wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 05:30 PM JST

PDB ID	:	6JLL
Title	:	XFEL structure of cyanobacterial photosystem II (2F state, dataset1)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2019-03-06
Resolution	:	2.15 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:

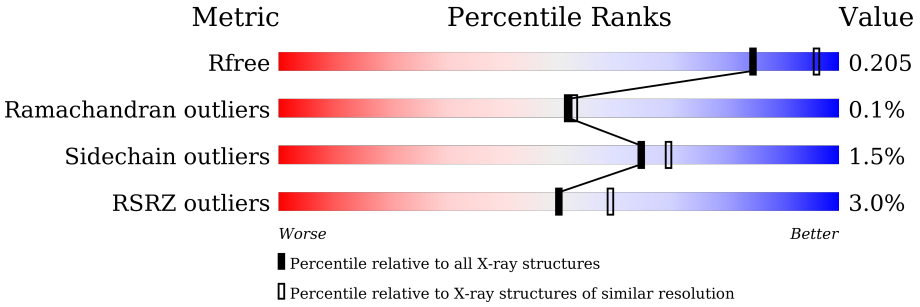
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	344	% 97%
1	a	344	3% 96%
2	B	505	% 99%
2	b	505	5% 99%
3	C	455	% 98%
3	c	455	% 99%
4	D	342	99%

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Mol	Chain	Length	Quality of chain
4	d	342	%, 99%
5	E	84	10%, 95%
5	e	84	12%, 95%
6	F	44	7%, 77%, 23%
6	f	44	5%, 70%, 27%
7	H	65	5%, 97%
7	h	65	3%, 98%
8	I	38	8%, 97%
8	i	38	5%, 95%
9	J	39	8%, 97%
9	j	39	10%, 97%
10	K	37	97%
10	k	37	95%, 5%
11	L	37	3%, 97%
11	l	37	3%, 100%
12	M	36	6%, 92%, 6%
12	m	36	89%, 6%, 6%
13	O	244	%, 98%
13	o	244	2%, 98%
14	T	32	3%, 88%, 6%, 6%
14	t	32	88%, 6%, 6%
15	U	104	91%, 7%
15	u	104	91%, 7%
16	V	137	100%
16	v	137	%, 100%

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Mol	Chain	Length	Quality of chain
17	Y	30	23% 93%
17	y	30	7% 90% 7%
18	X	40	10% 98%
18	x	40	10% 95% 5%
19	Z	62	11% 95% 5%
19	z	62	16% 94% 6%
20	R	34	53% 85% 12%

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	410	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	b	626	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 55675 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	3014	1963	496	537	18	0	54	0
1	a	334	3010	1964	494	534	18	0	56	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

- 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	504	4021	2639	667	702	13	0	10	0
2	b	503	4022	2644	664	701	13	0	12	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	3553	2322	592	626	13	0	14	0
3	c	455	3641	2382	606	639	14	0	20	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	See sequence details	UNP D0VWR7
C	20	SER	-	See sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	2849	1884	469	483	13	0	16	0
4	d	341	2849	1884	469	483	13	0	16	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	81	668	436	107	125	0	2	0
5	e	81	670	439	107	124	0	2	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	275	187	45	42	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	65	519	346	85	86	2	0	1	0
7	h	65	511	341	82	86	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	I	38	314	211	48	54	1	0	0	0
8	i	38	314	211	48	54	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	38	272	182	42	47	1	0	0	0
9	j	39	280	187	43	48	2	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	293	204	43	46	0	0	0
10	k	37	293	204	43	46	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	309	207	48	53	1	0	1	0
11	l	37	309	207	48	53	1	0	1	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	34	274	184	40	49	1	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	m	34	269	179	40	49	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	UNP P12312

- 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	1903	1191	315	392	5	0	8	0
			Total	C	N	O	S			
13	o	243	1891	1183	315	388	5	0	5	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	264	185	36	41	2	0	1	0
			Total	C	N	O	S			
14	t	30	264	185	36	41	2	0	1	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	774	491	129	154	0	0	0
			Total	C	N	O			
15	u	97	774	491	129	154	0	0	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	1085	689	181	211	4	0	2	0
			Total	C	N	O	S			
16	v	137	1077	684	178	211	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	215	142	37	33	3	0	0	0
17	y	29	215	142	37	33	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	X	39	287	191	46	50	0	0	0
18	x	38	281	188	45	48	0	0	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	479	328	72	77	2	0	0	0
19	z	62	479	328	72	77	2	0	0	0

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	R	30	239	163	41	35	98	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
21	A	1	2	2	0	1
21	a	1	1	1	0	1

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	A	2	4	4	0	2
22	U	1	1	1	0	0

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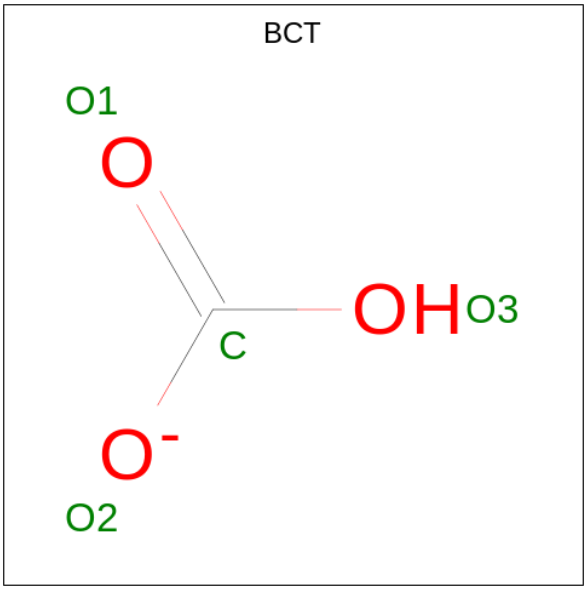
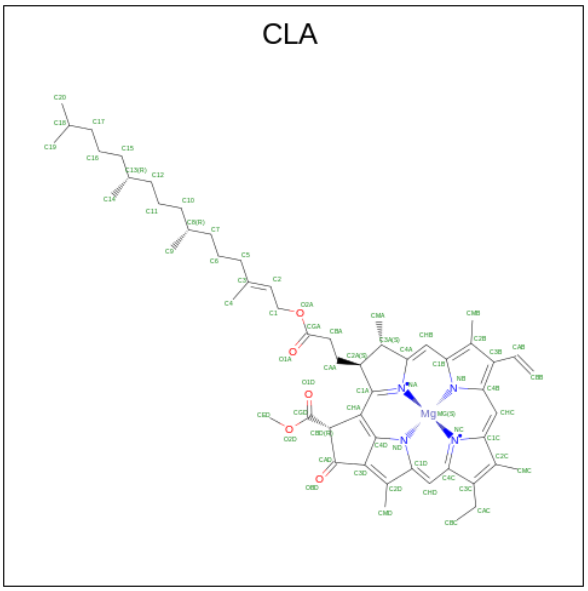
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	a	2	4	4	0	2
			Total	Cl		
22	v	1	1	1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	A	1	8	2	6	0	1
			Total	C	O		
23	a	1	8	2	6	0	1

- Molecule 24 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		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0

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

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

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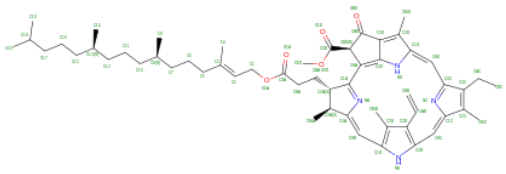
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

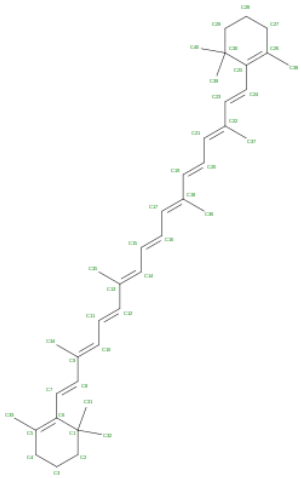
PHO



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	64	55	4	5	0	0
			Total	C	N	O		
25	A	1	128	110	8	10	0	1
			Total	C	N	O		
25	a	1	64	55	4	5	0	0
			Total	C	N	O		
25	a	1	128	110	8	10	0	1

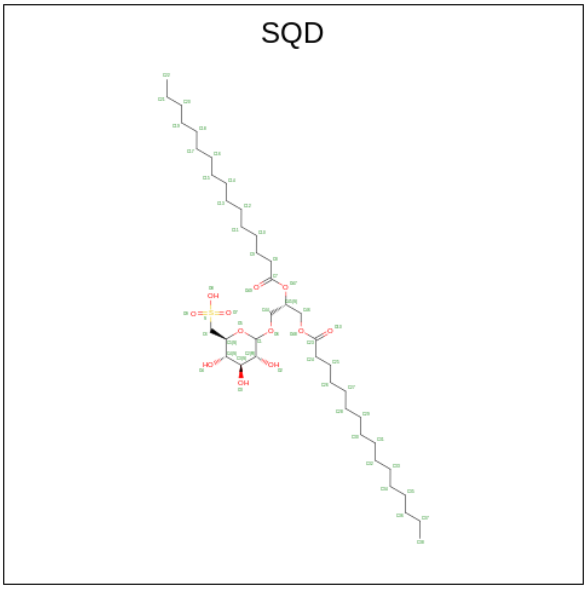
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



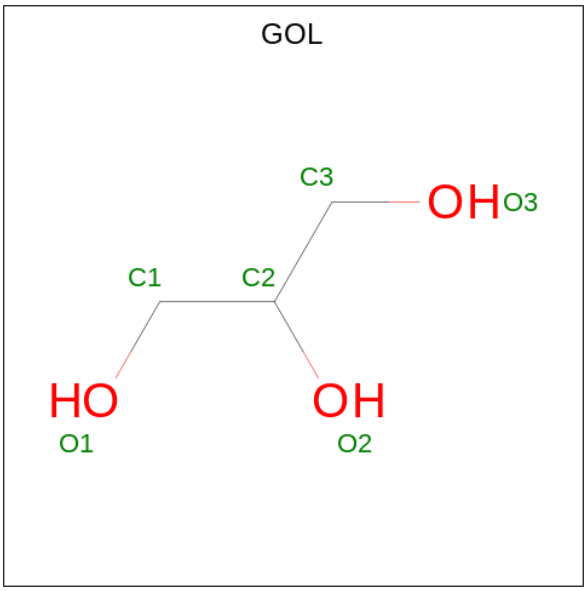
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
26	A	1	40	40	0	0
26	B	1	40	40	0	0
26	B	1	40	40	0	0
26	B	1	40	40	0	0
26	C	1	40	40	0	0
26	C	1	40	40	0	0
26	D	1	40	40	0	0
26	H	1	40	40	0	0
26	K	1	40	40	0	0
26	T	1	40	40	0	0
26	Y	1	40	40	0	0
26	a	1	40	40	0	0
26	b	1	40	40	0	0
26	b	1	40	40	0	0
26	b	1	40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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
			Total	C	O	S		
27	B	1	54	41	12	1	0	0
			Total	C	O	S		
27	F	1	43	30	12	1	0	0
			Total	C	O	S		
27	a	1	54	41	12	1	0	0
			Total	C	O	S		
27	a	1	54	41	12	1	0	0
			Total	C	O	S		
27	b	1	54	41	12	1	0	0
			Total	C	O	S		
27	f	1	43	30	12	1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
28	A	1	6	3	3		0	0
			Total	C	O			
28	A	1	6	3	3		0	0
			Total	C	O			
28	A	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	B	1	6	3	3		0	0
			Total	C	O			
28	C	1	6	3	3		0	0
			Total	C	O			
28	C	1	6	3	3		0	0
			Total	C	O			
28	O	1	6	3	3		0	0
			Total	C	O			
28	T	1	6	3	3		0	0

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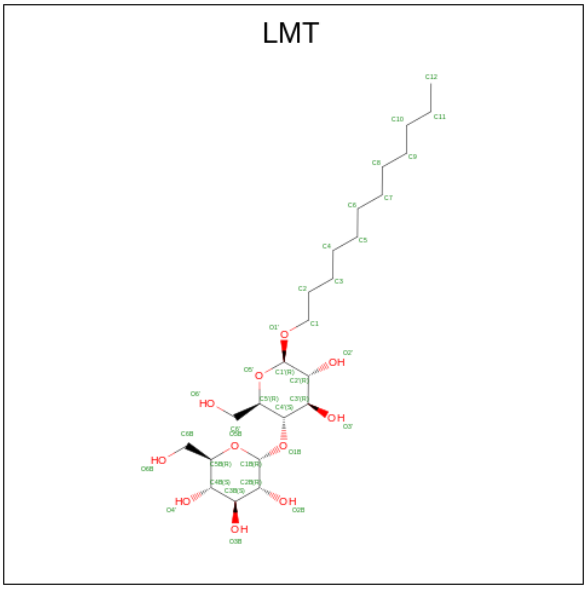
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	T	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	a	1	6	3	3	0	0
28	a	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	c	1	6	3	3	0	0
28	c	1	6	3	3	0	0
28	f	1	6	3	3	0	0
28	o	1	6	3	3	0	0
28	t	1	6	3	3	0	0
28	v	1	6	3	3	0	0
28	v	1	6	3	3	0	0
28	v	1	6	3	3	0	0

- Molecule 29 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		
29	A	1	35	24	11	0	0
			Total	C	O		
29	B	1	25	19	6	0	0
			Total	C	O		
29	C	1	35	24	11	0	0
			Total	C	O		
29	D	1	35	24	11	0	0
			Total	C	O		
29	F	1	35	24	11	0	0
			Total	C	O		
29	M	1	35	24	11	0	0
			Total	C	O		
29	M	1	35	24	11	0	0
			Total	C	O		
29	M	1	35	24	11	0	0
			Total	C	O		
29	T	1	25	19	6	0	0
			Total	C	O		
29	a	1	35	24	11	0	0
			Total	C	O		
29	a	1	35	24	11	0	0
			Total	C	O		
29	b	1	25	19	6	0	0

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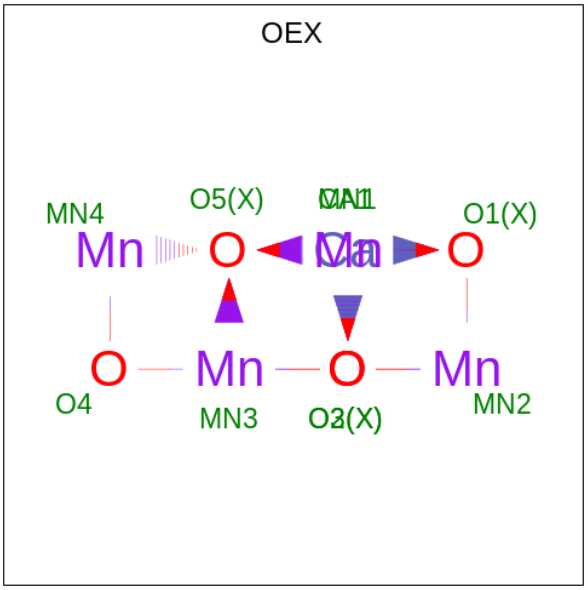
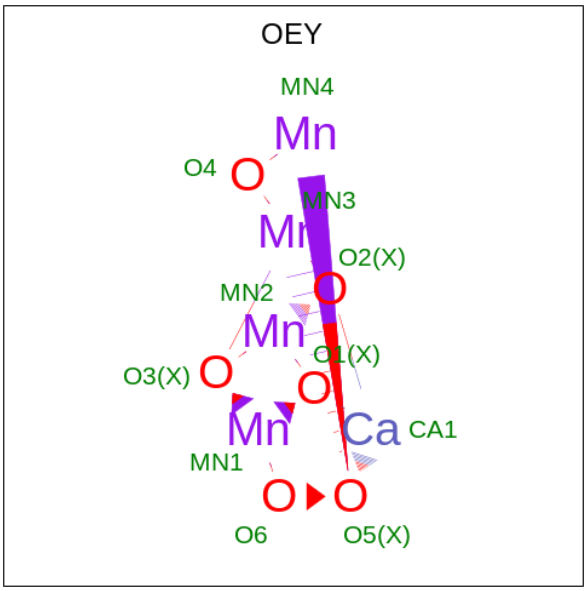
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	f	1	35	24	11	0	0
			Total	C	O		
29	m	1	35	24	11	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



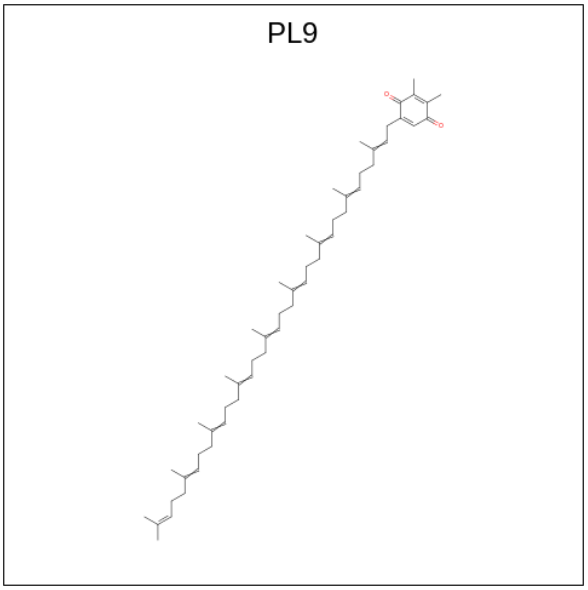
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
30	A	1	10	1	4	5	0	1
			Total	Ca	Mn	O		
30	a	1	10	1	4	5	0	1

- Molecule 31 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$).



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

- Molecule 32 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: $C_{53}H_{80}O_2$).



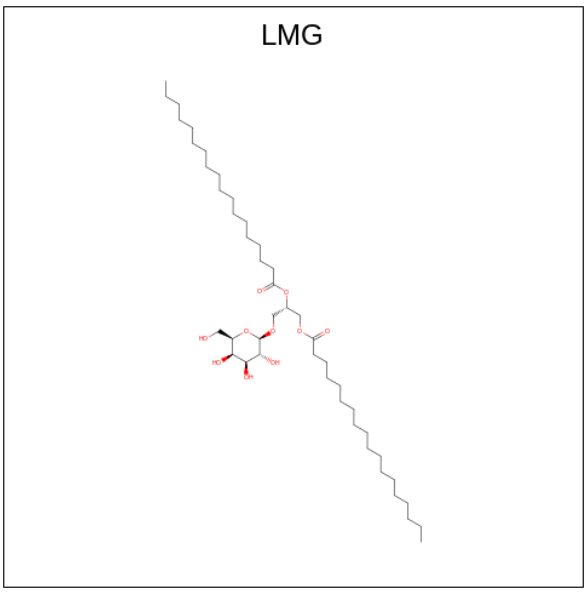
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 110 106 4	0	1
32	D	1	Total C O 110 106 4	0	1
32	a	1	Total C O 110 106 4	0	1
32	d	1	Total C O 110 106 4	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 28 23 5	0	0
33	B	1	Total C O 33 28 5	0	0
33	C	1	Total C O 34 29 5	0	0
33	D	2	Total C O 57 51 6	0	0
33	I	1	Total C O 40 35 5	0	0
33	J	1	Total C 10 10	0	0
33	M	1	Total C 10 10	0	0
33	X	1	Total C O 18 16 2	0	0
33	a	1	Total C O 30 25 5	0	0
33	b	1	Total C O 33 28 5	0	0
33	c	1	Total C O 32 27 5	0	0
33	d	3	Total C O 71 63 8	0	0
33	i	1	Total C O 40 35 5	0	0
33	j	1	Total C 10 10	0	0
33	m	1	Total C 10 10	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: $C_{45}H_{86}O_{10}$).

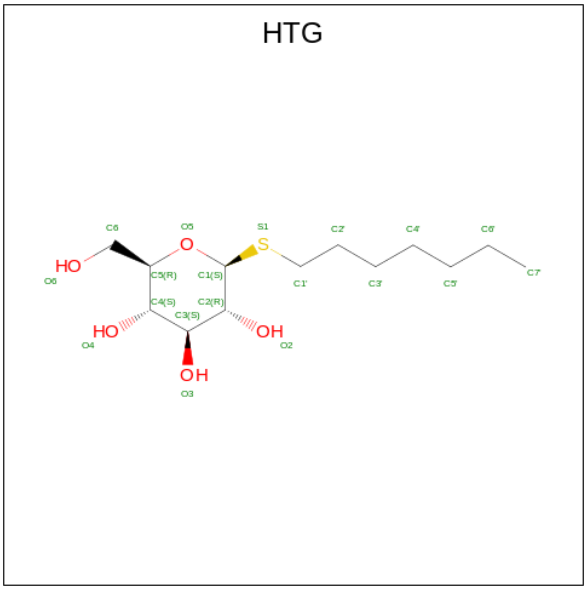


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	A	1	51	41	10	0	0
34	B	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	D	1	51	41	10	0	0
34	Z	1	37	27	10	0	0
34	a	1	51	41	10	0	0
34	b	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	j	1	51	41	10	0	0
34	z	1	39	29	10	0	0

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
35	B	1	1	1	0	0
35	C	1	1	1	0	0
35	F	1	1	1	0	0
35	O	1	1	1	0	0
35	b	1	1	1	0	0
35	c	2	2	2	0	0
35	f	1	1	1	0	0
35	o	1	1	1	0	0

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
36	B	1	19	13	5	1	0	0
			Total	C	O	S		
36	B	1	19	13	5	1	0	0
			Total	C	O	S		
36	B	1	19	13	5	1	0	0

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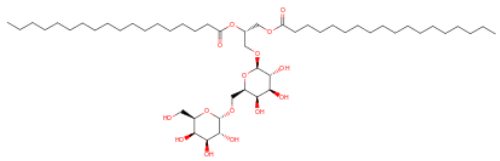
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
36	B	1	19	13	5	1	0	0
			Total	C	O	S		
36	B	1	19	13	5	1	0	0
			Total	C	O	S		
36	C	1	19	13	5	1	0	0
			Total	C	O	S		
36	C	1	19	13	5	1	0	0
			Total	C	O	S		
36	H	1	16	10	5	1	0	0
			Total	C	O	S		
36	V	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	c	1	19	13	5	1	0	0
			Total	C	O	S		
36	c	1	19	13	5	1	0	0
			Total	C	O	S		
36	d	1	16	10	5	1	0	0

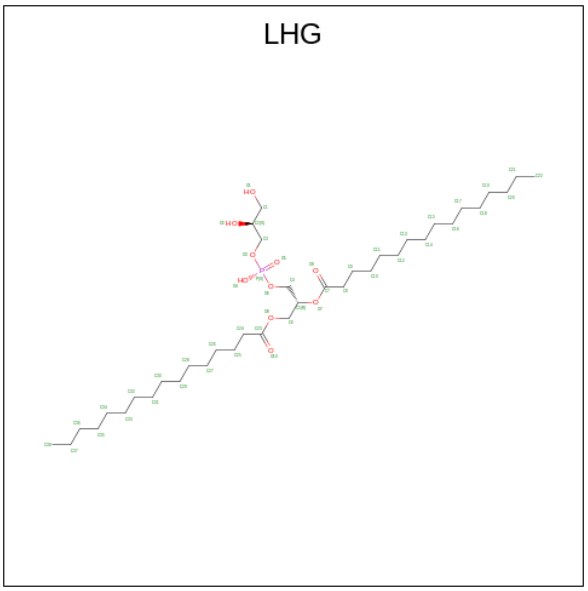
- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



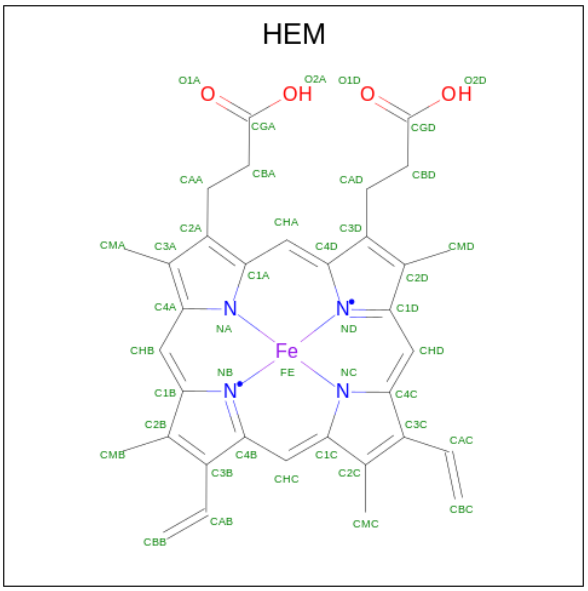
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
37	C	1	62	47	15	0	0
37	C	1	62	47	15	0	0
37	C	1	62	47	15	0	0
37	D	1	52	42	10	0	0
37	H	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	e	1	62	47	15	0	0
37	h	1	62	47	15	0	0

- Molecule 38 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		
38	D	1	49	38	10	1	0	0
			Total	C	O	P		
38	D	1	49	38	10	1	0	0
			Total	C	O	P		
38	D	1	49	38	10	1	0	0
			Total	C	O	P		
38	E	1	42	31	10	1	0	0
			Total	C	O	P		
38	L	1	49	38	10	1	0	0
			Total	C	O	P		
38	a	1	42	31	10	1	0	0
			Total	C	O	P		
38	d	1	49	38	10	1	0	0
			Total	C	O	P		
38	d	1	49	38	10	1	0	0
			Total	C	O	P		
38	d	1	49	38	10	1	0	0
			Total	C	O	P		
38	l	1	49	38	10	1	0	0

- Molecule 39 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		
39	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
39	V	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
39	e	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
39	v	1	43	34	1	4	4	0	0

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
40	J	1	1	1	0	0
			Total	Mg		
40	j	1	1	1	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	161	173	173	0	14
			Total	O		
41	B	290	294	294	0	4
			Total	O		
41	C	228	232	232	0	4

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	D	146	150	150	0	5
			Total	O		
41	E	30	30	30	0	0
			Total	O		
41	F	9	9	9	0	0
			Total	O		
41	H	48	49	49	0	1
			Total	O		
41	I	5	5	5	0	0
			Total	O		
41	J	10	10	10	0	0
			Total	O		
41	K	9	9	9	0	0
			Total	O		
41	L	13	14	14	0	1
			Total	O		
41	M	23	23	23	0	0
			Total	O		
41	O	178	180	180	0	2
			Total	O		
41	T	17	18	18	0	1
			Total	O		
41	U	77	77	77	0	0
			Total	O		
41	V	117	119	119	0	2
			Total	O		
41	Y	4	4	4	0	0
			Total	O		
41	X	6	6	6	0	0
			Total	O		
41	Z	1	1	1	0	0
			Total	O		
41	a	153	162	162	0	12
			Total	O		
41	b	266	269	269	0	3
			Total	O		
41	c	200	205	205	0	5
			Total	O		
41	d	129	132	132	0	3
			Total	O		
41	e	19	19	19	0	0

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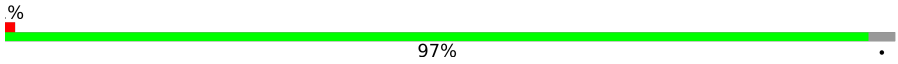
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	f	8	Total O 8 8	0	0
41	h	44	Total O 44 44	0	0
41	i	5	Total O 5 5	0	0
41	j	6	Total O 6 6	0	0
41	k	7	Total O 7 7	0	0
41	l	9	Total O 9 9	0	0
41	m	11	Total O 11 11	0	0
41	o	155	Total O 155 155	0	0
41	t	11	Total O 11 11	0	0
41	u	93	Total O 93 93	0	0
41	v	81	Total O 82 82	0	1
41	y	2	Total O 2 2	0	0
41	x	6	Total O 6 6	0	0

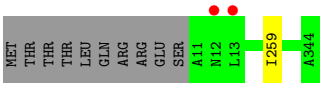
3 Residue-property plots (i)

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

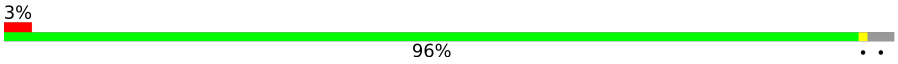
Chain A:





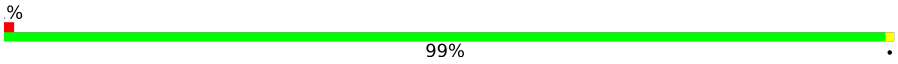
• Molecule 1: Photosystem II protein D1

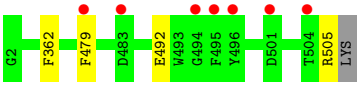
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

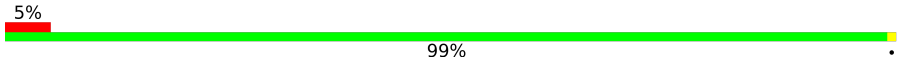
Chain B:

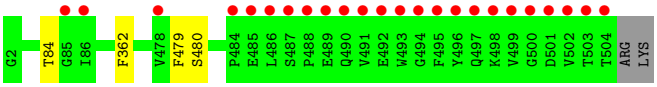




• Molecule 2: Photosystem II CP47 reaction center protein

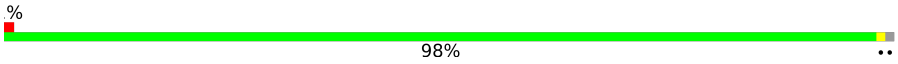
Chain b:



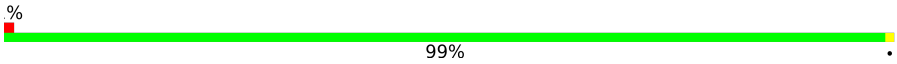


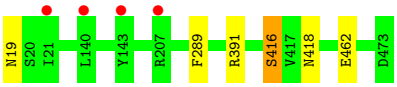
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

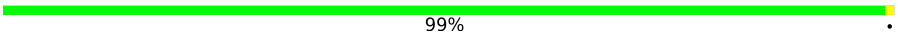


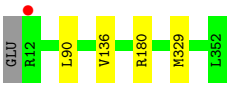
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 

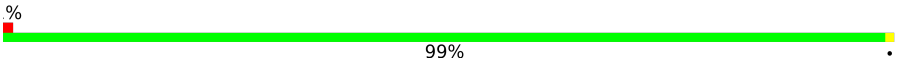


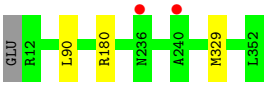
• Molecule 4: Photosystem II D2 protein

Chain D: 

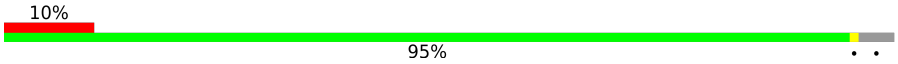


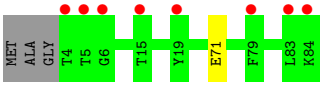
• Molecule 4: Photosystem II D2 protein

Chain d: 

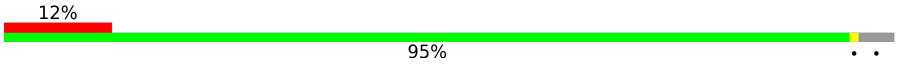


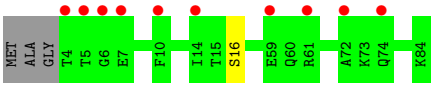
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 



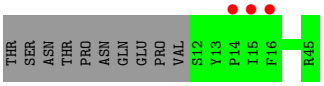
• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 



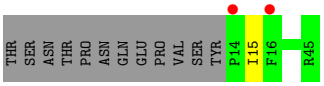
• Molecule 6: Cytochrome b559 subunit beta

Chain F:

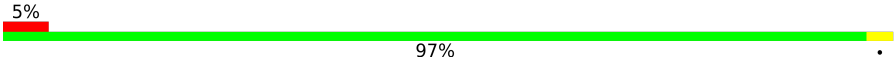


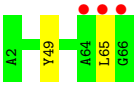
• Molecule 6: Cytochrome b559 subunit beta

Chain f:

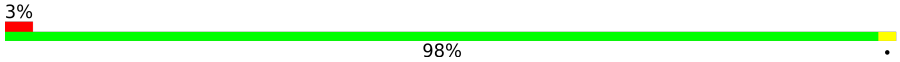


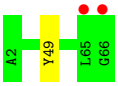
• Molecule 7: Photosystem II reaction center protein H

Chain H: 

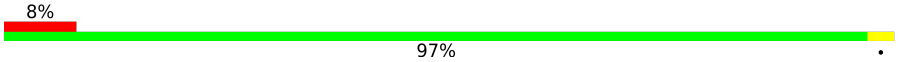


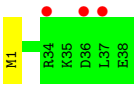
• Molecule 7: Photosystem II reaction center protein H

Chain h: 

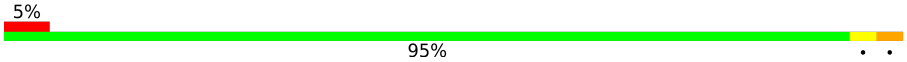


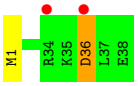
• Molecule 8: Photosystem II reaction center protein I

Chain I: 

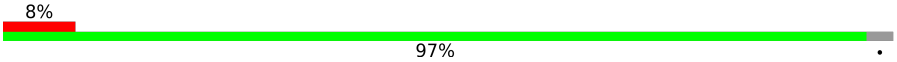


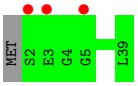
• Molecule 8: Photosystem II reaction center protein I

Chain i: 

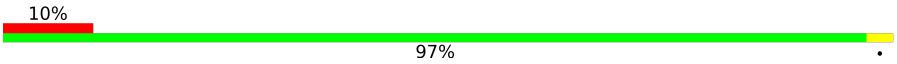


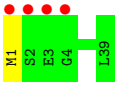
• Molecule 9: Photosystem II reaction center protein J

Chain J: 

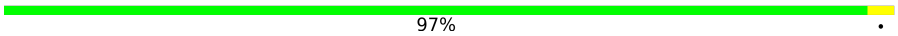


• Molecule 9: Photosystem II reaction center protein J

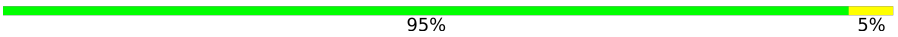
Chain j: 



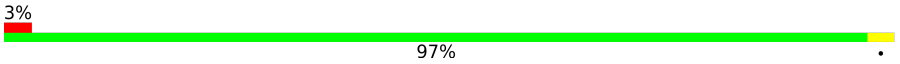
• Molecule 10: Photosystem II reaction center protein K

Chain K: 

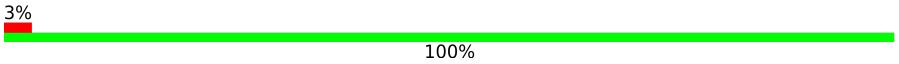
• Molecule 10: Photosystem II reaction center protein K

Chain k: 

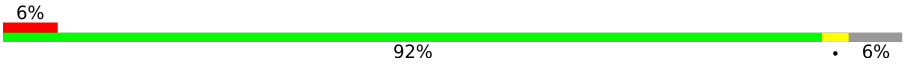
• Molecule 11: Photosystem II reaction center protein L

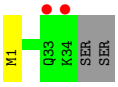
Chain L: 

• Molecule 11: Photosystem II reaction center protein L

Chain l: 

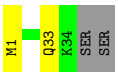
• Molecule 12: Photosystem II reaction center protein M

Chain M: 

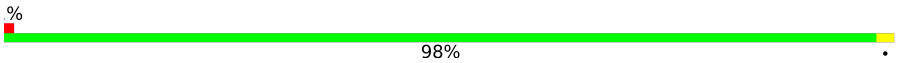


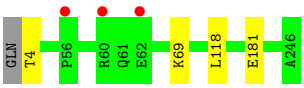
• Molecule 12: Photosystem II reaction center protein M

Chain m:

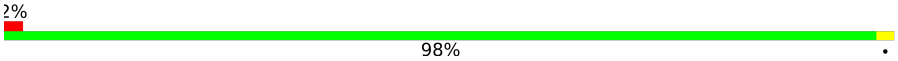


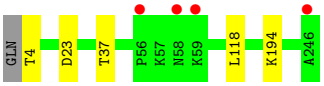
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 



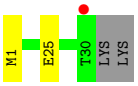
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 



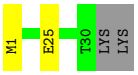
• Molecule 14: Photosystem II reaction center protein T

Chain T:



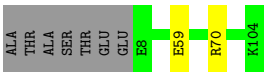
• Molecule 14: Photosystem II reaction center protein T

Chain t:



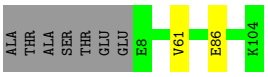
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



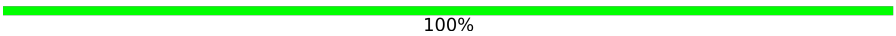
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



• Molecule 16: Cytochrome c-550

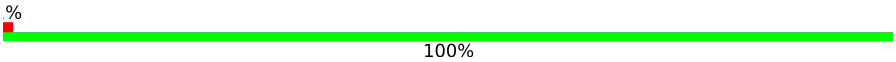
Chain V:



There are no outlier residues recorded for this chain.

