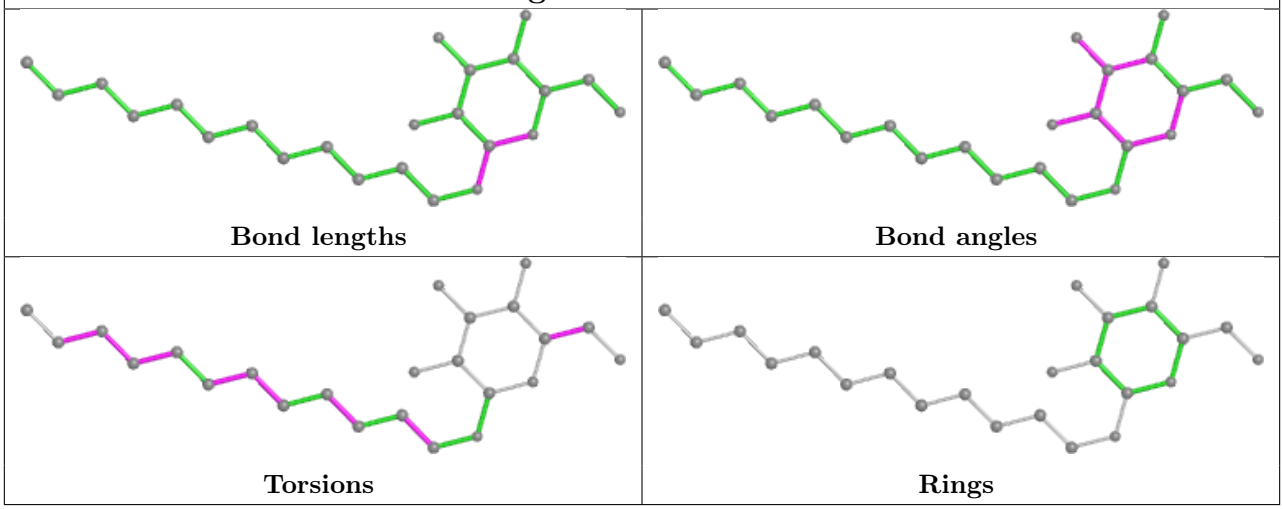
Ligand LMT Z 101

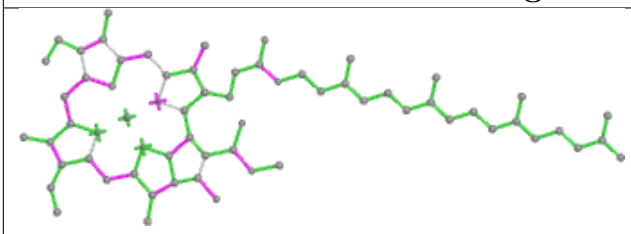
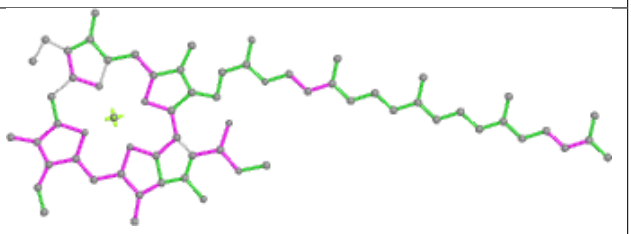
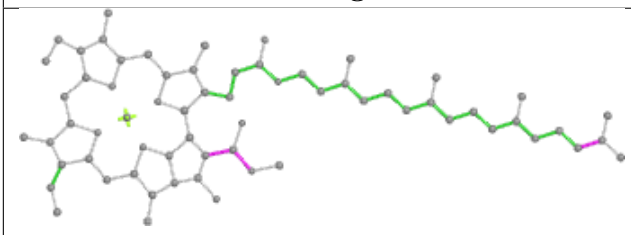
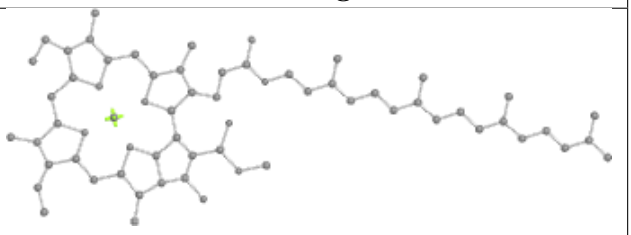


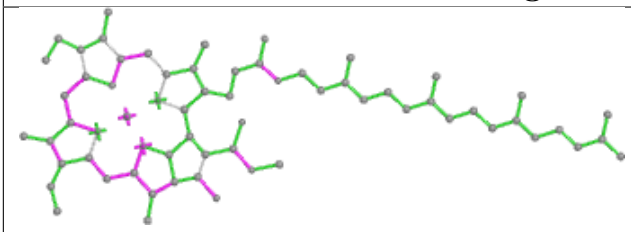
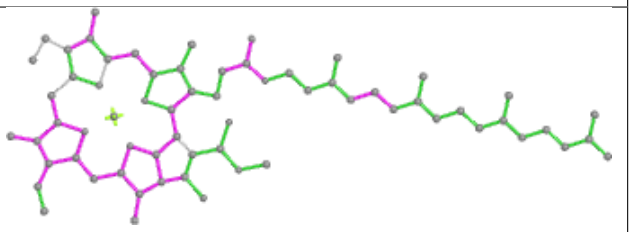
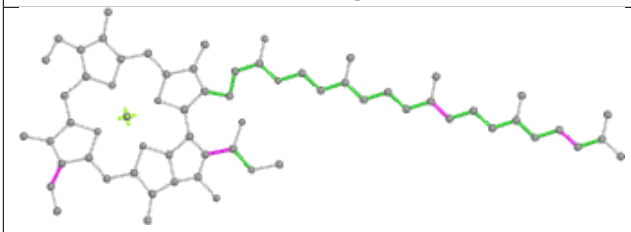
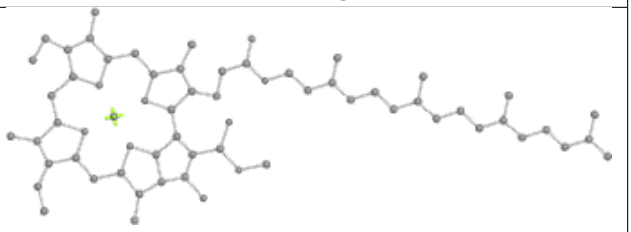
Ligand CLA a 409



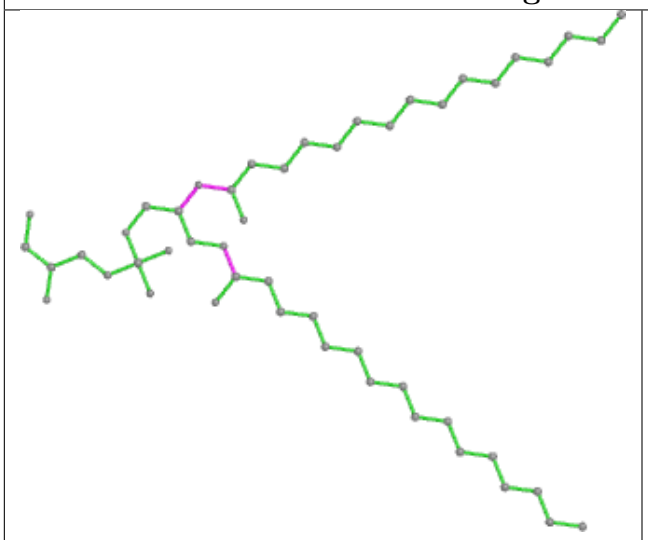
Ligand LMT t 102



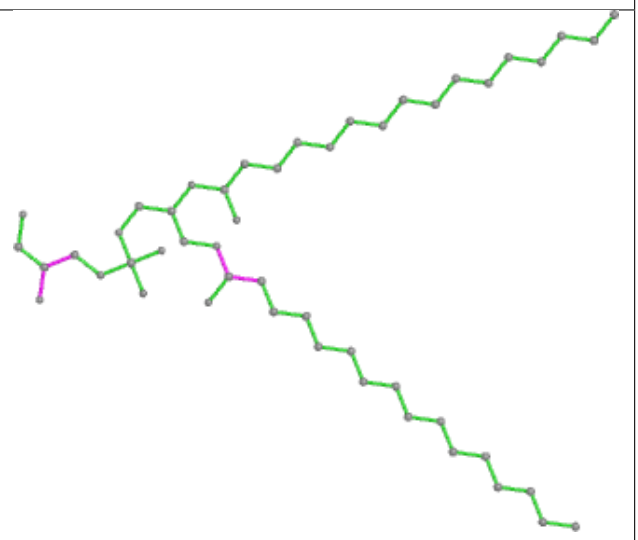
Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