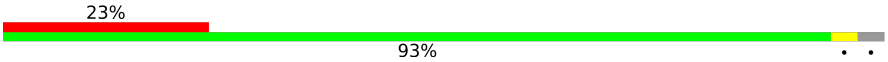
• Molecule 16: Cytochrome c-550

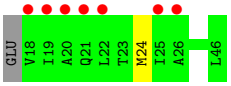
Chain v:



• Molecule 17: Photosystem II reaction center protein Ycf12

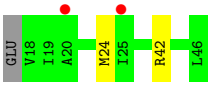
Chain Y:





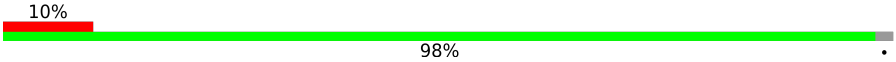
• Molecule 17: Photosystem II reaction center protein Ycf12

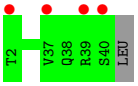
Chain y:



• Molecule 18: Photosystem II reaction center protein X

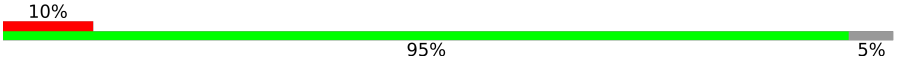
Chain X:

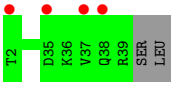




• Molecule 18: Photosystem II reaction center protein X

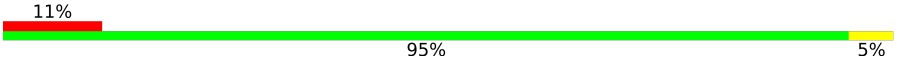
Chain x:

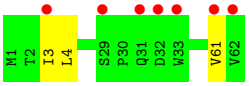




• Molecule 19: Photosystem II reaction center protein Z

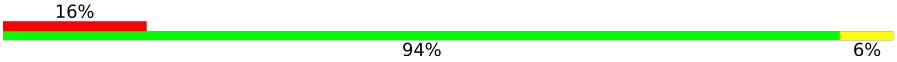
Chain Z:

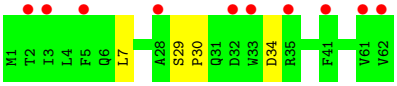




• Molecule 19: Photosystem II reaction center protein Z

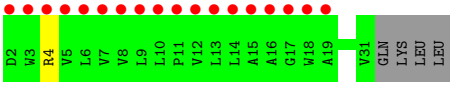
Chain z:





• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 178.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.9 (178.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.156 , 0.203 0.159 , 0.205	Depositor DCC
R_{free} test set	26822 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 76.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55675	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: PL9, OEY, CLA, BCT, GOL, OEX, HEM, LMT, HTG, PHO, FME, LHG, MG, BCR, DGD, CL, SQD, UNL, FE2, CA, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/3115	0.55	0/4242
1	a	0.44	0/3117	0.54	0/4245
2	B	0.44	0/4191	0.53	0/5709
2	b	0.42	0/4198	0.52	0/5720
3	C	0.39	0/3678	0.51	0/5007
3	c	0.38	0/3774	0.51	0/5135
4	D	0.48	0/2952	0.55	0/4021
4	d	0.45	0/2952	0.54	0/4021
5	E	0.34	0/693	0.49	0/944
5	e	0.33	0/695	0.49	0/948
6	F	0.41	0/284	0.51	0/387
6	f	0.40	0/265	0.52	0/360
7	H	0.36	0/535	0.55	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.35	0/311	0.49	0/419
8	i	0.34	0/311	0.45	0/419
9	J	0.33	0/278	0.41	0/376
9	j	0.35	0/286	0.45	0/386
10	K	0.34	0/303	0.50	0/416
10	k	0.34	0/303	0.50	0/416
11	L	0.44	0/319	0.48	0/433
11	l	0.43	0/319	0.46	0/433
12	M	0.48	0/270	0.57	0/368
12	m	0.43	0/262	0.54	0/357
13	O	0.38	0/1958	0.56	0/2654
13	o	0.37	0/1937	0.54	0/2625
14	T	0.49	0/266	0.54	0/362
14	t	0.49	0/266	0.52	0/362
15	U	0.38	0/785	0.53	0/1064
15	u	0.39	0/785	0.52	0/1064
16	V	0.39	0/1109	0.50	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.35	0/1098	0.50	0/1488
17	Y	0.35	0/216	0.50	0/289
17	y	0.30	0/216	0.43	0/289
18	X	0.34	0/290	0.45	0/392
18	x	0.30	0/284	0.46	0/384
19	Z	0.31	0/490	0.43	0/669
19	z	0.28	0/490	0.44	0/669
20	R	0.23	0/245	0.37	0/338
All	All	0.41	0/44370	0.52	0/60354

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	384/344 (112%)	380 (99%)	3 (1%)	1 (0%)	41	37
1	a	384/344 (112%)	378 (98%)	5 (1%)	1 (0%)	41	37
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	461/455 (101%)	450 (98%)	9 (2%)	2 (0%)	34	29
3	c	473/455 (104%)	459 (97%)	12 (2%)	2 (0%)	34	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	81 (100%)	0	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	245 (98%)	4 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	3
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5429/5384 (101%)	5309 (98%)	111 (2%)	9 (0%)	51	46

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP

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	311/279 (112%)	311 (100%)	0	100	100
1	a	311/279 (112%)	309 (99%)	2 (1%)	86	90
2	B	412/403 (102%)	408 (99%)	4 (1%)	76	81
2	b	413/403 (102%)	409 (99%)	4 (1%)	76	81
3	C	361/356 (101%)	356 (99%)	5 (1%)	67	72
3	c	371/356 (104%)	363 (98%)	8 (2%)	52	55
4	D	290/277 (105%)	286 (99%)	4 (1%)	67	72
4	d	290/277 (105%)	287 (99%)	3 (1%)	76	81
5	E	74/73 (101%)	73 (99%)	1 (1%)	67	72
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	72
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	31
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	33
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	42
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	32
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	37
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	11
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	44
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	37
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	53
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	51
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	9
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	9
15	U	84/89 (94%)	82 (98%)	2 (2%)	49	51
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	51
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	24
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	5
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	31
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	15
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	29
All	All	4504/4403 (102%)	4434 (98%)	70 (2%)	65	67

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	23	ASP
13	o	118	LEU
17	y	24	MET

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Mol	Chain	Res	Type
14	T	25[B]	GLU
14	T	25[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	53	ASN
4	d	61	HIS
3	c	373	ASN
4	d	83	ASN
4	D	83	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	t	1	14	8,9,10	0.79	0	7,9,11	2.41	4 (57%)
12	FME	m	1	12	8,9,10	0.66	0	7,9,11	1.33	1 (14%)
8	FME	i	1	8	8,9,10	0.60	0	7,9,11	1.21	1 (14%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.26	1 (14%)
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.30	1 (14%)
12	FME	M	1	12	8,9,10	0.67	0	7,9,11	1.39	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-3.87	116.87	122.82
14	t	1	FME	C-CA-N	2.86	114.89	109.73
14	T	1	FME	O-C-CA	-2.50	118.22	124.78
14	t	1	FME	O-C-CA	-2.43	118.40	124.78
14	t	1	FME	O1-CN-N	-2.33	119.13	125.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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 266 ligands modelled in this entry, 24 are monoatomic and 18 are unknown - leaving 224 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	$\#\|Z\| > 2$
28	GOL	B	629	-	5,5,5	0.36	0	5,5,5	0.33	0
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.07	3 (6%)
26	BCR	t	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.62	14 (25%)
28	GOL	V	202	-	5,5,5	0.37	0	5,5,5	0.28	0
24	CLA	B	614	-	65,73,73	2.06	15 (23%)	76,113,113	2.58	27 (35%)
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.18	6 (9%)
27	SQD	F	103	-	42,43,54	1.15	3 (7%)	51,54,65	1.64	11 (21%)
28	GOL	o	301	-	5,5,5	0.37	0	5,5,5	0.27	0
34	LMG	A	422	-	51,51,55	0.94	2 (3%)	59,59,63	1.13	5 (8%)
34	LMG	b	630	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
36	HTG	H	101	-	16,16,19	1.12	2 (12%)	20,21,24	1.22	1 (5%)
29	LMT	A	417	-	36,36,36	0.61	1 (2%)	47,47,47	1.25	3 (6%)
26	BCR	D	404	-	41,41,41	1.02	1 (2%)	56,56,56	1.80	11 (19%)
23	BCT	A	404[A]	21	2,3,3	0.63	0	2,3,3	1.09	0
34	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.13	4 (8%)
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.26	0
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
24	CLA	b	626	-	65,73,73	2.05	17 (26%)	76,113,113	2.74	28 (36%)
28	GOL	A	413	-	5,5,5	0.34	0	5,5,5	0.25	0
32	PL9	d	405[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.55	13 (19%)
28	GOL	V	203	-	5,5,5	0.35	0	5,5,5	0.43	0
36	HTG	b	608	-	19,19,19	1.03	2 (10%)	23,24,24	1.48	2 (8%)
26	BCR	C	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.49	9 (16%)
26	BCR	C	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.55	10 (17%)
29	LMT	M	103	-	36,36,36	0.52	1 (2%)	47,47,47	0.99	3 (6%)
34	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	0.98	3 (5%)
28	GOL	b	605	-	5,5,5	0.37	0	5,5,5	0.30	0
24	CLA	b	616	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	27 (35%)
24	CLA	b	624	-	65,73,73	2.03	15 (23%)	76,113,113	2.88	29 (38%)
27	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.41	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	SQD	A	412	-	53,54,54	0.97	3 (5%)	62,65,65	1.53	11 (17%)
34	LMG	c	523	-	51,51,55	0.96	2 (3%)	59,59,63	1.22	8 (13%)
29	LMT	b	631	-	25,25,36	0.52	0	30,30,47	0.67	0
31	OEY	a	418[B]	3,1,41	0,16,16	-	-	-		
36	HTG	B	633	-	19,19,19	1.01	2 (10%)	23,24,24	1.43	2 (8%)
26	BCR	b	627	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	5 (8%)
24	CLA	b	617	41	65,73,73	1.96	16 (24%)	76,113,113	2.82	25 (32%)
24	CLA	c	506	-	65,73,73	2.06	17 (26%)	76,113,113	2.66	25 (32%)
24	CLA	C	507	41	65,73,73	2.02	15 (23%)	76,113,113	2.71	27 (35%)
34	LMG	B	622	-	51,51,55	0.93	2 (3%)	59,59,63	1.08	4 (6%)
24	CLA	C	504	41	65,73,73	2.06	17 (26%)	76,113,113	2.84	28 (36%)
24	CLA	c	515	3	65,73,73	2.03	16 (24%)	76,113,113	2.66	25 (32%)
38	LHG	D	407	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.47	9 (16%)
24	CLA	C	511	3	65,73,73	2.07	15 (23%)	76,113,113	2.70	28 (36%)
23	BCT	A	404[B]	21	2,3,3	0.63	0	2,3,3	1.02	0
27	SQD	b	601	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	9 (14%)
24	CLA	c	508	41	65,73,73	2.07	17 (26%)	76,113,113	2.85	31 (40%)
38	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.98	2 (3%)
24	CLA	d	401	41	65,73,73	2.08	17 (26%)	76,113,113	2.77	30 (39%)
28	GOL	v	202	-	5,5,5	0.35	0	5,5,5	0.25	0
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	6 (7%)
32	PL9	d	405[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.61	16 (23%)
24	CLA	C	510	-	65,73,73	2.10	16 (24%)	76,113,113	2.65	28 (36%)
28	GOL	A	414	-	5,5,5	0.46	0	5,5,5	0.53	0
28	GOL	C	525	-	5,5,5	0.39	0	5,5,5	0.67	0
28	GOL	C	524	-	5,5,5	0.38	0	5,5,5	0.77	0
24	CLA	d	403	-	65,73,73	2.04	17 (26%)	76,113,113	2.82	28 (36%)
37	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.98	5 (6%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.10	2 (3%)
24	CLA	B	610	-	65,73,73	2.04	16 (24%)	76,113,113	2.69	27 (35%)
26	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	11 (19%)
28	GOL	V	205	-	5,5,5	0.34	0	5,5,5	0.37	0
24	CLA	b	621	-	65,73,73	2.00	15 (23%)	76,113,113	2.77	27 (35%)
24	CLA	b	618	-	65,73,73	2.12	16 (24%)	76,113,113	2.64	29 (38%)
28	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	PHO	a	420[A]	-	51,69,69	1.85	8 (15%)	47,99,99	1.96	10 (21%)
38	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.84	3 (5%)
28	GOL	v	203	-	5,5,5	0.40	0	5,5,5	0.26	0
29	LMT	a	404	-	36,36,36	0.48	1 (2%)	47,47,47	1.20	3 (6%)
36	HTG	C	523	-	19,19,19	1.03	2 (10%)	23,24,24	1.81	4 (17%)
28	GOL	b	603	-	5,5,5	0.43	0	5,5,5	0.47	0
24	CLA	c	505	-	65,73,73	2.04	16 (24%)	76,113,113	2.66	26 (34%)
24	CLA	b	622	-	65,73,73	2.09	16 (24%)	76,113,113	2.67	29 (38%)
39	HEM	F	102	6,5	41,50,50	1.25	4 (9%)	45,82,82	1.95	9 (20%)
26	BCR	b	629	-	41,41,41	1.08	1 (2%)	56,56,56	1.22	6 (10%)
37	DGD	H	103	-	63,63,67	0.88	3 (4%)	77,77,81	1.05	7 (9%)
39	HEM	V	206	16	41,50,50	1.40	6 (14%)	45,82,82	1.73	9 (20%)
28	GOL	T	102	-	5,5,5	0.39	0	5,5,5	0.26	0
36	HTG	d	411	-	16,16,19	1.13	2 (12%)	20,21,24	1.90	2 (10%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.94	1 (2%)
26	BCR	a	413	-	41,41,41	1.04	1 (2%)	56,56,56	1.17	7 (12%)
36	HTG	c	524	-	19,19,19	1.04	2 (10%)	23,24,24	1.53	2 (8%)
37	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.96	2 (2%)
24	CLA	c	517	-	65,73,73	2.03	16 (24%)	76,113,113	2.76	29 (38%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.05	4 (7%)
38	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.07	3 (5%)
24	CLA	A	406	41	65,73,73	2.03	15 (23%)	76,113,113	2.89	31 (40%)
25	PHO	a	411	-	51,69,69	1.86	9 (17%)	47,99,99	1.67	8 (17%)
30	OEX	a	417[A]	3,1,41	0,15,15	-	-	-		
24	CLA	d	402	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	27 (35%)
24	CLA	B	609	-	65,73,73	2.05	17 (26%)	76,113,113	2.70	29 (38%)
29	LMT	B	635	-	25,25,36	0.51	0	30,30,47	0.87	1 (3%)
26	BCR	T	103	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	16 (28%)
26	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.61	8 (14%)
25	PHO	a	420[B]	-	51,69,69	1.86	8 (15%)	47,99,99	1.81	9 (19%)
24	CLA	a	410	41	65,73,73	2.03	15 (23%)	76,113,113	2.80	29 (38%)
32	PL9	a	416[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.91	20 (29%)
36	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.57	2 (8%)
26	BCR	B	620	-	41,41,41	1.06	1 (2%)	56,56,56	1.52	8 (14%)
26	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.56	10 (17%)
23	BCT	a	419[A]	-	2,3,3	0.66	0	2,3,3	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	B	603	-	65,73,73	2.08	16 (24%)	76,113,113	2.84	30 (39%)
26	BCR	k	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.45	10 (17%)
26	BCR	K	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.55	13 (23%)
36	HTG	b	609	-	19,19,19	1.06	2 (10%)	23,24,24	1.23	3 (13%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.14	0
32	PL9	D	405[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.65	20 (29%)
24	CLA	b	611	41	65,73,73	2.08	15 (23%)	76,113,113	2.76	25 (32%)
26	BCR	c	527	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	9 (16%)
36	HTG	B	625	-	19,19,19	1.07	2 (10%)	23,24,24	1.87	4 (17%)
28	GOL	O	301	-	5,5,5	0.37	0	5,5,5	0.41	0
24	CLA	c	509	-	65,73,73	2.00	15 (23%)	76,113,113	2.64	26 (34%)
31	OEY	A	419[B]	3,1,41	0,16,16	-	-	-		
28	GOL	B	631	-	5,5,5	0.37	0	5,5,5	0.30	0
34	LMG	Z	101	-	37,37,55	0.95	2 (5%)	45,45,63	1.38	6 (13%)
38	LHG	a	422	-	41,41,48	1.02	2 (4%)	44,47,54	0.95	3 (6%)
36	HTG	b	632	-	19,19,19	0.77	1 (5%)	23,24,24	1.29	2 (8%)
24	CLA	B	612	-	65,73,73	1.99	16 (24%)	76,113,113	2.84	27 (35%)
28	GOL	t	102	-	5,5,5	0.47	0	5,5,5	0.16	0
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.97	4 (5%)
24	CLA	C	509	-	65,73,73	2.14	16 (24%)	76,113,113	2.75	28 (36%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.93	1 (3%)
24	CLA	a	412	-	65,73,73	2.05	15 (23%)	76,113,113	2.79	30 (39%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.13	3 (6%)
24	CLA	c	511	41	65,73,73	2.04	16 (24%)	76,113,113	2.72	24 (31%)
37	DGD	c	521	-	63,63,67	0.87	2 (3%)	77,77,81	1.08	6 (7%)
24	CLA	B	611	41	65,73,73	2.11	17 (26%)	76,113,113	2.69	30 (39%)
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.45	10 (16%)
28	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.26	0
36	HTG	c	525	-	19,19,19	1.02	2 (10%)	23,24,24	1.47	2 (8%)
24	CLA	B	616	-	65,73,73	1.99	16 (24%)	76,113,113	2.78	29 (38%)
37	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	0.92	4 (5%)
28	GOL	T	101	-	5,5,5	0.50	0	5,5,5	0.19	0
24	CLA	B	604	-	65,73,73	2.09	17 (26%)	76,113,113	2.77	26 (34%)
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	1.01	3 (6%)
24	CLA	b	620	41	65,73,73	2.07	16 (24%)	76,113,113	2.73	27 (35%)
28	GOL	V	201	35	5,5,5	0.36	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	20 (29%)
24	CLA	C	512	-	65,73,73	2.03	16 (24%)	76,113,113	2.75	26 (34%)
28	GOL	A	415	-	5,5,5	0.41	0	5,5,5	0.21	0
34	LMG	D	412	40	51,51,55	0.89	2 (3%)	59,59,63	1.00	3 (5%)
23	BCT	a	419[B]	21	2,3,3	0.66	0	2,3,3	0.74	0
26	BCR	b	628	-	41,41,41	0.96	1 (2%)	56,56,56	1.34	9 (16%)
39	HEM	e	102	6,5	41,50,50	1.28	5 (12%)	45,82,82	1.77	9 (20%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	8 (14%)
26	BCR	H	102	-	41,41,41	1.10	1 (2%)	56,56,56	1.44	9 (16%)
28	GOL	b	607	-	5,5,5	0.37	0	5,5,5	0.31	0
28	GOL	v	201	-	5,5,5	0.34	0	5,5,5	0.25	0
26	BCR	A	411	-	41,41,41	1.04	1 (2%)	56,56,56	1.21	5 (8%)
32	PL9	D	405[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.71	20 (29%)
24	CLA	c	514	-	65,73,73	2.07	16 (24%)	76,113,113	2.74	29 (38%)
25	PHO	A	409[A]	-	51,69,69	1.88	8 (15%)	47,99,99	1.82	9 (19%)
24	CLA	C	501	-	65,73,73	2.03	16 (24%)	76,113,113	2.73	25 (32%)
34	LMG	j	101	40	51,51,55	0.92	2 (3%)	59,59,63	0.94	4 (6%)
24	CLA	b	623	-	65,73,73	2.08	16 (24%)	76,113,113	2.66	26 (34%)
36	HTG	b	633	-	19,19,19	1.16	2 (10%)	23,24,24	1.91	4 (17%)
27	SQD	a	414	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	12 (19%)
24	CLA	B	605	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	26 (34%)
28	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.28	0
24	CLA	B	606	-	65,73,73	2.00	15 (23%)	76,113,113	2.84	27 (35%)
26	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.39	8 (14%)
24	CLA	D	402	-	65,73,73	1.98	17 (26%)	76,113,113	2.84	28 (36%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	5 (6%)
24	CLA	a	409	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	32 (42%)
24	CLA	b	615	-	65,73,73	2.02	15 (23%)	76,113,113	2.90	24 (31%)
26	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.51	11 (19%)
27	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.22	4 (6%)
28	GOL	f	101	35	5,5,5	0.32	0	5,5,5	0.36	0
28	GOL	a	401	-	5,5,5	0.48	0	5,5,5	0.50	0
24	CLA	B	607	-	65,73,73	2.05	17 (26%)	76,113,113	2.82	29 (38%)
24	CLA	c	507	-	65,73,73	2.05	16 (24%)	76,113,113	2.74	25 (32%)
24	CLA	C	502	-	65,73,73	2.02	16 (24%)	76,113,113	2.69	27 (35%)
28	GOL	B	626	-	5,5,5	0.43	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	HTG	B	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.24	1 (4%)
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.05	4 (7%)
24	CLA	c	516	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	27 (35%)
24	CLA	B	617	-	65,73,73	2.04	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	C	506	-	65,73,73	2.05	16 (24%)	76,113,113	2.68	27 (35%)
25	PHO	A	409[B]	-	51,69,69	1.91	8 (15%)	47,99,99	1.75	9 (19%)
32	PL9	A	420[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
28	GOL	B	636	-	5,5,5	0.40	0	5,5,5	0.53	0
29	LMT	a	421	-	36,36,36	0.46	0	47,47,47	0.83	1 (2%)
24	CLA	C	508	-	65,73,73	2.10	16 (24%)	76,113,113	2.75	28 (36%)
24	CLA	c	513	-	65,73,73	2.11	16 (24%)	76,113,113	2.70	27 (35%)
28	GOL	c	502	-	5,5,5	0.41	0	5,5,5	0.51	0
24	CLA	B	602	41	65,73,73	2.07	14 (21%)	76,113,113	2.76	24 (31%)
25	PHO	A	408	-	51,69,69	1.82	8 (15%)	47,99,99	1.69	7 (14%)
36	HTG	b	602	-	19,19,19	0.92	1 (5%)	23,24,24	1.18	2 (8%)
39	HEM	v	205	16	41,50,50	1.29	6 (14%)	45,82,82	1.77	9 (20%)
24	CLA	C	513	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	28 (36%)
30	OEX	A	418[A]	3,1,41	0,15,15	-	-	-		
24	CLA	C	503	-	65,73,73	2.06	16 (24%)	76,113,113	2.68	24 (31%)
24	CLA	A	405	-	65,73,73	2.04	15 (23%)	76,113,113	2.67	26 (34%)
24	CLA	A	410	-	65,73,73	2.07	16 (24%)	76,113,113	2.71	32 (42%)
34	LMG	a	415	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	4 (6%)
36	HTG	V	207	-	19,19,19	1.05	2 (10%)	23,24,24	1.25	3 (13%)
24	CLA	b	613	-	65,73,73	2.01	16 (24%)	76,113,113	2.75	30 (39%)
24	CLA	B	615	-	65,73,73	2.01	16 (24%)	76,113,113	2.86	28 (36%)
24	CLA	B	608	41	65,73,73	2.03	16 (24%)	76,113,113	2.74	30 (39%)
24	CLA	A	407	41	65,73,73	2.01	16 (24%)	76,113,113	2.77	29 (38%)
28	GOL	b	604	-	5,5,5	0.36	0	5,5,5	0.25	0
24	CLA	c	512	-	65,73,73	2.08	16 (24%)	76,113,113	2.69	29 (38%)
28	GOL	c	501	-	5,5,5	0.32	0	5,5,5	0.31	0
29	LMT	f	103	-	36,36,36	0.46	0	47,47,47	0.83	1 (2%)
34	LMG	c	522	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	5 (8%)
24	CLA	b	612	-	65,73,73	2.05	17 (26%)	76,113,113	2.79	27 (35%)
24	CLA	b	619	-	65,73,73	2.03	15 (23%)	76,113,113	2.77	27 (35%)
37	DGD	D	406	-	52,52,67	1.00	3 (5%)	60,60,81	1.16	4 (6%)
24	CLA	b	625	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	PL9	A	420[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.76	22 (32%)
29	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.92	1 (2%)
29	LMT	M	104	-	36,36,36	0.46	0	47,47,47	0.87	1 (2%)
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	0.99	1 (2%)
36	HTG	B	624	-	19,19,19	0.83	1 (5%)	23,24,24	1.48	3 (13%)
24	CLA	B	613	-	65,73,73	2.04	16 (24%)	76,113,113	2.88	28 (36%)
24	CLA	D	403	-	65,73,73	2.06	17 (26%)	76,113,113	2.77	28 (36%)
36	HTG	B	632	-	19,19,19	1.09	2 (10%)	23,24,24	1.36	3 (13%)
38	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	4 (7%)
24	CLA	b	614	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	26 (34%)
28	GOL	B	627	-	5,5,5	0.33	0	5,5,5	0.44	0
24	CLA	c	510	-	65,73,73	2.05	16 (24%)	76,113,113	2.73	27 (35%)
24	CLA	C	505	-	65,73,73	2.03	16 (24%)	76,113,113	2.64	24 (31%)
38	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	4 (7%)

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
28	GOL	B	629	-	-	1/4/4/4	-
38	LHG	E	101	-	-	20/46/46/53	-
26	BCR	t	101	-	-	2/29/63/63	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	B	614	-	1/1/15/20	3/37/115/115	-
27	SQD	A	416	-	-	15/49/69/69	0/1/1/1
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
28	GOL	o	301	-	-	0/4/4/4	-
34	LMG	A	422	-	-	20/46/66/70	0/1/1/1
34	LMG	b	630	-	-	10/46/66/70	0/1/1/1
36	HTG	H	101	-	-	0/7/27/30	0/1/1/1
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
34	LMG	z	101	-	-	14/34/54/70	0/1/1/1
28	GOL	V	204	-	-	1/4/4/4	-
37	DGD	e	101	-	-	27/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	626	-	1/1/15/20	9/37/115/115	-
28	GOL	A	413	-	-	1/4/4/4	-
32	PL9	d	405[A]	-	-	8/53/73/73	0/1/1/1
28	GOL	V	203	-	-	2/4/4/4	-
36	HTG	b	608	-	-	1/10/30/30	0/1/1/1
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
34	LMG	C	519	-	-	13/46/66/70	0/1/1/1
28	GOL	b	605	-	-	1/4/4/4	-
24	CLA	b	616	-	1/1/15/20	9/37/115/115	-
24	CLA	b	624	-	1/1/15/20	19/37/115/115	-
27	SQD	f	102	-	-	14/38/58/69	0/1/1/1
27	SQD	A	412	-	-	8/49/69/69	0/1/1/1
34	LMG	c	523	-	-	3/46/66/70	0/1/1/1
29	LMT	b	631	-	-	4/17/37/61	0/1/1/2
36	HTG	B	633	-	-	0/10/30/30	0/1/1/1
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
24	CLA	b	617	41	1/1/15/20	0/37/115/115	-
24	CLA	c	506	-	-	4/37/115/115	-
24	CLA	C	507	41	1/1/15/20	7/37/115/115	-
34	LMG	B	622	-	-	9/46/66/70	0/1/1/1
24	CLA	C	504	41	1/1/15/20	5/37/115/115	-
24	CLA	c	515	3	1/1/15/20	6/37/115/115	-
38	LHG	D	407	-	-	13/53/53/53	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	C	511	3	1/1/15/20	3/37/115/115	-
27	SQD	b	601	-	-	22/49/69/69	0/1/1/1
24	CLA	c	508	41	1/1/15/20	5/37/115/115	-
38	LHG	d	408	-	-	11/53/53/53	-
24	CLA	d	401	41	1/1/15/20	6/37/115/115	-
28	GOL	v	202	-	-	2/4/4/4	-
37	DGD	C	516	-	-	15/51/91/95	0/2/2/2
32	PL9	d	405[B]	-	-	5/53/73/73	0/1/1/1
24	CLA	C	510	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	C	525	-	-	0/4/4/4	-
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	d	403	-	1/1/15/20	3/37/115/115	-
37	DGD	C	517	-	-	17/51/91/95	0/2/2/2
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	V	205	-	-	2/4/4/4	-
24	CLA	b	621	-	-	3/37/115/115	-
24	CLA	b	618	-	-	2/37/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
25	PHO	a	420[A]	-	-	1/37/103/103	0/5/6/6
38	LHG	D	408	-	-	12/53/53/53	-
28	GOL	v	203	-	-	2/4/4/4	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
36	HTG	C	523	-	-	3/10/30/30	0/1/1/1
28	GOL	b	603	-	-	0/4/4/4	-
24	CLA	c	505	-	1/1/15/20	2/37/115/115	-
24	CLA	b	622	-	1/1/15/20	1/37/115/115	-
39	HEM	F	102	6,5	-	7/12/54/54	-
26	BCR	b	629	-	-	0/29/63/63	0/2/2/2
37	DGD	H	103	-	-	13/51/91/95	0/2/2/2
39	HEM	V	206	16	-	4/12/54/54	-
28	GOL	T	102	-	-	2/4/4/4	-
36	HTG	d	411	-	-	1/7/27/30	0/1/1/1
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
36	HTG	c	524	-	-	3/10/30/30	0/1/1/1
37	DGD	c	520	-	-	18/51/91/95	0/2/2/2
24	CLA	c	517	-	-	4/37/115/115	-
38	LHG	L	101	-	-	17/53/53/53	-
38	LHG	D	409	-	-	12/53/53/53	-
24	CLA	A	406	41	1/1/15/20	6/37/115/115	-
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	402	-	1/1/15/20	3/37/115/115	-
24	CLA	B	609	-	-	1/37/115/115	-
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
26	BCR	T	103	-	-	3/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
25	PHO	a	420[B]	-	-	3/37/103/103	0/5/6/6
24	CLA	a	410	41	-	6/37/115/115	-
32	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/15/20	5/37/115/115	-
26	BCR	k	101	-	-	2/29/63/63	0/2/2/2
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
36	HTG	b	609	-	-	0/10/30/30	0/1/1/1
28	GOL	B	630	-	-	4/4/4/4	-
32	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
24	CLA	b	611	41	1/1/15/20	17/37/115/115	-
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
36	HTG	B	625	-	-	4/10/30/30	0/1/1/1
28	GOL	O	301	-	-	2/4/4/4	-
24	CLA	c	509	-	1/1/15/20	2/37/115/115	-
28	GOL	B	631	-	-	1/4/4/4	-
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
38	LHG	a	422	-	-	19/46/46/53	-
36	HTG	b	632	-	-	3/10/30/30	0/1/1/1
24	CLA	B	612	-	1/1/15/20	0/37/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
24	CLA	C	509	-	1/1/15/20	11/37/115/115	-
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
24	CLA	a	412	-	1/1/15/20	9/37/115/115	-
29	LMT	C	521	-	-	11/21/61/61	0/2/2/2
24	CLA	c	511	41	1/1/15/20	4/37/115/115	-
37	DGD	c	521	-	-	15/51/91/95	0/2/2/2
24	CLA	B	611	41	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
28	GOL	b	606	-	-	2/4/4/4	-
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
37	DGD	C	518	-	-	11/51/91/95	0/2/2/2
28	GOL	T	101	-	-	2/4/4/4	-
24	CLA	B	604	-	1/1/15/20	6/37/115/115	-
29	LMT	m	102	-	-	7/21/61/61	0/2/2/2
24	CLA	b	620	41	1/1/15/20	6/37/115/115	-
28	GOL	V	201	35	-	2/4/4/4	-
32	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
24	CLA	C	512	-	1/1/15/20	8/37/115/115	-
28	GOL	A	415	-	-	2/4/4/4	-
34	LMG	D	412	40	-	7/46/66/70	0/1/1/1
26	BCR	b	628	-	-	1/29/63/63	0/2/2/2
39	HEM	e	102	6,5	-	7/12/54/54	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
26	BCR	H	102	-	-	1/29/63/63	0/2/2/2
28	GOL	b	607	-	-	3/4/4/4	-
28	GOL	v	201	-	-	2/4/4/4	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
32	PL9	D	405[B]	-	-	7/53/73/73	0/1/1/1
24	CLA	c	514	-	1/1/15/20	9/37/115/115	-
25	PHO	A	409[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	C	501	-	1/1/15/20	5/37/115/115	-
34	LMG	j	101	40	-	11/46/66/70	0/1/1/1
24	CLA	b	623	-	1/1/15/20	2/37/115/115	-
36	HTG	b	633	-	-	5/10/30/30	0/1/1/1
27	SQD	a	414	-	-	14/49/69/69	0/1/1/1
24	CLA	B	605	-	1/1/15/20	6/37/115/115	-
28	GOL	a	402	-	-	2/4/4/4	-
24	CLA	B	606	-	1/1/15/20	5/37/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	D	402	-	1/1/15/20	1/37/115/115	-
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	409	-	1/1/15/20	4/37/115/115	-
24	CLA	b	615	-	1/1/15/20	4/37/115/115	-
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
27	SQD	a	405	-	-	17/49/69/69	0/1/1/1
28	GOL	f	101	35	-	3/4/4/4	-
28	GOL	a	401	-	-	0/4/4/4	-
24	CLA	B	607	-	1/1/15/20	4/37/115/115	-
24	CLA	c	507	-	-	4/37/115/115	-
24	CLA	C	502	-	1/1/15/20	8/37/115/115	-
28	GOL	B	626	-	-	1/4/4/4	-
36	HTG	B	623	-	-	4/10/30/30	0/1/1/1
38	LHG	d	406	-	-	10/53/53/53	-
24	CLA	c	516	-	1/1/15/20	9/37/115/115	-
24	CLA	B	617	-	1/1/15/20	6/37/115/115	-
24	CLA	C	506	-	1/1/15/20	8/37/115/115	-
25	PHO	A	409[B]	-	-	1/37/103/103	0/5/6/6
32	PL9	A	420[A]	-	-	10/53/73/73	0/1/1/1
28	GOL	B	636	-	-	0/4/4/4	-
29	LMT	a	421	-	-	4/21/61/61	0/2/2/2
24	CLA	C	508	-	1/1/15/20	5/37/115/115	-
24	CLA	c	513	-	1/1/15/20	11/37/115/115	-
28	GOL	c	502	-	-	1/4/4/4	-
24	CLA	B	602	41	1/1/15/20	12/37/115/115	-
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
39	HEM	v	205	16	-	4/12/54/54	-
24	CLA	C	513	-	1/1/15/20	7/37/115/115	-
24	CLA	C	503	-	1/1/15/20	2/37/115/115	-
24	CLA	A	405	-	1/1/15/20	7/37/115/115	-
24	CLA	A	410	-	1/1/15/20	7/37/115/115	-
34	LMG	a	415	-	-	16/46/66/70	0/1/1/1
36	HTG	V	207	-	-	3/10/30/30	0/1/1/1
24	CLA	b	613	-	1/1/15/20	5/37/115/115	-
24	CLA	B	615	-	1/1/15/20	15/37/115/115	-
24	CLA	B	608	41	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	407	41	-	2/37/115/115	-
28	GOL	b	604	-	-	0/4/4/4	-
24	CLA	c	512	-	1/1/15/20	4/37/115/115	-
28	GOL	c	501	-	-	0/4/4/4	-
29	LMT	f	103	-	-	10/21/61/61	0/2/2/2
34	LMG	c	522	-	-	15/46/66/70	0/1/1/1
24	CLA	b	612	-	1/1/15/20	3/37/115/115	-
24	CLA	b	619	-	1/1/15/20	4/37/115/115	-
37	DGD	D	406	-	-	21/47/67/95	0/1/1/2
24	CLA	b	625	-	1/1/15/20	4/37/115/115	-
32	PL9	A	420[B]	-	-	10/53/73/73	0/1/1/1
29	LMT	F	101	-	-	3/21/61/61	0/2/2/2
29	LMT	M	104	-	-	7/21/61/61	0/2/2/2
29	LMT	D	401	-	-	8/21/61/61	0/2/2/2
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
24	CLA	B	613	-	1/1/15/20	3/37/115/115	-
24	CLA	D	403	-	1/1/15/20	7/37/115/115	-
36	HTG	B	632	-	-	3/10/30/30	0/1/1/1
38	LHG	l	101	-	-	15/53/53/53	-
24	CLA	b	614	-	1/1/15/20	6/37/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	c	510	-	1/1/15/20	15/37/115/115	-
24	CLA	C	505	-	1/1/15/20	5/37/115/115	-
38	LHG	d	407	-	-	10/53/53/53	-

The worst 5 of 1349 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	CLA	C3B-C2B	6.68	1.49	1.40
24	B	613	CLA	C3B-C2B	6.54	1.49	1.40
24	C	509	CLA	C3B-C2B	6.51	1.49	1.40
24	B	603	CLA	C3B-C2B	6.46	1.49	1.40
25	A	409[A]	PHO	C3B-C2B	6.46	1.49	1.40

The worst 5 of 2644 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	C1D-ND-C4D	-10.41	98.94	106.33
24	a	410	CLA	C1D-ND-C4D	-10.25	99.06	106.33
24	B	613	CLA	C1D-ND-C4D	-10.11	99.15	106.33
24	B	606	CLA	C1D-ND-C4D	-9.96	99.26	106.33
24	C	503	CLA	C1D-ND-C4D	-9.86	99.33	106.33

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	410	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 1308 torsion outliers are listed below:

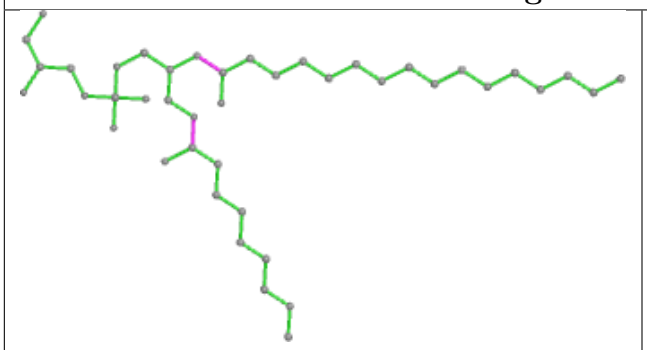
Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

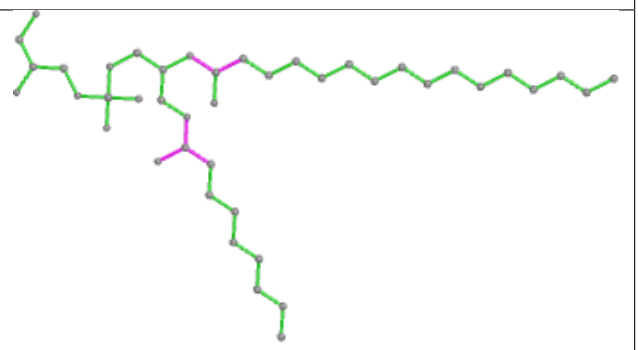
No monomer is involved in short contacts.

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

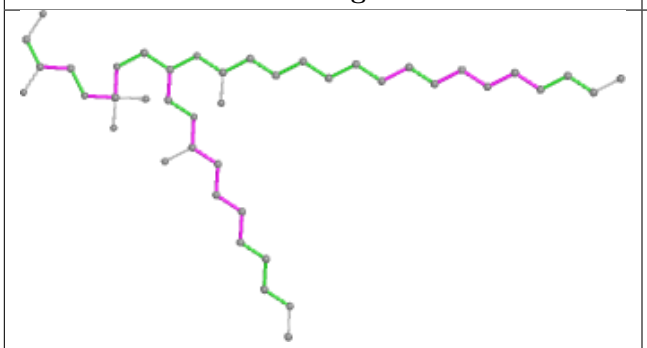
Ligand LHG E 101



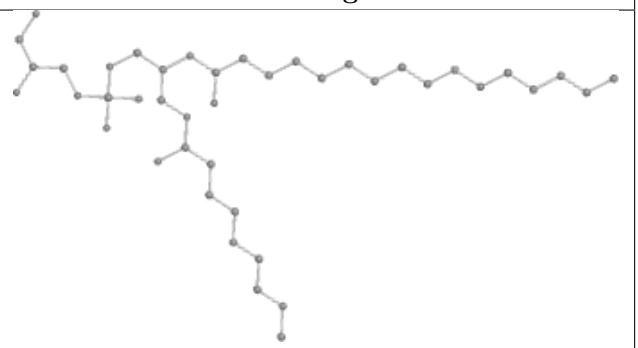
Bond lengths



Bond angles

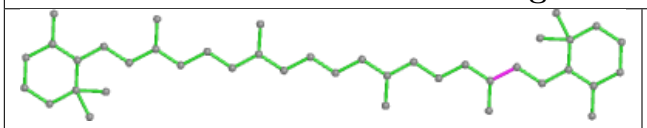


Torsions



Rings

Ligand BCR t 101



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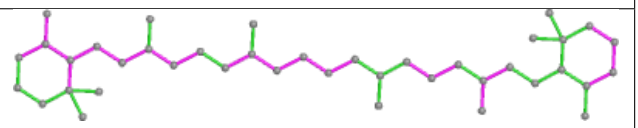
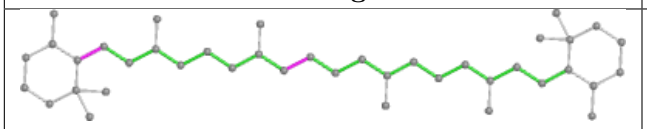
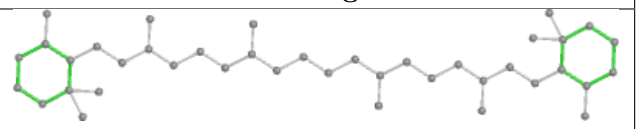


Bond angles

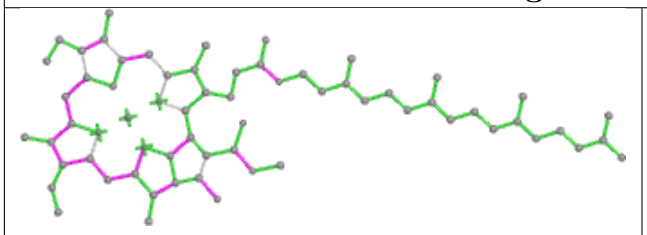


Torsions



Rings

Ligand CLA B 614



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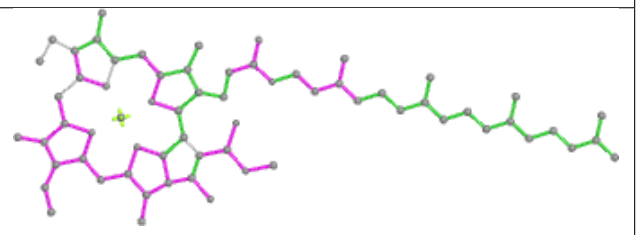
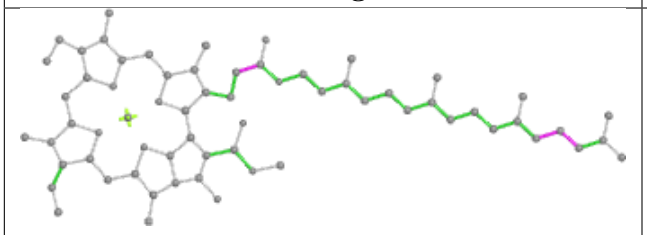


Bond angles



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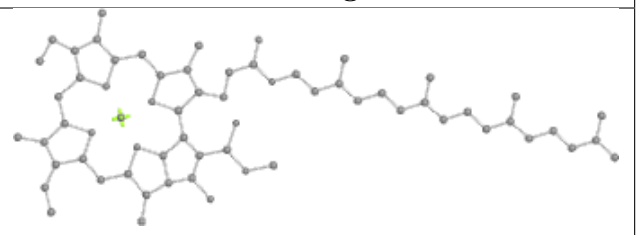
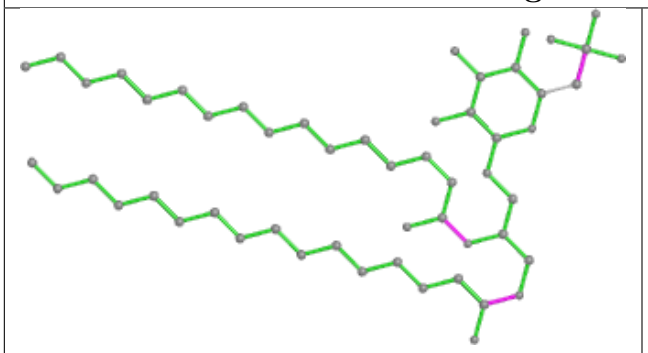
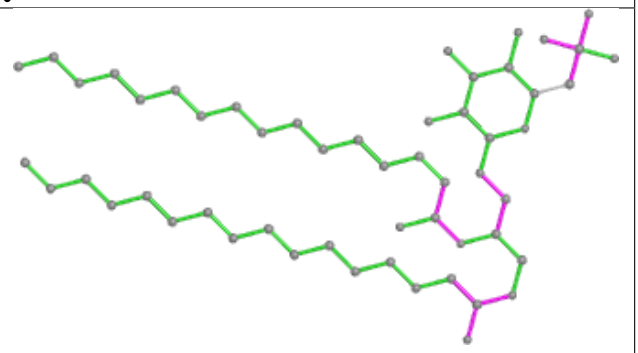


Rings

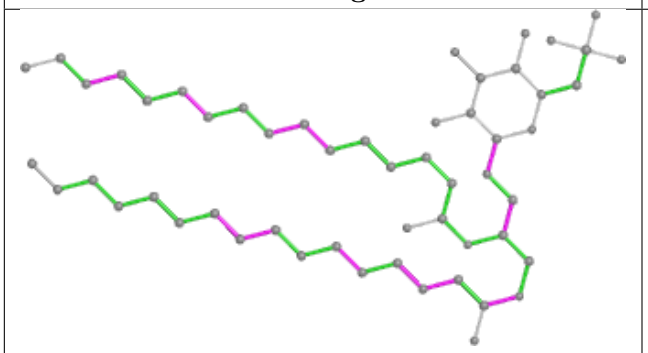
Ligand SQD A 416



Bond lengths



Bond angles



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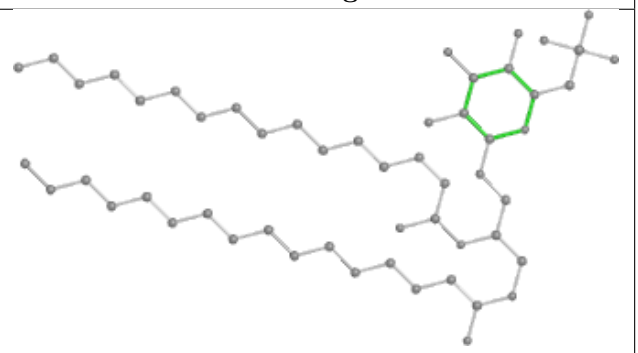
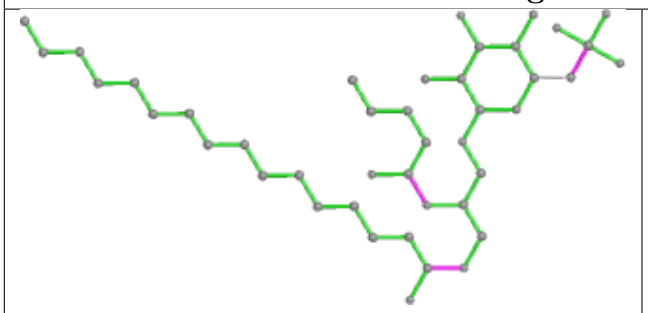


Rings

Ligand SQD F 103



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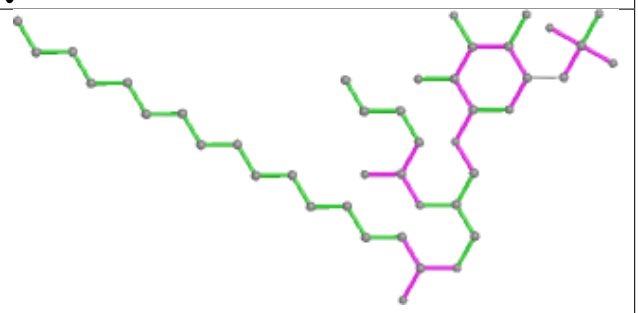
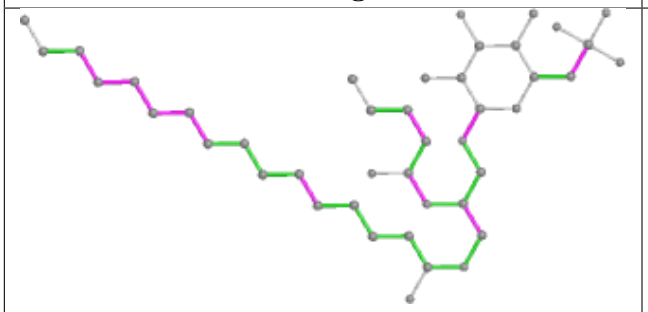


Bond angles



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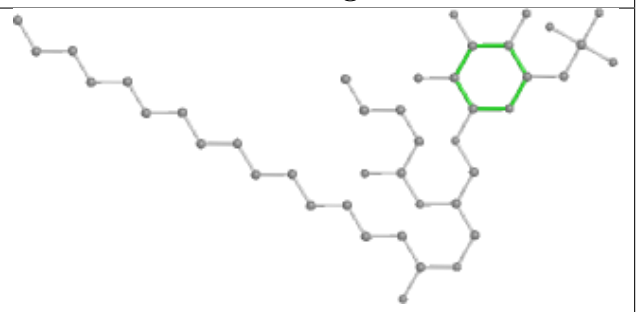
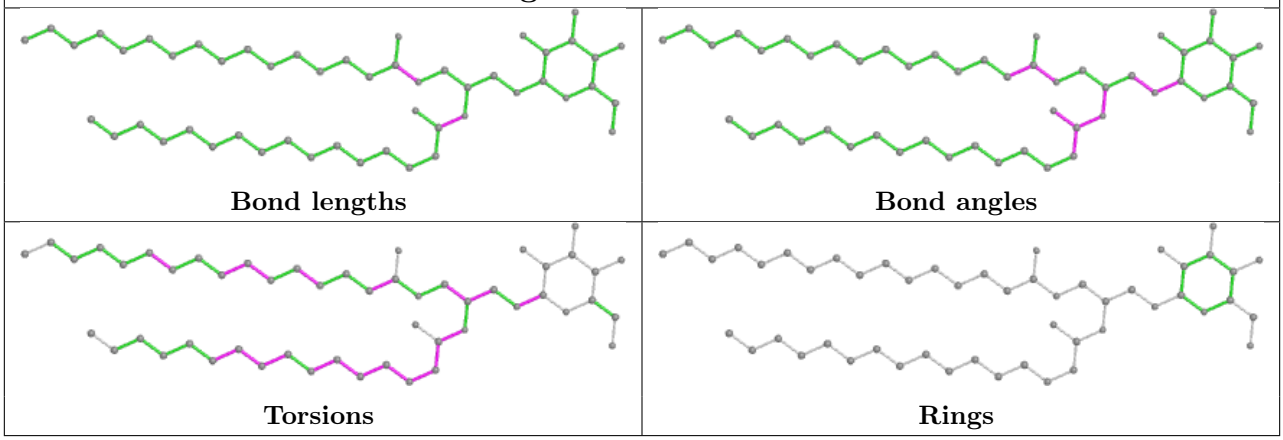
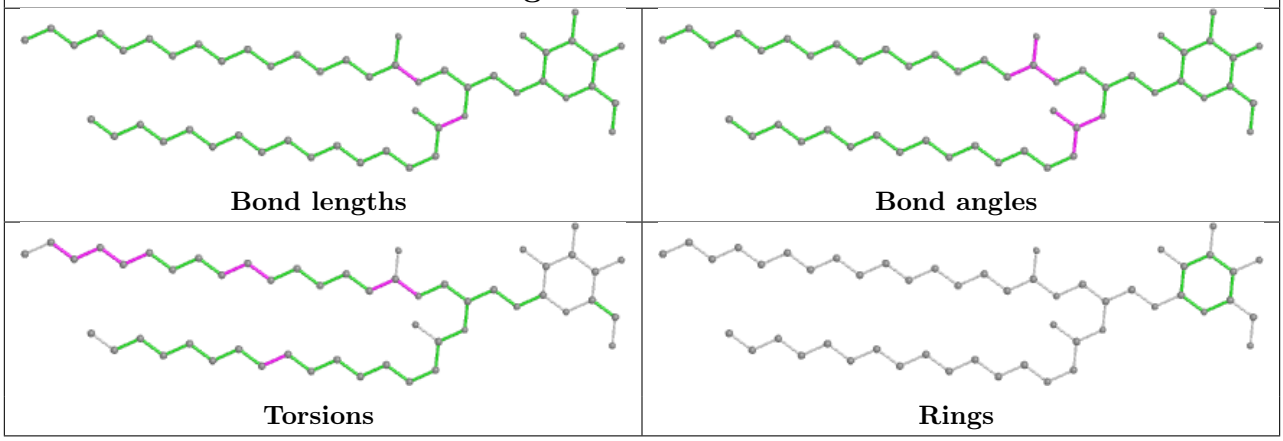


Rings

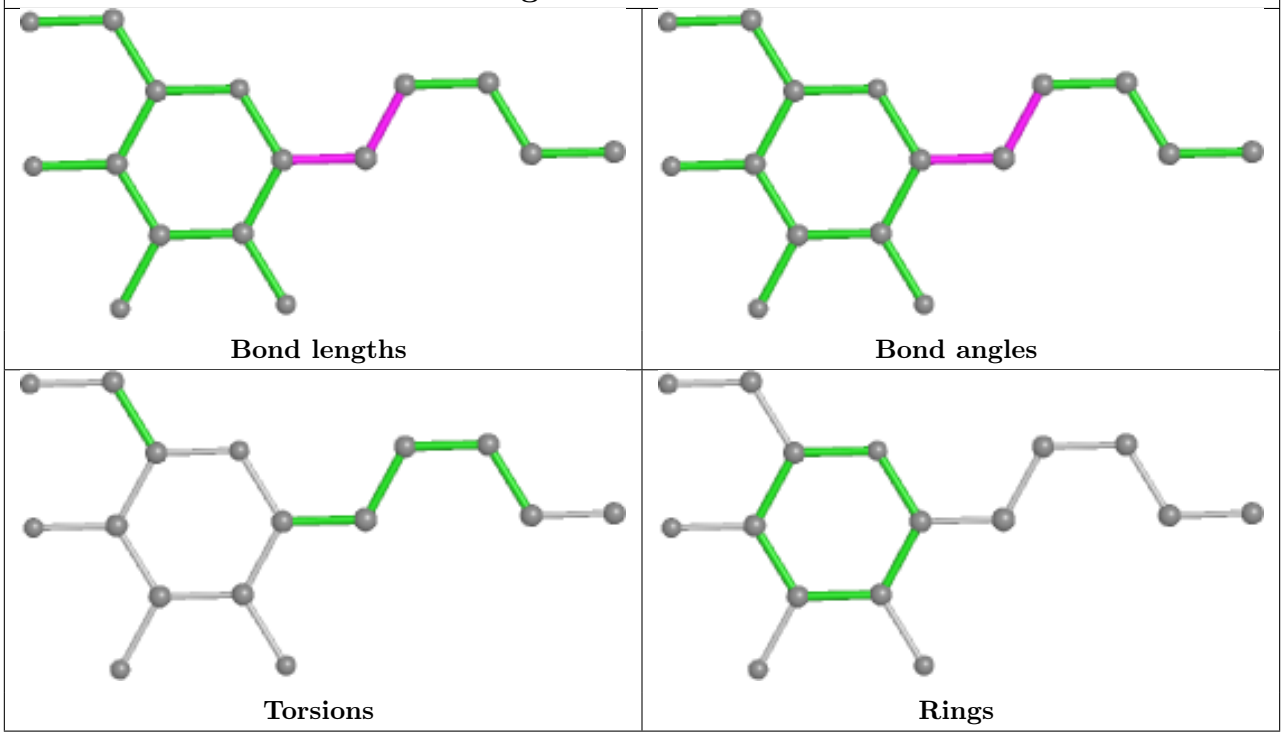
Ligand LMG A 422



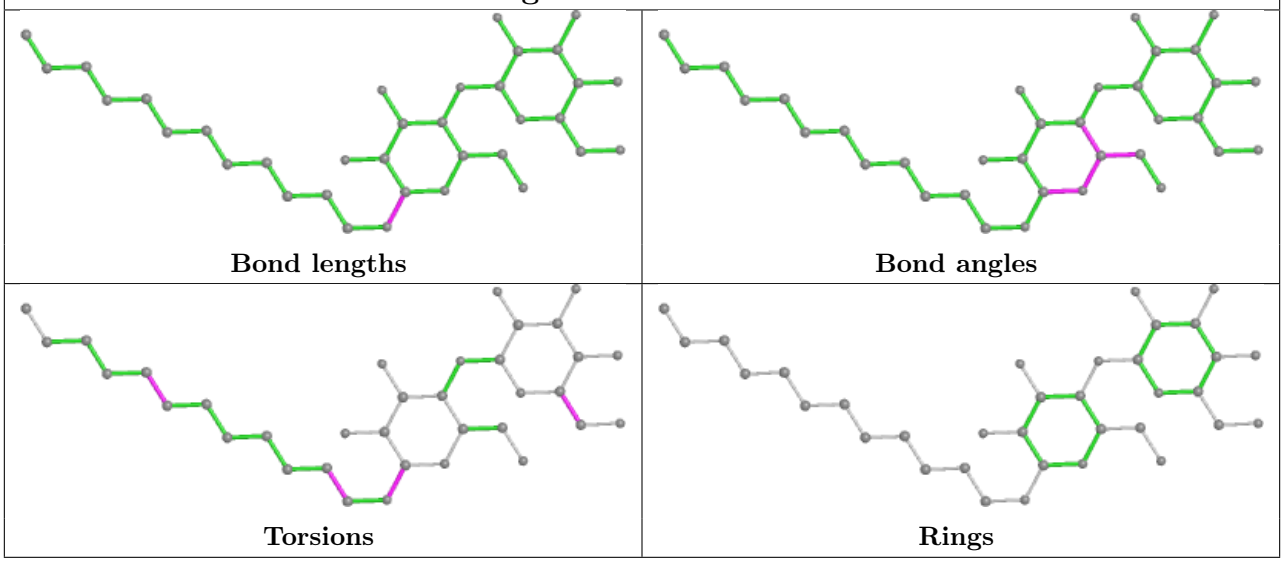
Ligand LMG b 630



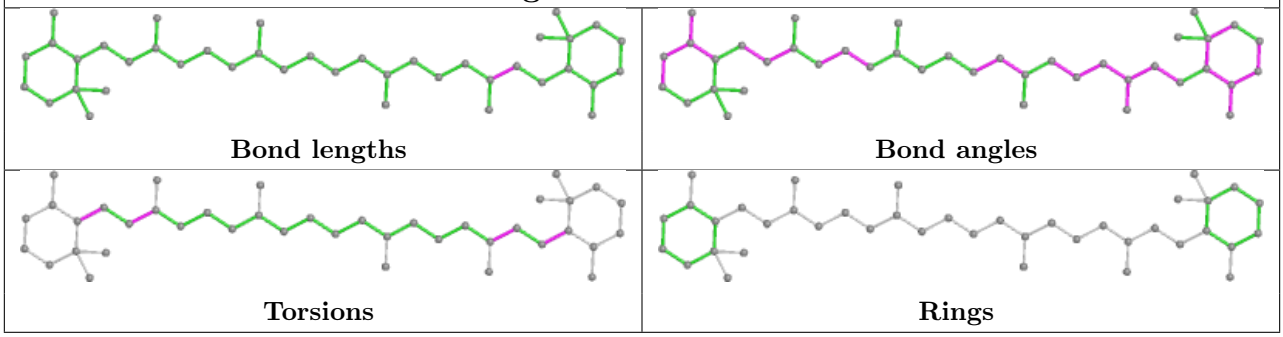
Ligand HTG H 101



Ligand LMT A 417



Ligand BCR D 404



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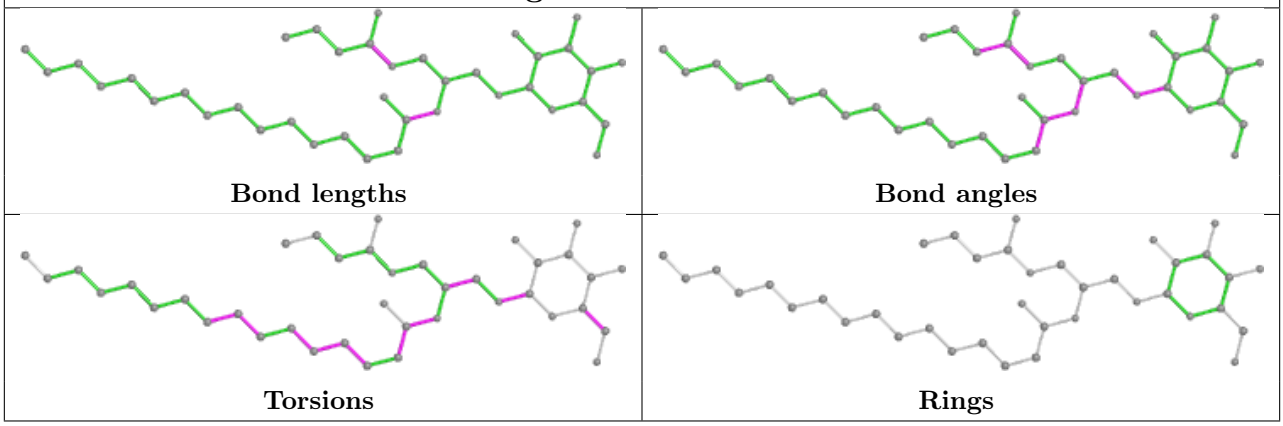
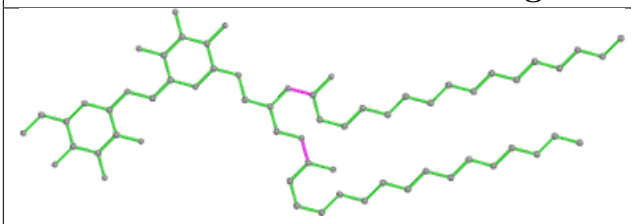
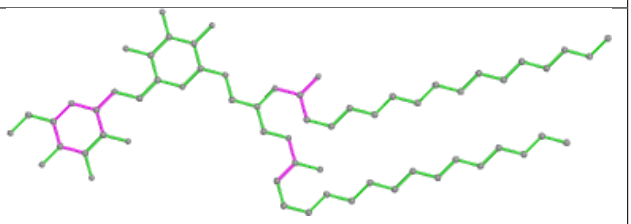


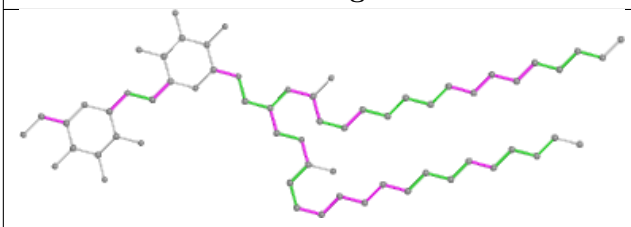
Ligand DGD e 101



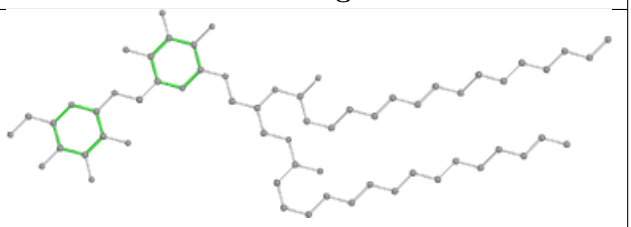
Bond lengths



Bond angles

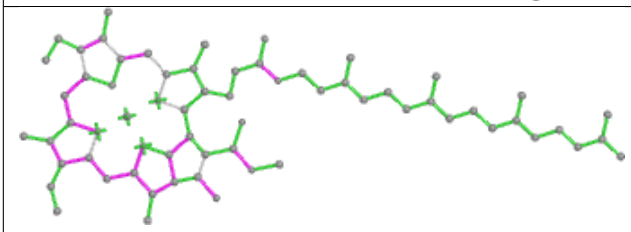


Torsions

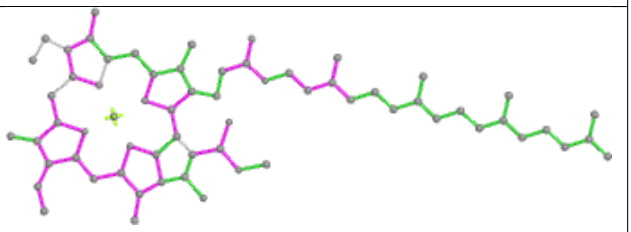


Rings

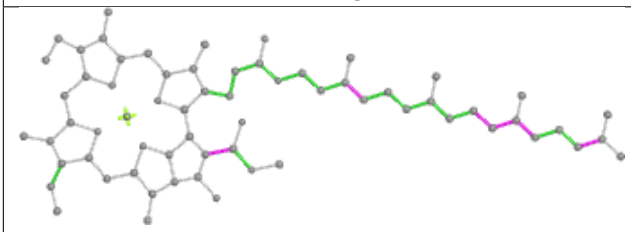
Ligand CLA b 626



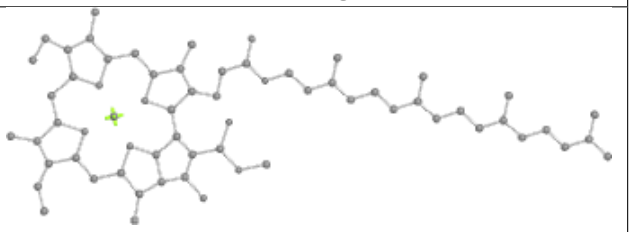
Bond lengths



Bond angles

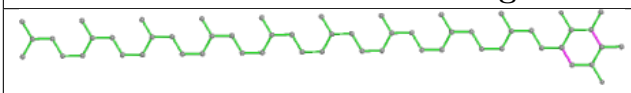


Torsions

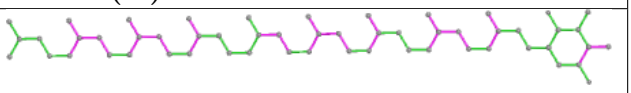


Rings

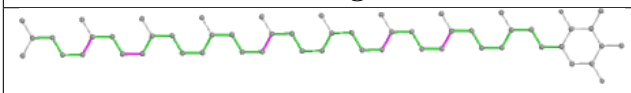
Ligand PL9 d 405 (A)



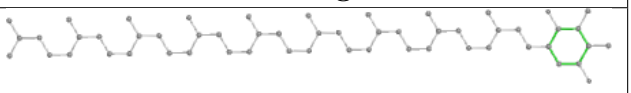
Bond lengths



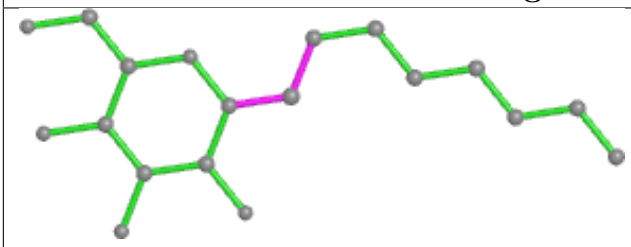
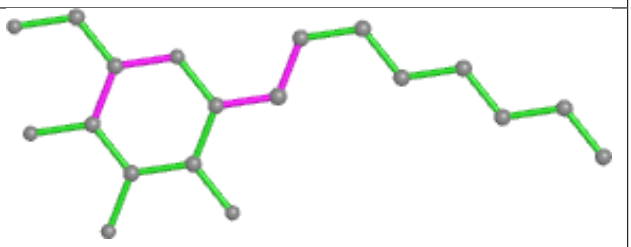
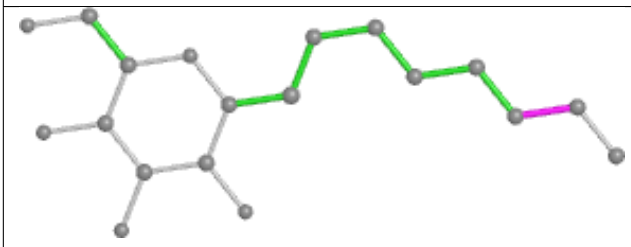
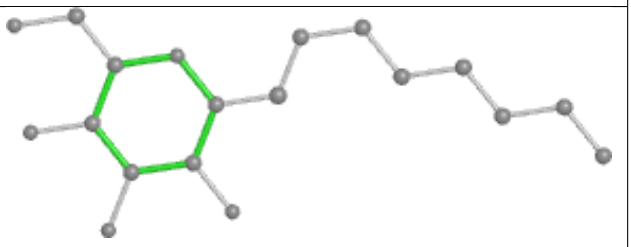
Bond angles

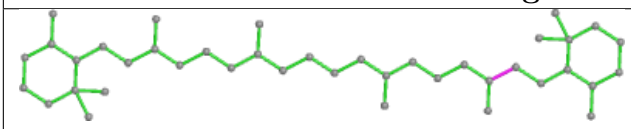
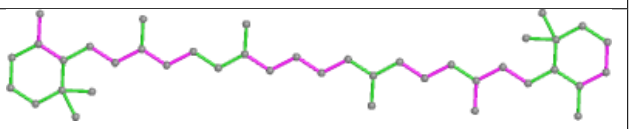
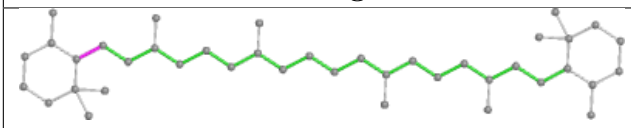
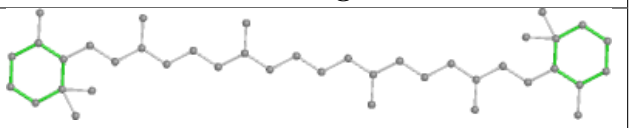


Torsions



Rings

Ligand HTG b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

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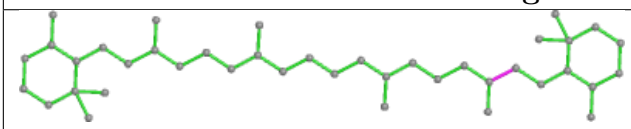
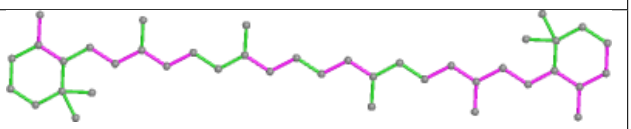
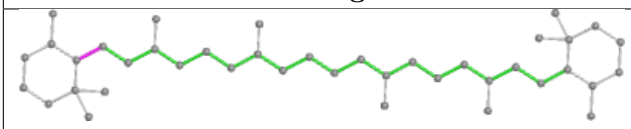
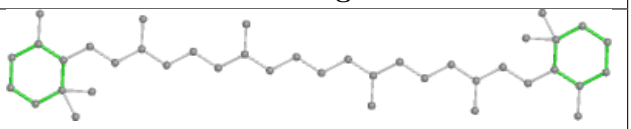
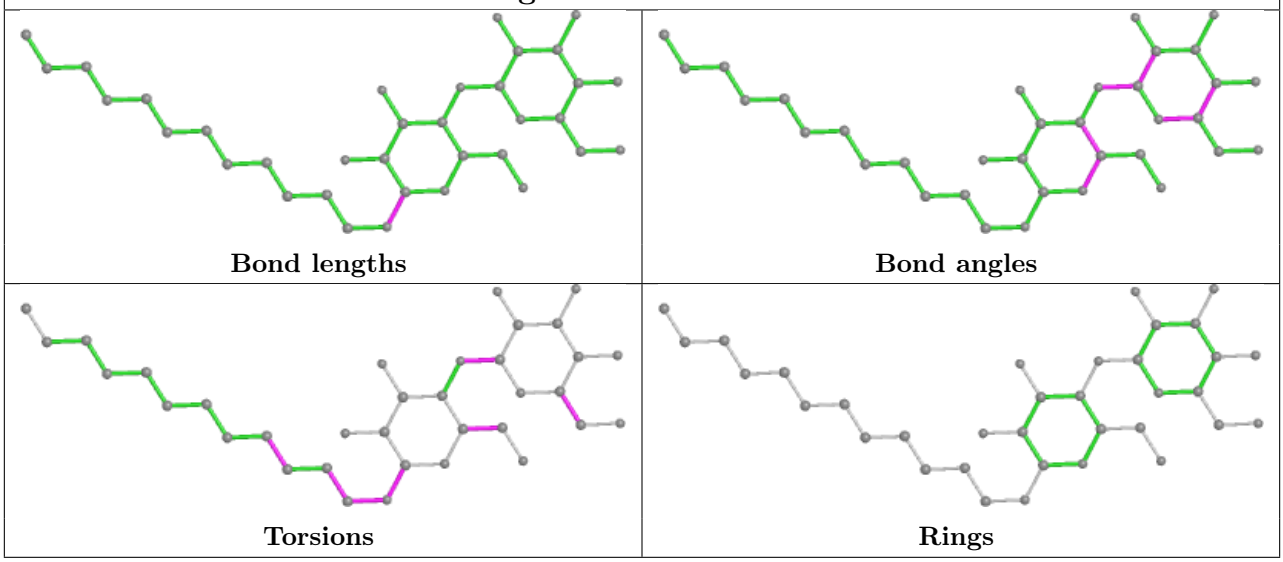
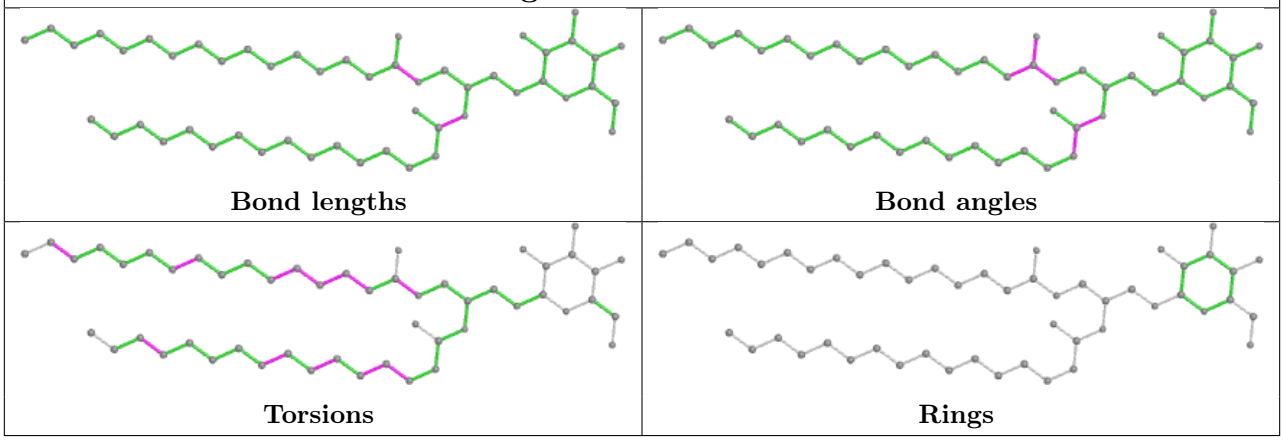
 Bond lengths	 Bond angles
 Torsions	 Rings

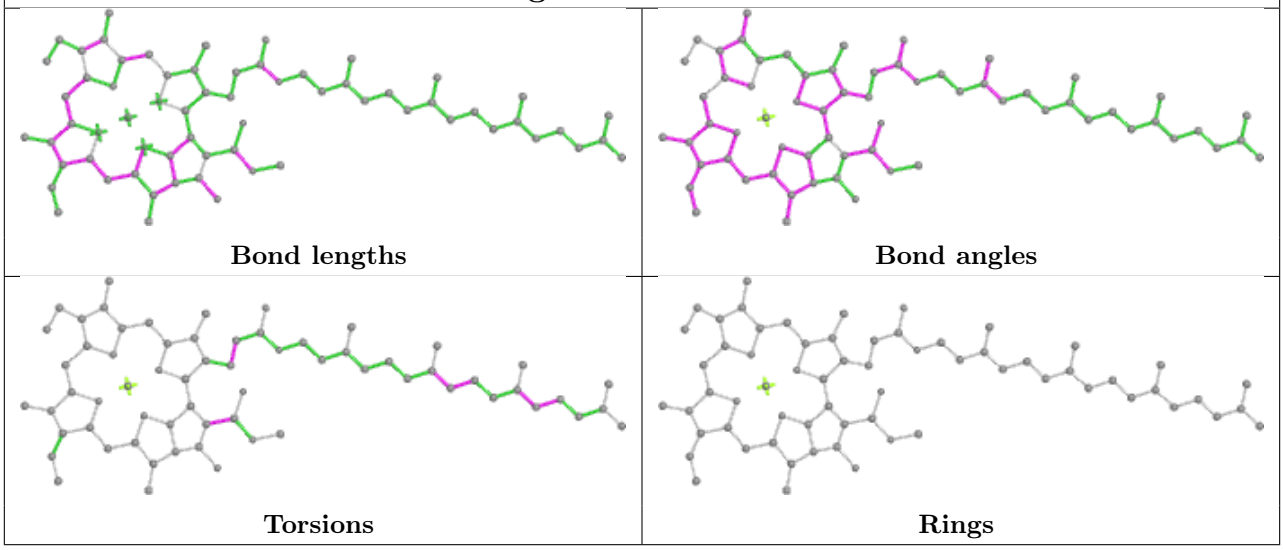
Ligand LMT M 103

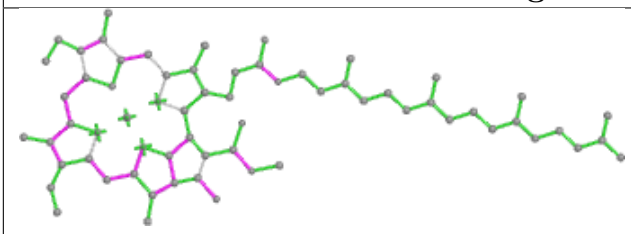
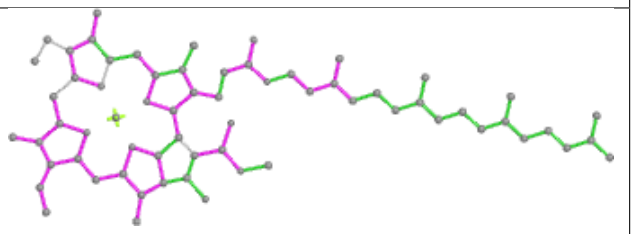
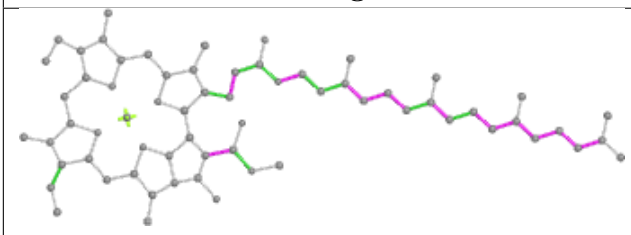
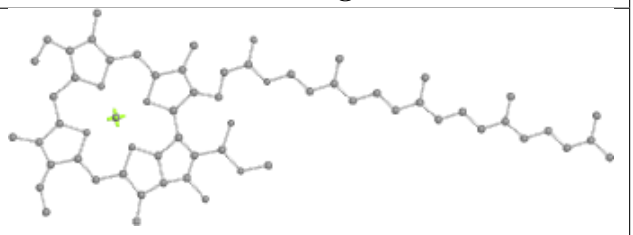