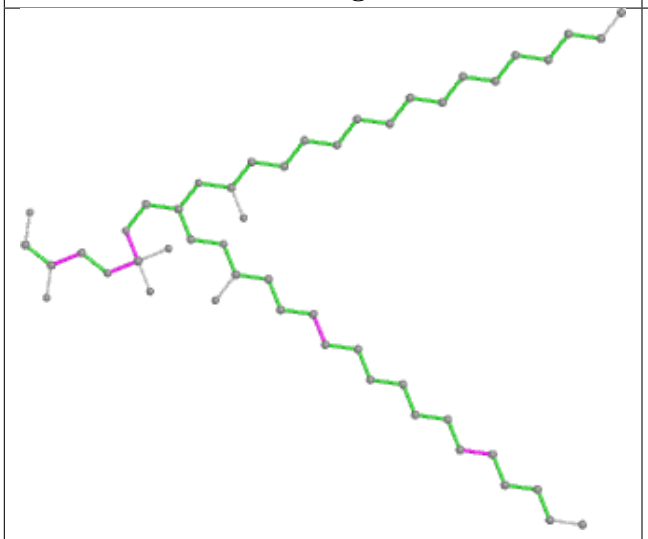
Ligand LHG D 410



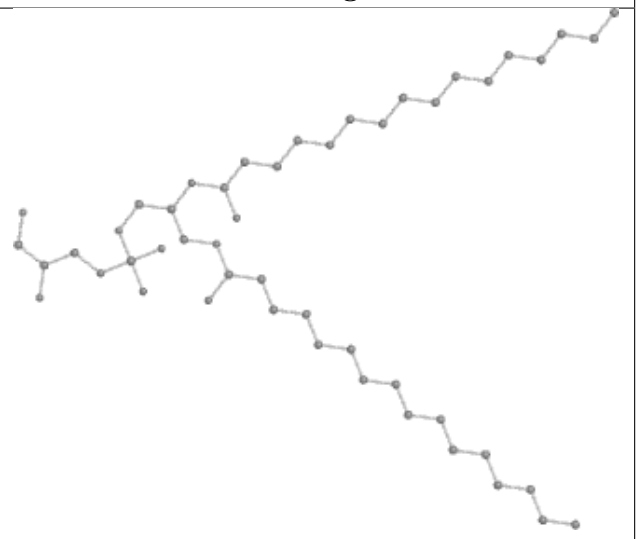
Bond lengths



Bond angles

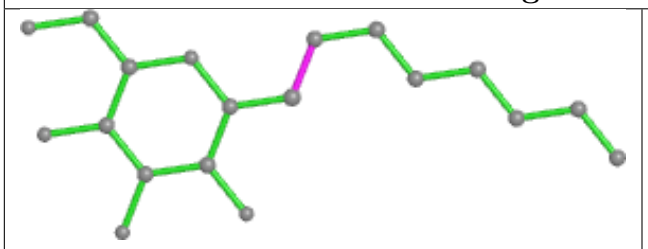


Torsions

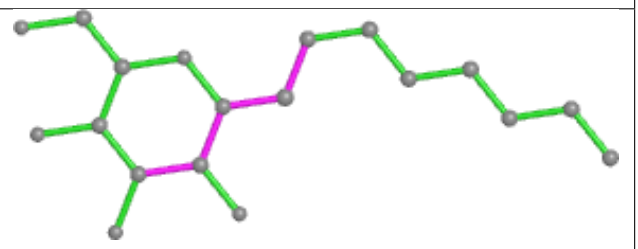


Rings

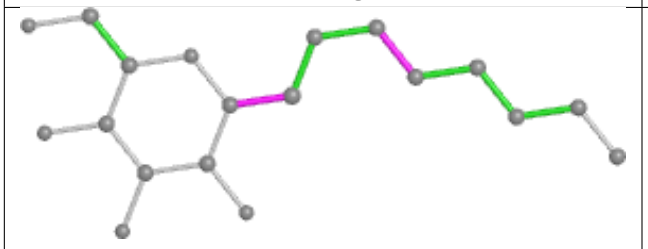
Ligand HTG B 624



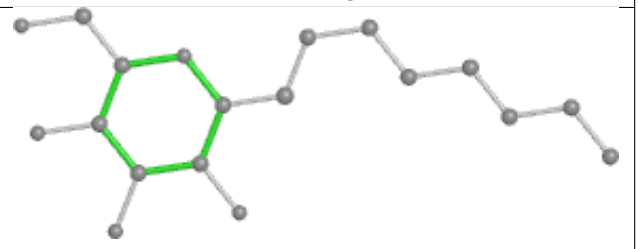
Bond lengths



Bond angles

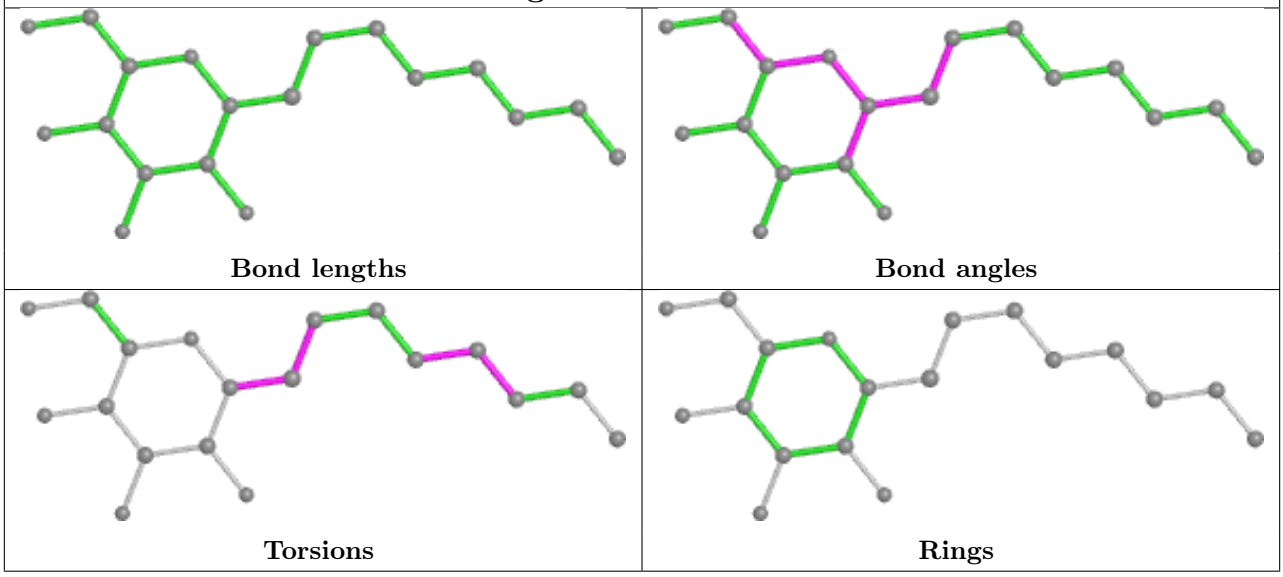


Torsions

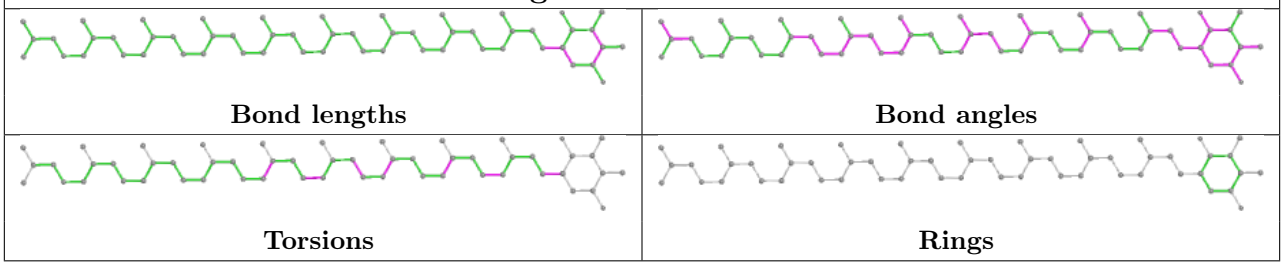


Rings

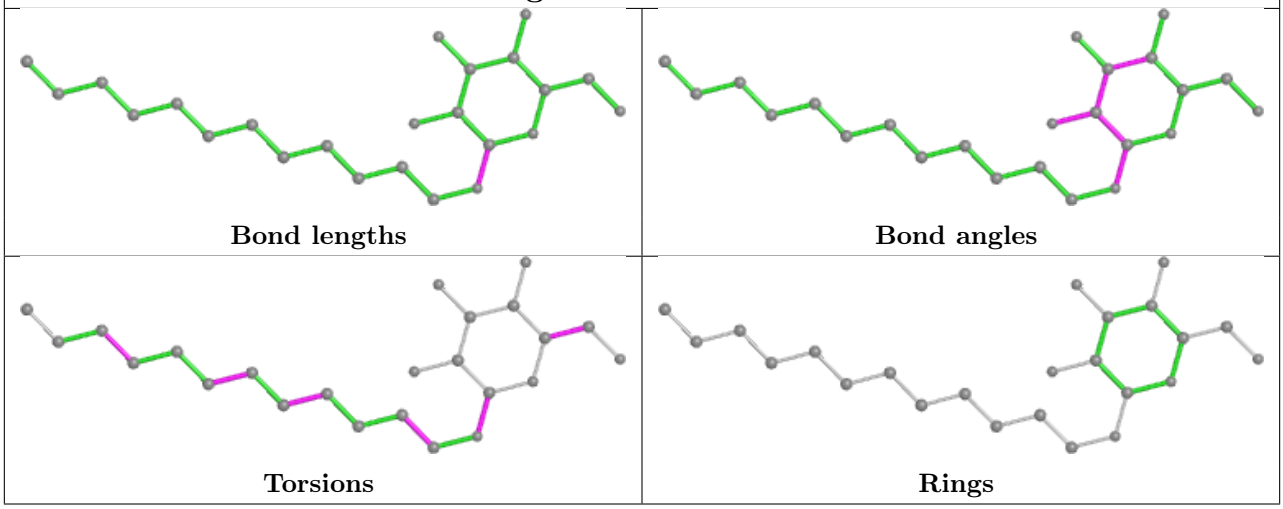
Ligand HTG c 523



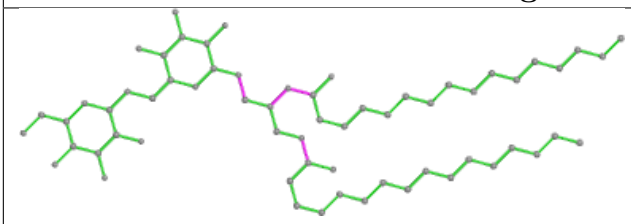
Ligand PL9 A 410



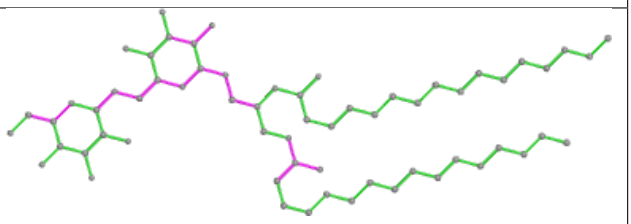
Ligand LMT J 102



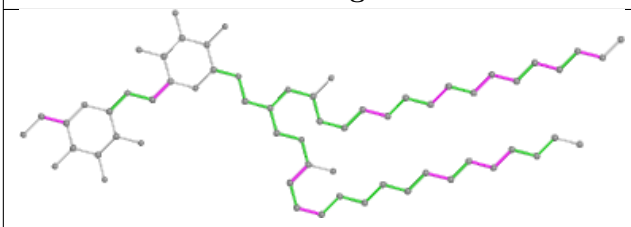
Ligand DGD C 517



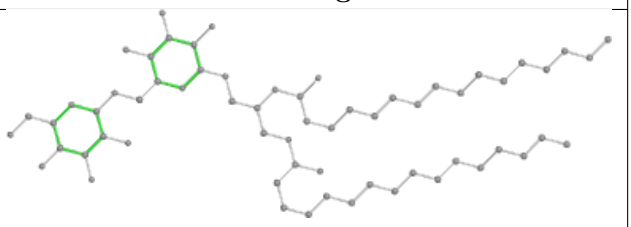
Bond lengths



Bond angles

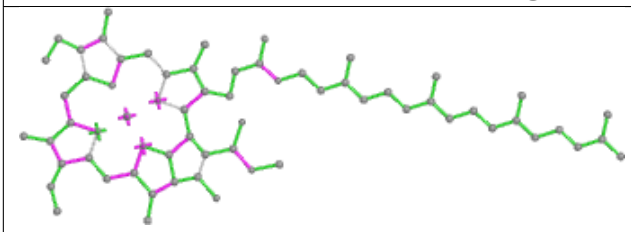


Torsions

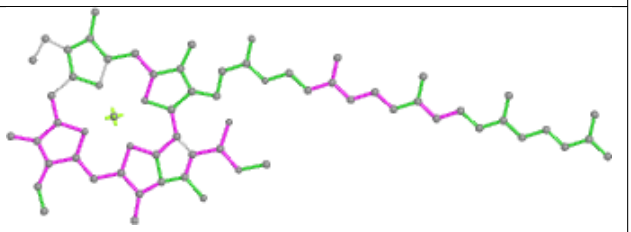


Rings

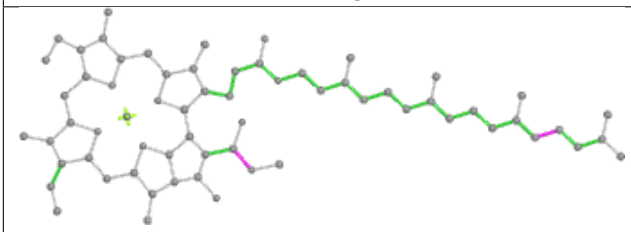
Ligand CLA B 609



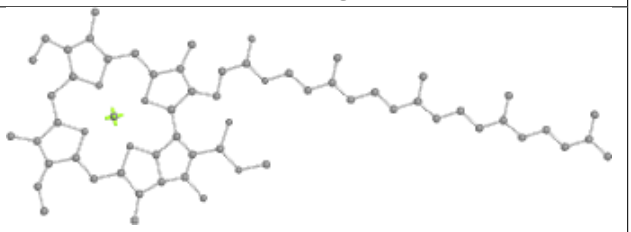
Bond lengths



Bond angles

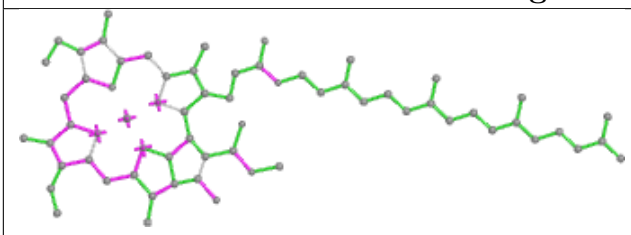


Torsions

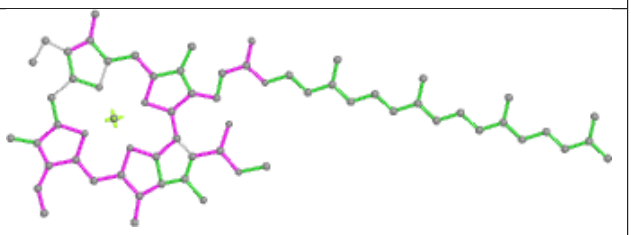


Rings

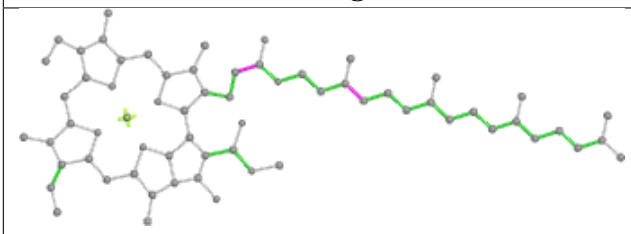
Ligand CLA c 506



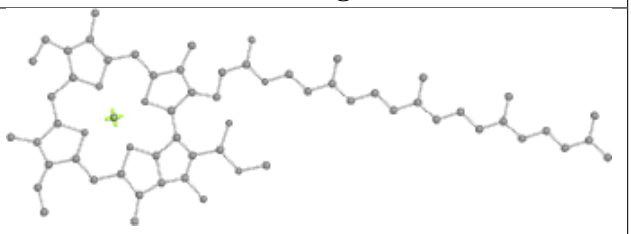
Bond lengths



Bond angles

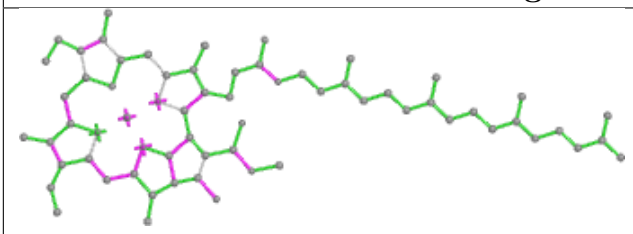


Torsions

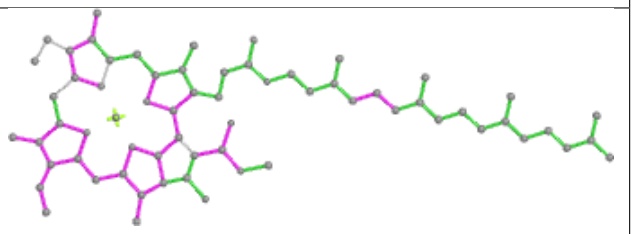


Rings

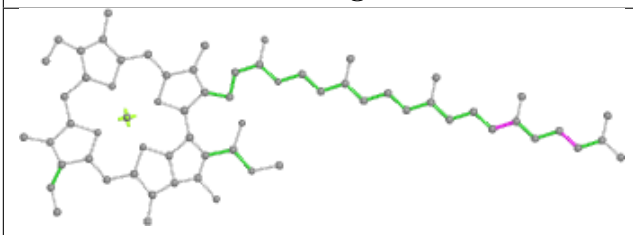
Ligand CLA B 612



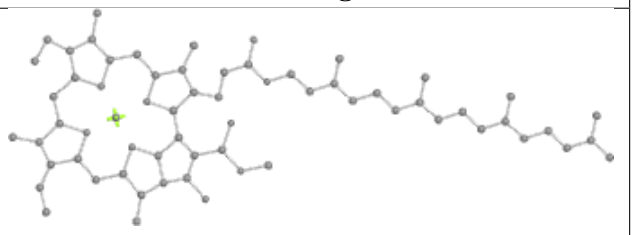
Bond lengths



Bond angles

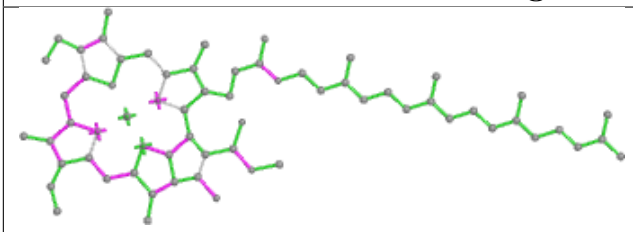


Torsions

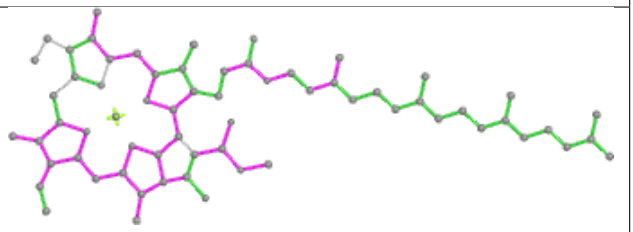


Rings

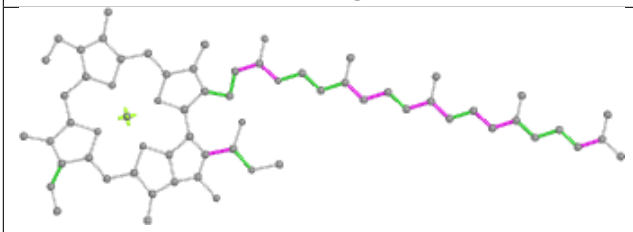
Ligand CLA b 605



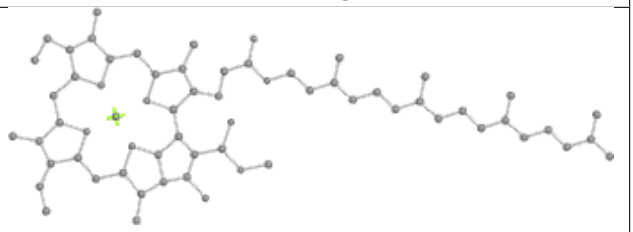
Bond lengths



Bond angles

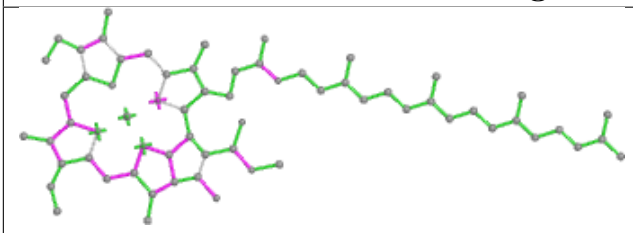


Torsions

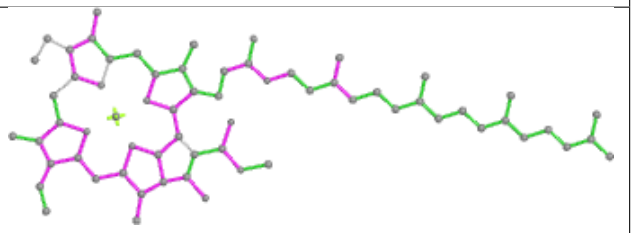


Rings

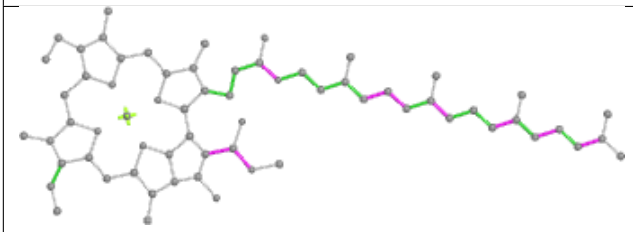
Ligand CLA c 514



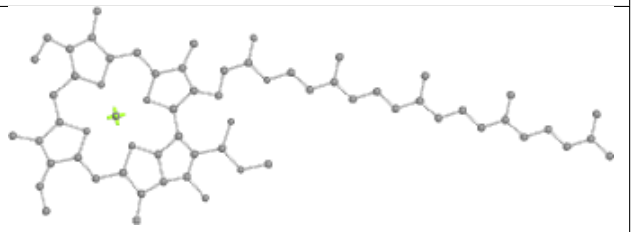
Bond lengths



Bond angles

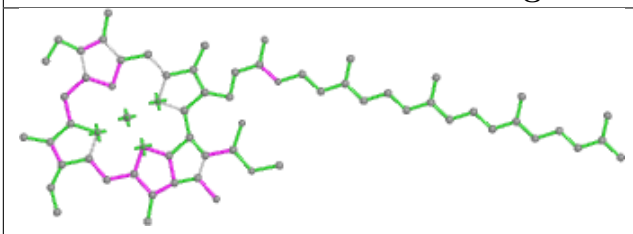


Torsions

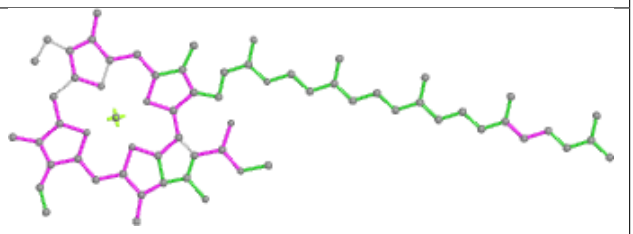


Rings

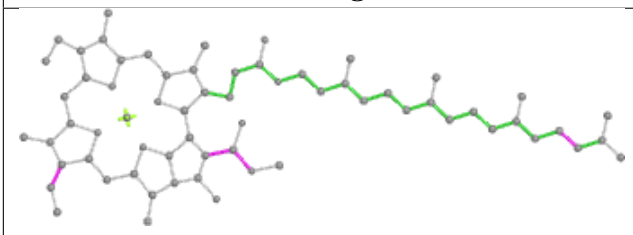
Ligand CLA A 405



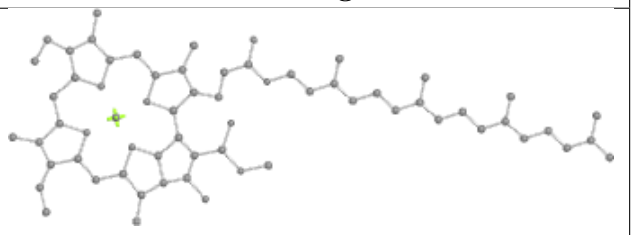
Bond lengths



Bond angles

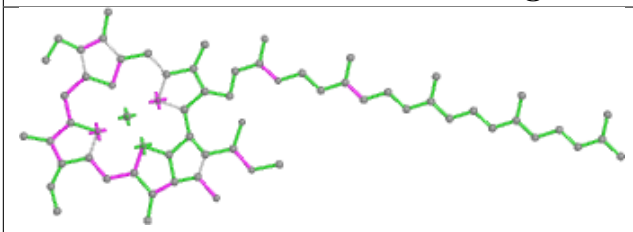


Torsions

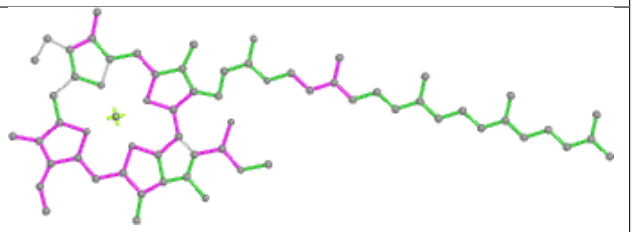


Rings

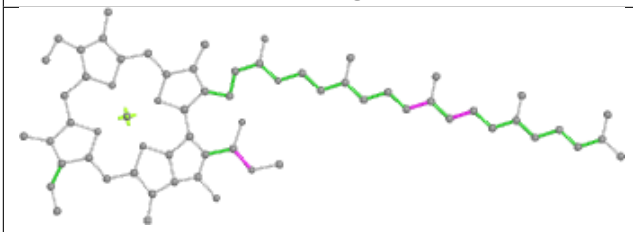
Ligand CLA C 503



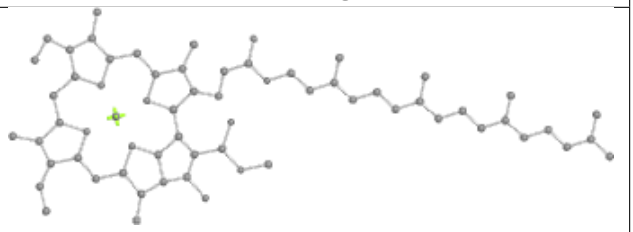
Bond lengths



Bond angles

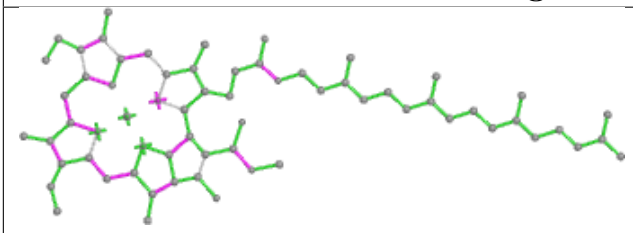


Torsions

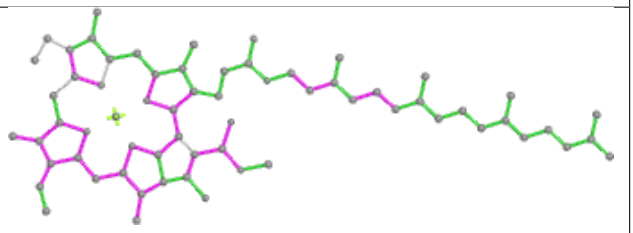


Rings

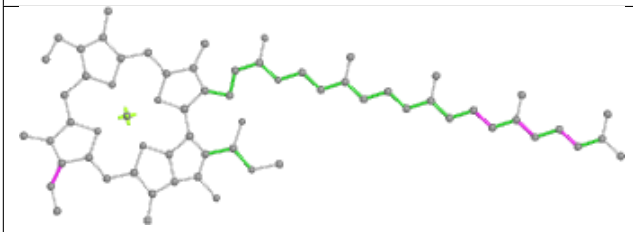
Ligand CLA b 615



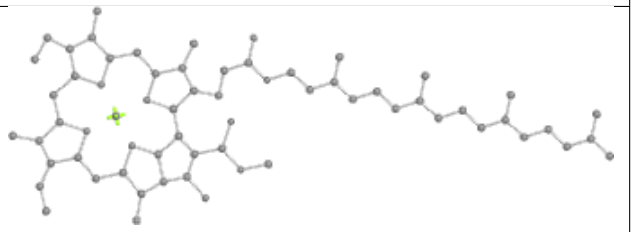
Bond lengths



Bond angles

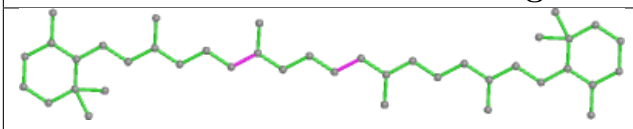


Torsions

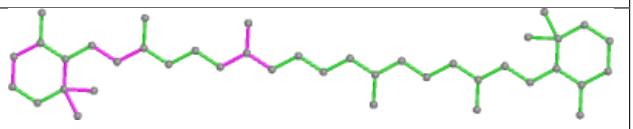


Rings

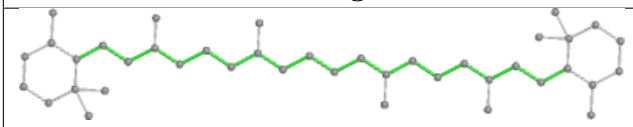
Ligand BCR k 101



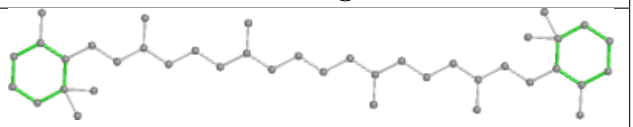
Bond lengths



Bond angles

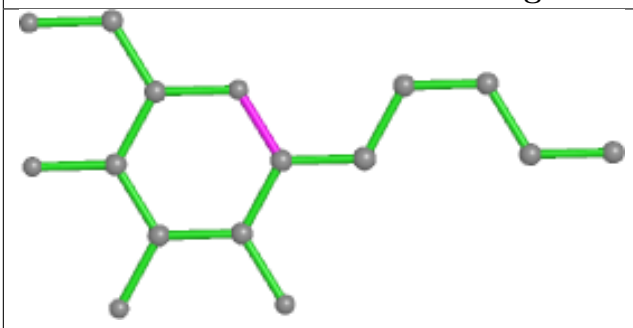


Torsions

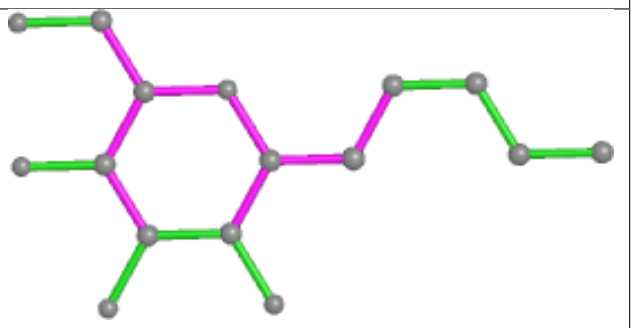


Rings

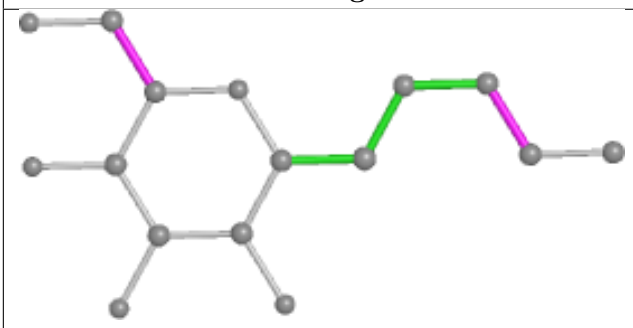
Ligand HTG d 413



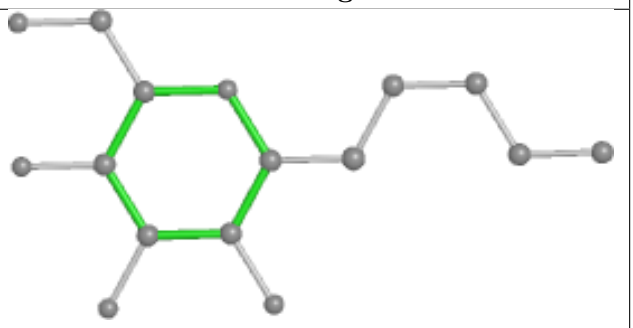
Bond lengths



Bond angles

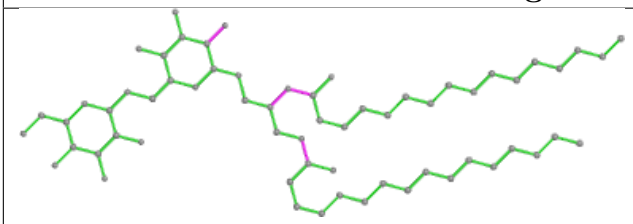


Torsions

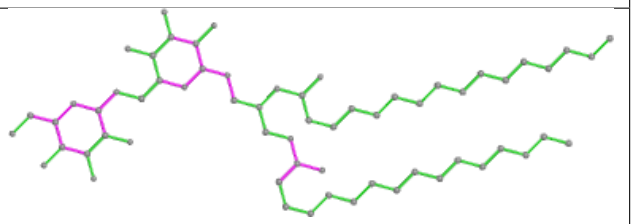


Rings

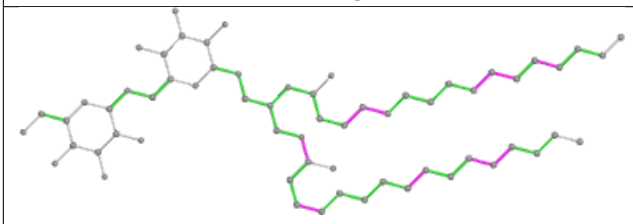
Ligand DGD c 519



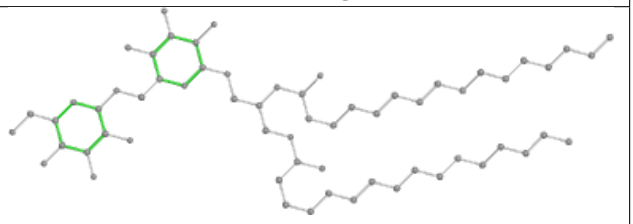
Bond lengths



Bond angles

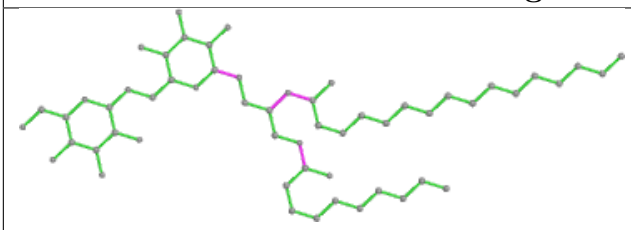


Torsions

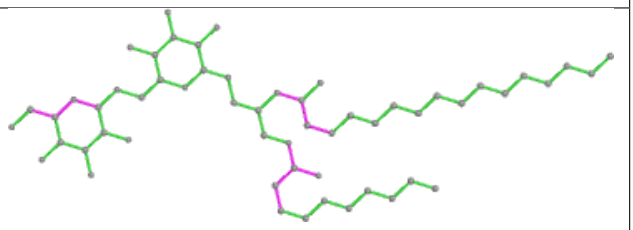


Rings

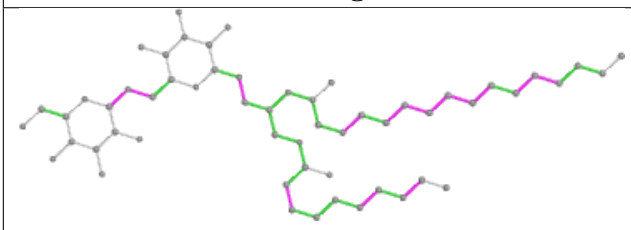
Ligand DGD c 518



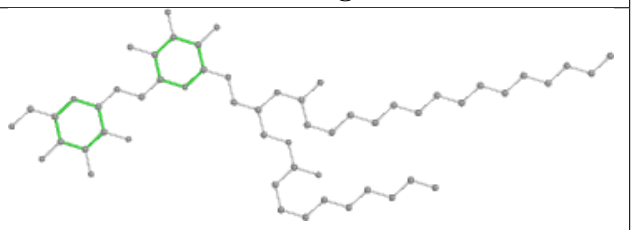
Bond lengths



Bond angles

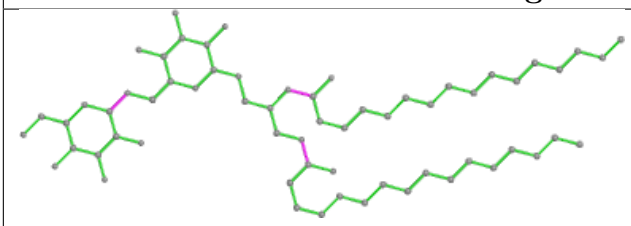


Torsions

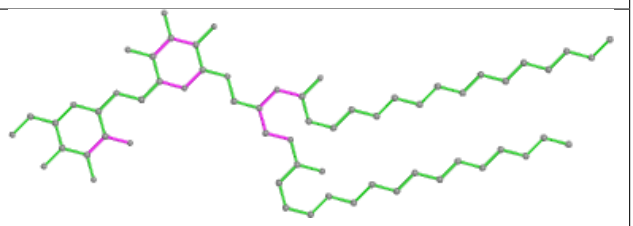


Rings

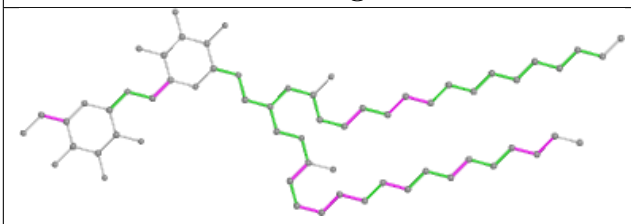
Ligand DGD c 517



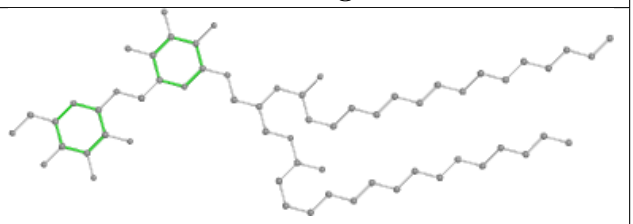
Bond lengths



Bond angles

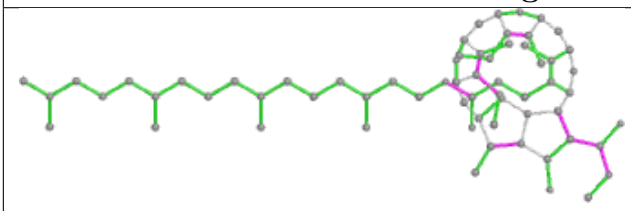


Torsions

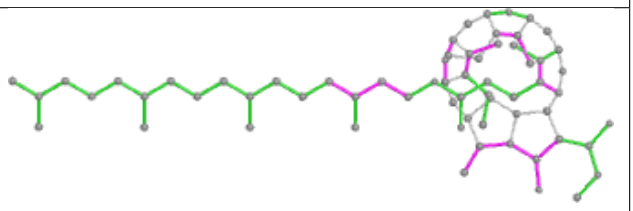


Rings

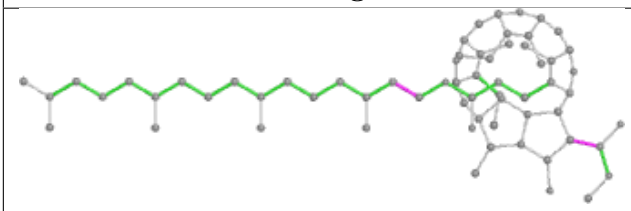
Ligand PHO A 407



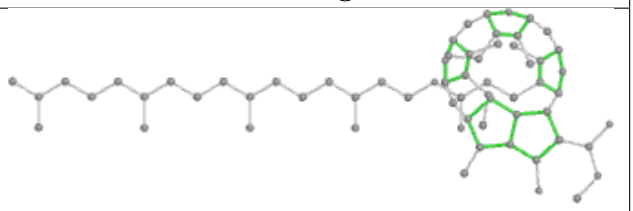
Bond lengths



Bond angles

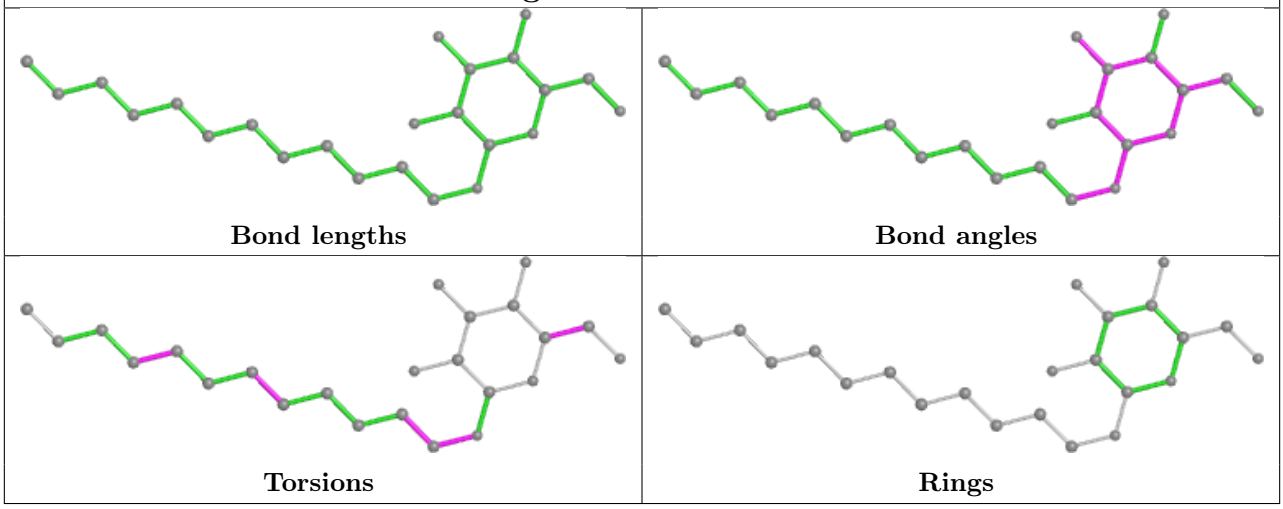


Torsions

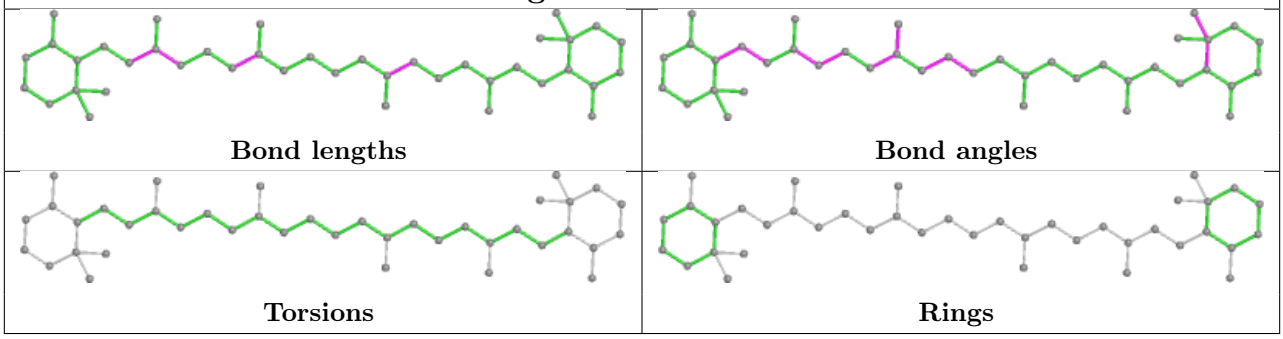


Rings

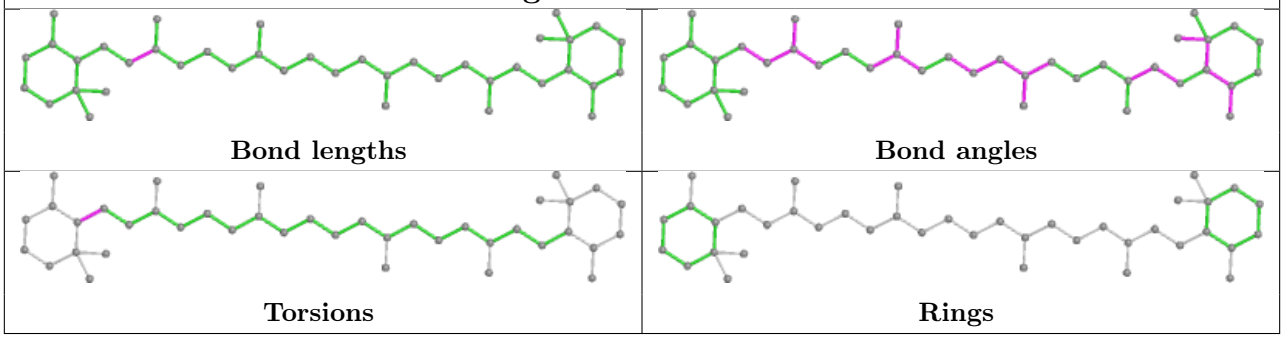
Ligand LMT T 102



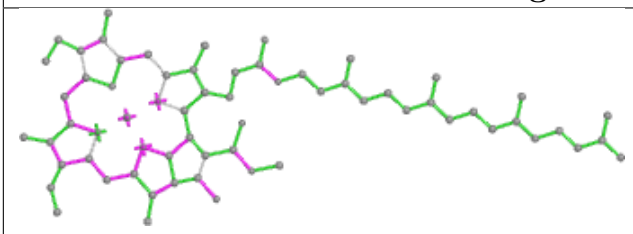
Ligand BCR a 410



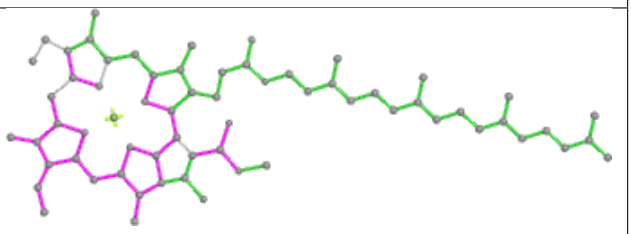
Ligand BCR Y 101



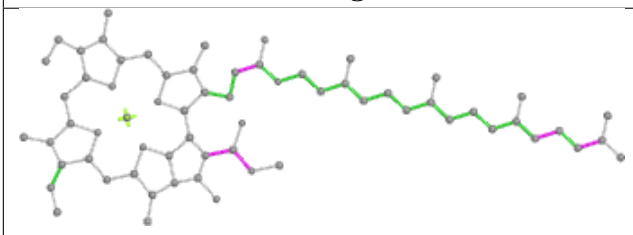
Ligand CLA c 502



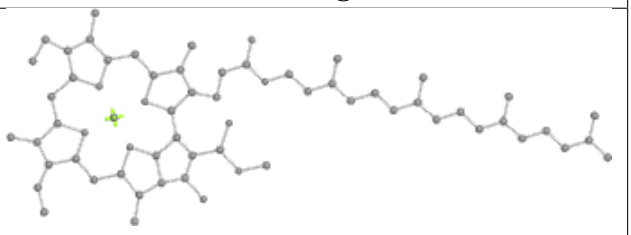
Bond lengths



Bond angles

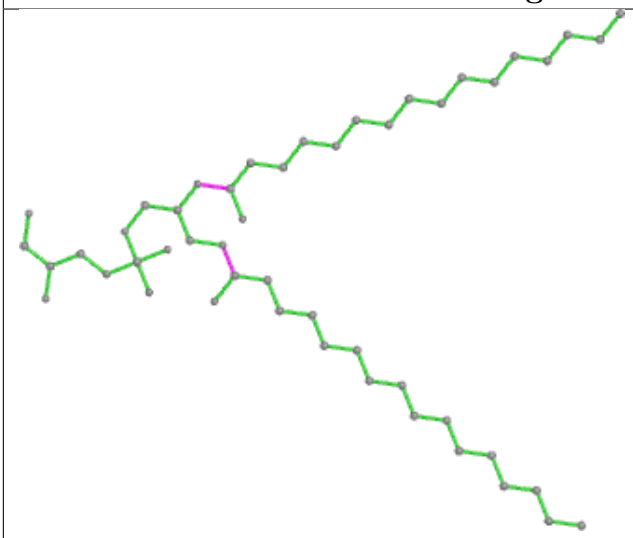


Torsions

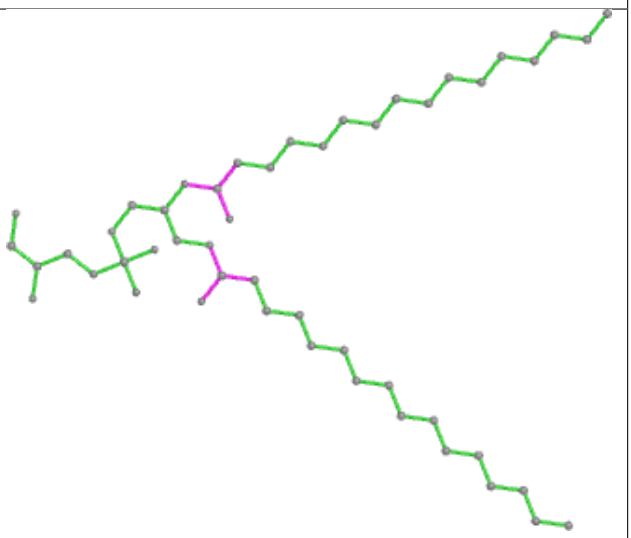


Rings

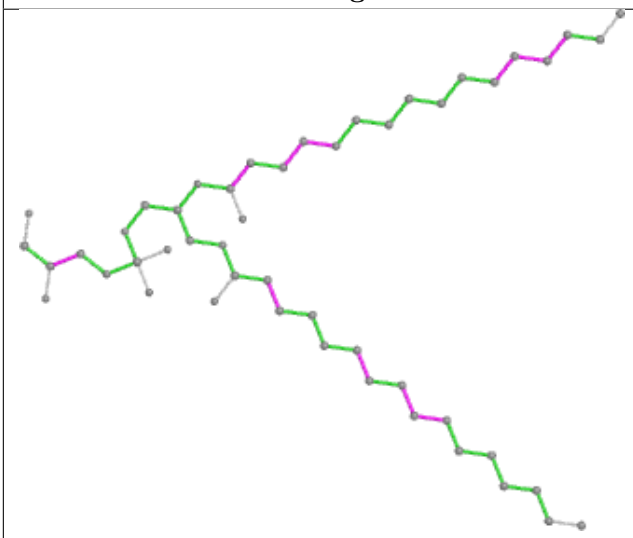
Ligand LHG d 409



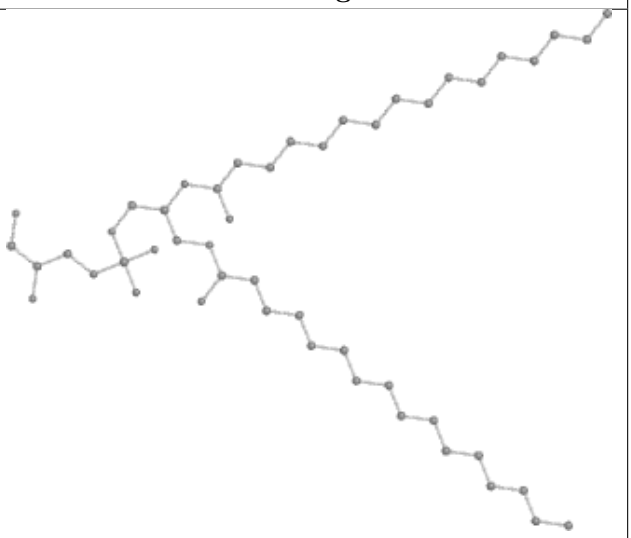
Bond lengths



Bond angles

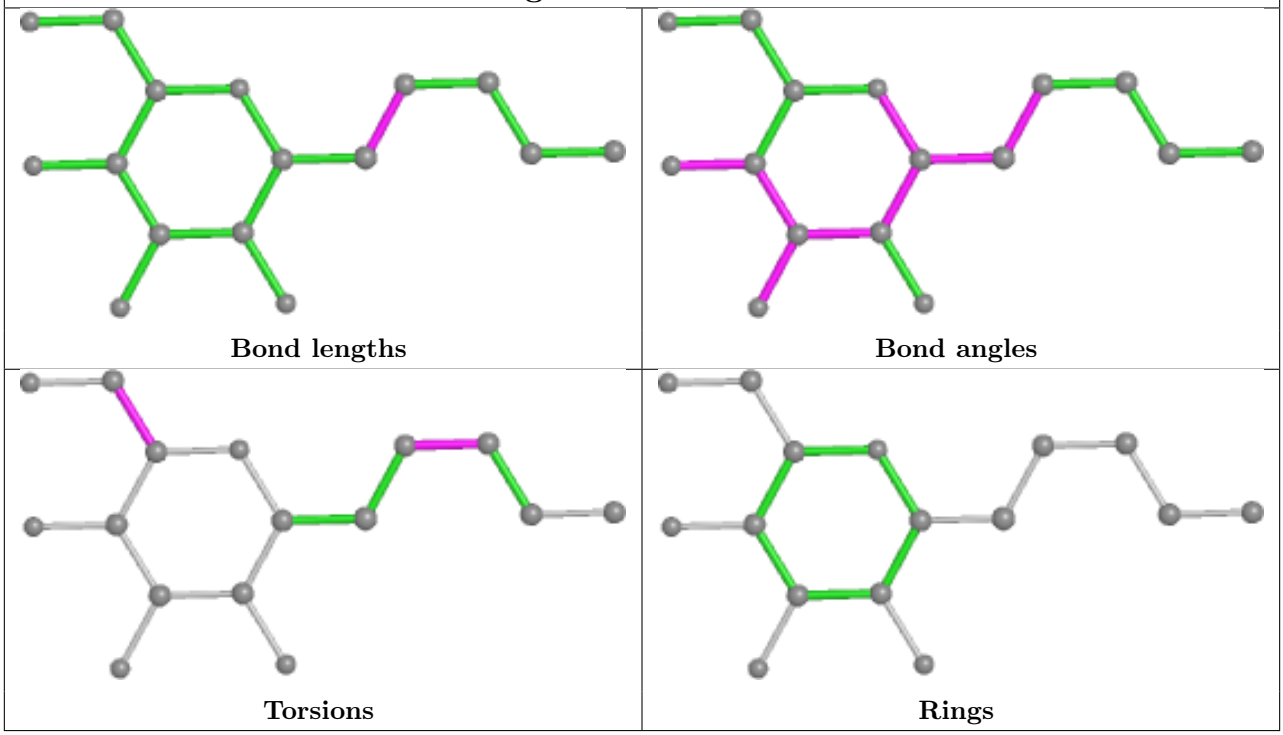


Torsions

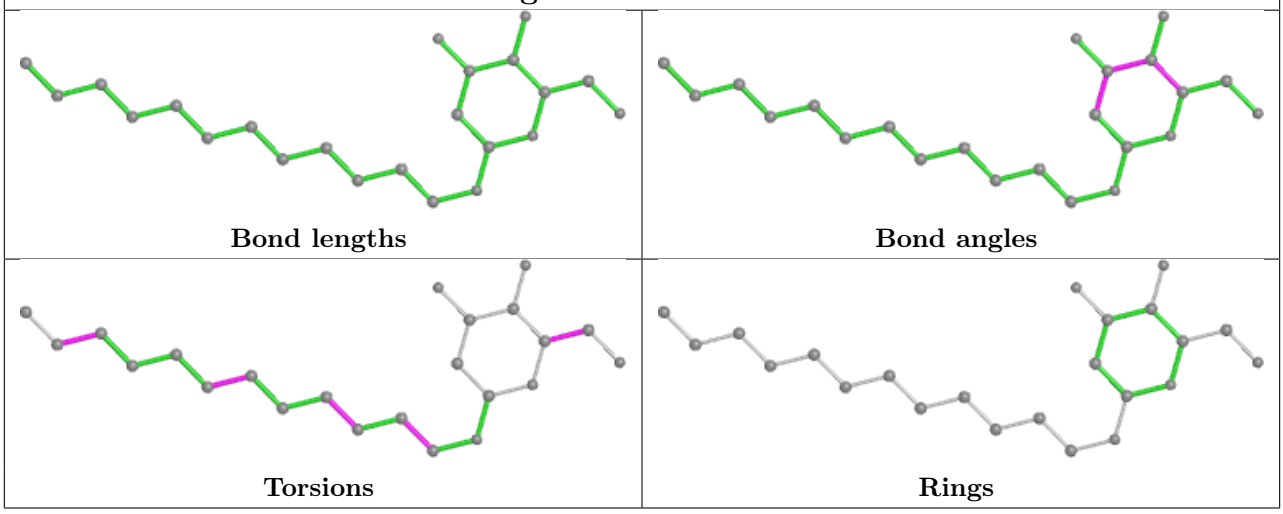


Rings

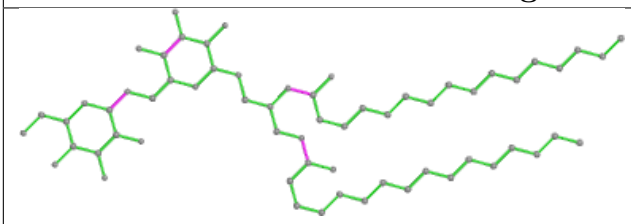
Ligand HTG v 208



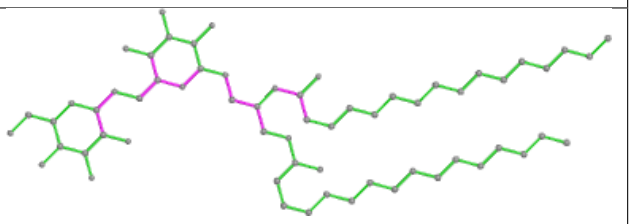
Ligand LMT m 103



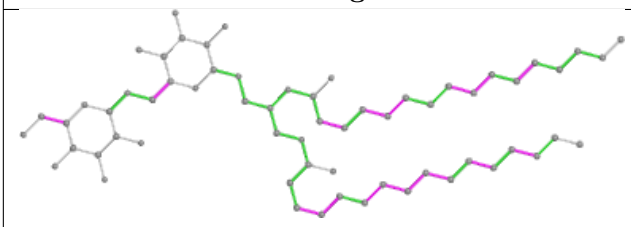
Ligand DGD C 515



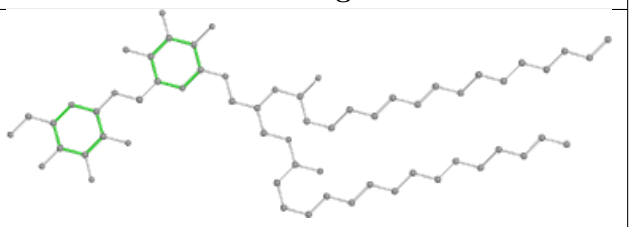
Bond lengths



Bond angles

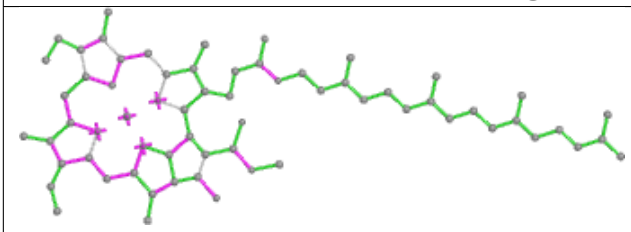


Torsions

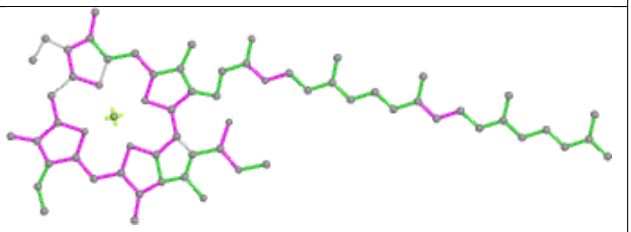


Rings

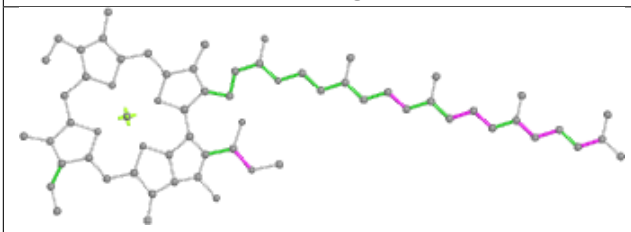
Ligand CLA B 616



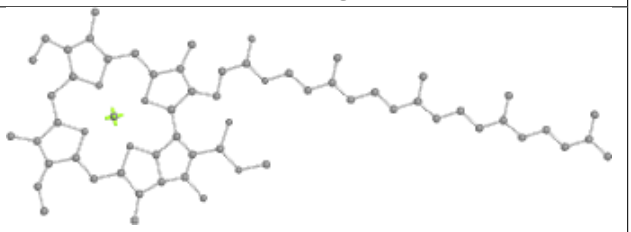
Bond lengths



Bond angles

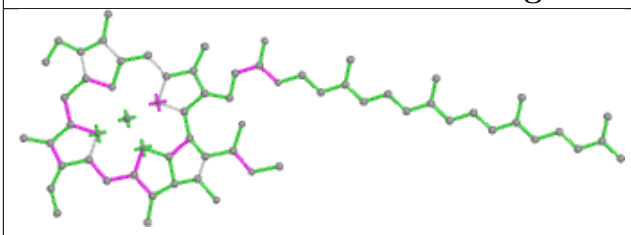


Torsions

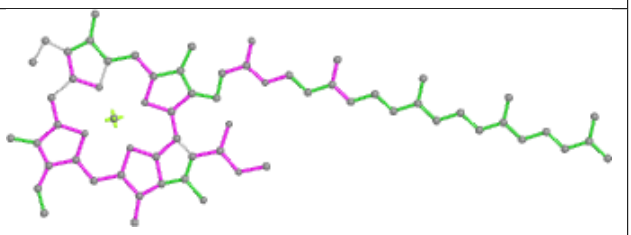


Rings

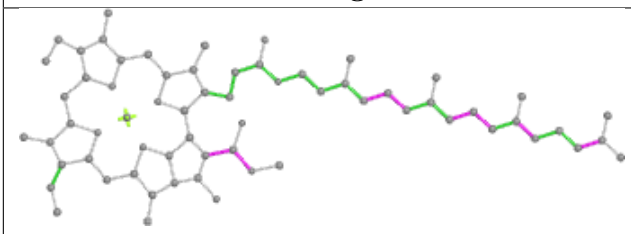
Ligand CLA B 615



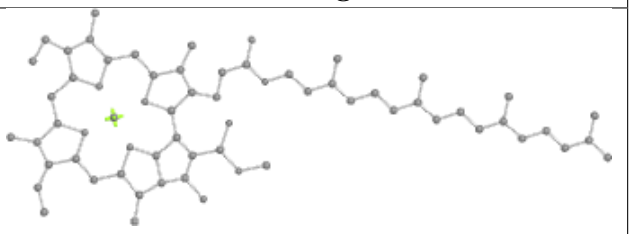
Bond lengths



Bond angles

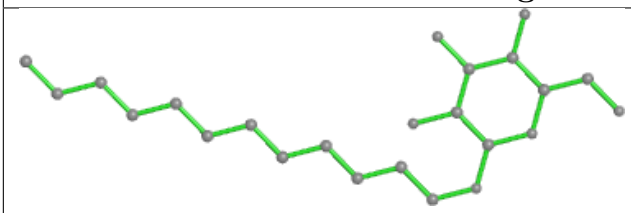


Torsions

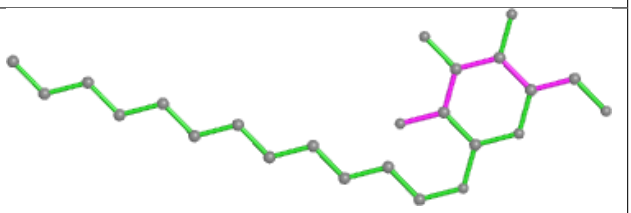


Rings

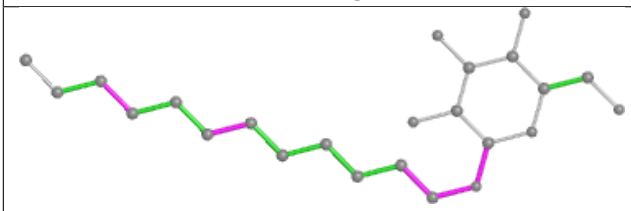
Ligand LMT M 102



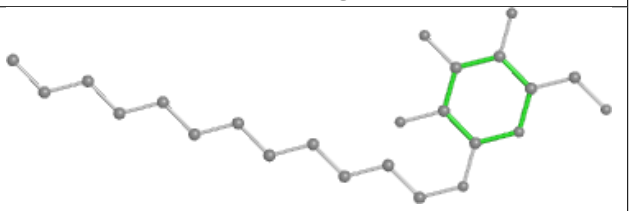
Bond lengths



Bond angles

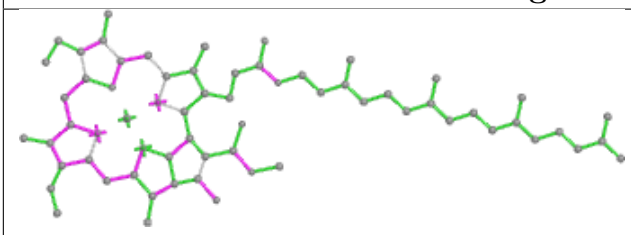


Torsions

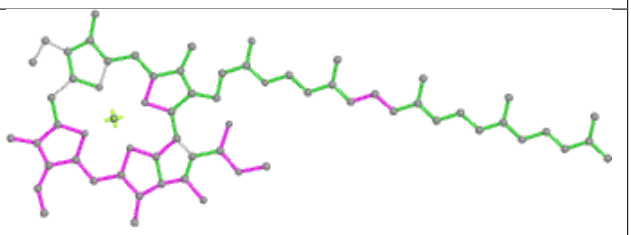


Rings

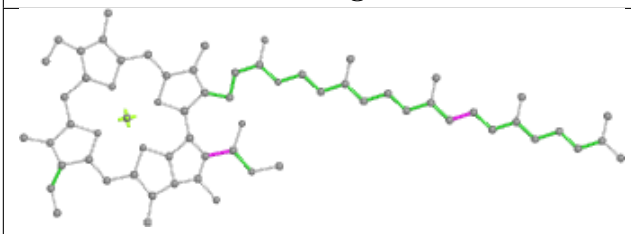
Ligand CLA c 504



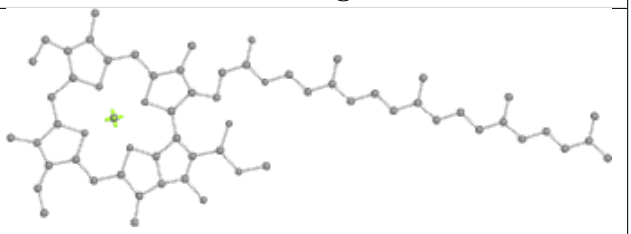
Bond lengths



Bond angles

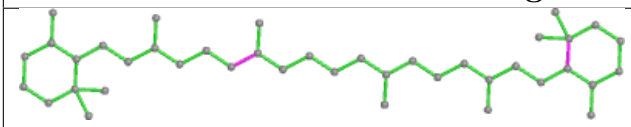


Torsions

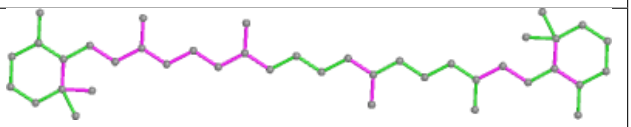


Rings

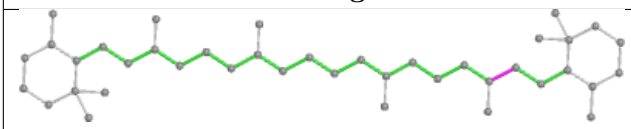
Ligand BCR d 406



Bond lengths



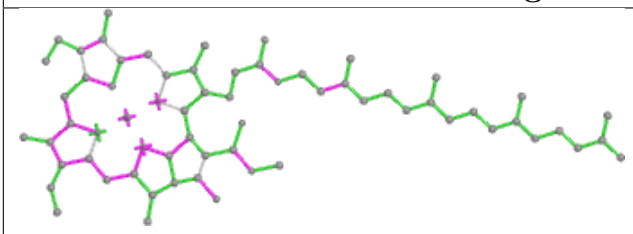
Bond angles



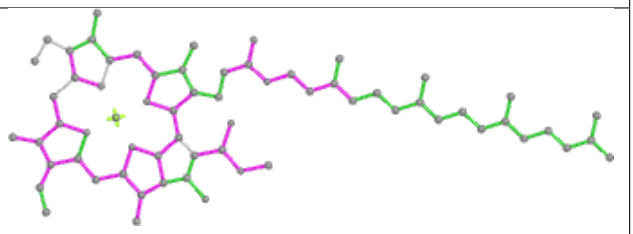
Torsions

Rings

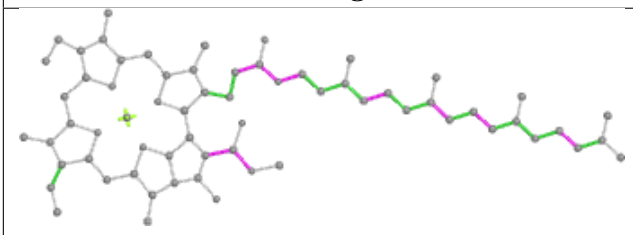
Ligand CLA B 602



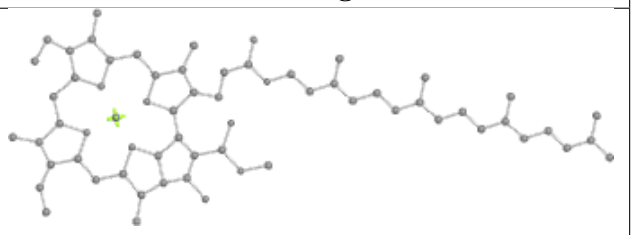
Bond lengths



Bond angles

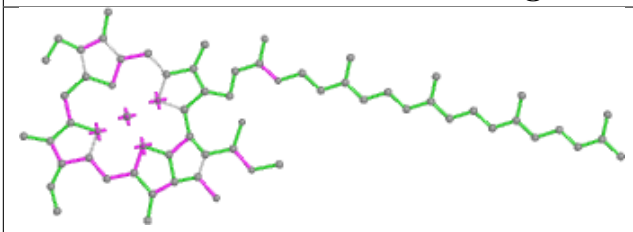


Torsions

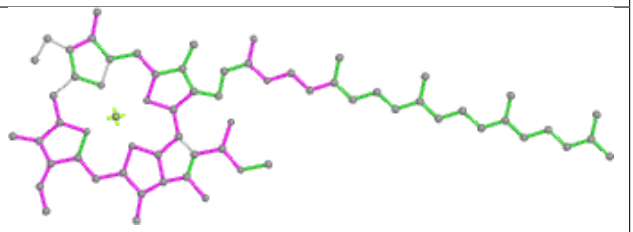


Rings

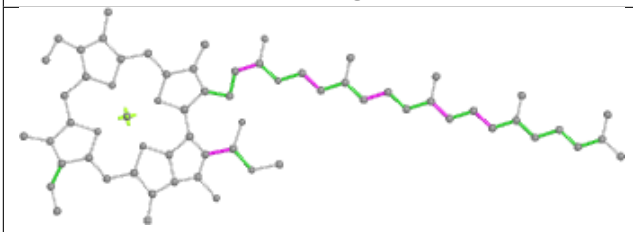
Ligand CLA C 512



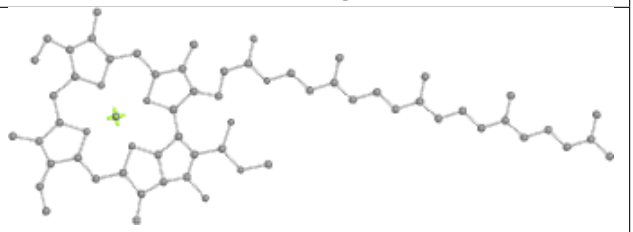
Bond lengths



Bond angles

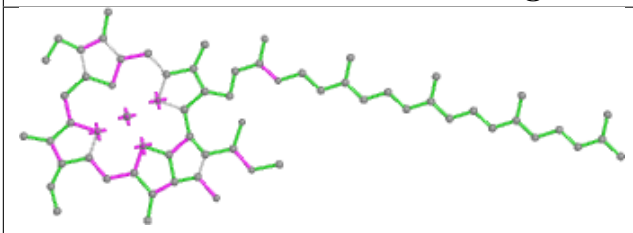


Torsions

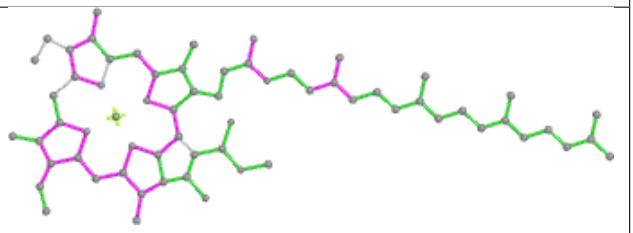


Rings

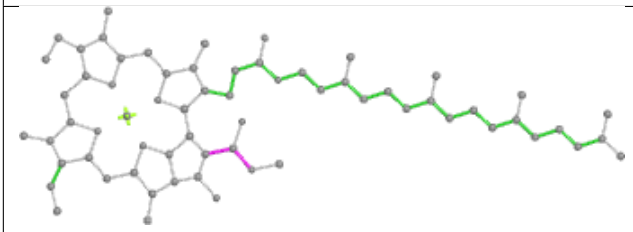
Ligand CLA C 508



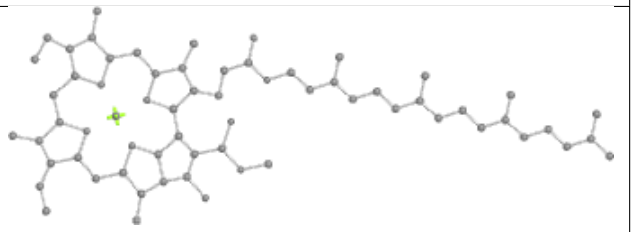
Bond lengths



Bond angles

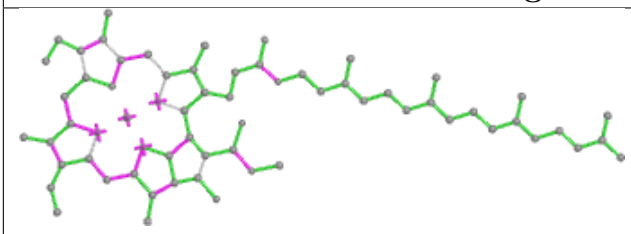


Torsions

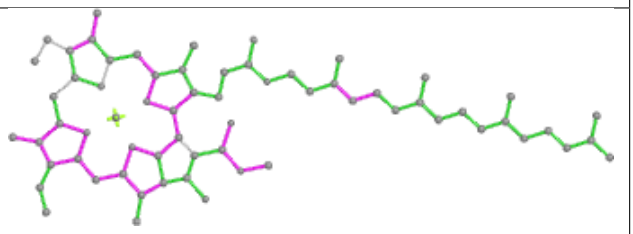


Rings

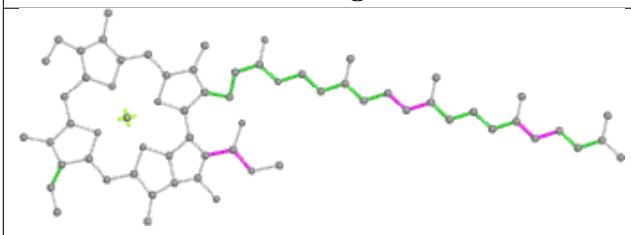
Ligand CLA C 504



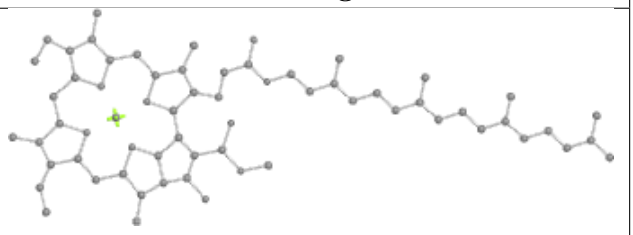
Bond lengths



Bond angles

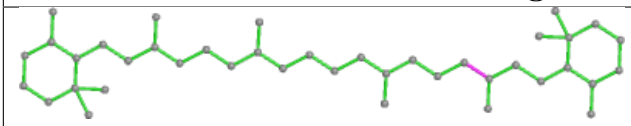


Torsions

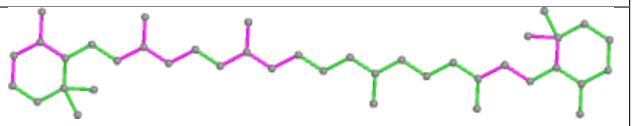


Rings

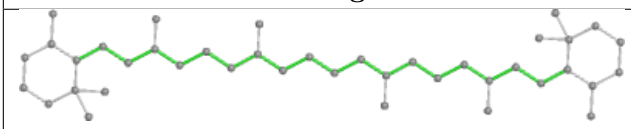
Ligand BCR c 515



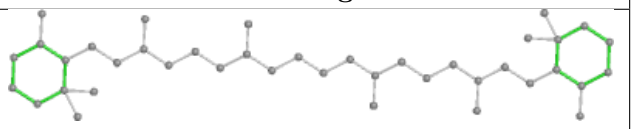
Bond lengths



Bond angles

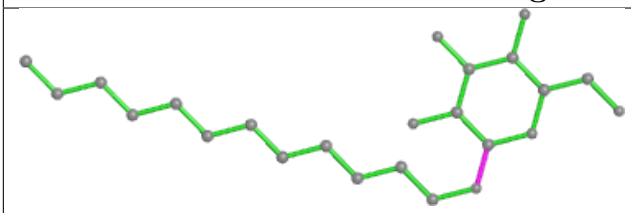


Torsions

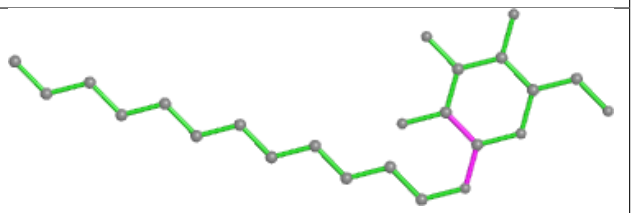


Rings

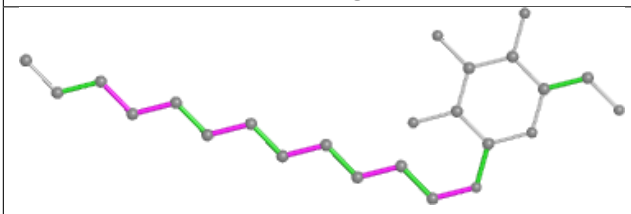
Ligand LMT l 101



Bond lengths



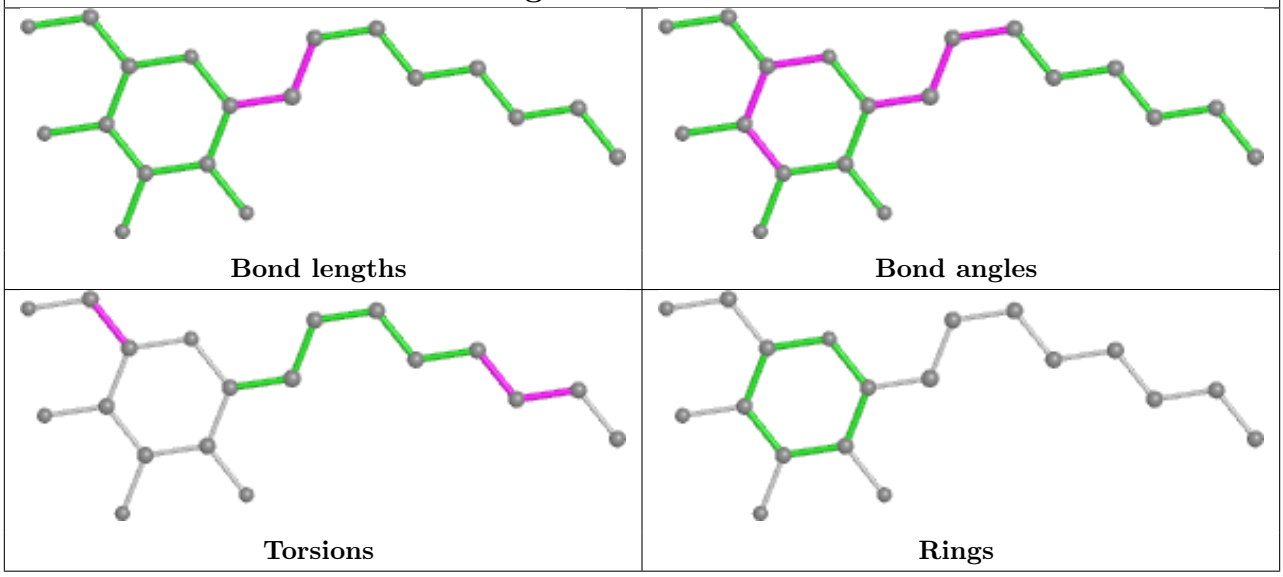
Bond angles



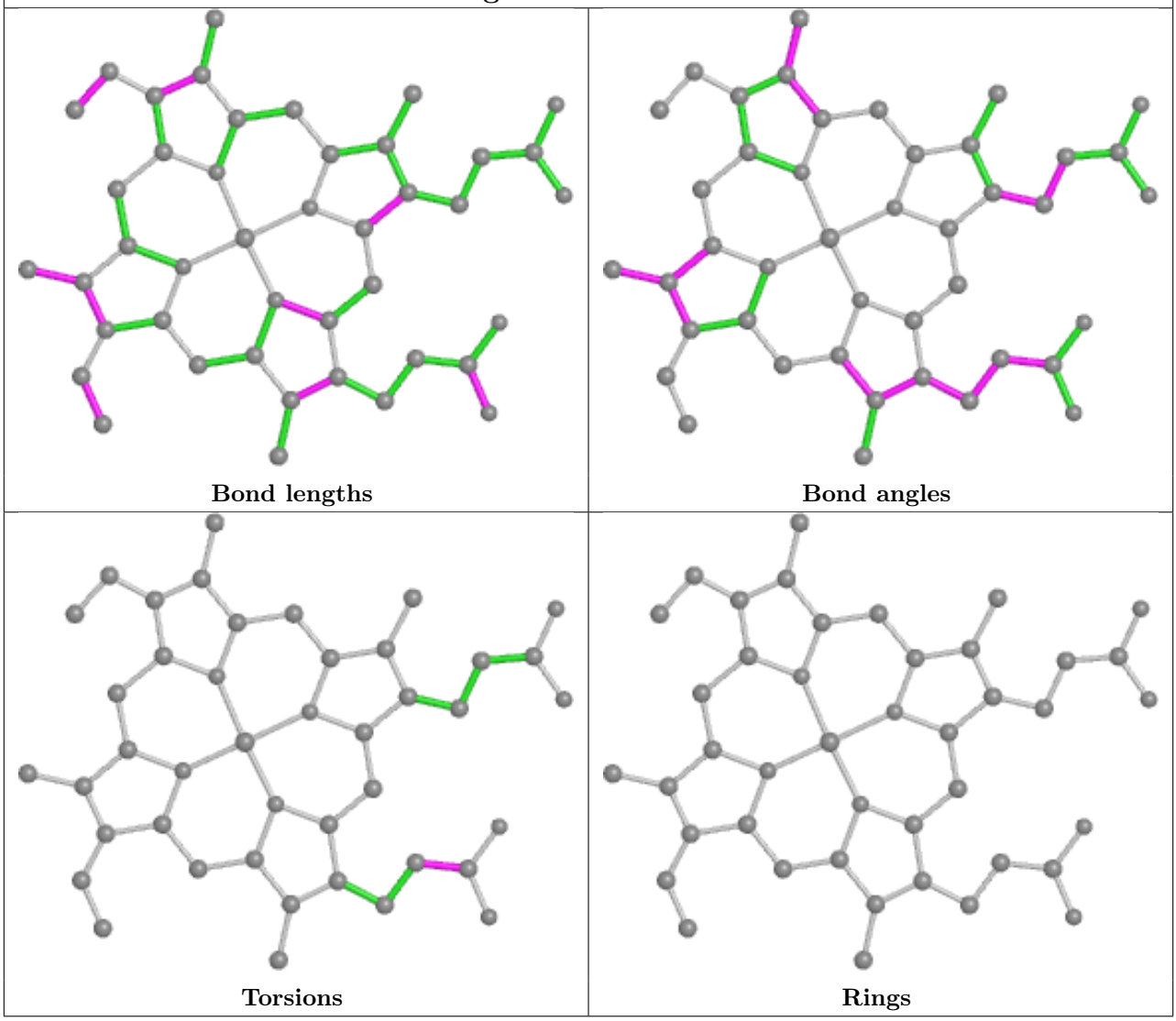
Torsions

Rings

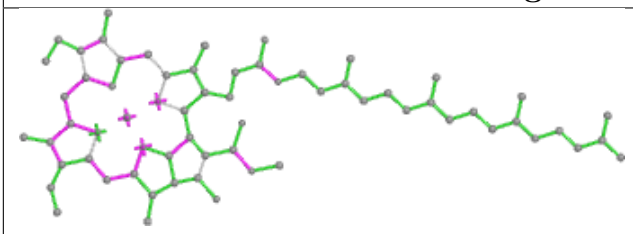
Ligand HTG b 601



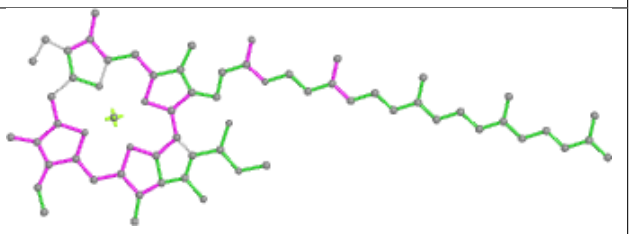
Ligand HEC v 202



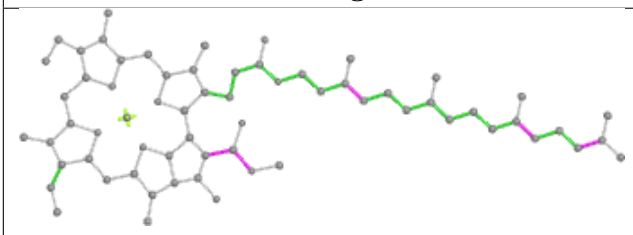
Ligand CLA B 606



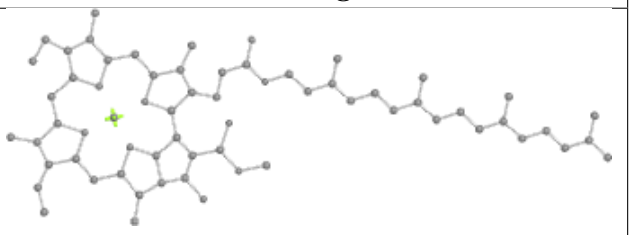
Bond lengths



Bond angles

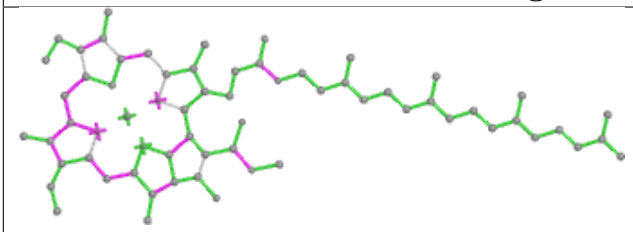


Torsions

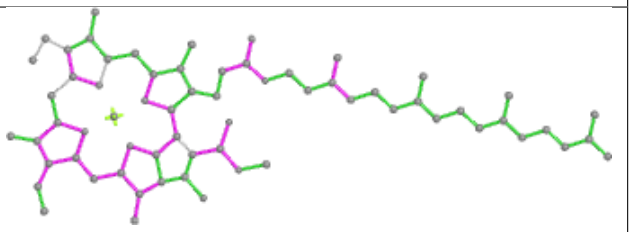


Rings

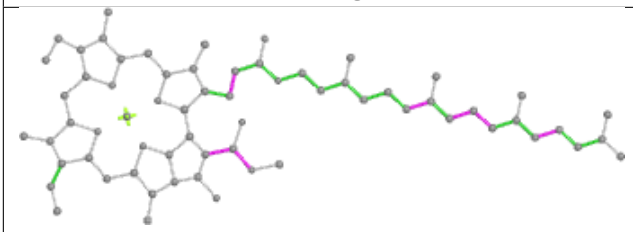
Ligand CLA b 610



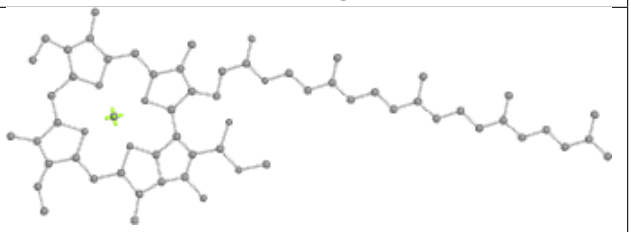
Bond lengths



Bond angles

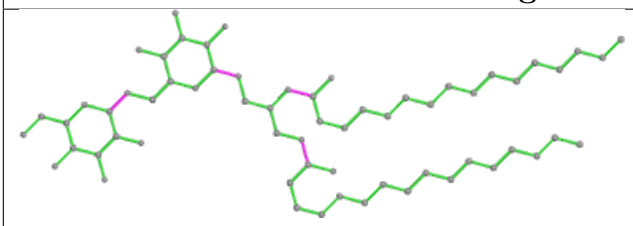


Torsions

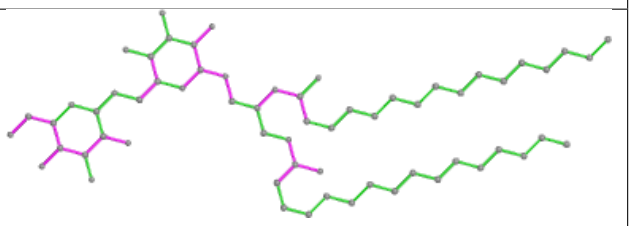


Rings

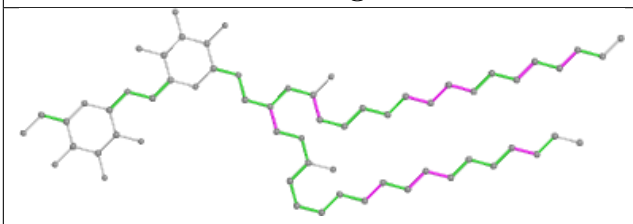
Ligand DGD H 101



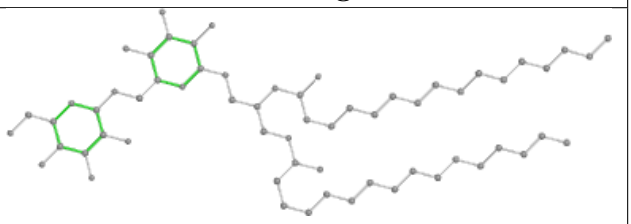
Bond lengths



Bond angles

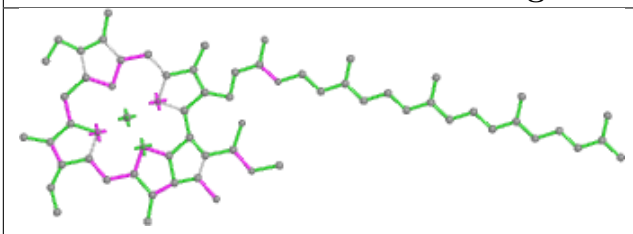


Torsions

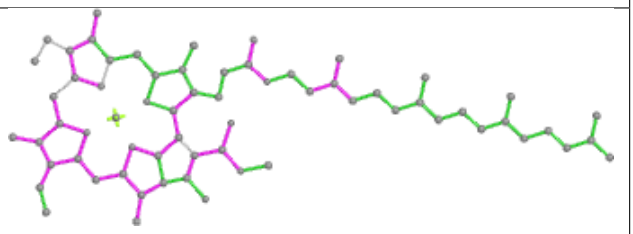


Rings

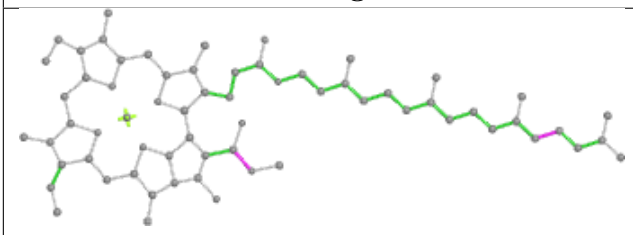
Ligand CLA b 612



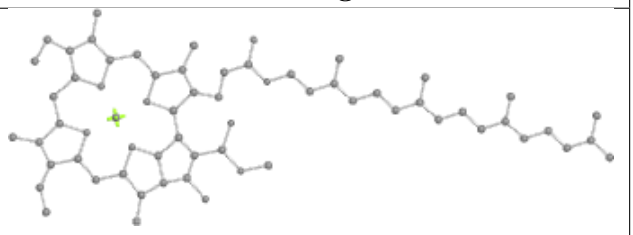
Bond lengths



Bond angles

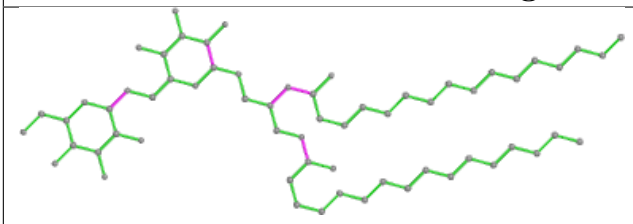


Torsions

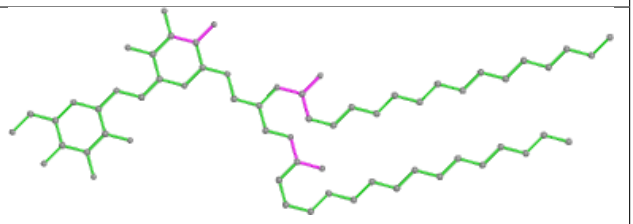


Rings

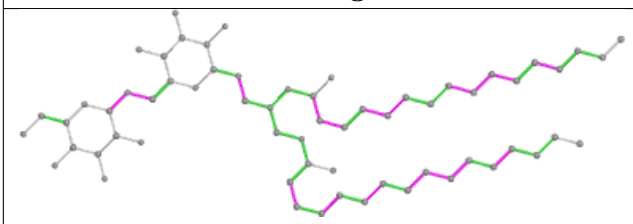
Ligand DGD C 516



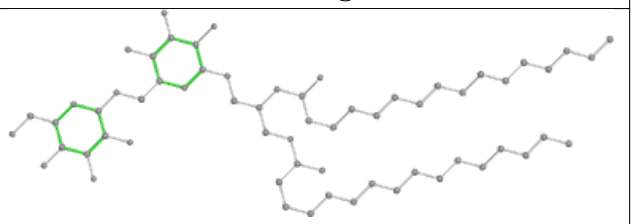
Bond lengths



Bond angles

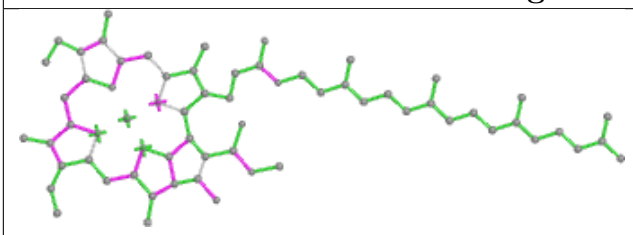


Torsions

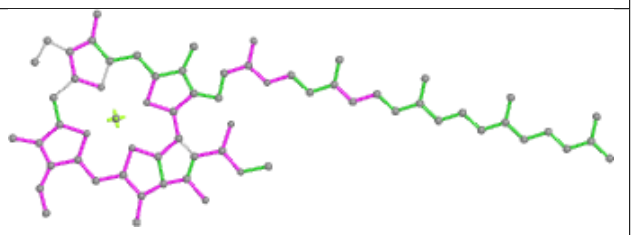


Rings

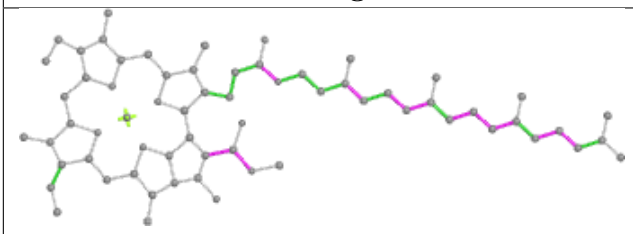
Ligand CLA b 620



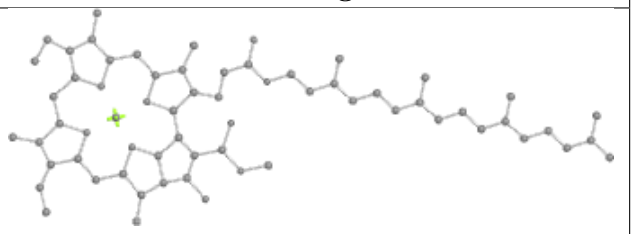
Bond lengths



Bond angles

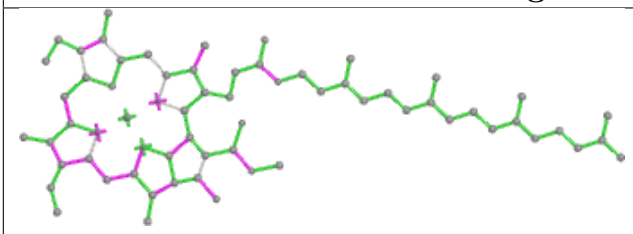


Torsions

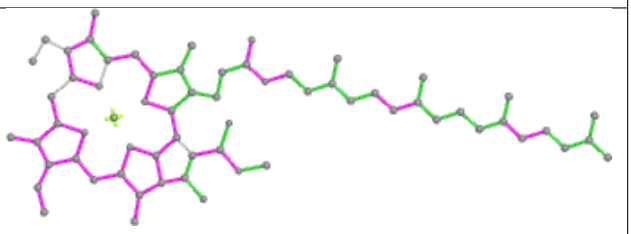


Rings

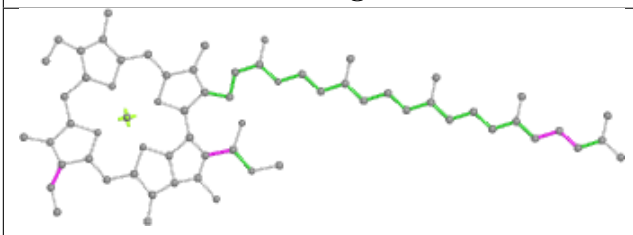
Ligand CLA d 403



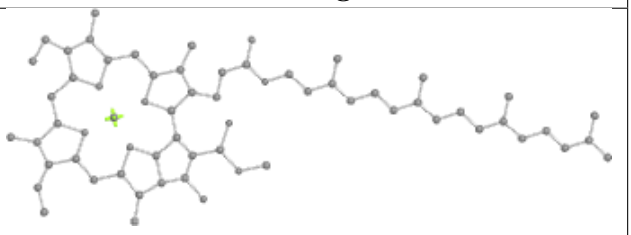
Bond lengths



Bond angles

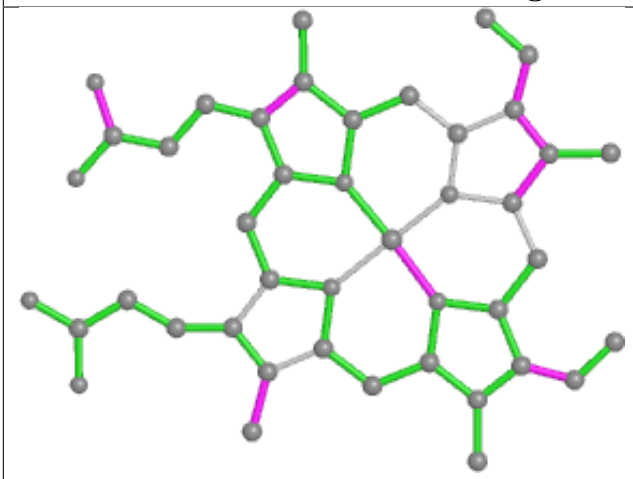


Torsions

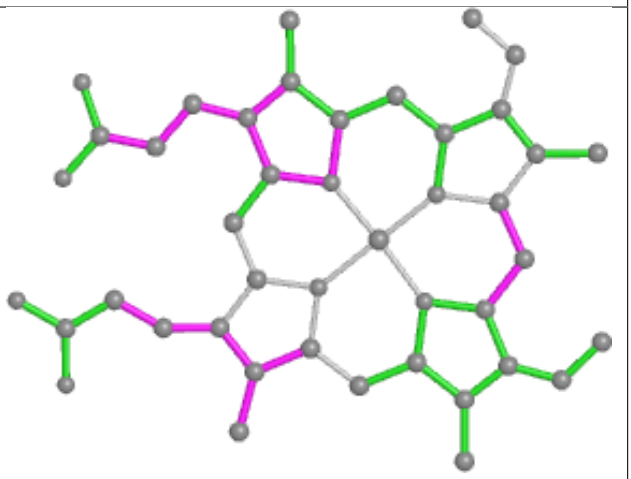


Rings

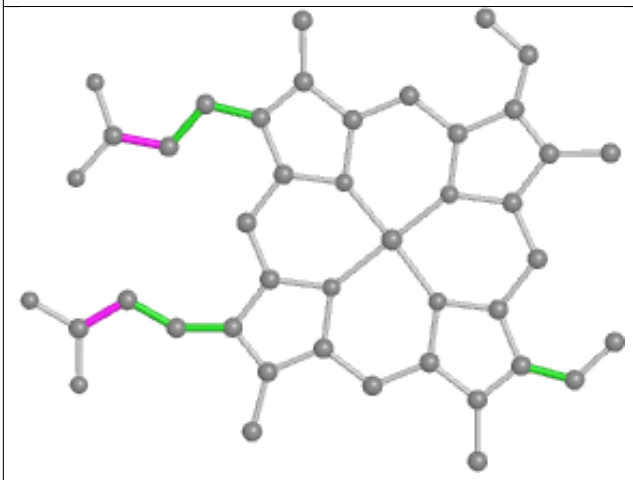
Ligand HEM f 101



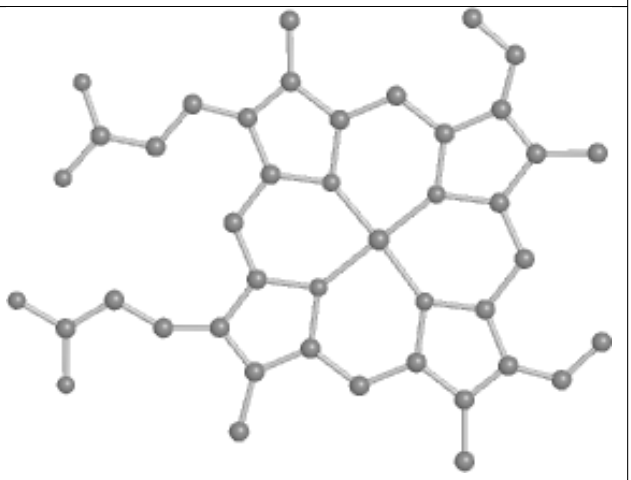
Bond lengths



Bond angles

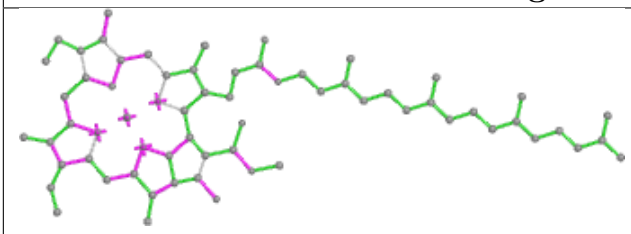


Torsions

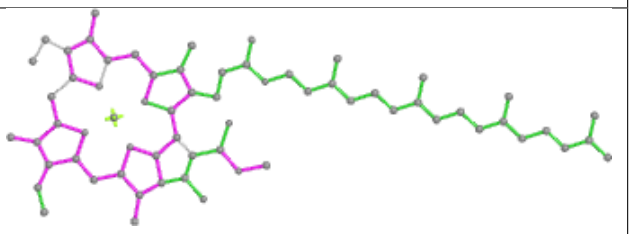


Rings

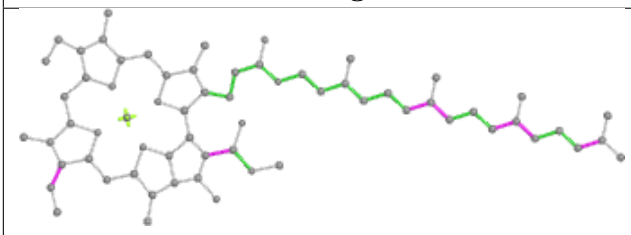
Ligand CLA a 407



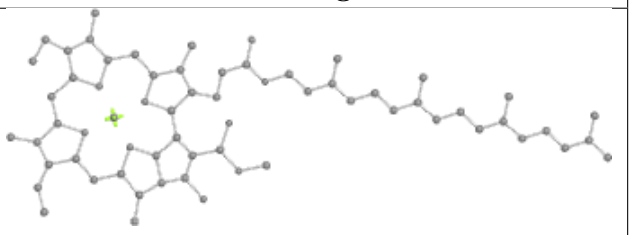
Bond lengths



Bond angles

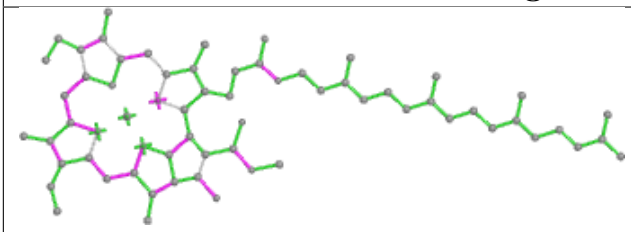


Torsions

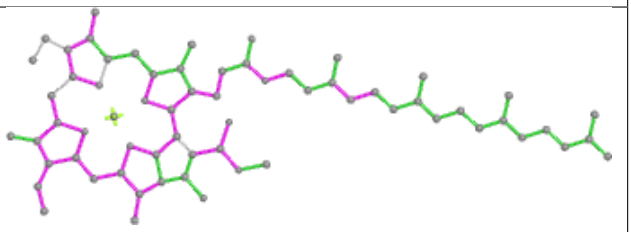


Rings

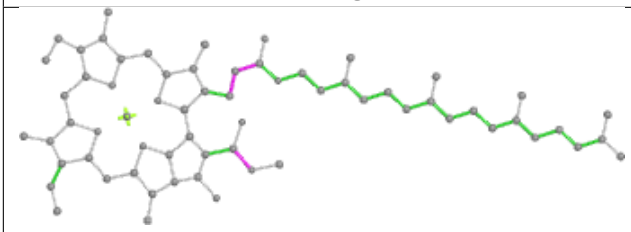
Ligand CLA C 501



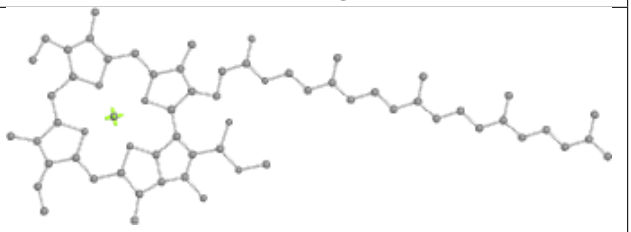
Bond lengths



Bond angles

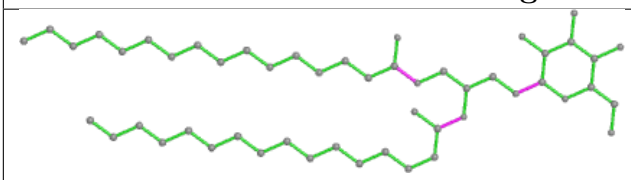


Torsions

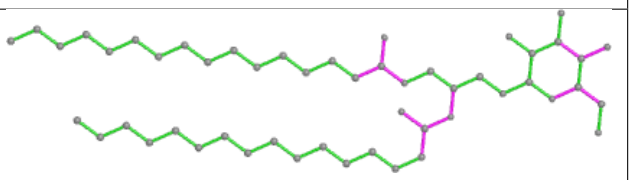


Rings

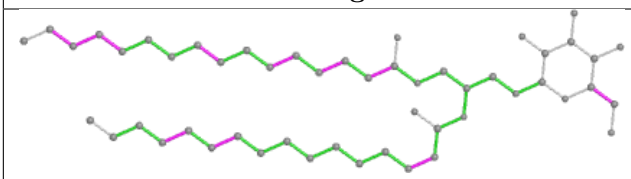
Ligand LMG B 622



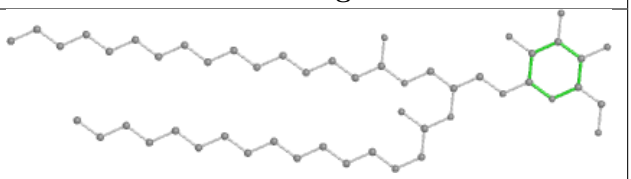
Bond lengths



Bond angles

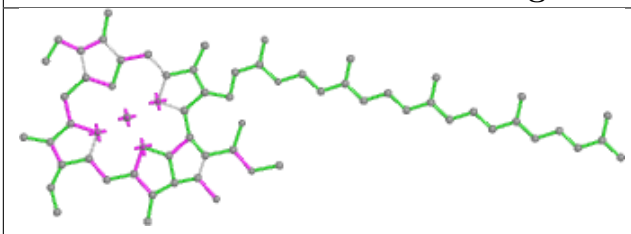


Torsions

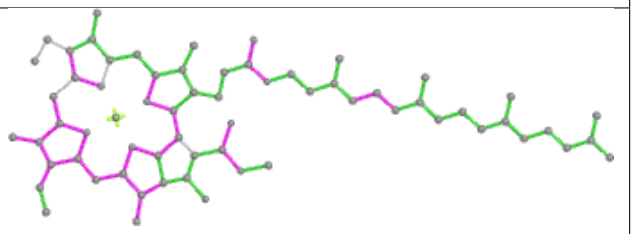


Rings

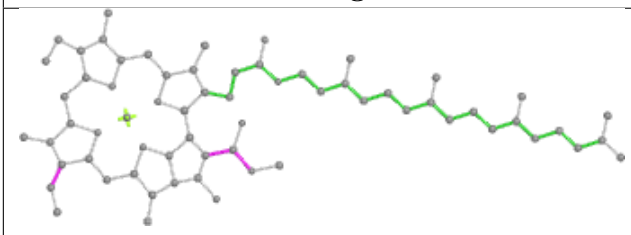
Ligand CLA a 406



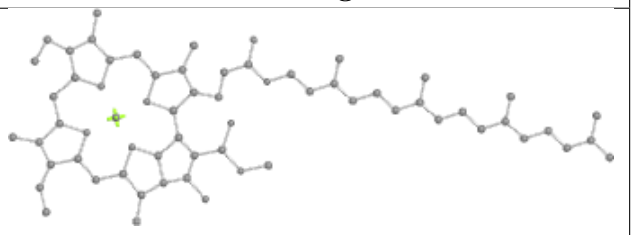
Bond lengths



Bond angles

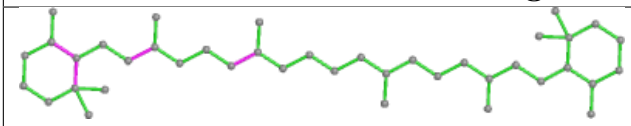


Torsions

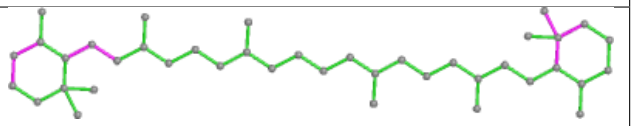


Rings

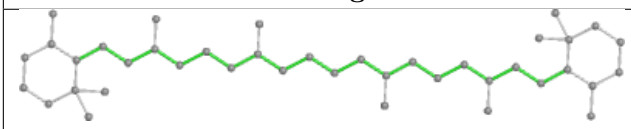
Ligand BCR b 622



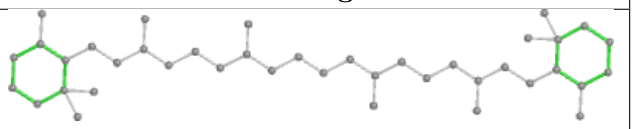
Bond lengths



Bond angles

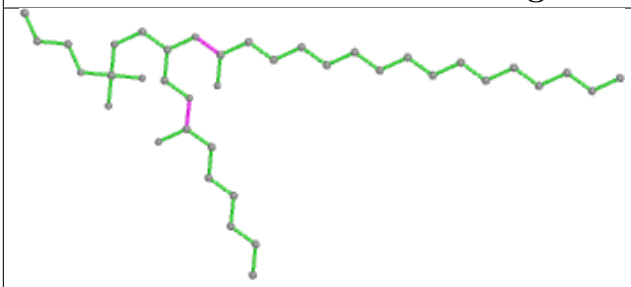


Torsions

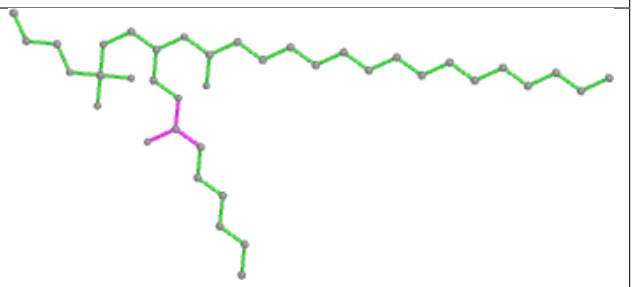


Rings

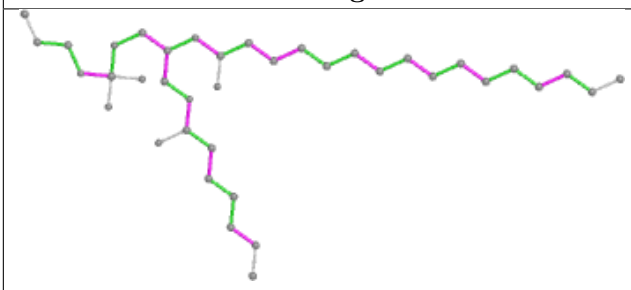
Ligand LHG e 101



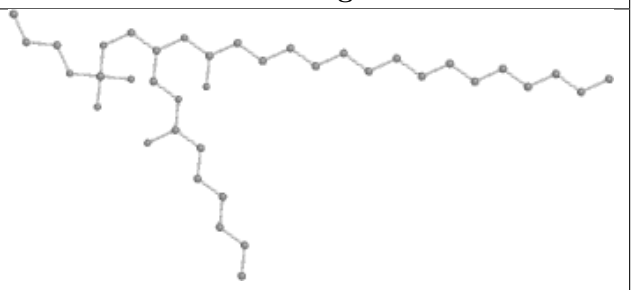
Bond lengths



Bond angles

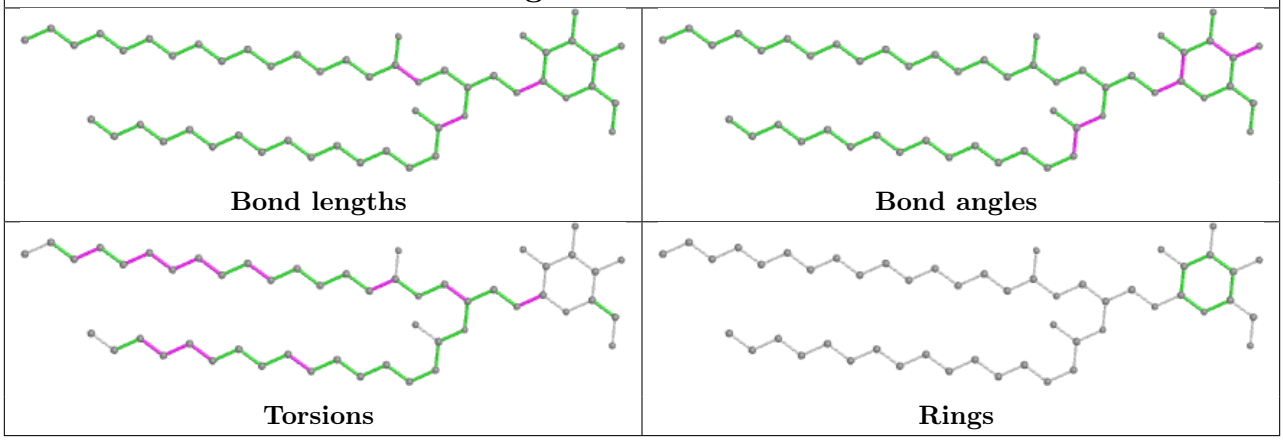


Torsions

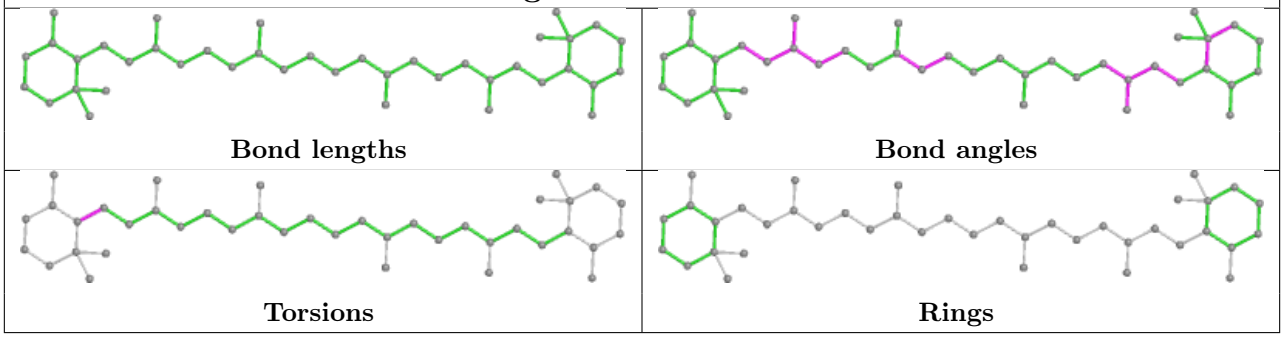


Rings

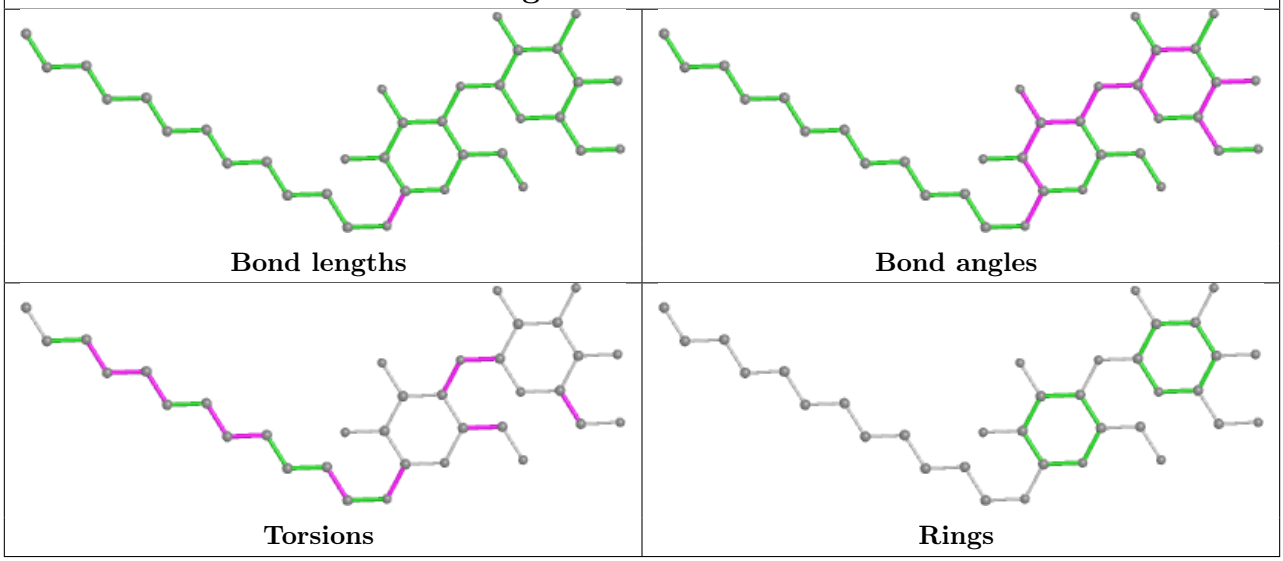
Ligand LMG a 412



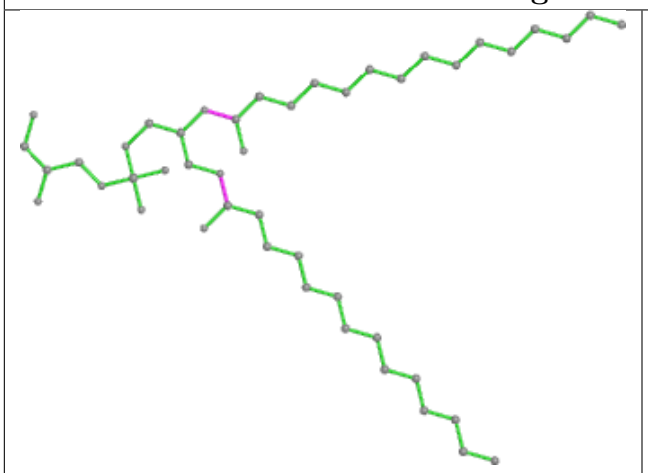
Ligand BCR B 618



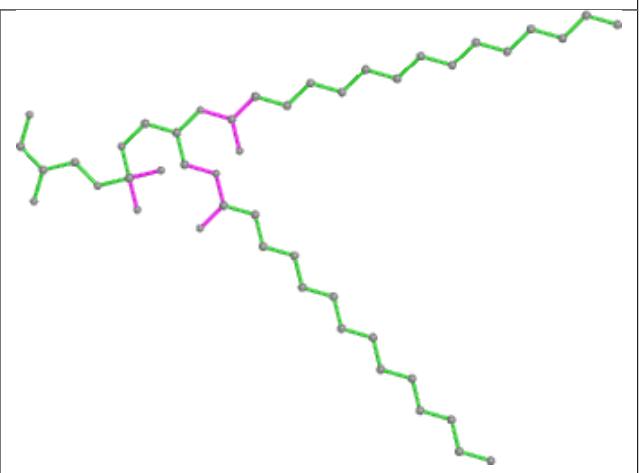
Ligand LMT C 520



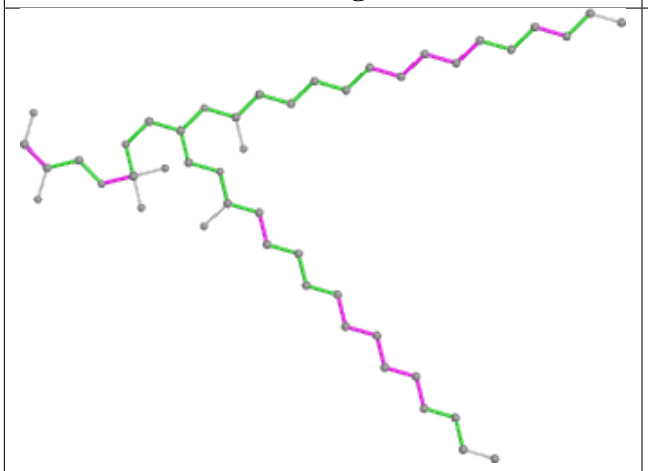
Ligand LHG f 102



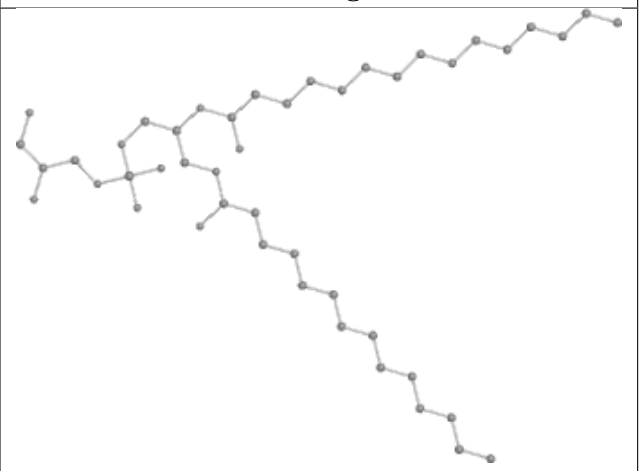
Bond lengths



Bond angles

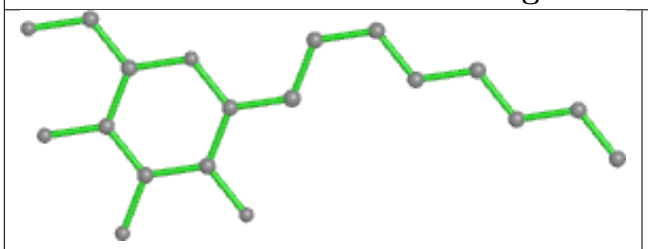


Torsions

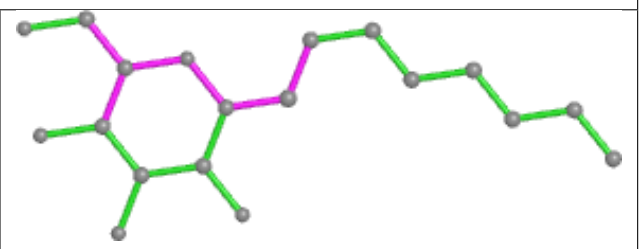


Rings

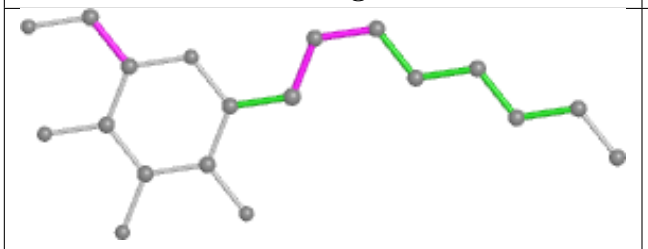
Ligand HTG C 521



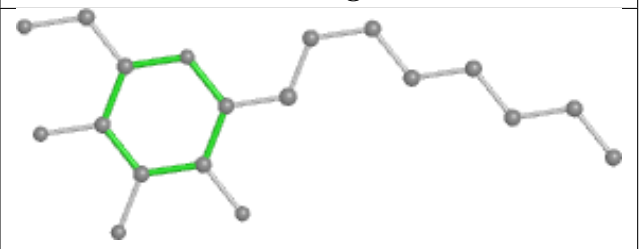
Bond lengths



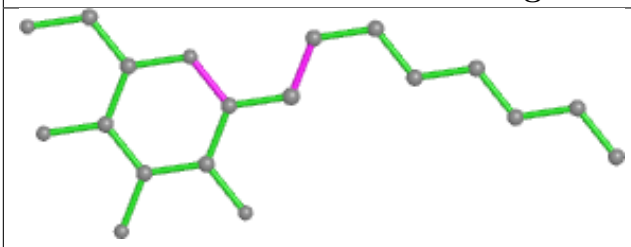
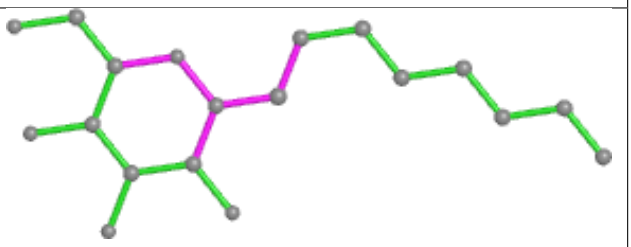
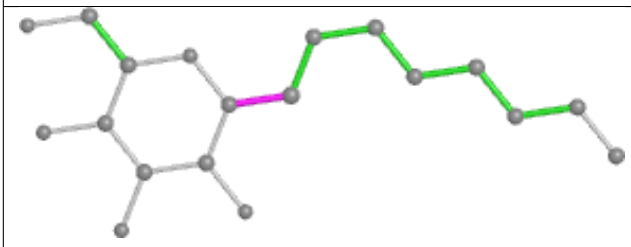
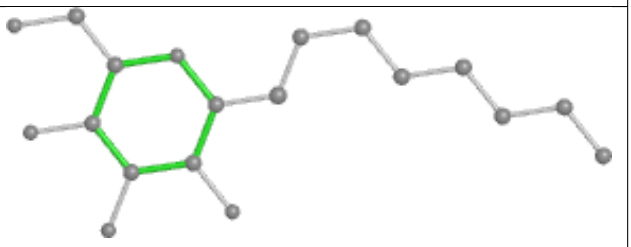
Bond angles

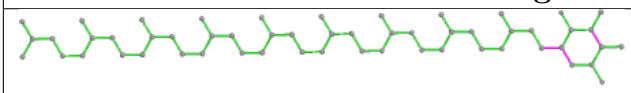
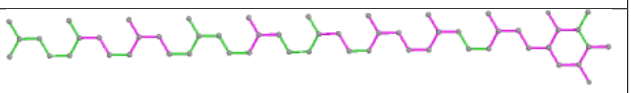
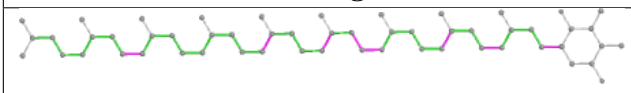
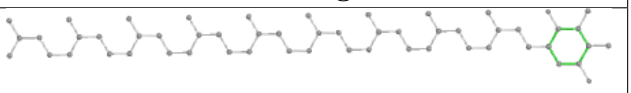


Torsions

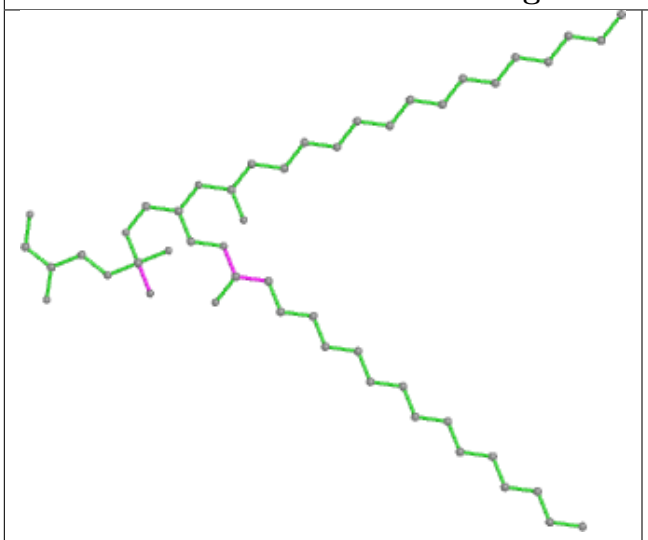


Rings

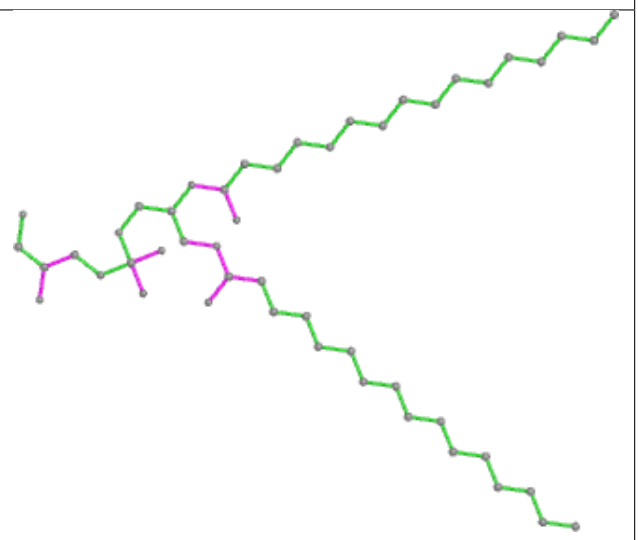
Ligand HTG b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 a 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