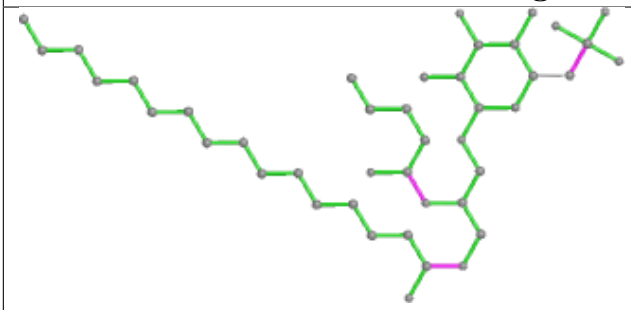
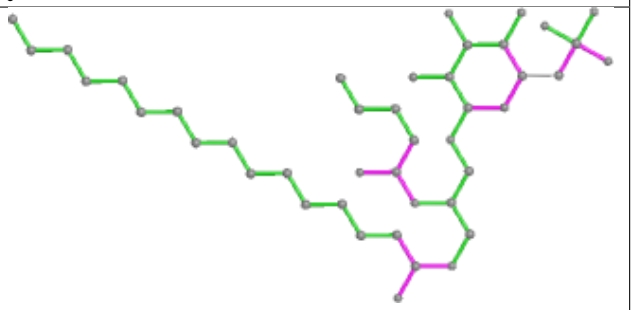
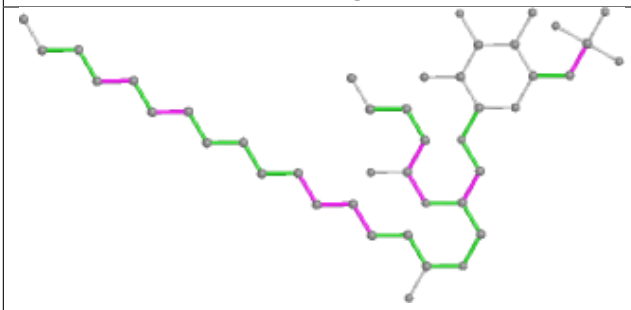
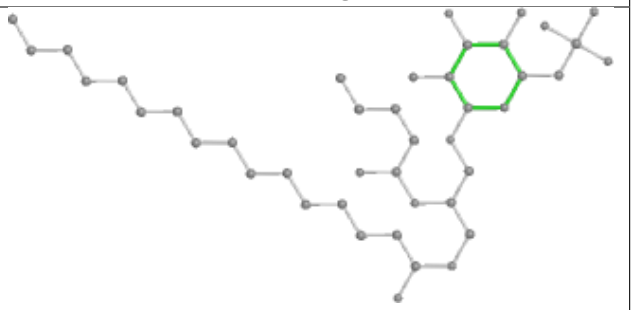
Ligand LMG C 519



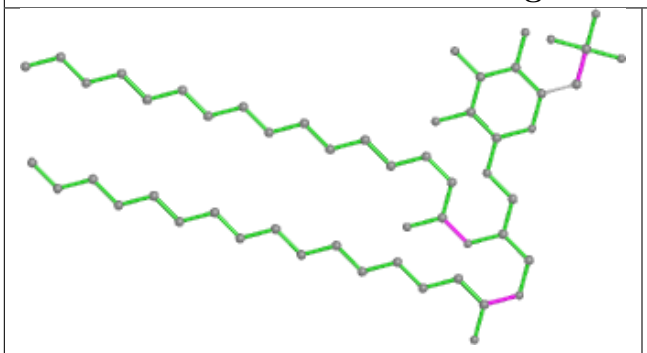
Ligand CLA b 616



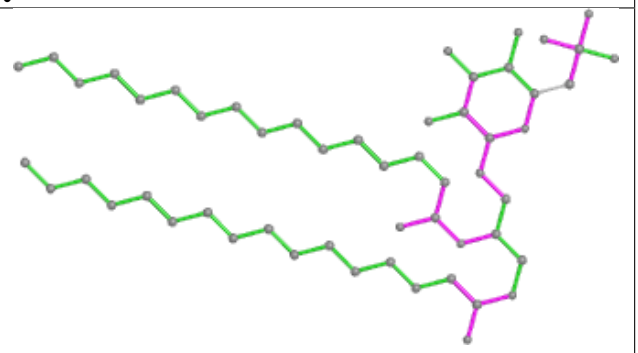
Ligand CLA b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

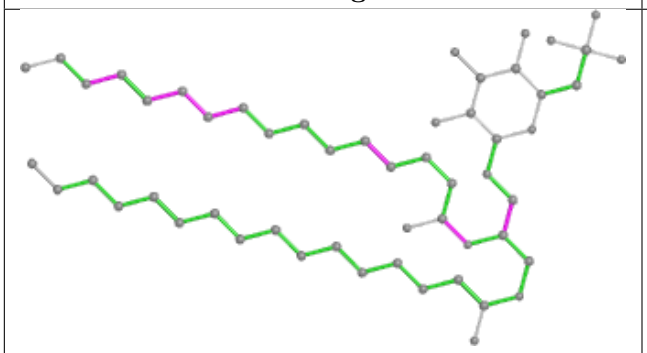
Ligand SQD A 412



Bond lengths



Bond angles



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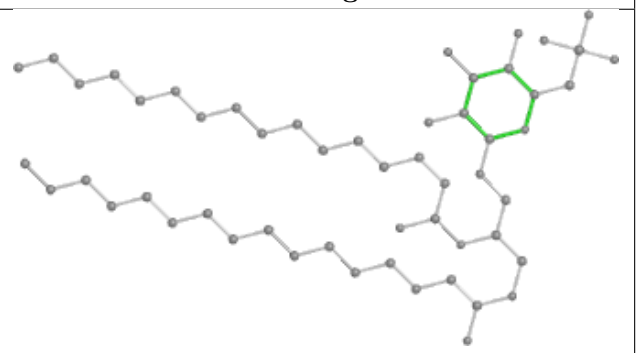
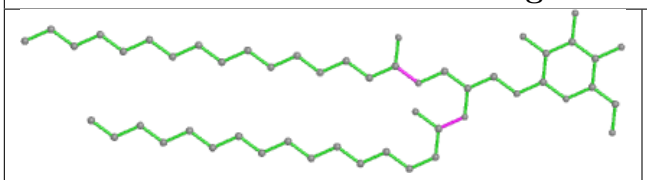


Rings

Ligand LMG c 523



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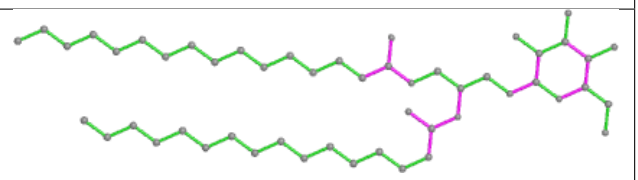

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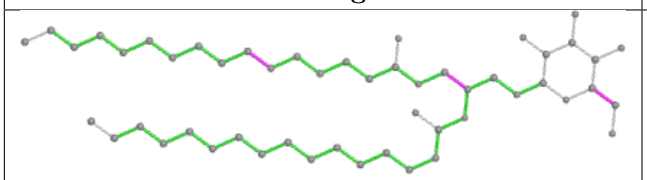

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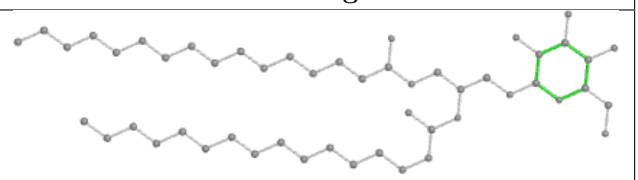
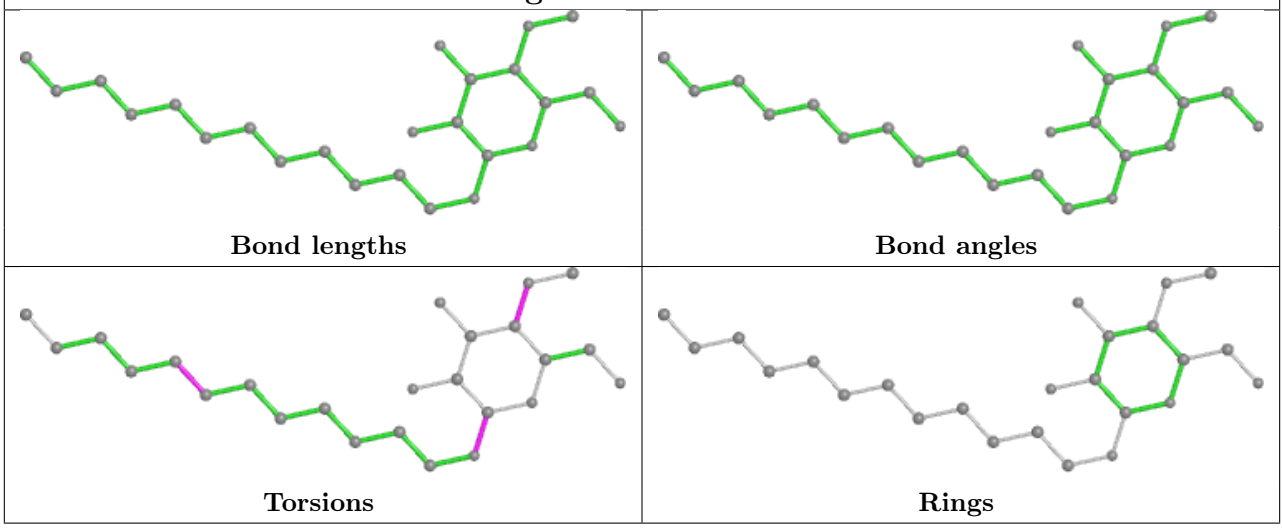
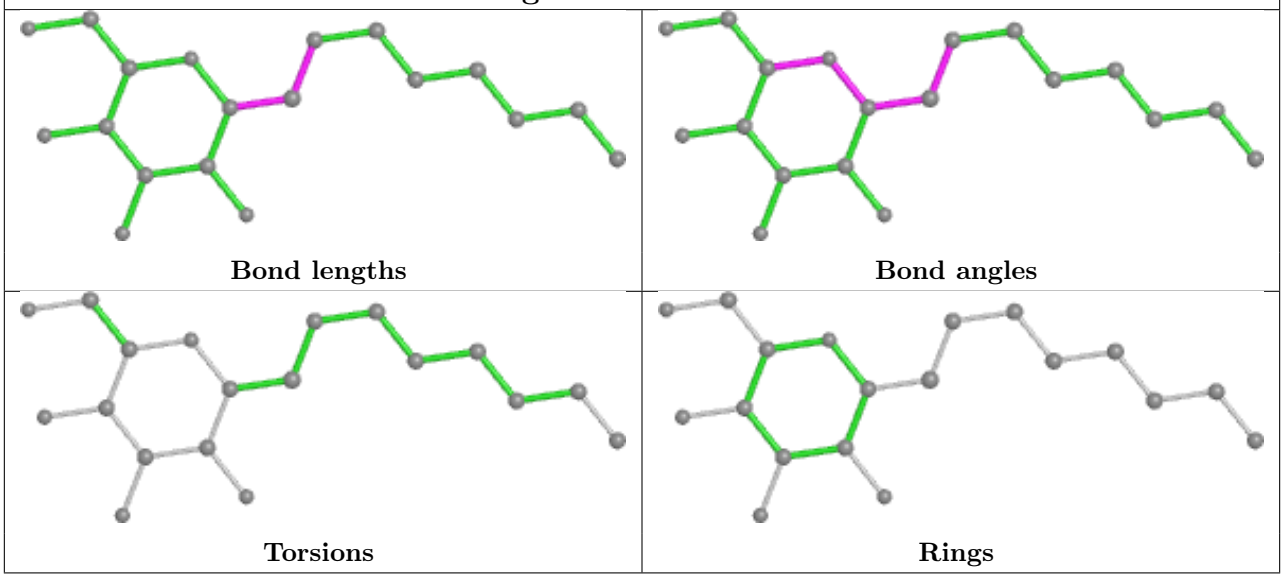


Rings

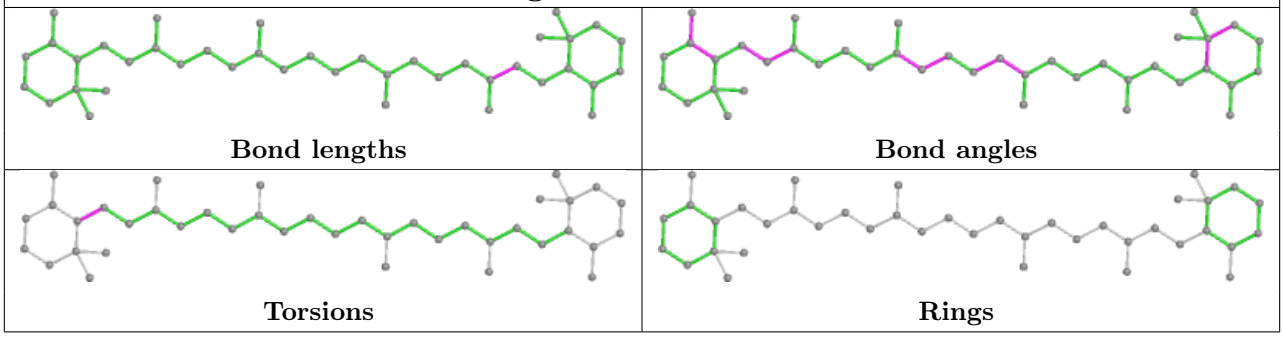
Ligand LMT b 631



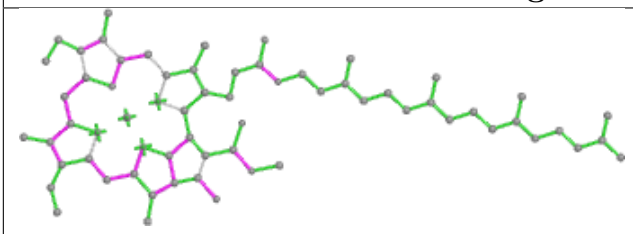
Ligand HTG B 633



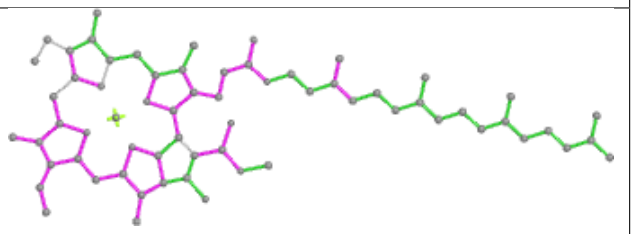
Ligand BCR b 627



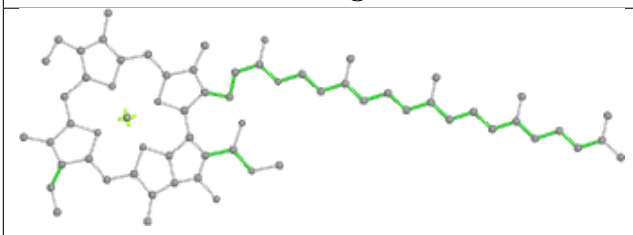
Ligand CLA b 617



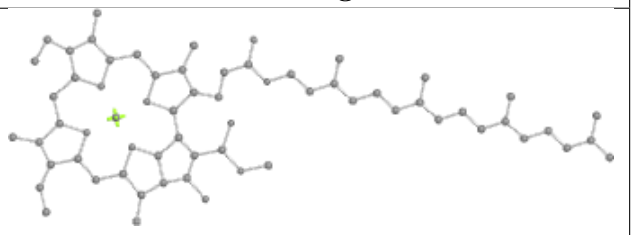
Bond lengths



Bond angles

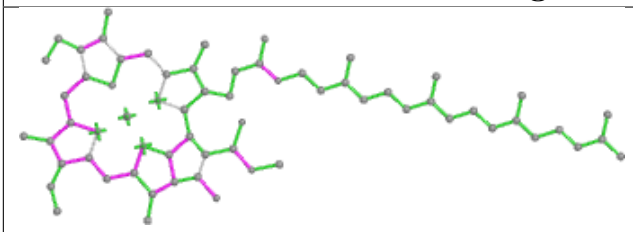


Torsions



Rings

Ligand CLA c 506



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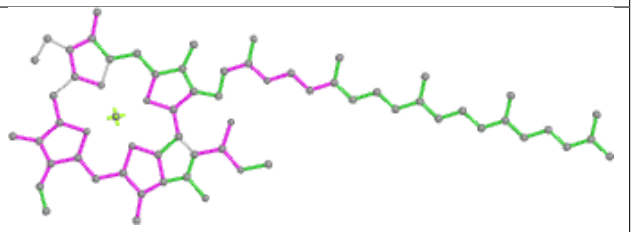
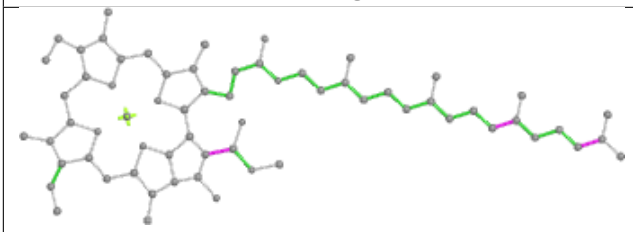


Bond angles



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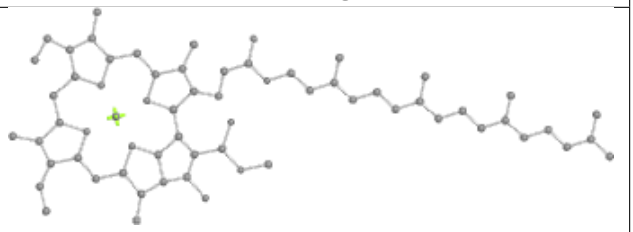
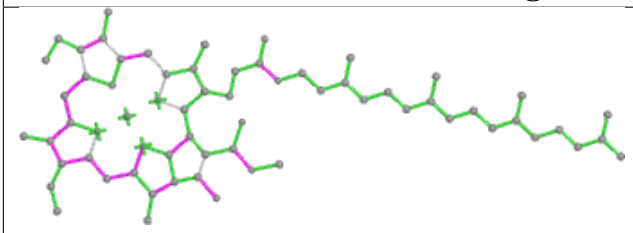


Rings

Ligand CLA C 507



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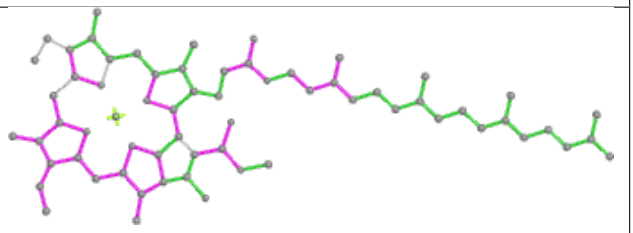

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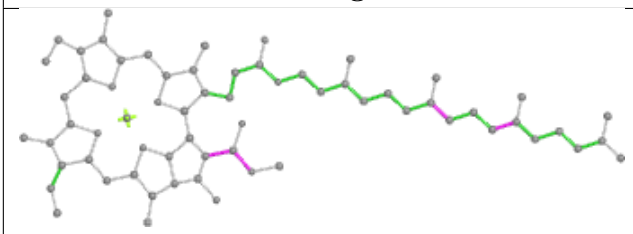

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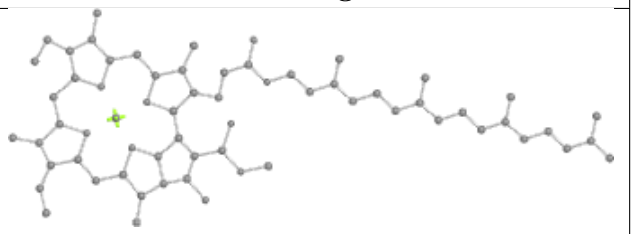
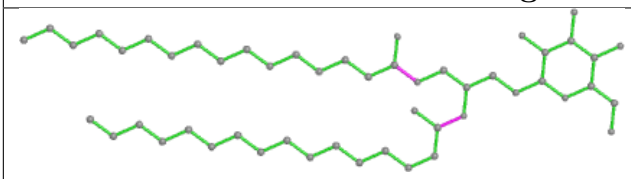


Rings

Ligand LMG B 622



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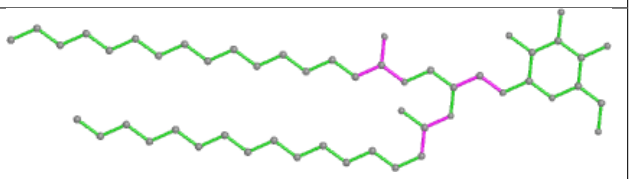
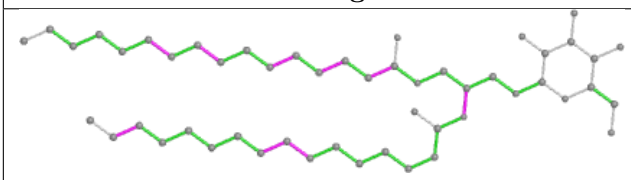


Bond angles



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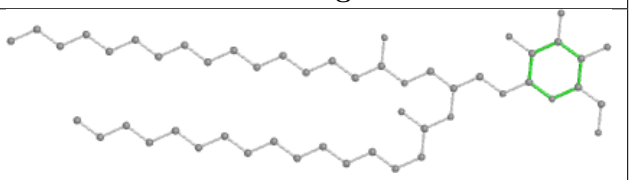
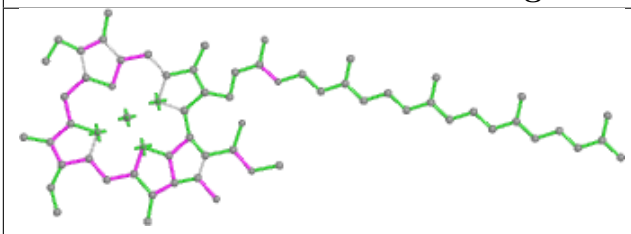


Rings

Ligand CLA C 504



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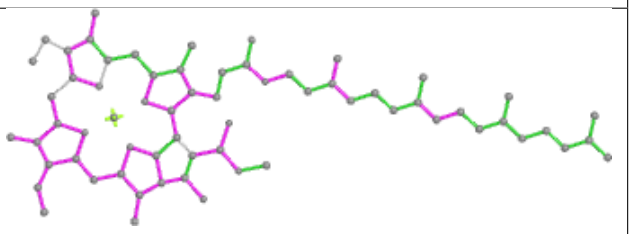
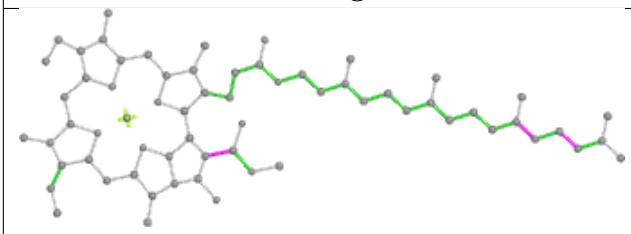


Bond angles



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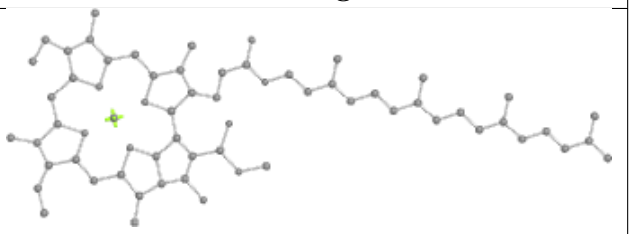
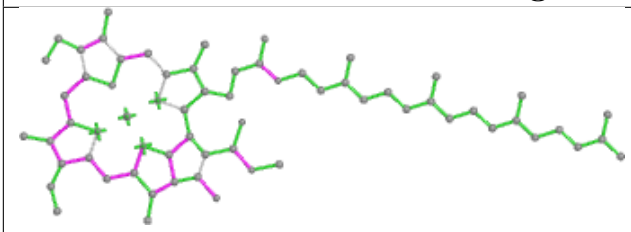


Rings

Ligand CLA c 515



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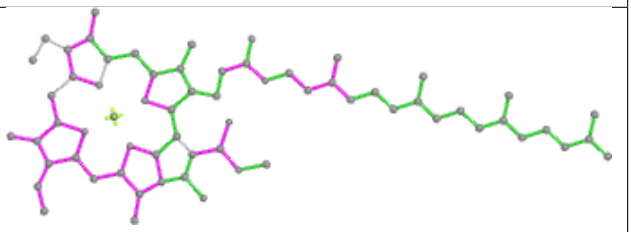
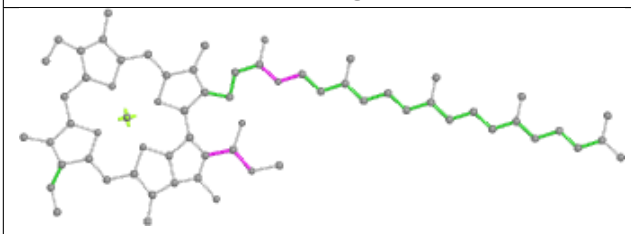
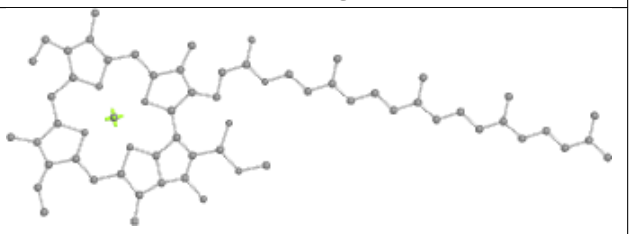


Bond angles

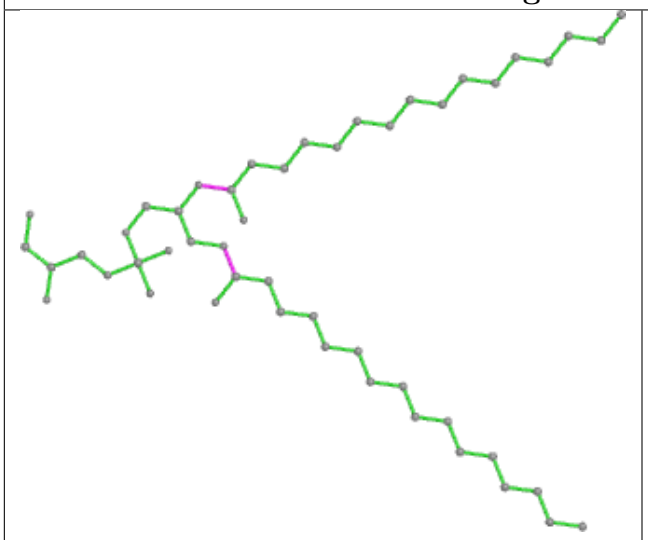


Torsions



Rings

Ligand LHG D 407



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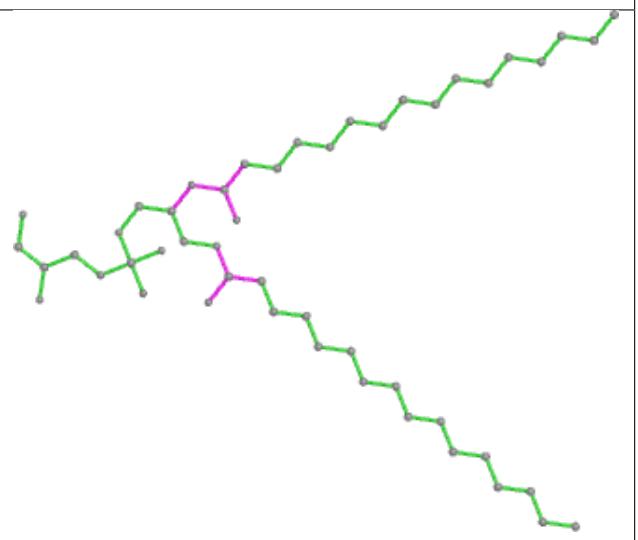
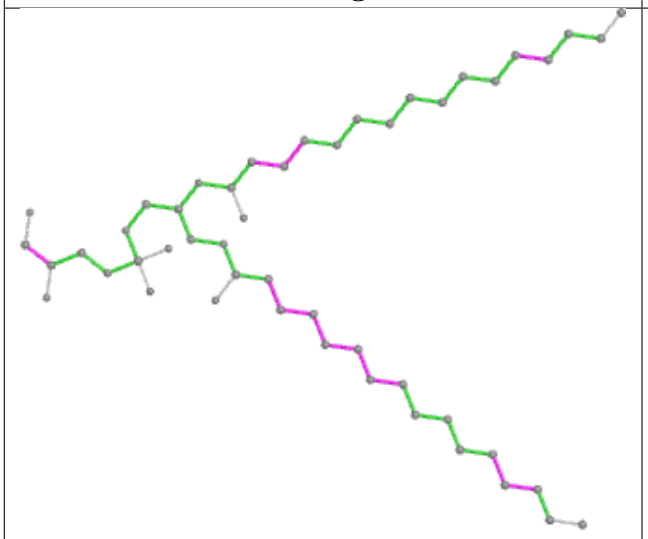
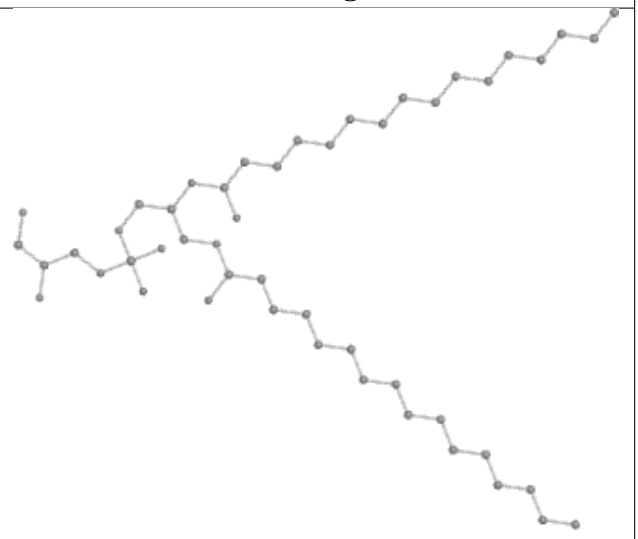


Bond angles

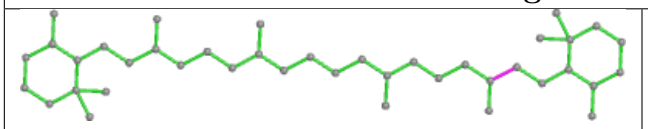


Torsions

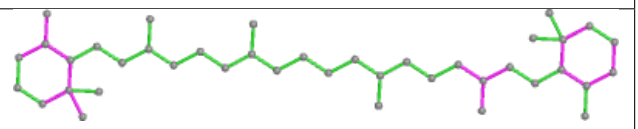


Rings

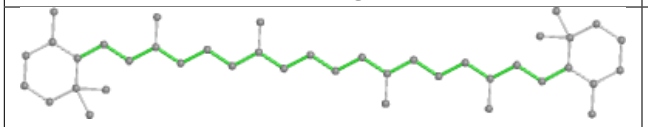
Ligand BCR B 619



Bond lengths



Bond angles



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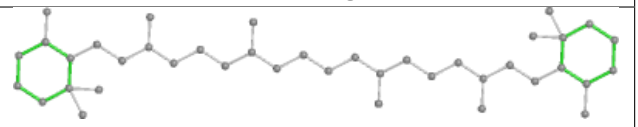
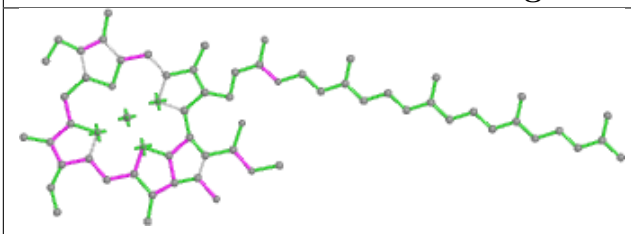
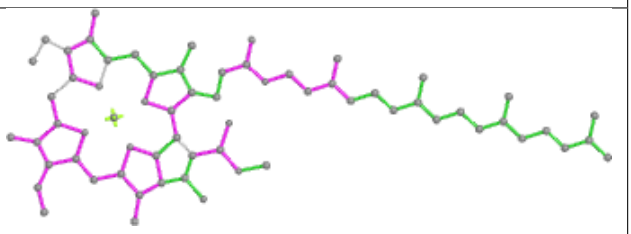


Rings

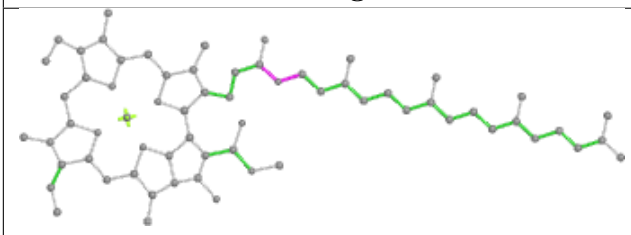
Ligand CLA C 511



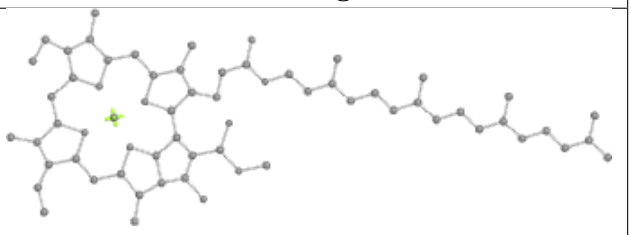
Bond lengths



Bond angles

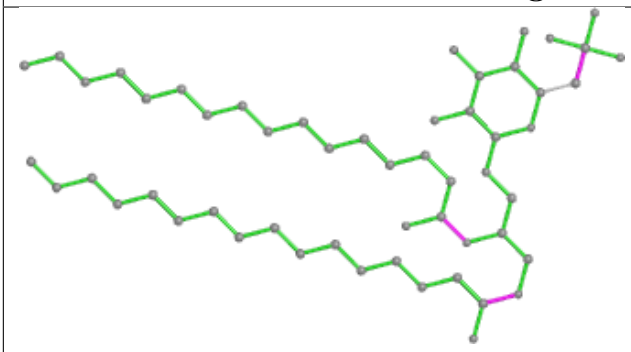


Torsions

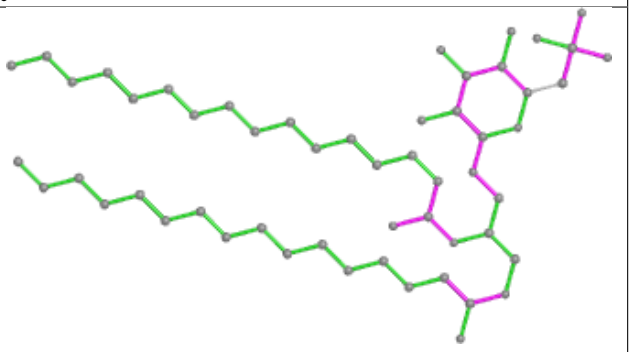


Rings

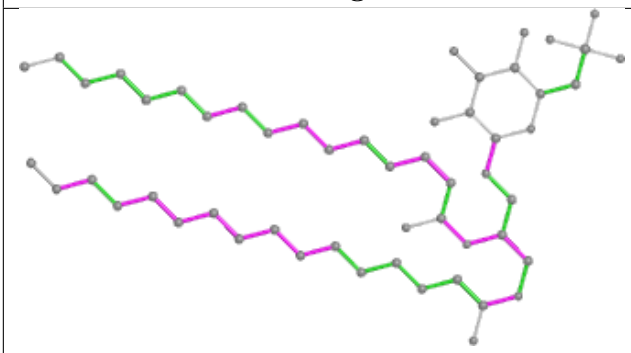
Ligand SQD b 601



Bond lengths



Bond angles



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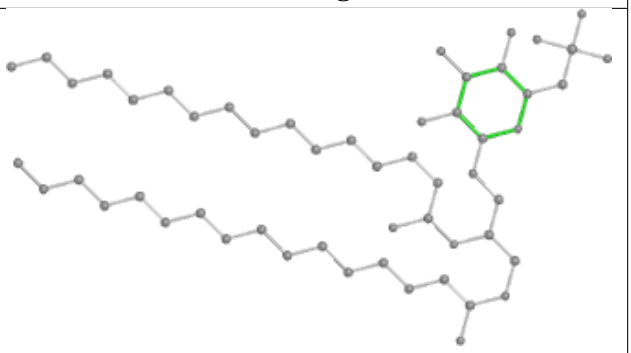
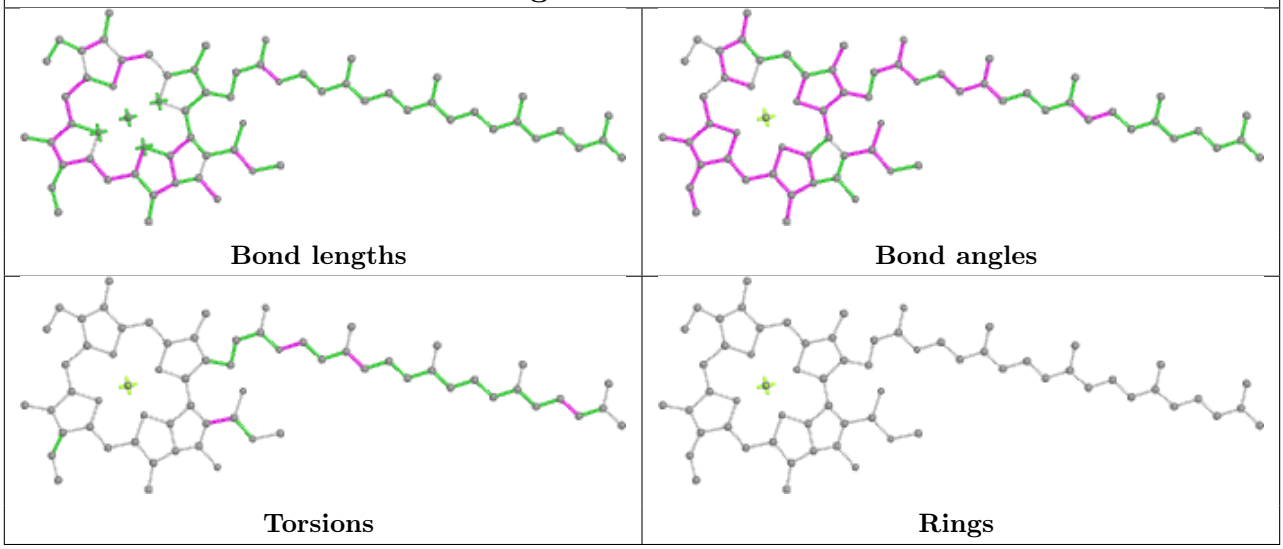
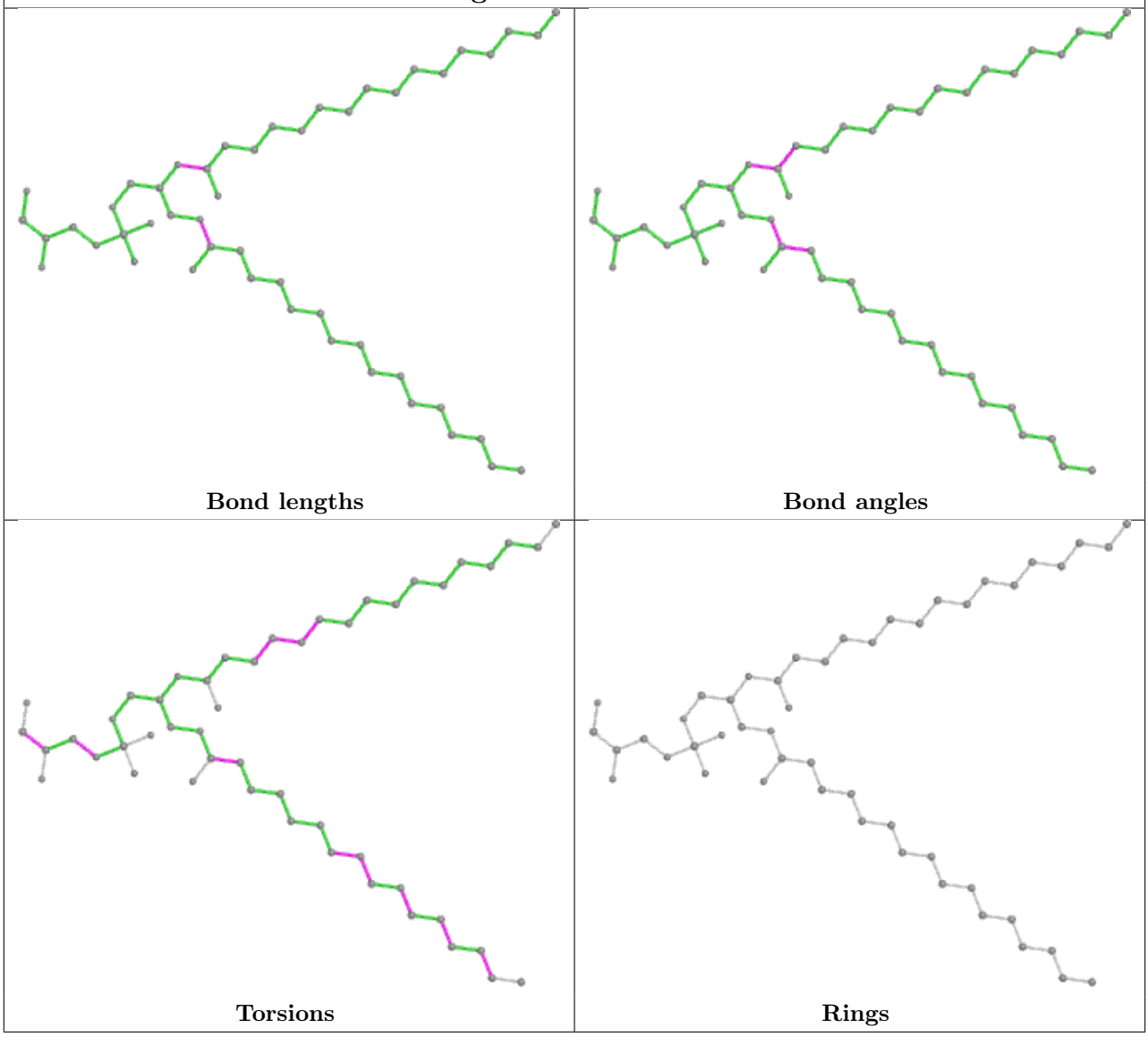


Rings

Ligand CLA c 508



Ligand LHG d 408



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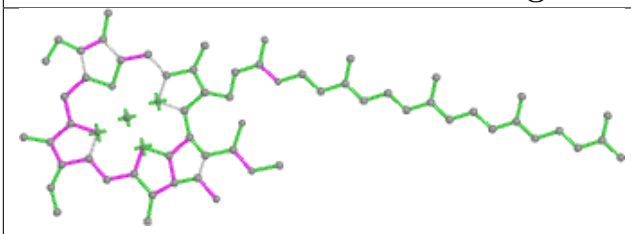
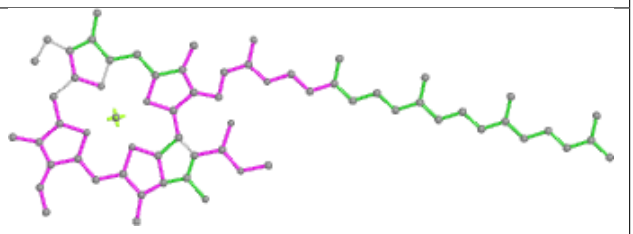
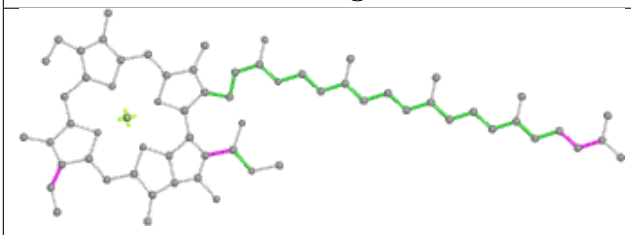


Bond lengths



Bond angles



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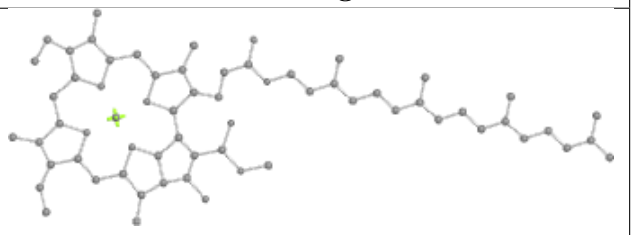
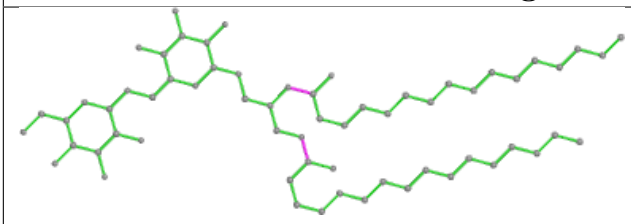


Rings

Ligand DGD C 516



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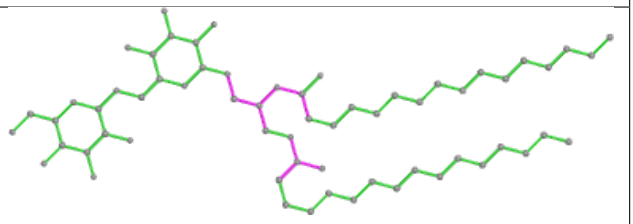
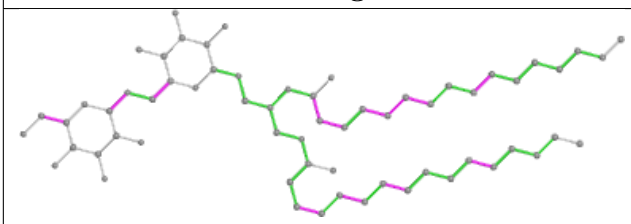


Bond angles



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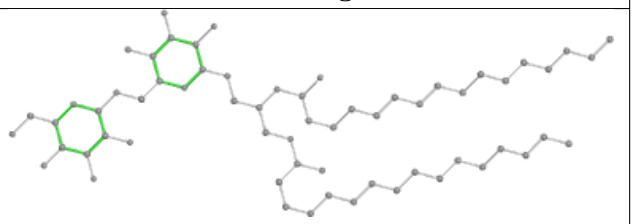
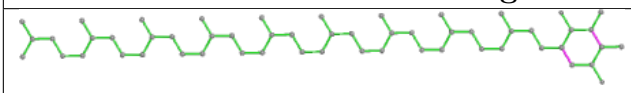


Rings

Ligand PL9 d 405 (B)



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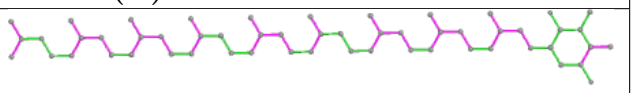
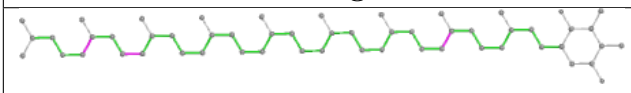


Bond angles



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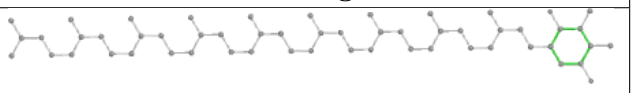
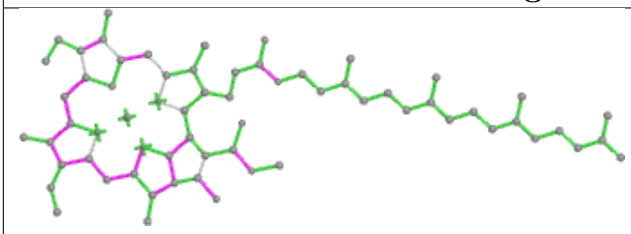


Rings

Ligand CLA C 510



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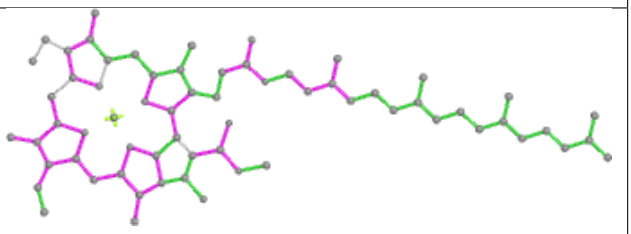
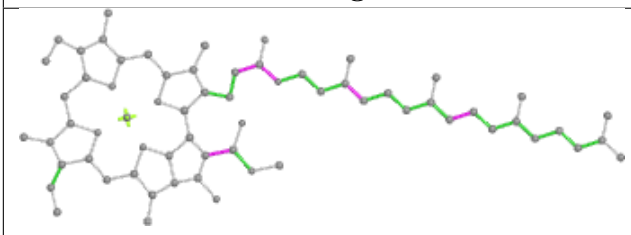


Bond angles



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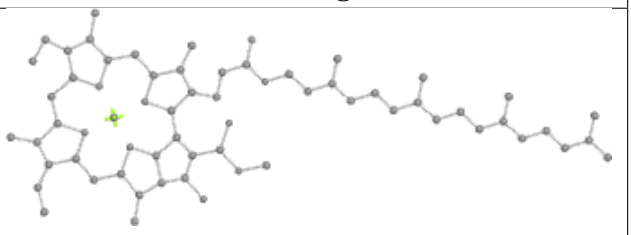
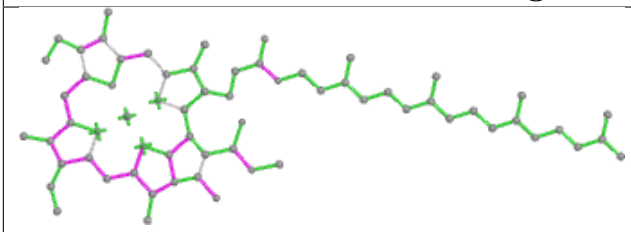


Rings

Ligand CLA d 403



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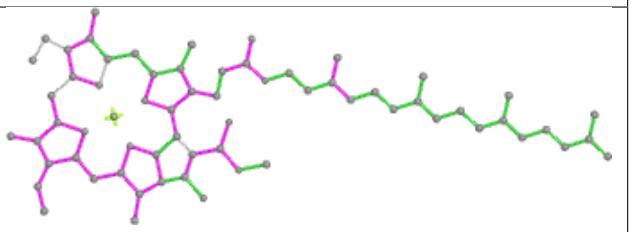
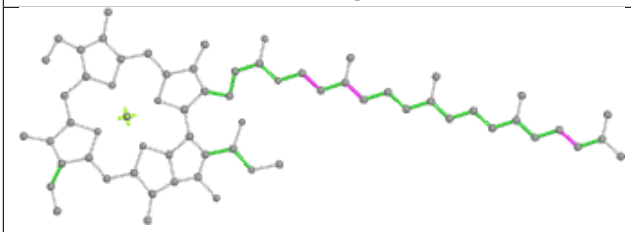


Bond angles



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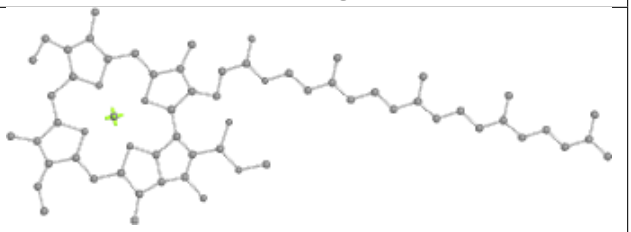
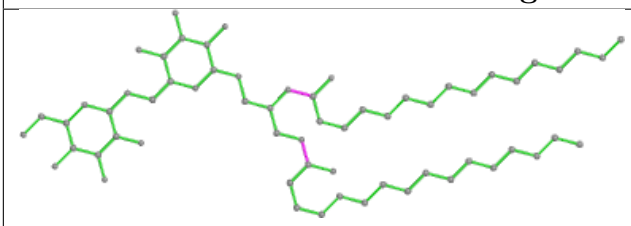


Rings

Ligand DGD C 517



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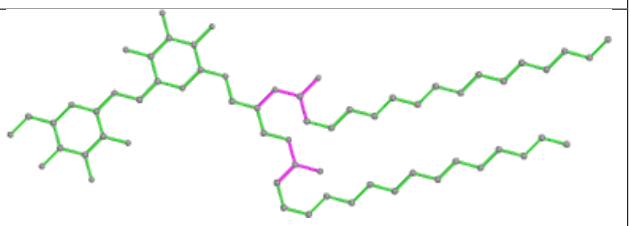
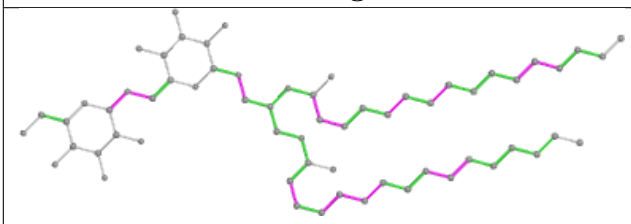


Bond angles



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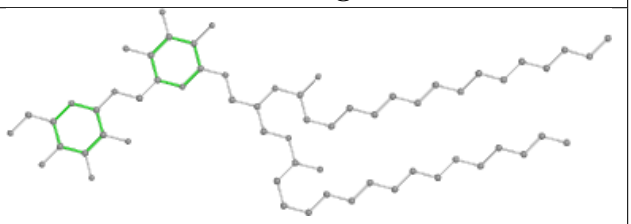
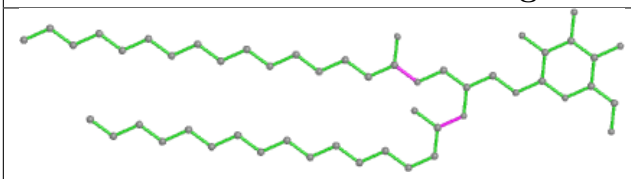


Rings

Ligand LMG C 520



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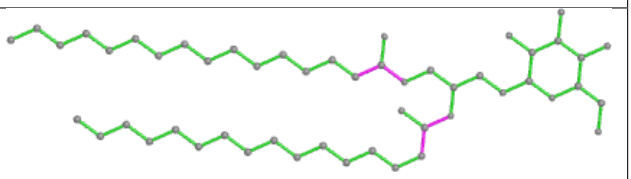
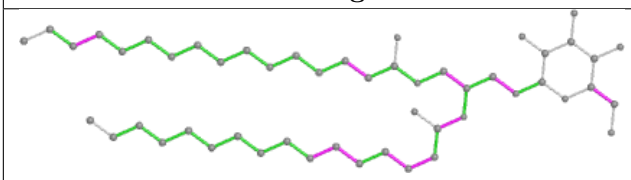


Bond angles



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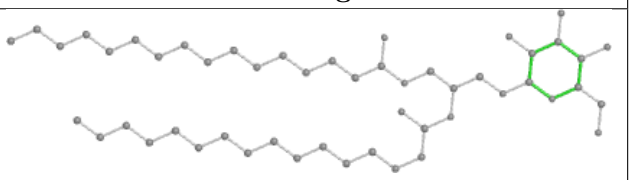
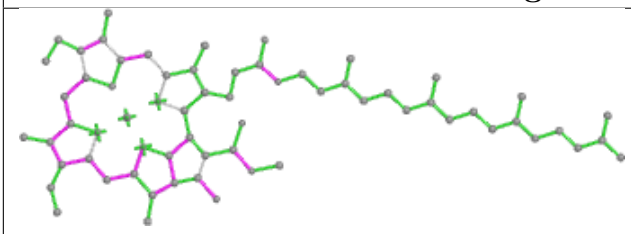


Rings

Ligand CLA B 610



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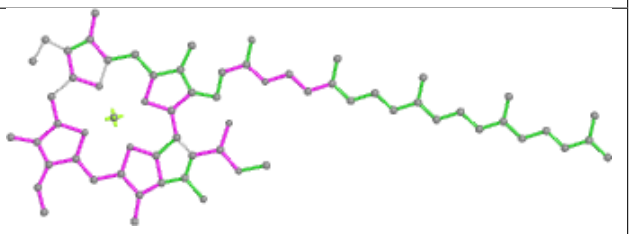
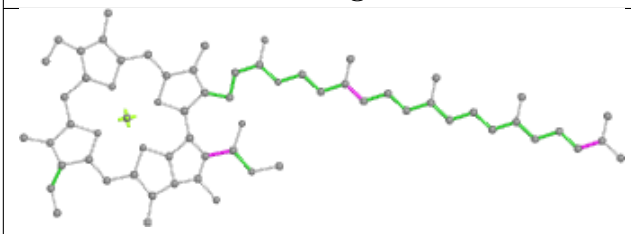


Bond angles



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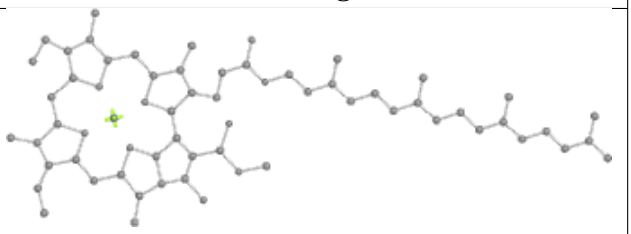
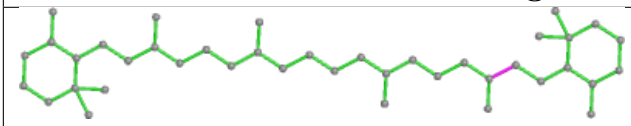


Rings

Ligand BCR y 101



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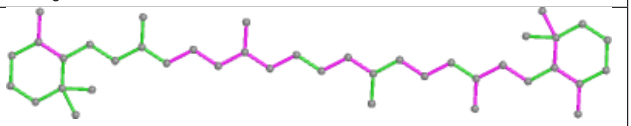
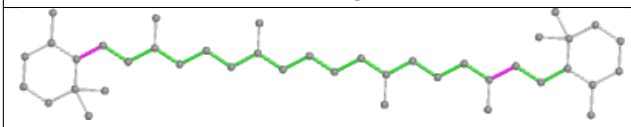


Bond angles



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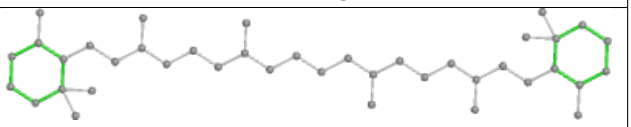
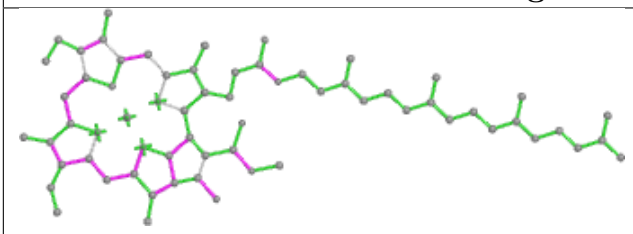


Rings

Ligand CLA b 621



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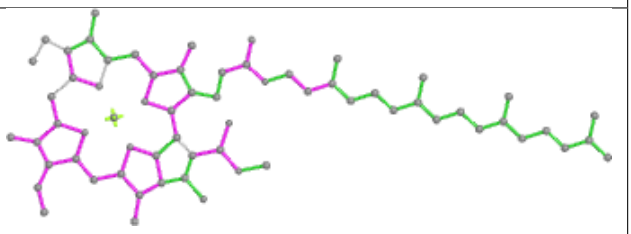
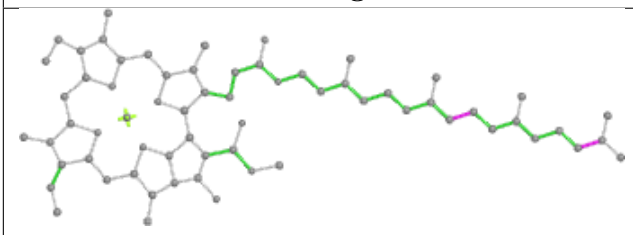
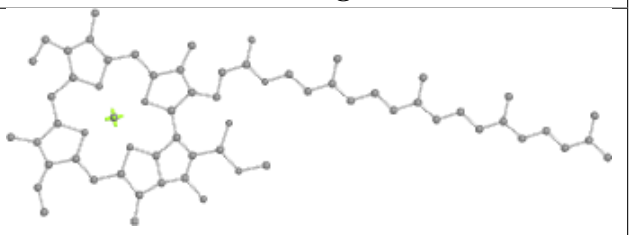


Bond angles

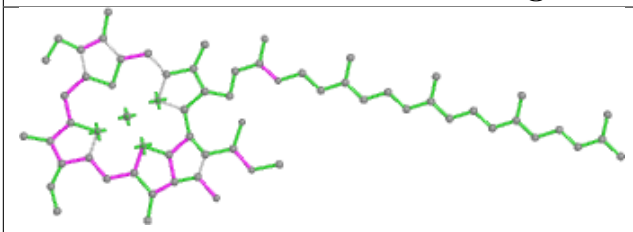


Torsions



Rings

Ligand CLA b 618



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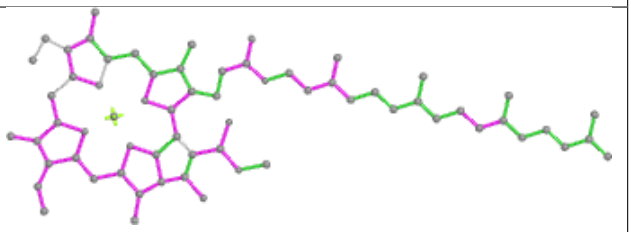
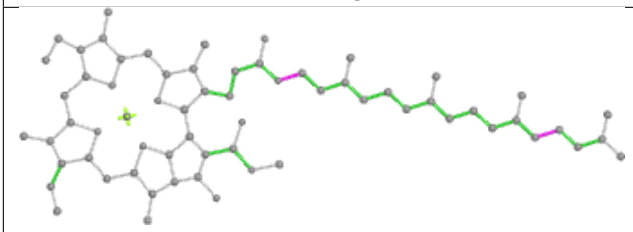
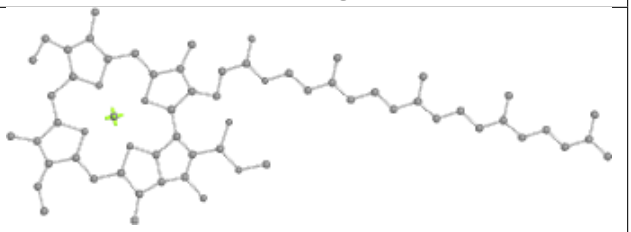


Bond angles

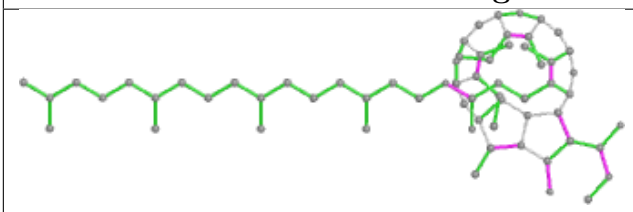


Torsions

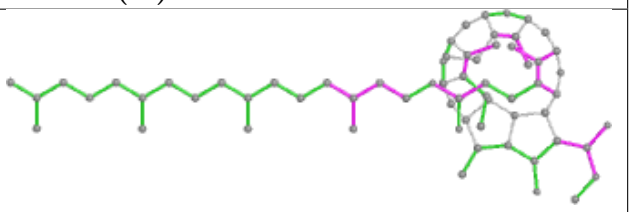


Rings

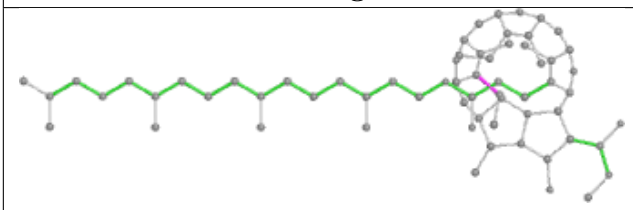
Ligand PHO a 420 (A)



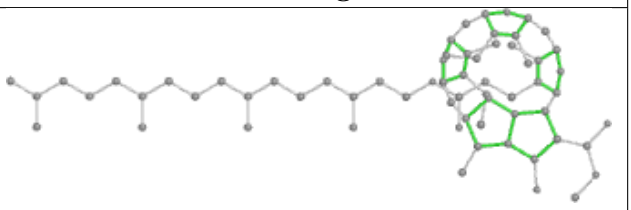
Bond lengths



Bond angles

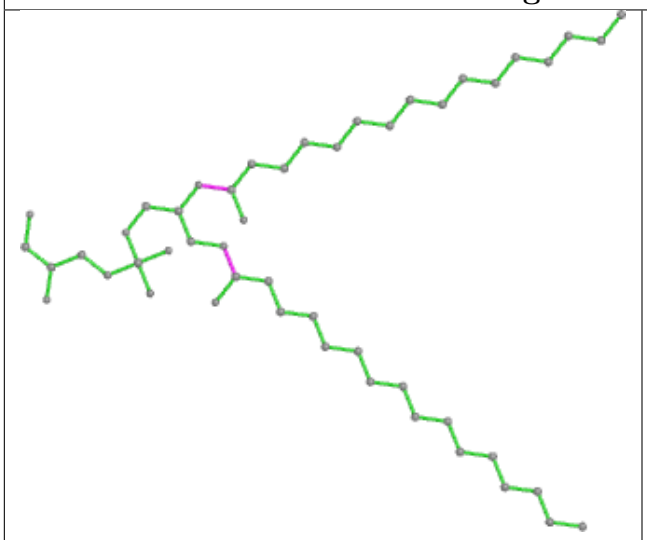


Torsions

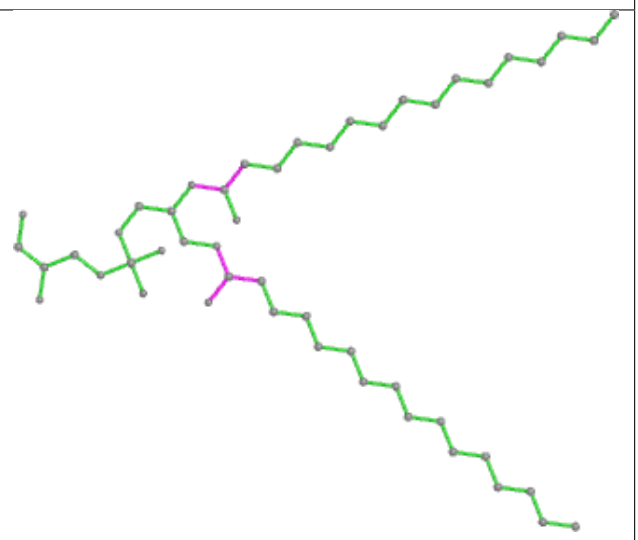


Rings

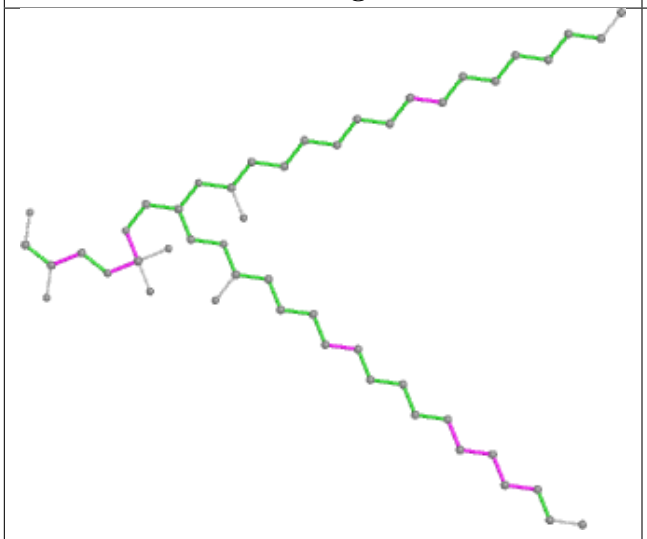
Ligand LHG D 408



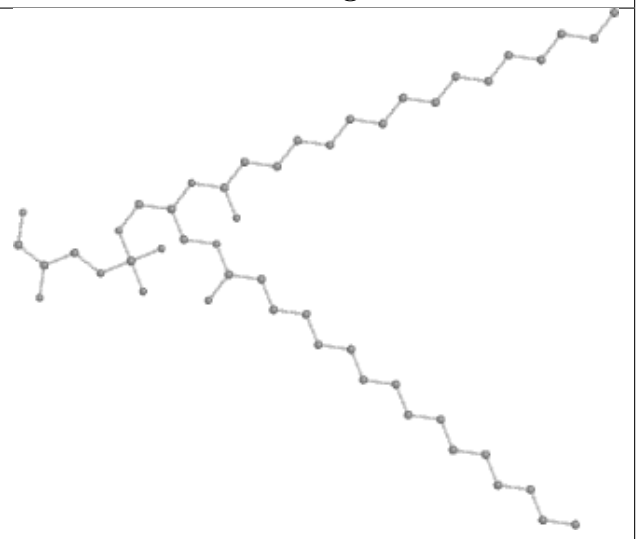
Bond lengths



Bond angles

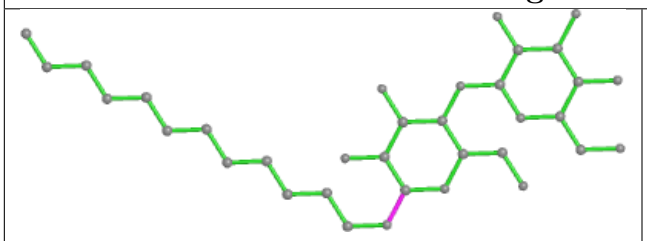


Torsions

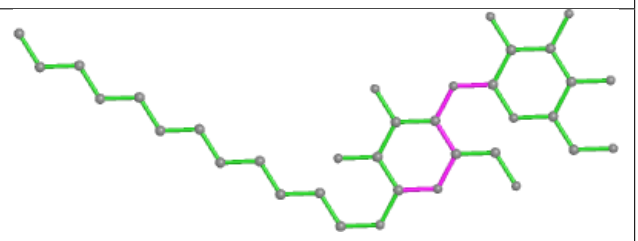


Rings

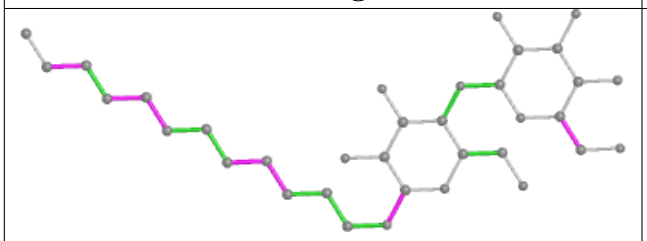
Ligand LMT a 404



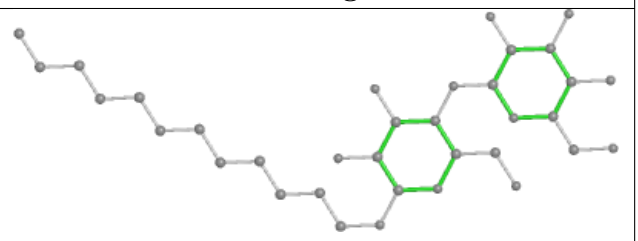
Bond lengths



Bond angles

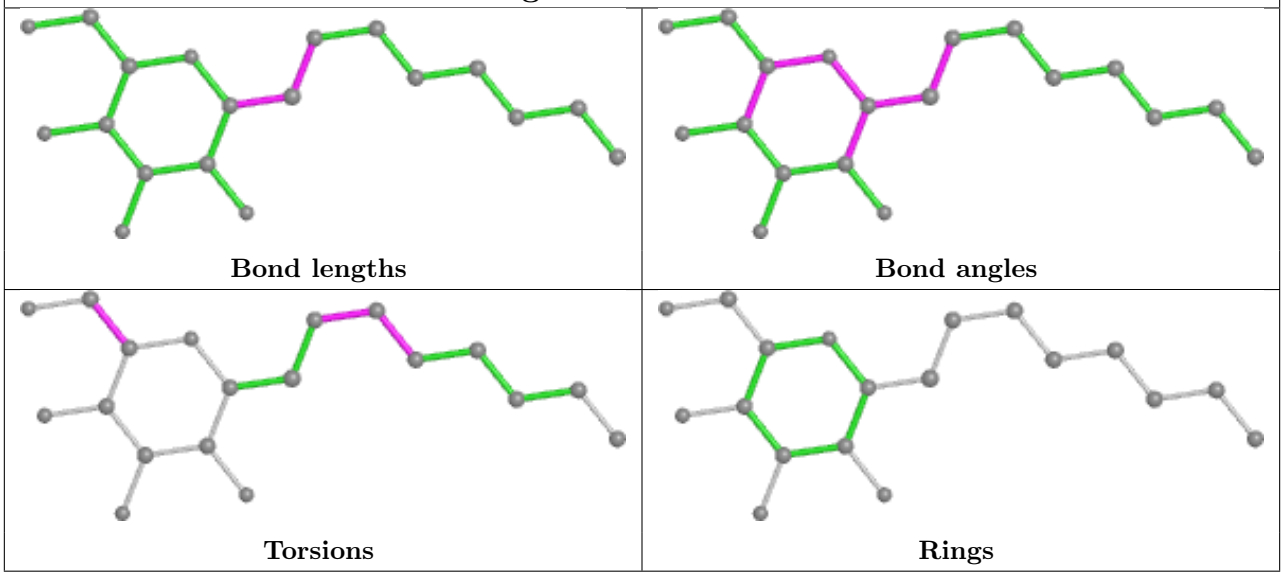


Torsions

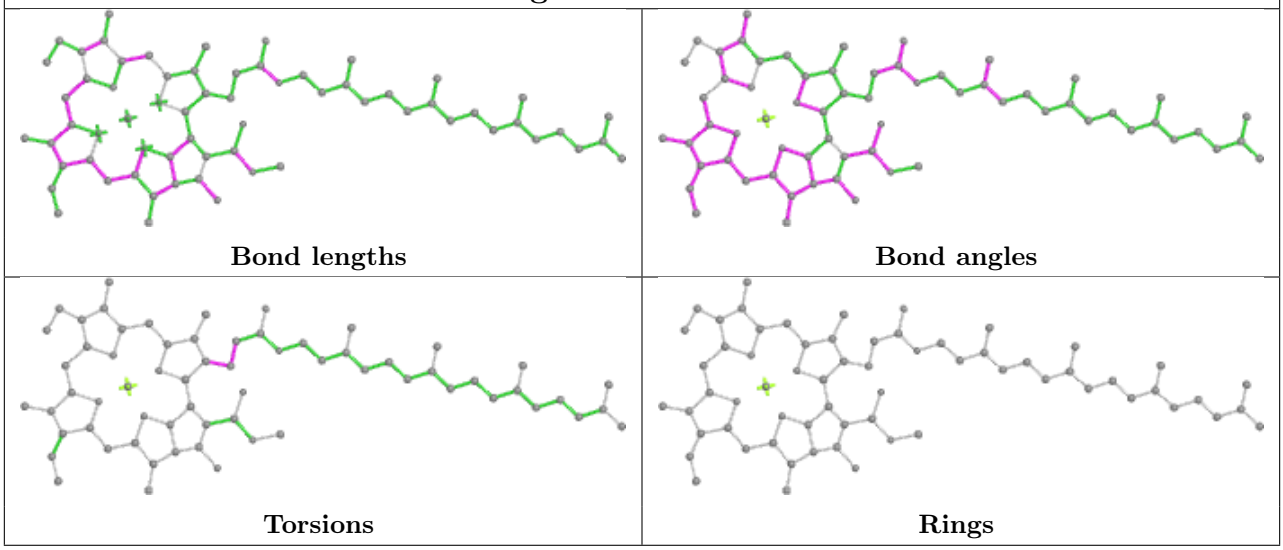


Rings

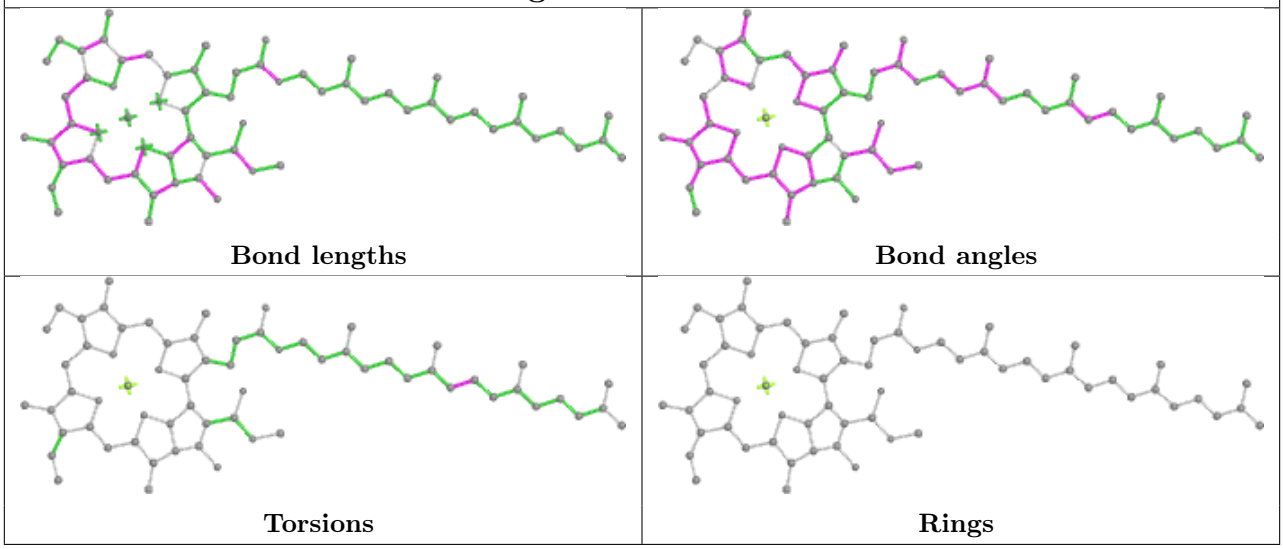
Ligand HTG C 523



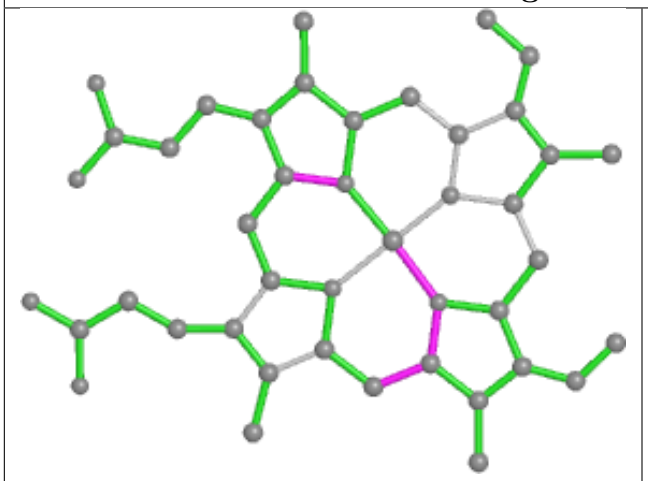
Ligand CLA c 505



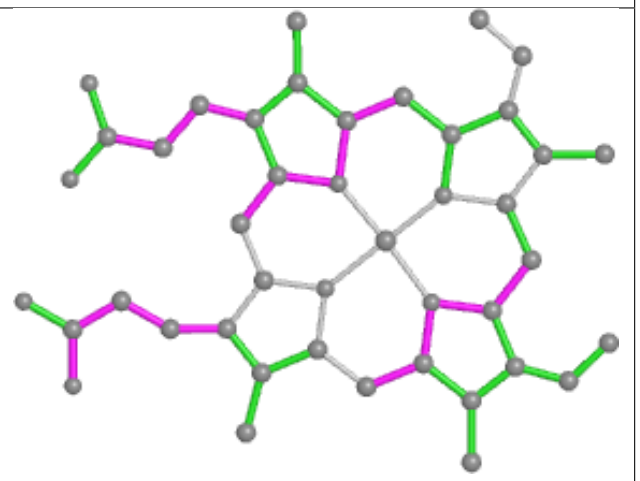
Ligand CLA b 622



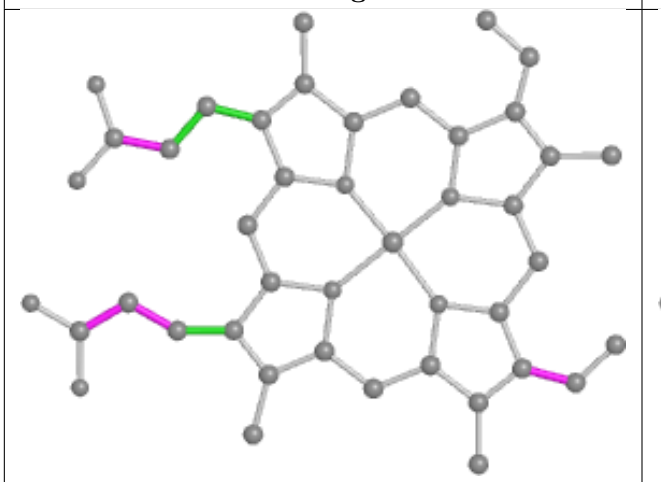
Ligand HEM F 102



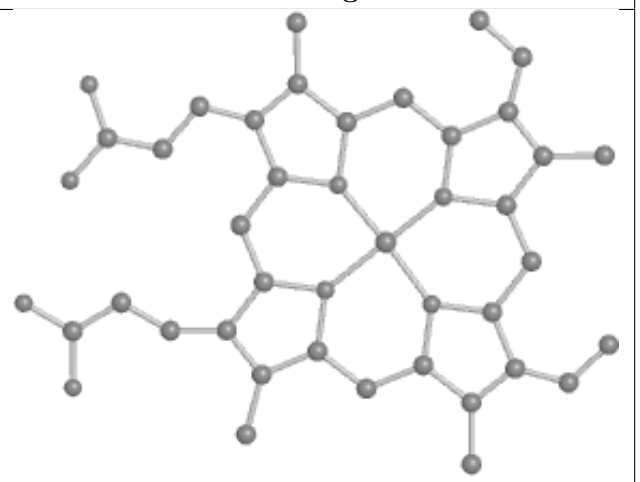
Bond lengths



Bond angles

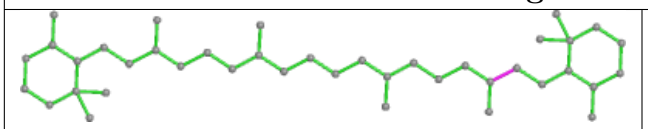


Torsions



Rings

Ligand BCR b 629



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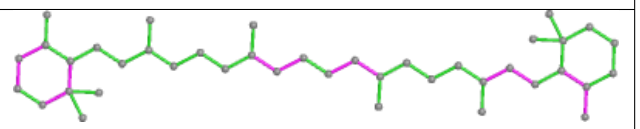
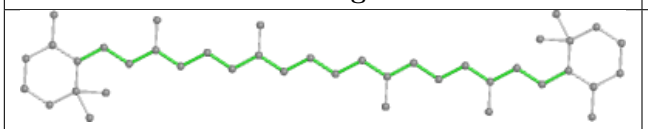
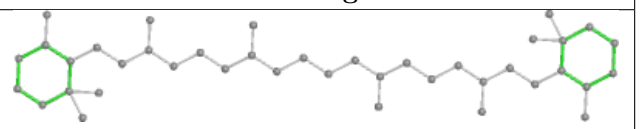