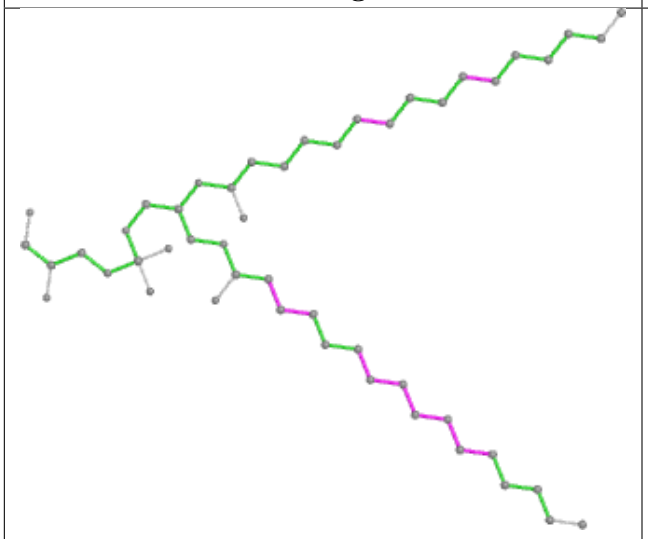
Ligand LHG D 409



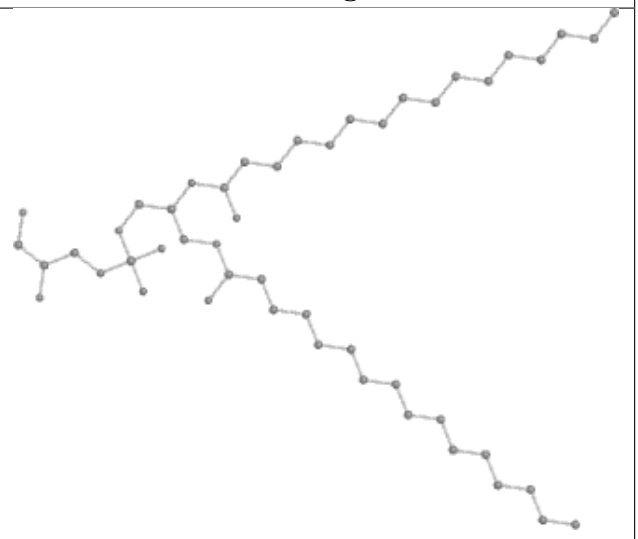
Bond lengths



Bond angles

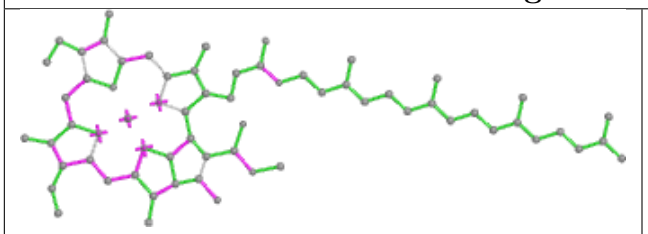


Torsions

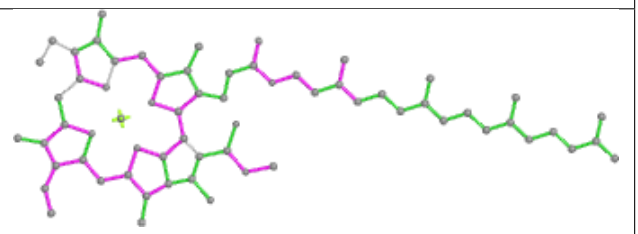


Rings

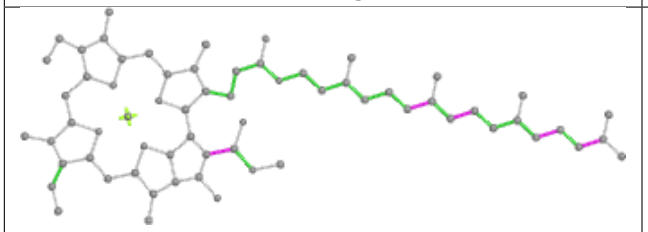
Ligand CLA D 405



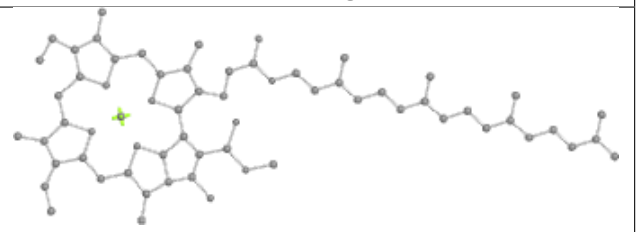
Bond lengths



Bond angles

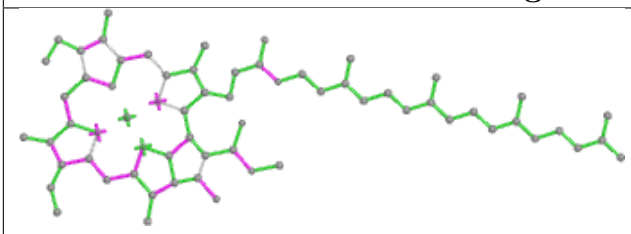


Torsions

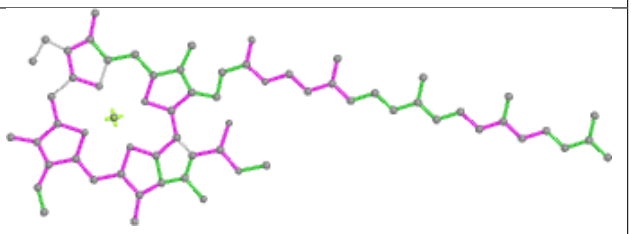


Rings

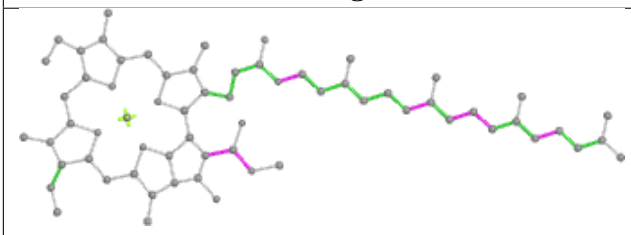
Ligand CLA C 509



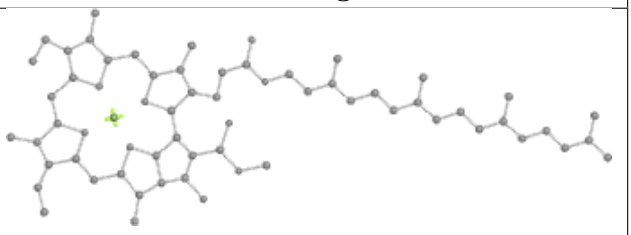
Bond lengths



Bond angles

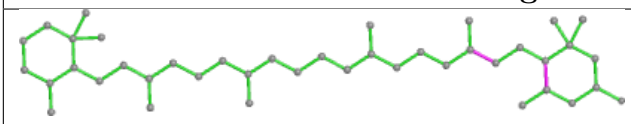


Torsions

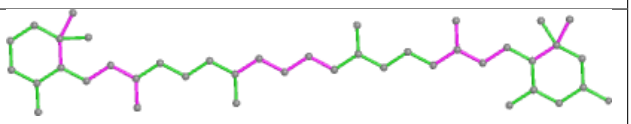


Rings

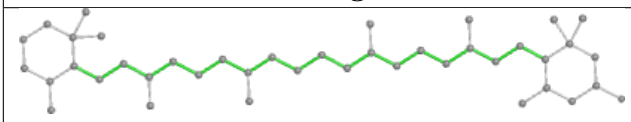
Ligand RRX H 102



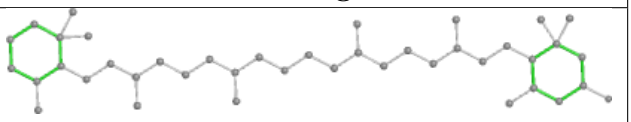
Bond lengths



Bond angles

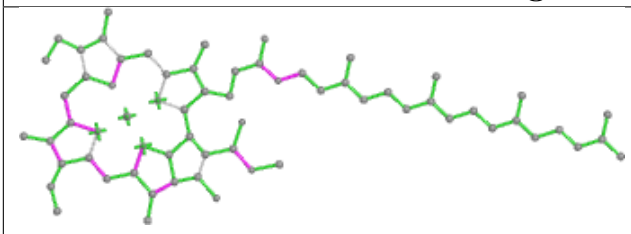


Torsions

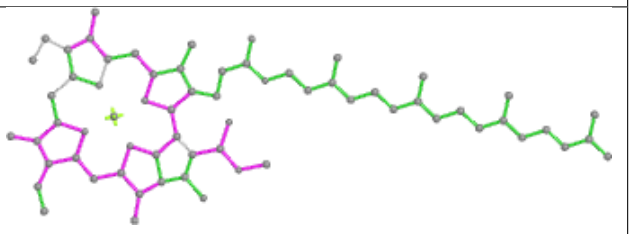


Rings

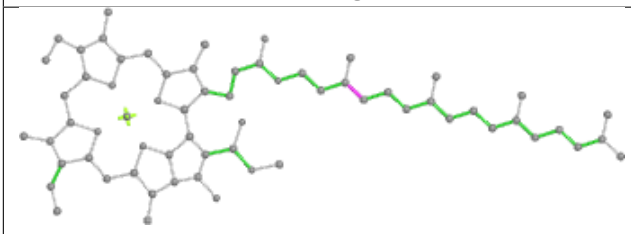
Ligand CLA b 609



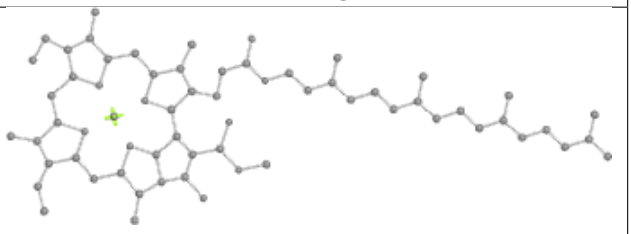
Bond lengths



Bond angles

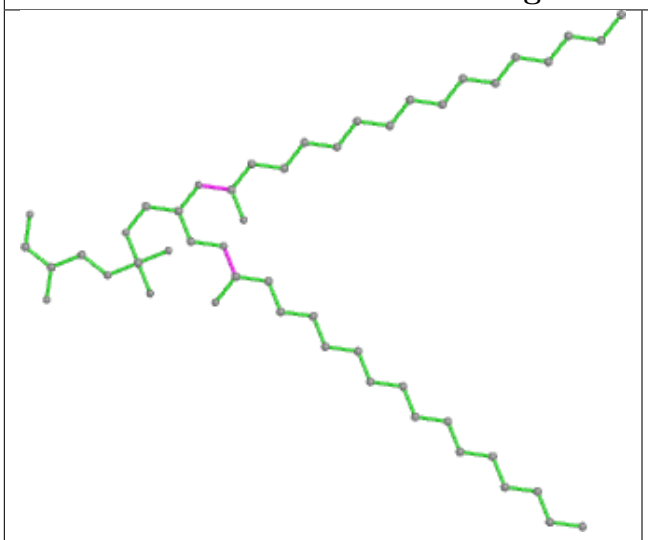


Torsions

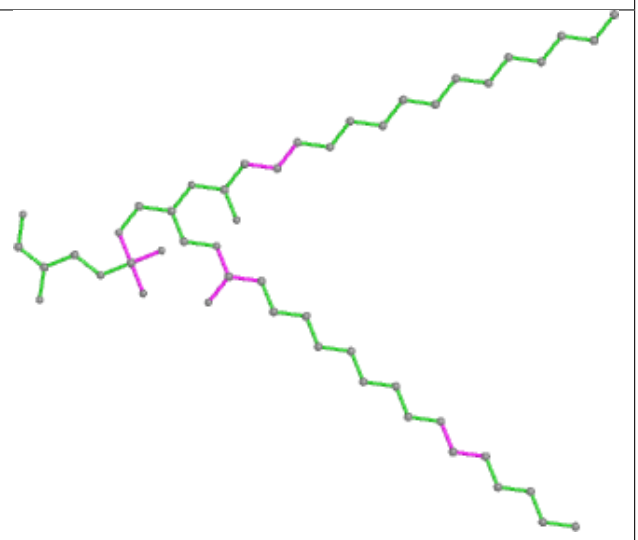


Rings

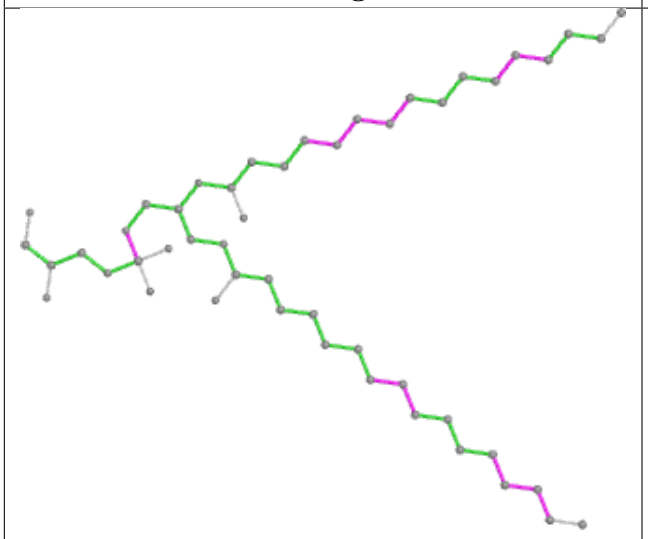
Ligand LHG B 621



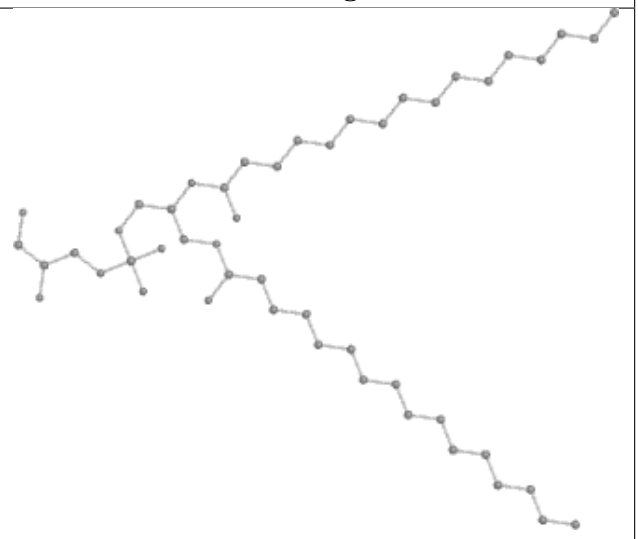
Bond lengths



Bond angles

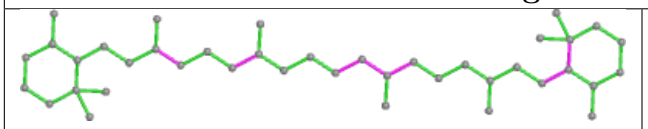


Torsions

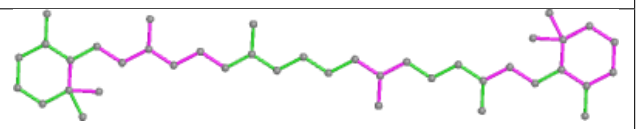


Rings

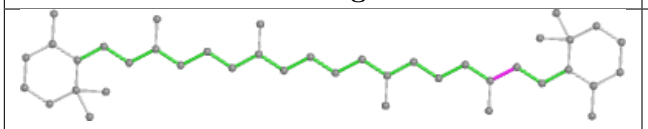
Ligand BCR D 406



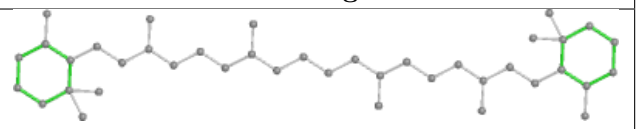
Bond lengths



Bond angles

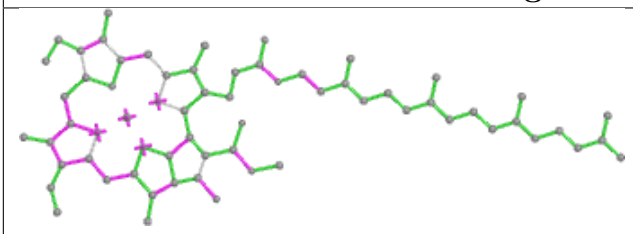


Torsions

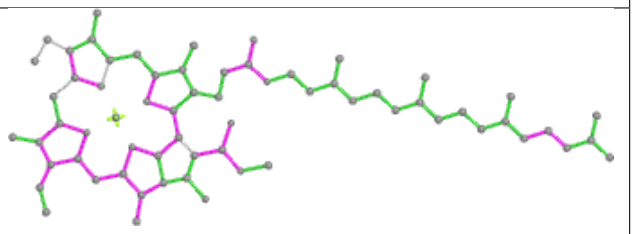


Rings

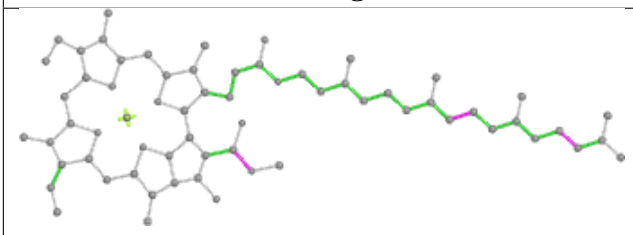
Ligand CLA B 611



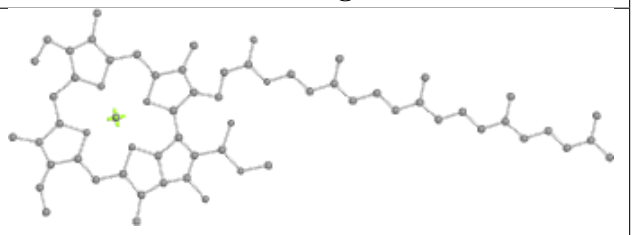
Bond lengths



Bond angles

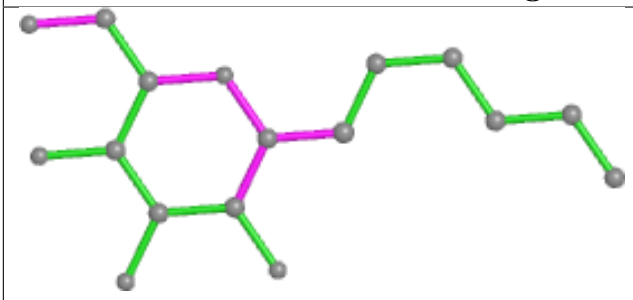


Torsions

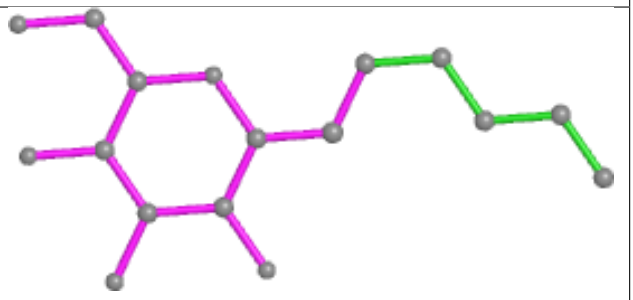


Rings

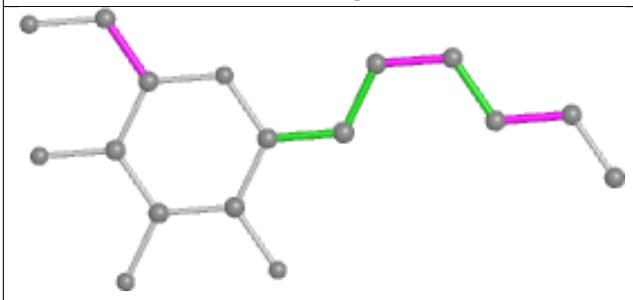
Ligand HTG b 640



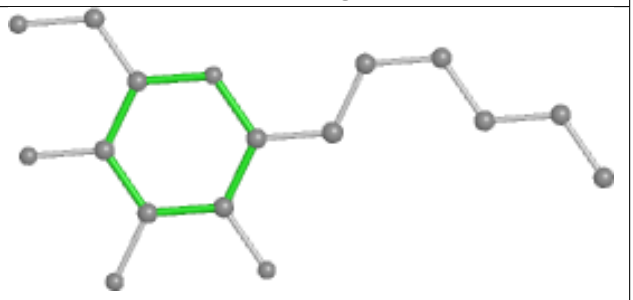
Bond lengths



Bond angles

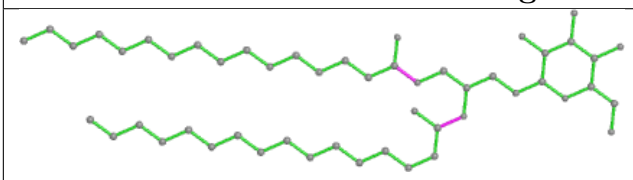


Torsions

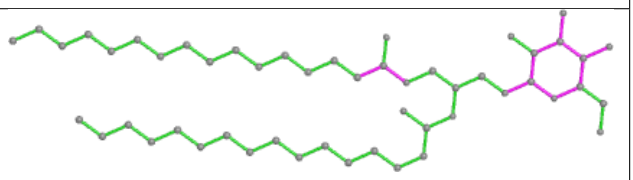


Rings

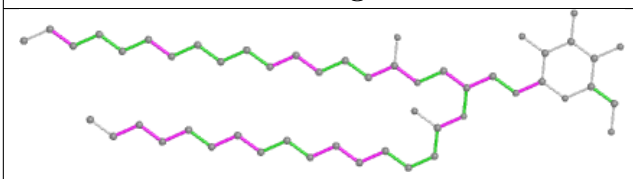
Ligand LMG A 411



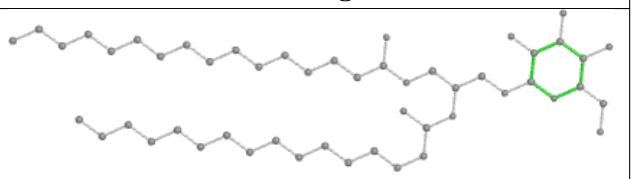
Bond lengths



Bond angles

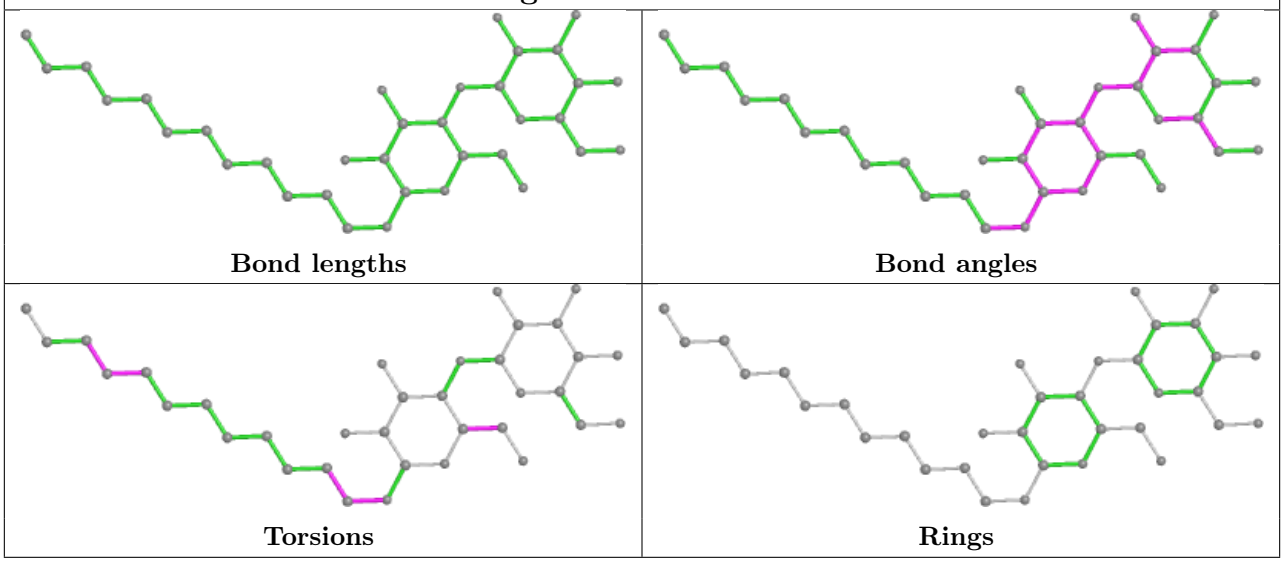


Torsions

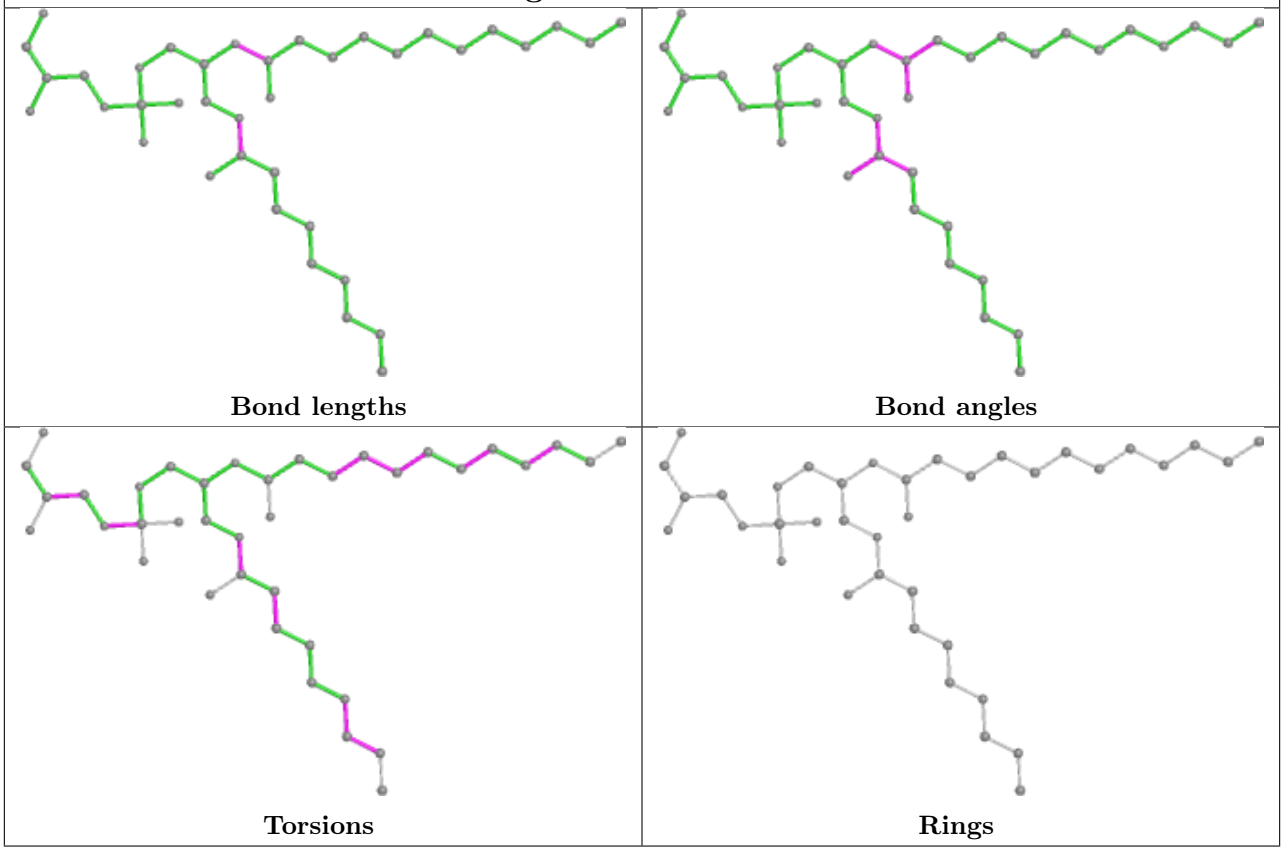


Rings

Ligand LMT m 101



Ligand LHG F 103



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%)	-0.79	3 (0%)	84	86	24, 33, 56, 90	0
1	a	334/334 (100%)	-0.78	4 (1%)	79	82	27, 35, 59, 92	0
2	B	505/505 (100%)	-0.58	11 (2%)	62	66	23, 38, 68, 90	0
2	b	504/505 (99%)	-0.47	23 (4%)	32	38	29, 39, 71, 131	0
3	C	451/455 (99%)	-0.64	4 (0%)	84	86	28, 41, 60, 115	0
3	c	455/455 (100%)	-0.53	8 (1%)	68	72	32, 45, 62, 110	0
4	D	341/342 (99%)	-0.76	5 (1%)	73	77	25, 34, 52, 118	0
4	d	341/342 (99%)	-0.78	7 (2%)	63	68	27, 35, 56, 98	0
5	E	80/81 (98%)	0.21	7 (8%)	10	12	37, 58, 90, 102	0
5	e	81/81 (100%)	0.27	9 (11%)	5	7	40, 54, 83, 105	0
6	F	34/34 (100%)	0.07	4 (11%)	4	5	36, 46, 86, 115	0
6	f	32/34 (94%)	-0.39	1 (3%)	49	55	38, 46, 70, 77	0
7	H	63/63 (100%)	-0.34	2 (3%)	47	54	34, 46, 59, 106	0
7	h	63/63 (100%)	-0.24	4 (6%)	20	24	35, 49, 66, 85	0
8	I	34/37 (91%)	-0.41	1 (2%)	51	57	36, 47, 67, 90	0
8	i	36/37 (97%)	-0.26	2 (5%)	24	29	38, 49, 90, 96	0
9	J	37/40 (92%)	-0.28	3 (8%)	12	15	32, 50, 104, 120	0
9	j	40/40 (100%)	-0.42	1 (2%)	57	62	39, 52, 67, 90	0
10	K	37/37 (100%)	-0.48	0	100	100	41, 49, 62, 73	0
10	k	37/37 (100%)	-0.44	0	100	100	44, 52, 74, 77	0
11	L	36/36 (100%)	-0.46	3 (8%)	11	14	26, 32, 77, 105	0
11	l	35/36 (97%)	-0.51	2 (5%)	23	29	29, 33, 69, 106	0
12	M	32/34 (94%)	-0.81	1 (3%)	49	55	31, 35, 55, 89	0
12	m	33/34 (97%)	-0.52	2 (6%)	21	26	32, 37, 76, 89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	-0.24	10 (4%)	37	43	28, 45, 73, 129	0
13	o	243/243 (100%)	-0.13	19 (7%)	13	17	29, 47, 80, 114	0
14	T	29/30 (96%)	-0.58	1 (3%)	45	51	28, 35, 58, 126	0
14	t	29/30 (96%)	-0.65	1 (3%)	45	51	29, 34, 61, 103	0
15	U	97/97 (100%)	-0.45	2 (2%)	63	68	30, 40, 60, 89	0
15	u	97/97 (100%)	-0.43	1 (1%)	82	85	34, 42, 63, 108	0
16	V	137/137 (100%)	-0.66	0	100	100	29, 39, 58, 77	0
16	v	137/137 (100%)	-0.28	5 (3%)	42	49	36, 49, 70, 90	0
17	Y	29/29 (100%)	0.56	3 (10%)	6	8	48, 62, 85, 111	0
17	y	29/29 (100%)	0.57	5 (17%)	1	1	53, 69, 83, 94	0
18	X	39/39 (100%)	0.07	4 (10%)	6	8	41, 51, 80, 108	0
18	x	38/39 (97%)	-0.09	4 (10%)	6	8	42, 52, 97, 107	0
19	Z	62/62 (100%)	0.11	9 (14%)	2	3	46, 59, 102, 129	0
19	z	62/62 (100%)	0.47	12 (19%)	1	1	57, 73, 113, 130	0
All	All	5246/5270 (99%)	-0.49	183 (3%)	44	50	23, 41, 73, 131	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	12	SER	9.3
18	X	40	SER	8.9
14	T	30	THR	7.0
2	b	486	LEU	7.0
7	H	64	ALA	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.93	0.13	39,42,73,78	0
12	FME	m	1	10/11	0.94	0.13	40,46,74,76	0
8	FME	I	1	10/11	0.95	0.08	36,43,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.96	0.08	31,41,67,75	0
8	FME	i	1	10/11	0.97	0.08	40,45,49,51	0
14	FME	T	1	10/11	0.98	0.06	35,40,67,76	0
4	HSK	d	336[B]	11/12	0.99	0.06	35,42,52,56	8
4	HSK	D	336[B]	11/12	0.99	0.07	35,37,42,45	8
4	HSK	D	336[A]	10/12	0.99	0.07	32,36,37,37	7
4	HSK	d	336[A]	10/12	0.99	0.06	35,38,42,42	7

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
27	UNL	J	103	16/-	0.42	0.27	74,97,111,112	0
27	UNL	b	603	16/-	0.47	0.26	73,94,114,115	0
27	UNL	I	102	14/-	0.52	0.22	82,96,101,101	0
27	UNL	j	104	16/-	0.52	0.27	77,91,113,115	0
32	HTG	D	413	16/19	0.52	0.33	80,99,115,116	0
28	LMT	m	103	23/35	0.53	0.23	59,80,125,127	0
32	HTG	C	536	19/19	0.53	0.32	79,117,138,138	0
28	LMT	J	102	24/35	0.53	0.26	62,83,124,131	0
27	UNL	B	625	15/-	0.54	0.23	83,93,115,120	0
27	UNL	c	525	5/-	0.56	0.16	72,83,84,84	0
32	HTG	B	624	19/19	0.56	0.40	65,99,109,114	0
32	HTG	b	602	19/19	0.56	0.20	71,113,132,135	0
33	DGD	d	408	48/66	0.56	0.30	70,100,122,132	0
27	UNL	C	524	26/-	0.58	0.24	76,97,109,120	0
32	HTG	C	522	19/19	0.58	0.33	61,92,117,117	0
28	LMT	a	401	35/35	0.59	0.33	38,67,86,100	35
28	LMT	A	415	35/35	0.59	0.27	54,88,106,116	0
27	UNL	e	103	11/-	0.60	0.33	67,81,102,104	0
28	LMT	l	101	24/35	0.61	0.23	59,76,130,142	0
27	UNL	i	101	16/-	0.61	0.23	82,85,100,101	0
27	UNL	E	103	16/-	0.62	0.25	78,88,108,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	HTG	d	413	16/19	0.63	0.32	66,100,118,131	0
33	DGD	D	408	45/66	0.63	0.25	70,93,120,129	0
27	UNL	K	103	10/-	0.63	0.23	78,89,97,98	0
32	HTG	c	541	15/19	0.64	0.37	74,104,117,120	0
32	HTG	U	203	14/19	0.64	0.48	76,107,133,154	0
27	UNL	I	101	16/-	0.65	0.21	78,88,102,110	0
27	UNL	H	104	7/-	0.65	0.18	78,82,85,88	0
28	LMT	j	102	23/35	0.67	0.21	71,81,105,108	0
27	UNL	u	201	13/-	0.68	0.26	57,67,80,84	0
28	LMT	M	101	35/35	0.68	0.21	43,73,83,90	0
28	LMT	m	101	35/35	0.68	0.23	38,70,81,85	0
28	LMT	m	102	25/35	0.68	0.26	45,72,116,124	0
28	LMT	F	102	24/35	0.68	0.25	60,97,113,121	0
27	UNL	a	415	40/-	0.69	0.24	75,97,121,124	0
28	LMT	t	102	24/35	0.69	0.20	67,87,121,126	0
32	HTG	c	524	9/19	0.70	0.19	73,79,97,114	0
32	HTG	B	629	19/19	0.70	0.20	59,118,133,135	0
27	UNL	A	414	28/-	0.70	0.23	76,94,110,114	0
27	UNL	j	103	33/-	0.70	0.24	67,112,139,141	0
32	HTG	b	627	19/19	0.70	0.25	69,91,106,109	0
34	GOL	e	104	6/6	0.70	0.23	72,77,81,84	0
26	LMG	c	521	51/55	0.71	0.23	51,93,114,122	0
29	DMS	c	540	4/4	0.71	0.33	99,101,109,120	0
27	UNL	i	102	14/-	0.71	0.23	91,101,109,109	0
26	LMG	C	519	48/55	0.71	0.23	52,89,111,119	0
29	DMS	O	312	4/4	0.72	0.29	78,88,109,113	0
27	UNL	c	527	16/-	0.72	0.24	73,83,115,120	0
27	UNL	c	526	32/-	0.72	0.24	67,94,116,119	0
28	LMT	b	626	25/35	0.72	0.20	62,76,105,114	0
27	UNL	Z	102	6/-	0.73	0.19	71,83,89,90	0
27	UNL	A	413	7/-	0.74	0.21	84,90,95,96	0
31	LHG	E	101	49/49	0.74	0.25	60,95,130,135	0
27	UNL	E	102	13/-	0.75	0.18	81,91,100,100	0
29	DMS	c	538	4/4	0.75	0.19	70,106,108,128	0
27	UNL	U	201	14/-	0.76	0.23	54,74,82,82	0
28	LMT	T	102	24/35	0.76	0.20	43,78,107,110	0
32	HTG	c	523	19/19	0.76	0.23	86,101,115,118	0
27	UNL	e	102	8/-	0.77	0.18	77,82,84,84	0
28	LMT	z	101	32/35	0.77	0.18	53,88,118,138	0
28	LMT	M	102	24/35	0.77	0.15	51,70,94,108	0
27	UNL	T	103	13/-	0.78	0.28	80,89,96,101	0
27	UNL	a	414	8/-	0.78	0.16	77,81,86,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DMS	a	418	4/4	0.78	0.19	97,107,116,118	0
29	DMS	O	309	4/4	0.79	0.33	80,106,109,118	0
27	UNL	B	630	16/-	0.80	0.18	69,81,89,89	0
27	UNL	b	641	40/-	0.80	0.18	60,77,94,97	0
27	UNL	B	643	40/-	0.80	0.20	60,76,101,112	0
27	UNL	A	412	8/-	0.80	0.16	64,74,78,79	0
29	DMS	d	416	4/4	0.81	0.24	99,114,115,118	0
27	UNL	i	104	14/-	0.81	0.18	69,80,99,101	0
31	LHG	e	101	38/49	0.81	0.23	63,94,111,113	0
28	LMT	Z	101	35/35	0.81	0.19	48,88,101,103	0
27	UNL	a	413	8/-	0.81	0.15	76,83,90,95	0
34	GOL	D	417	6/6	0.81	0.21	63,70,73,74	0
27	UNL	A	421	40/-	0.81	0.16	56,78,120,123	0
27	UNL	d	417	36/-	0.82	0.15	49,87,101,107	0
29	DMS	a	419	4/4	0.82	0.27	96,109,116,119	0
29	DMS	D	419	4/4	0.82	0.22	96,114,118,120	0
27	UNL	C	523	9/-	0.82	0.13	75,77,85,87	0
27	UNL	A	420	36/-	0.82	0.15	41,86,102,108	0
29	DMS	v	207	4/4	0.82	0.20	75,78,83,99	0
27	UNL	B	627	16/-	0.83	0.17	53,64,87,88	0
28	LMT	C	520	35/35	0.83	0.23	71,97,104,104	0
29	DMS	B	640	4/4	0.83	0.31	70,86,87,96	0
32	HTG	B	642	18/19	0.83	0.22	25,38,48,49	18
27	UNL	X	101	16/-	0.83	0.16	47,53,78,80	0
34	GOL	b	636	6/6	0.83	0.31	61,76,83,103	0
29	DMS	c	532	4/4	0.83	0.22	64,81,98,107	0
29	DMS	c	534	4/4	0.84	0.26	80,90,95,100	0
29	DMS	A	419	4/4	0.84	0.22	94,96,101,109	0
29	DMS	V	207	4/4	0.84	0.29	85,97,101,104	0
26	LMG	a	412	51/55	0.84	0.14	51,69,85,98	0
32	HTG	b	640	17/19	0.84	0.20	27,44,57,61	17
25	PL9	A	410	55/55	0.84	0.19	51,77,105,110	0
27	UNL	b	628	36/-	0.84	0.17	50,73,110,135	0
29	DMS	O	306	4/4	0.85	0.25	76,88,93,106	0
29	DMS	O	308	4/4	0.85	0.24	67,71,84,97	0
27	UNL	B	626	40/-	0.85	0.15	46,68,109,118	0
26	LMG	A	411	51/55	0.85	0.15	54,68,92,105	0
28	LMT	B	623	35/35	0.85	0.16	56,68,85,93	0
27	UNL	H	103	7/-	0.85	0.11	69,72,89,93	0
25	PL9	a	411	55/55	0.85	0.18	54,73,105,110	0
28	LMT	c	522	35/35	0.85	0.26	65,89,117,127	0
27	UNL	h	103	8/-	0.85	0.17	66,79,89,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	UNL	t	103	16/-	0.85	0.19	71,86,109,110	0
29	DMS	I	105	4/4	0.85	0.41	76,86,99,99	0
32	HTG	b	601	19/19	0.85	0.15	57,66,80,92	0
26	LMG	C	518	49/55	0.86	0.18	42,73,104,111	0
29	DMS	O	310	4/4	0.86	0.29	70,98,98,109	0
29	DMS	c	536	4/4	0.86	0.37	97,97,105,115	0
26	LMG	c	520	38/55	0.86	0.14	43,70,87,91	0
29	DMS	c	539	4/4	0.86	0.16	106,108,113,115	0
32	HTG	v	208	16/19	0.87	0.23	60,80,108,119	0
32	HTG	B	628	19/19	0.87	0.14	47,69,90,102	0
26	LMG	B	622	51/55	0.87	0.13	48,60,79,84	0
27	UNL	a	421	40/-	0.87	0.12	55,75,110,112	0
29	DMS	O	304	4/4	0.87	0.44	85,104,105,105	0
29	DMS	u	203	4/4	0.87	0.31	48,83,83,92	0
32	HTG	C	521	19/19	0.88	0.19	70,88,102,103	0
27	UNL	x	101	16/-	0.88	0.20	56,65,93,94	0
32	HTG	C	535	9/19	0.88	0.15	72,80,85,97	0
27	UNL	I	104	13/-	0.88	0.16	57,66,93,95	0
29	DMS	b	633	4/4	0.89	0.17	77,78,82,98	0
27	UNL	I	103	16/-	0.89	0.22	47,62,98,98	0
29	DMS	o	307	4/4	0.89	0.31	63,84,93,93	0
29	DMS	o	310	4/4	0.89	0.25	73,80,91,101	0
27	UNL	i	103	16/-	0.89	0.21	50,59,84,85	0
33	DGD	h	101	62/66	0.89	0.14	35,47,64,65	0
29	DMS	a	416	4/4	0.89	0.19	75,83,103,104	0
22	CLA	B	602	65/65	0.89	0.13	39,52,116,127	0
27	UNL	b	629	16/-	0.89	0.13	48,62,81,82	0
26	LMG	b	625	49/55	0.90	0.12	47,57,79,86	0
29	DMS	o	306	4/4	0.90	0.35	87,88,103,119	0
31	LHG	f	102	46/49	0.90	0.14	52,78,107,120	0
24	BCR	d	406	40/40	0.90	0.11	30,42,75,76	0
29	DMS	C	529	4/4	0.90	0.33	90,90,93,97	0
29	DMS	V	206	4/4	0.90	0.39	61,85,90,90	0
22	CLA	C	513	65/65	0.90	0.11	46,58,99,105	0
38	RRX	h	102	41/41	0.90	0.12	38,46,63,72	0
29	DMS	v	204	4/4	0.91	0.27	89,92,96,99	0
29	DMS	v	206	4/4	0.91	0.20	63,73,80,85	0
22	CLA	b	605	65/65	0.91	0.14	41,60,107,122	0
30	CA	v	209	1/1	0.91	0.19	90,90,90,90	0
22	CLA	b	620	65/65	0.91	0.11	32,44,112,139	0
27	UNL	D	414	16/-	0.91	0.17	44,53,66,73	0
29	DMS	O	307	4/4	0.91	0.25	87,92,93,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	D	406	40/40	0.91	0.10	32,40,73,76	0
24	BCR	K	101	40/40	0.91	0.16	36,47,54,58	0
29	DMS	B	639	4/4	0.91	0.27	75,84,91,94	0
24	BCR	K	102	40/40	0.91	0.10	42,53,57,60	0
33	DGD	H	101	62/66	0.91	0.13	34,46,55,59	0
29	DMS	U	202	4/4	0.91	0.15	40,61,69,82	0
29	DMS	C	527	4/4	0.91	0.15	75,76,79,93	0
24	BCR	T	101	40/40	0.91	0.11	40,52,78,83	0
29	DMS	C	534	4/4	0.91	0.30	67,81,87,87	0
24	BCR	c	515	40/40	0.91	0.11	50,62,69,70	0
32	HTG	O	302	19/19	0.91	0.12	41,57,74,75	0
29	DMS	O	311	4/4	0.92	0.15	80,88,88,91	0
29	DMS	h	104	4/4	0.92	0.19	103,104,106,109	0
32	HTG	o	301	19/19	0.92	0.11	49,58,70,73	0
31	LHG	F	103	38/49	0.92	0.15	56,82,111,112	0
33	DGD	C	516	62/66	0.92	0.11	31,45,103,116	0
29	DMS	B	634	4/4	0.92	0.35	83,86,86,94	0
29	DMS	C	532	4/4	0.92	0.25	58,72,80,81	0
22	CLA	B	617	65/65	0.92	0.12	31,43,129,145	0
29	DMS	u	202	4/4	0.92	0.17	48,69,70,82	0
24	BCR	t	101	40/40	0.92	0.10	36,52,72,74	0
29	DMS	D	420	4/4	0.92	0.33	93,98,108,110	0
29	DMS	a	417	4/4	0.92	0.35	69,78,88,92	0
38	RRX	H	102	41/41	0.92	0.11	36,42,56,60	0
27	UNL	d	414	16/-	0.92	0.17	44,56,84,88	0
26	LMG	d	412	47/55	0.93	0.12	37,47,99,103	0
29	DMS	B	633	4/4	0.93	0.15	94,98,98,100	0
29	DMS	E	104	4/4	0.93	0.28	91,95,98,105	0
29	DMS	e	105	4/4	0.93	0.33	80,93,97,97	0
22	CLA	c	507	65/65	0.93	0.10	42,51,109,121	0
29	DMS	B	635	4/4	0.93	0.21	90,94,95,106	0
34	GOL	c	533	6/6	0.93	0.25	58,62,76,81	0
32	HTG	V	202	19/19	0.93	0.27	50,62,107,107	0
24	BCR	y	101	40/40	0.93	0.09	40,47,57,59	0
29	DMS	o	309	4/4	0.93	0.26	70,78,79,91	0
29	DMS	B	638	4/4	0.94	0.27	43,55,65,71	0
29	DMS	O	303	4/4	0.94	0.19	72,84,93,96	0
29	DMS	V	208	4/4	0.94	0.11	83,84,90,91	0
22	CLA	C	506	65/65	0.94	0.10	39,55,121,136	0
29	DMS	O	305	4/4	0.94	0.17	77,88,91,93	0
22	CLA	C	512	65/65	0.94	0.09	39,51,96,105	0
22	CLA	c	513	65/65	0.94	0.10	43,56,94,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	Y	101	40/40	0.94	0.10	37,43,55,57	0
29	DMS	b	637	4/4	0.94	0.18	71,82,87,95	0
33	DGD	c	518	56/66	0.94	0.09	37,45,80,86	0
29	DMS	u	204	4/4	0.94	0.09	70,83,95,98	0
29	DMS	b	638	4/4	0.94	0.23	80,89,92,92	0
29	DMS	A	418	4/4	0.94	0.23	82,92,94,95	0
24	BCR	b	623	40/40	0.94	0.09	33,44,60,61	0
22	CLA	c	514	65/65	0.94	0.11	44,66,111,118	0
24	BCR	c	516	40/40	0.94	0.09	37,46,57,58	0
22	CLA	b	610	65/65	0.94	0.09	31,42,81,83	0
29	DMS	V	204	4/4	0.94	0.13	68,73,75,90	0
29	DMS	b	634	4/4	0.95	0.20	73,77,82,89	0
29	DMS	b	635	4/4	0.95	0.22	70,71,71,73	0
22	CLA	c	508	65/65	0.95	0.09	34,44,68,76	0
29	DMS	v	203	4/4	0.95	0.18	76,78,80,82	0
29	DMS	D	418	4/4	0.95	0.24	83,92,96,114	0
29	DMS	v	205	4/4	0.95	0.16	61,68,69,70	0
29	DMS	b	639	4/4	0.95	0.27	87,93,94,106	0
26	LMG	D	412	47/55	0.95	0.10	34,44,84,95	0
22	CLA	C	508	65/65	0.95	0.09	33,39,105,122	0
31	LHG	D	409	49/49	0.95	0.10	37,48,64,69	0
31	LHG	D	411	44/49	0.95	0.11	35,44,110,117	0
29	DMS	c	535	4/4	0.95	0.21	84,92,99,112	0
29	DMS	B	636	4/4	0.95	0.25	65,83,88,91	0
31	LHG	d	411	44/49	0.95	0.13	37,47,109,121	0
33	DGD	C	517	62/66	0.95	0.08	27,42,77,83	0
29	DMS	c	537	4/4	0.95	0.31	85,94,103,106	0
29	DMS	V	205	4/4	0.95	0.25	77,79,80,89	0
21	CL	v	201	1/1	0.95	0.26	93,93,93,93	0
33	DGD	c	519	62/66	0.95	0.09	32,45,73,87	0
24	BCR	B	618	40/40	0.95	0.08	31,39,51,54	0
24	BCR	B	619	40/40	0.95	0.08	30,40,55,70	0
34	GOL	C	533	6/6	0.95	0.17	46,53,57,61	0
29	DMS	B	641	4/4	0.95	0.25	65,66,71,83	0
29	DMS	A	416	4/4	0.95	0.21	71,73,77,85	0
22	CLA	C	507	65/65	0.95	0.10	37,44,68,75	0
29	DMS	C	531	4/4	0.95	0.12	86,87,90,92	0
29	DMS	a	420	4/4	0.95	0.17	87,90,91,93	0
22	CLA	D	405	65/65	0.95	0.09	31,39,114,126	0
39	MG	K	104	1/1	0.95	0.09	56,56,56,56	0
22	CLA	c	512	65/65	0.96	0.10	40,49,56,65	0
22	CLA	C	503	65/65	0.96	0.08	33,41,47,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	B	603	65/65	0.96	0.08	30,38,46,50	0
22	CLA	d	405	65/65	0.96	0.08	31,43,111,120	0
24	BCR	A	409	40/40	0.96	0.08	28,35,42,44	0
22	CLA	a	409	65/65	0.96	0.11	29,37,126,135	0
22	CLA	B	607	65/65	0.96	0.09	32,39,71,87	0
24	BCR	B	620	40/40	0.96	0.08	31,41,57,60	0
24	BCR	C	514	40/40	0.96	0.09	35,46,60,63	0
29	DMS	V	203	4/4	0.96	0.15	74,84,87,92	0
22	CLA	b	606	65/65	0.96	0.09	32,37,48,59	0
29	DMS	B	637	4/4	0.96	0.12	69,73,81,82	0
22	CLA	B	611	65/65	0.96	0.09	30,37,44,57	0
22	CLA	b	611	65/65	0.96	0.07	26,32,50,58	0
22	CLA	b	614	65/65	0.96	0.07	30,40,46,51	0
22	CLA	b	616	65/65	0.96	0.08	29,36,44,50	0
24	BCR	a	410	40/40	0.96	0.07	32,39,45,46	0
29	DMS	C	528	4/4	0.96	0.25	74,81,82,82	0
33	DGD	C	515	62/66	0.96	0.11	30,41,105,109	0
24	BCR	b	621	40/40	0.96	0.07	36,42,55,58	0
24	BCR	b	622	40/40	0.96	0.08	29,44,58,67	0
30	CA	V	209	1/1	0.96	0.15	93,93,93,93	0
30	CA	c	501	1/1	0.96	0.10	62,62,62,62	0
29	DMS	b	631	4/4	0.96	0.08	66,78,80,82	0
29	DMS	b	632	4/4	0.96	0.12	63,72,72,73	0
22	CLA	b	619	65/65	0.96	0.08	32,42,59,67	0
22	CLA	C	509	65/65	0.96	0.10	33,42,68,76	0
22	CLA	c	504	65/65	0.96	0.08	34,47,56,58	0
22	CLA	c	505	65/65	0.96	0.07	35,40,74,82	0
22	CLA	C	510	65/65	0.96	0.08	33,40,52,66	0
22	CLA	A	408	65/65	0.96	0.09	25,34,110,115	0
29	DMS	c	530	4/4	0.96	0.17	70,88,95,104	0
22	CLA	c	509	65/65	0.96	0.08	34,41,100,113	0
22	CLA	c	510	65/65	0.96	0.10	30,42,76,81	0
25	PL9	d	407	55/55	0.96	0.08	27,34,46,55	0
31	LHG	b	624	49/49	0.97	0.09	33,42,65,76	0
31	LHG	d	409	49/49	0.97	0.12	40,47,64,70	0
31	LHG	d	410	49/49	0.97	0.11	27,38,58,73	0
29	DMS	C	530	4/4	0.97	0.16	40,54,55,58	0
22	CLA	C	504	65/65	0.97	0.07	32,38,72,74	0
23	PHO	A	407	64/64	0.97	0.07	25,30,33,38	0
23	PHO	D	404	64/64	0.97	0.08	25,34,41,45	0
23	PHO	a	408	64/64	0.97	0.07	27,33,38,42	0
29	DMS	c	531	4/4	0.97	0.27	90,91,96,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	607	65/65	0.97	0.07	29,36,47,51	0
22	CLA	b	608	65/65	0.97	0.08	29,35,75,79	0
22	CLA	C	505	65/65	0.97	0.07	34,41,54,60	0
22	CLA	B	608	65/65	0.97	0.08	24,31,47,62	0
22	CLA	b	612	65/65	0.97	0.07	26,35,44,49	0
22	CLA	b	613	65/65	0.97	0.10	35,40,50,54	0
22	CLA	B	610	65/65	0.97	0.10	33,41,49,54	0
22	CLA	B	604	65/65	0.97	0.07	26,34,44,55	0
29	DMS	d	415	4/4	0.97	0.18	64,70,75,87	0
22	CLA	b	617	65/65	0.97	0.08	30,35,74,80	0
22	CLA	b	618	65/65	0.97	0.09	29,36,123,128	0
22	CLA	B	614	65/65	0.97	0.07	26,32,69,94	0
29	DMS	o	304	4/4	0.97	0.14	85,86,87,87	0
29	DMS	o	305	4/4	0.97	0.31	88,91,92,102	0
22	CLA	B	615	65/65	0.97	0.07	27,36,115,119	0
22	CLA	c	502	65/65	0.97	0.07	38,43,56,64	0
29	DMS	o	308	4/4	0.97	0.26	71,77,85,85	0
22	CLA	c	503	65/65	0.97	0.07	31,38,55,64	0
22	CLA	C	511	65/65	0.97	0.09	36,44,50,53	0
29	DMS	o	311	4/4	0.97	0.20	80,91,94,116	0
29	DMS	B	632	4/4	0.97	0.09	53,54,55,69	0
22	CLA	B	616	65/65	0.97	0.07	32,39,61,67	0
22	CLA	c	506	65/65	0.97	0.07	34,43,57,71	0
24	BCR	k	101	40/40	0.97	0.12	41,48,56,58	0
33	DGD	c	517	62/66	0.97	0.09	32,46,93,108	0
22	CLA	B	605	65/65	0.97	0.08	26,33,65,73	0
22	CLA	D	403	65/65	0.97	0.08	23,28,49,53	0
22	CLA	C	501	65/65	0.97	0.08	32,41,55,66	0
25	PL9	D	407	55/55	0.97	0.08	26,35,43,54	0
22	CLA	a	406	65/65	0.97	0.10	25,31,40,56	0
22	CLA	c	511	65/65	0.97	0.08	30,40,54,58	0
29	DMS	C	525	4/4	0.97	0.10	42,51,52,58	0
31	LHG	B	621	49/49	0.97	0.10	33,41,61,65	0
29	DMS	C	526	4/4	0.97	0.20	60,61,66,69	0
36	BCT	d	401[A]	4/4	0.97	0.12	50,52,55,67	4
36	BCT	d	401[B]	4/4	0.97	0.12	21,31,31,38	4
37	HEM	F	101	43/43	0.97	0.09	43,52,63,69	0
22	CLA	a	407	65/65	0.97	0.08	25,33,104,120	0
22	CLA	C	502	65/65	0.97	0.07	30,36,52,61	0
39	MG	J	101	1/1	0.97	0.04	45,45,45,45	0
22	CLA	A	404	65/65	0.97	0.09	22,28,40,59	0
39	MG	k	102	1/1	0.97	0.13	61,61,61,61	0

Continued on next page...

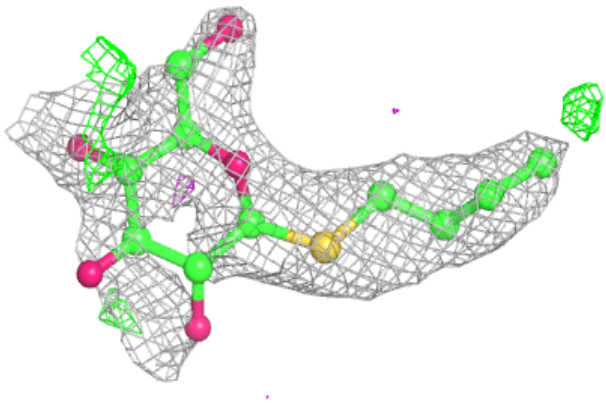
Continued from previous page...

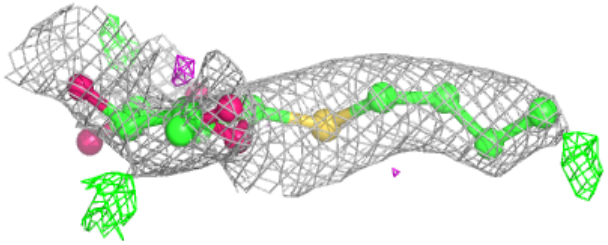
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	CA	O	301	1/1	0.98	0.05	57,57,57,57	0
22	CLA	B	613	65/65	0.98	0.07	28,33,40,43	0
30	CA	b	604	1/1	0.98	0.07	63,63,63,63	0
23	PHO	d	404	64/64	0.98	0.09	27,34,41,48	0
30	CA	o	302	1/1	0.98	0.07	58,58,58,58	0
29	DMS	c	528	4/4	0.98	0.10	41,54,55,56	0
29	DMS	c	529	4/4	0.98	0.16	52,56,57,67	0
22	CLA	A	405	65/65	0.98	0.07	22,27,39,48	0
31	LHG	D	410	49/49	0.98	0.12	30,38,53,67	0
22	CLA	b	615	65/65	0.98	0.08	25,33,52,55	0
22	CLA	B	609	65/65	0.98	0.07	28,35,44,47	0
22	CLA	b	609	65/65	0.98	0.09	28,33,47,48	0
22	CLA	d	402	65/65	0.98	0.09	25,30,48,56	0
36	BCT	D	402[A]	4/4	0.98	0.16	24,36,36,40	4
36	BCT	D	402[B]	4/4	0.98	0.16	36,44,46,50	4
29	DMS	D	415	4/4	0.98	0.11	65,68,77,91	0
29	DMS	b	630	4/4	0.98	0.10	37,40,40,42	0
29	DMS	D	416	4/4	0.98	0.17	68,80,85,89	0
37	HEM	f	101	43/43	0.98	0.07	42,50,58,63	0
22	CLA	d	403	65/65	0.98	0.07	26,29,43,53	0
22	CLA	B	606	65/65	0.98	0.09	28,34,51,56	0
22	CLA	A	406	65/65	0.98	0.06	24,33,95,113	0
22	CLA	B	612	65/65	0.98	0.07	25,32,48,55	0
39	MG	j	101	1/1	0.98	0.06	50,50,50,50	0
29	DMS	B	631	4/4	0.98	0.09	31,35,36,42	0
40	HEC	V	201	43/43	0.98	0.10	28,32,39,44	0
40	HEC	v	202	43/43	0.98	0.09	37,44,49,57	0
30	CA	B	601	1/1	0.99	0.10	60,60,60,60	0
21	CL	A	402	1/1	0.99	0.04	31,31,31,31	0
29	DMS	o	303	4/4	0.99	0.05	31,40,41,44	0
21	CL	a	404	1/1	0.99	0.02	35,35,35,35	0
21	CL	a	405	1/1	0.99	0.06	34,34,34,34	0
20	OEX	a	402	10/10	0.99	0.04	28,33,39,41	0
29	DMS	A	417	4/4	0.99	0.07	32,36,37,38	0
35	FE2	D	401	1/1	1.00	0.06	41,41,41,41	0
35	FE2	a	403	1/1	1.00	0.07	40,40,40,40	0
21	CL	A	403	1/1	1.00	0.04	29,29,29,29	0
20	OEX	A	401	10/10	1.00	0.04	28,31,39,40	0

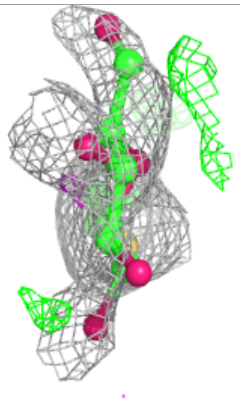
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG D 413:

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

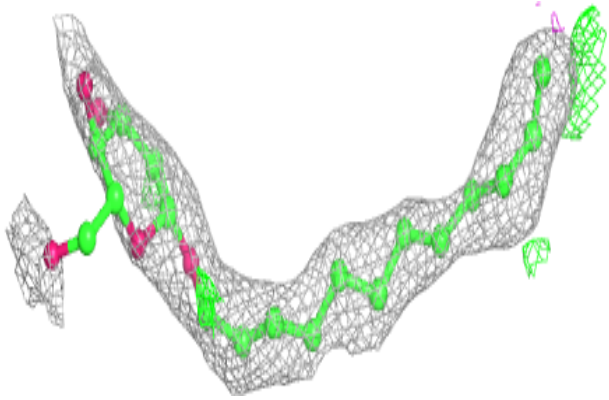


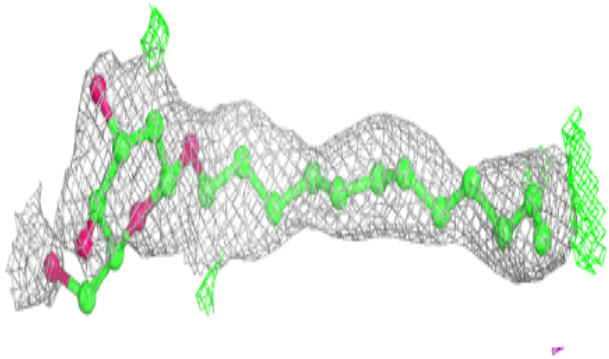


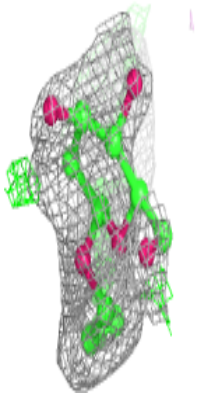


Electron density around LMT m 103:

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

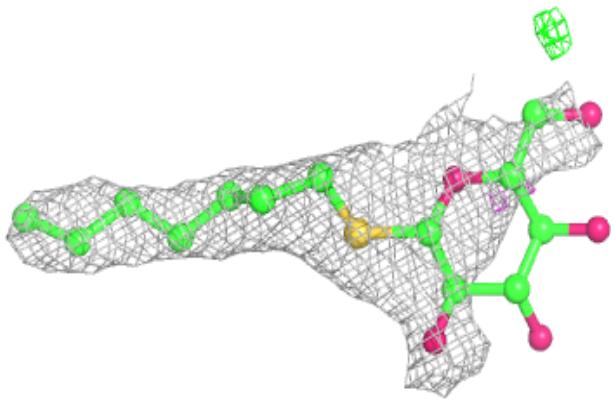


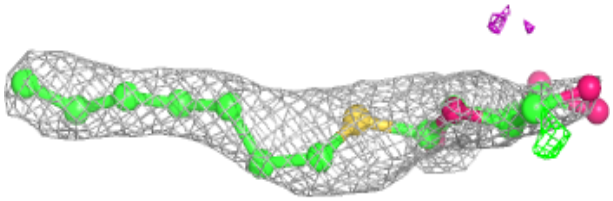


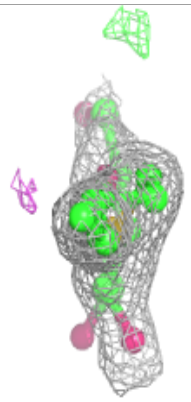


Electron density around HTG C 536:

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

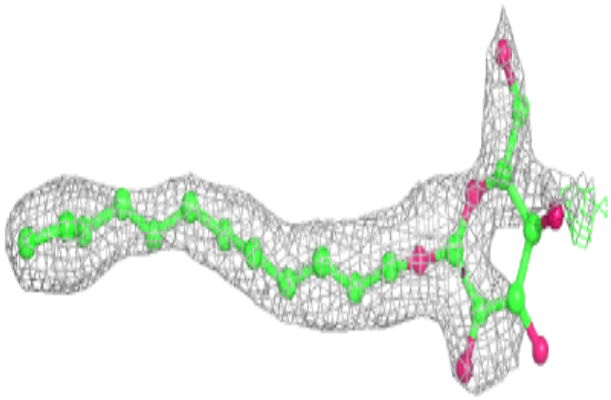


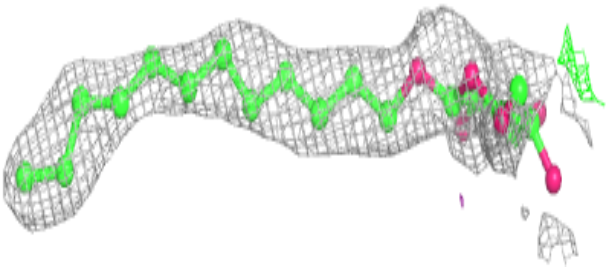




Electron density around LMT J 102:

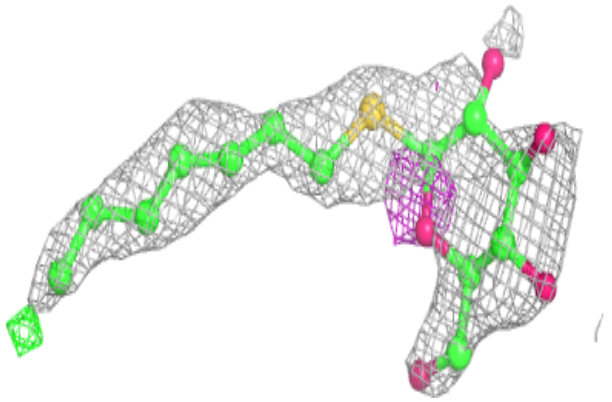
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

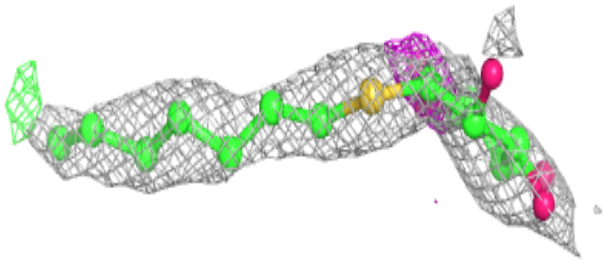


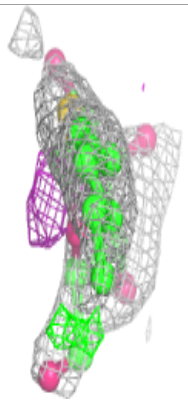


Electron density around HTG B 624:

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

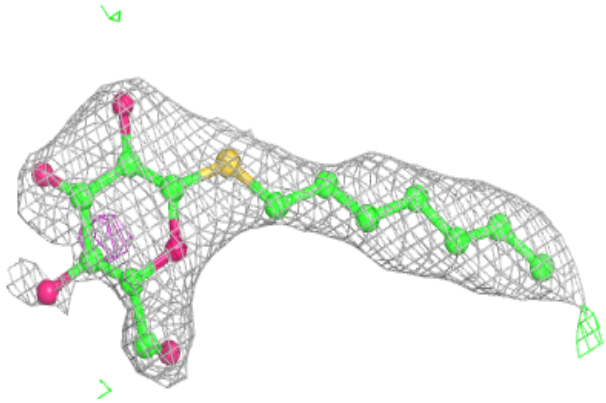


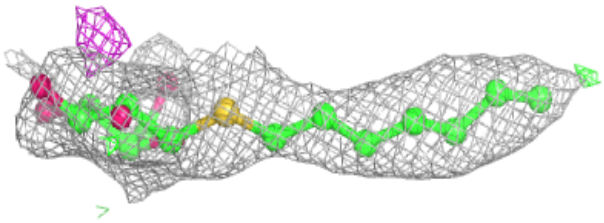


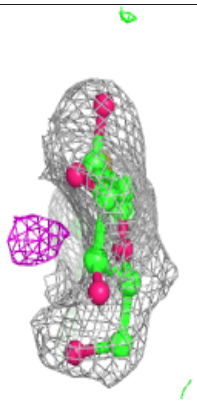


Electron density around HTG b 602:

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

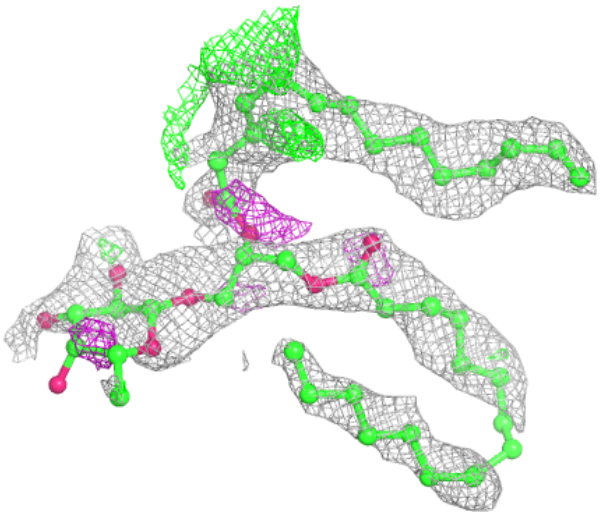


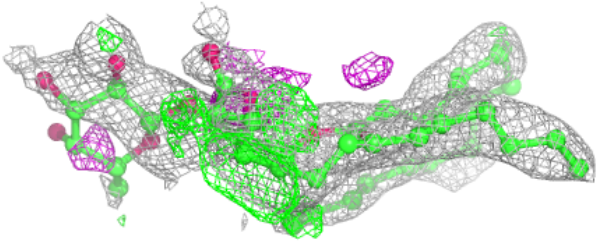


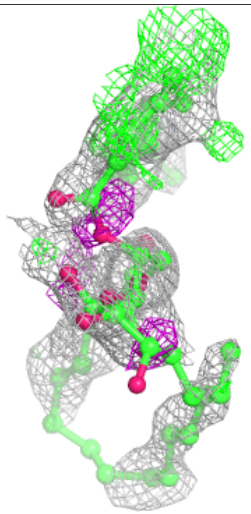


Electron density around DGD d 408:

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

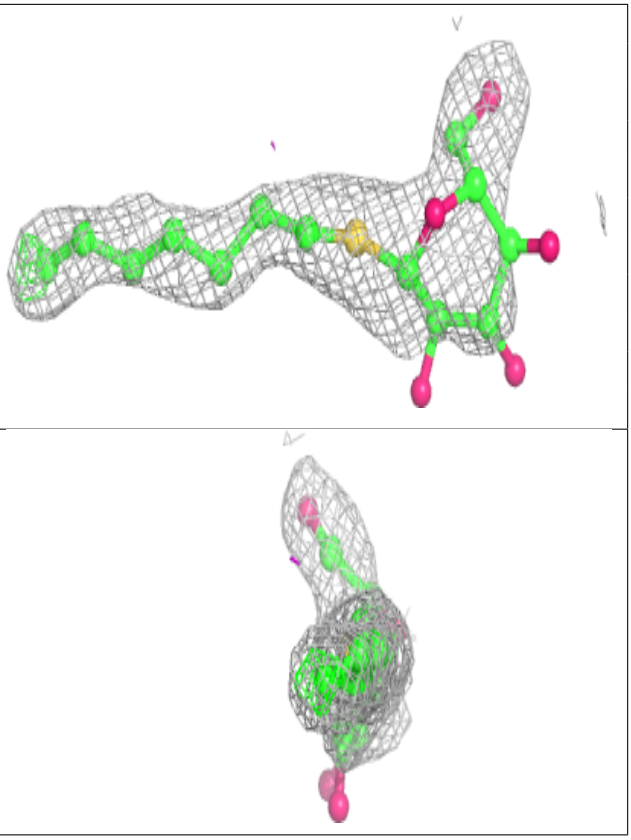


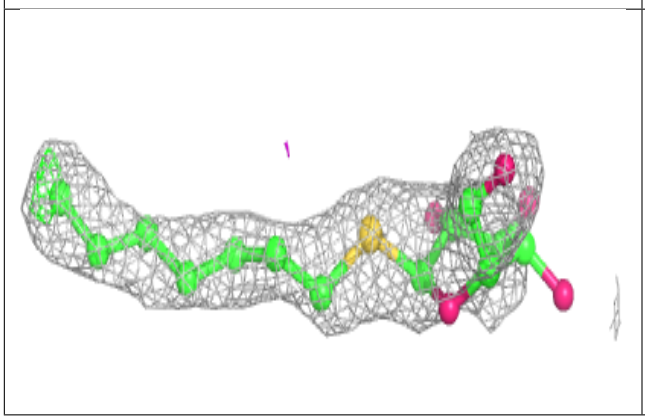




Electron density around HTG C 522:

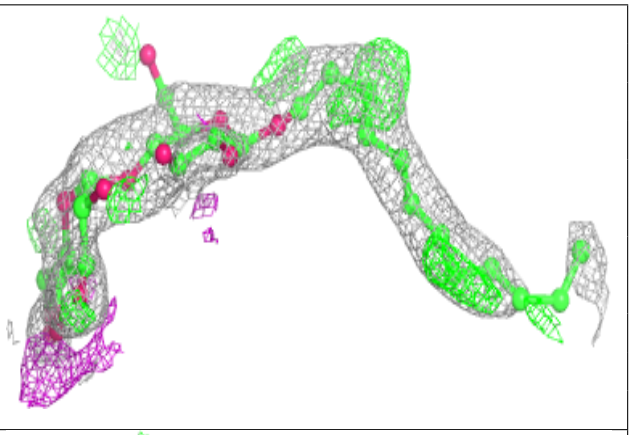
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

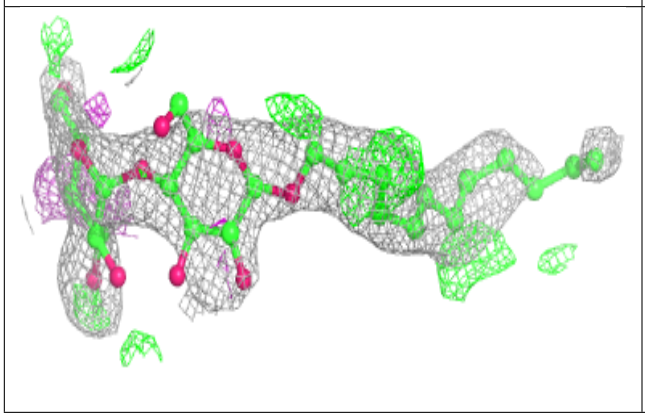




Electron density around LMT a 401:

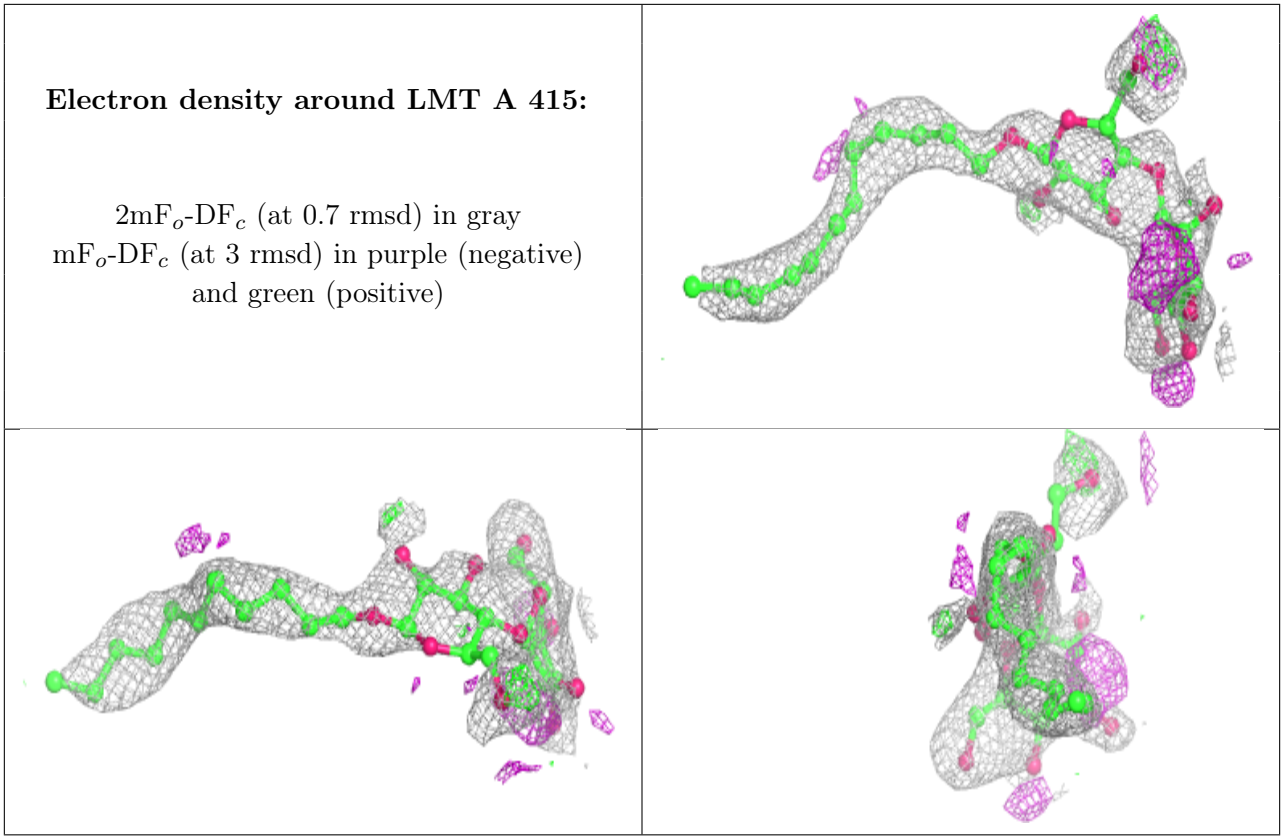
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





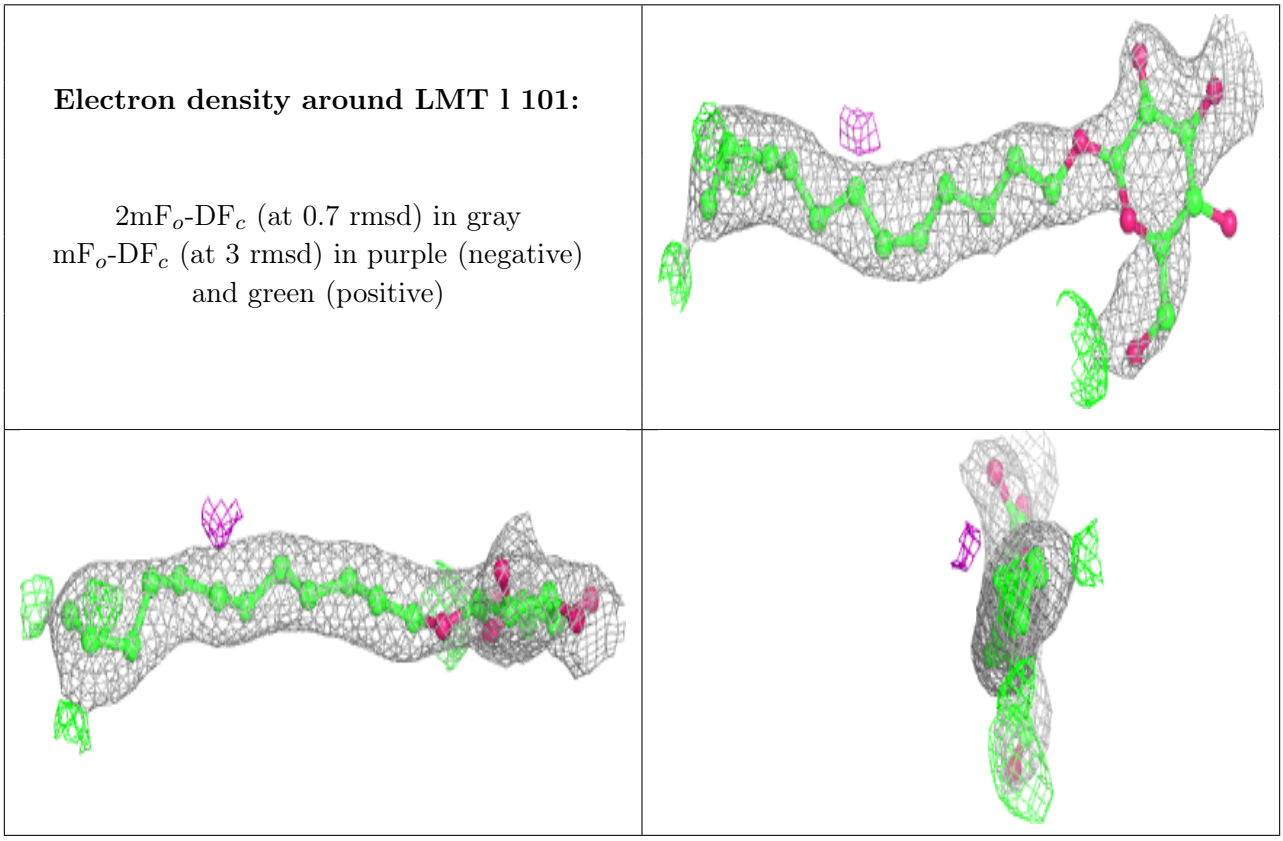
Electron density around LMT A 415:

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



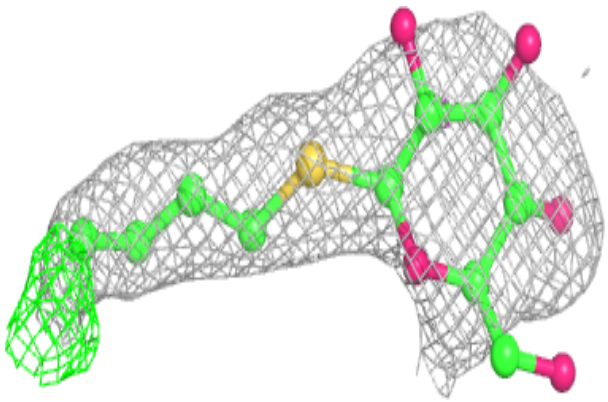
Electron density around LMT l 101:

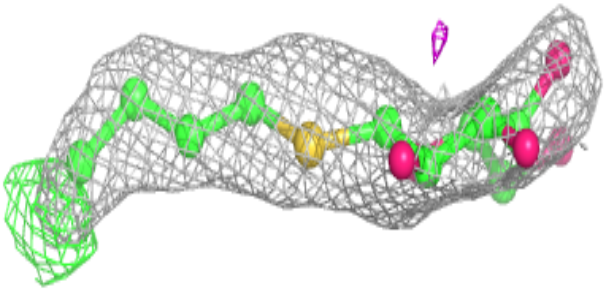
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

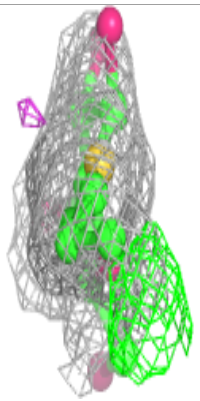


Electron density around HTG d 413:

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

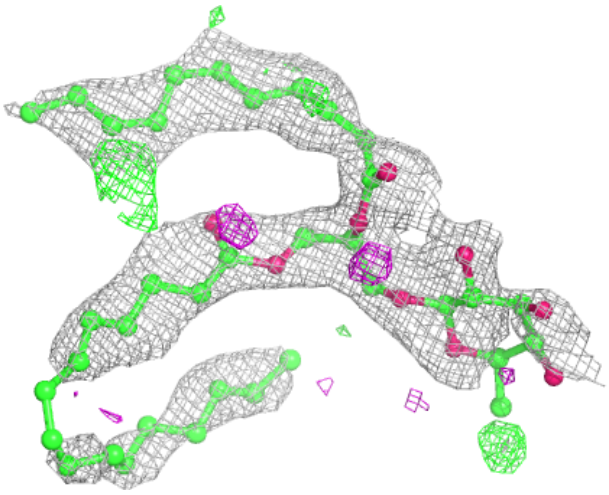


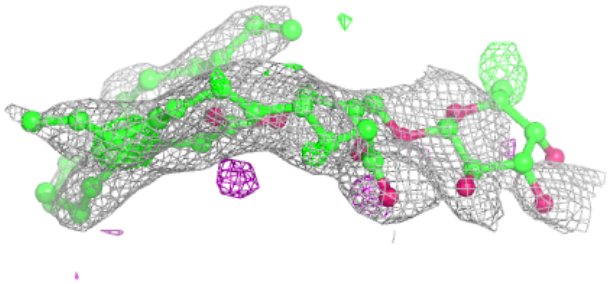


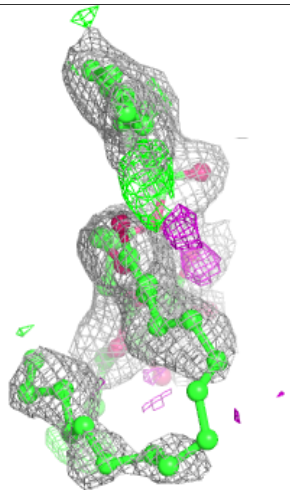


Electron density around DGD D 408:

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

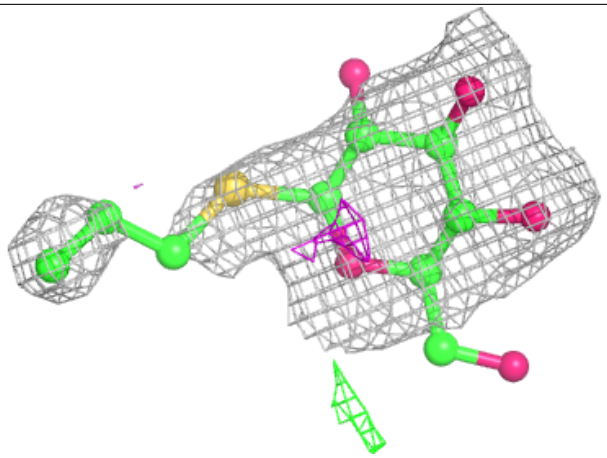


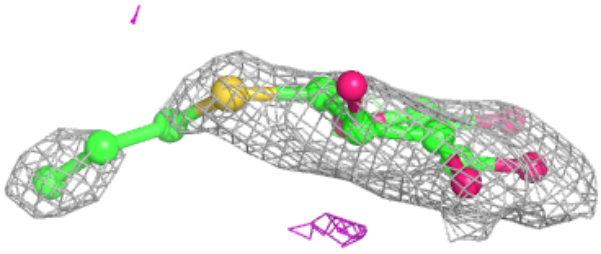


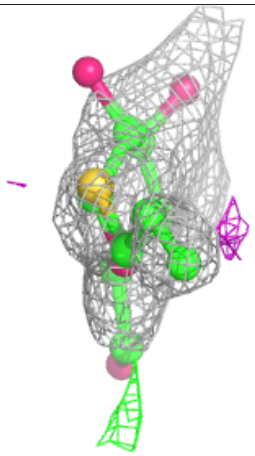


Electron density around HTG c 541:

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

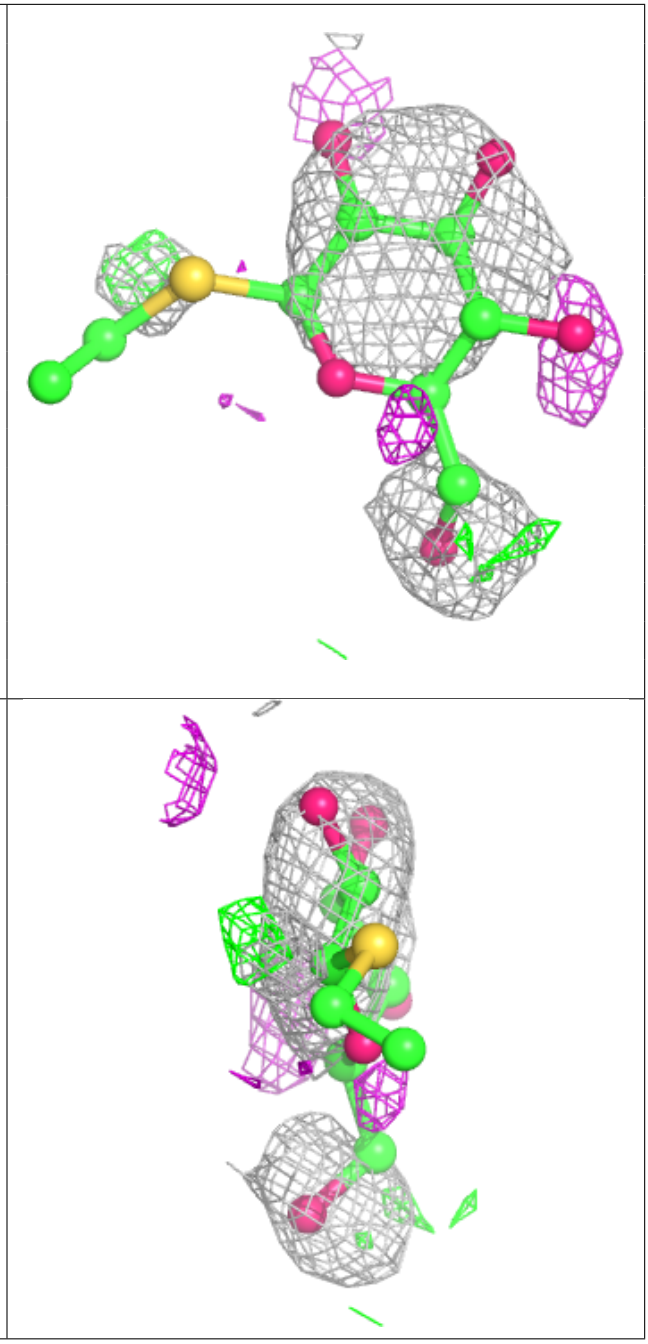






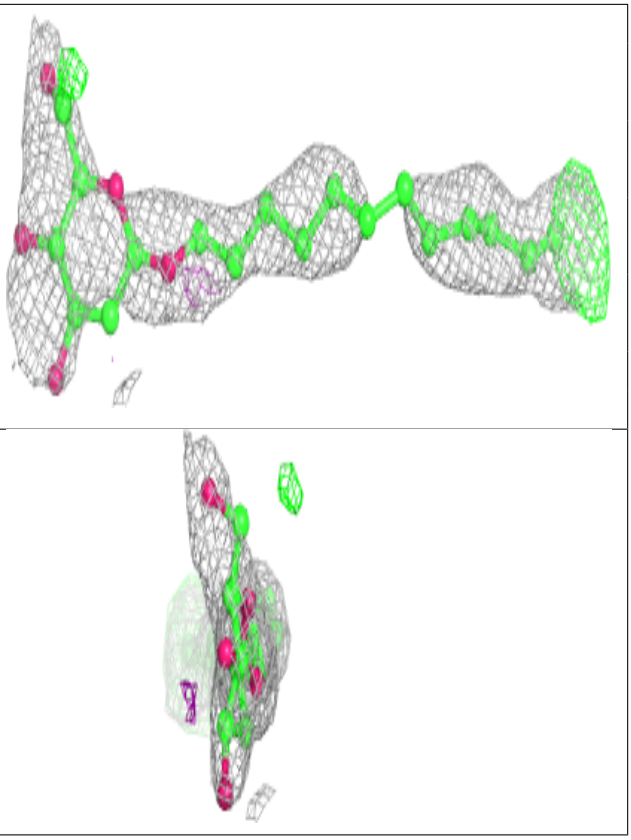
Electron density around HTG U 203:

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



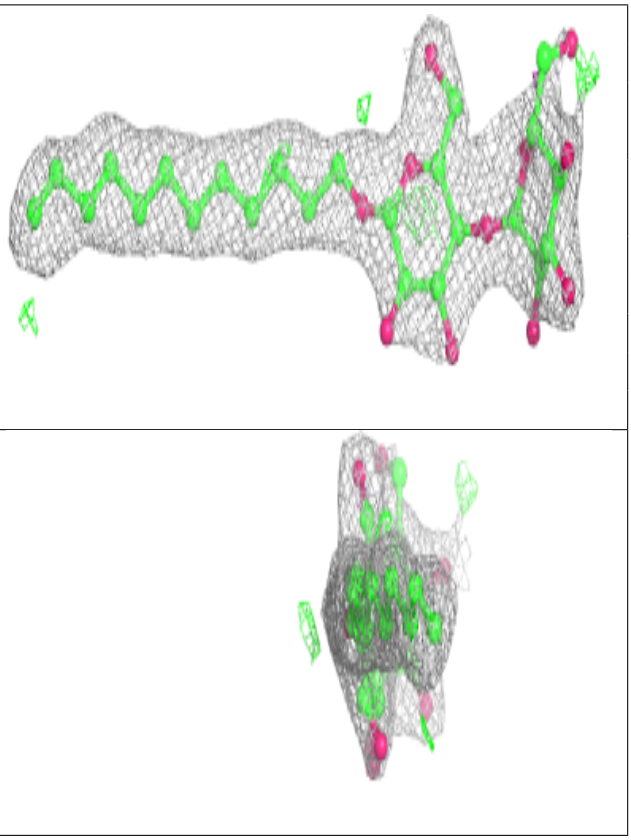
Electron density around LMT j 102:

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



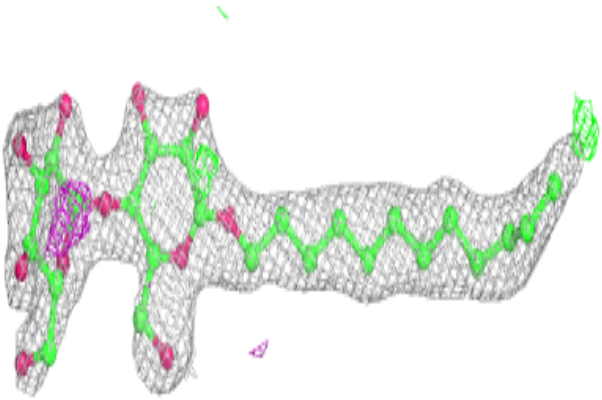
Electron density around LMT M 101:

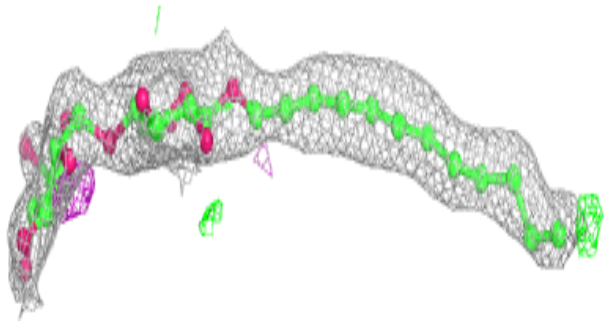
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

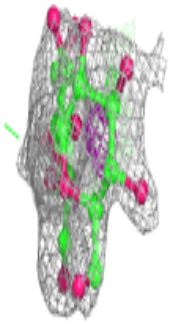


Electron density around LMT m 101:

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

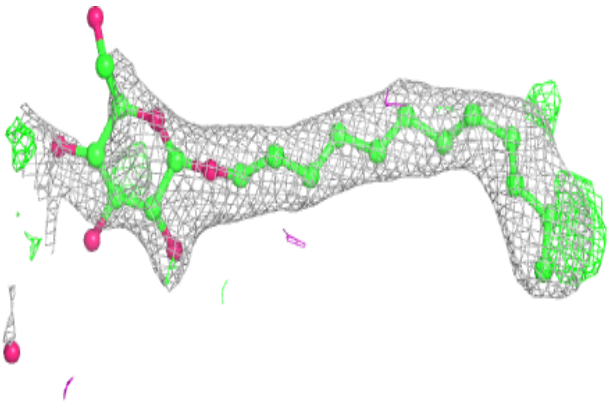


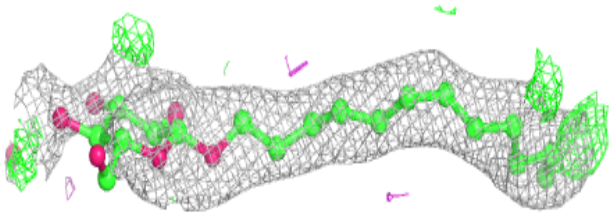


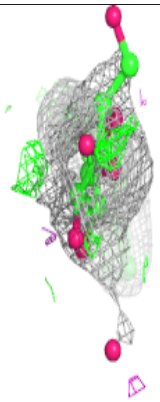


Electron density around LMT m 102:

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

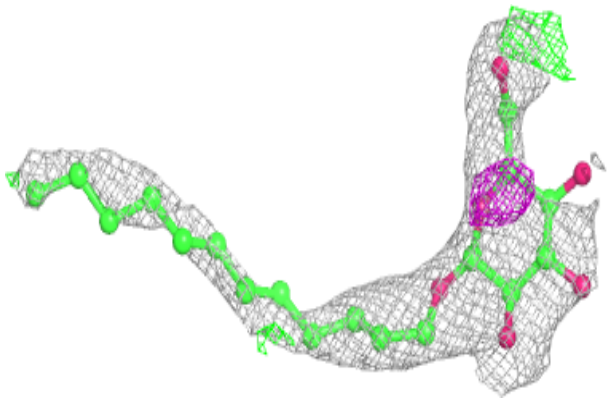


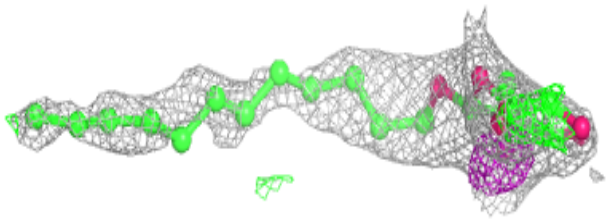


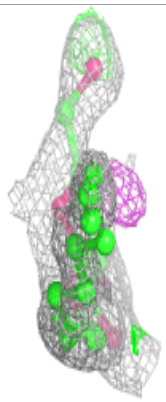


Electron density around LMT F 102:

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

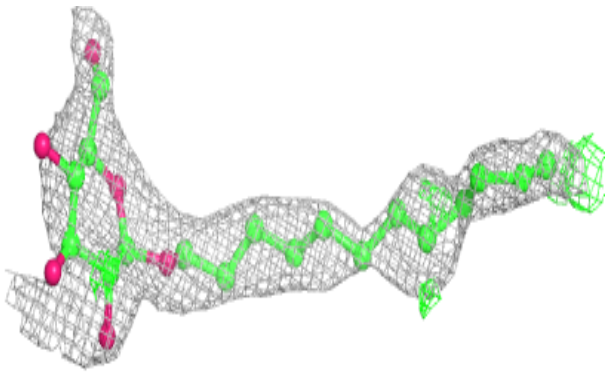


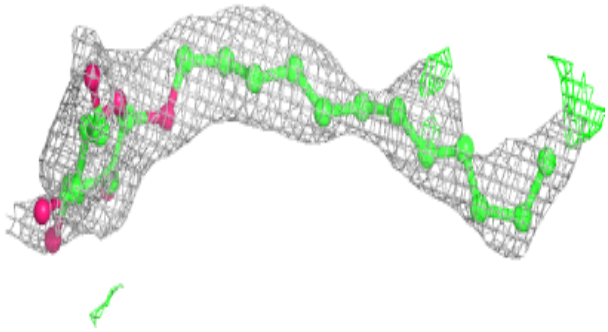


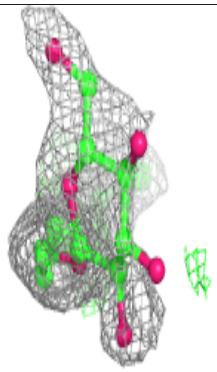


Electron density around LMT t 102:

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

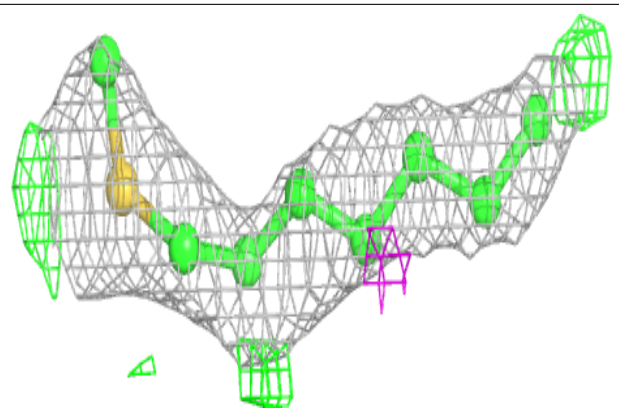


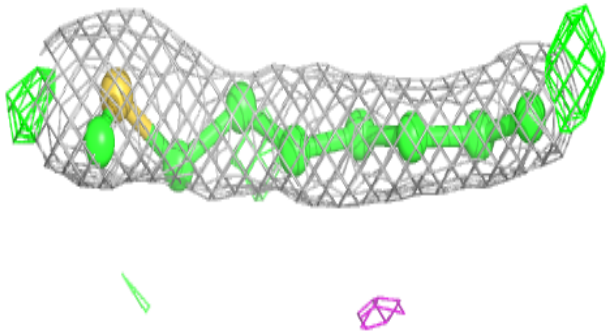


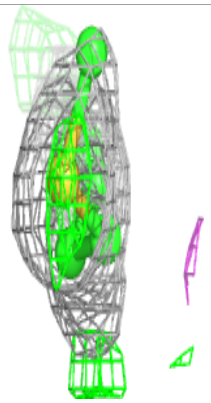


Electron density around HTG c 524:

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

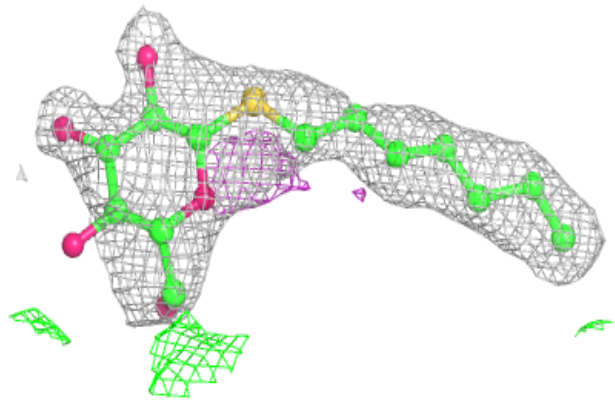


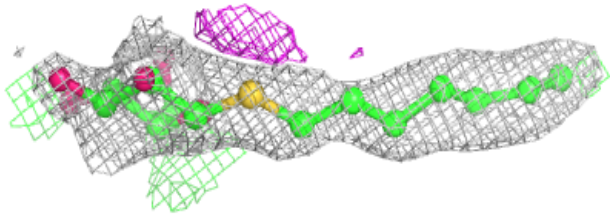


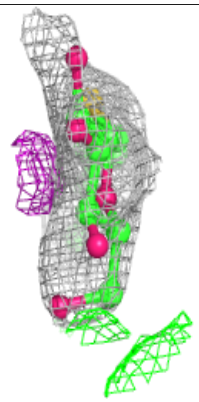


Electron density around HTG B 629:

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

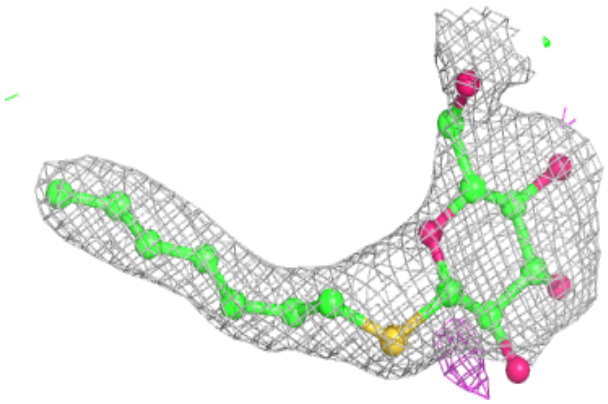


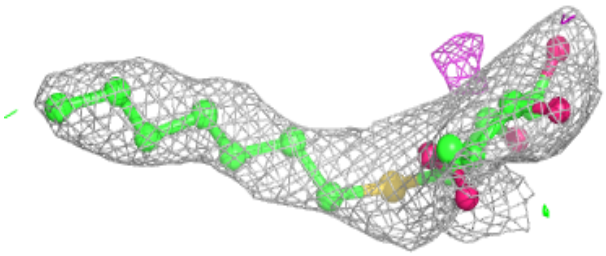


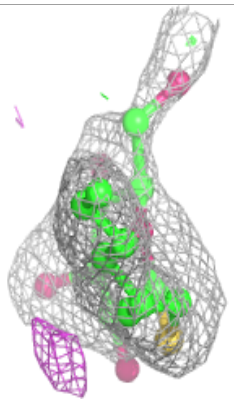


Electron density around HTG b 627:

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

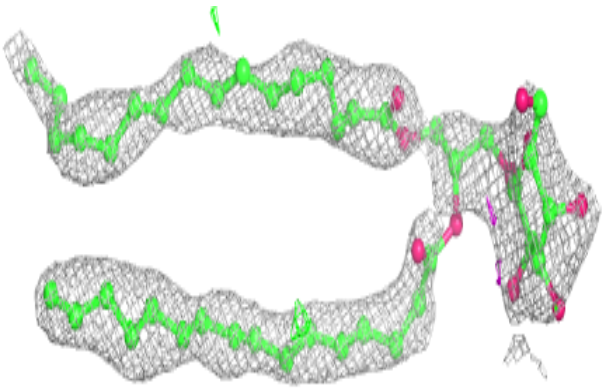


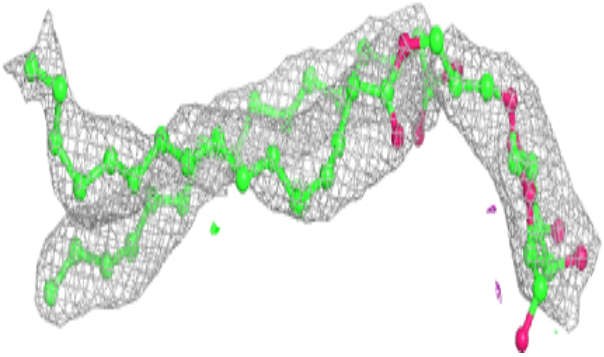


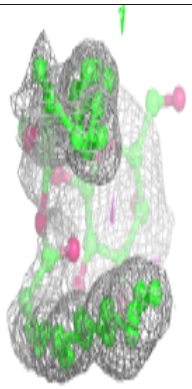


Electron density around LMG c 521:

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

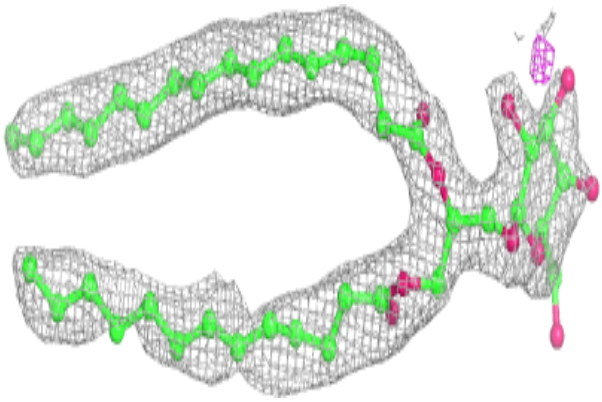


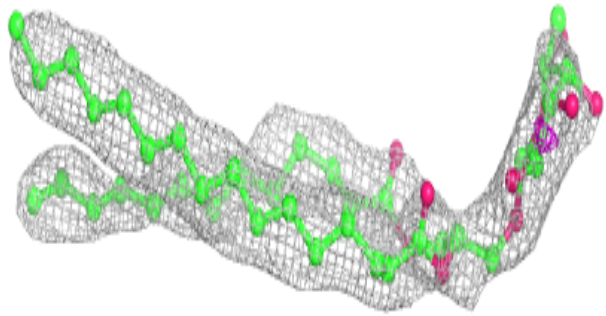


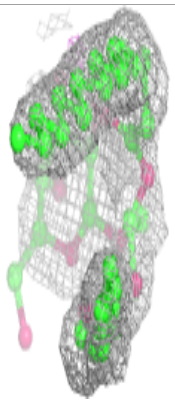


Electron density around LMG C 519:

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

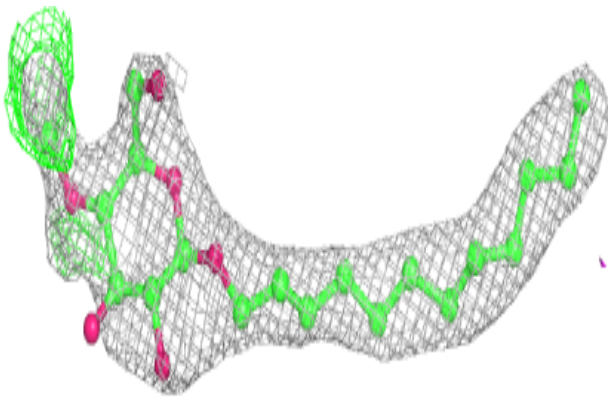


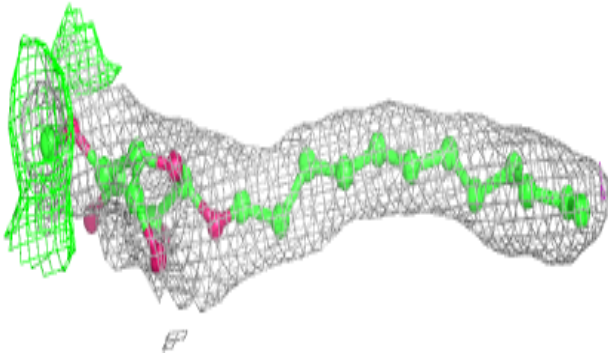


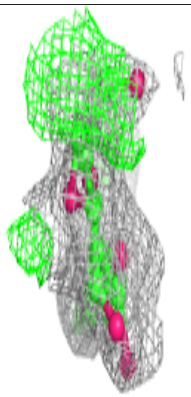


Electron density around LMT b 626:

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

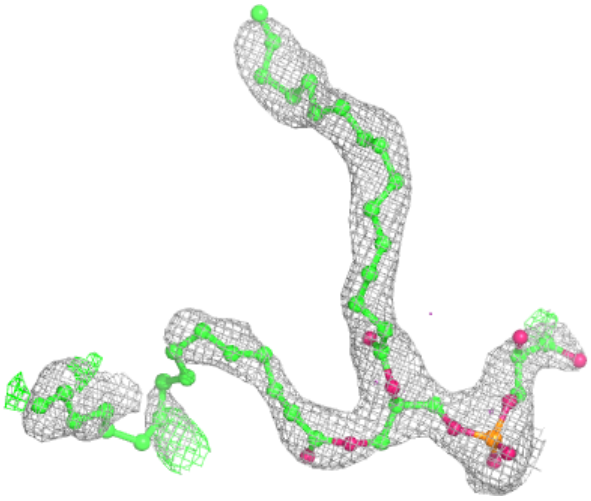


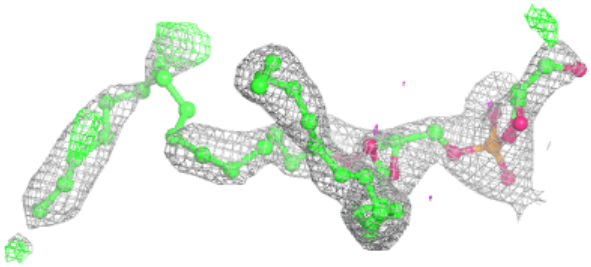


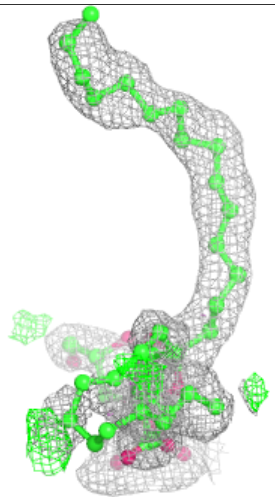


Electron density around LHG E 101:

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

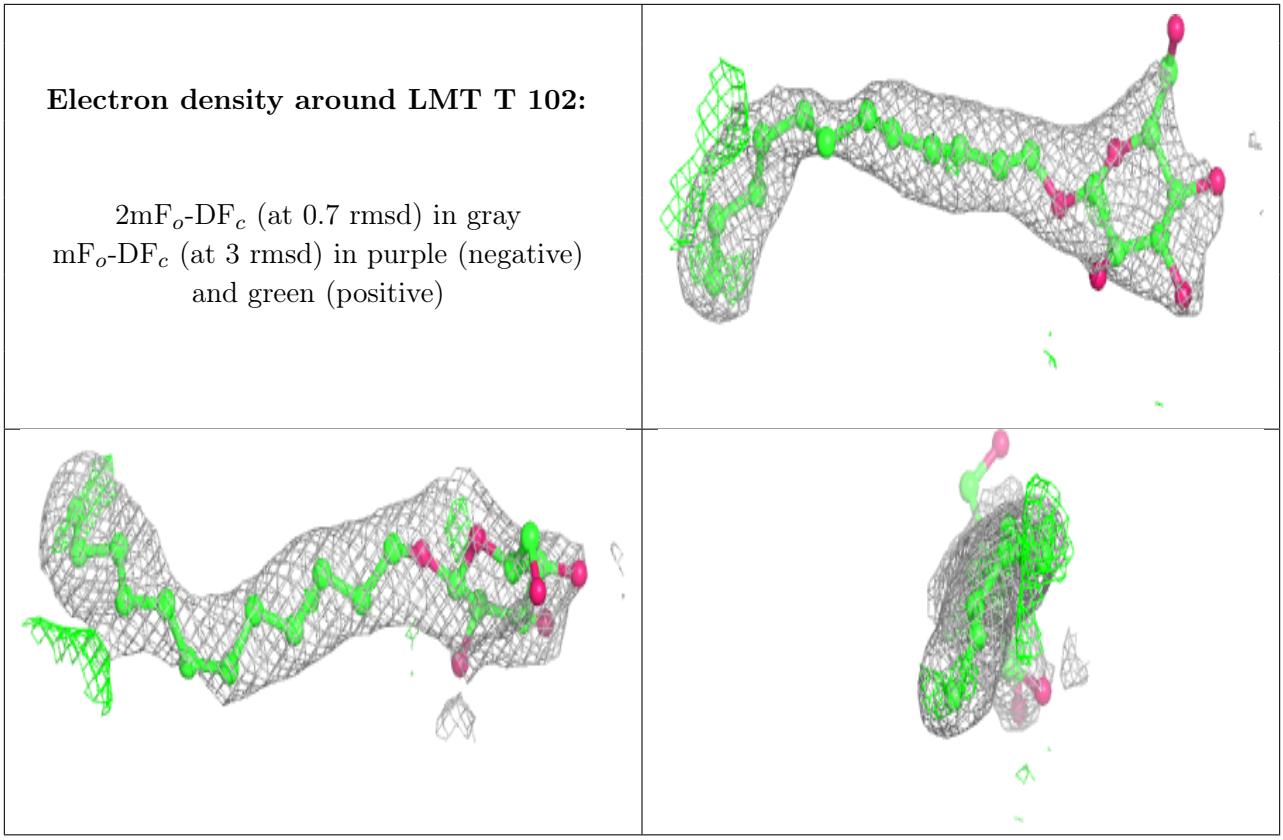






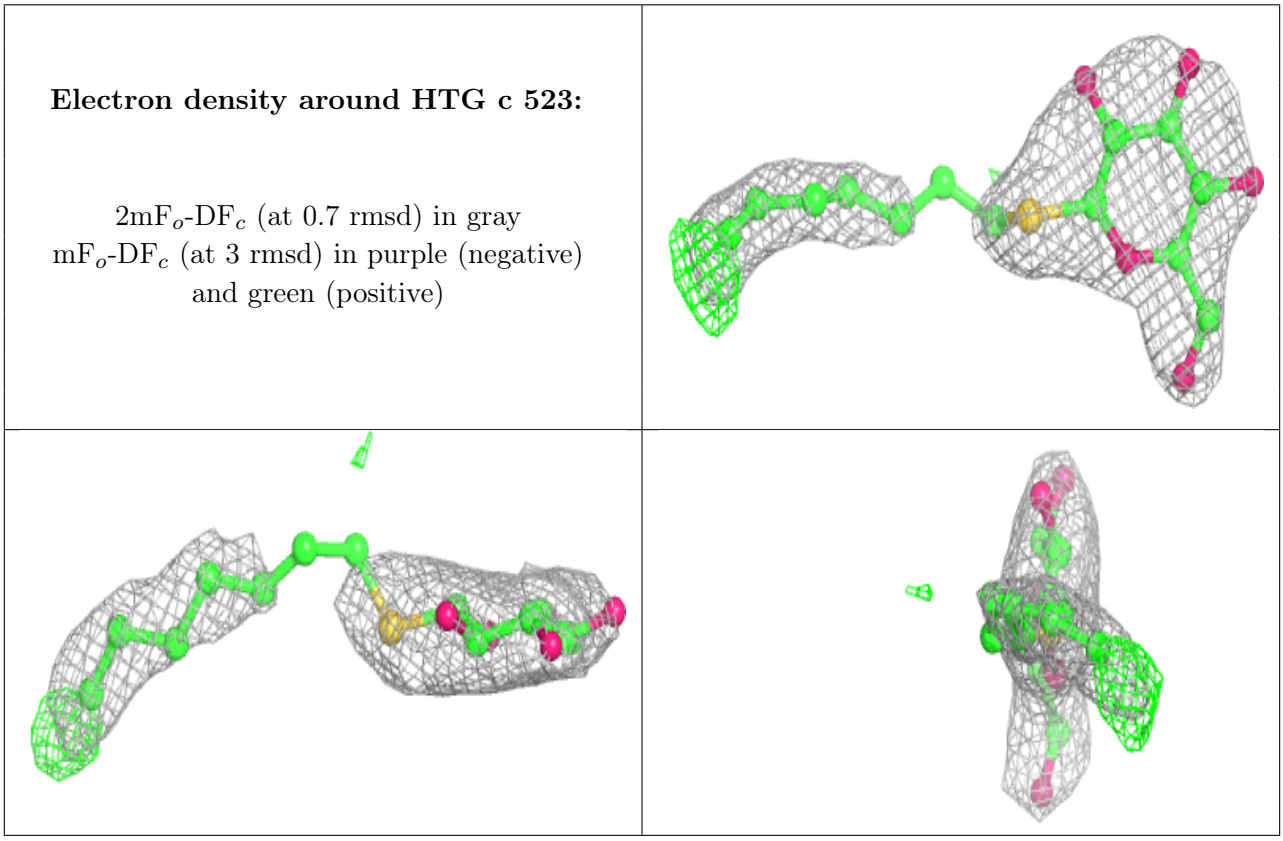
Electron density around LMT T 102:

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



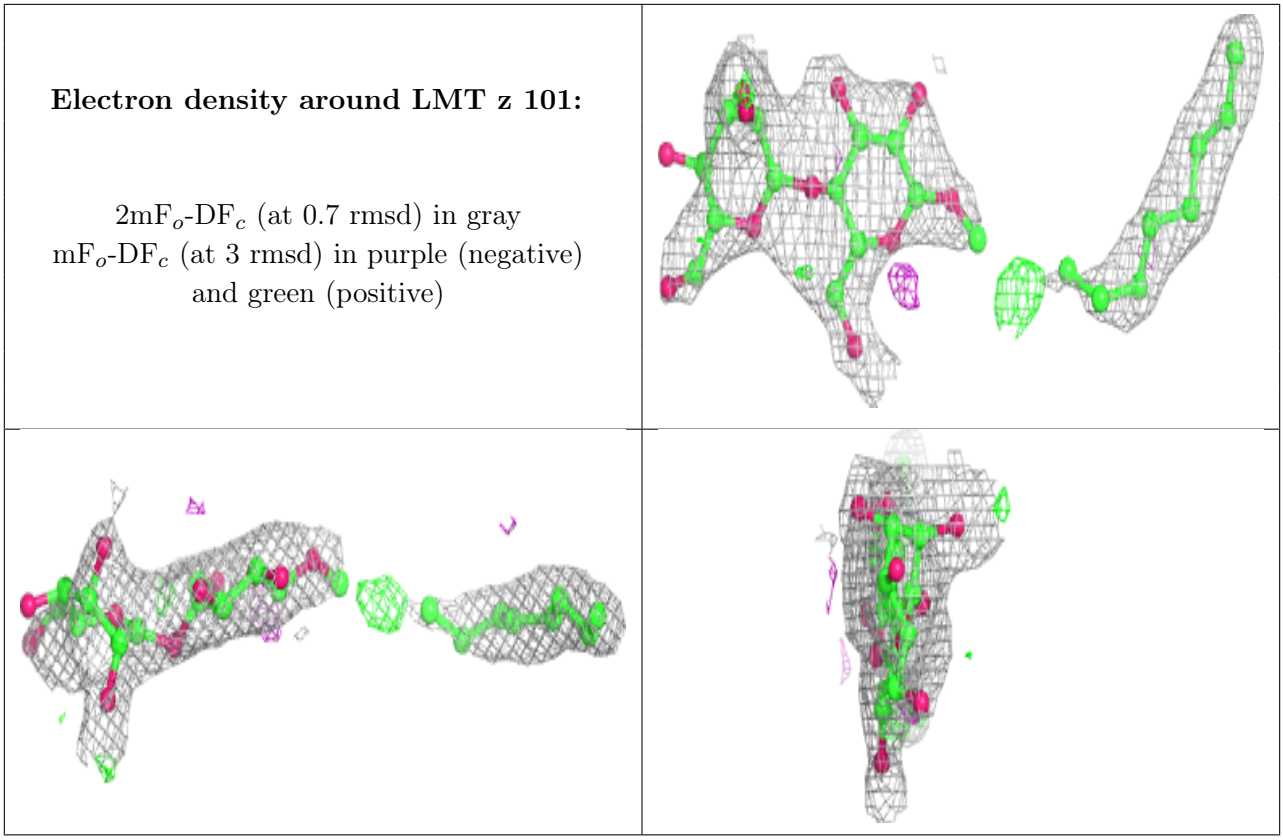
Electron density around HTG c 523:

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



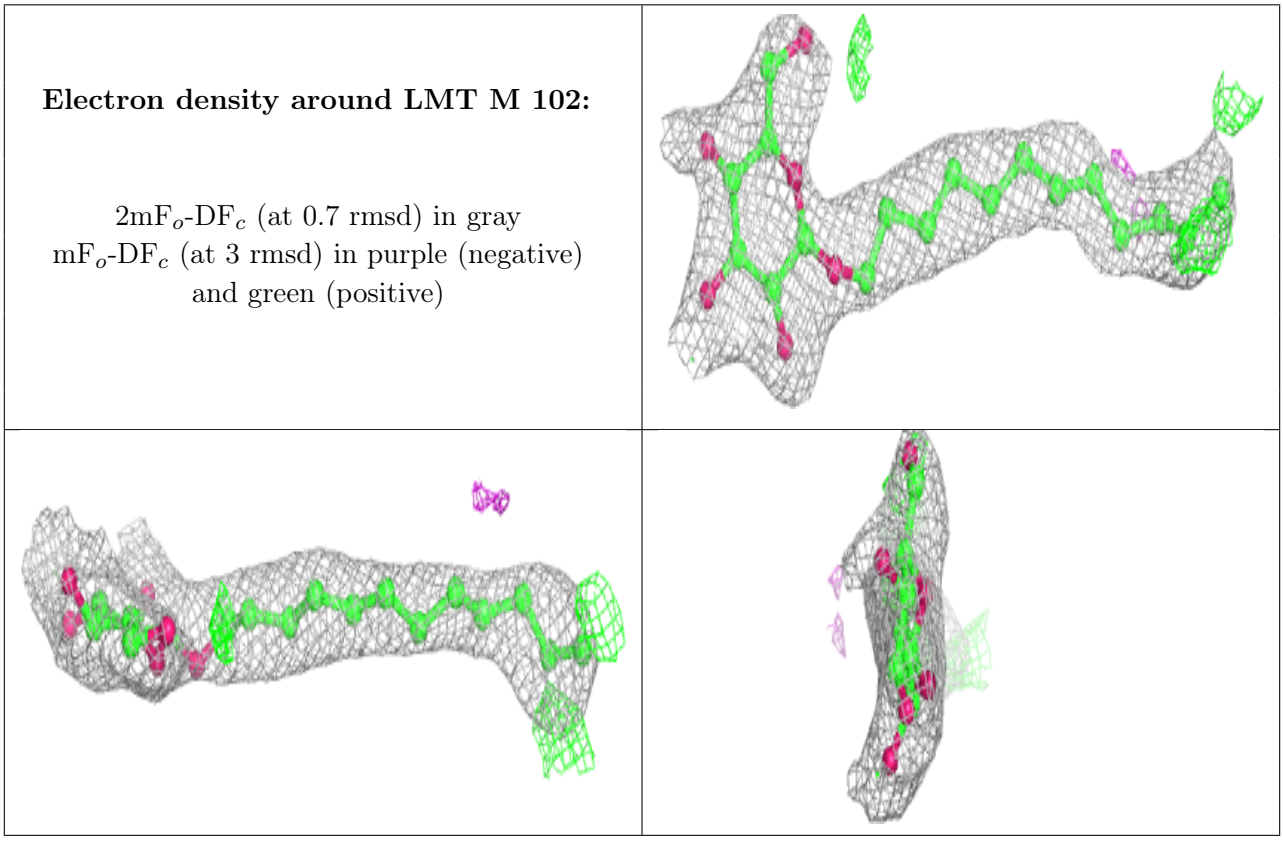
Electron density around LMT z 101:

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



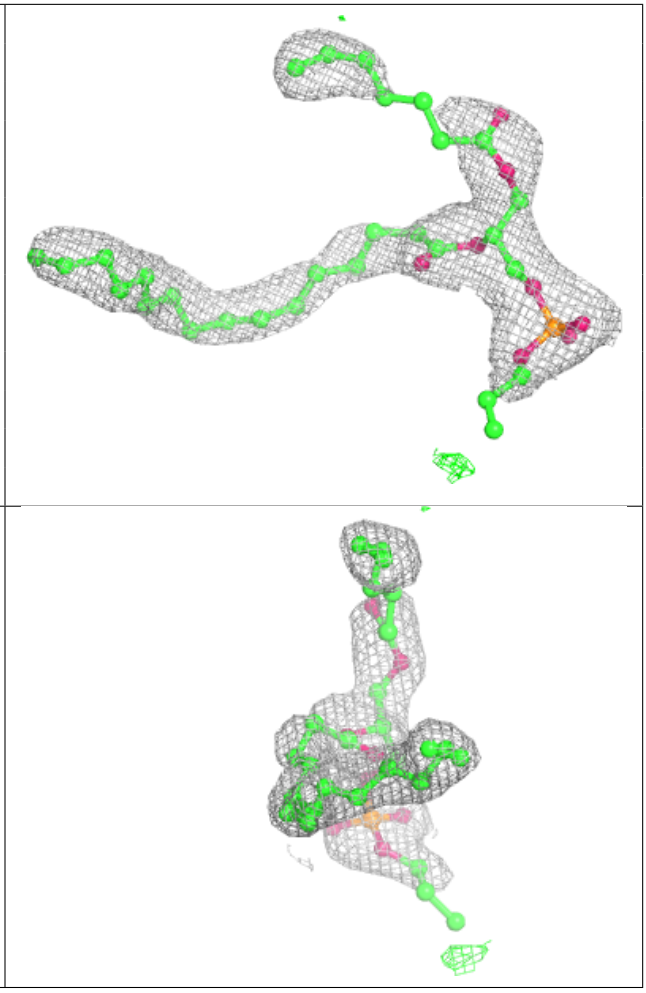
Electron density around LMT M 102:

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



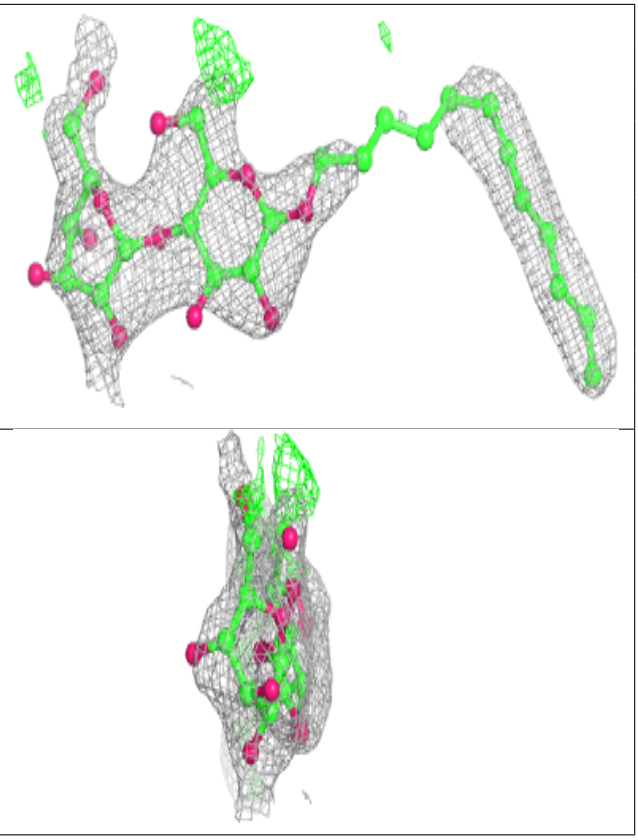
Electron density around LHG e 101:

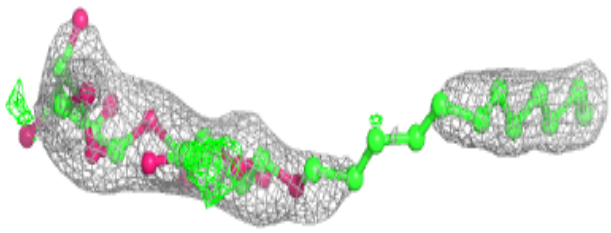
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMT Z 101:

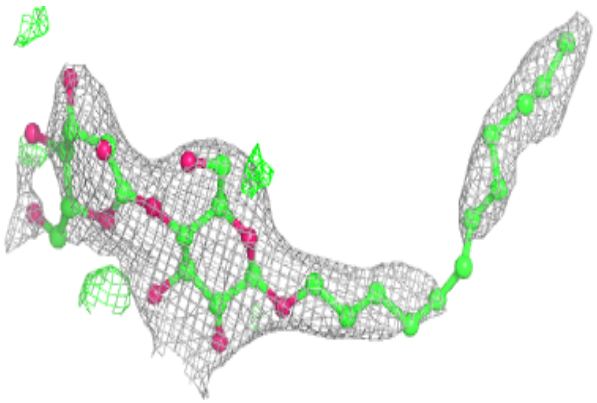
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

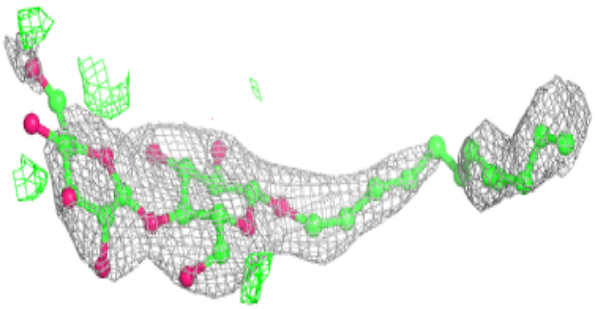


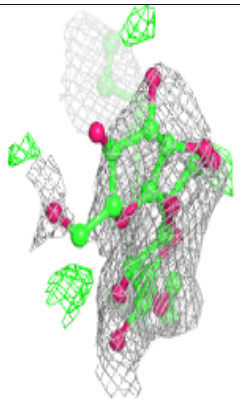


Electron density around LMT C 520:

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

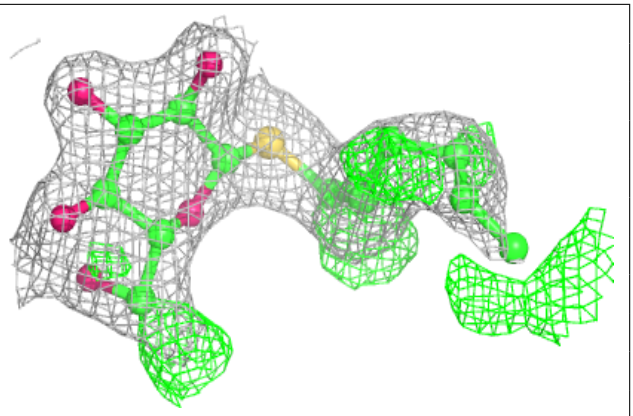


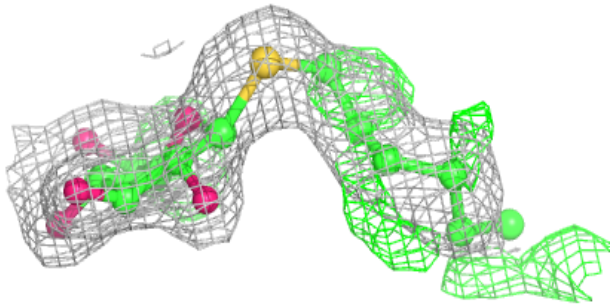


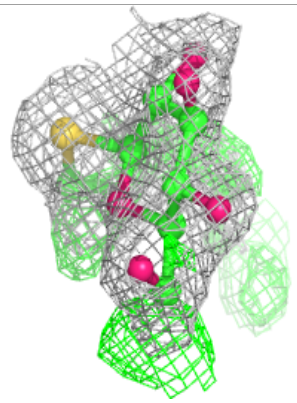


Electron density around HTG B 642:

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

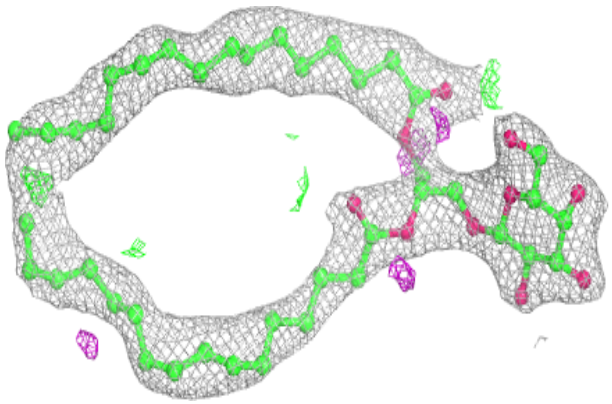


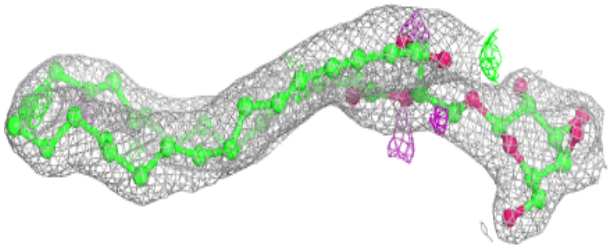


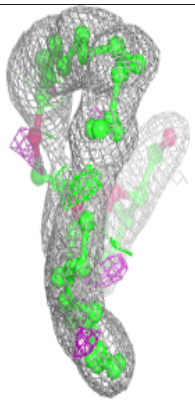


Electron density around LMG a 412:

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

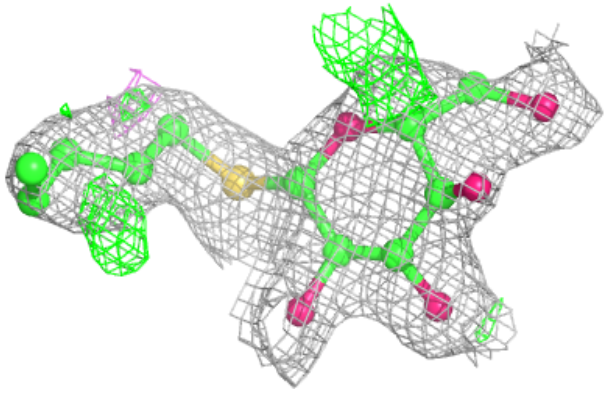


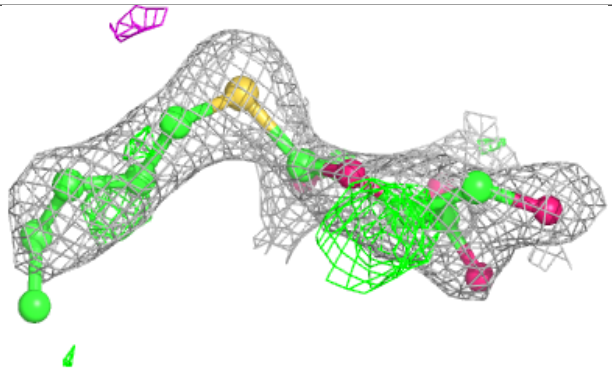


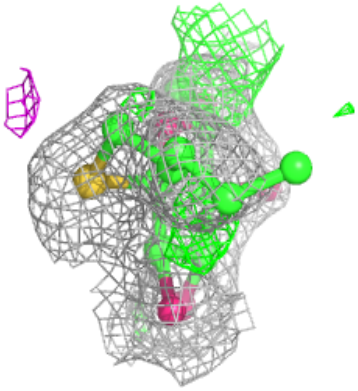


Electron density around HTG b 640:

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

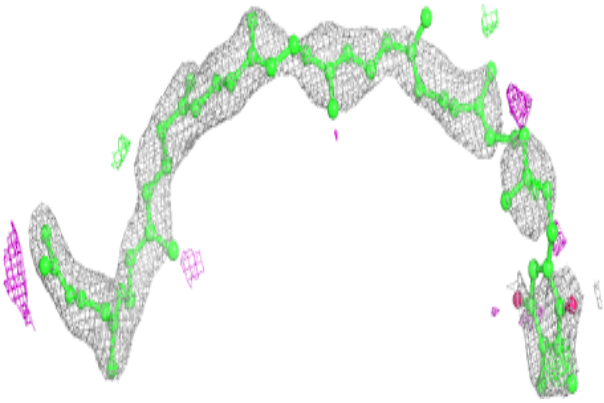


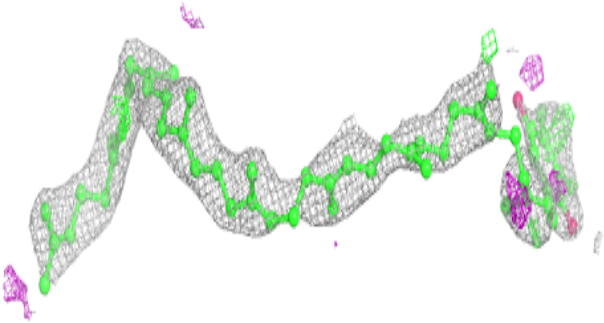


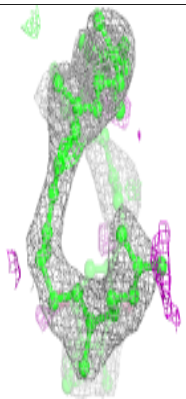


Electron density around PL9 A 410:

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

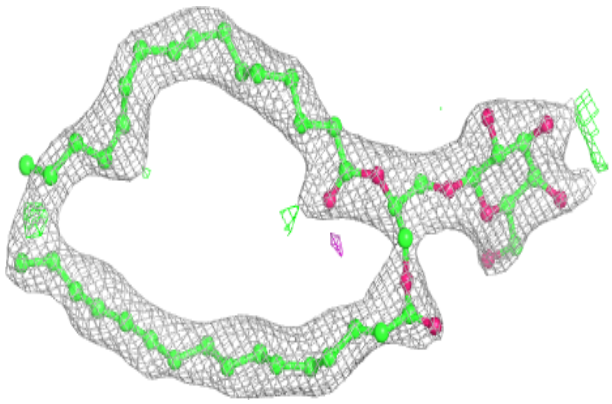


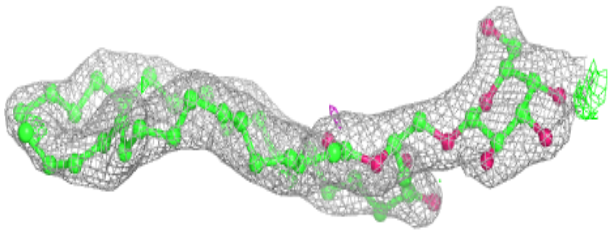


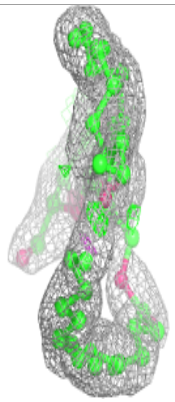


Electron density around LMG A 411:

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

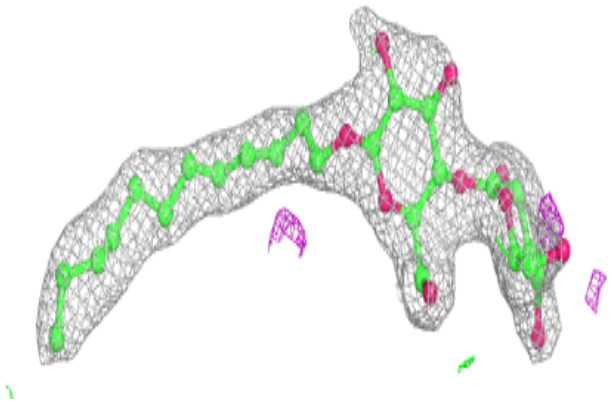


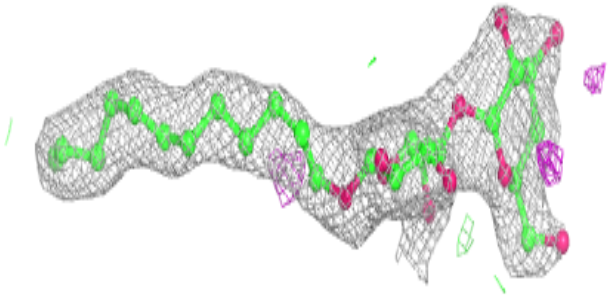


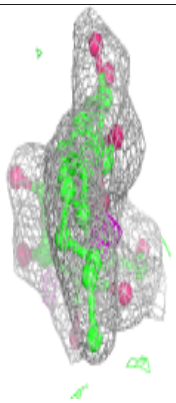


Electron density around LMT B 623:

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

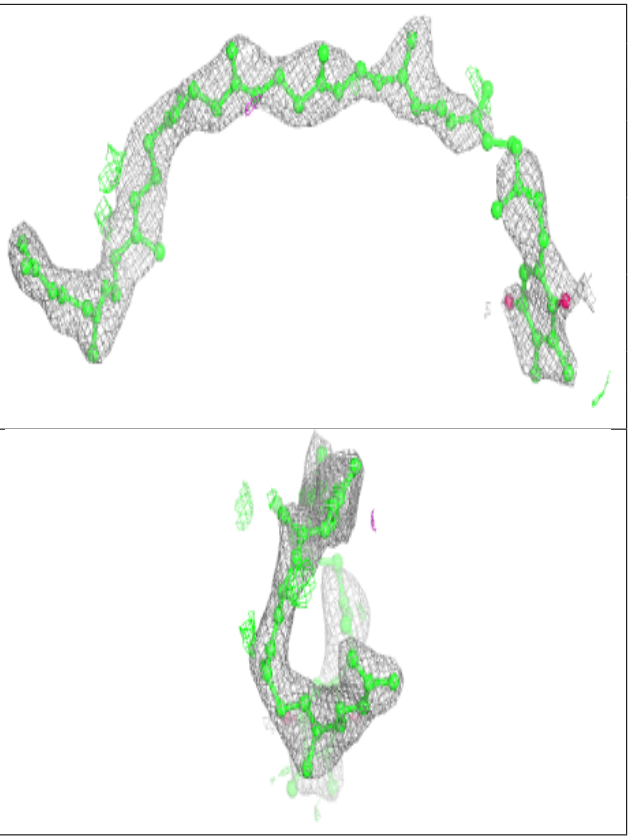






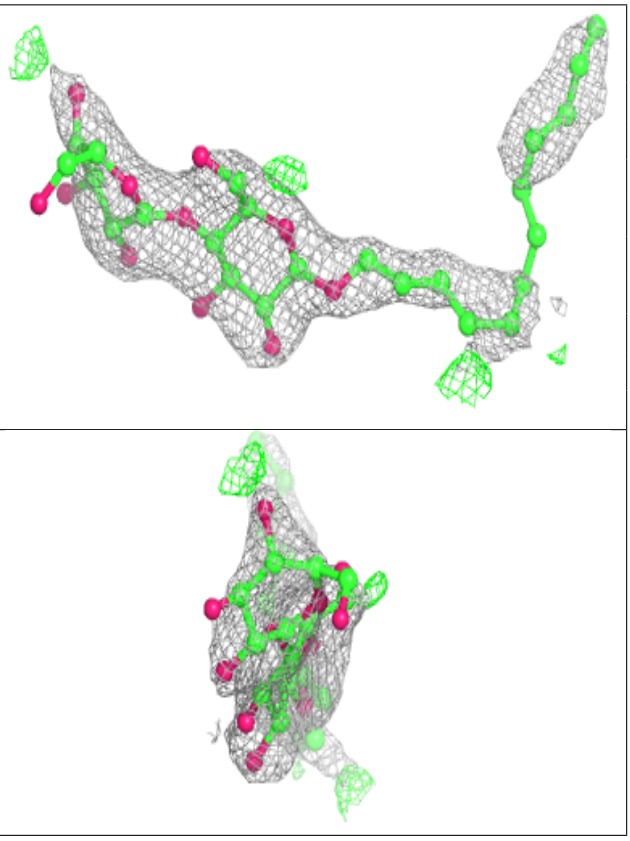
Electron density around PL9 a 411:

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



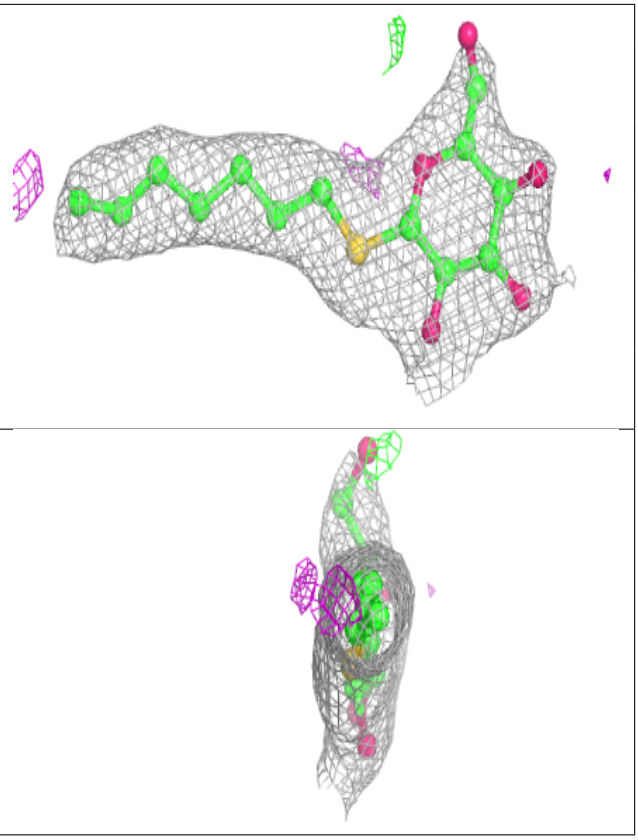
Electron density around LMT c 522:

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



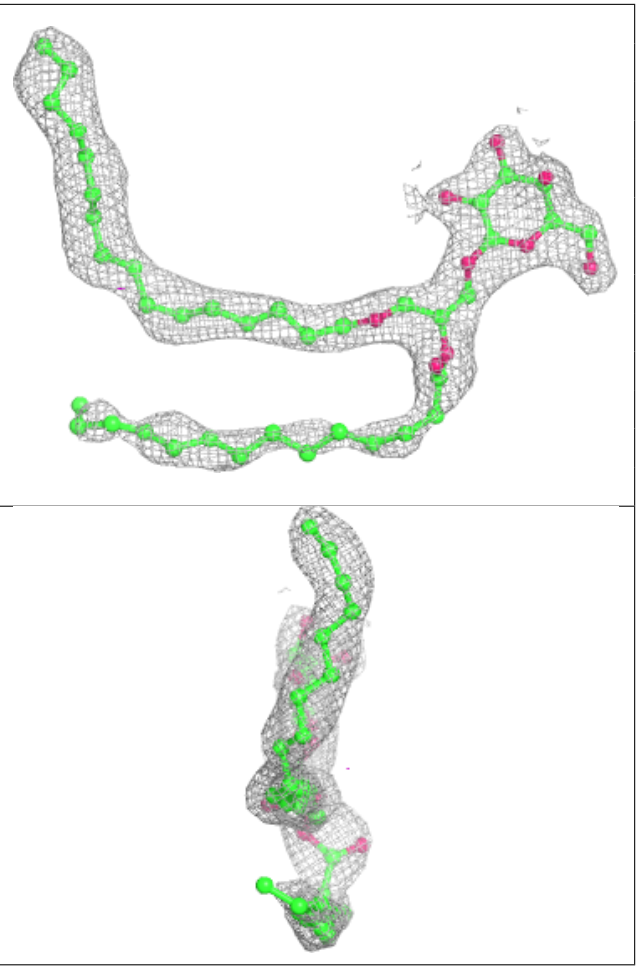
Electron density around HTG b 601:

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



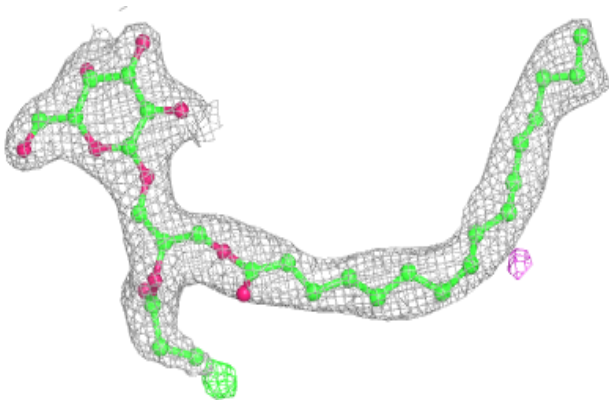
Electron density around LMG C 518:

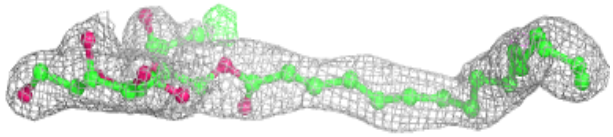
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

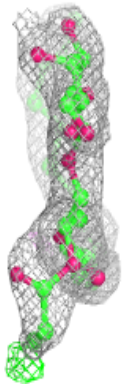


Electron density around LMG c 520:

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

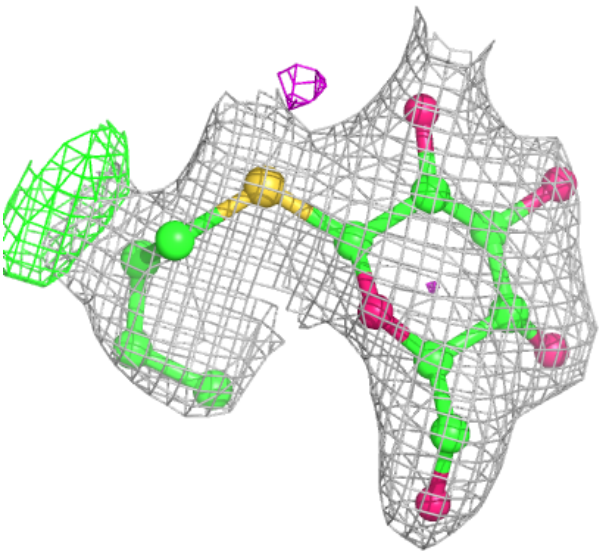


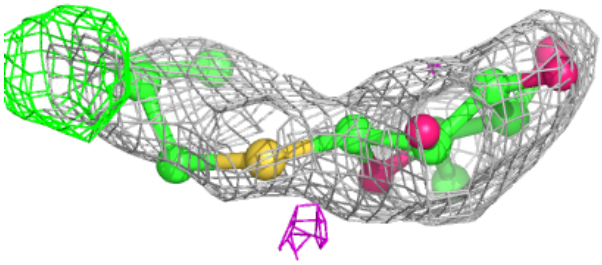


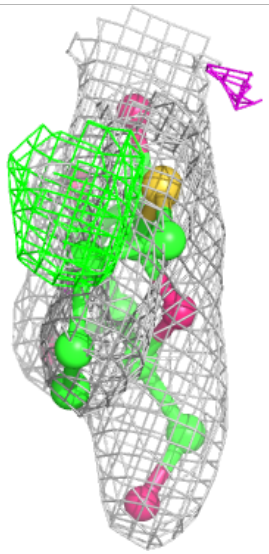


Electron density around HTG v 208:

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

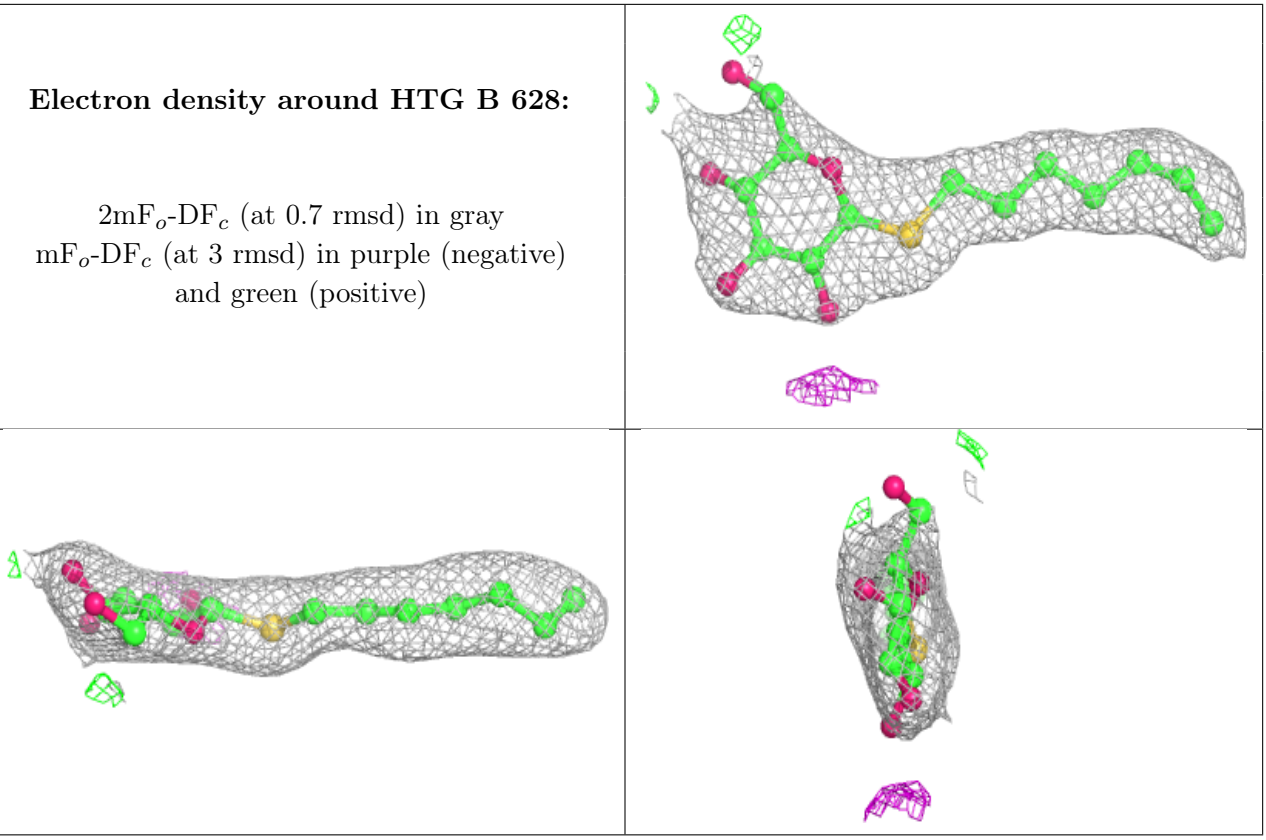






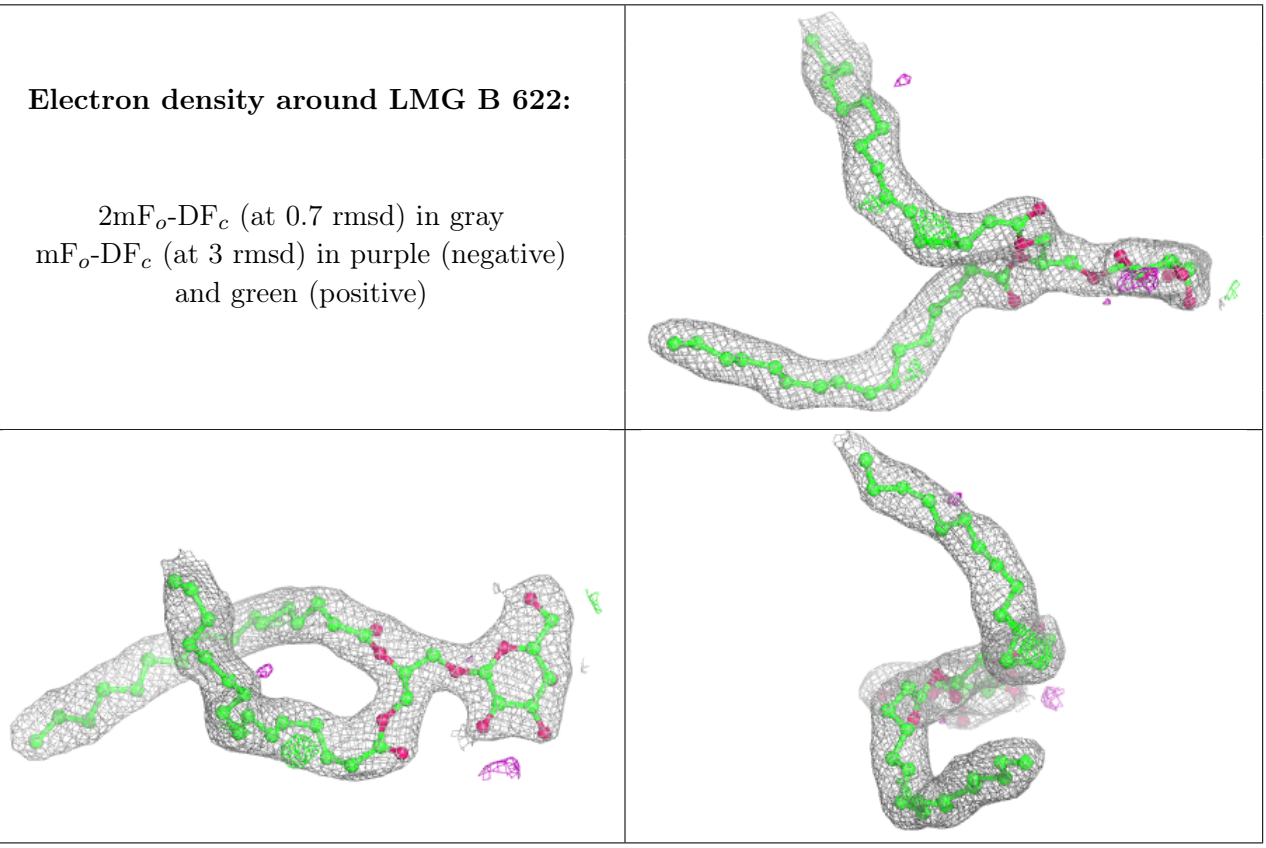
Electron density around HTG B 628:

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



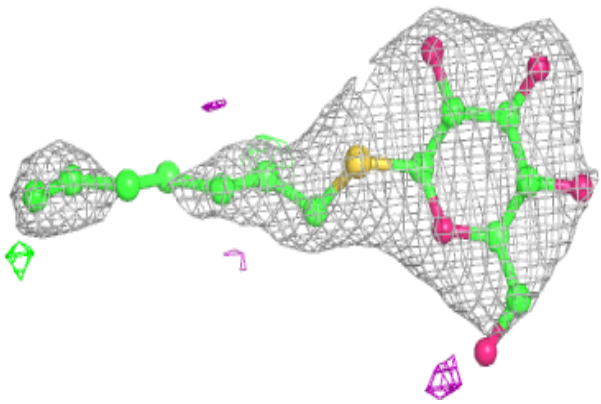
Electron density around LMG B 622:

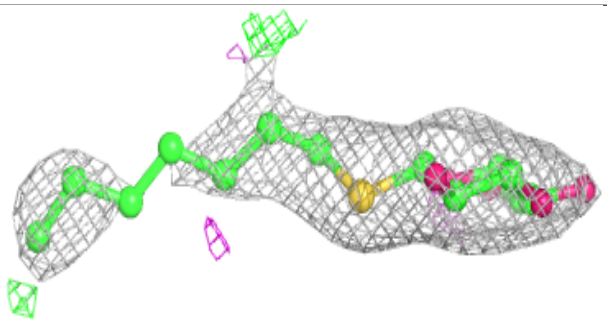
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

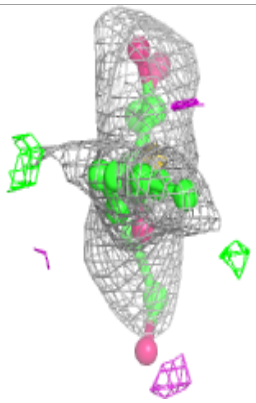


Electron density around HTG C 521:

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

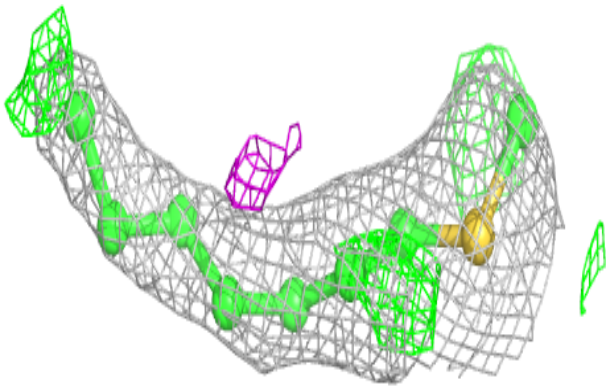


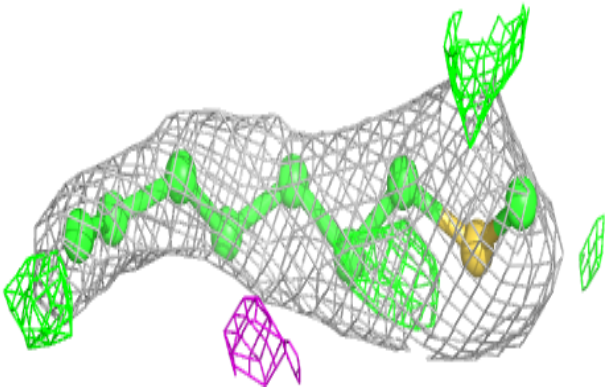


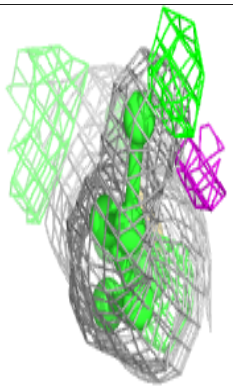


Electron density around HTG C 535:

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

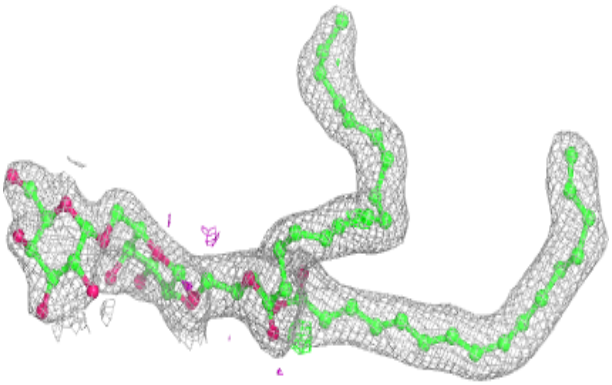


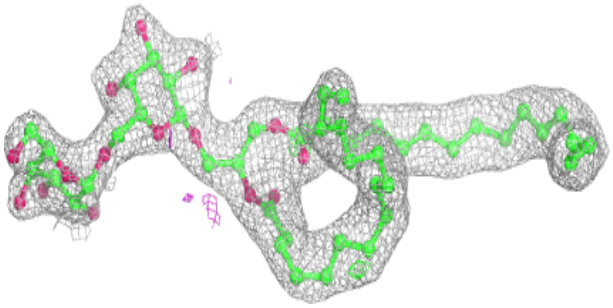


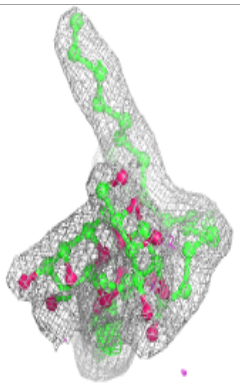


Electron density around DGD h 101:

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

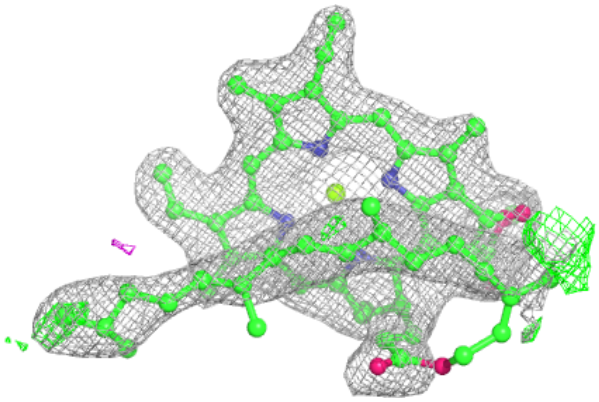


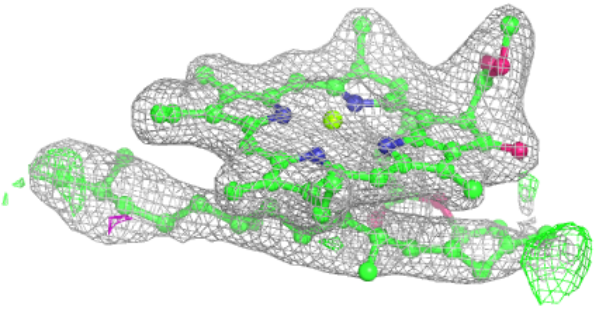


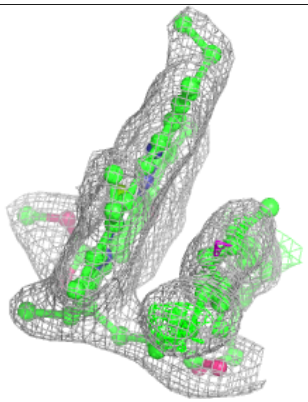


Electron density around CLA B 602:

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

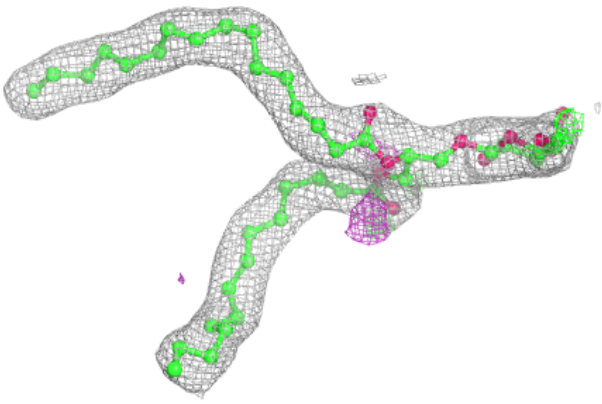


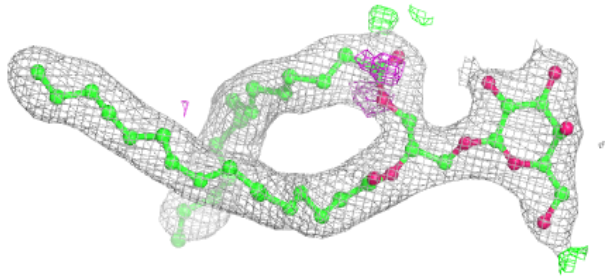


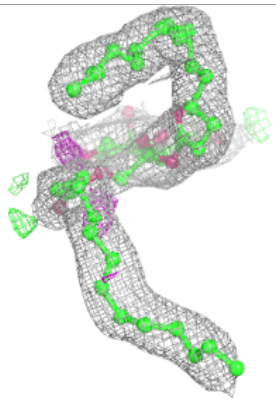


Electron density around LMG b 625:

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

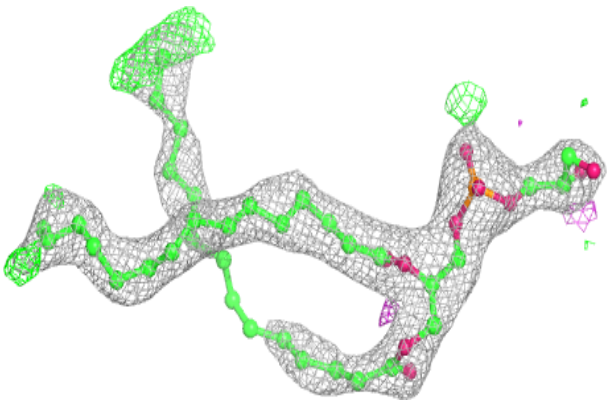


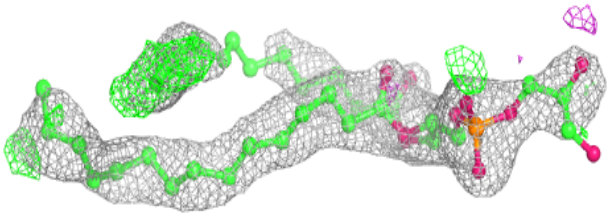


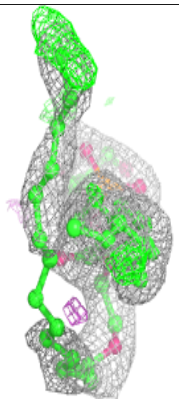


Electron density around LHG f 102:

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

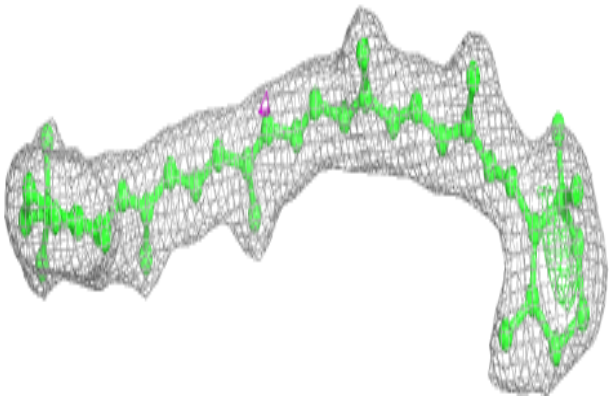


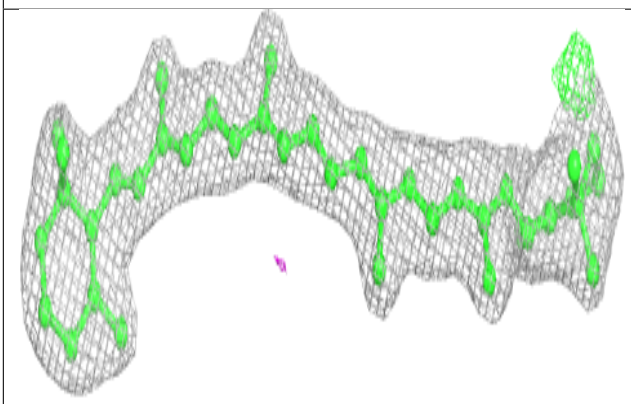


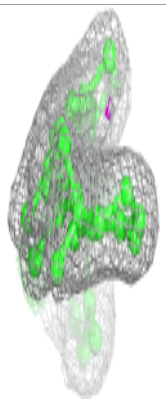


Electron density around BCR d 406:

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

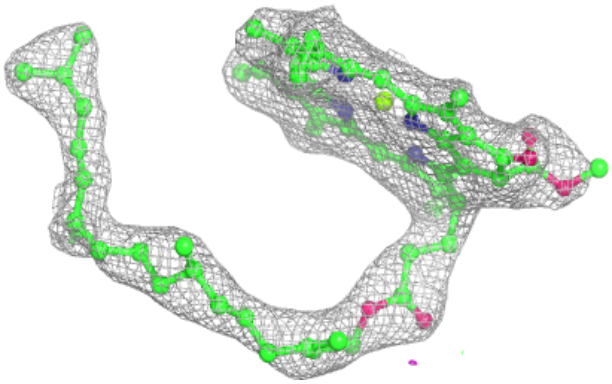


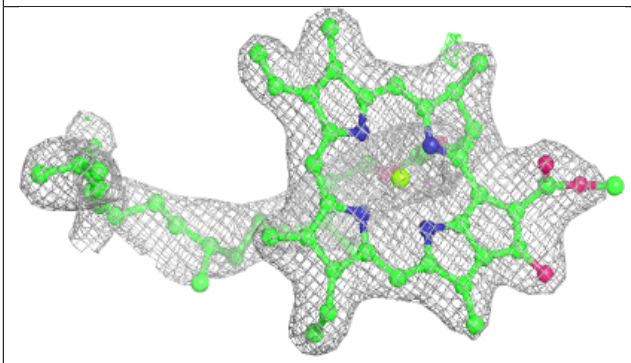


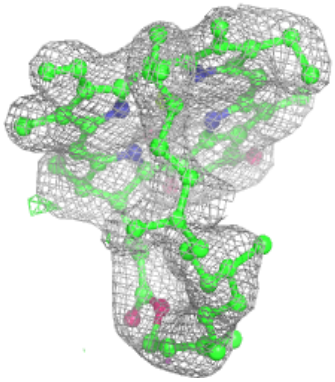


Electron density around CLA C 513:

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

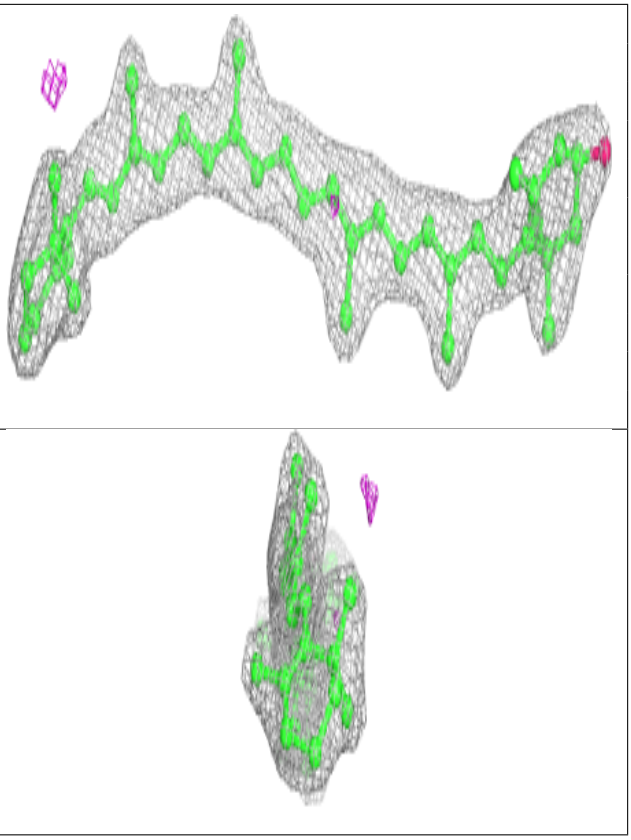






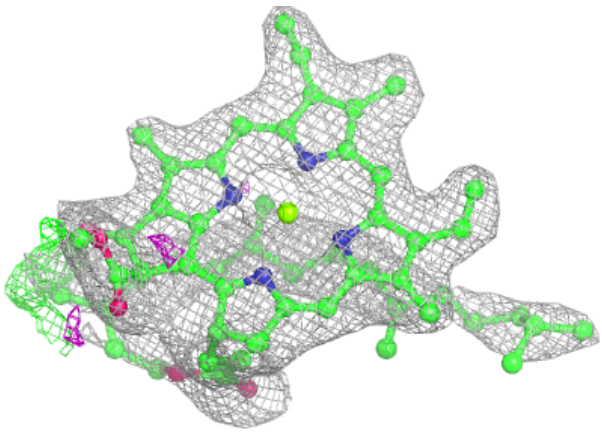
Electron density around RRX h 102:

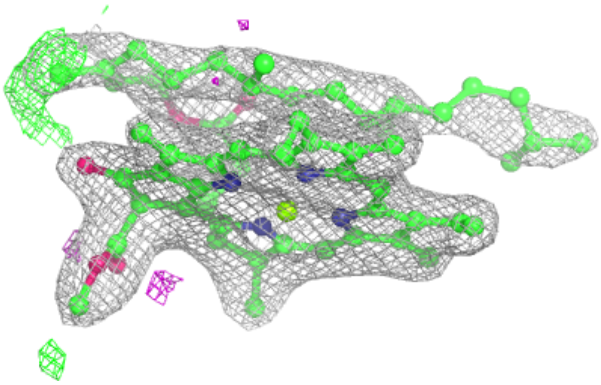
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

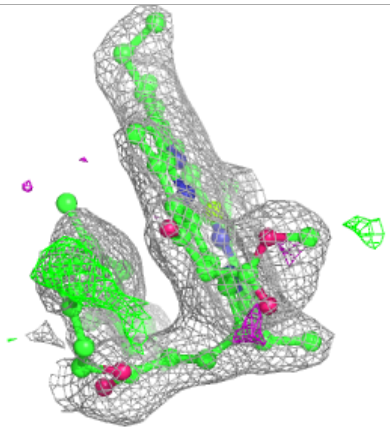


Electron density around CLA b 605:

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

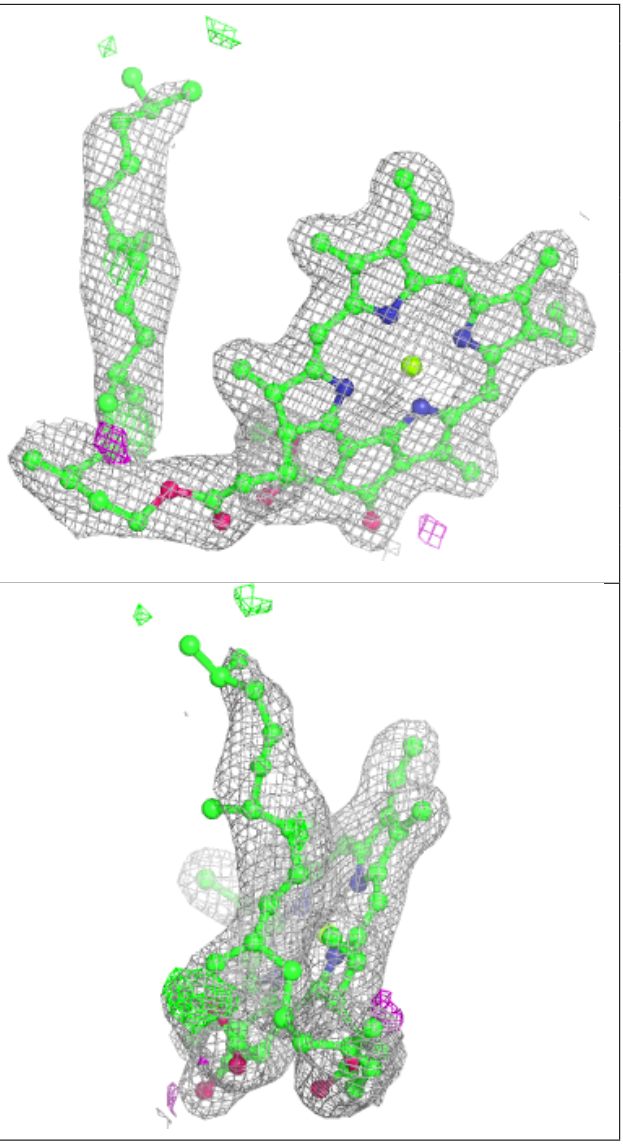






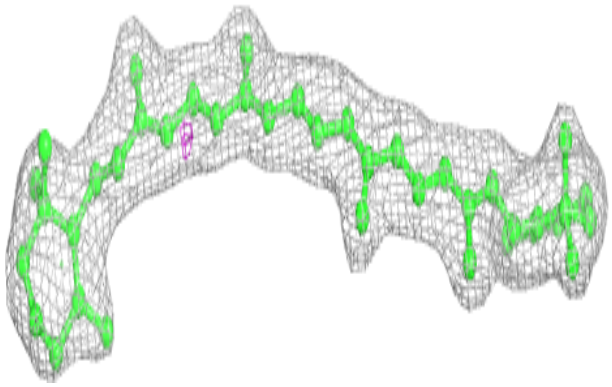
Electron density around CLA b 620:

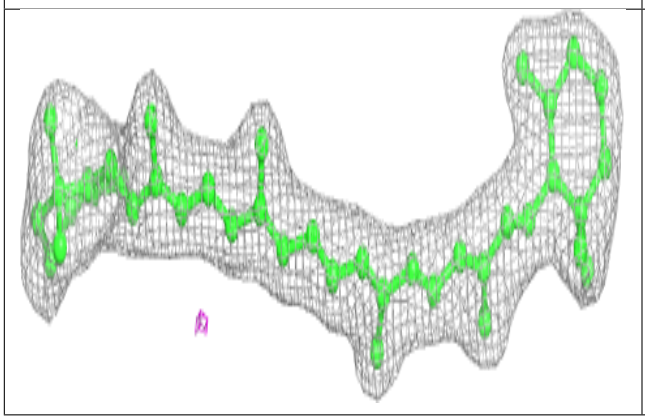
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

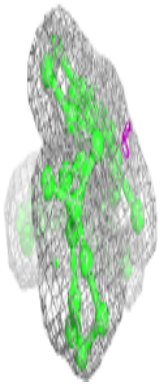


Electron density around BCR D 406:

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

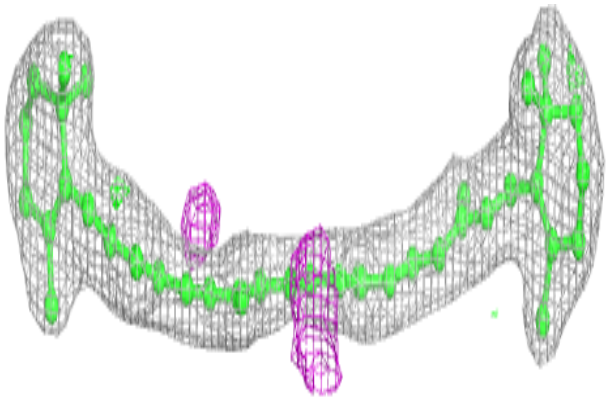


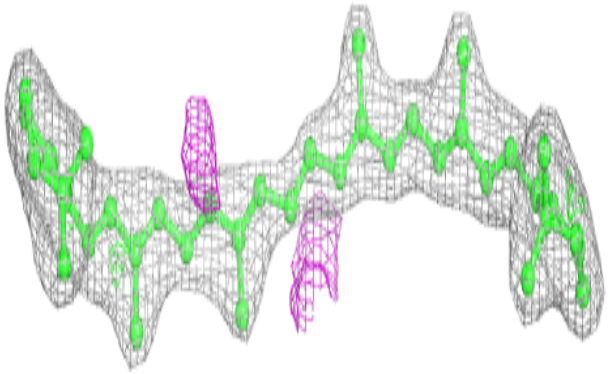


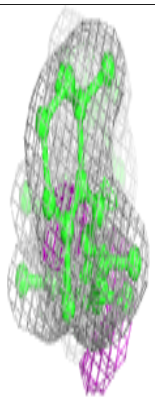


Electron density around BCR K 101:

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

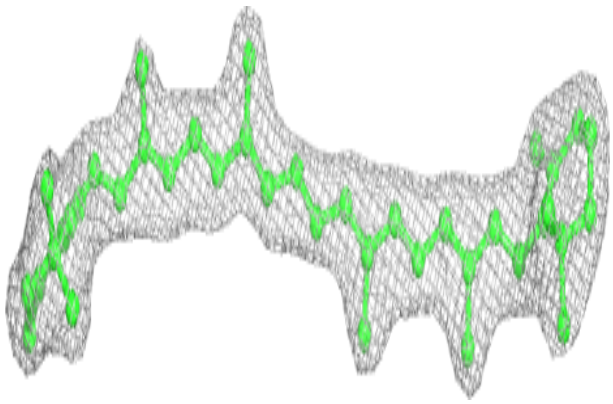


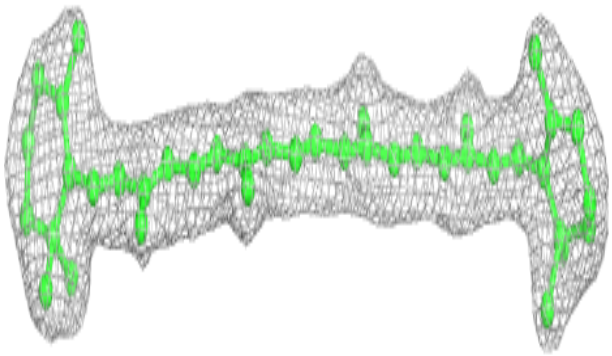


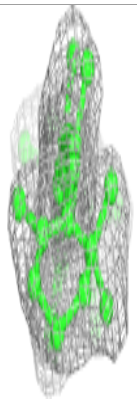


Electron density around BCR K 102:

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

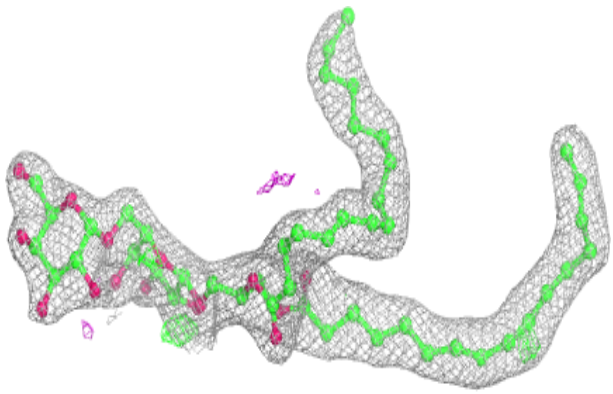


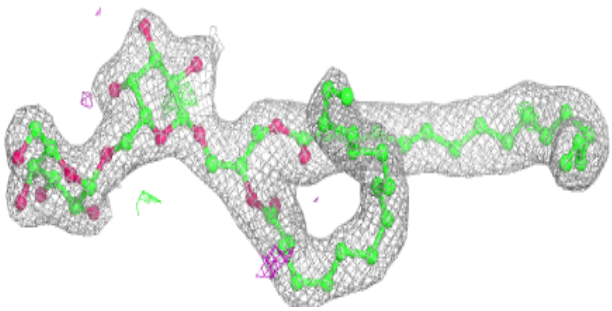




Electron density around DGD H 101:

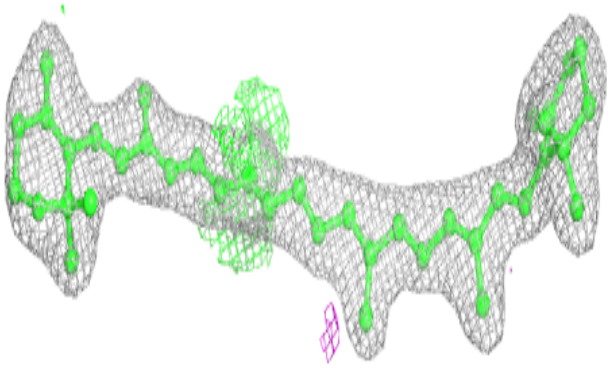
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

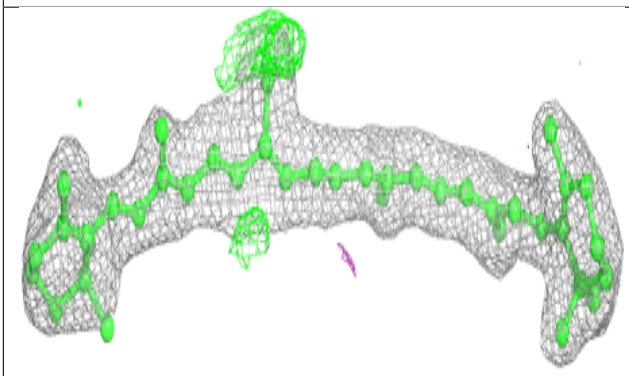


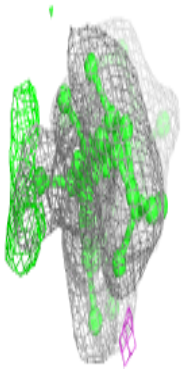


Electron density around BCR T 101:

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

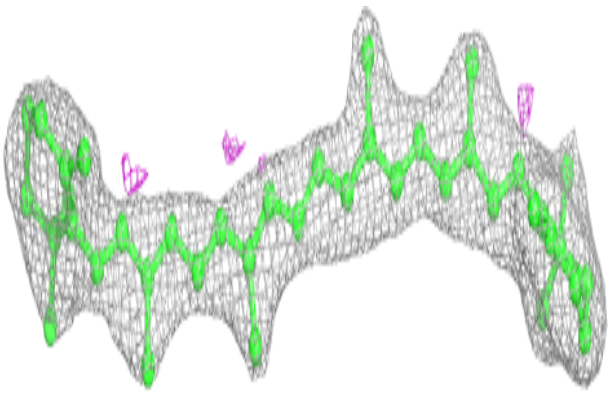


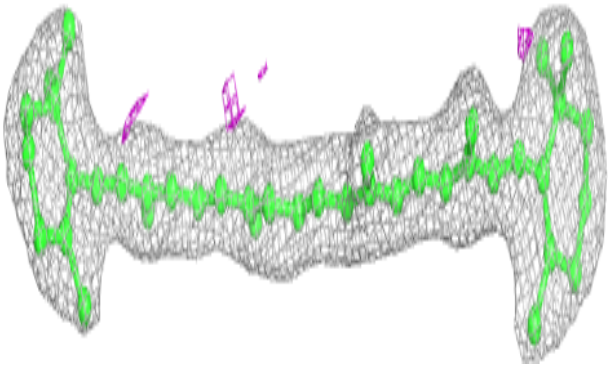


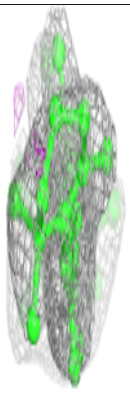


Electron density around BCR c 515:

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

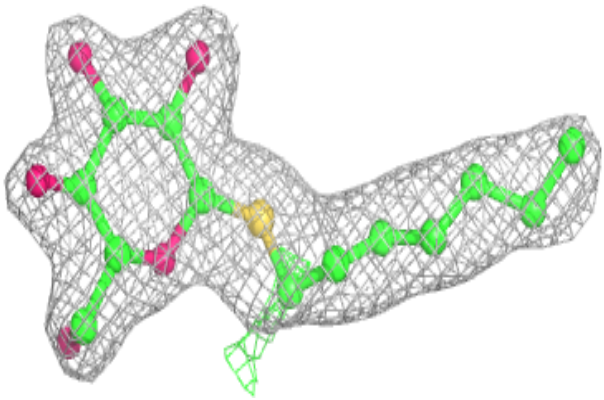


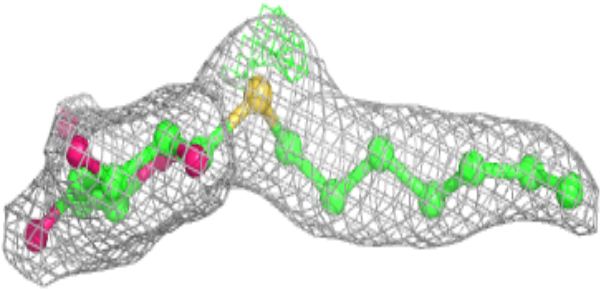


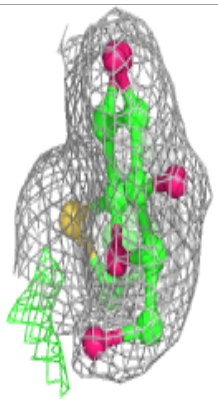


Electron density around HTG O 302:

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

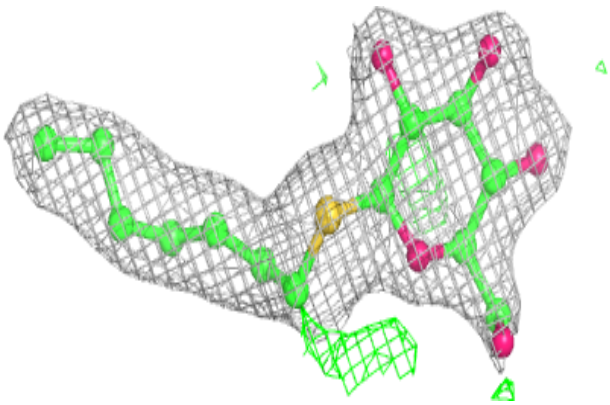


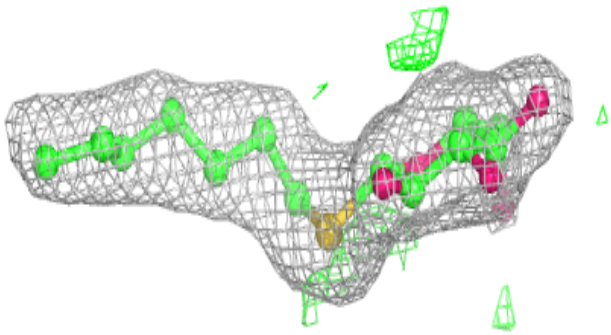


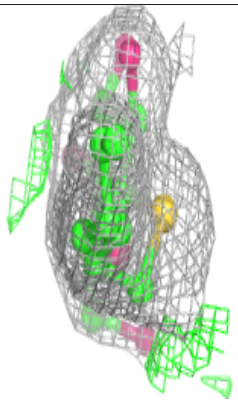


Electron density around HTG o 301:

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

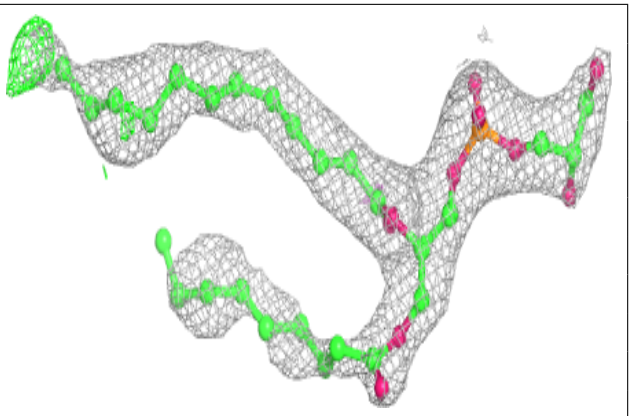


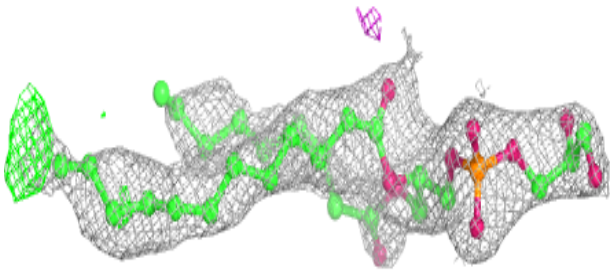


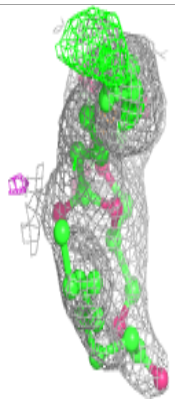


Electron density around LHG F 103:

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

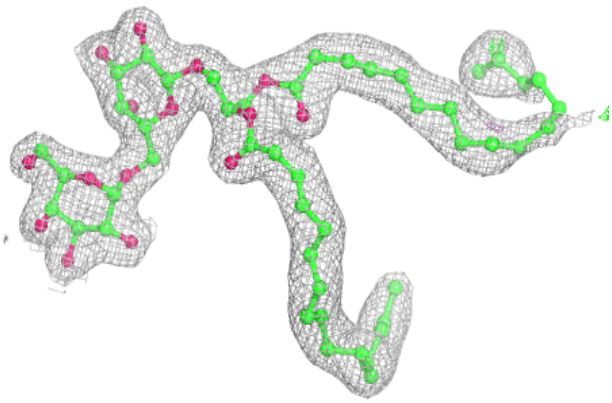


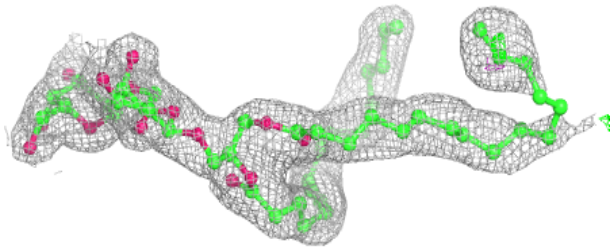


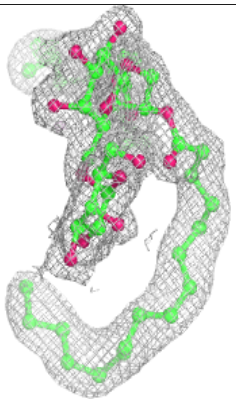


Electron density around DGD C 516:

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

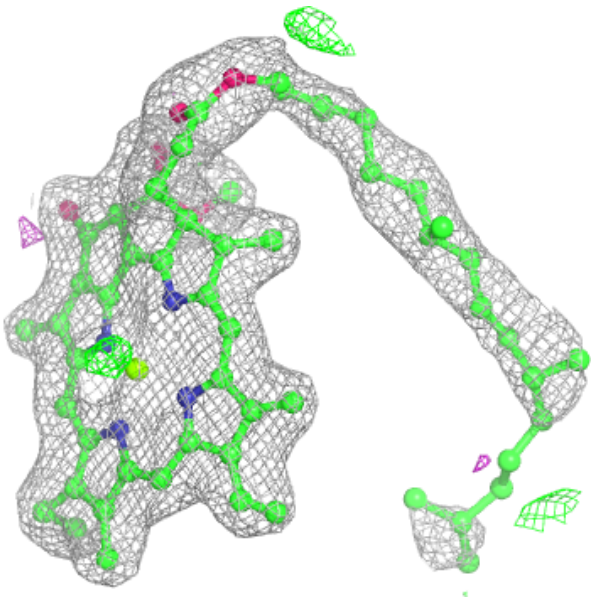


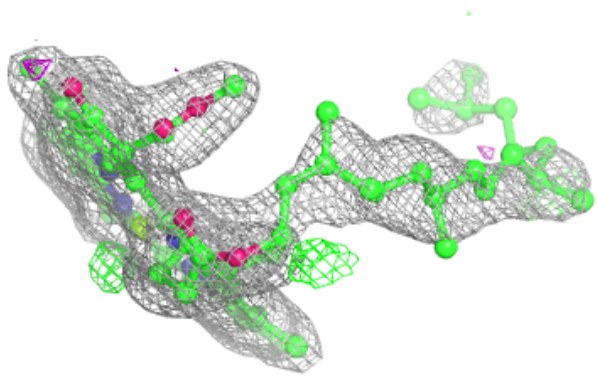


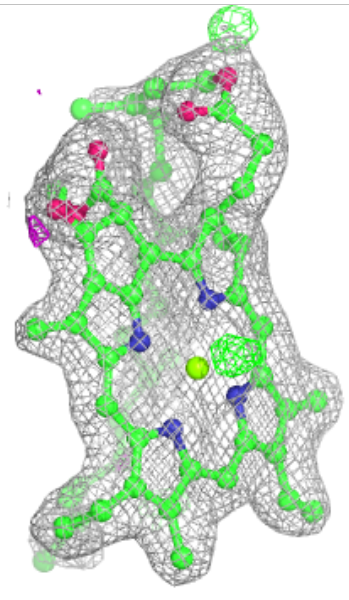


Electron density around CLA B 617:

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

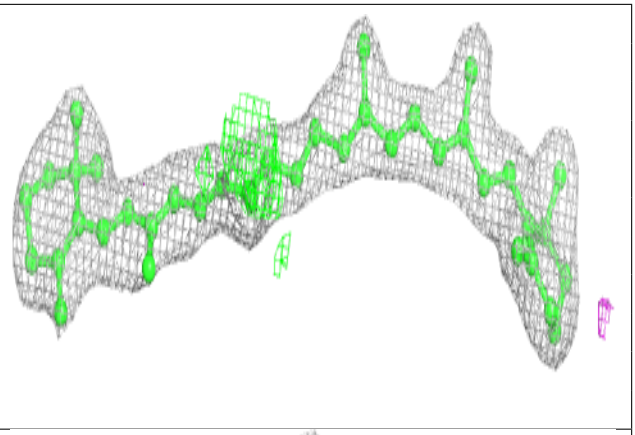


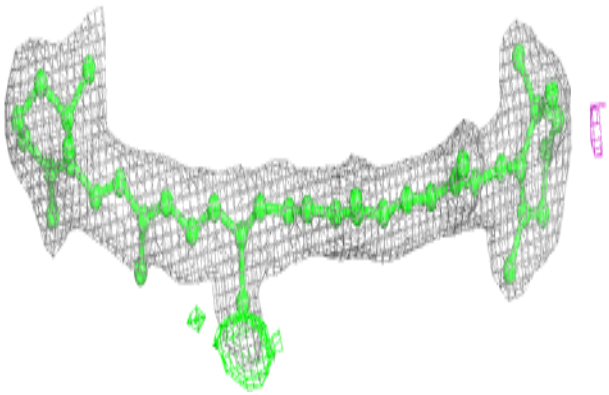


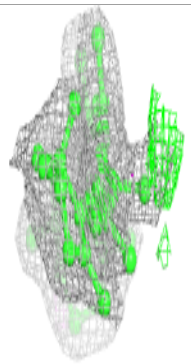


Electron density around BCR t 101:

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

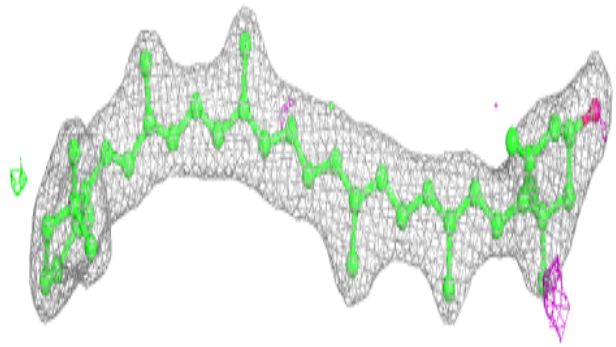


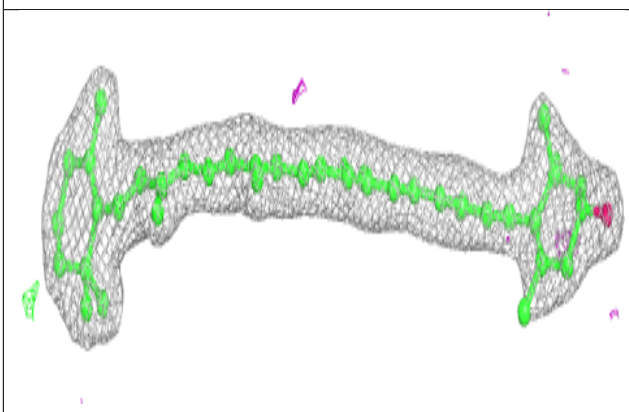


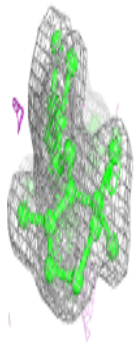


Electron density around RRX H 102:

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

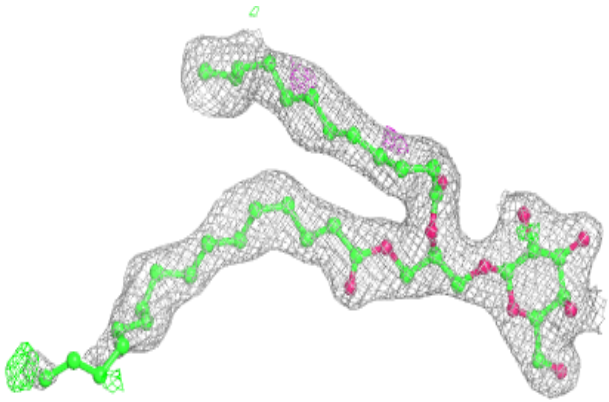


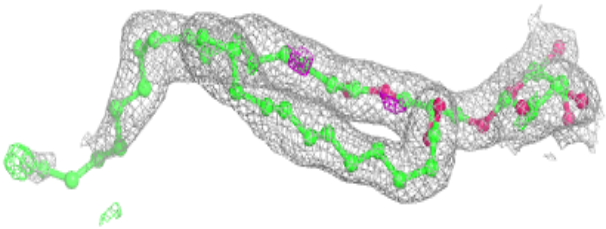




Electron density around LMG d 412:

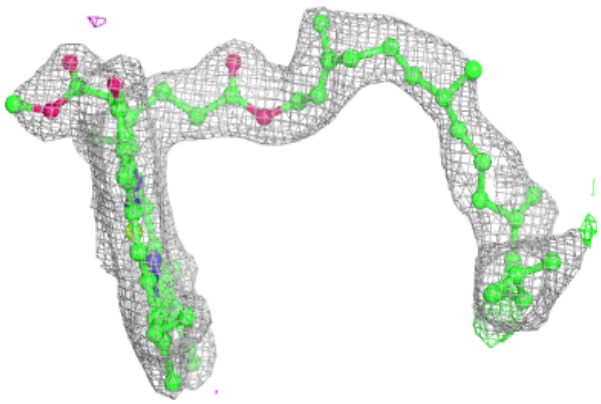
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

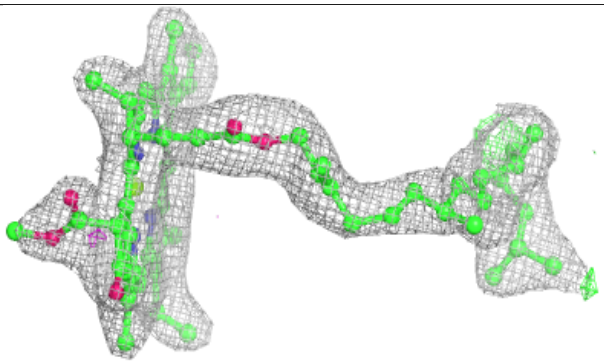


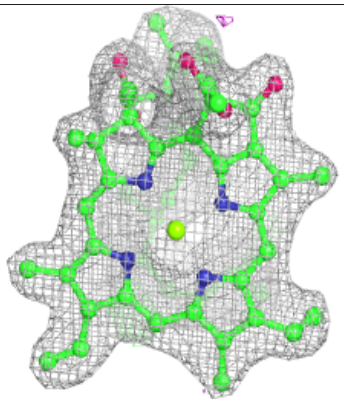


Electron density around CLA c 507:

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

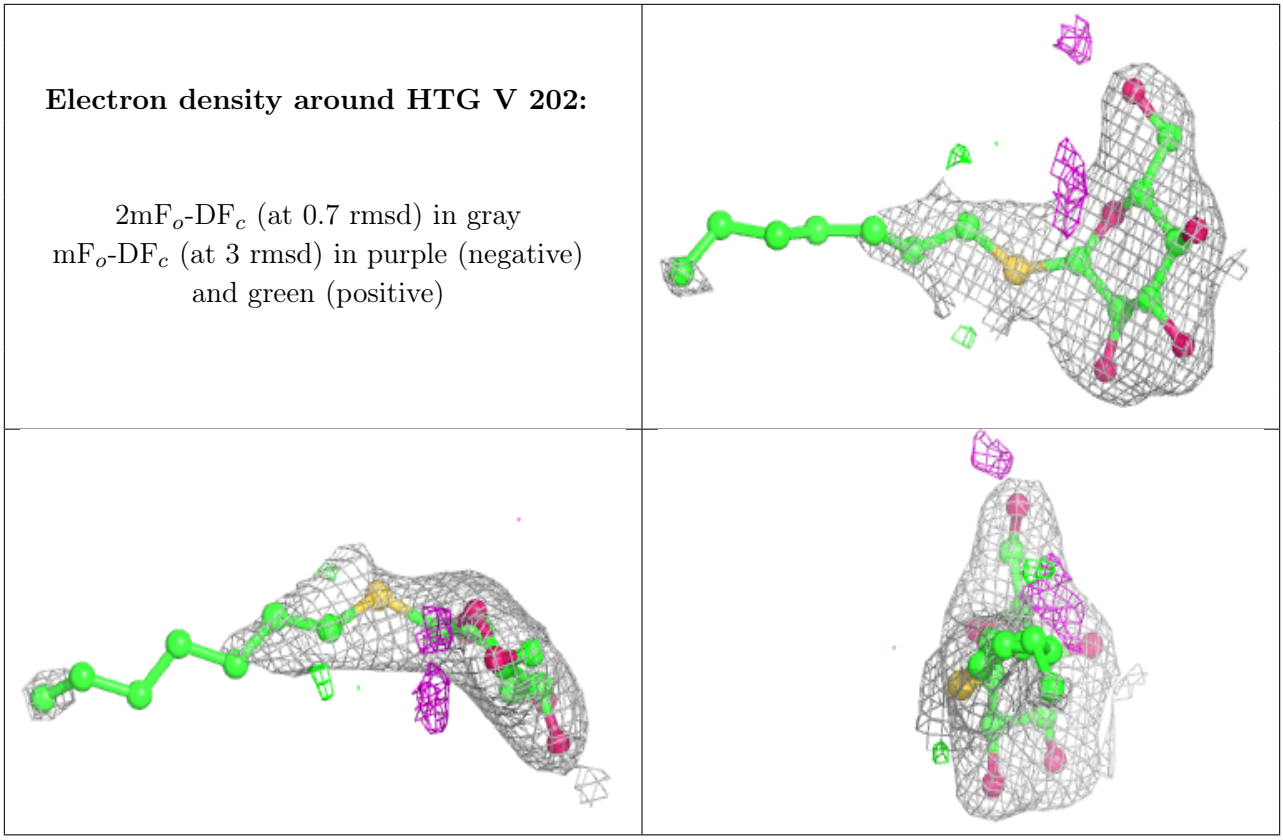






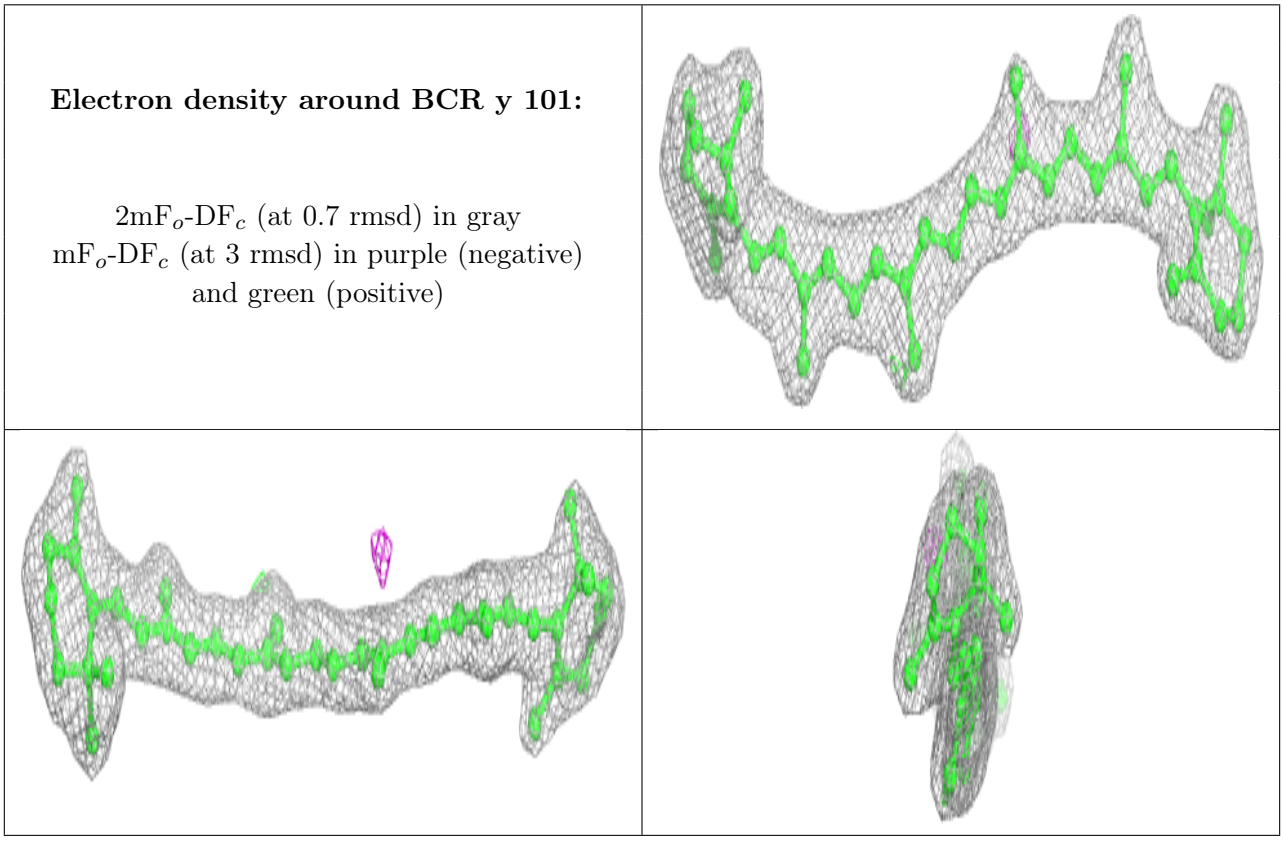
Electron density around HTG V 202:

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



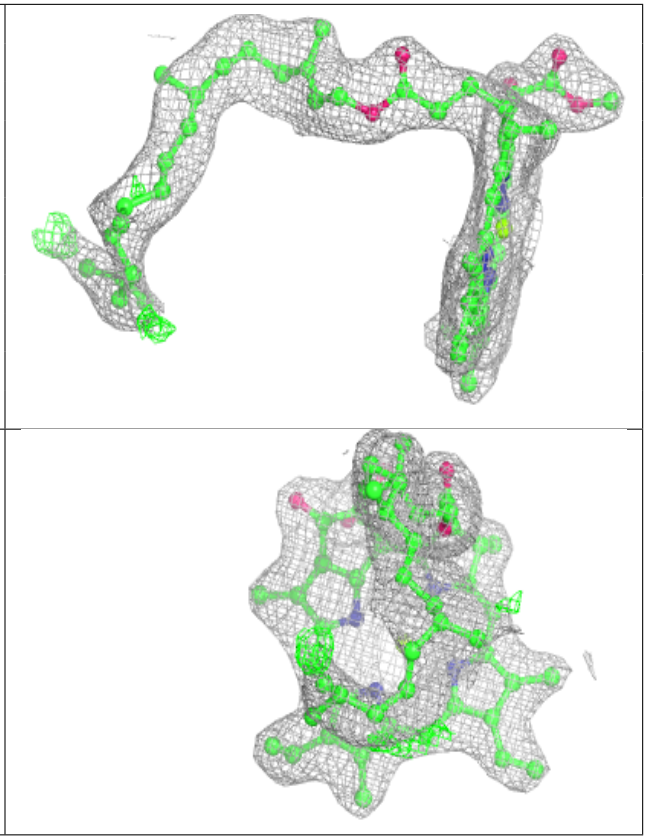
Electron density around BCR y 101:

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



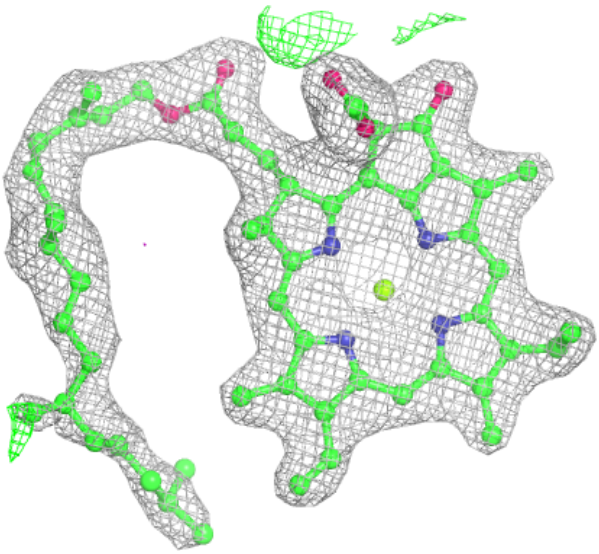
Electron density around CLA C 506:

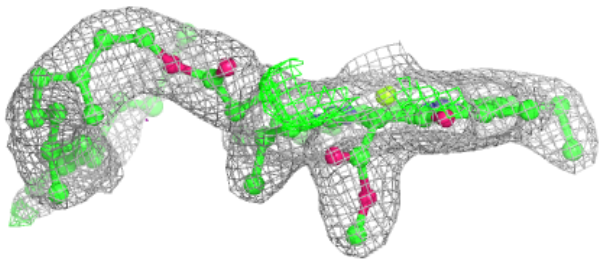
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

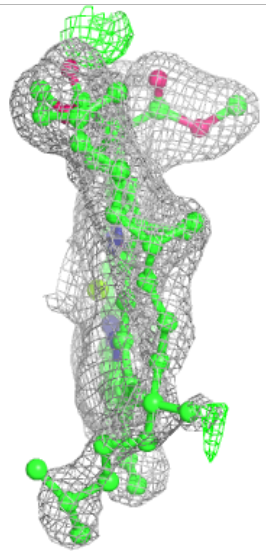


Electron density around CLA C 512:

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

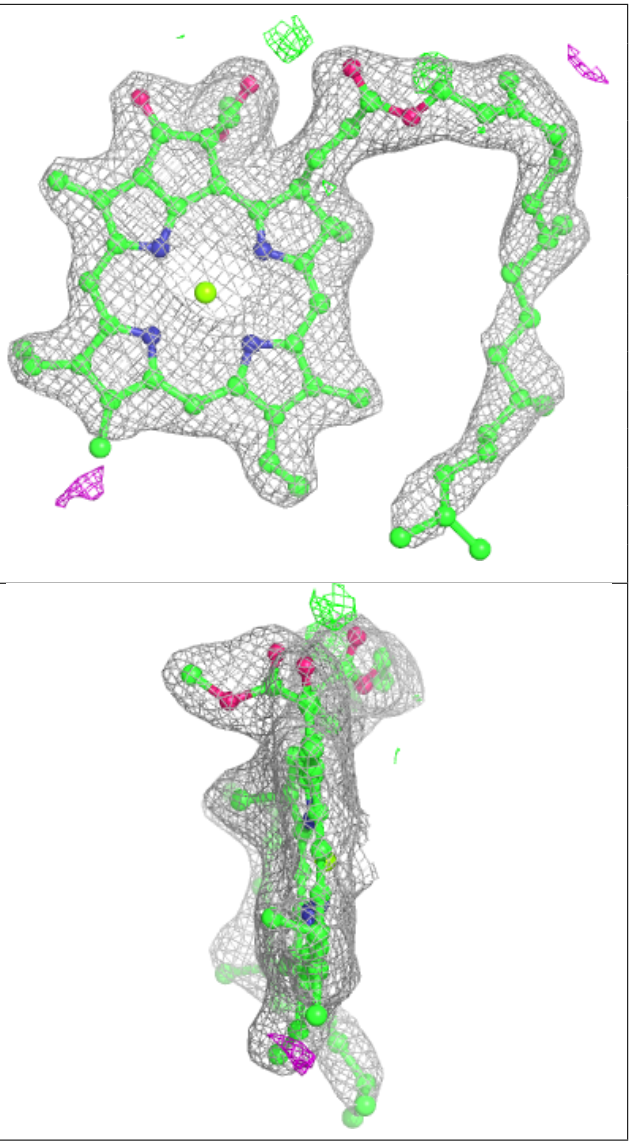






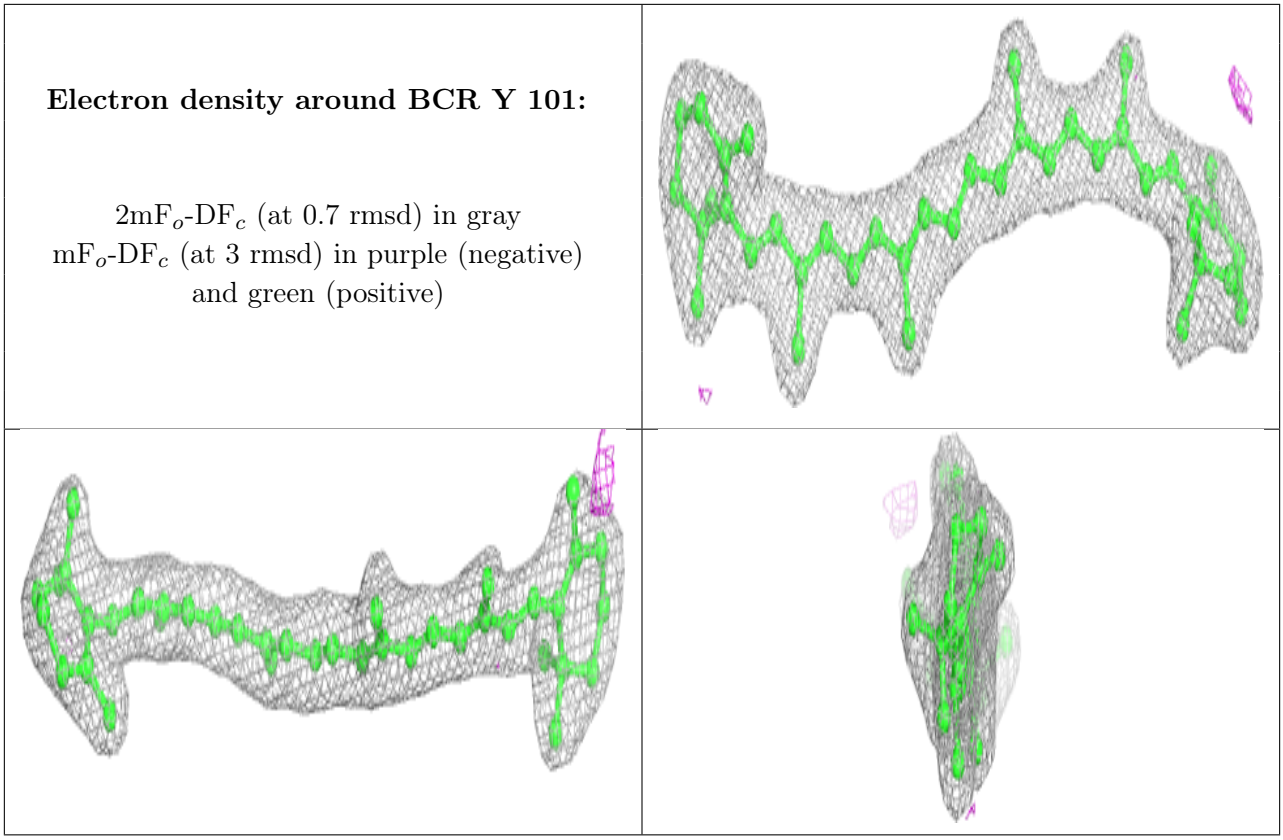
Electron density around CLA c 513:

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



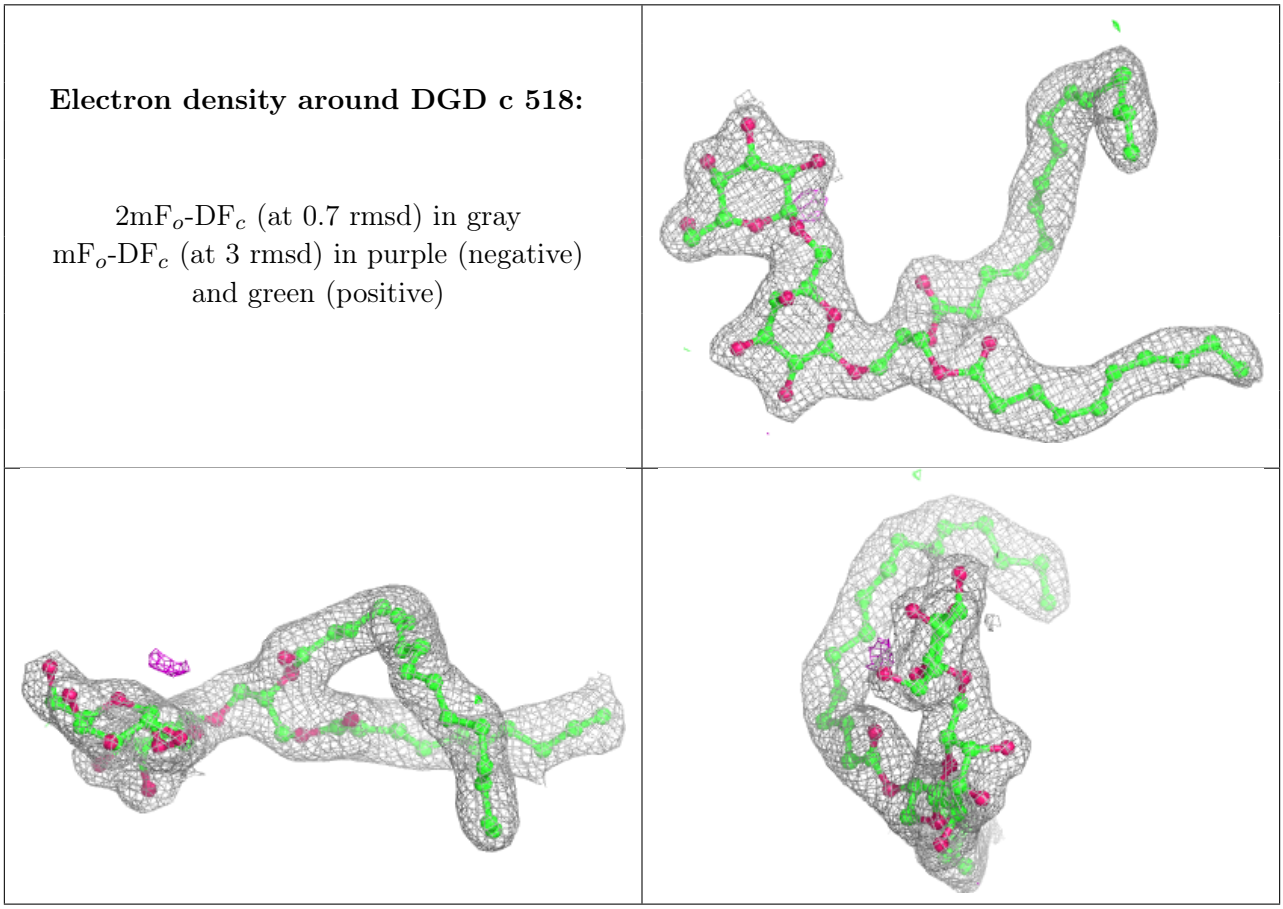
Electron density around BCR Y 101:

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



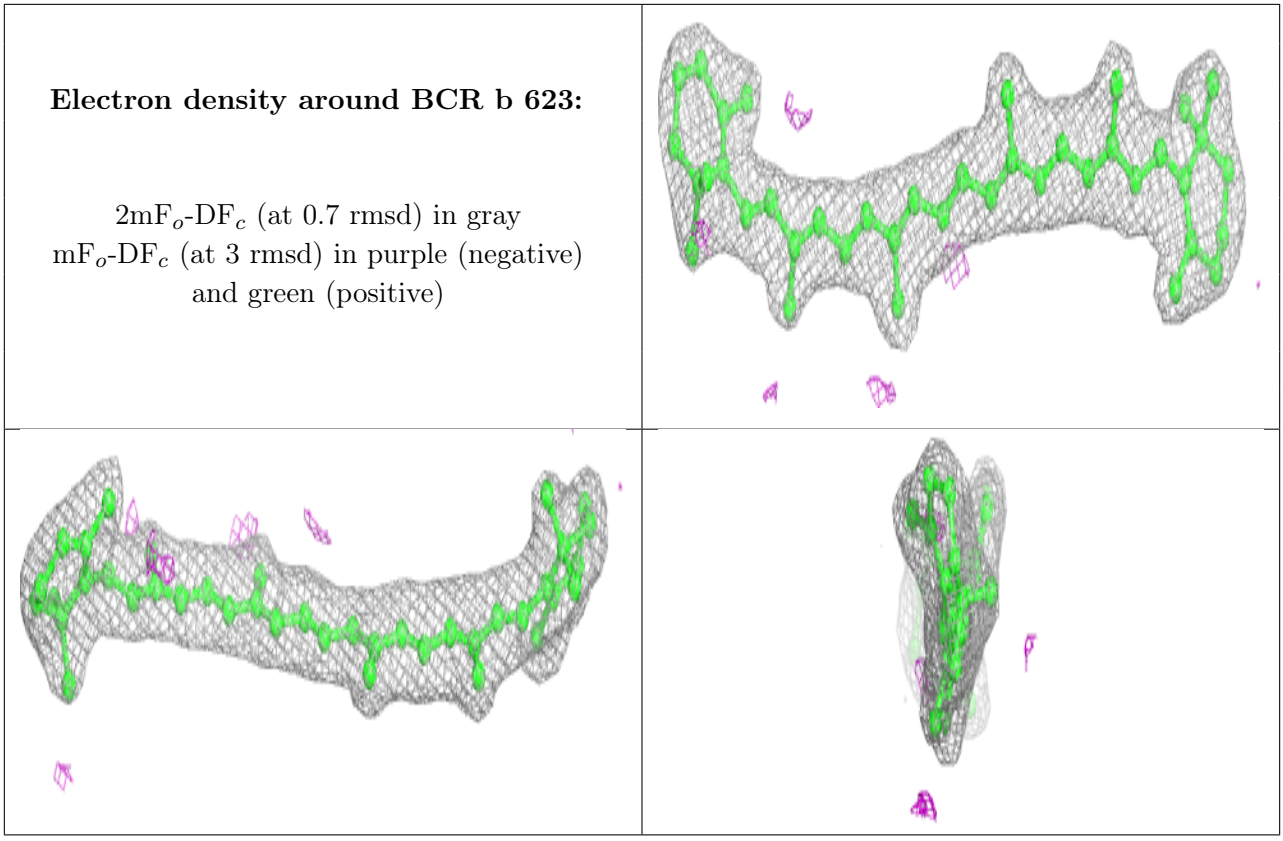
Electron density around DGD c 518:

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



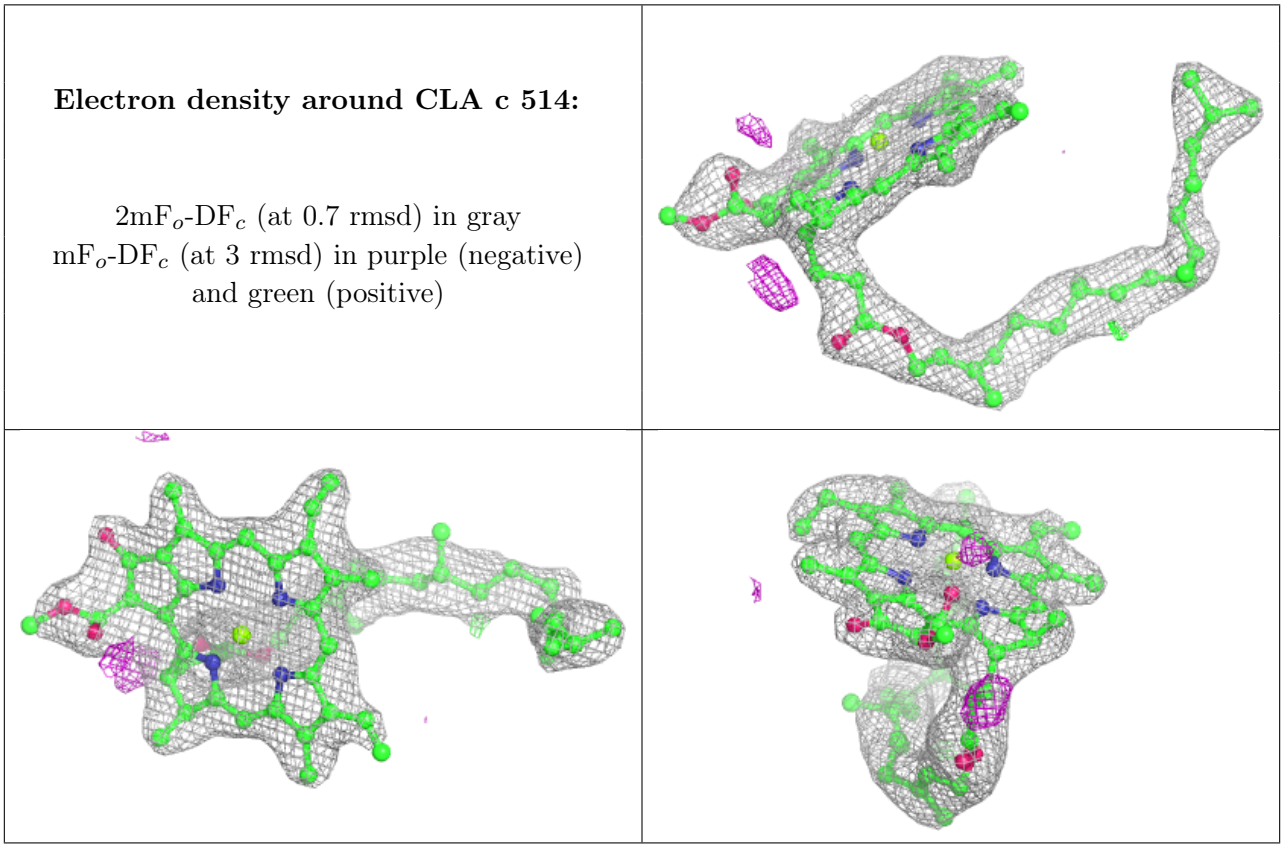
Electron density around BCR b 623:

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



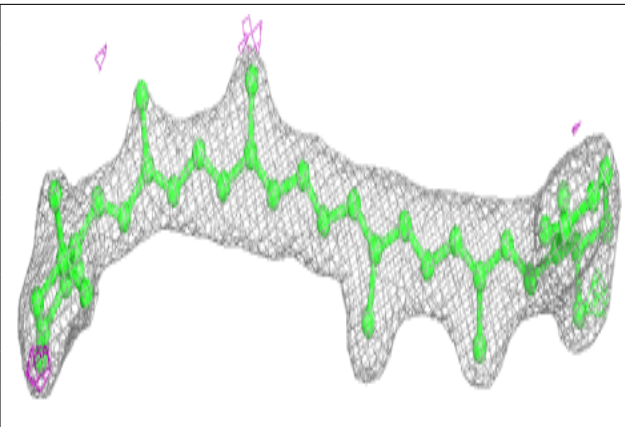
Electron density around CLA c 514:

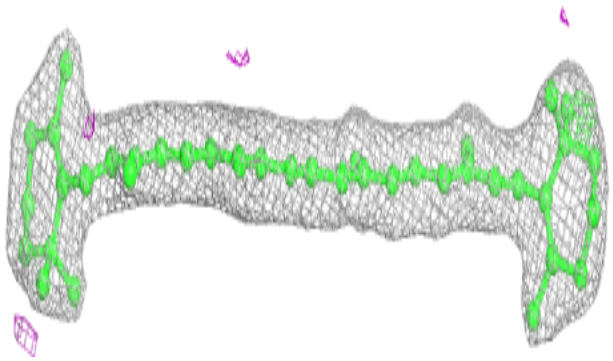
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

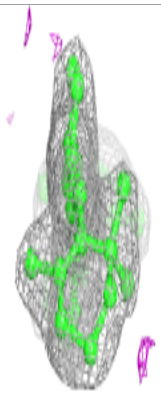


Electron density around BCR c 516:

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

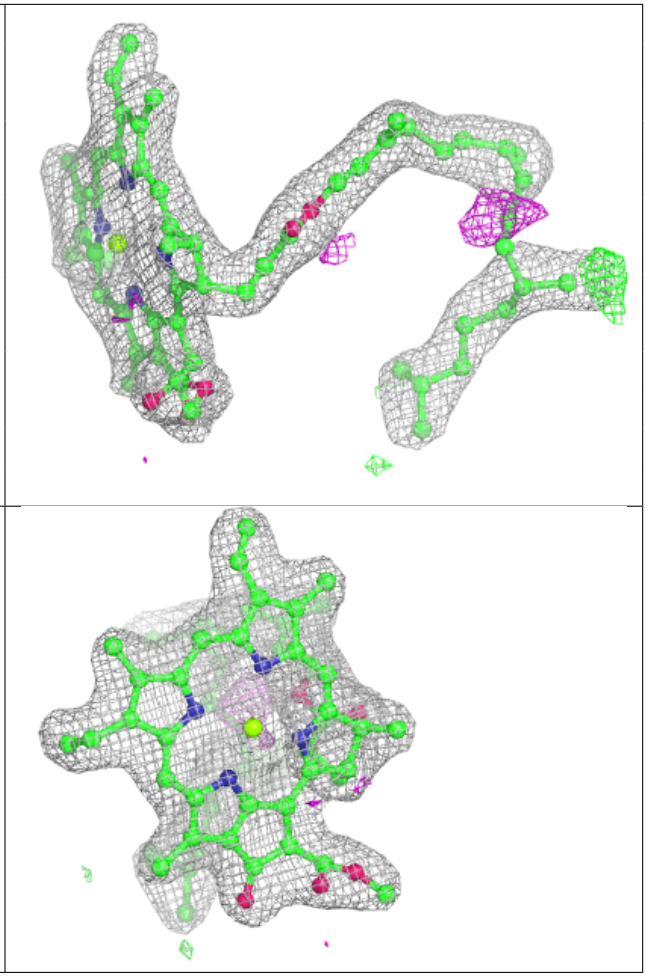






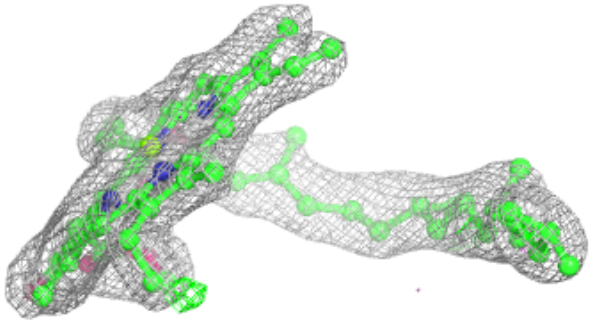
Electron density around CLA b 610:

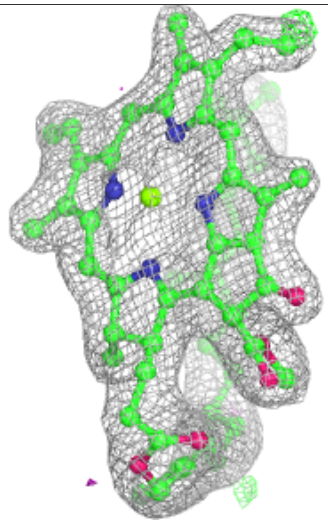
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 508:

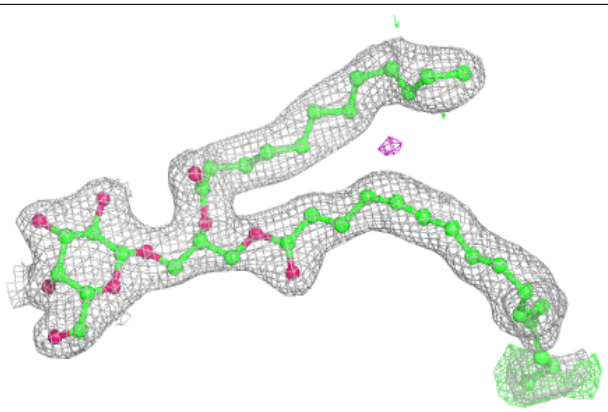
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

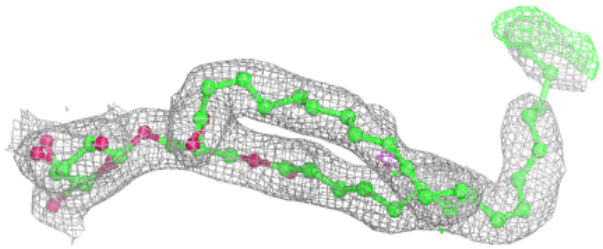


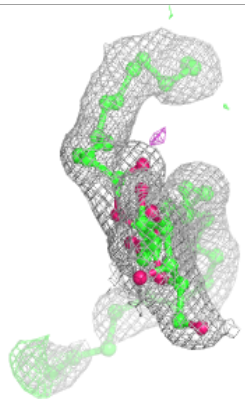


Electron density around LMG D 412:

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

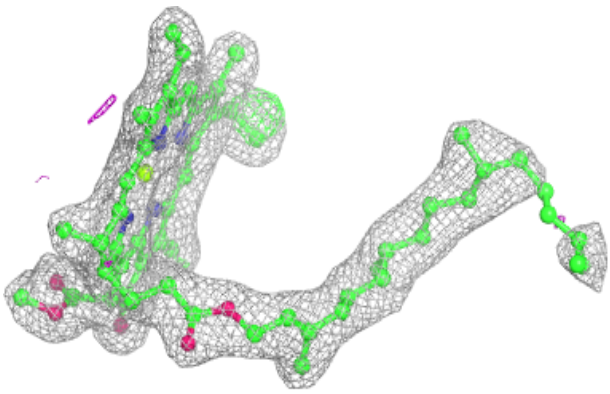


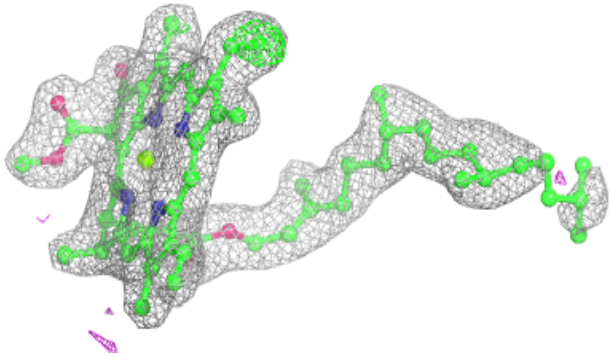


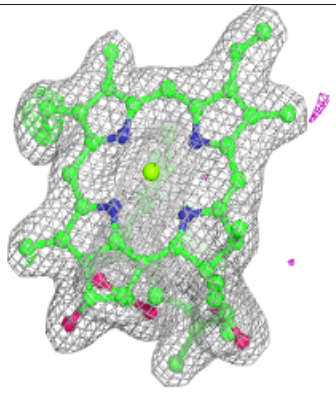


Electron density around CLA C 508:

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

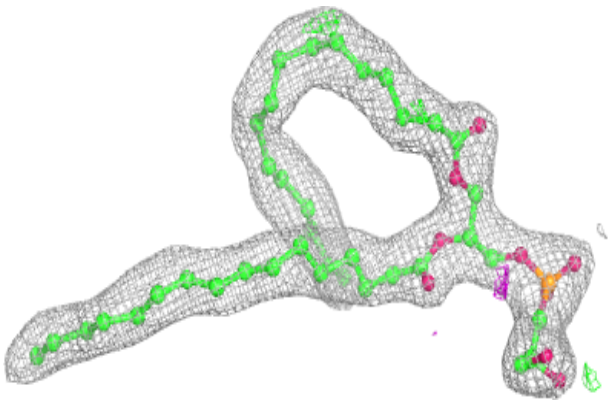


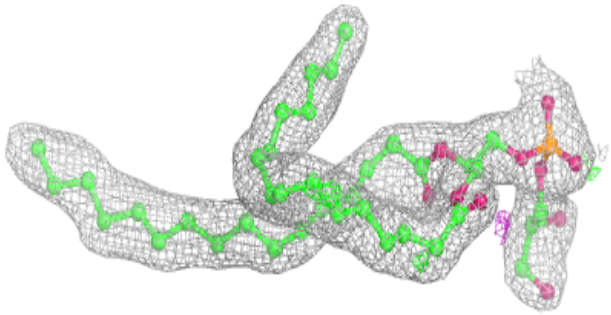


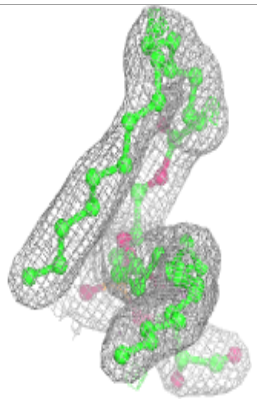


Electron density around LHG D 409:

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

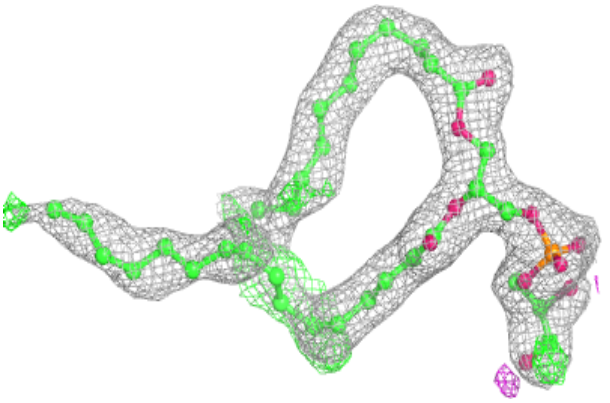


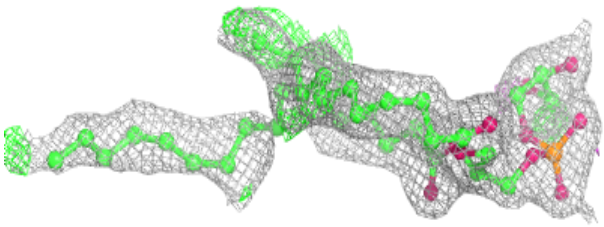


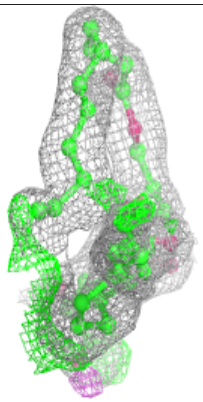


Electron density around LHG D 411:

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

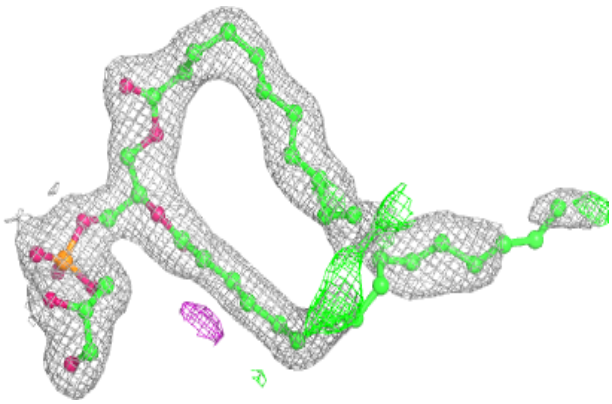


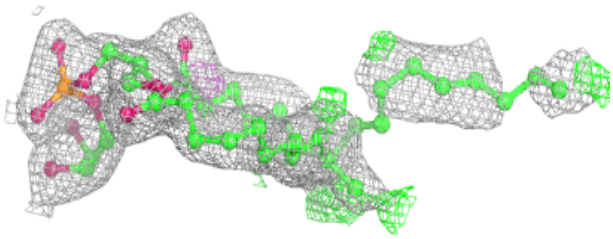


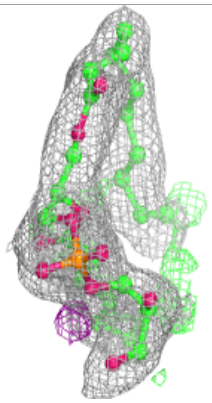


Electron density around LHG d 411:

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

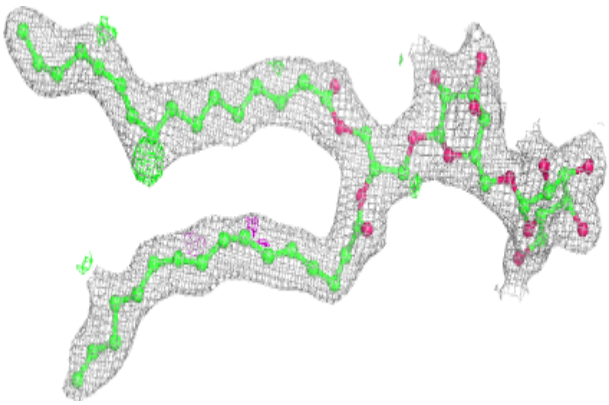


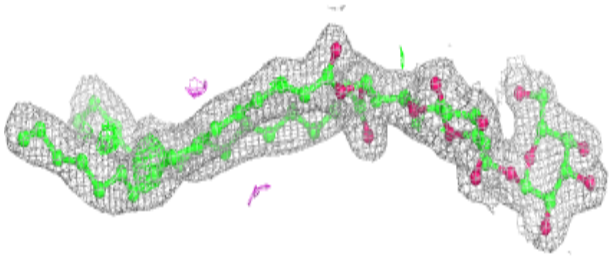


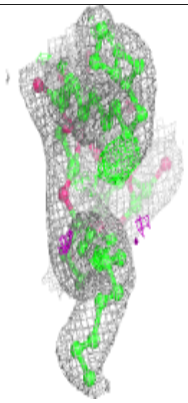


Electron density around DGD C 517:

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

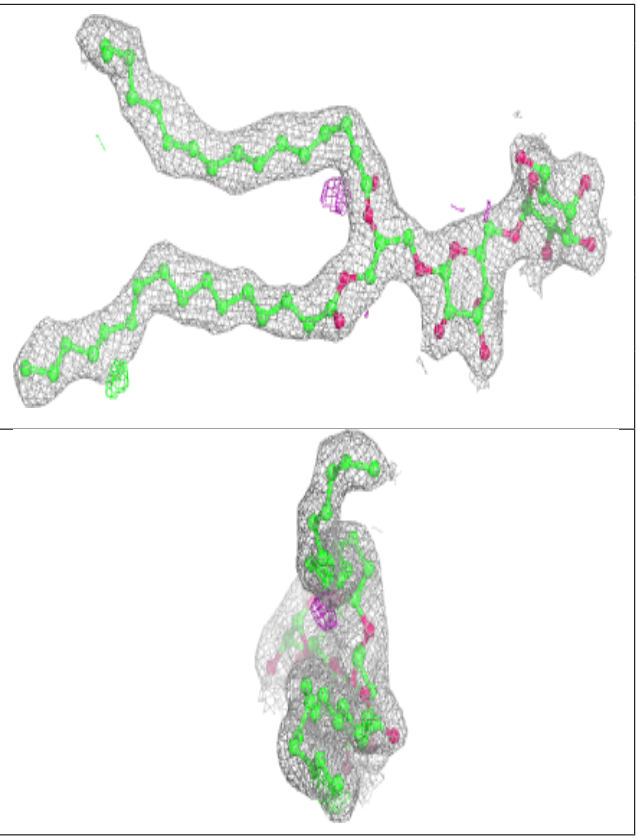






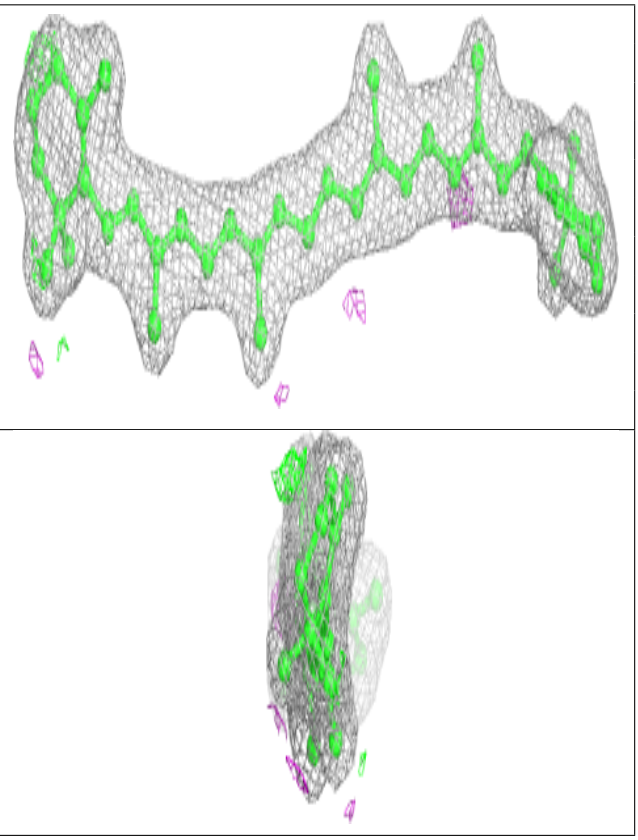
Electron density around DGD c 519:

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



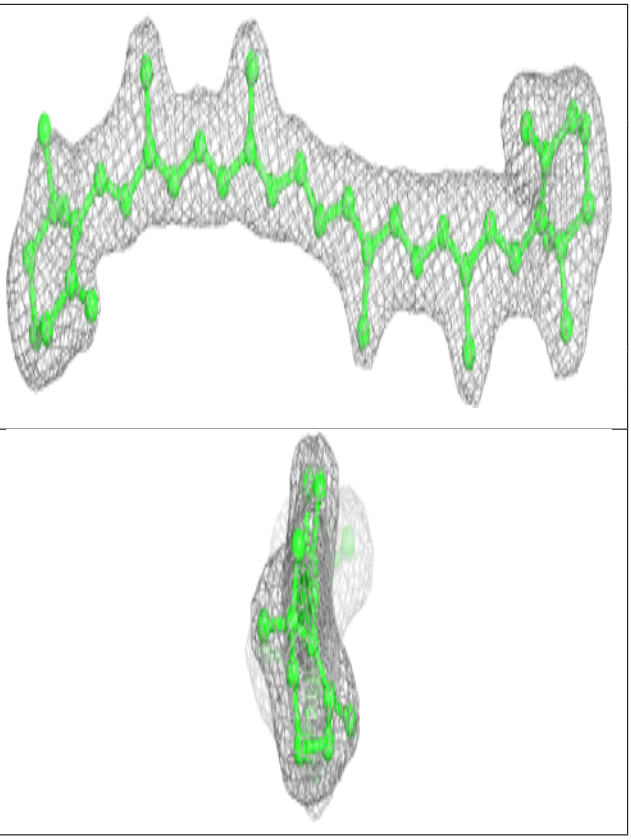
Electron density around BCR B 618:

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



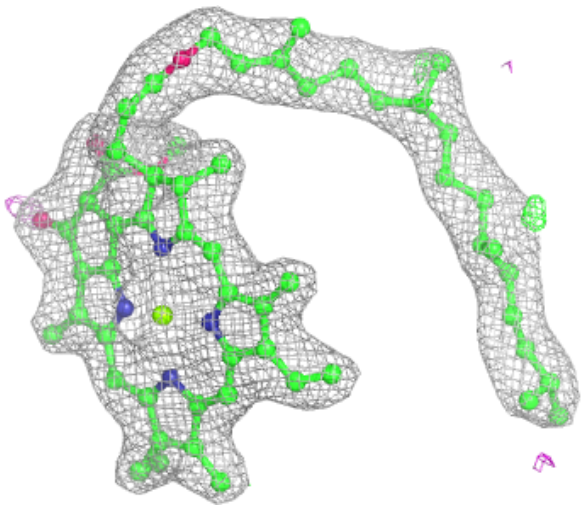
Electron density around BCR B 619:

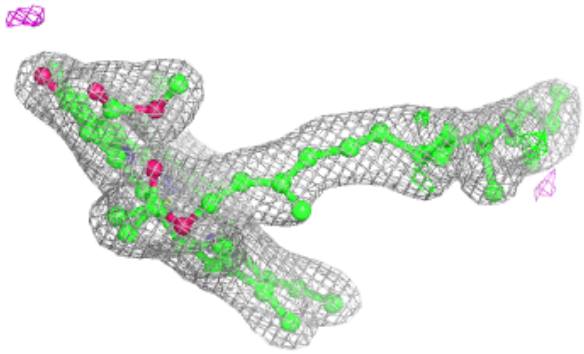
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

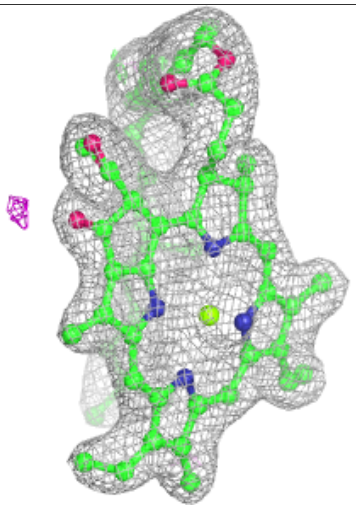


Electron density around CLA C 507:

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

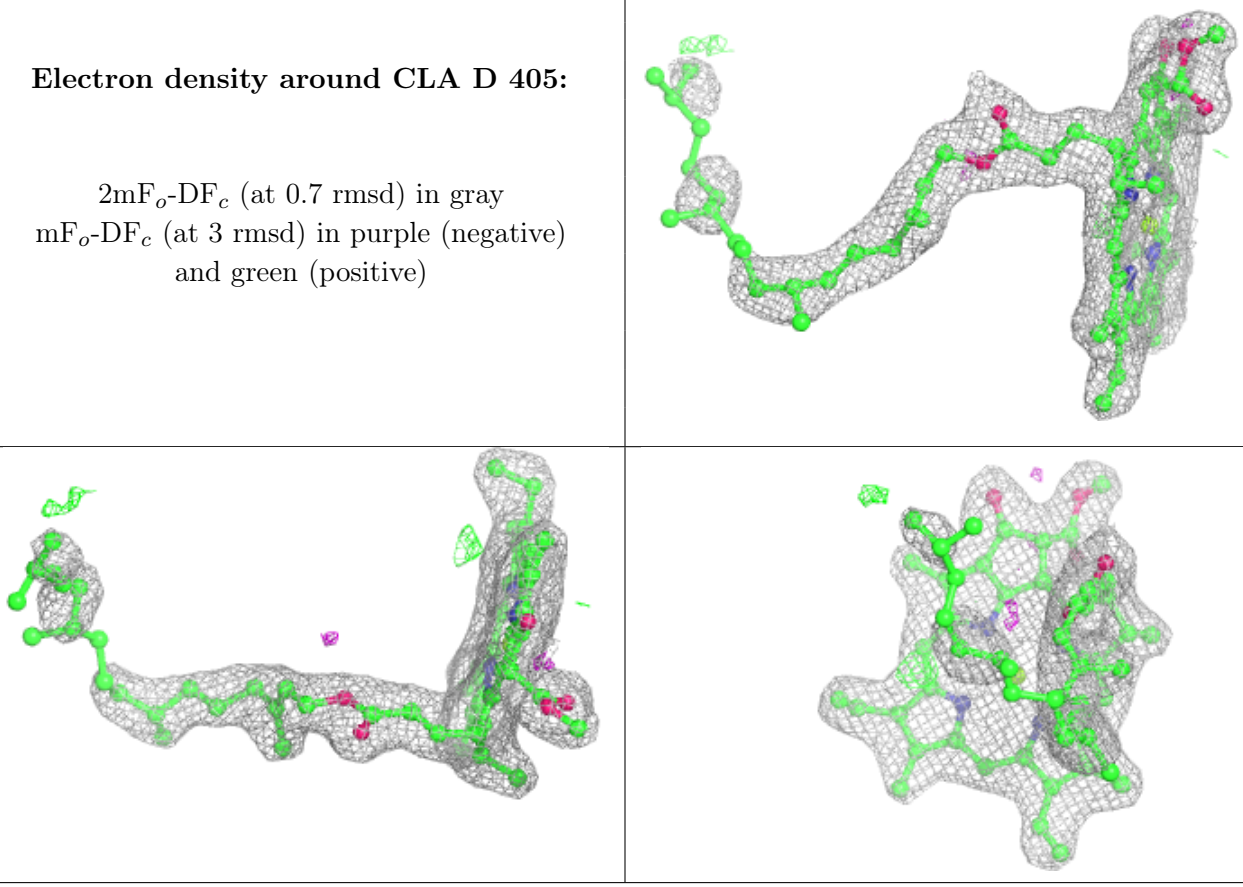






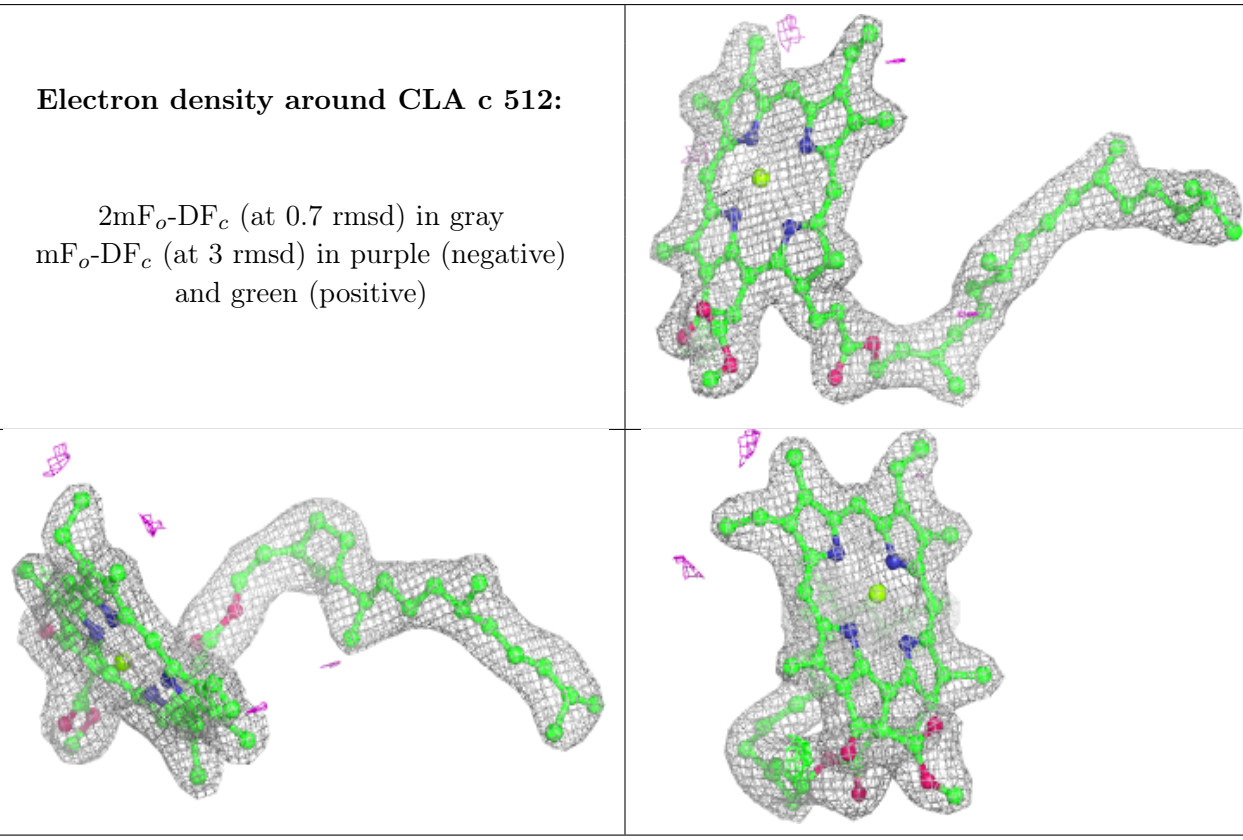
Electron density around CLA D 405:

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



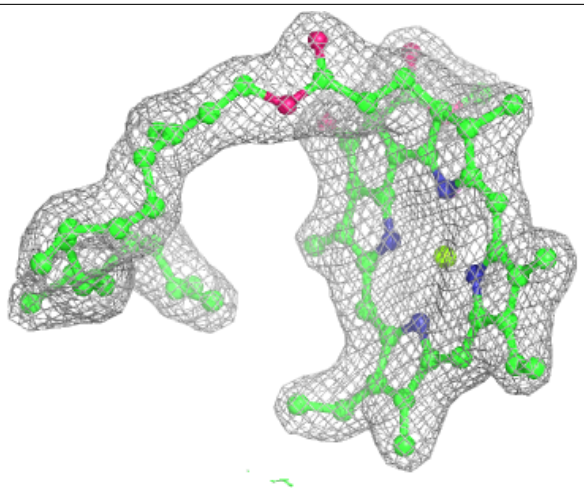
Electron density around CLA c 512:

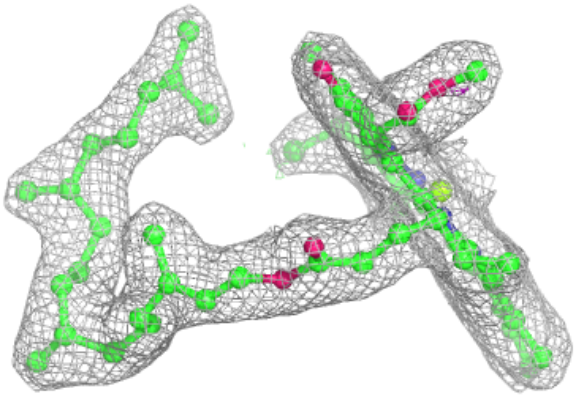
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

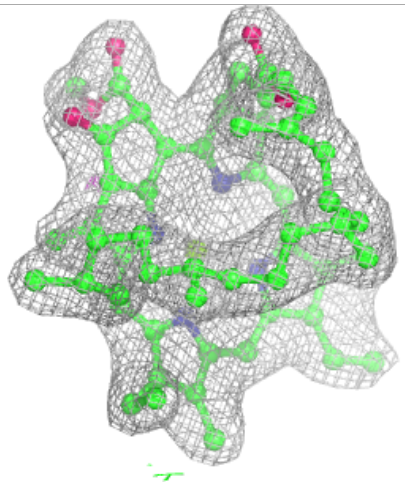


Electron density around CLA C 503:

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

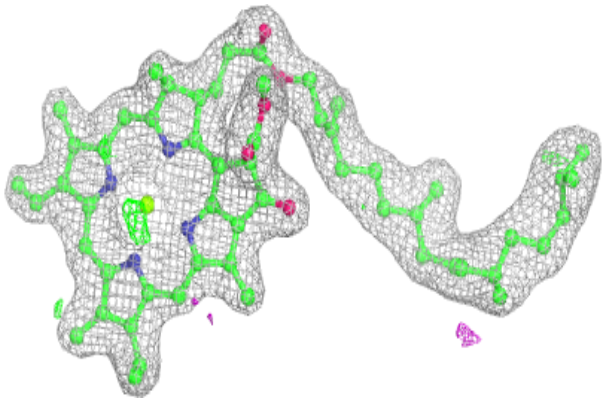


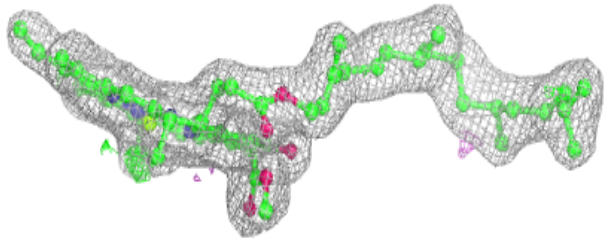


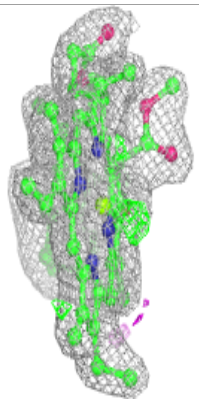


Electron density around CLA B 603:

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

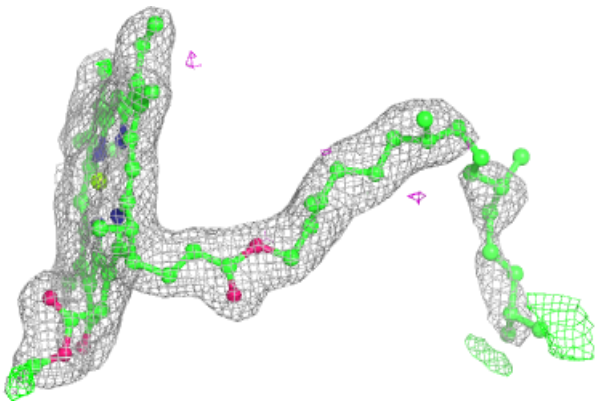


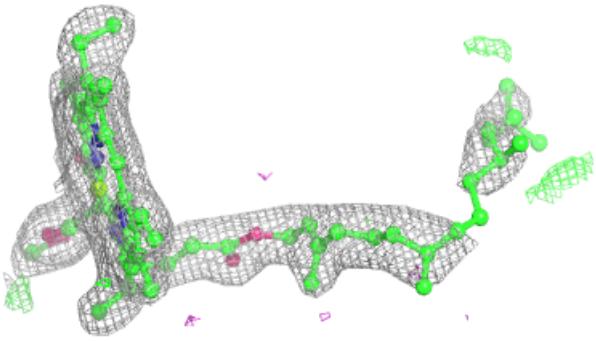


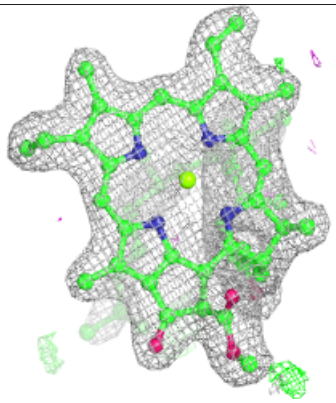


Electron density around CLA d 405:

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

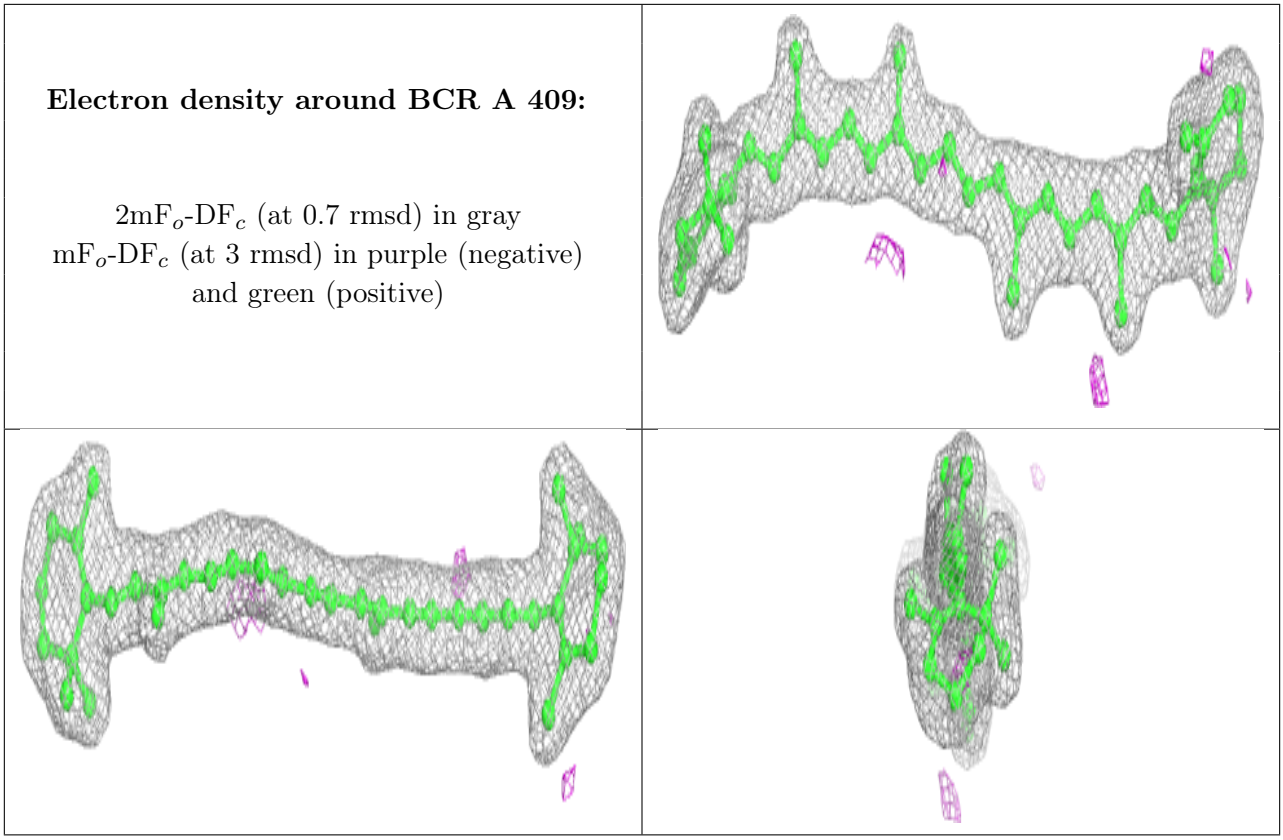






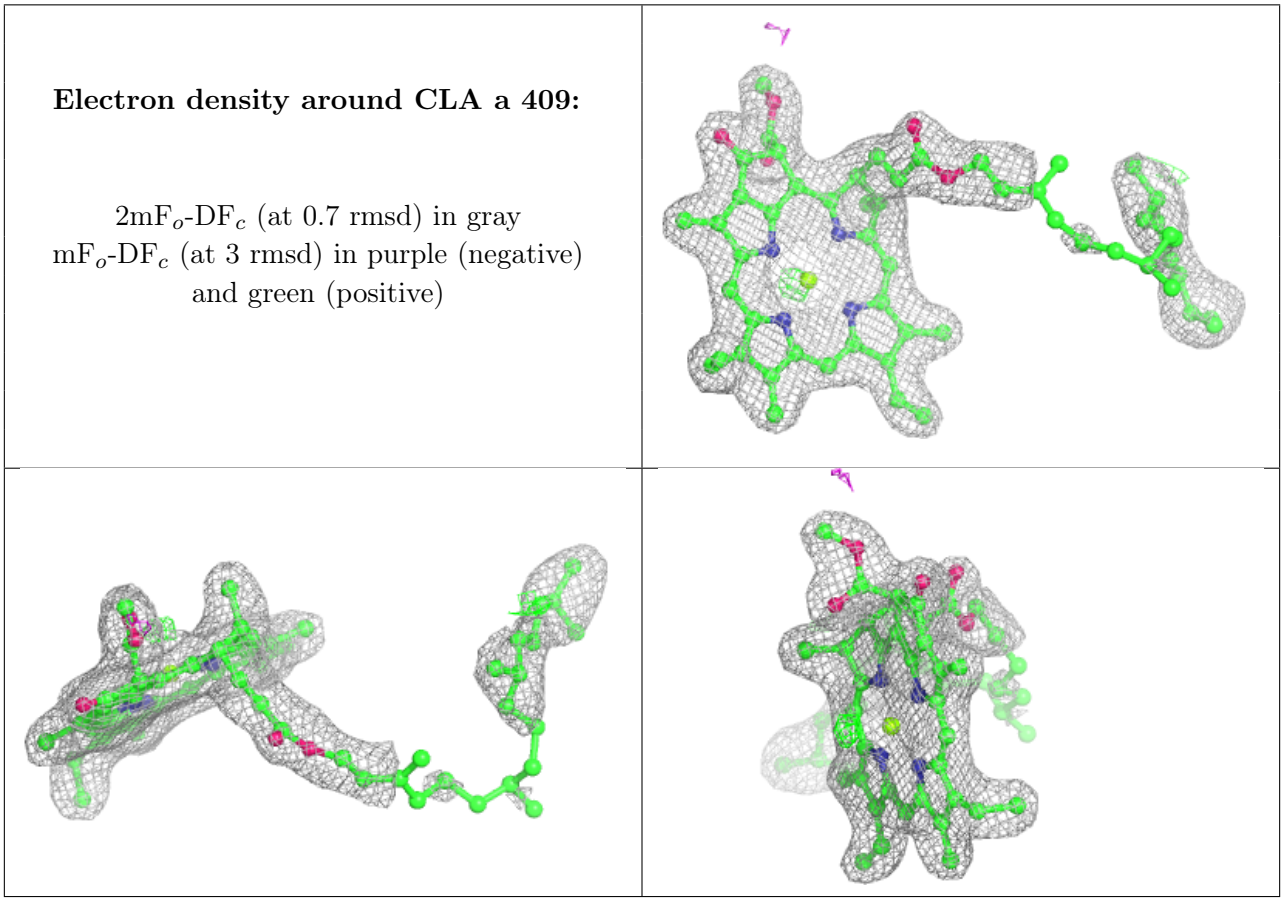
Electron density around BCR A 409:

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



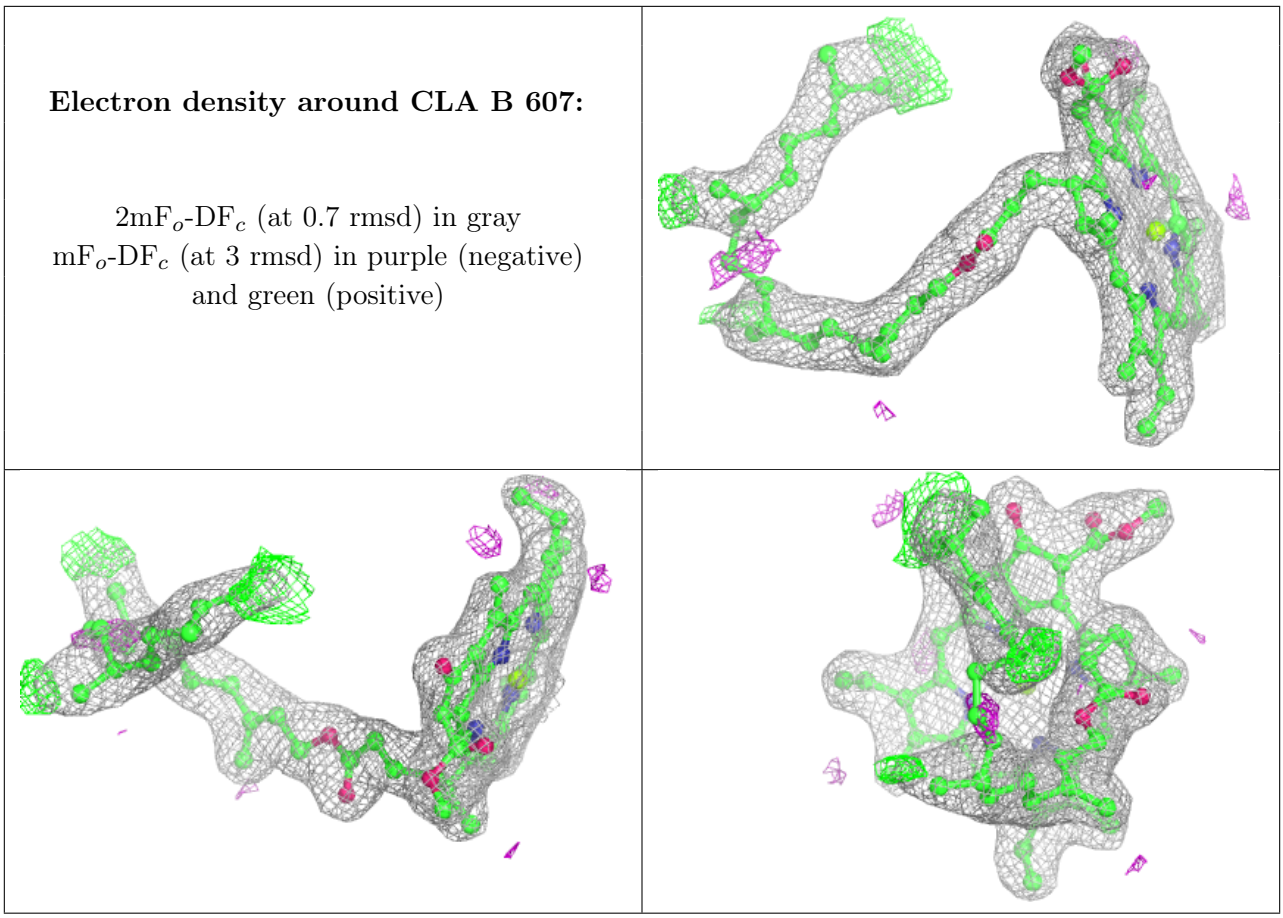
Electron density around CLA a 409:

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



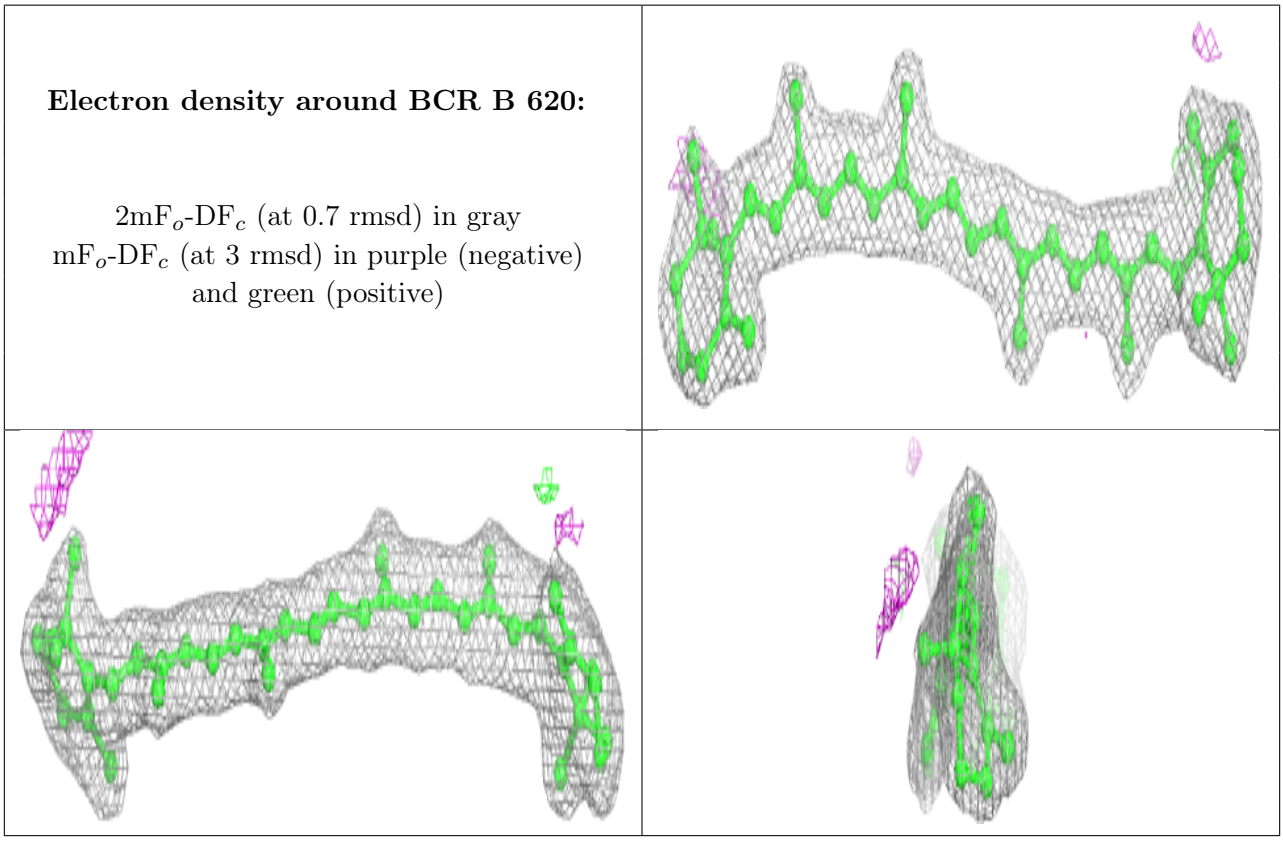
Electron density around CLA B 607:

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



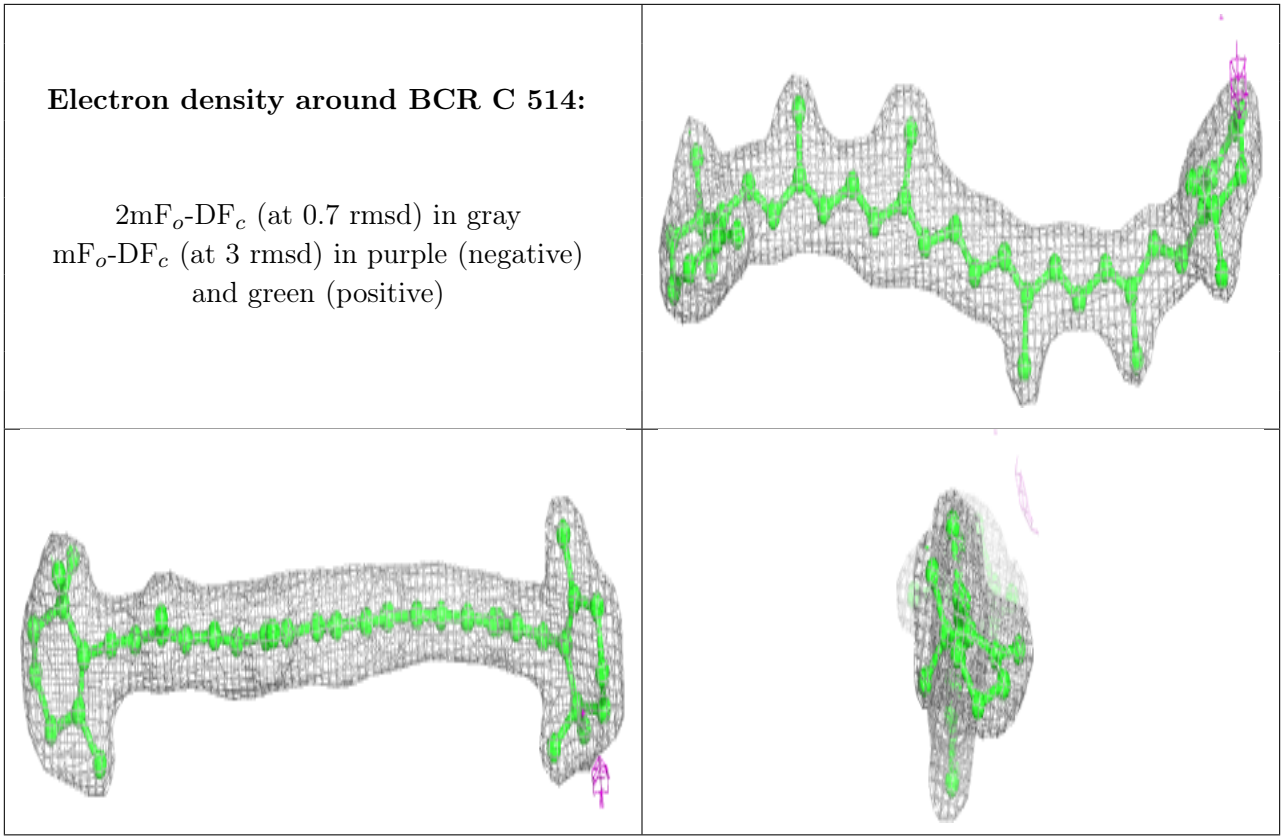
Electron density around BCR B 620:

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



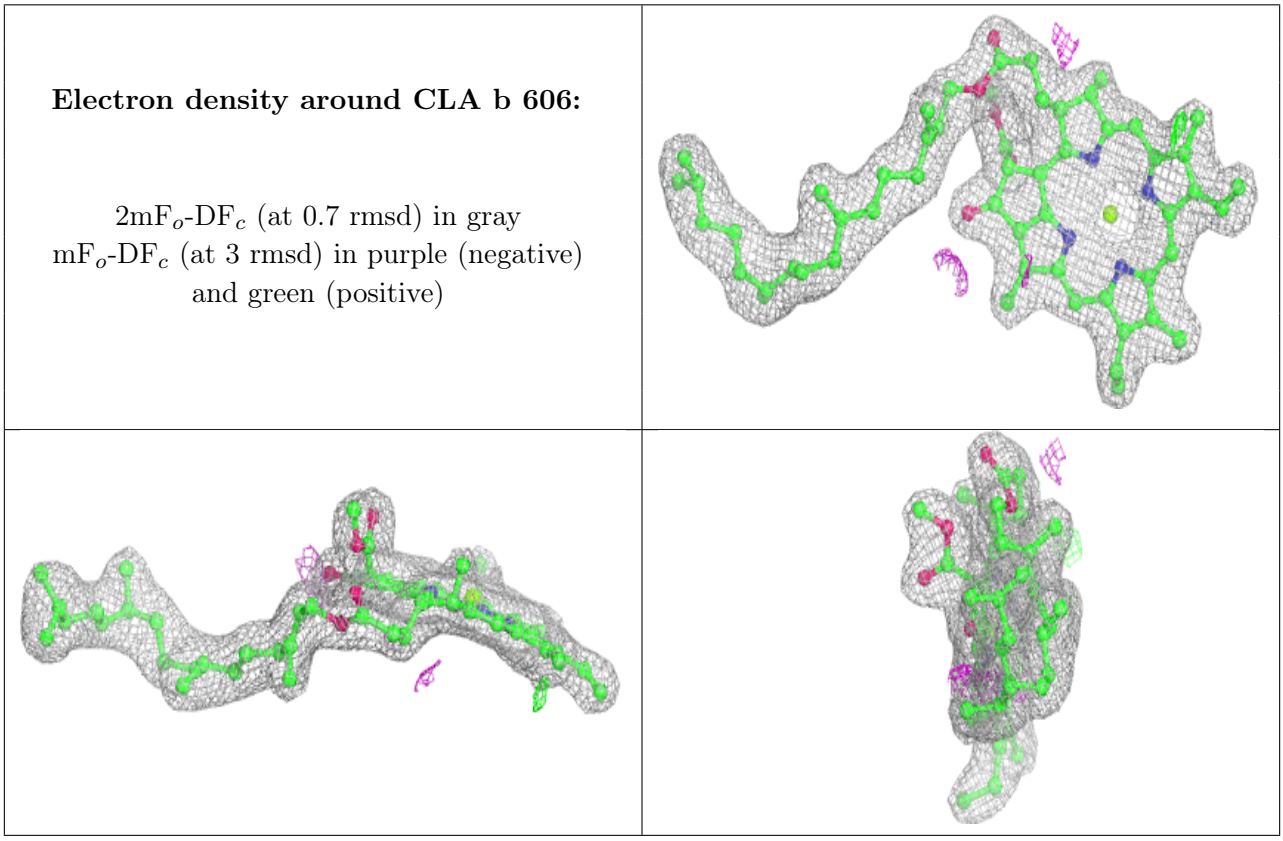
Electron density around BCR C 514:

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



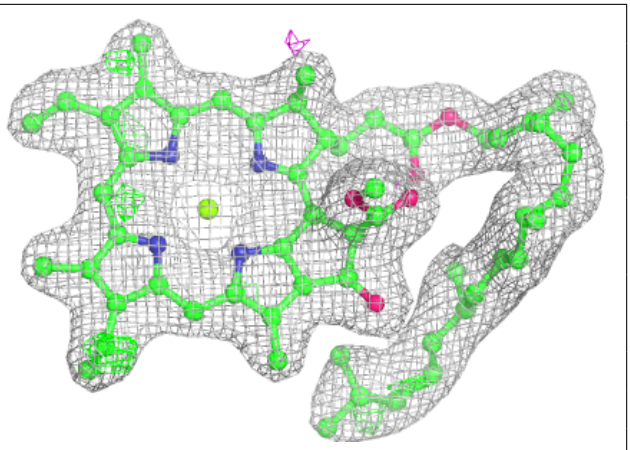
Electron density around CLA b 606:

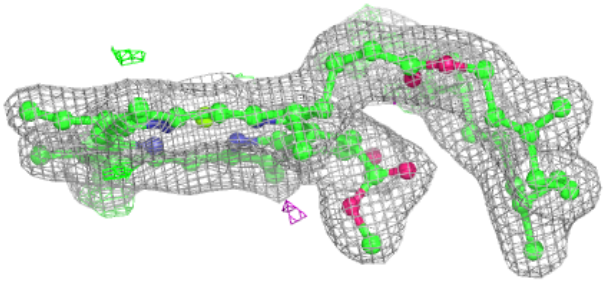
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

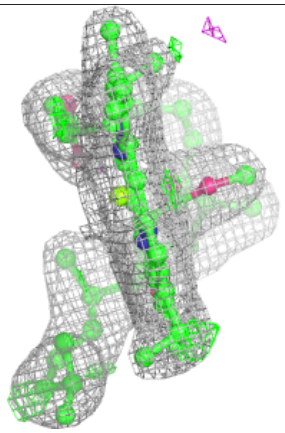


Electron density around CLA B 611:

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

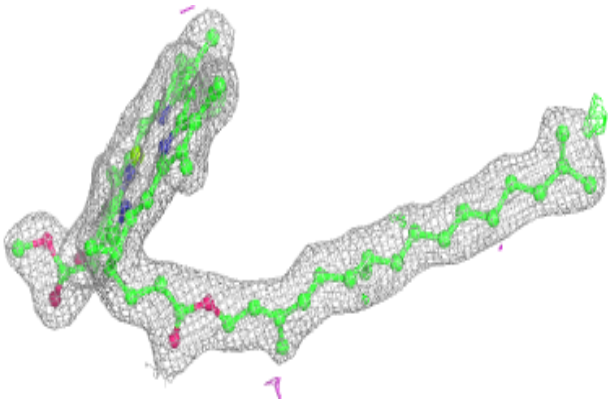


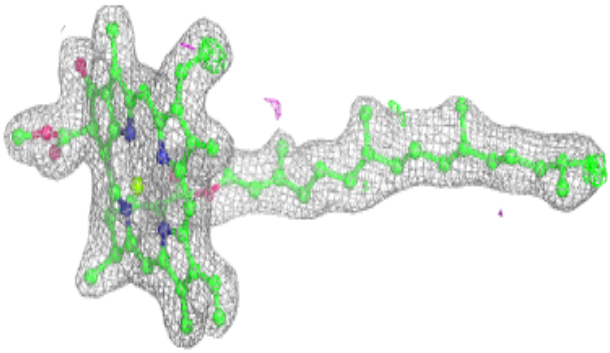


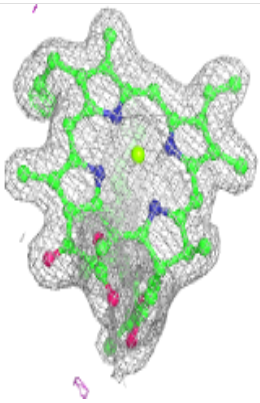


Electron density around CLA b 611:

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

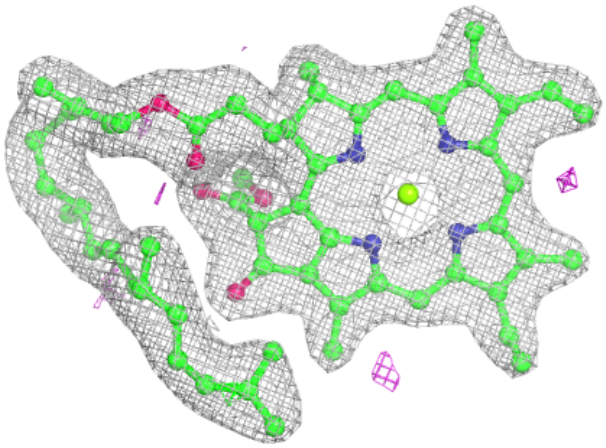


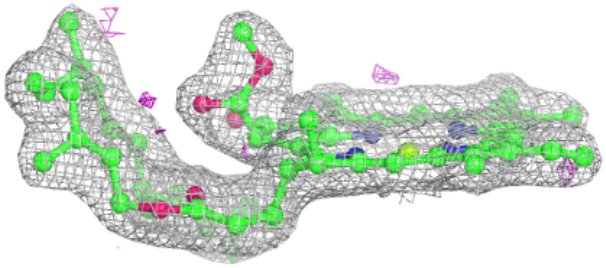


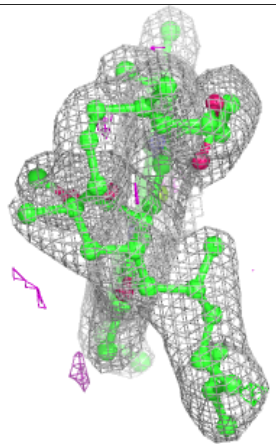


Electron density around CLA b 614:

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

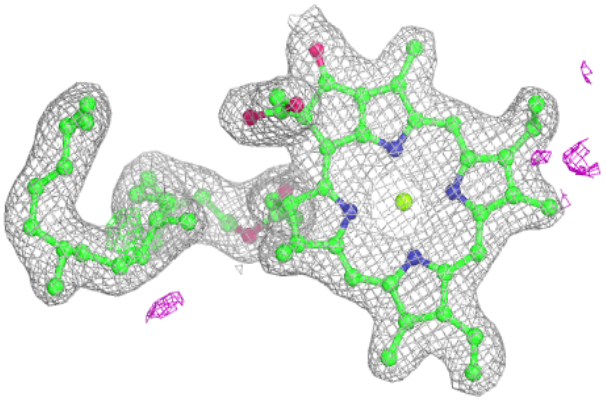


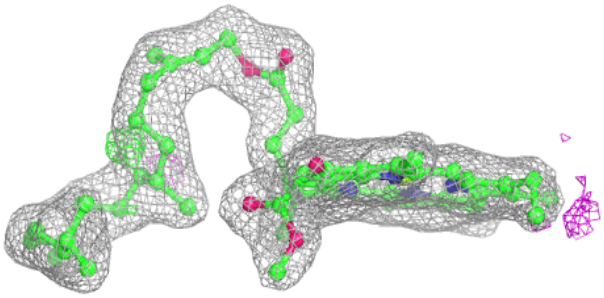


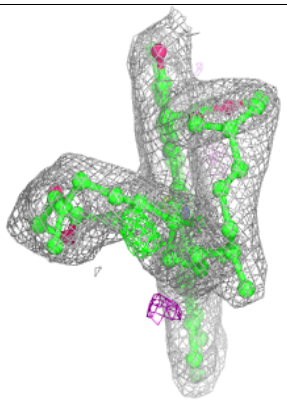


Electron density around CLA b 616:

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

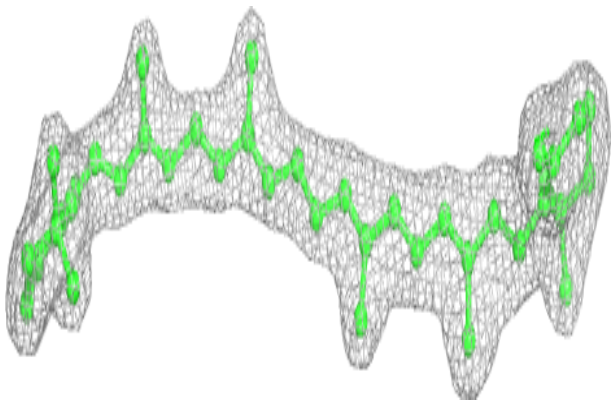


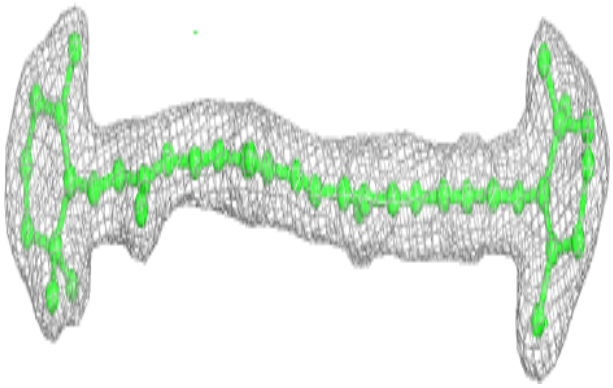


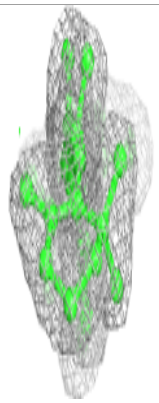


Electron density around BCR a 410:

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

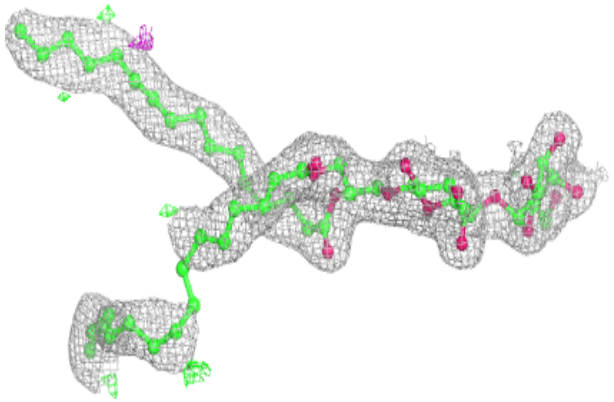


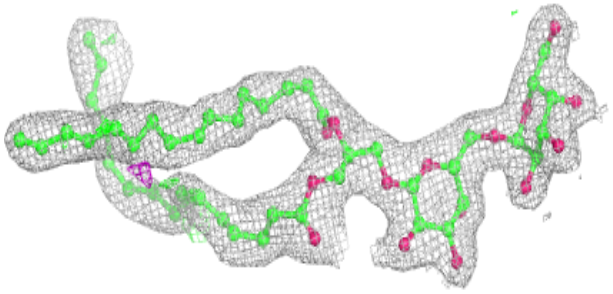


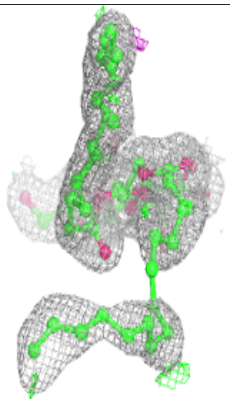


Electron density around DGD C 515:

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

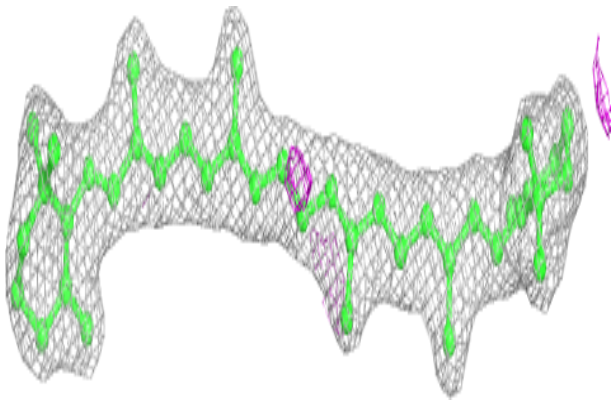


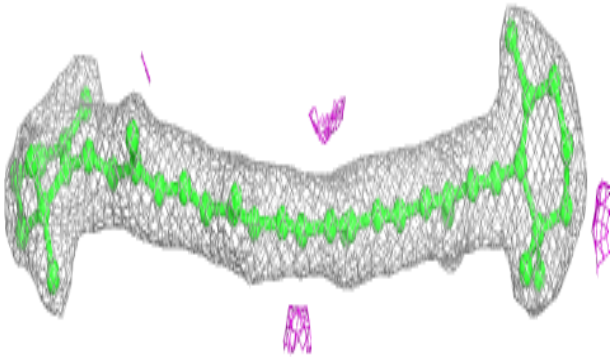


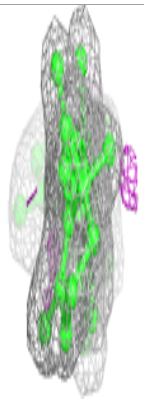


Electron density around BCR b 621:

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

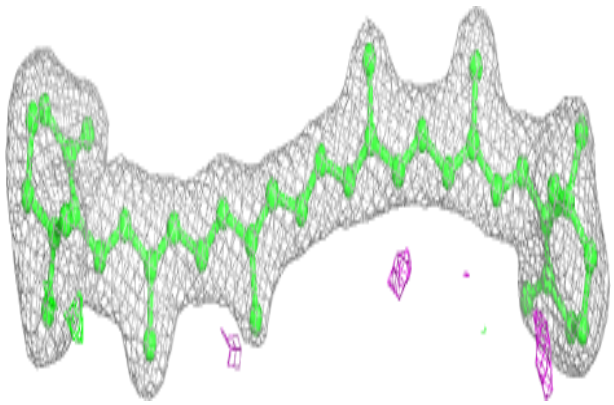


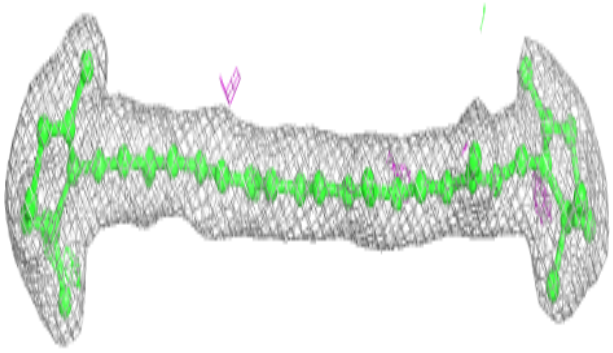


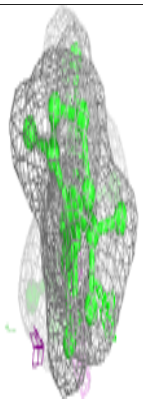


Electron density around BCR b 622:

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

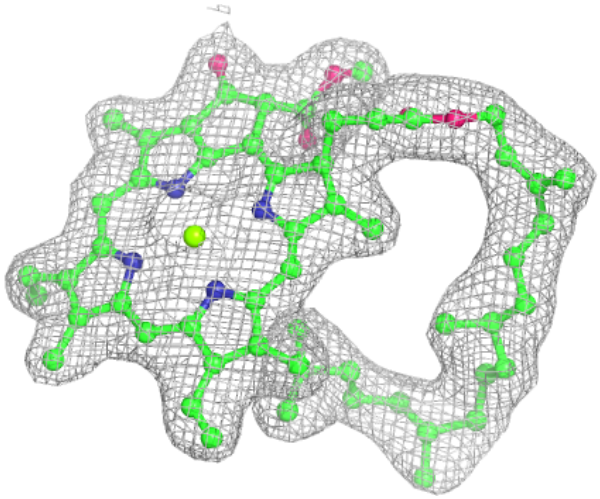


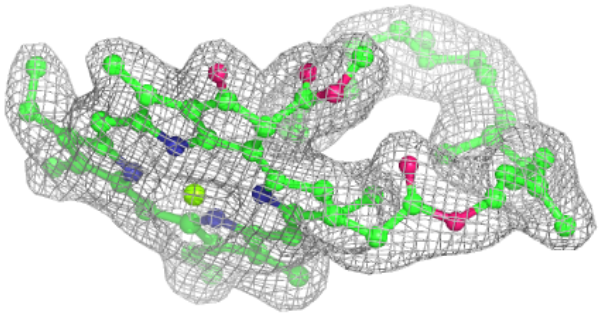


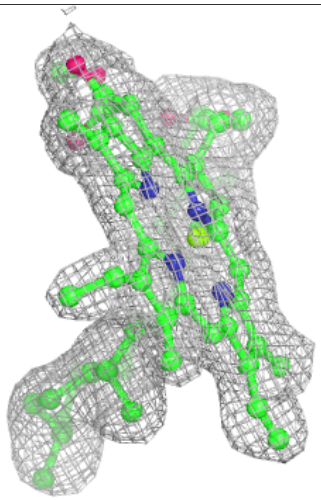


Electron density around CLA b 619:

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

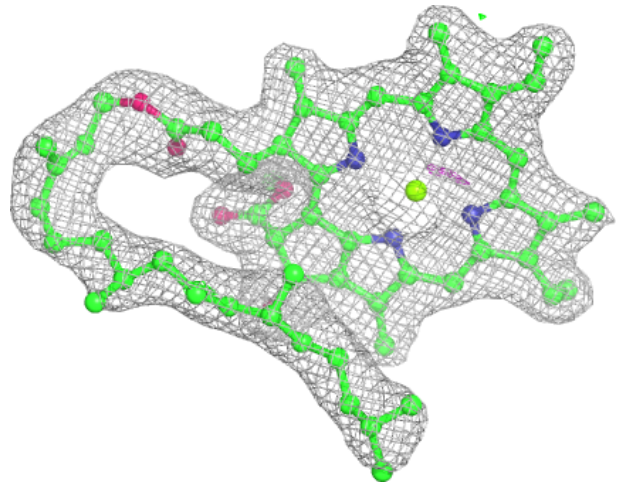


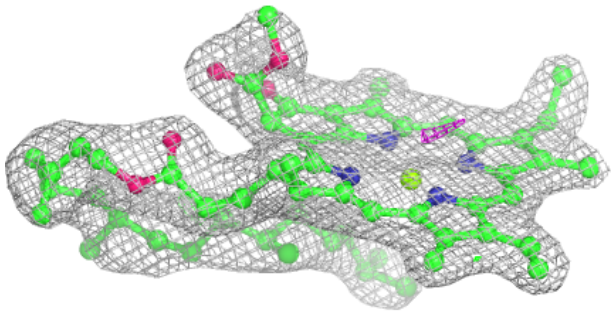


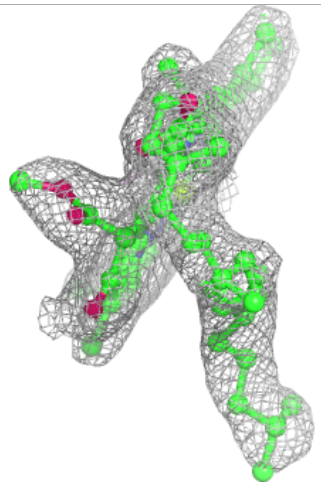


Electron density around CLA C 509:

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

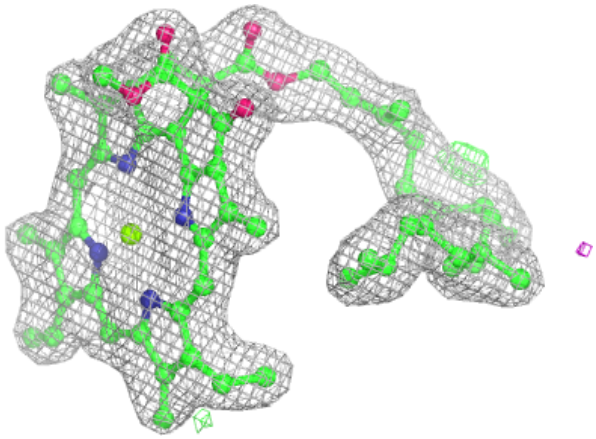


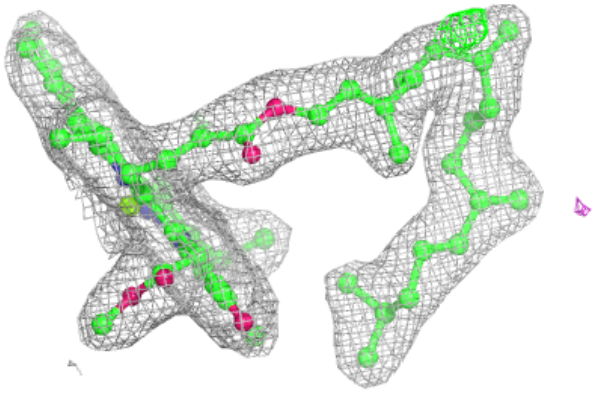


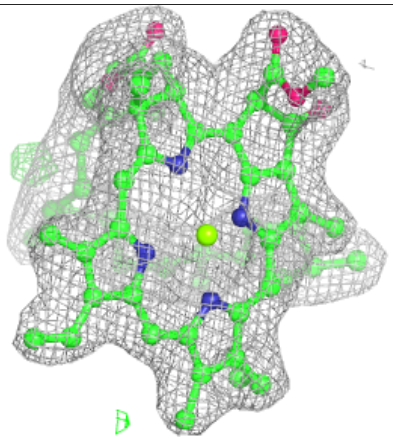


Electron density around CLA c 504:

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

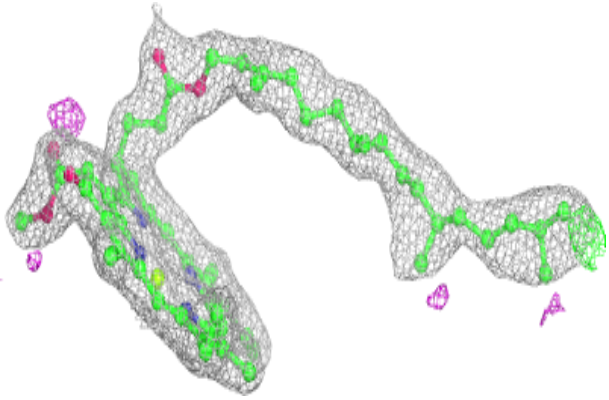


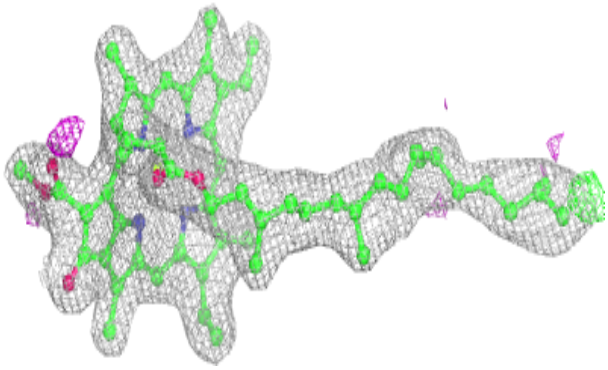


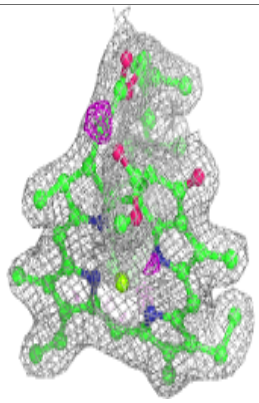


Electron density around CLA c 505:

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

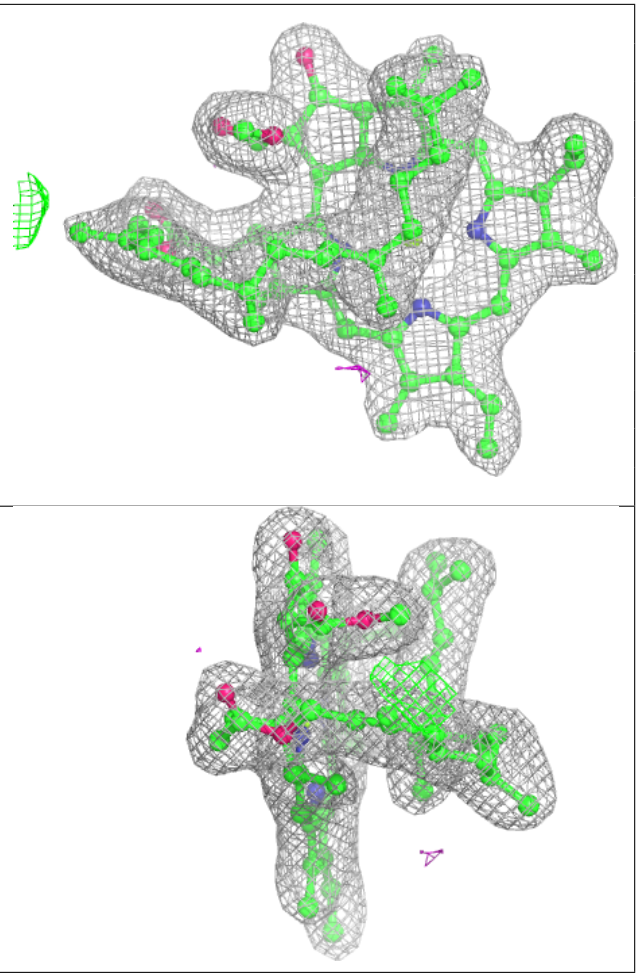






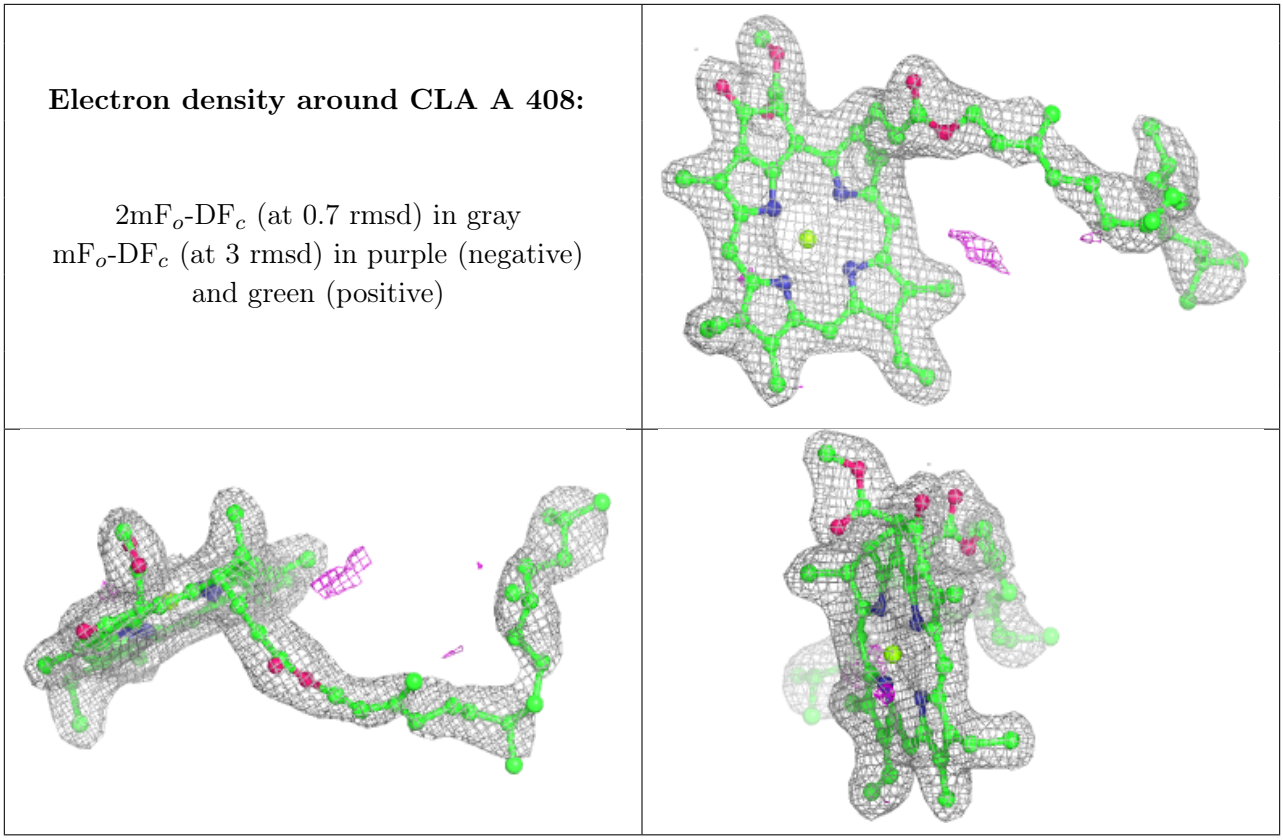
Electron density around CLA C 510:

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



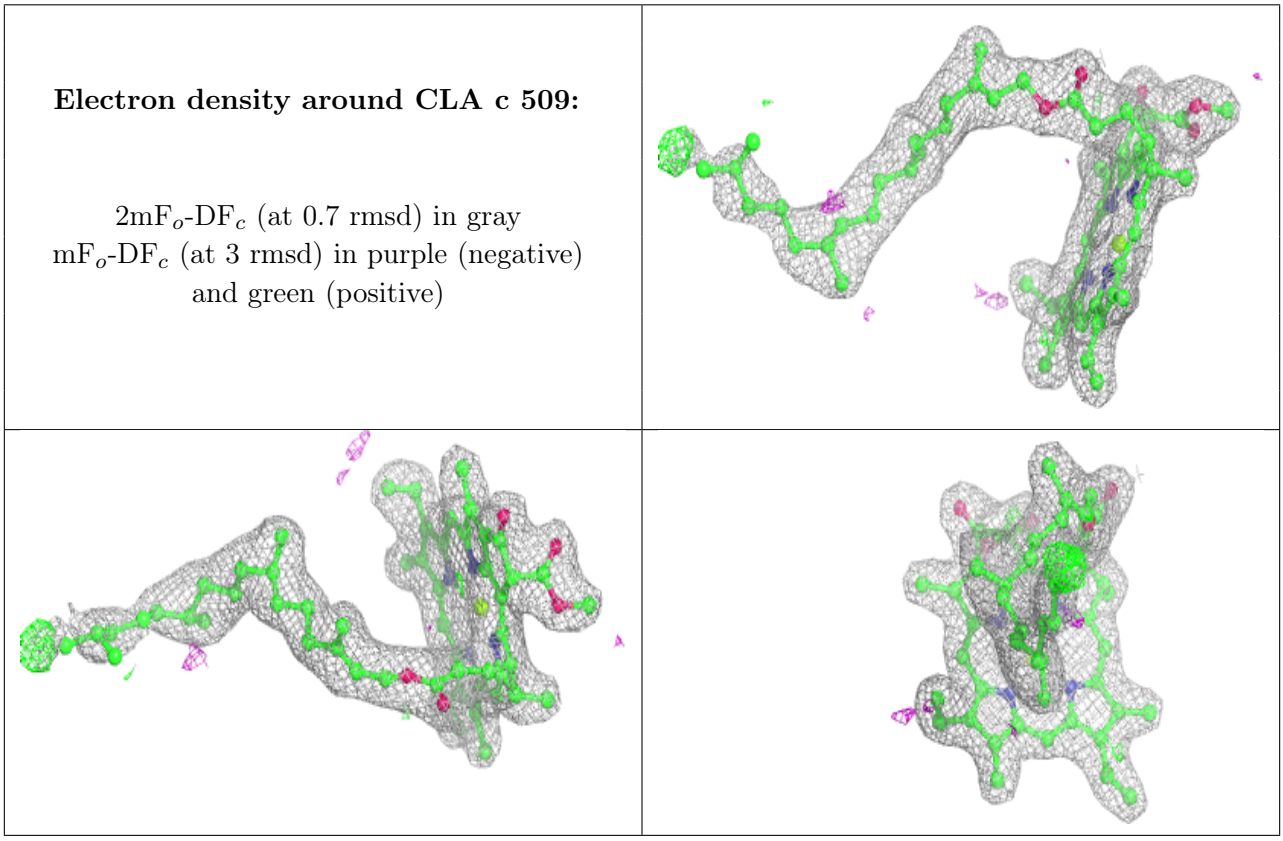
Electron density around CLA A 408:

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



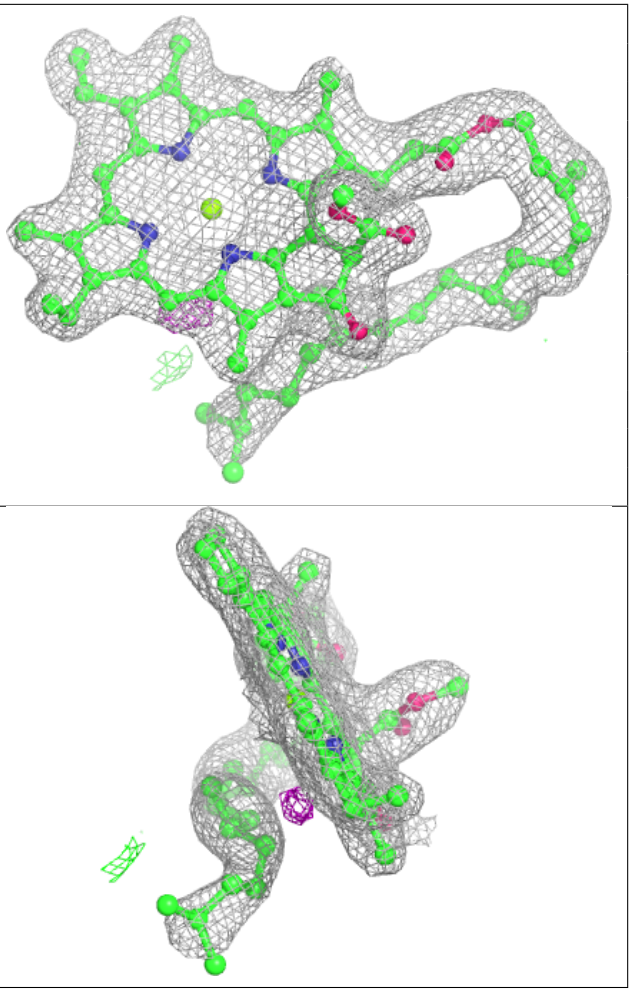
Electron density around CLA c 509:

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



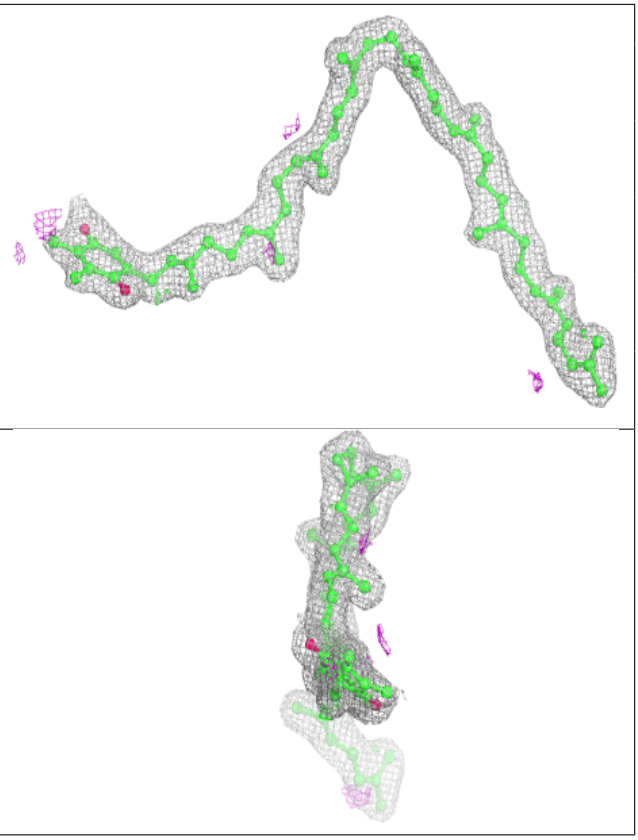
Electron density around CLA c 510:

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



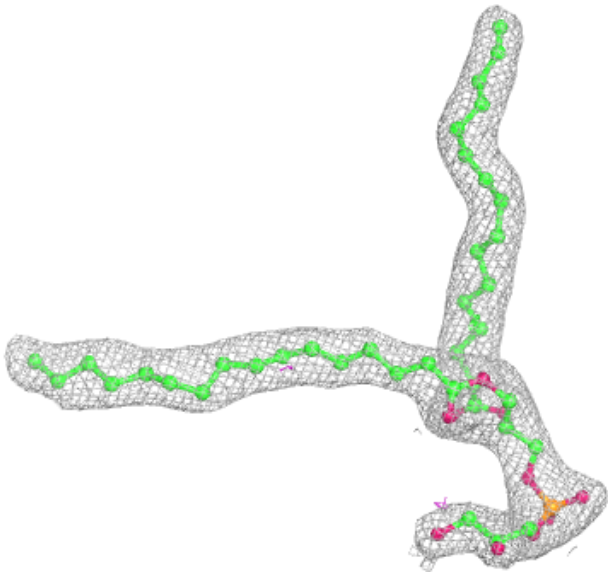
Electron density around PL9 d 407:

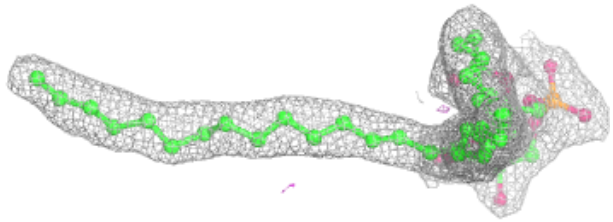
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

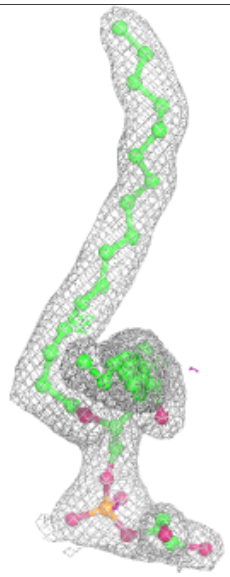


Electron density around LHG b 624:

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

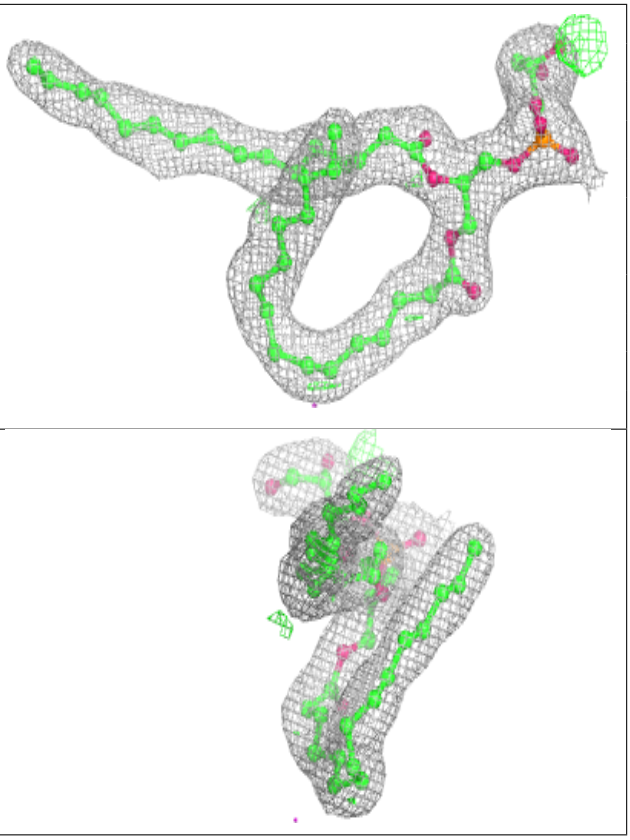






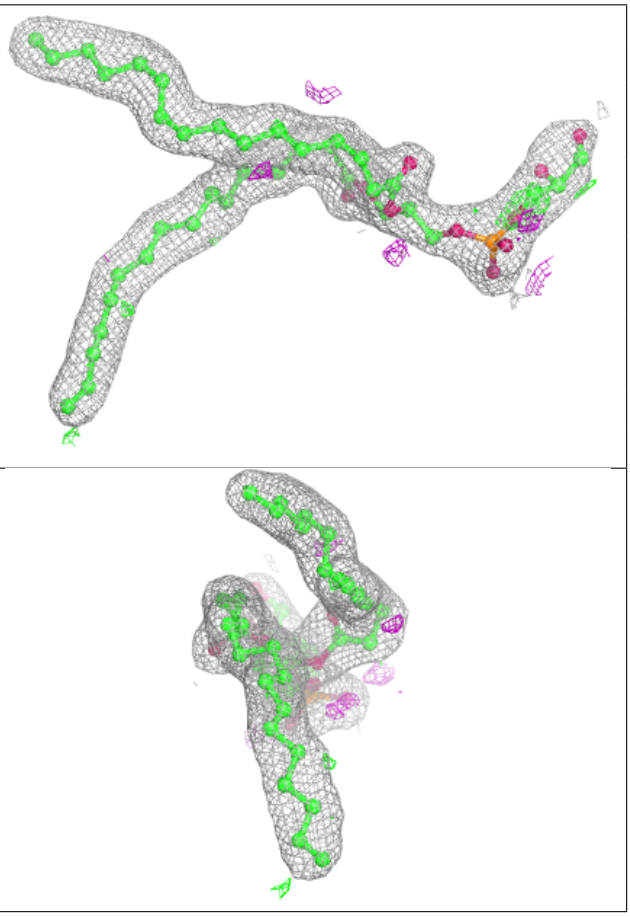
Electron density around LHG d 409:

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



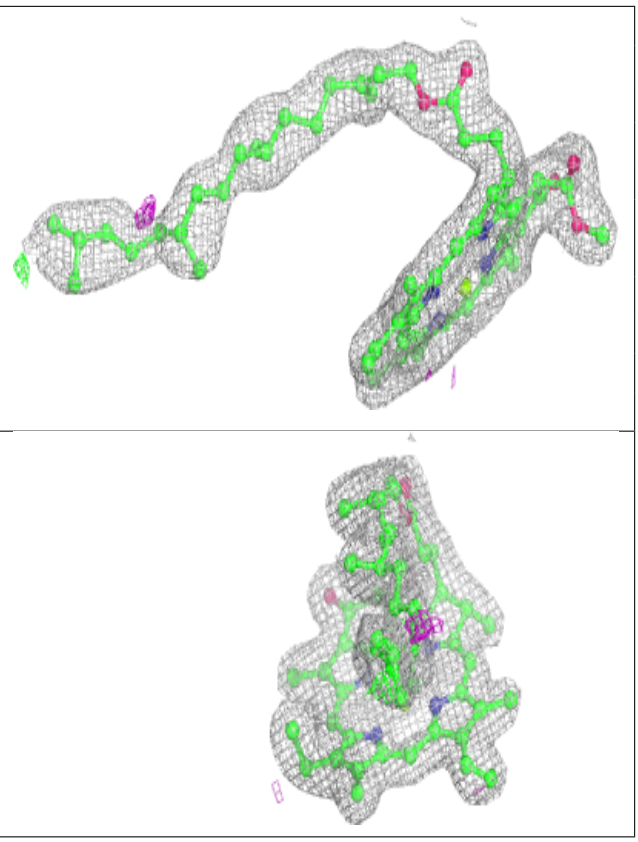
Electron density around LHG d 410:

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



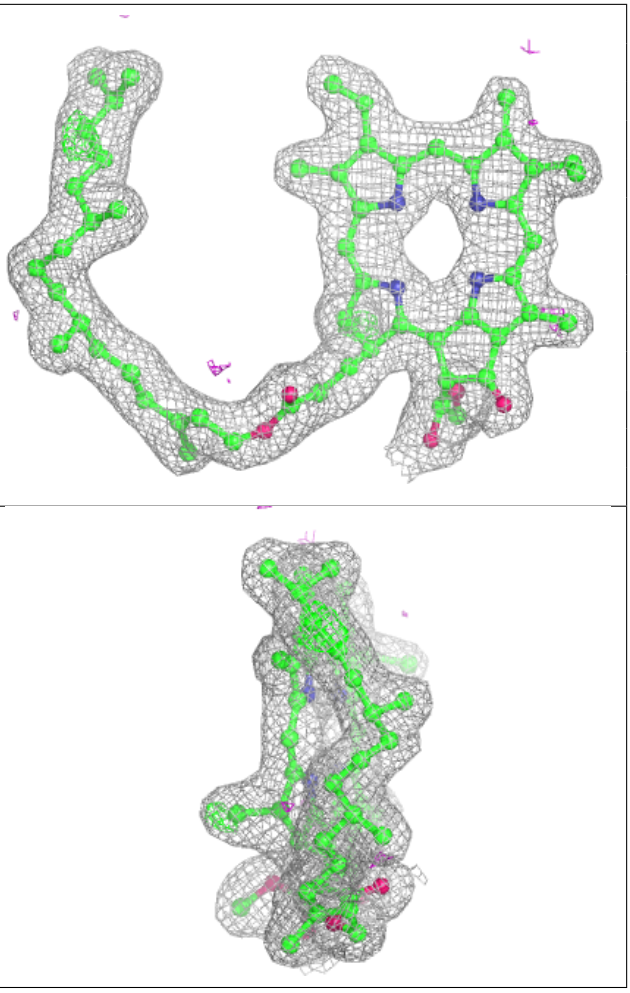
Electron density around CLA C 504:

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



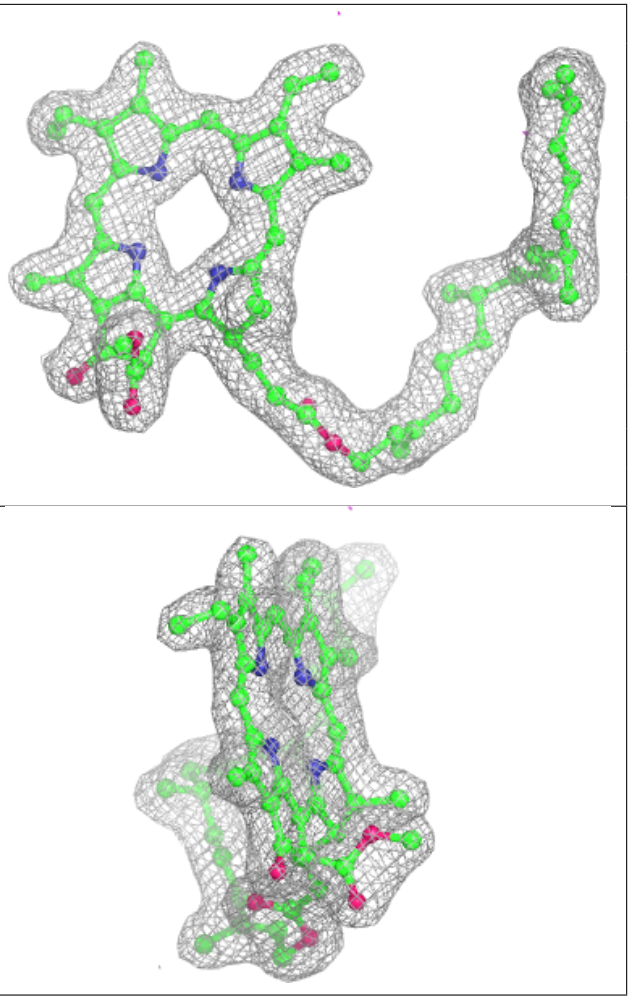
Electron density around PHO A 407:

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



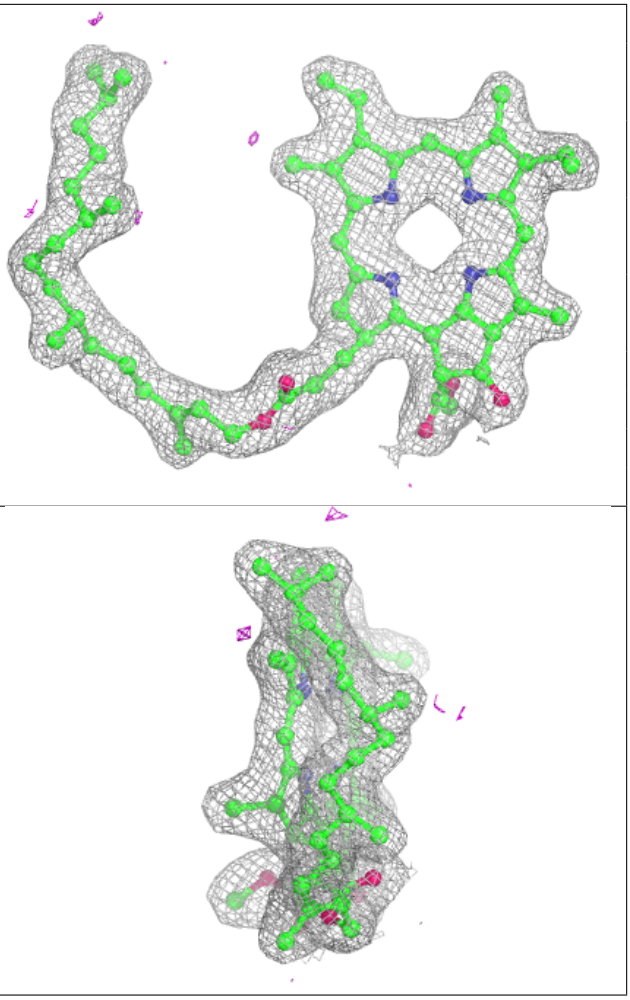
Electron density around PHO D 404:

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



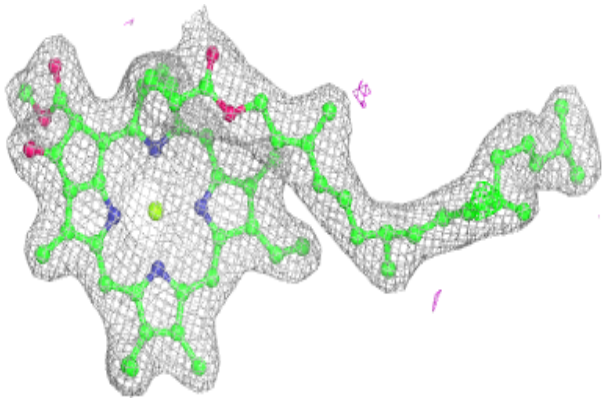
Electron density around PHO a 408:

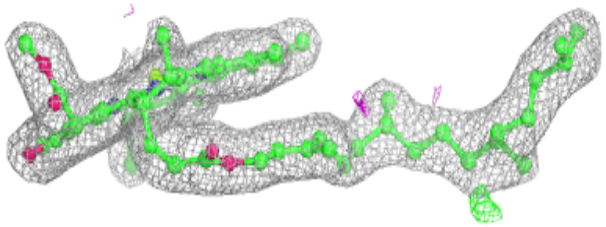
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

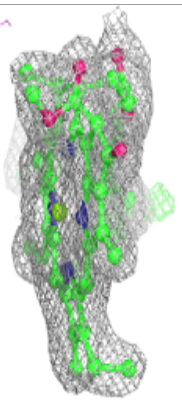


Electron density around CLA b 607:

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

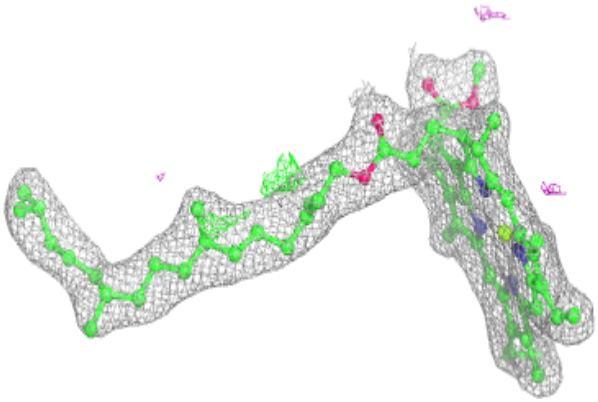


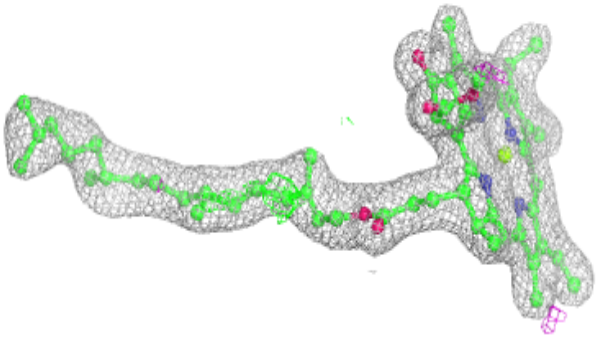




Electron density around CLA b 608:

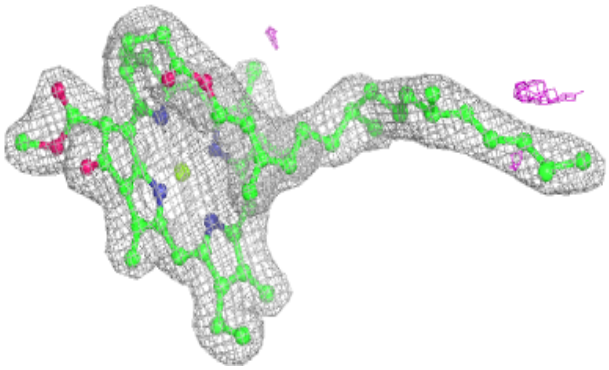
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

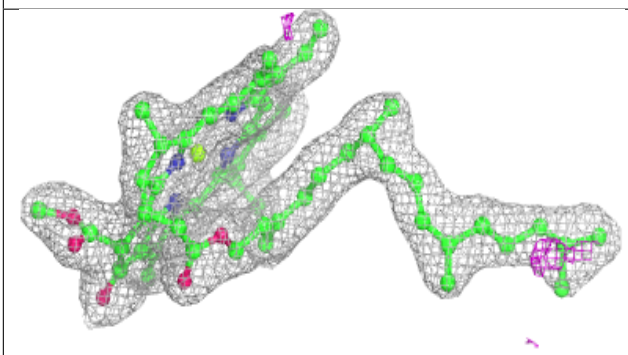


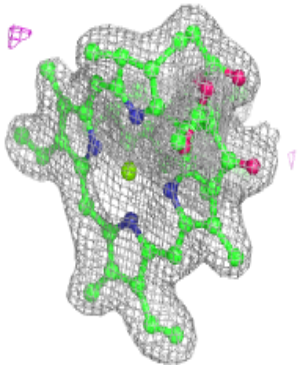


Electron density around CLA C 505:

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

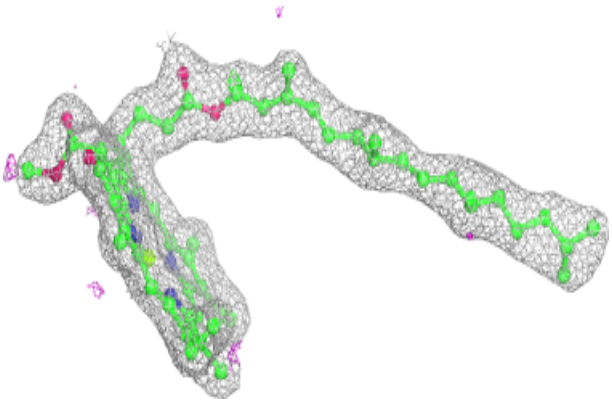


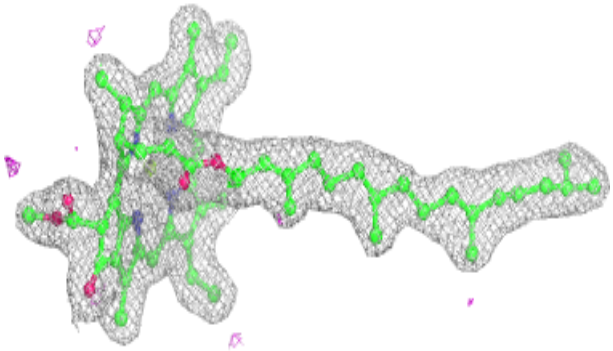


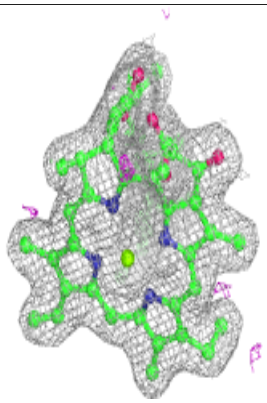


Electron density around CLA B 608:

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

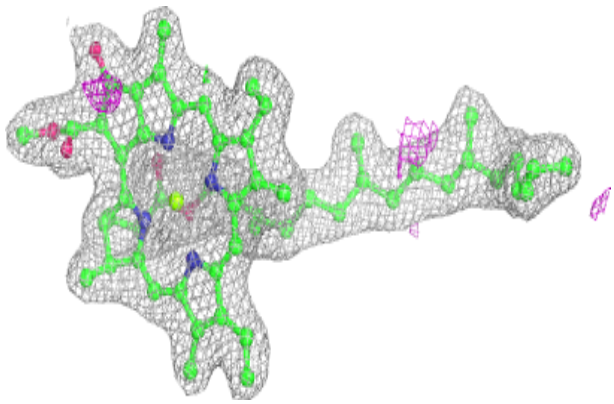


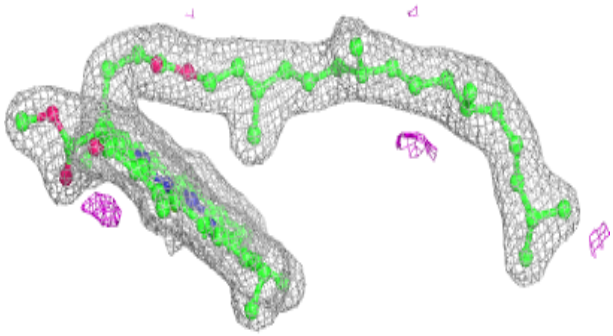


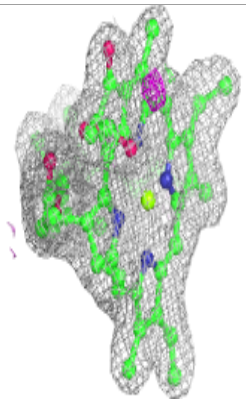


Electron density around CLA b 612:

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

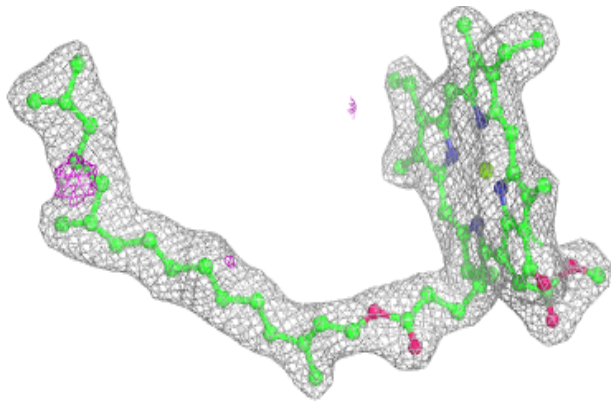


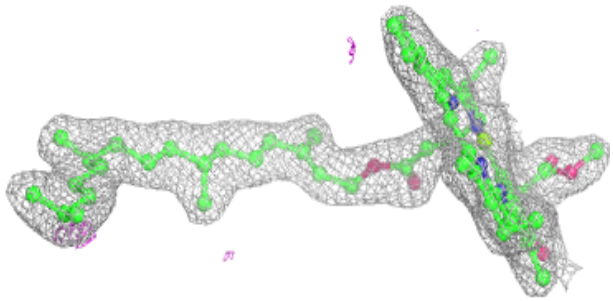


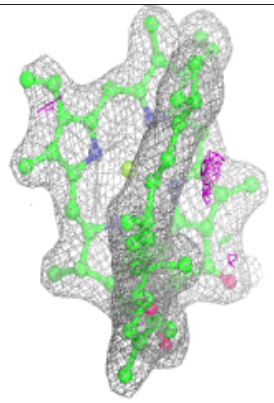


Electron density around CLA b 613:

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

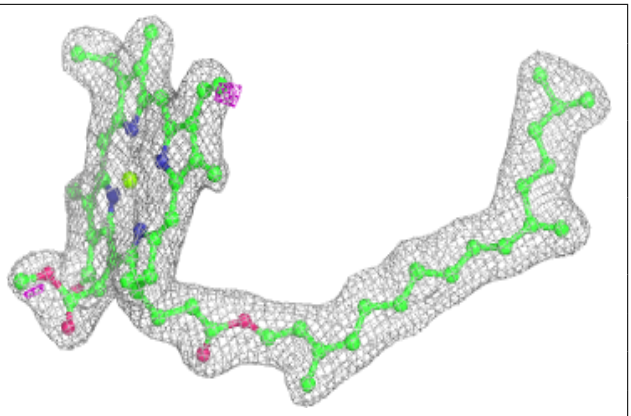


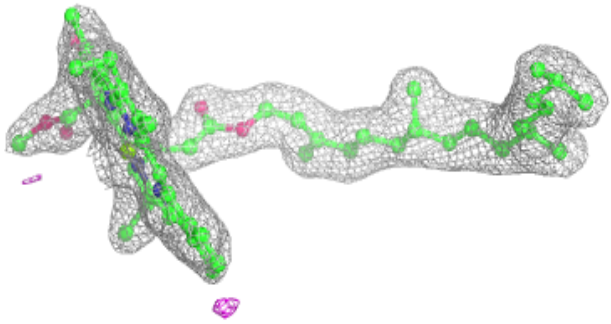


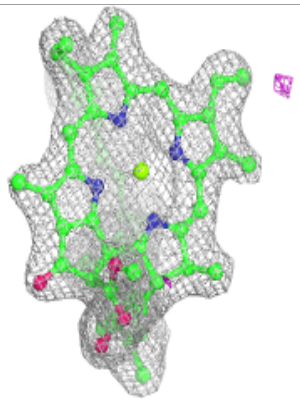


Electron density around CLA B 610:

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

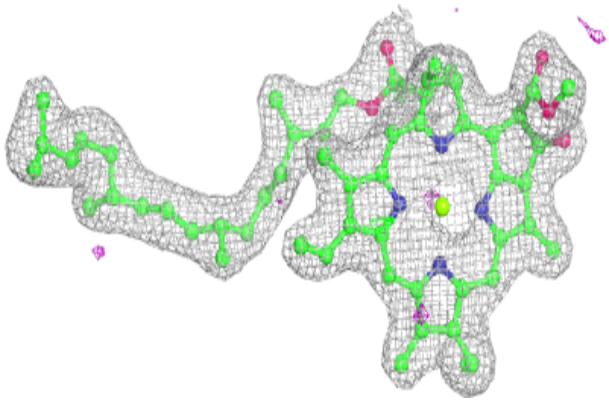


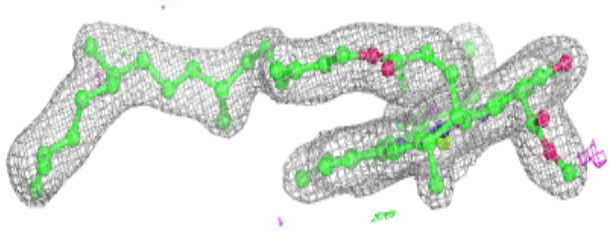


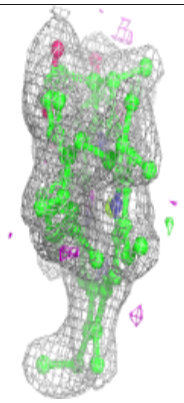


Electron density around CLA B 604:

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

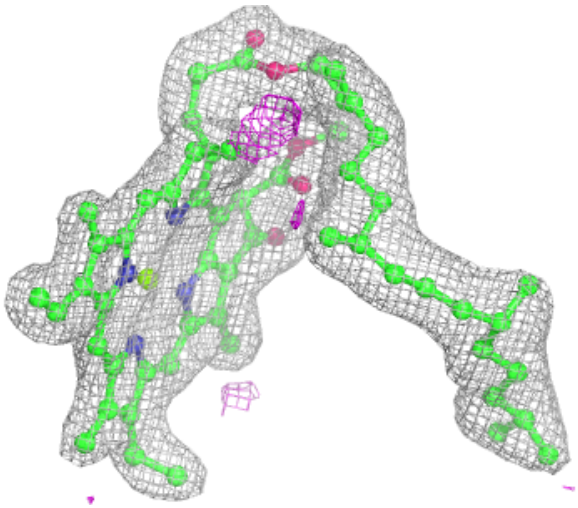


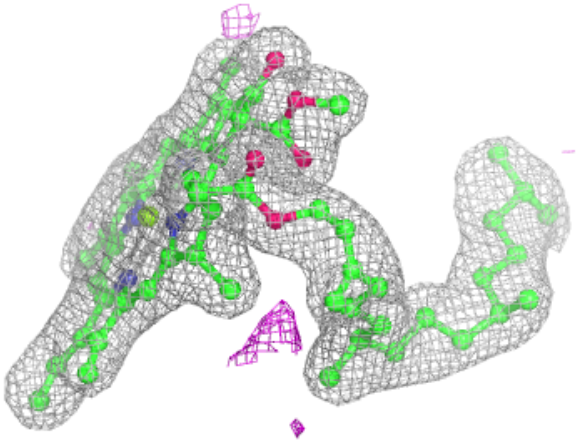


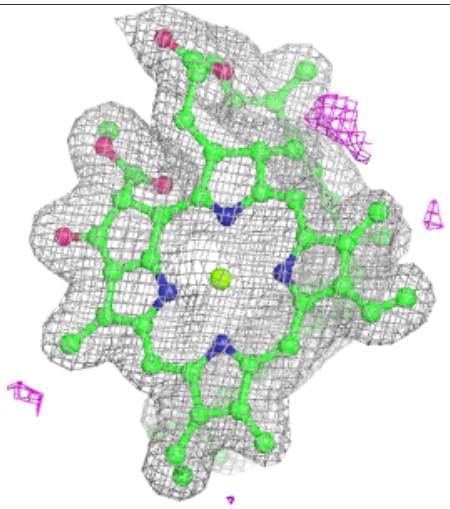


Electron density around CLA b 617:

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

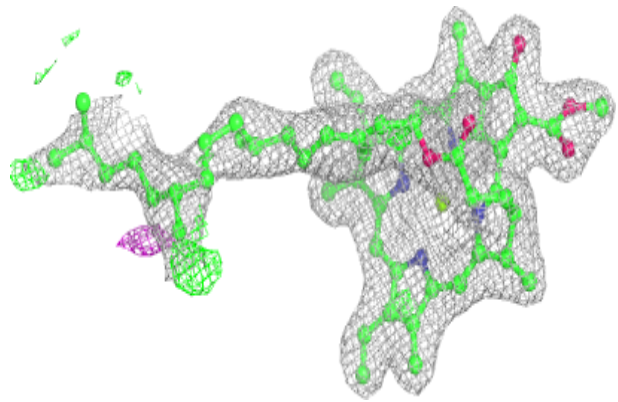


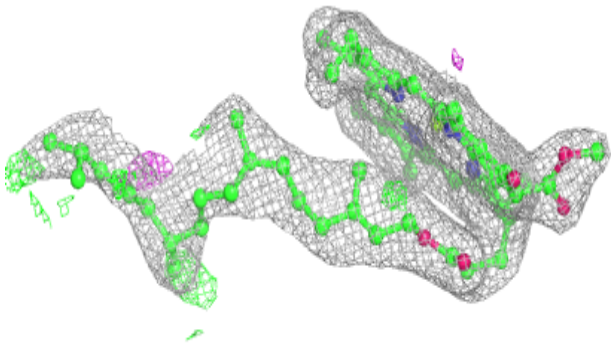


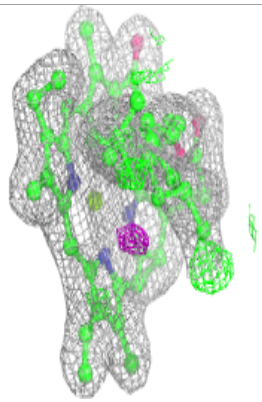


Electron density around CLA b 618:

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

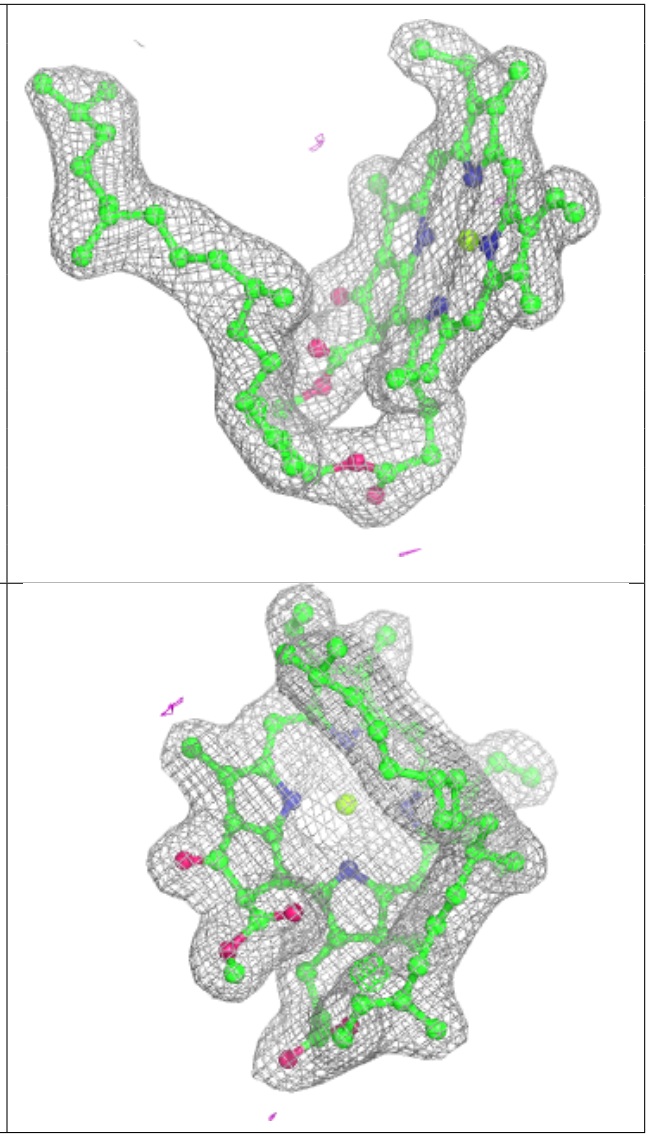






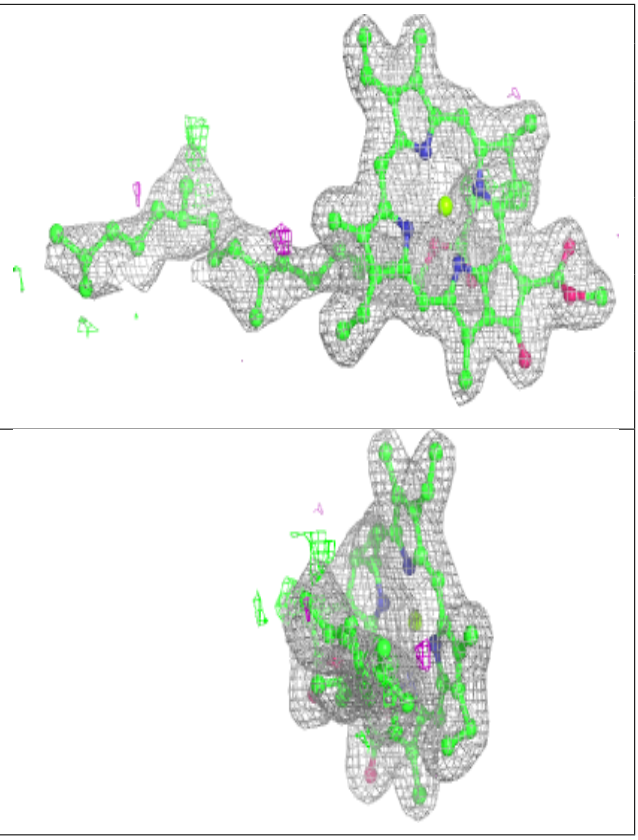
Electron density around CLA B 614:

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



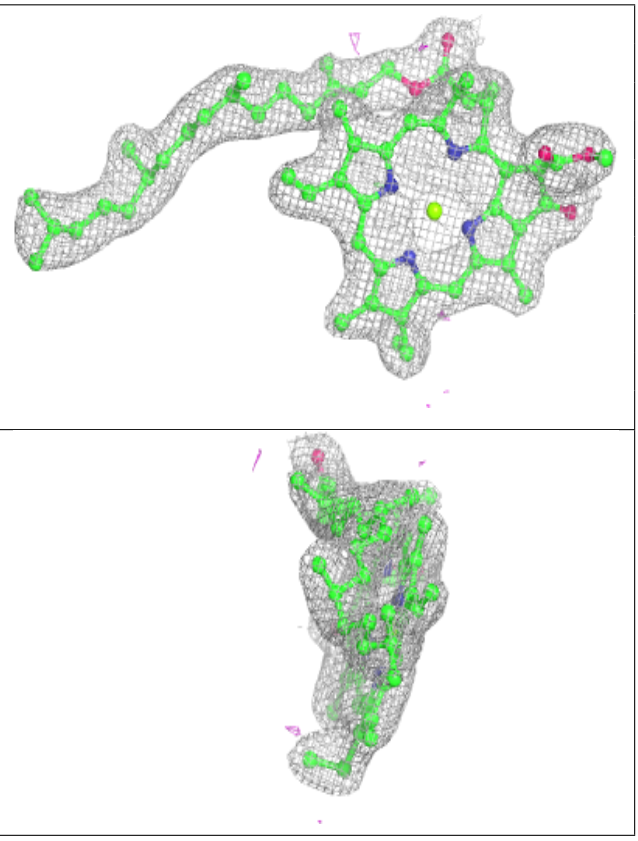
Electron density around CLA B 615:

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



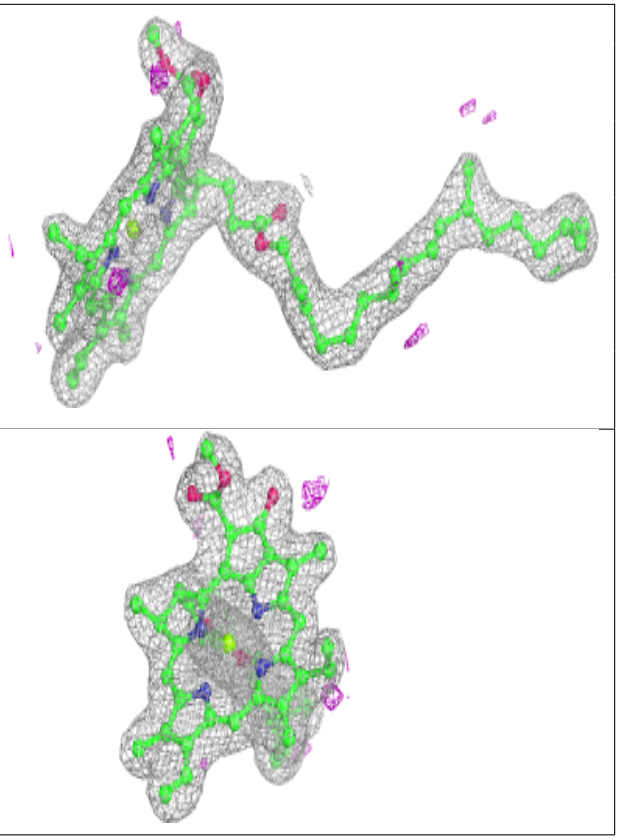
Electron density around CLA c 502:

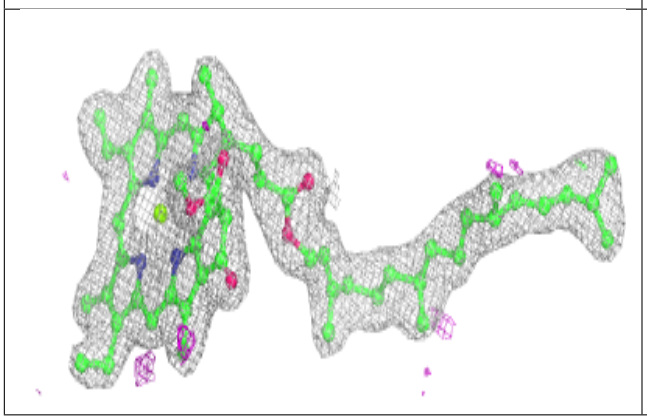
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 503:

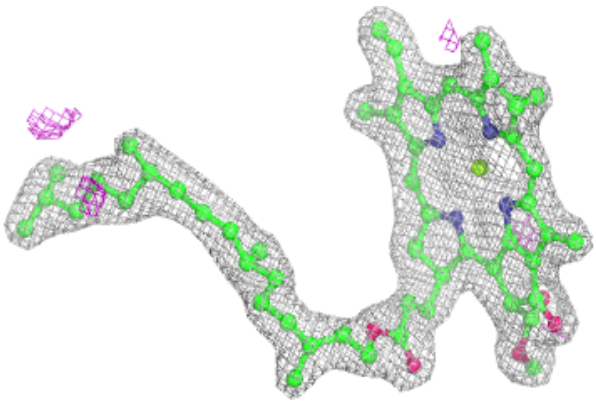
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

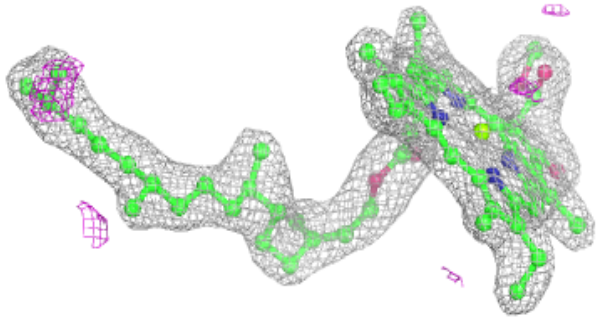


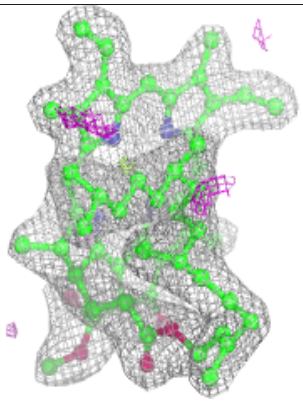


Electron density around CLA C 511:

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

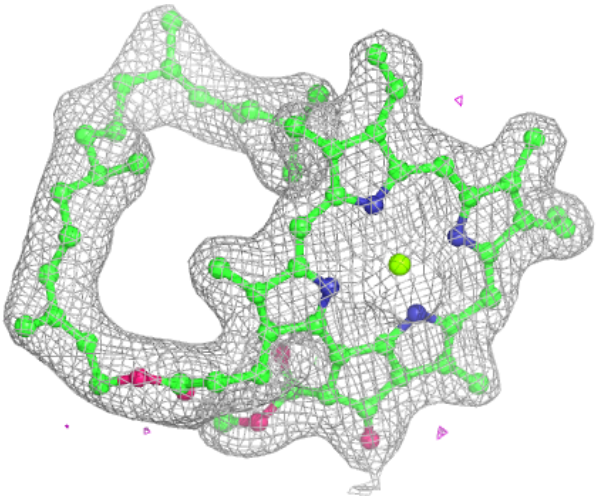


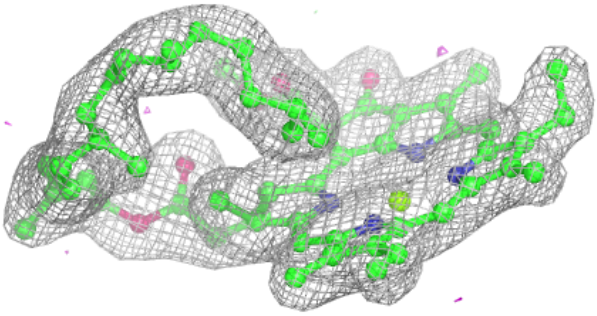


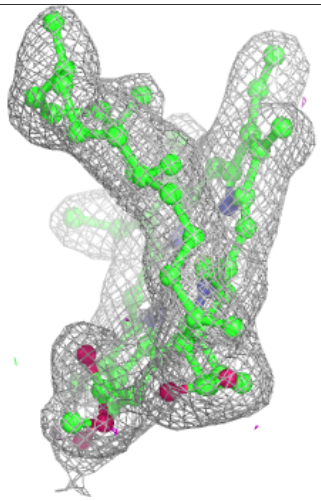


Electron density around CLA B 616:

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

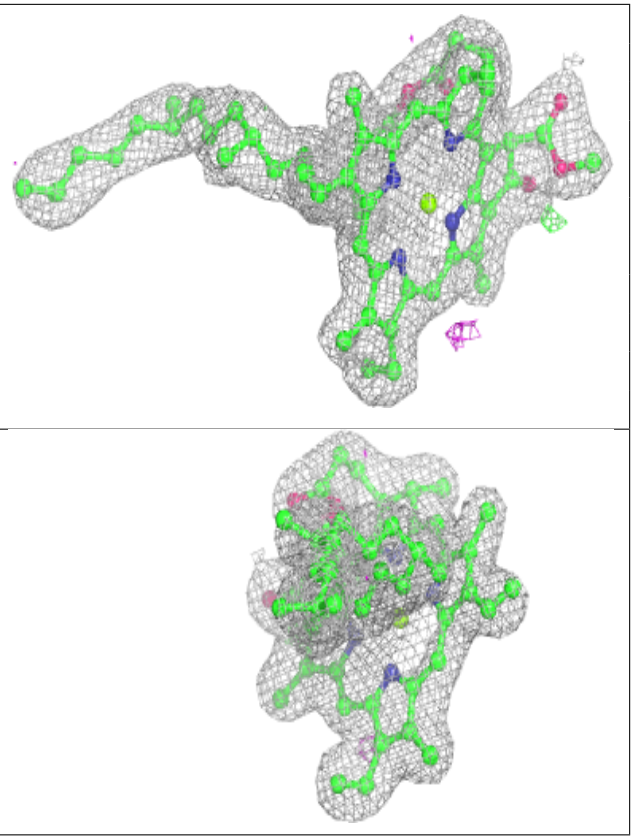






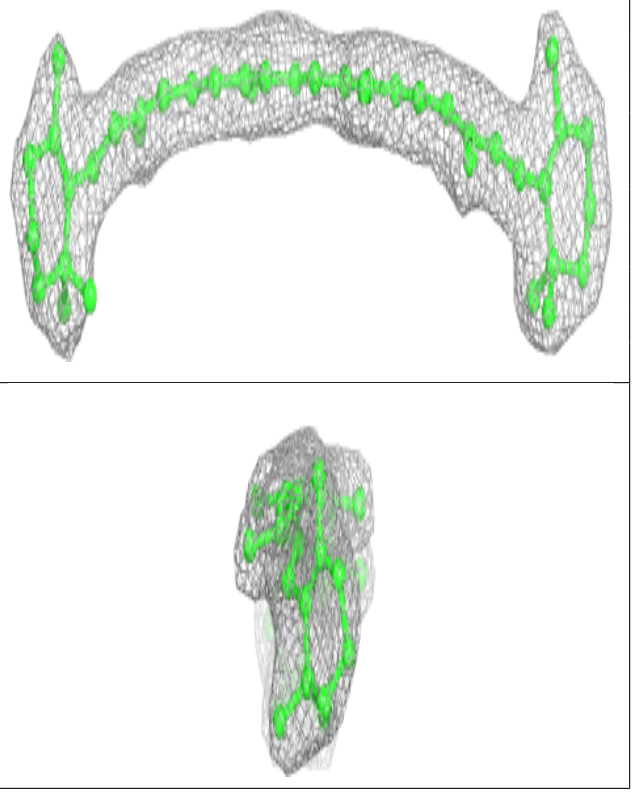
Electron density around CLA c 506:

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



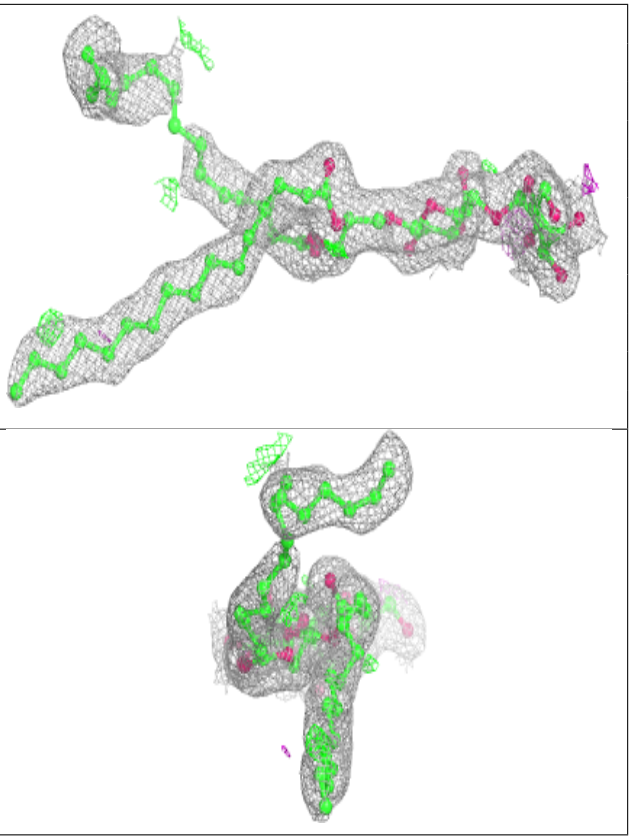
Electron density around BCR k 101:

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



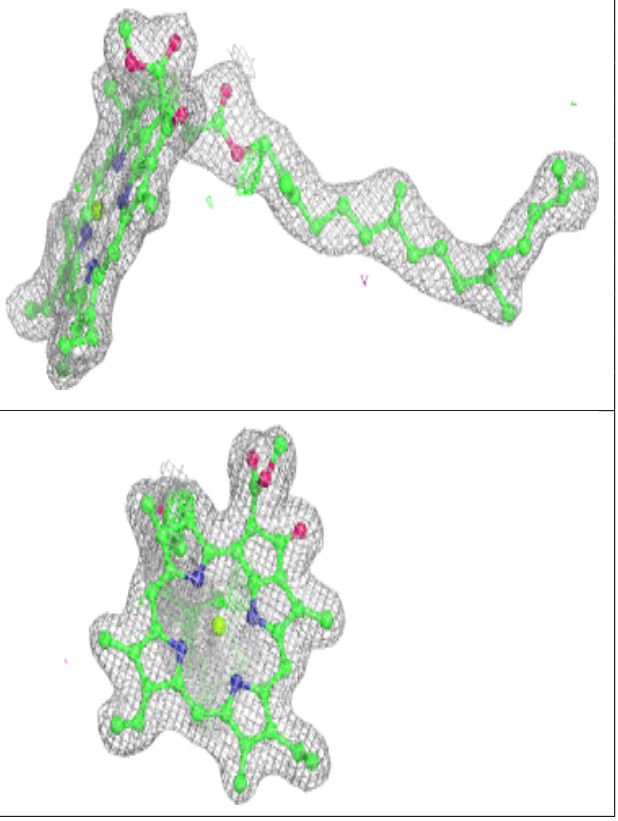
Electron density around DGD c 517:

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



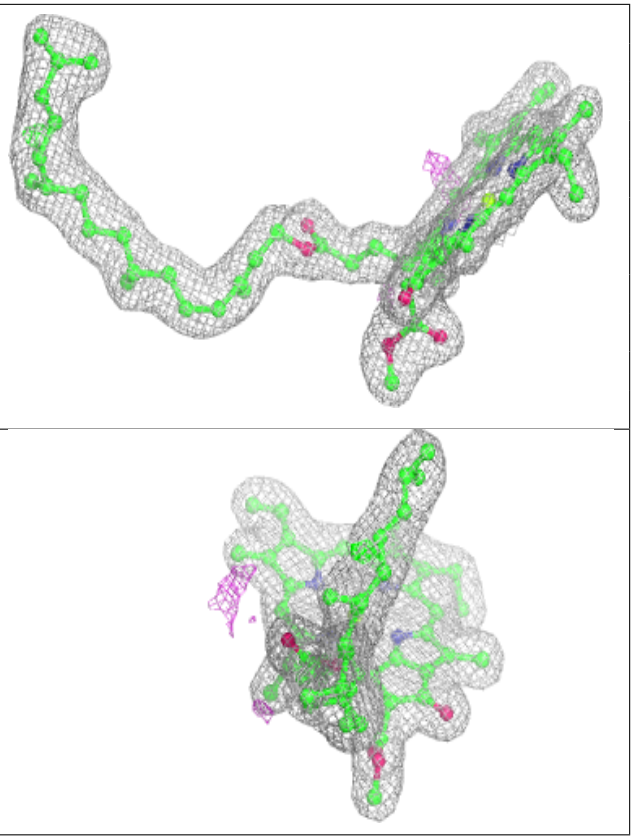
Electron density around CLA B 605:

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



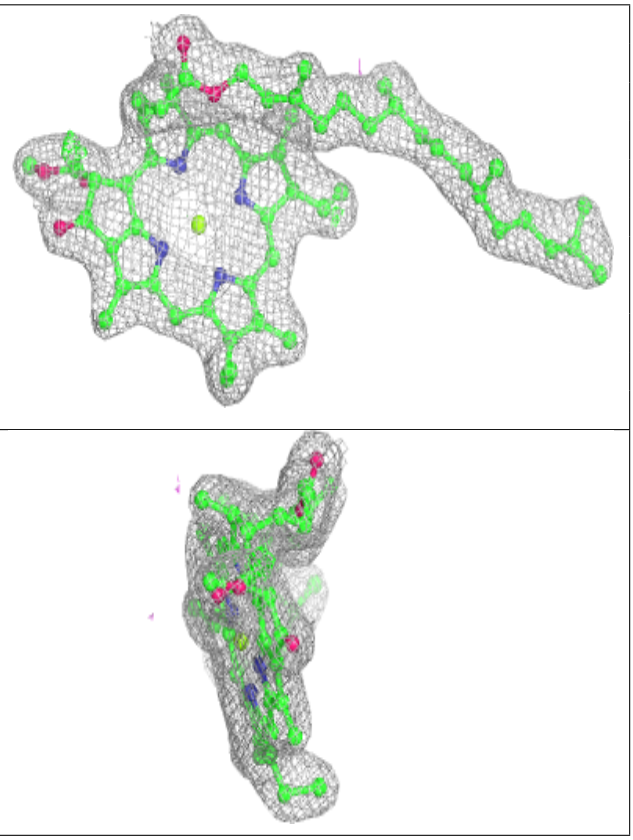
Electron density around CLA D 403:

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



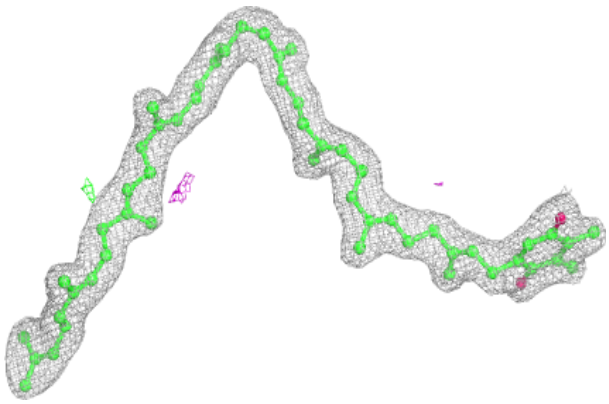
Electron density around CLA C 501:

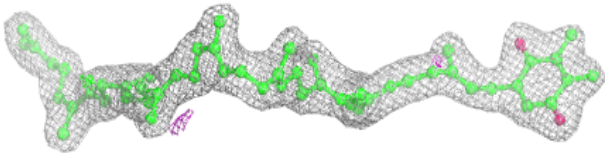
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

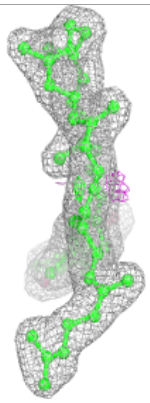


Electron density around PL9 D 407:

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

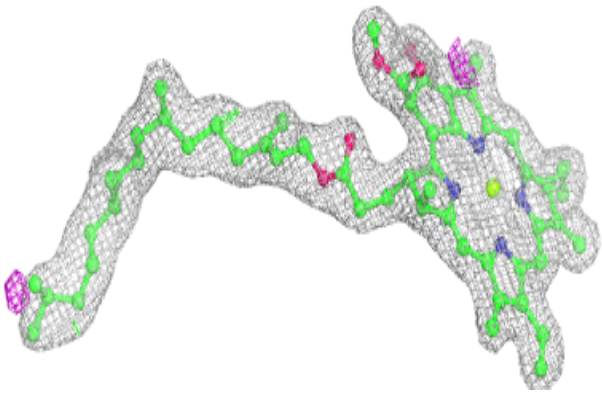


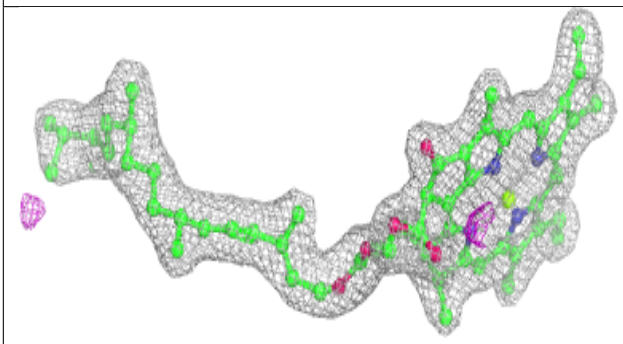


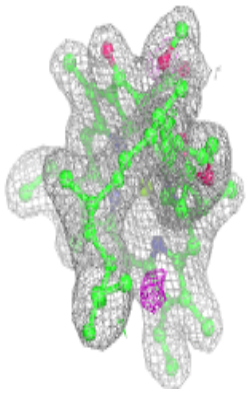


Electron density around CLA a 406:

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

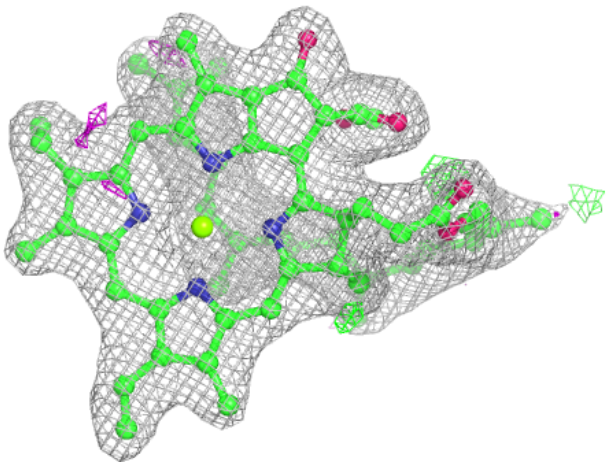


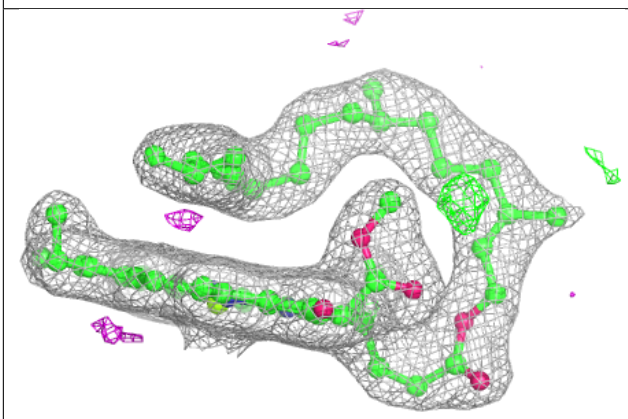


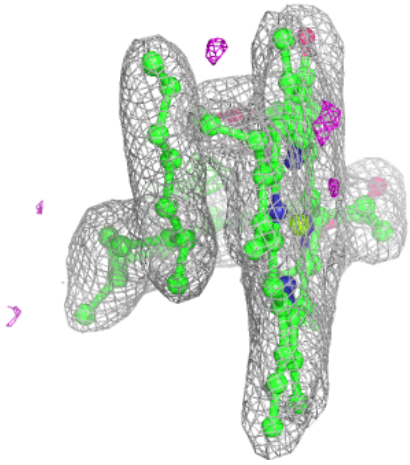


Electron density around CLA c 511:

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

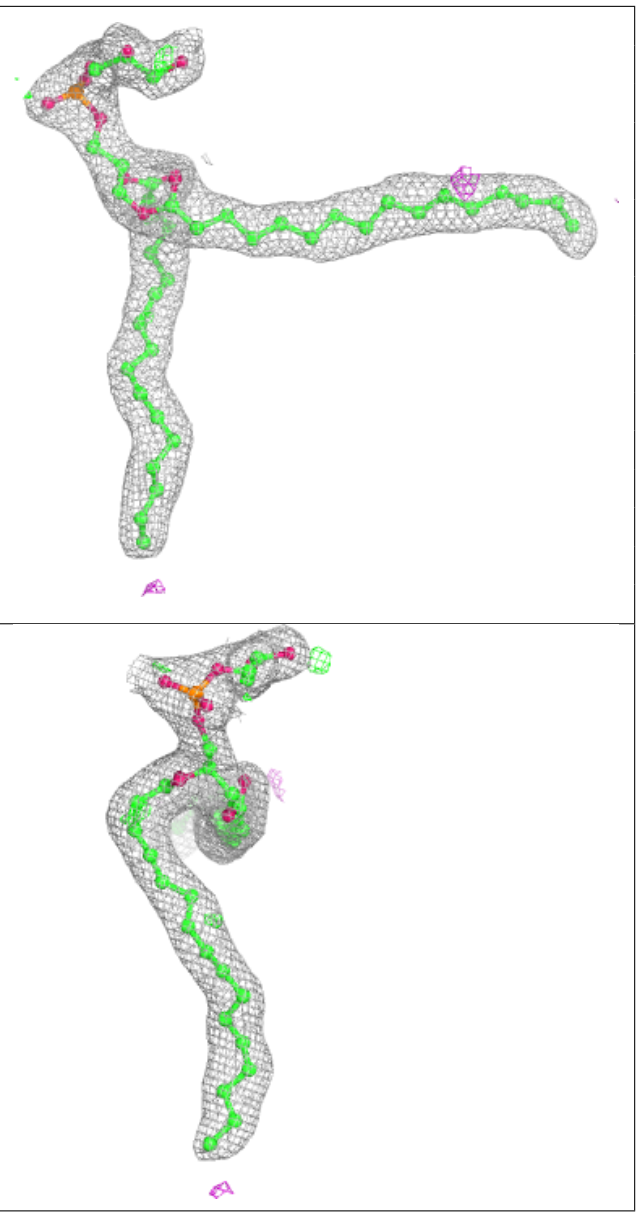


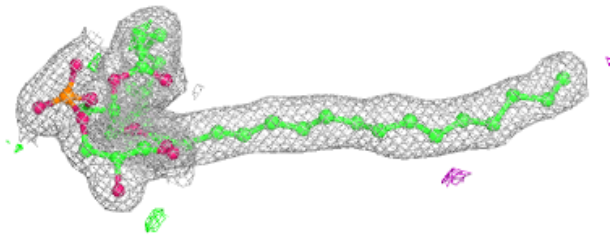




Electron density around LHG B 621:

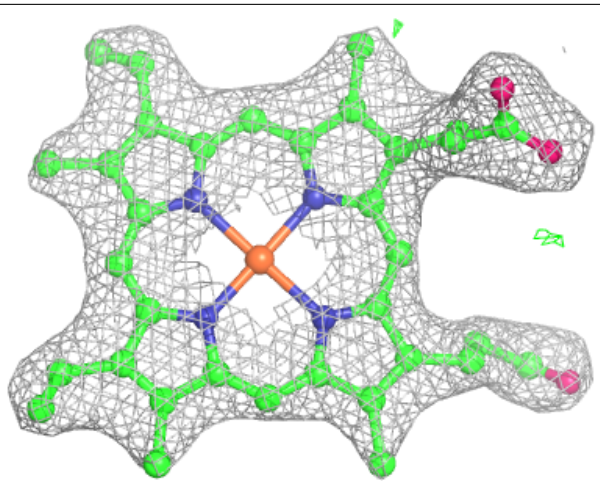
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

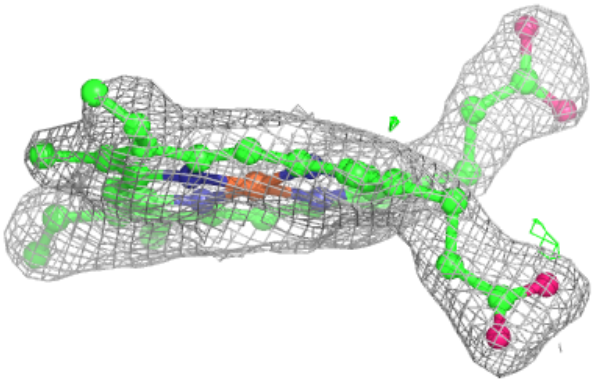


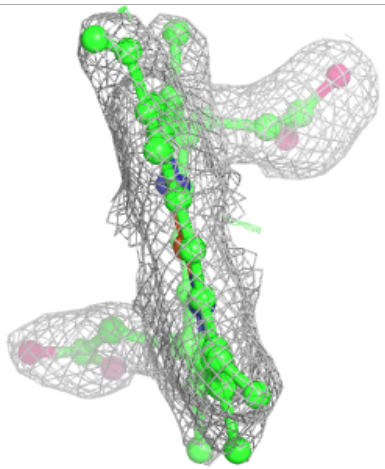


Electron density around HEM F 101:

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

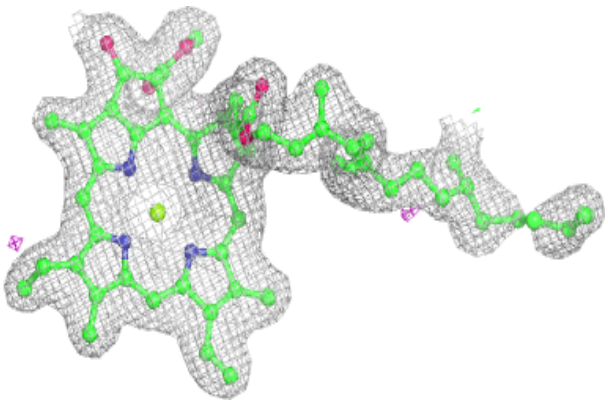


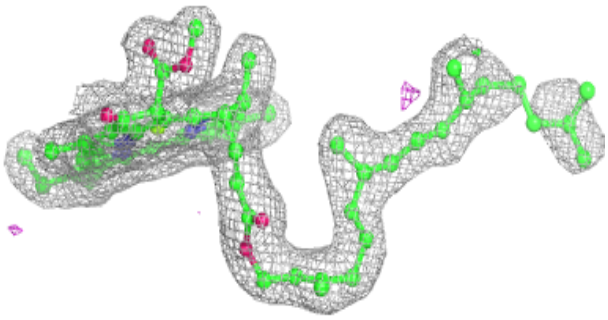


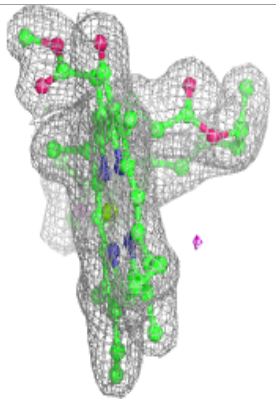


Electron density around CLA a 407:

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

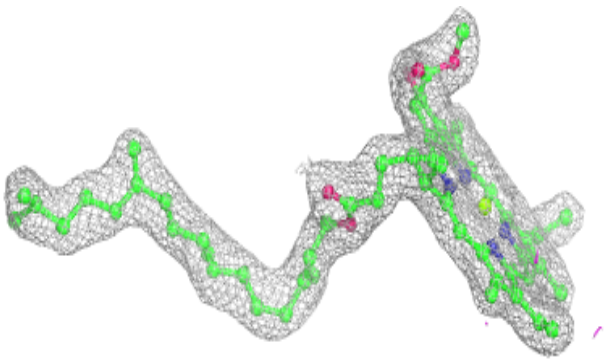


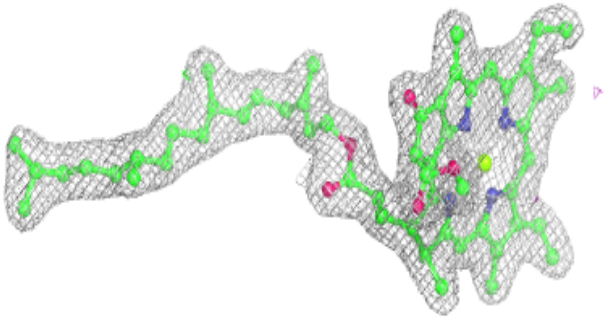


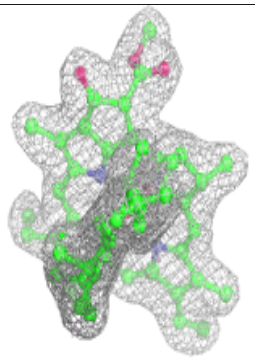


Electron density around CLA C 502:

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

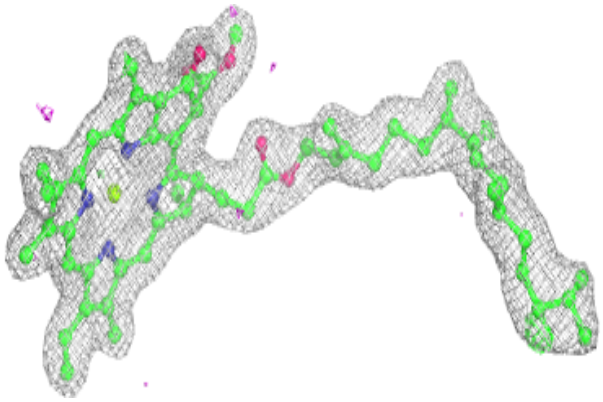


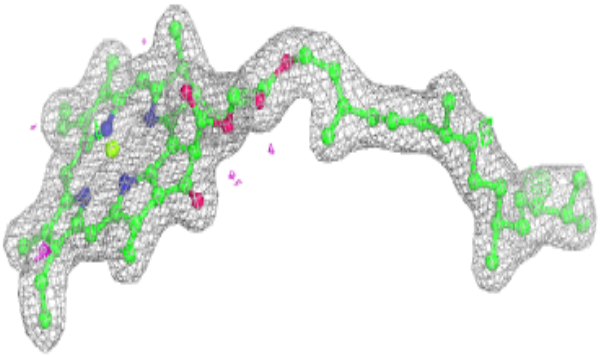


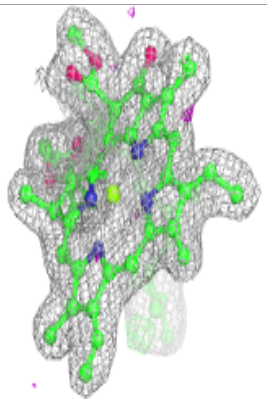


Electron density around CLA A 404:

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

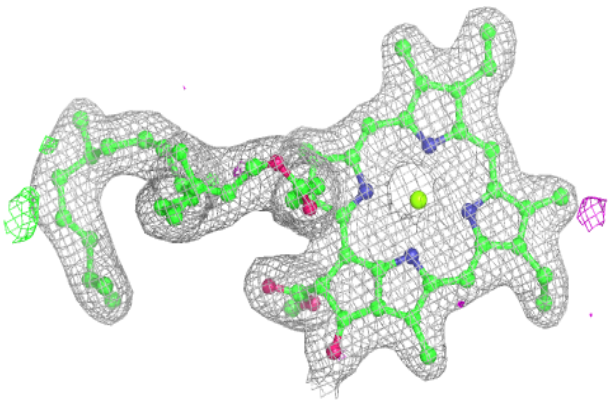


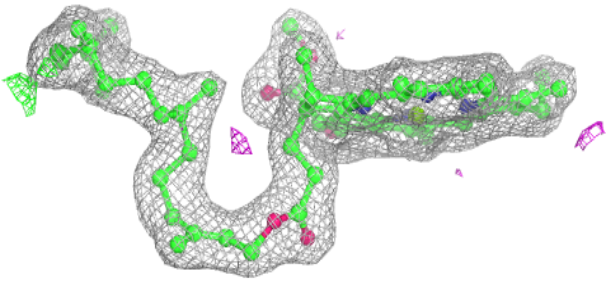


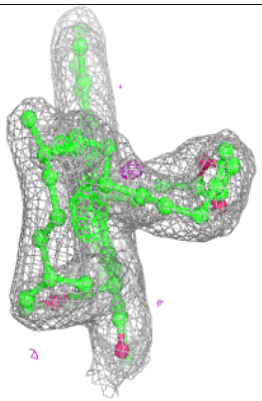


Electron density around CLA B 613:

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

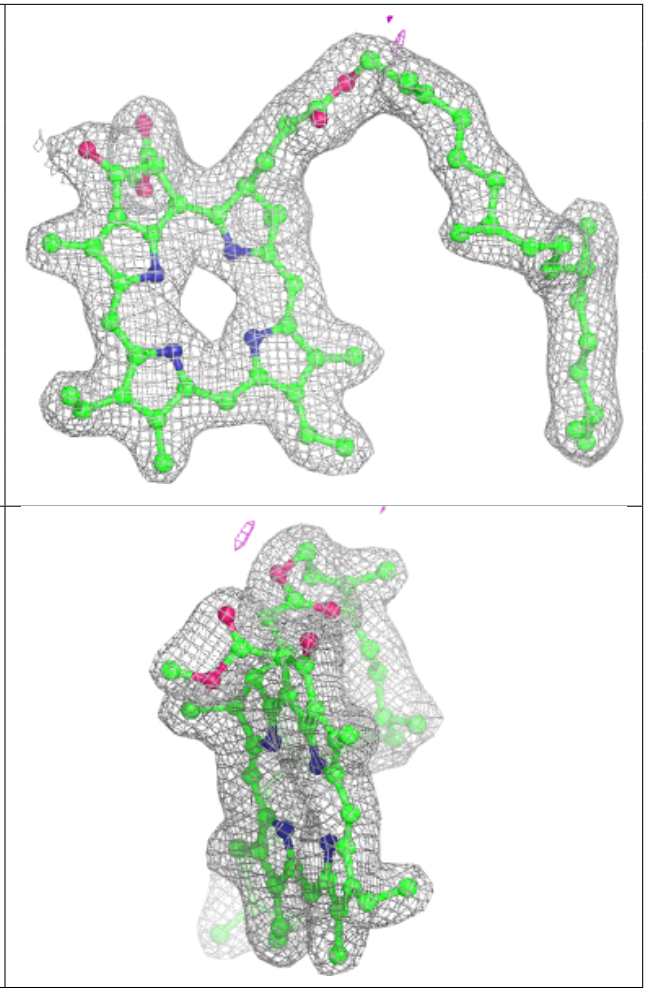






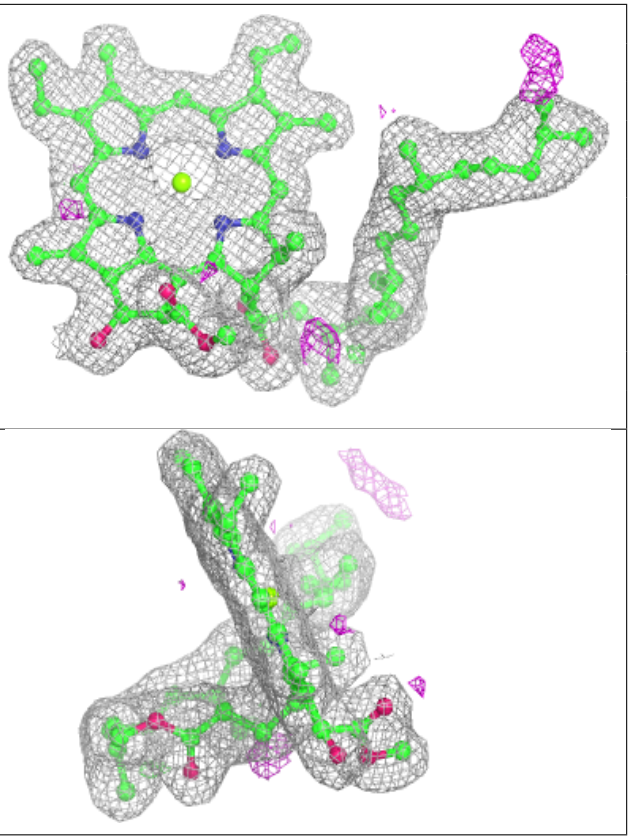
Electron density around PHO d 404:

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



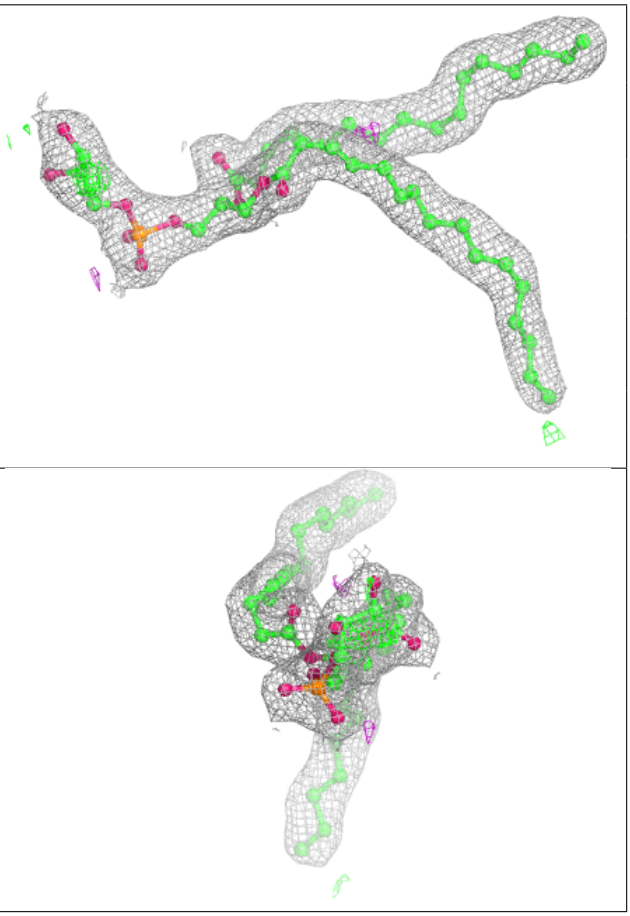
Electron density around CLA A 405:

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



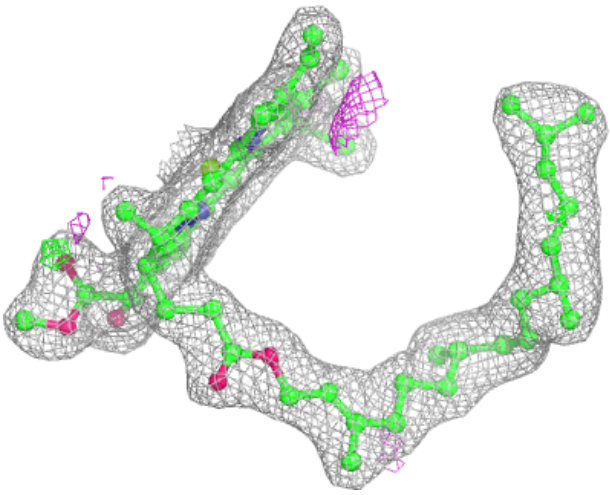
Electron density around LHG D 410:

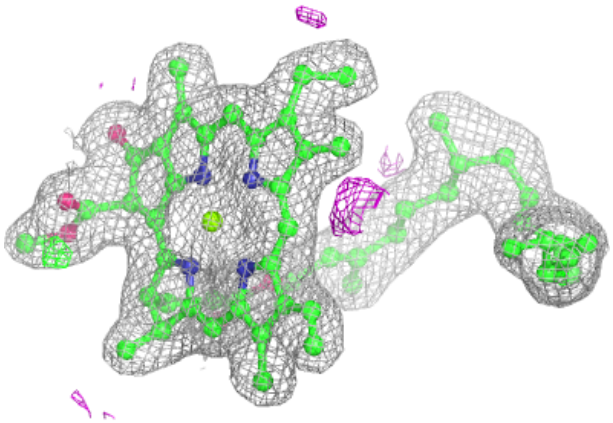
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

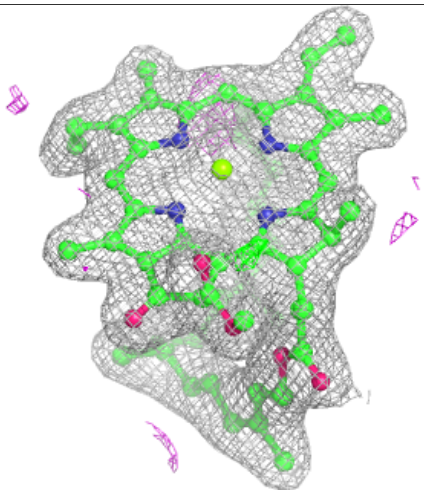


Electron density around CLA b 615:

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

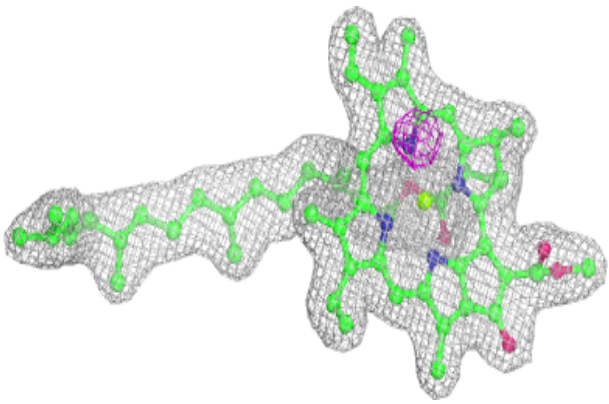


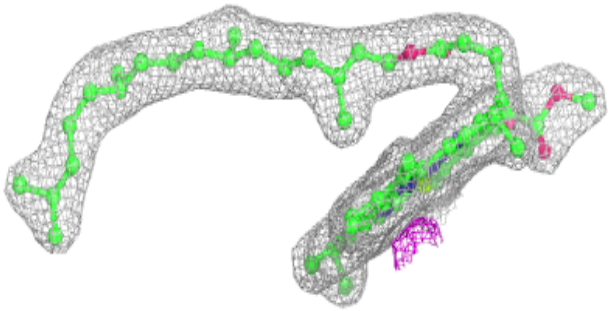


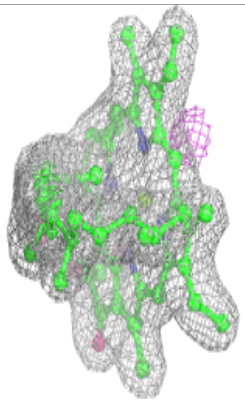


Electron density around CLA B 609:

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

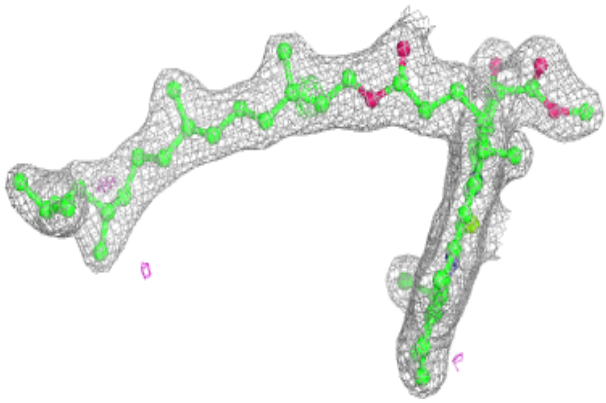


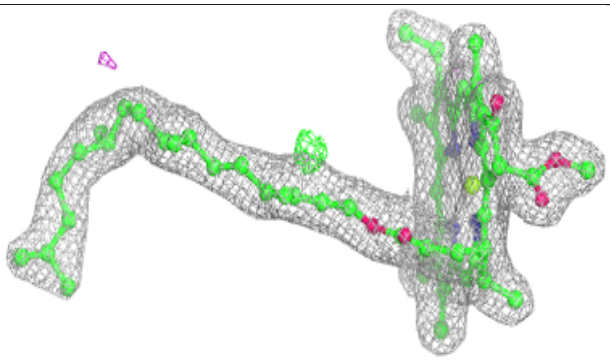


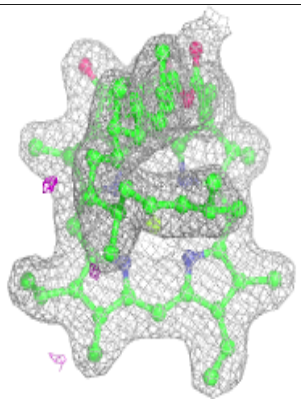


Electron density around CLA b 609:

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

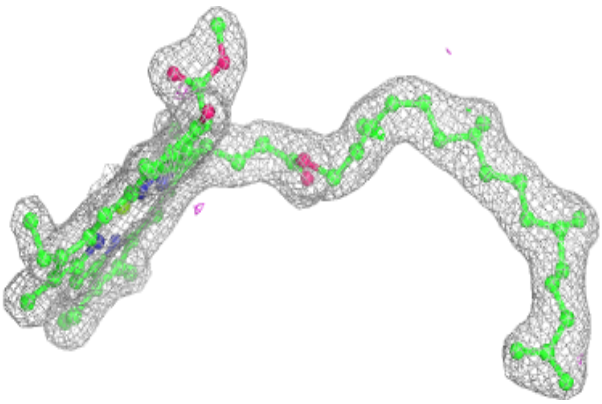


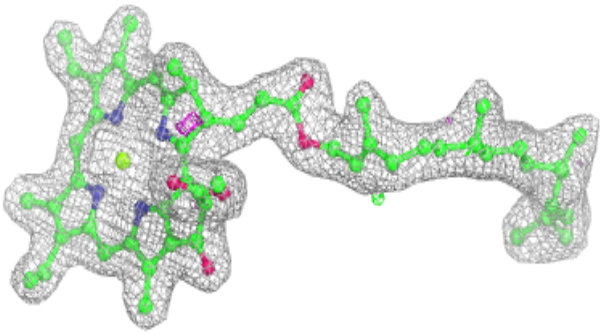


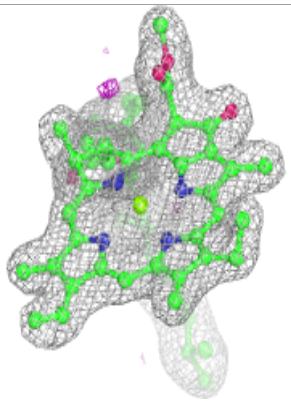


Electron density around CLA d 402:

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

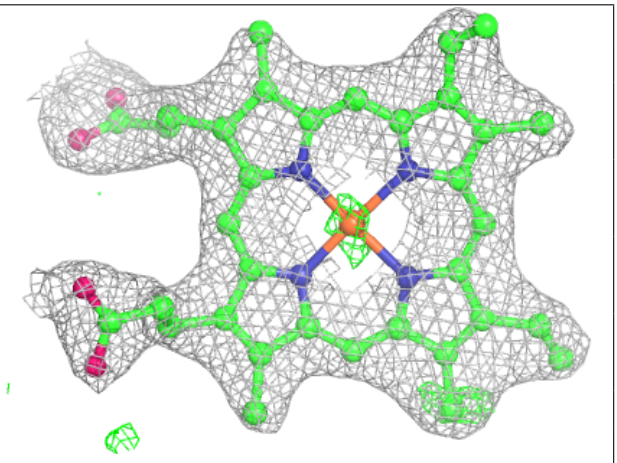


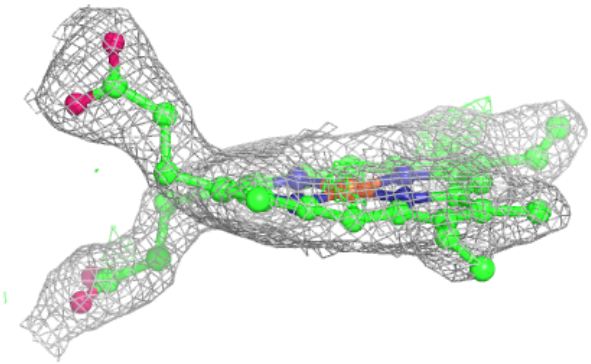


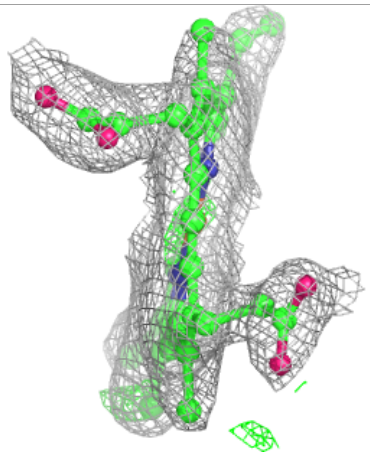


Electron density around HEM f 101:

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

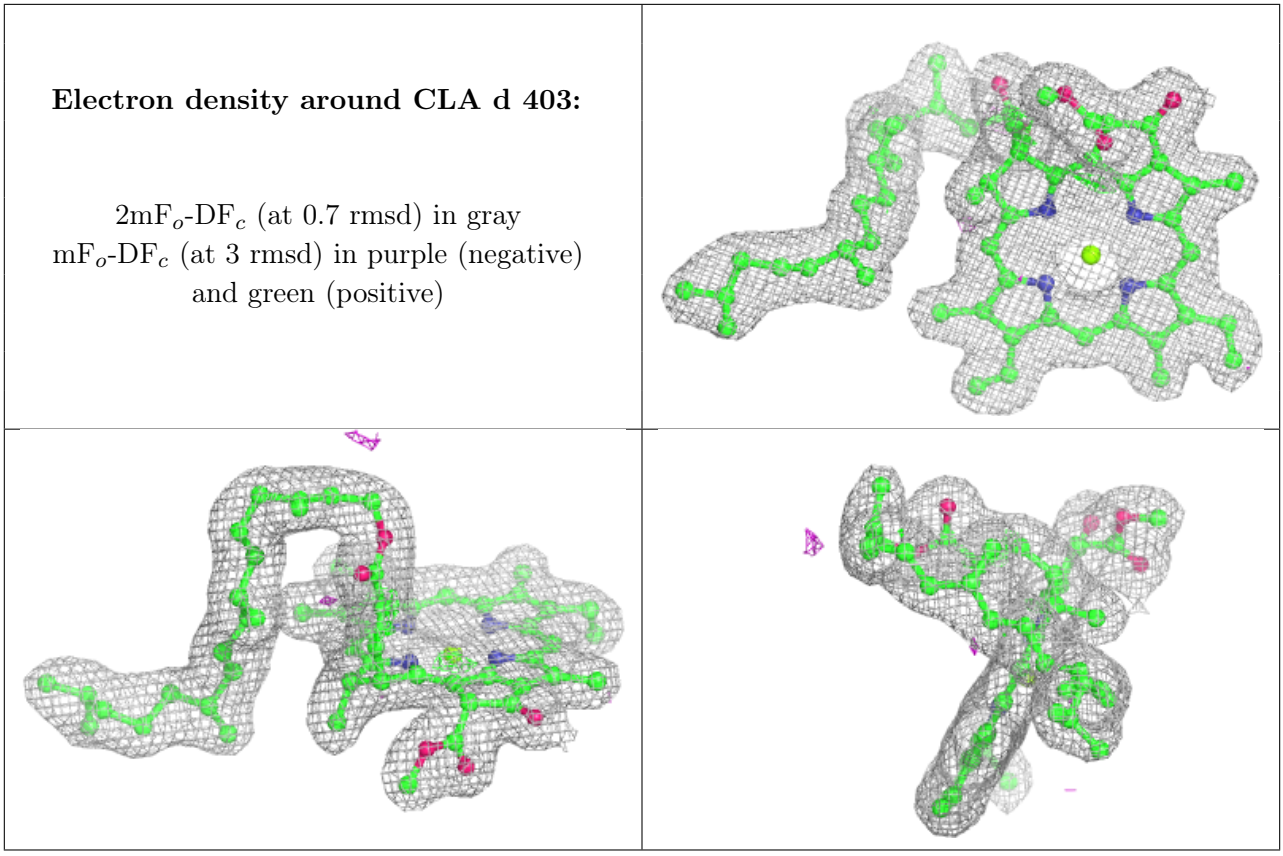






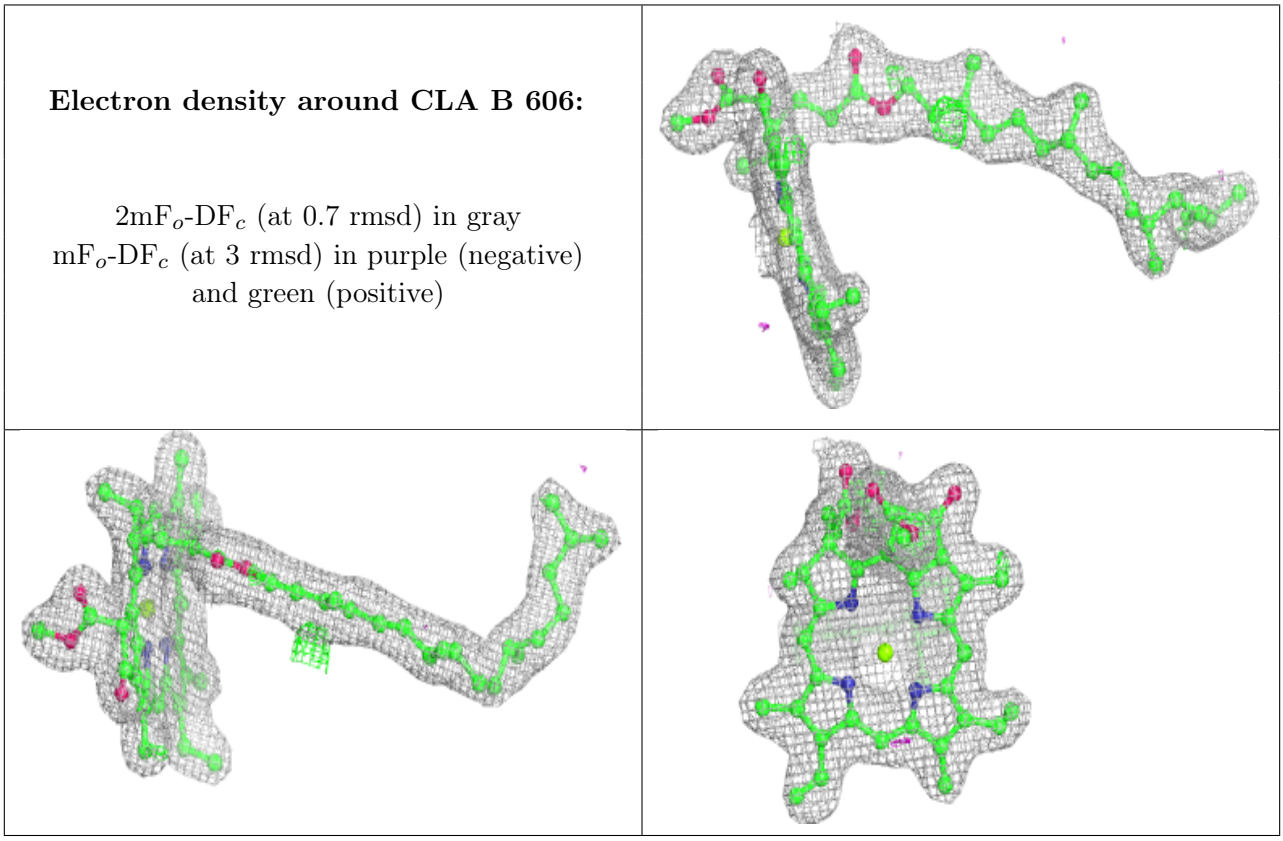
Electron density around CLA d 403:

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



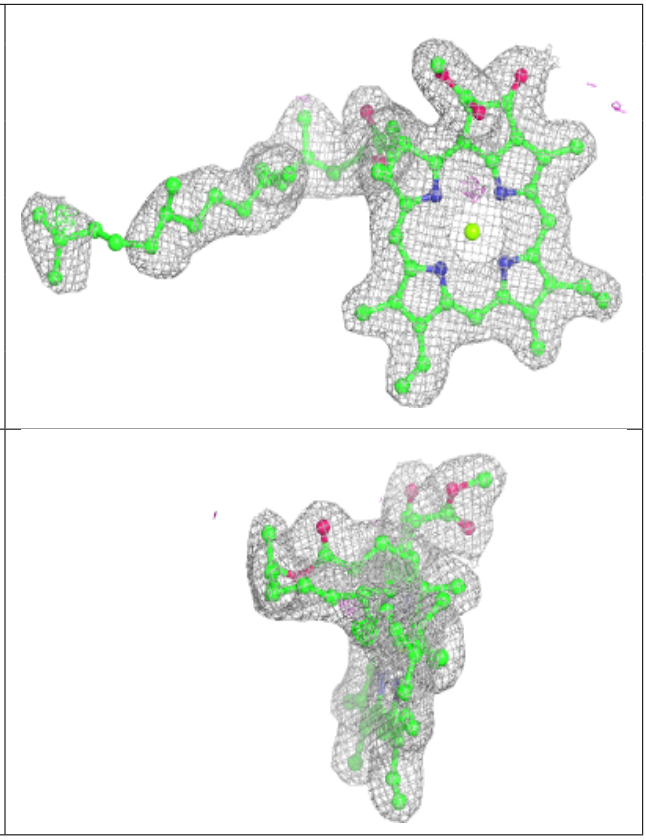
Electron density around CLA B 606:

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



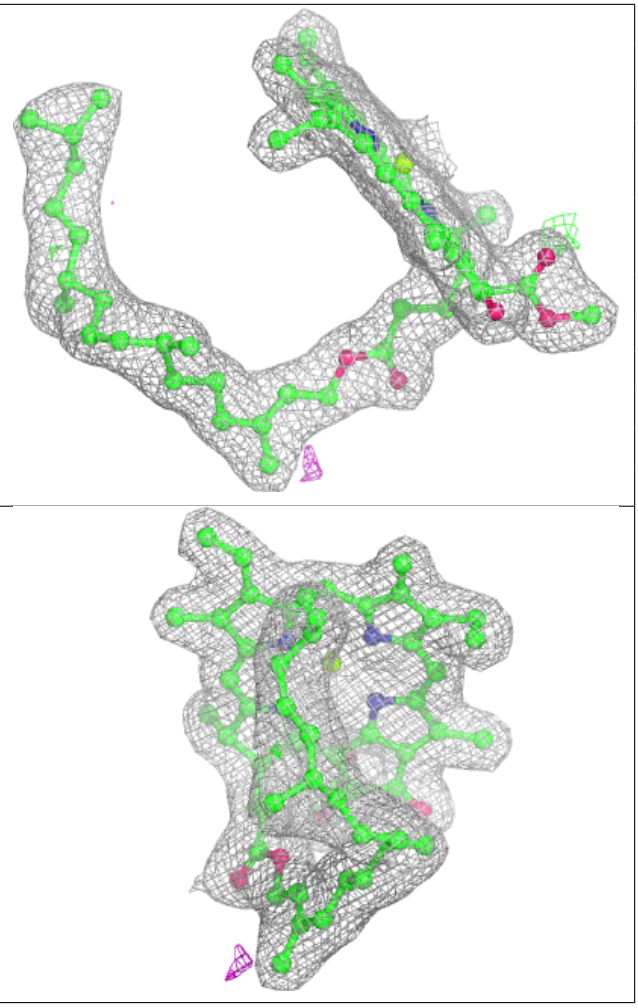
Electron density around CLA A 406:

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



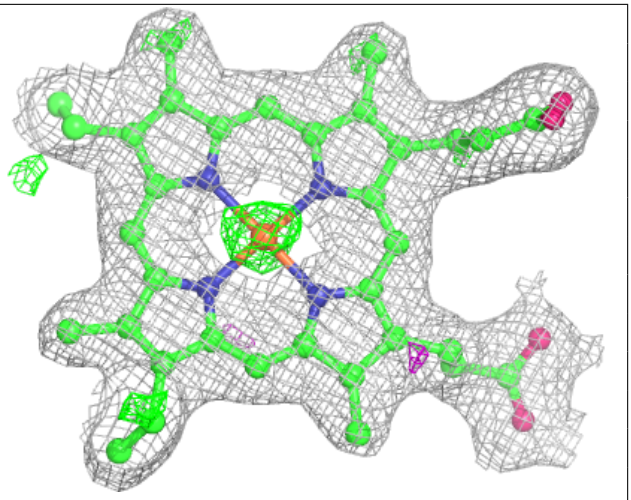
Electron density around CLA B 612:

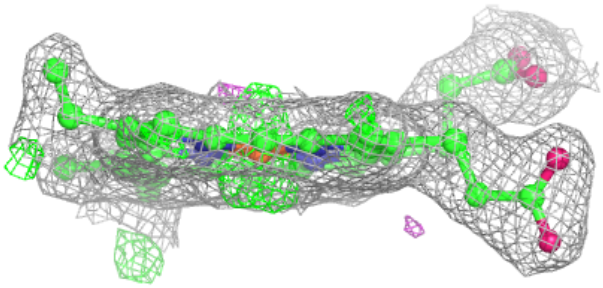
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

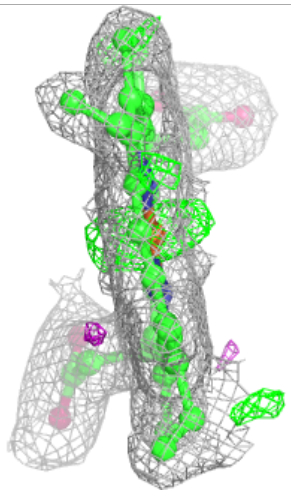


Electron density around HEC V 201:

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

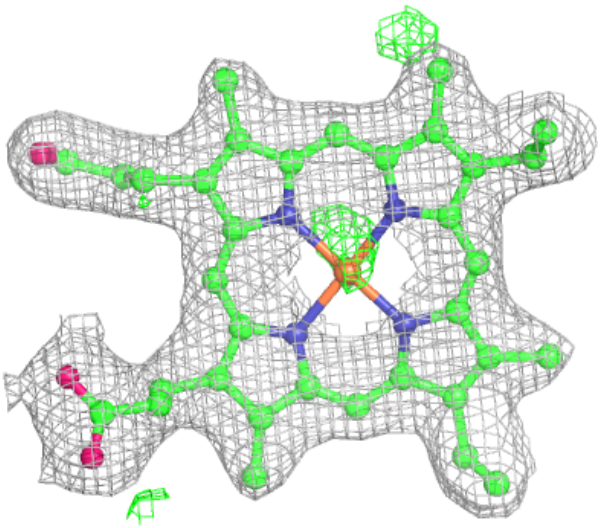


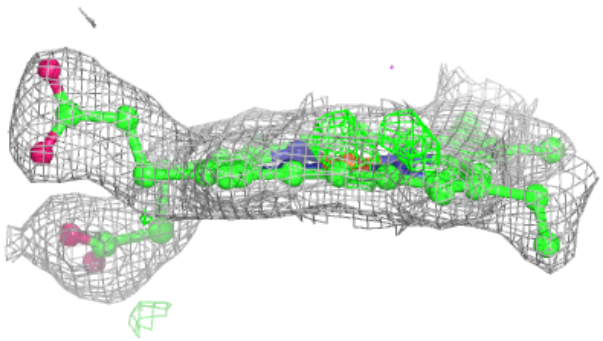


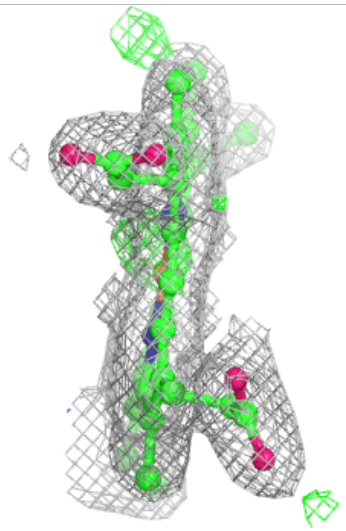


Electron density around HEC v 202:

$2mF_o$-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.