Bond angles

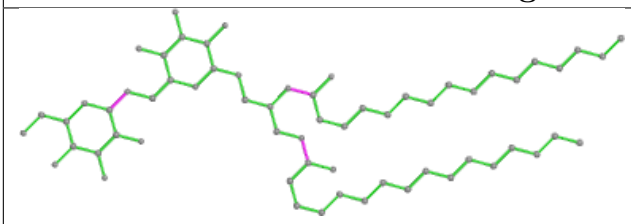


Torsions

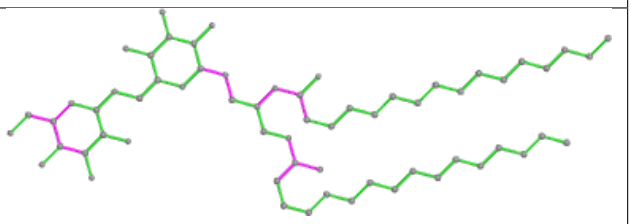


Rings

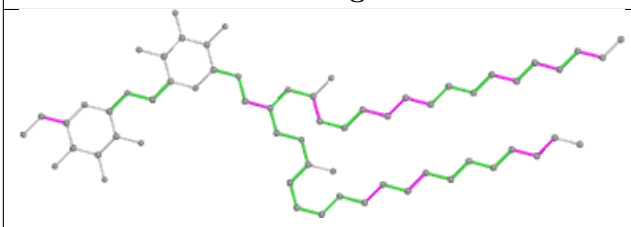
Ligand DGD H 103



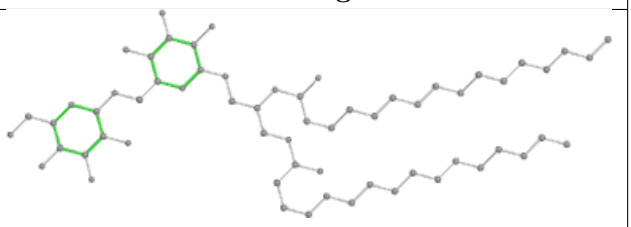
Bond lengths



Bond angles

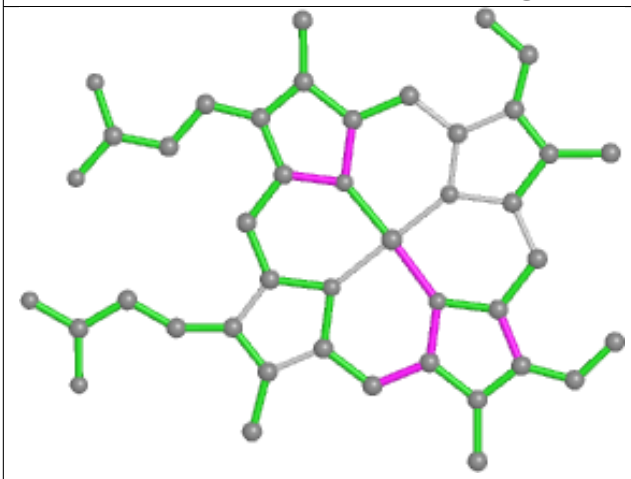


Torsions

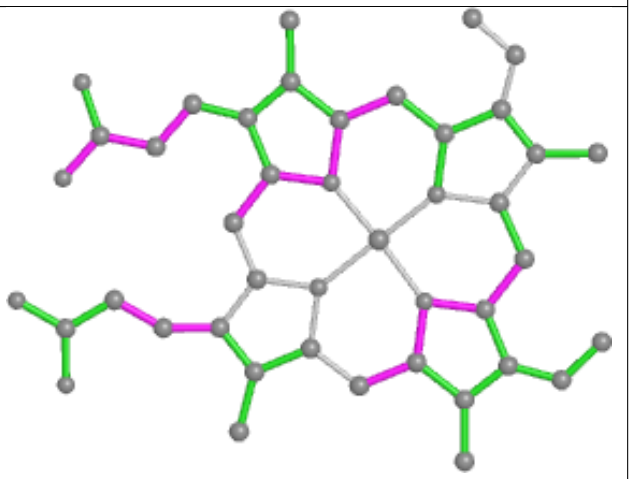


Rings

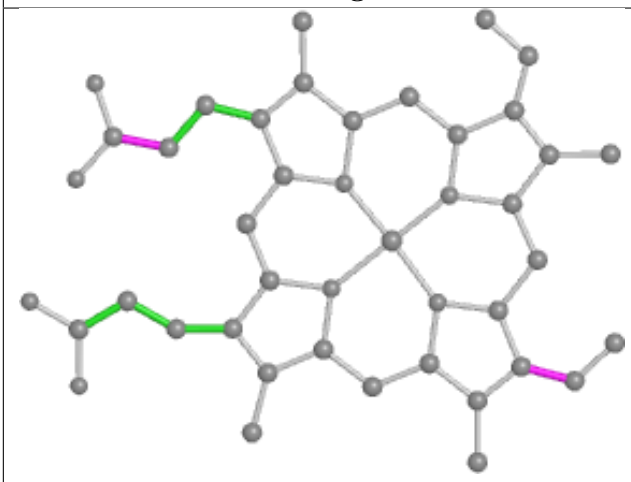
Ligand HEM V 206



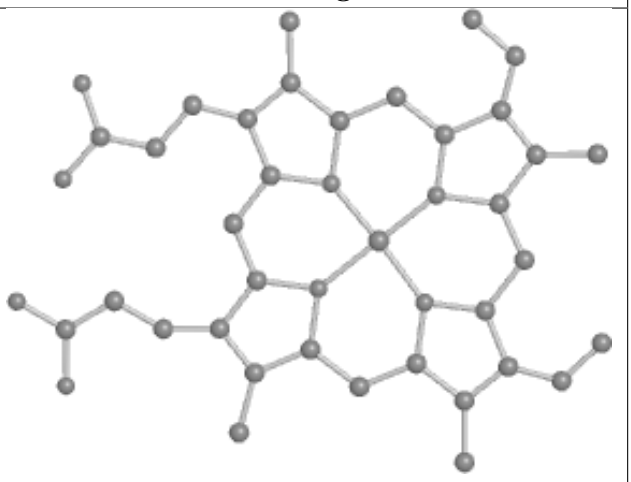
Bond lengths



Bond angles

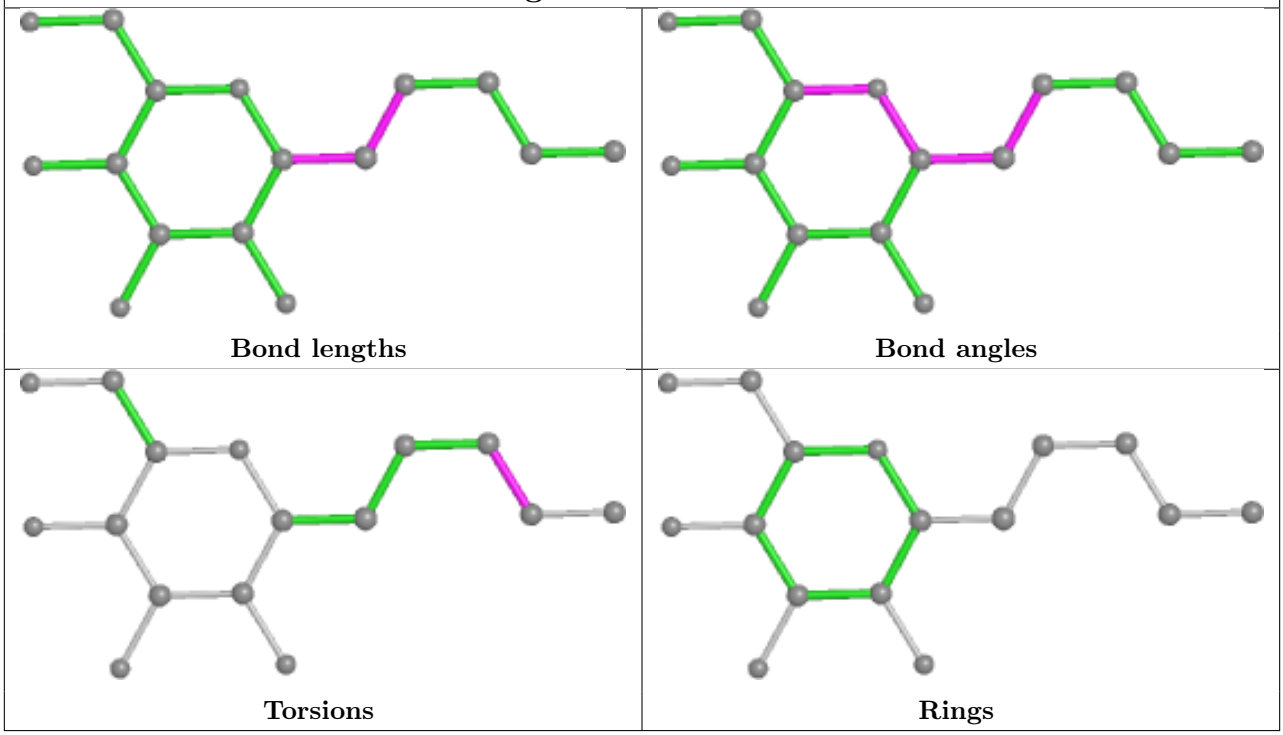


Torsions

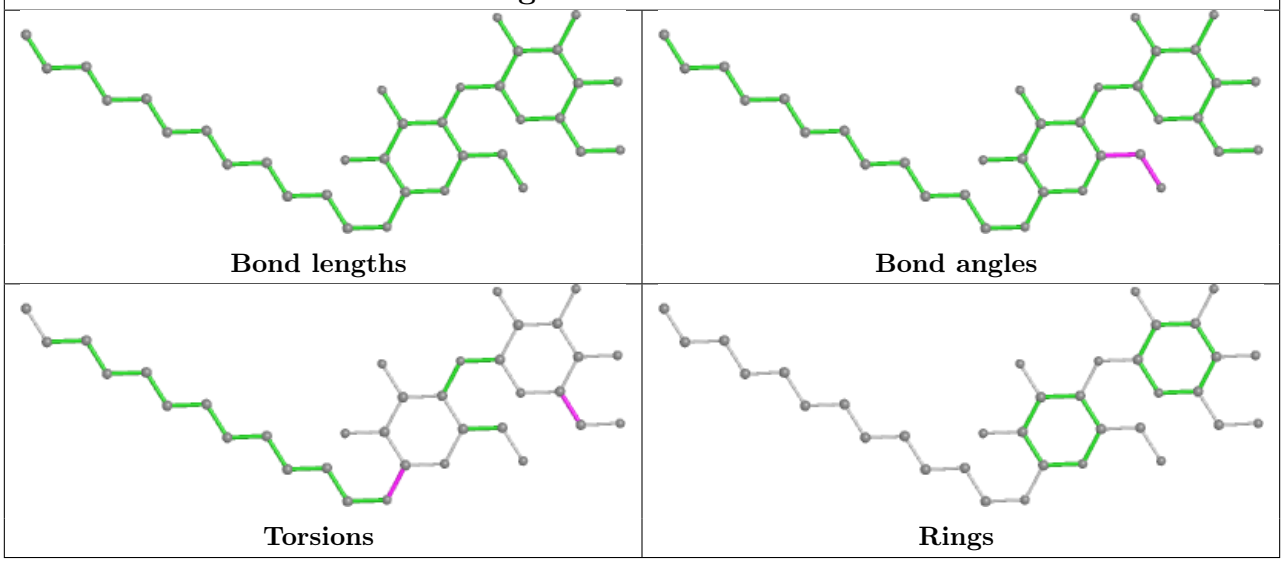


Rings

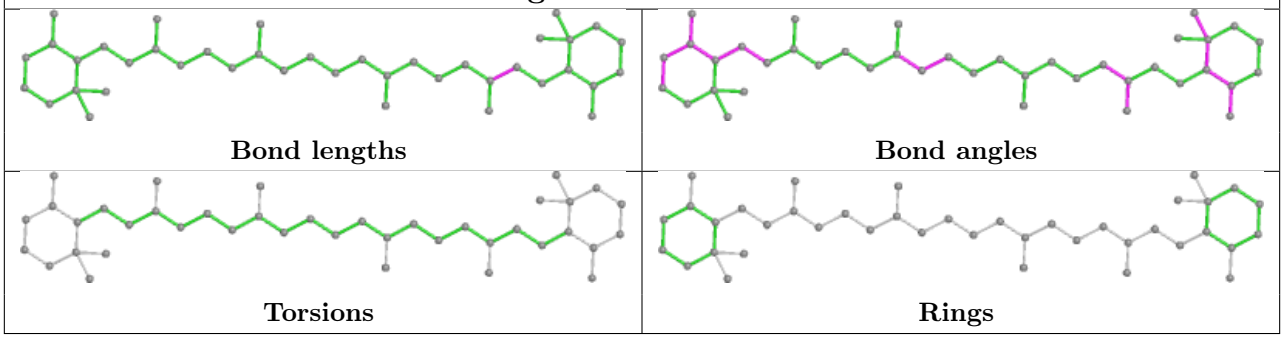
Ligand HTG d 411



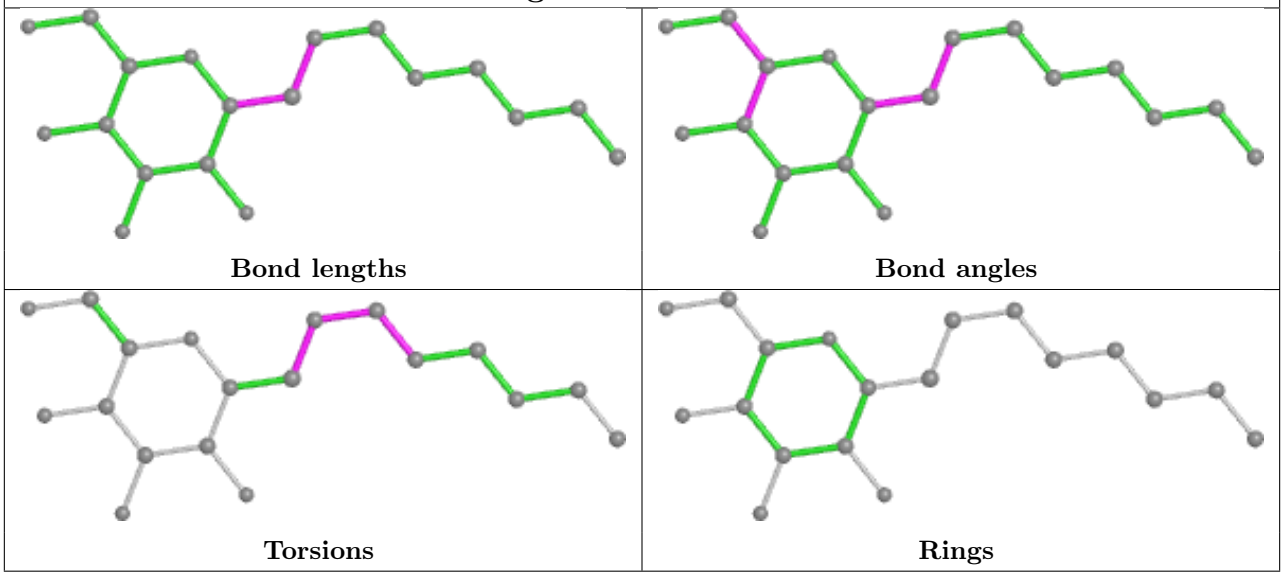
Ligand LMT M 101



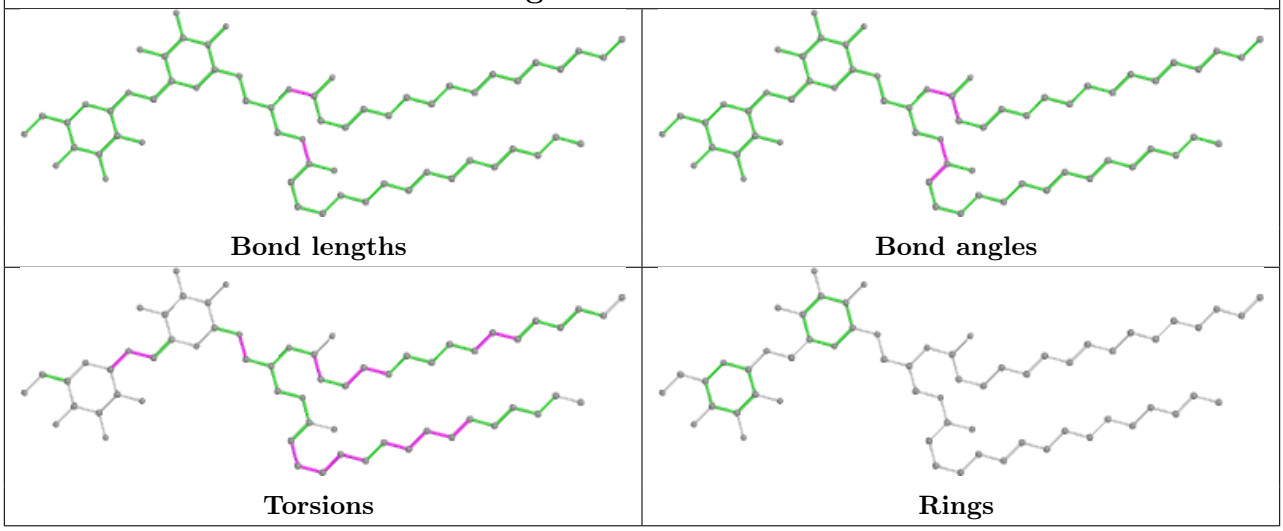
Ligand BCR a 413



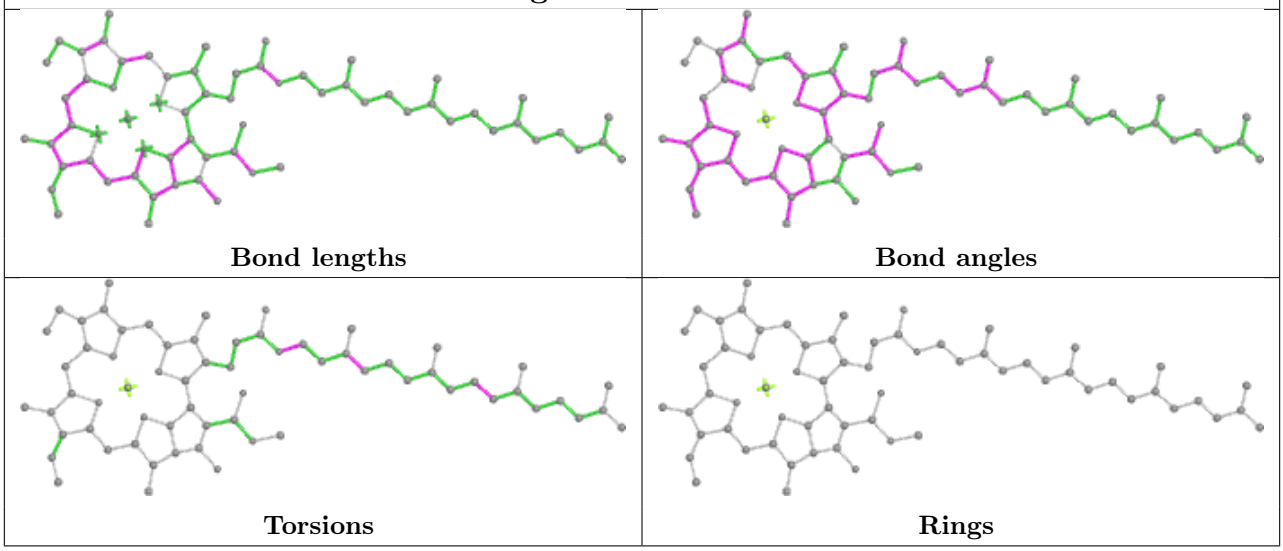
Ligand HTG c 524



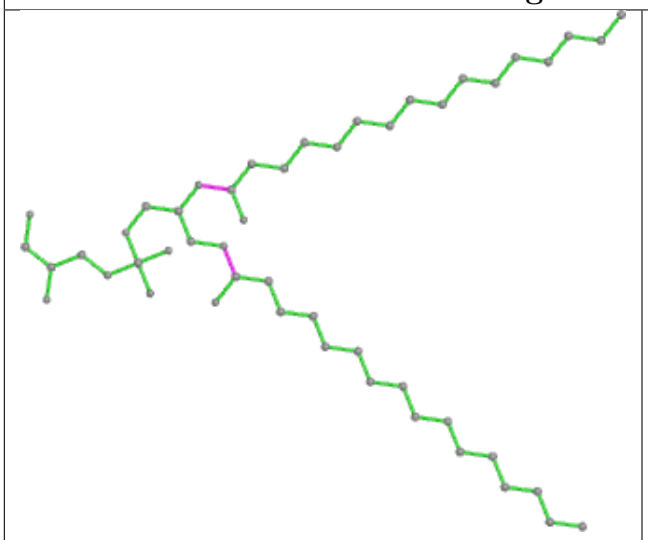
Ligand DGD c 520



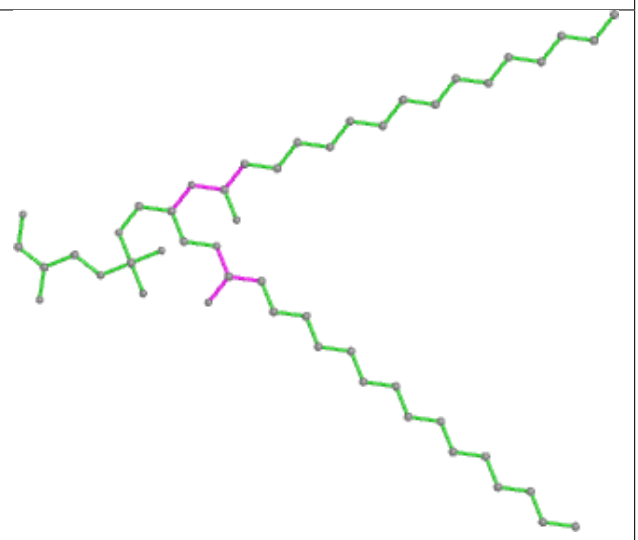
Ligand CLA c 517



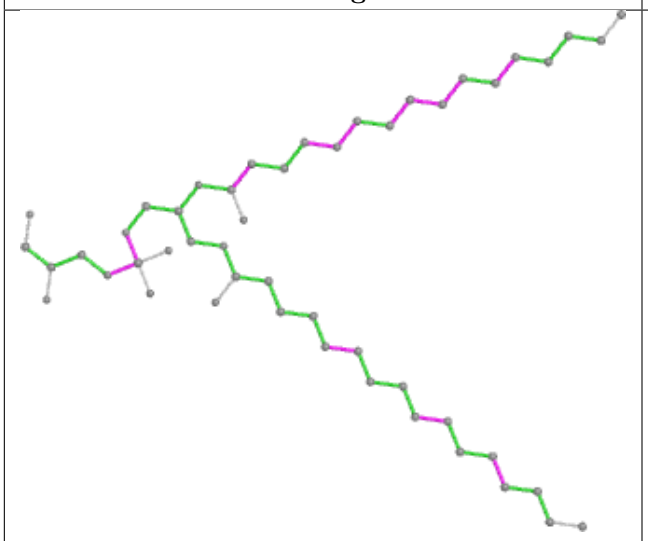
Ligand LHG L 101



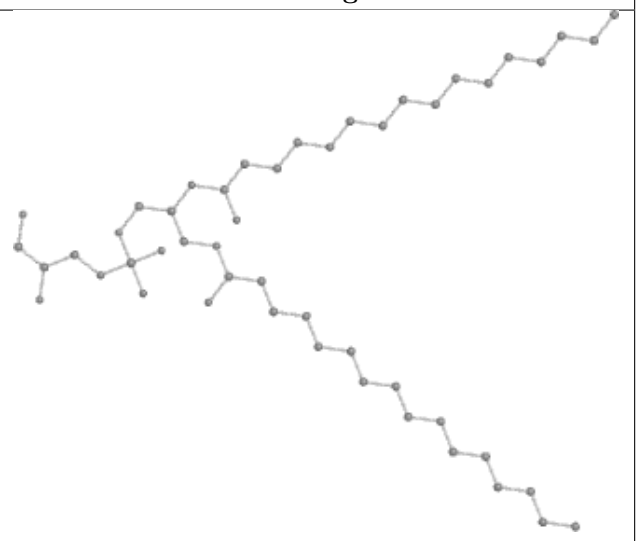
Bond lengths



Bond angles

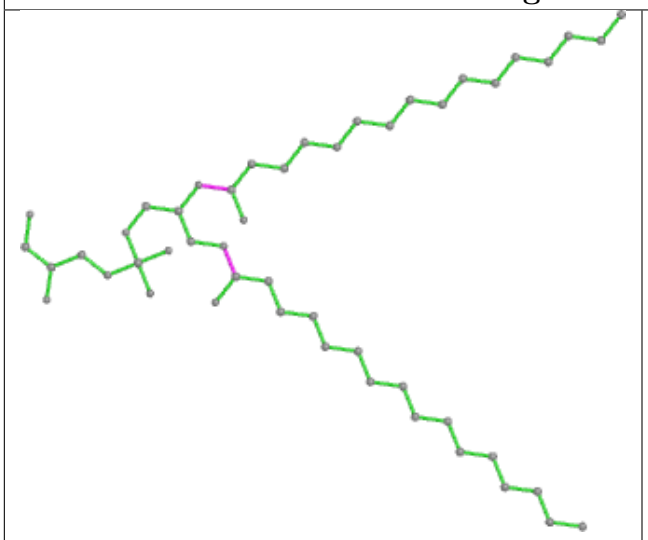


Torsions

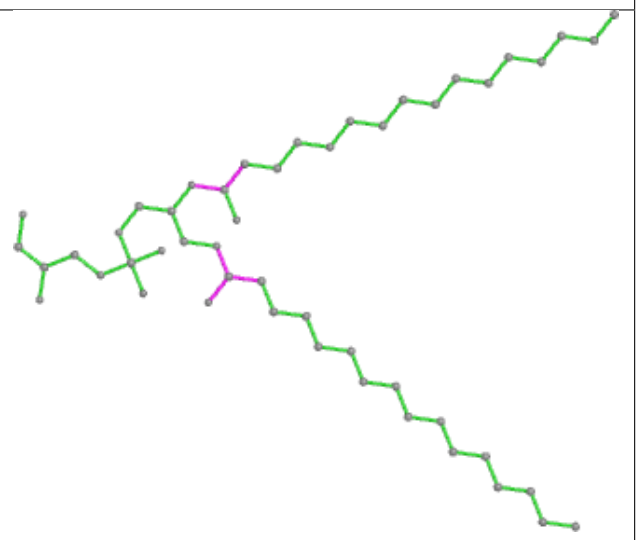


Rings

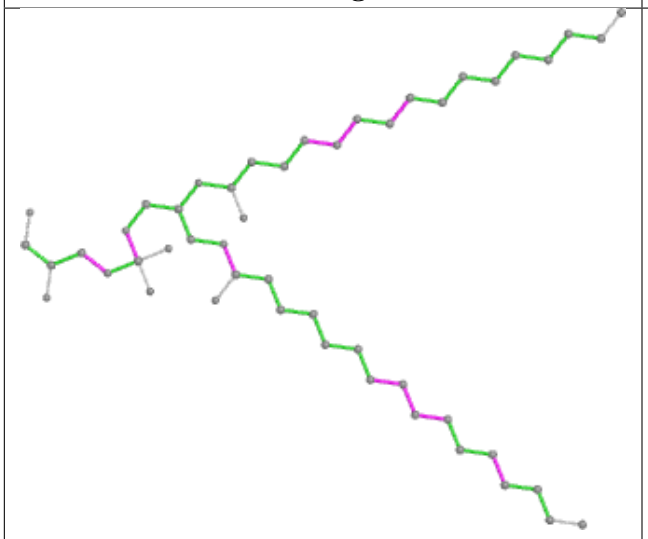
Ligand LHG D 409



Bond lengths



Bond angles



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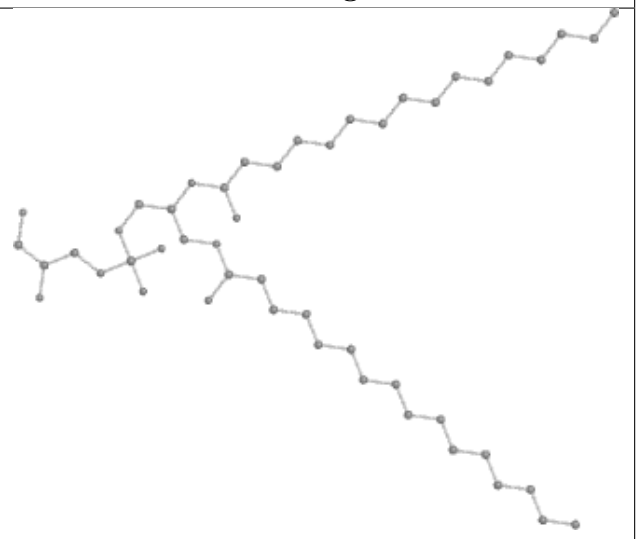
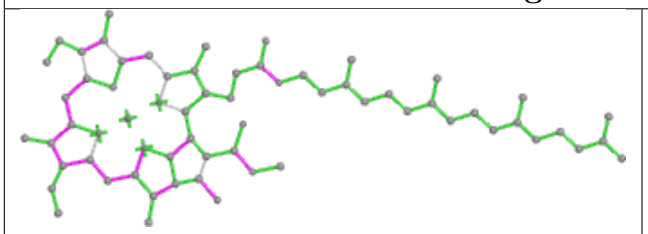
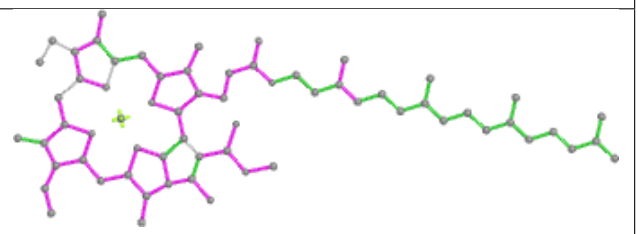


Rings

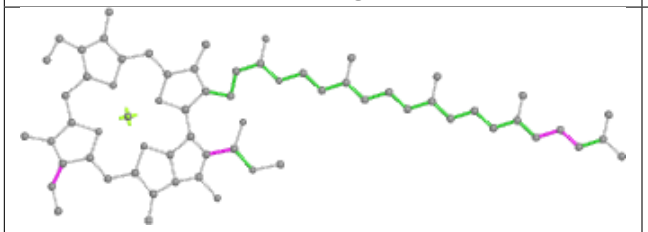
Ligand CLA A 406



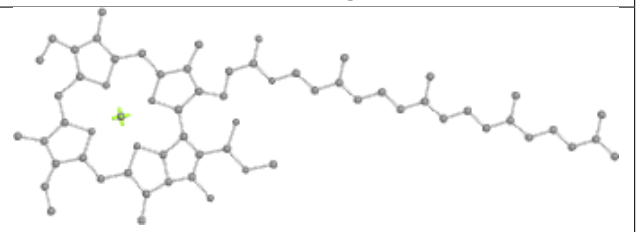
Bond lengths



Bond angles

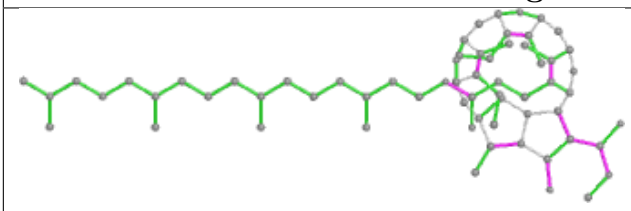


Torsions

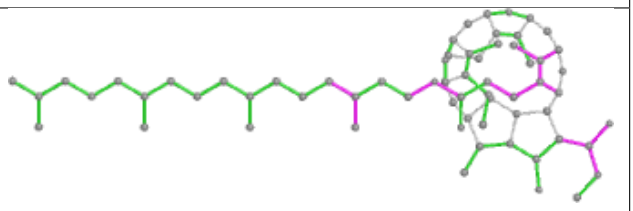


Rings

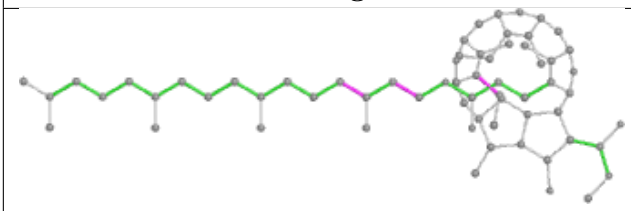
Ligand PHO a 411



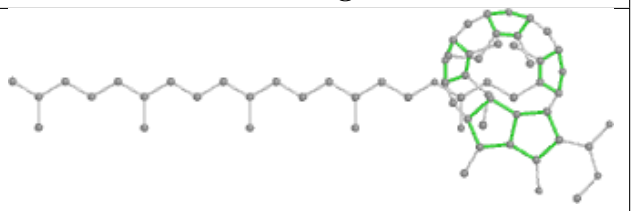
Bond lengths



Bond angles

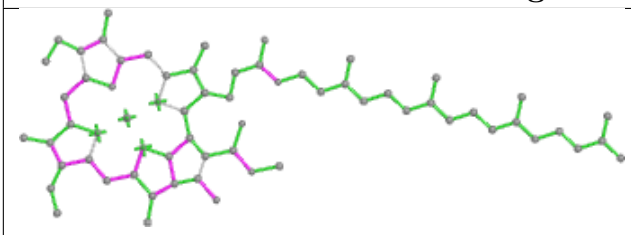


Torsions

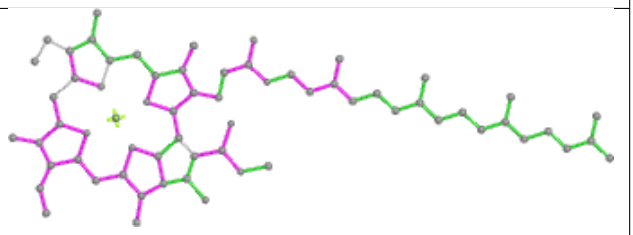


Rings

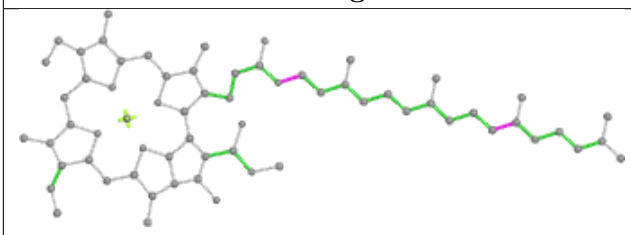
Ligand CLA d 402



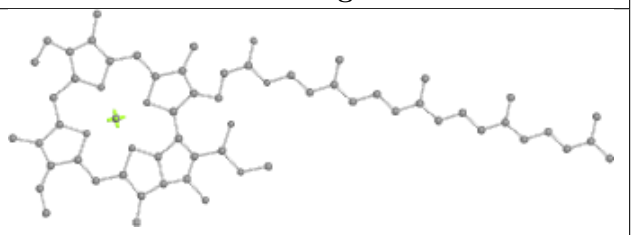
Bond lengths



Bond angles

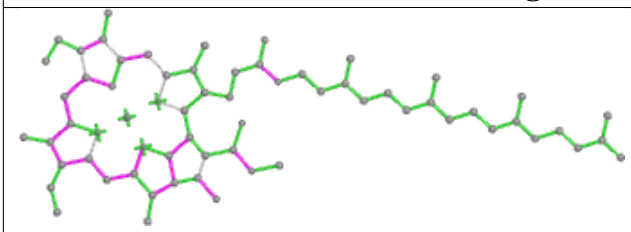


Torsions

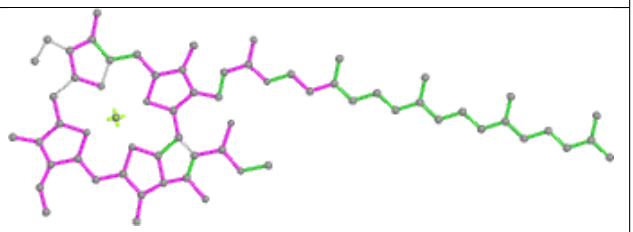


Rings

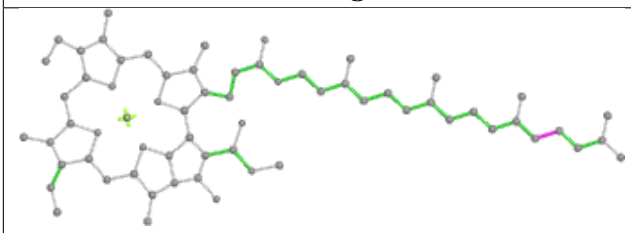
Ligand CLA B 609



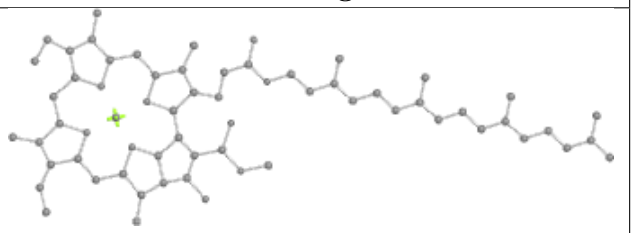
Bond lengths



Bond angles

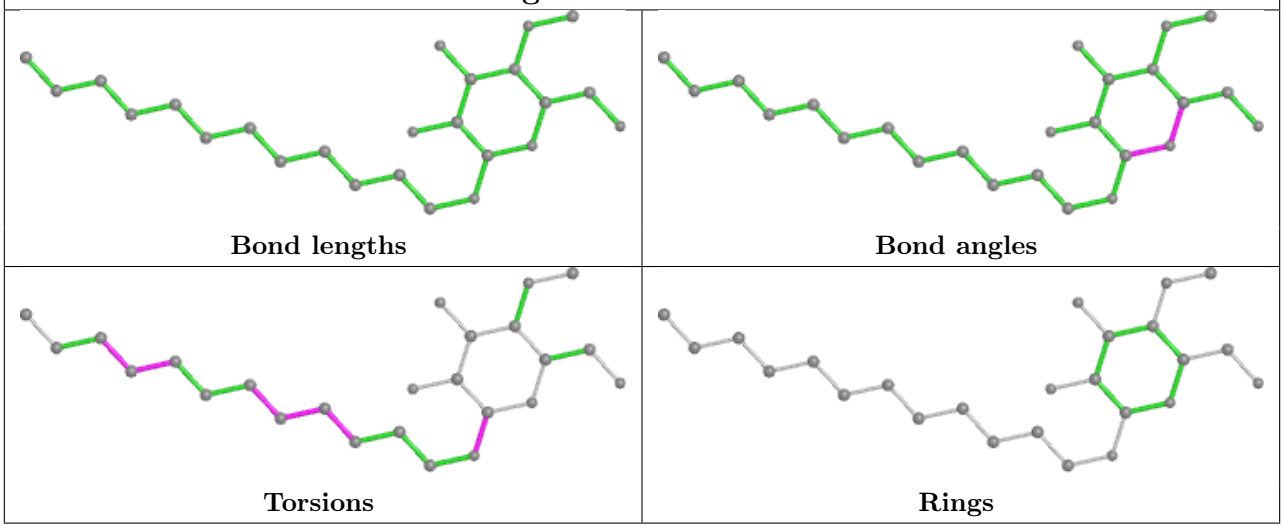


Torsions

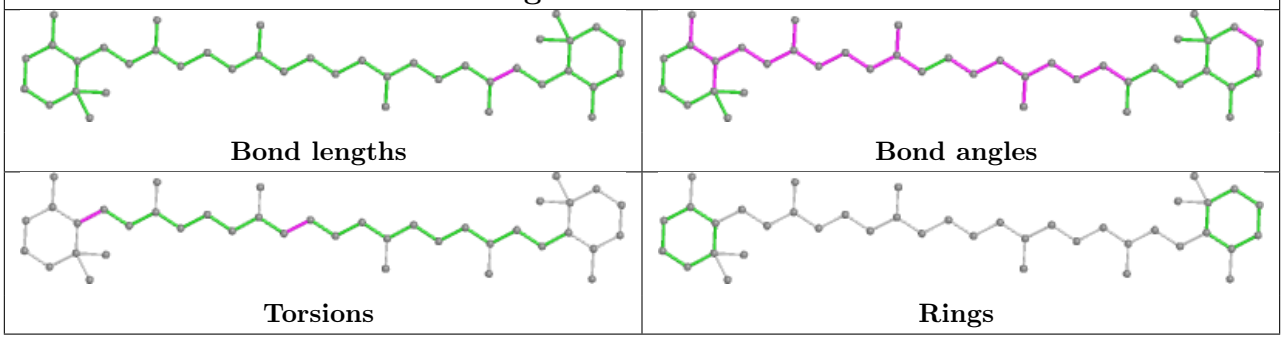


Rings

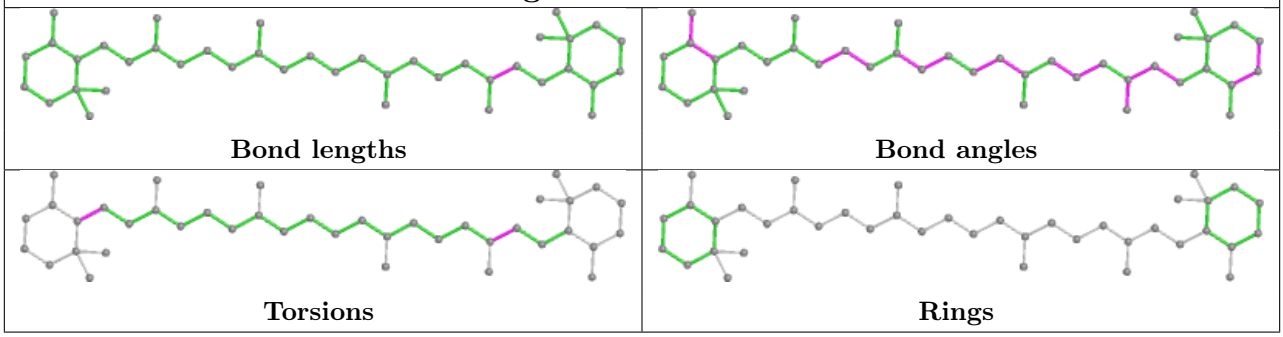
Ligand LMT B 635



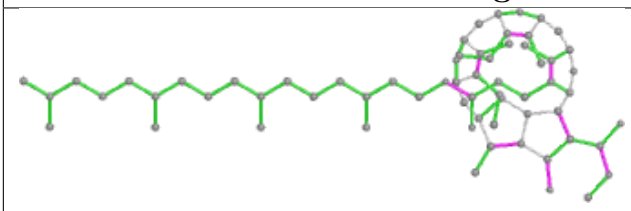
Ligand BCR T 103



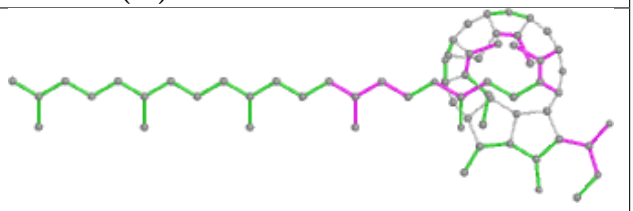
Ligand BCR Y 101



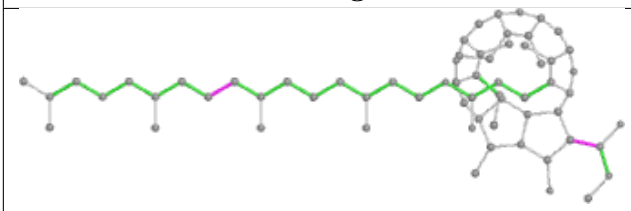
Ligand PHO a 420 (B)



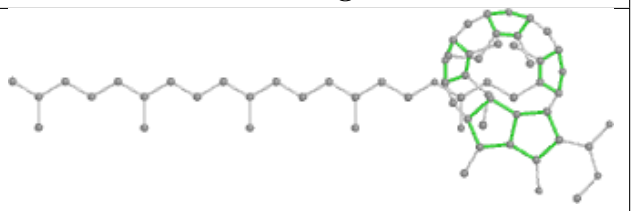
Bond lengths



Bond angles

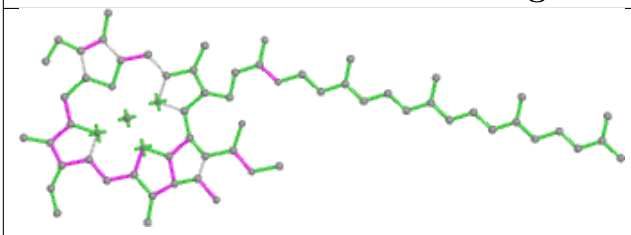


Torsions

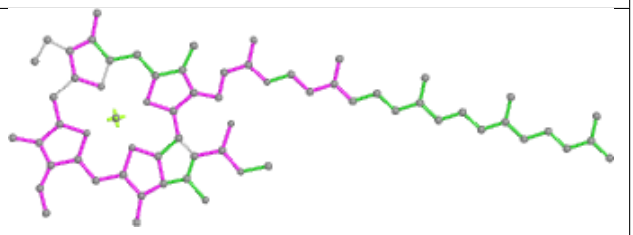


Rings

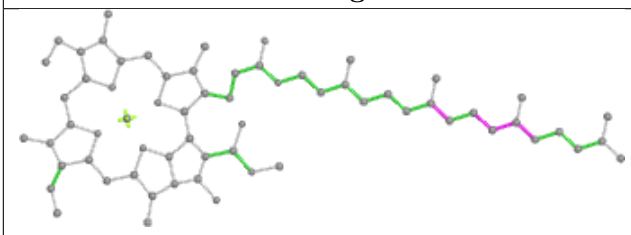
Ligand CLA a 410



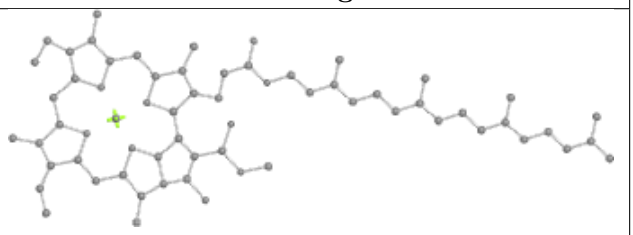
Bond lengths



Bond angles

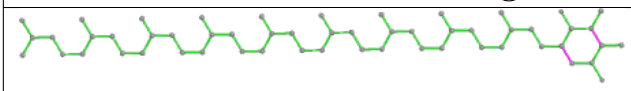


Torsions

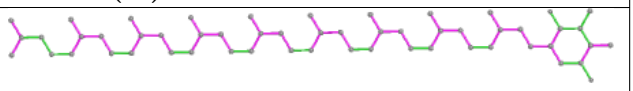


Rings

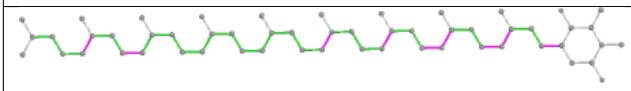
Ligand PL9 a 416 (A)



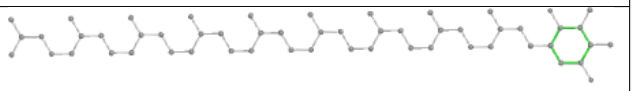
Bond lengths



Bond angles

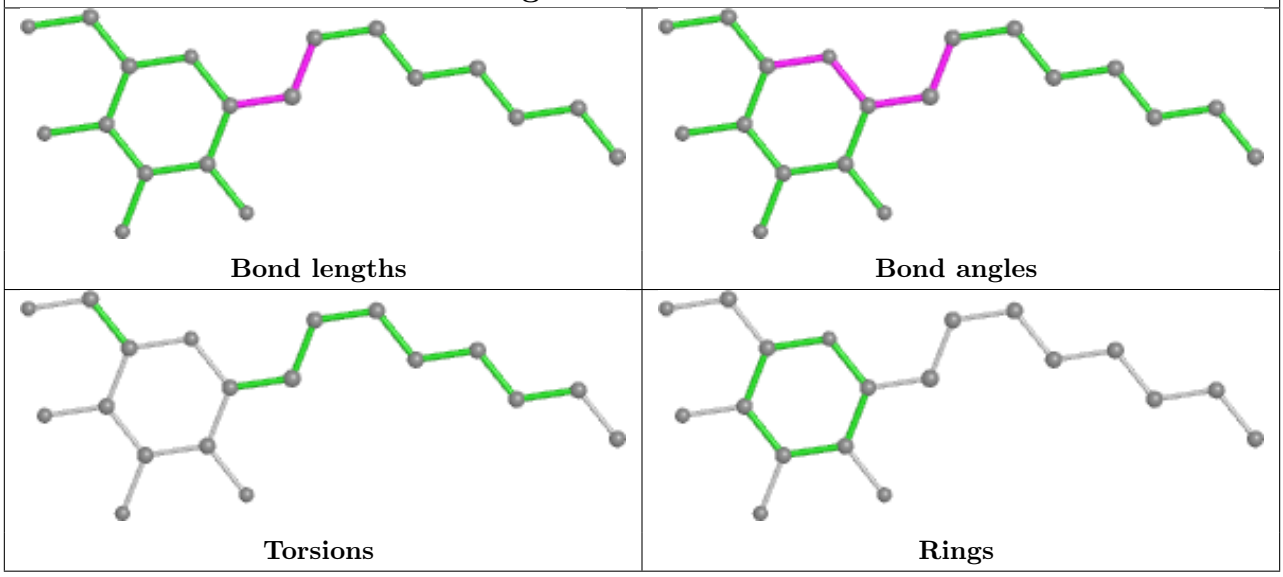


Torsions

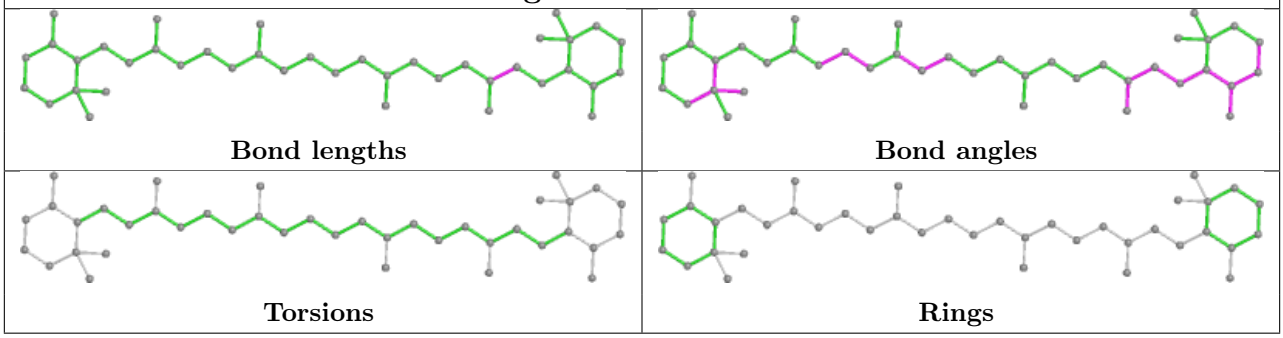


Rings

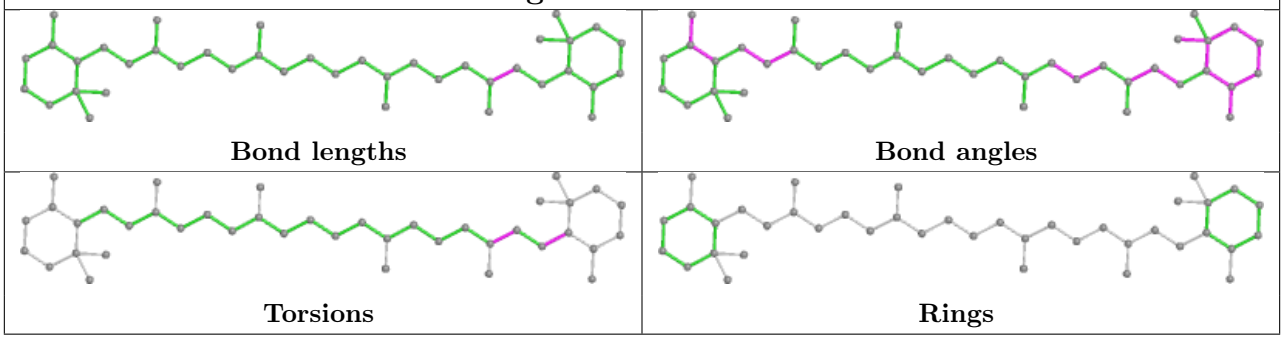
Ligand HTG C 522



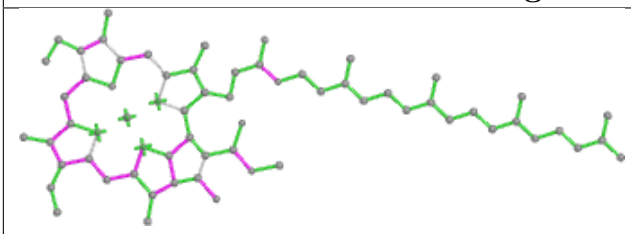
Ligand BCR B 620



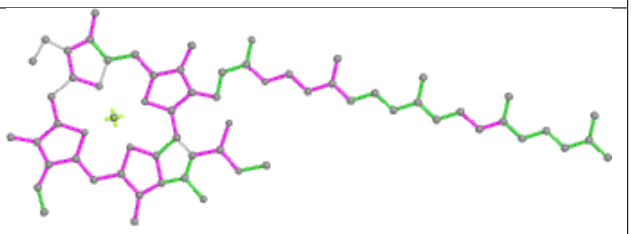
Ligand BCR d 404



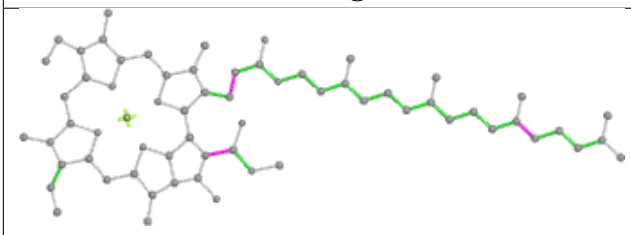
Ligand CLA B 603



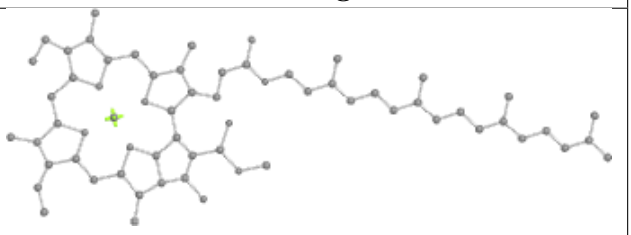
Bond lengths



Bond angles

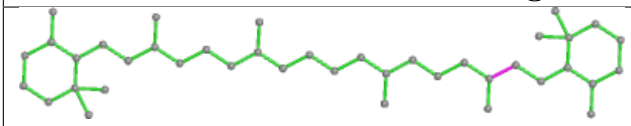


Torsions

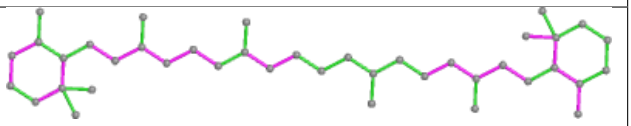


Rings

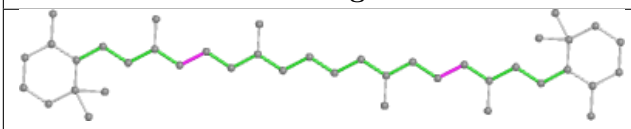
Ligand BCR k 101



Bond lengths



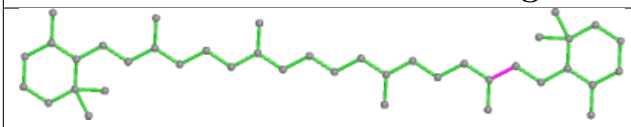
Bond angles



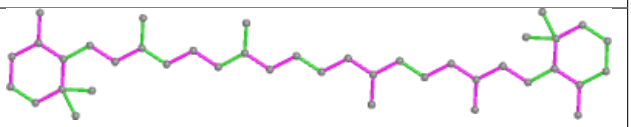
Torsions

Rings

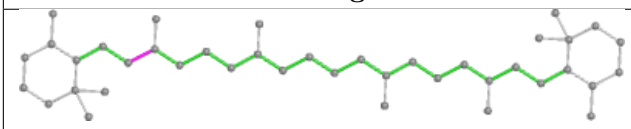
Ligand BCR K 101



Bond lengths



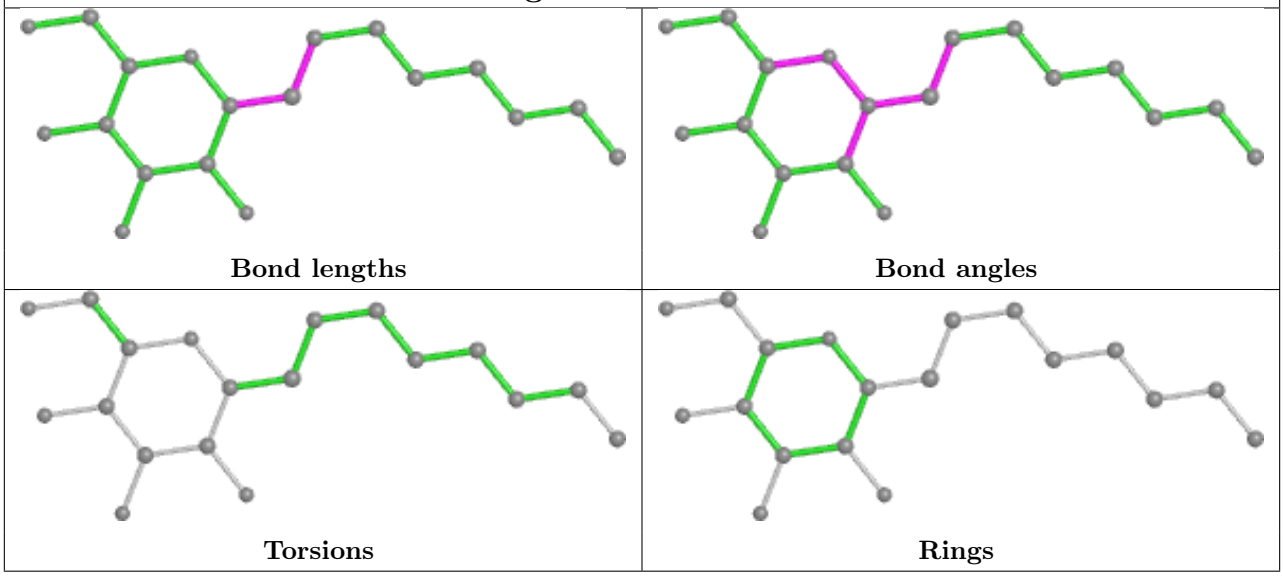
Bond angles



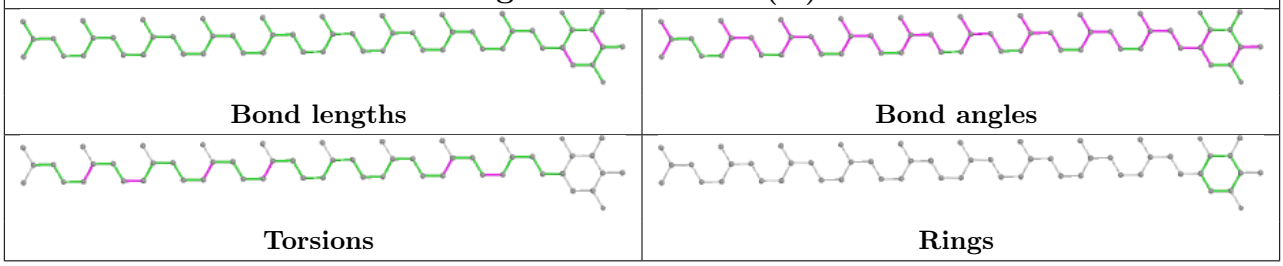
Torsions

Rings

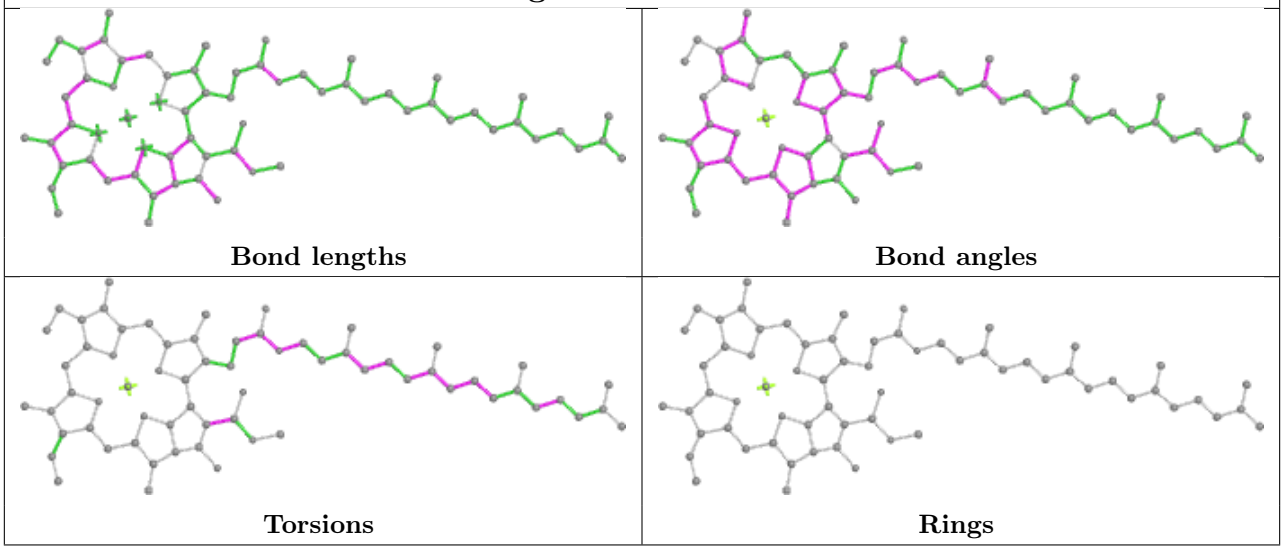
Ligand HTG b 609



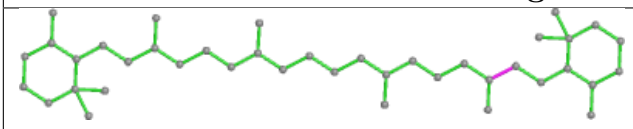
Ligand PL9 D 405 (A)



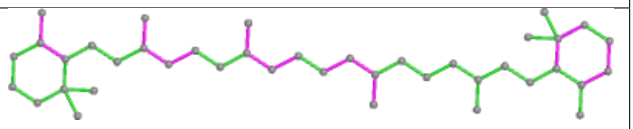
Ligand CLA b 611



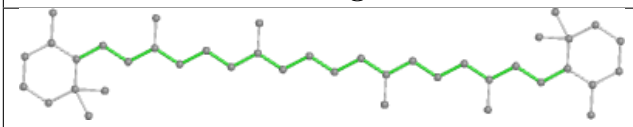
Ligand BCR c 527



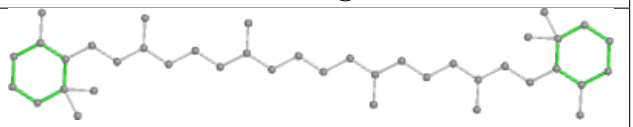
Bond lengths



Bond angles

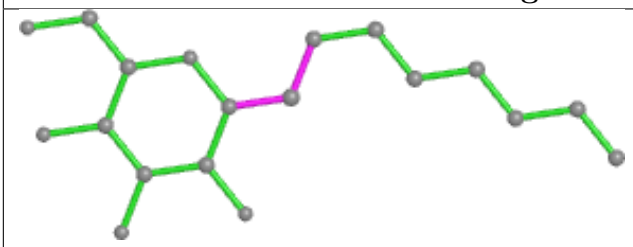


Torsions

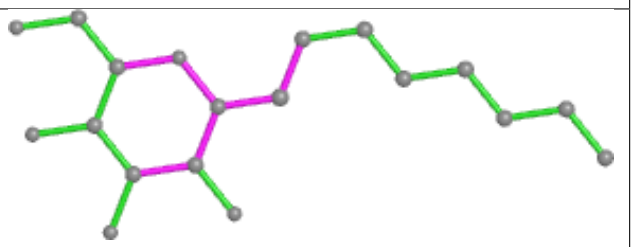


Rings

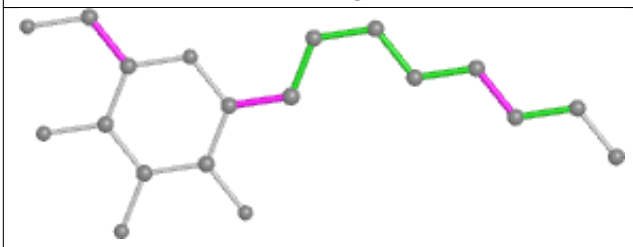
Ligand HTG B 625



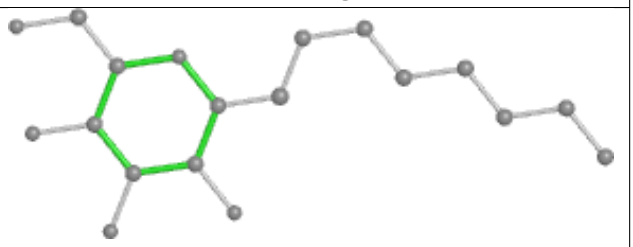
Bond lengths



Bond angles

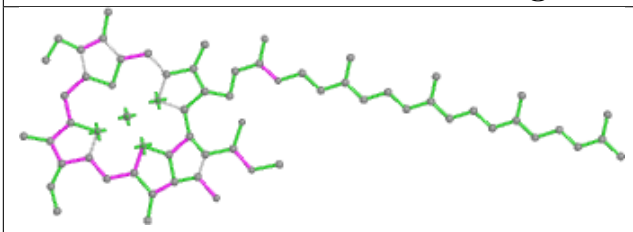


Torsions

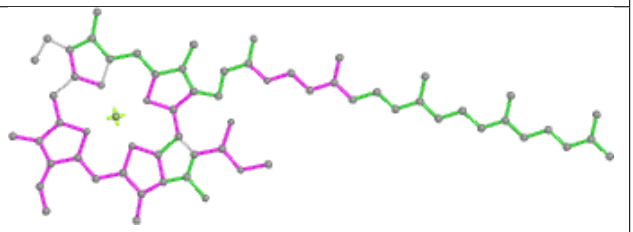


Rings

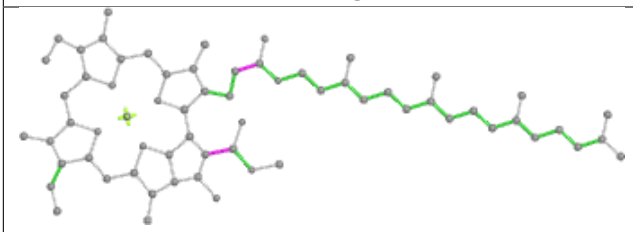
Ligand CLA c 509



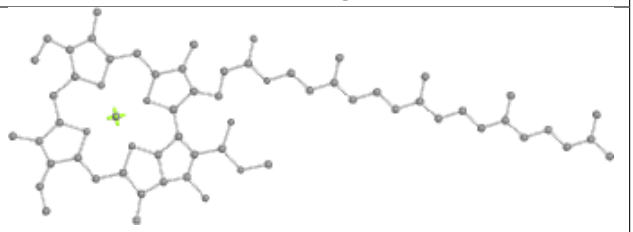
Bond lengths



Bond angles

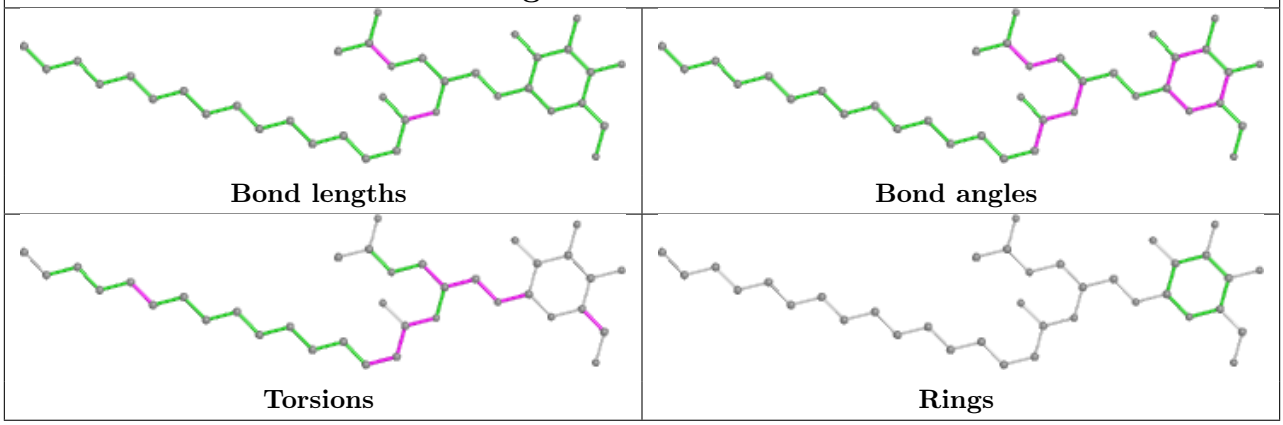


Torsions

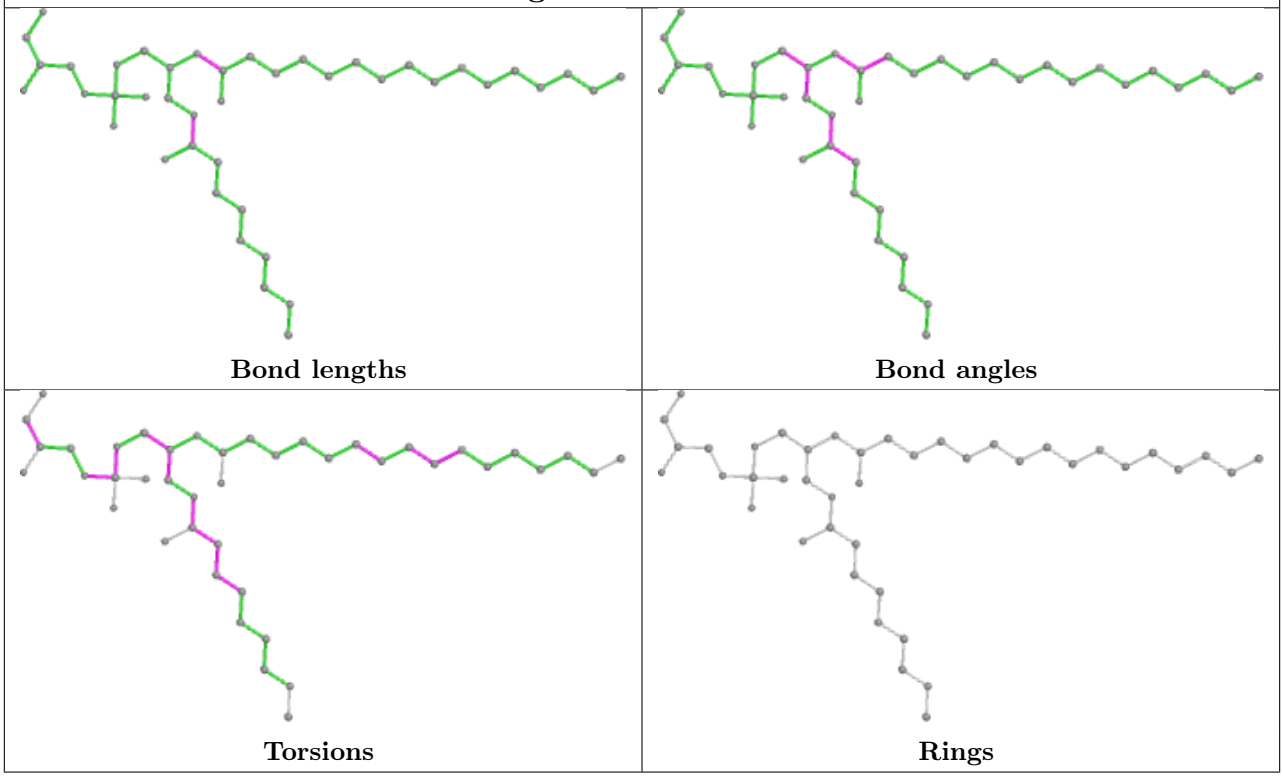


Rings

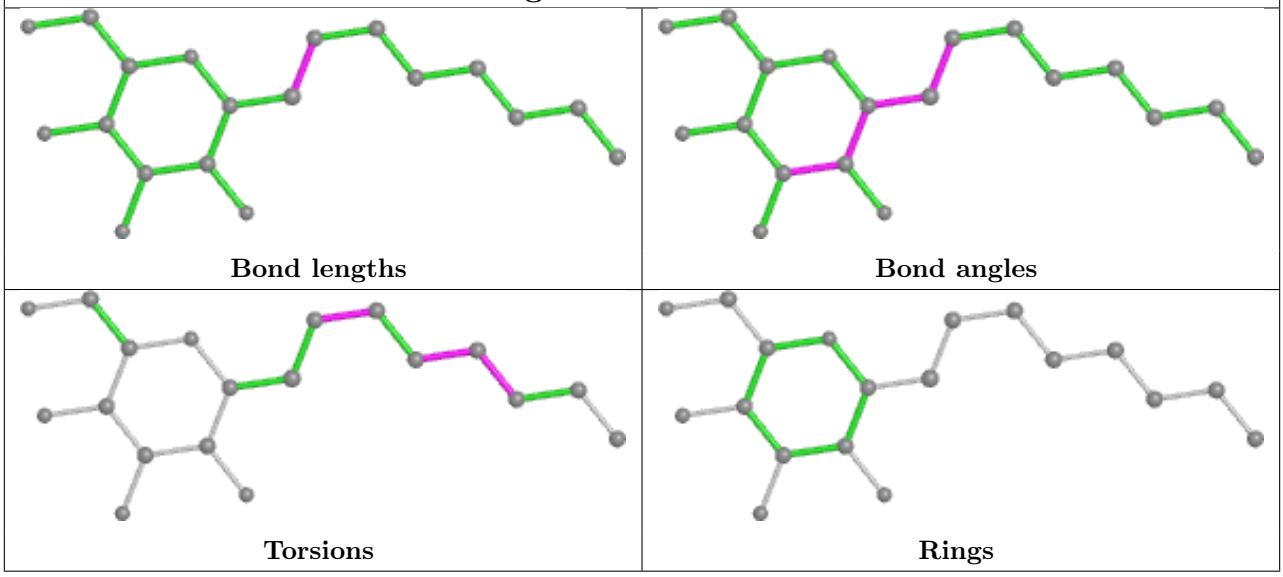
Ligand LMG Z 101



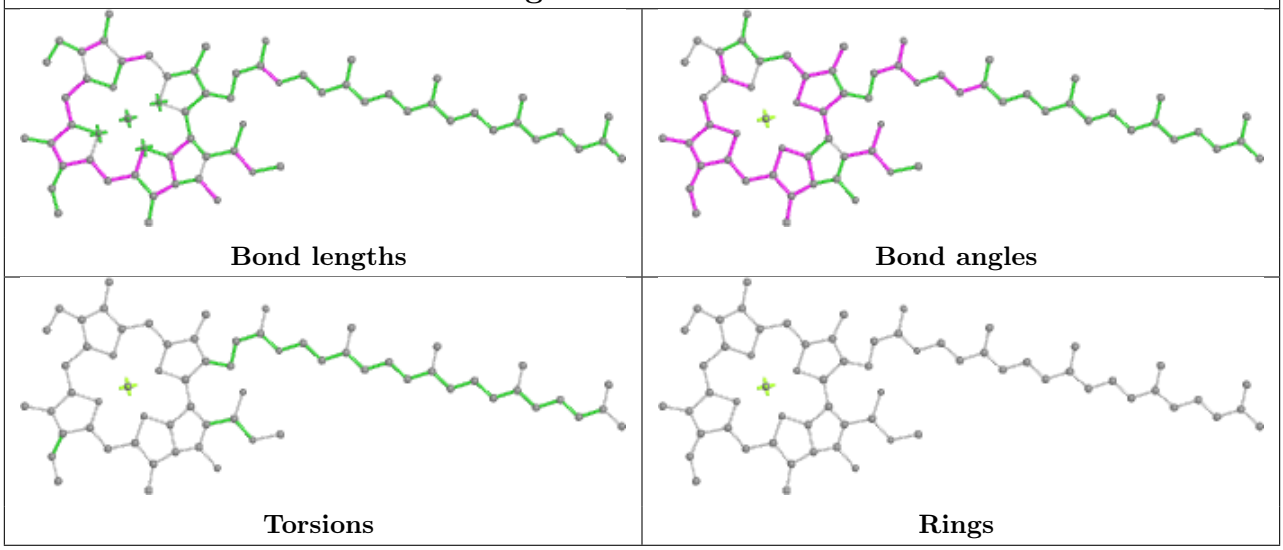
Ligand LHG a 422



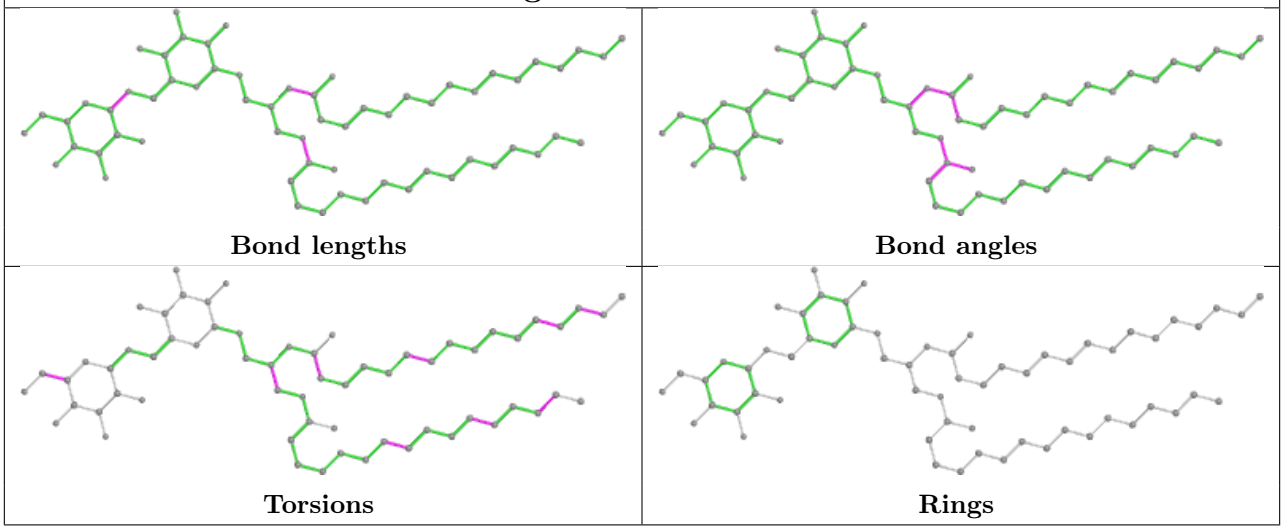
Ligand HTG b 632



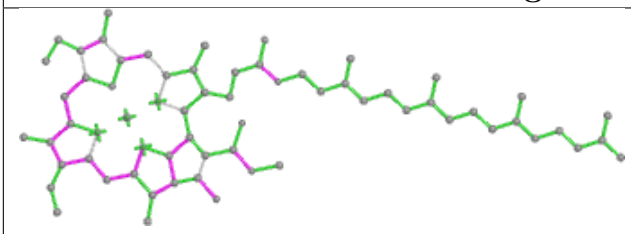
Ligand CLA B 612



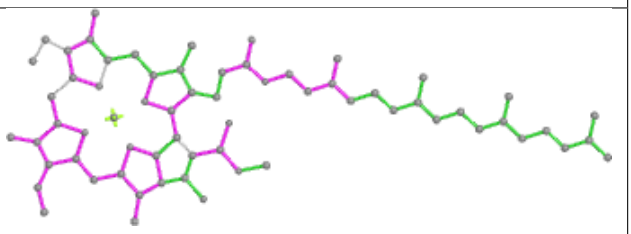
Ligand DGD h 102



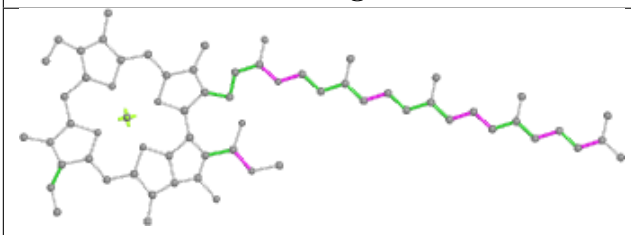
Ligand CLA C 509



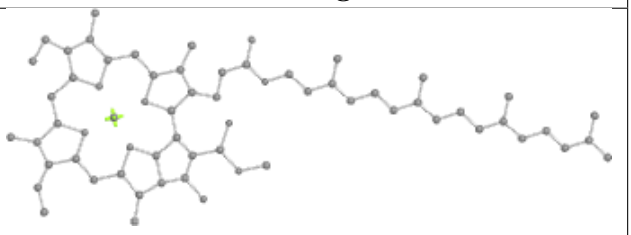
Bond lengths



Bond angles

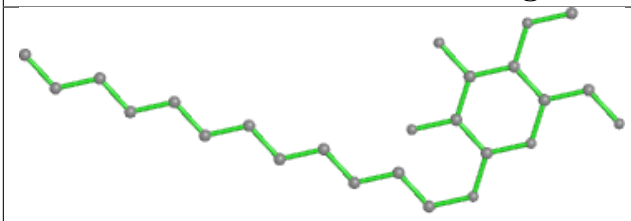


Torsions



Rings

Ligand LMT T 104



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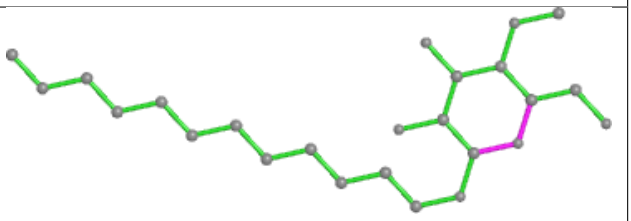
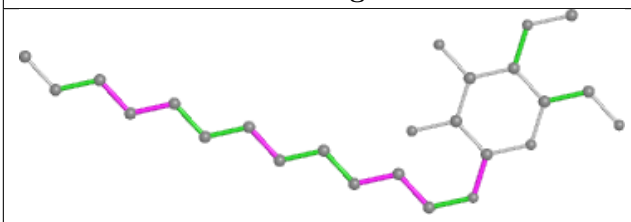


Bond angles



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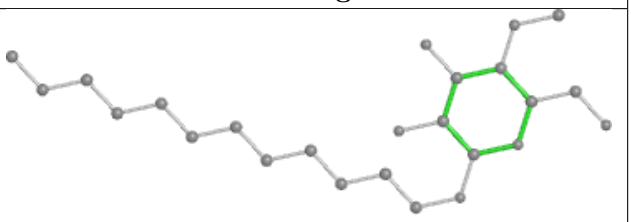
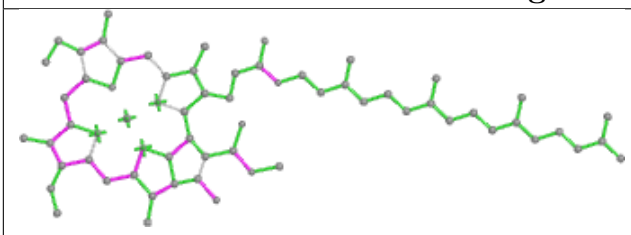
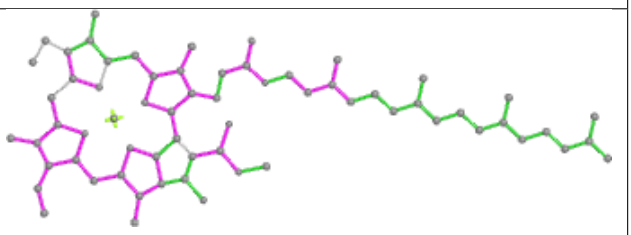


Rings

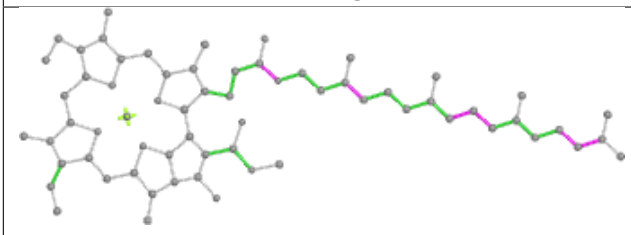
Ligand CLA a 412



Bond lengths



Bond angles



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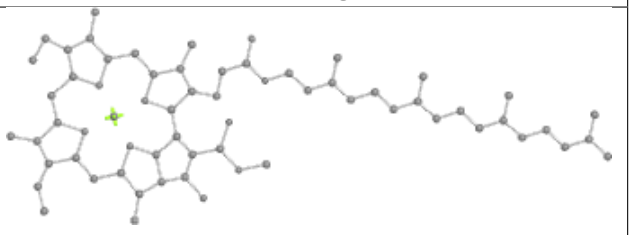
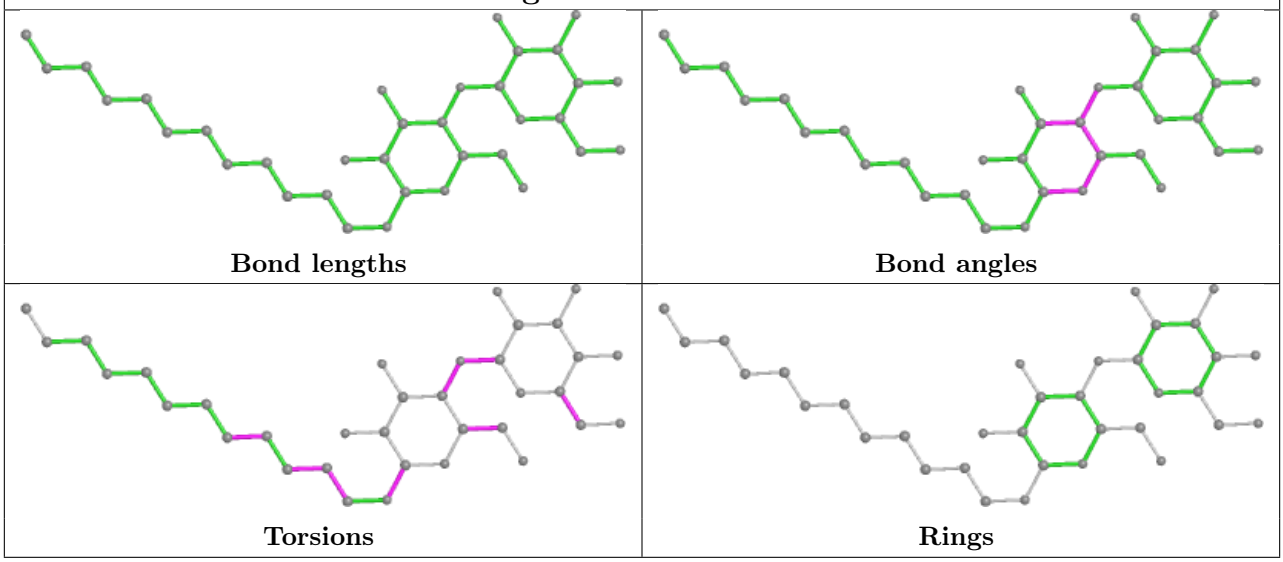
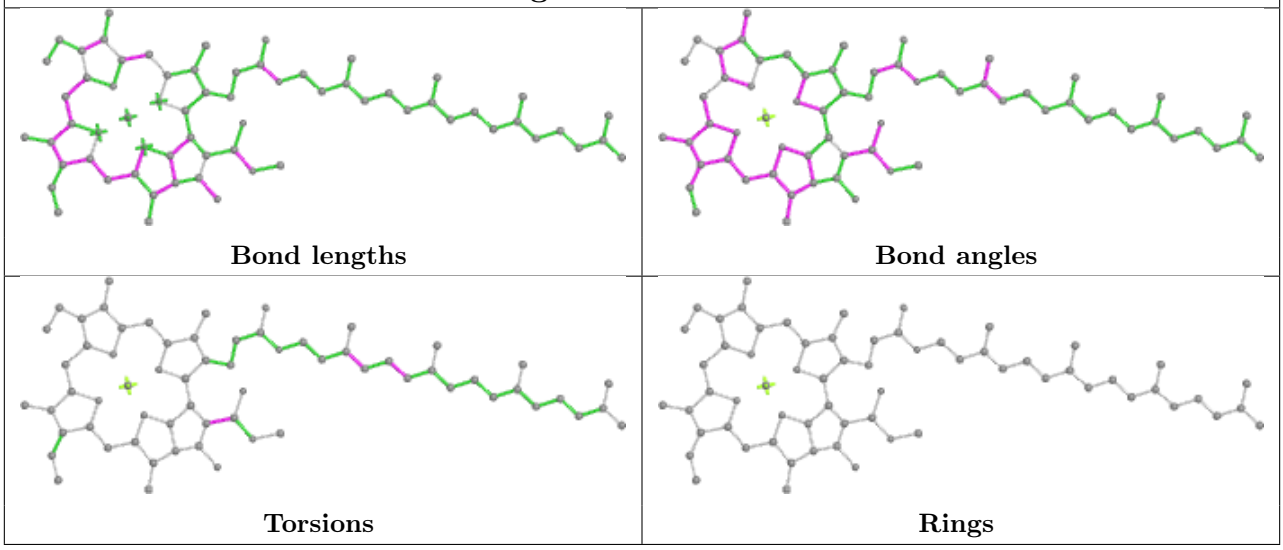


Rings

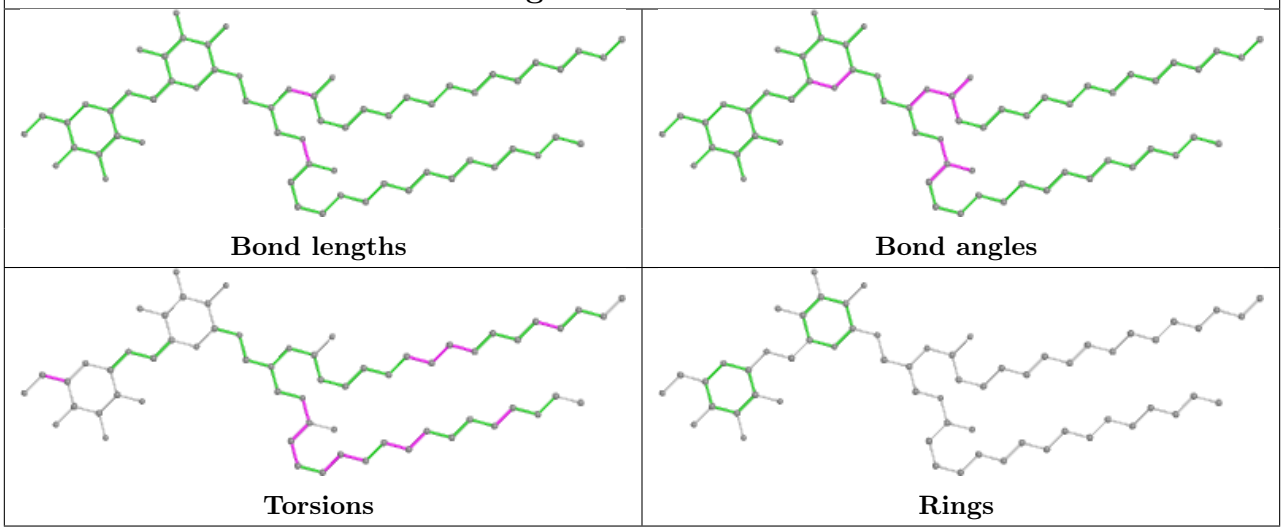
Ligand LMT C 521



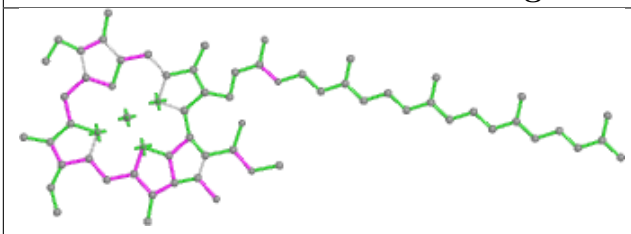
Ligand CLA c 511



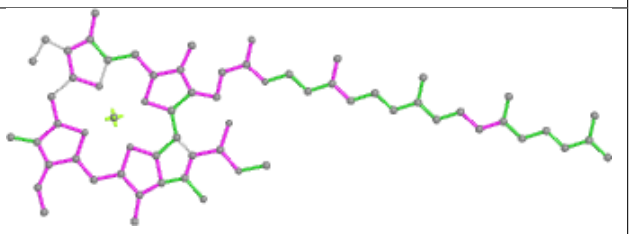
Ligand DGD c 521



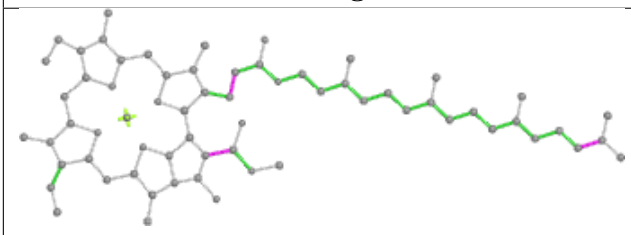
Ligand CLA B 611



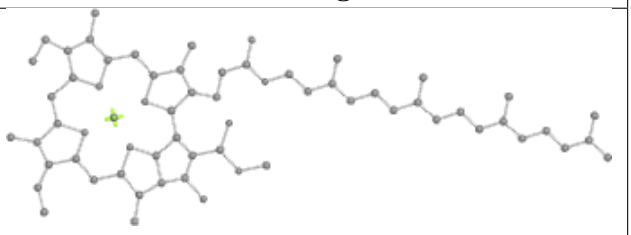
Bond lengths



Bond angles

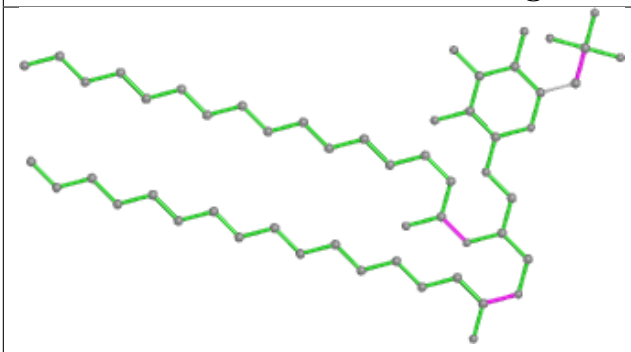


Torsions

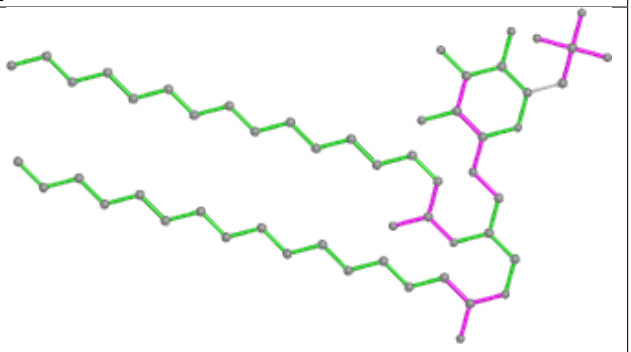


Rings

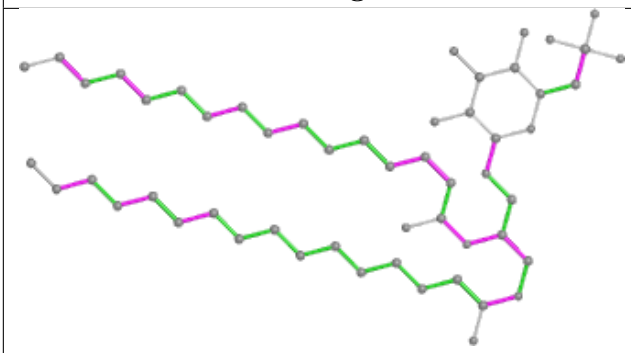
Ligand SQD B 621



Bond lengths



Bond angles



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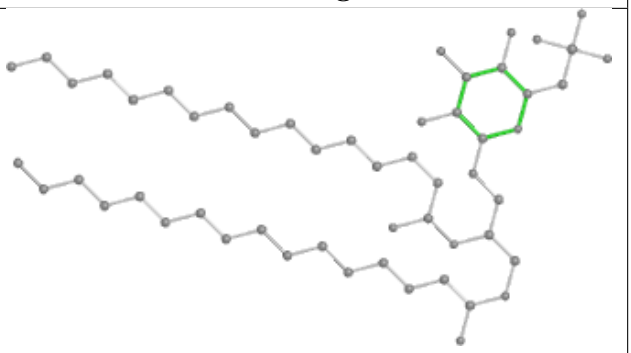
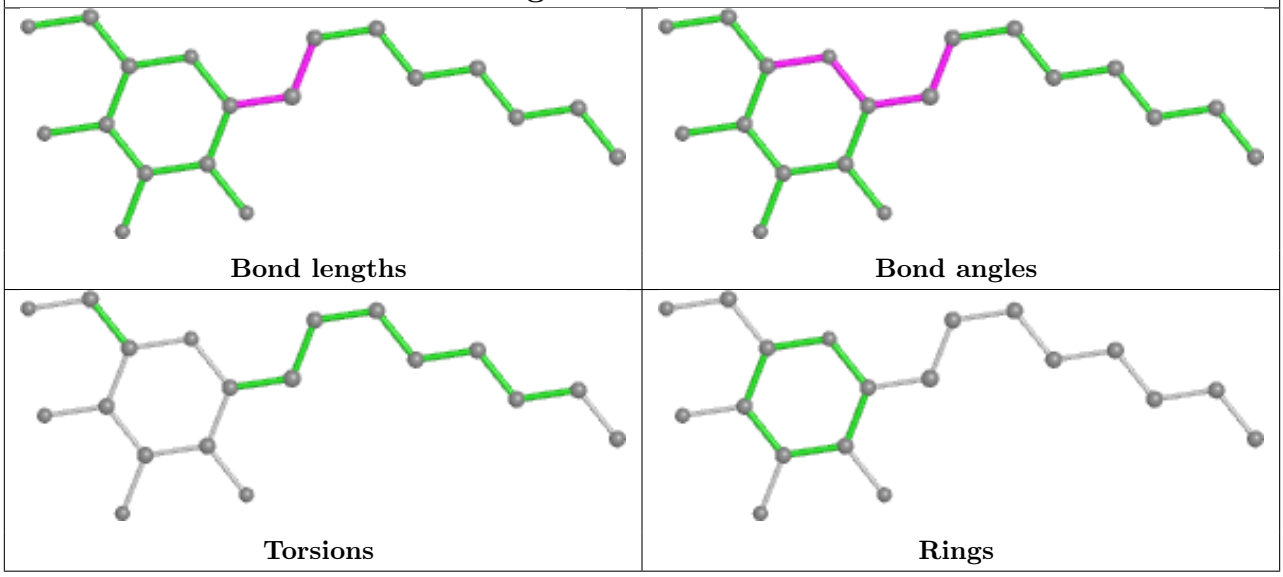
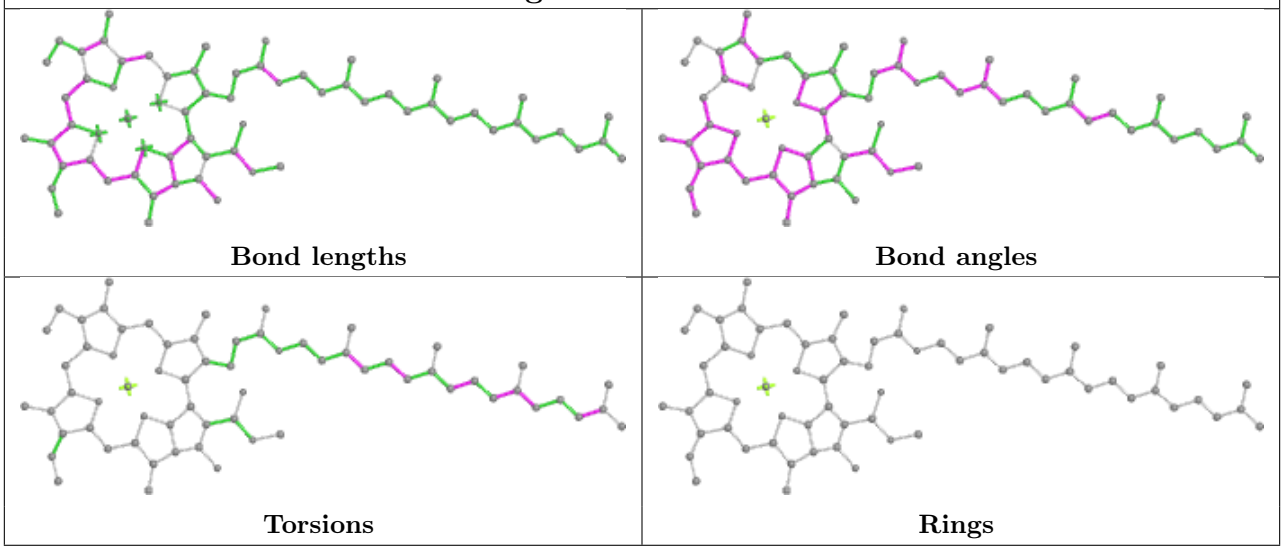


Rings

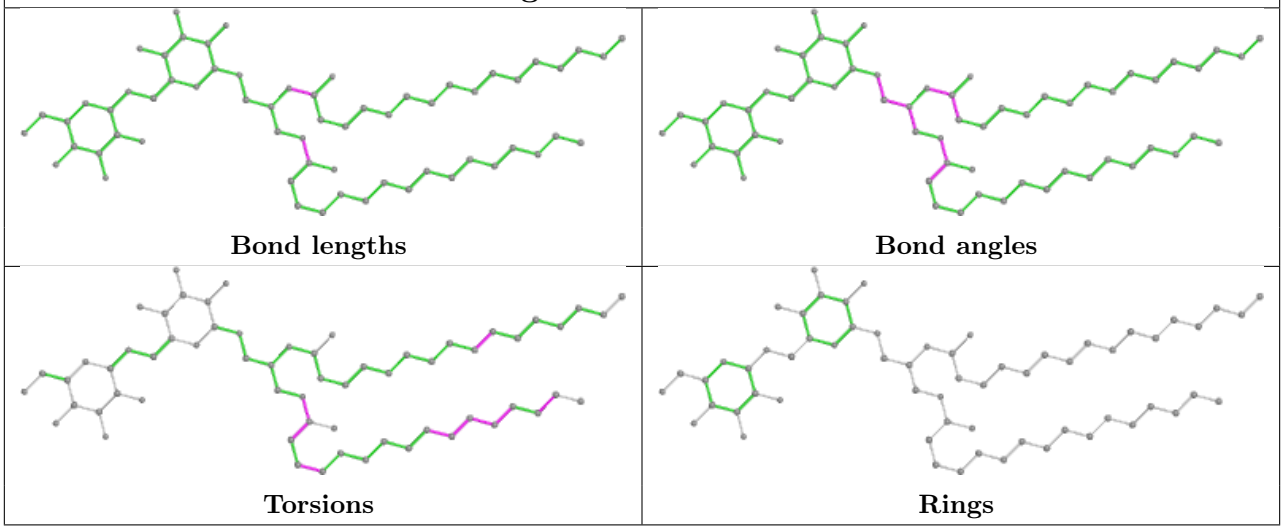
Ligand HTG c 525



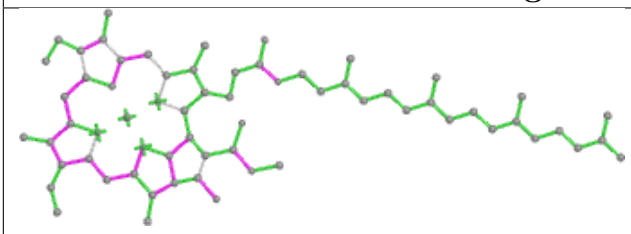
Ligand CLA B 616



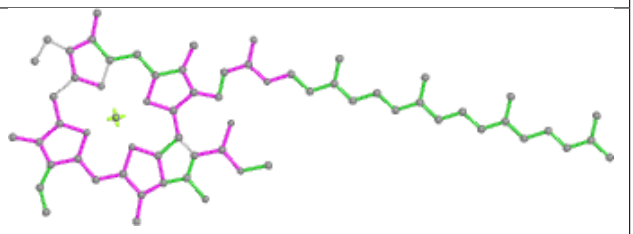
Ligand DGD C 518



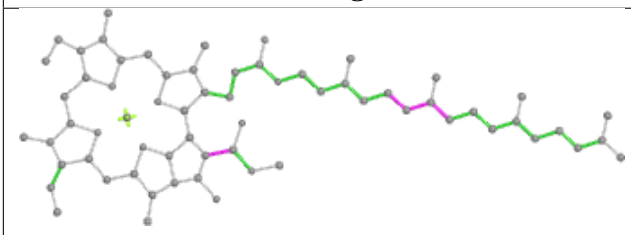
Ligand CLA B 604



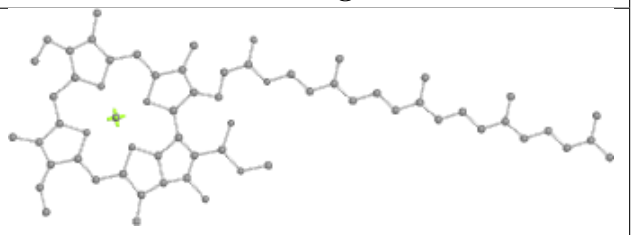
Bond lengths



Bond angles

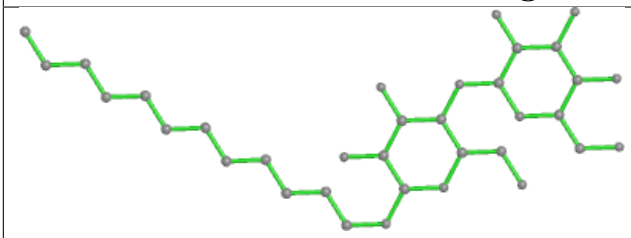


Torsions



Rings

Ligand LMT m 102



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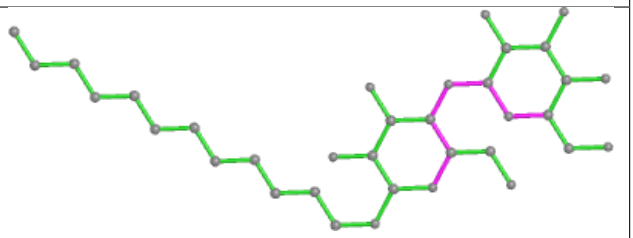
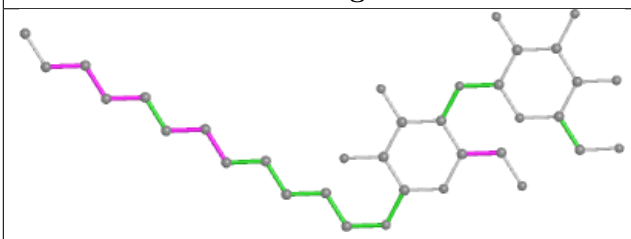
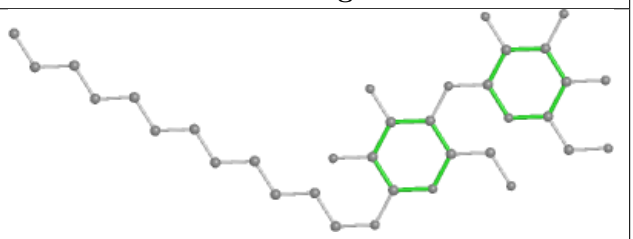


Bond angles

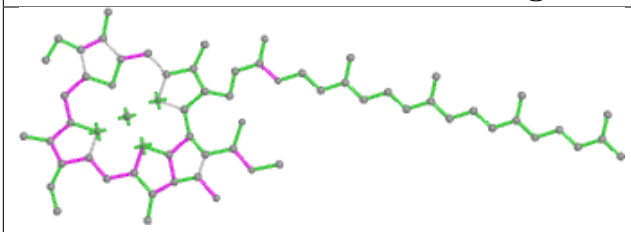


Torsions

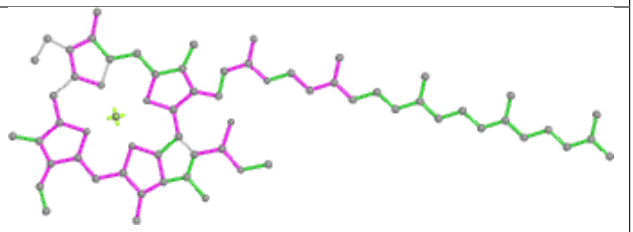


Rings

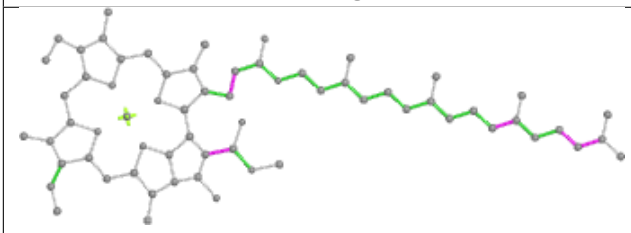
Ligand CLA b 620



Bond lengths



Bond angles



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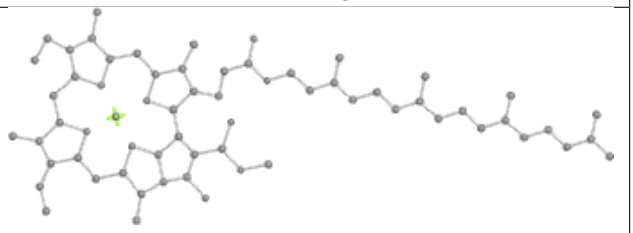
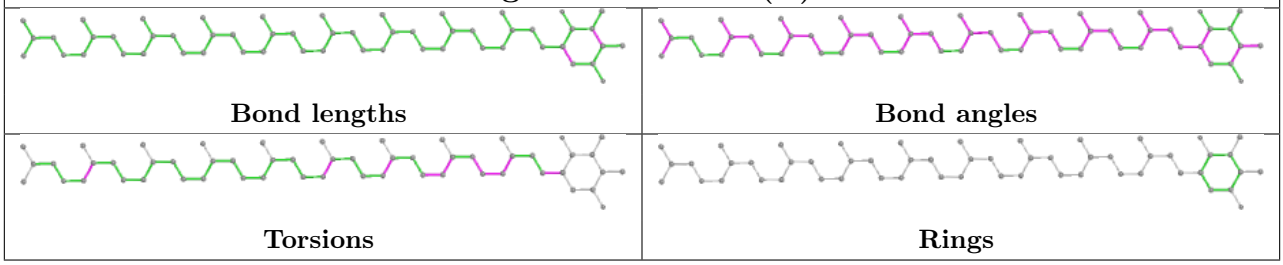
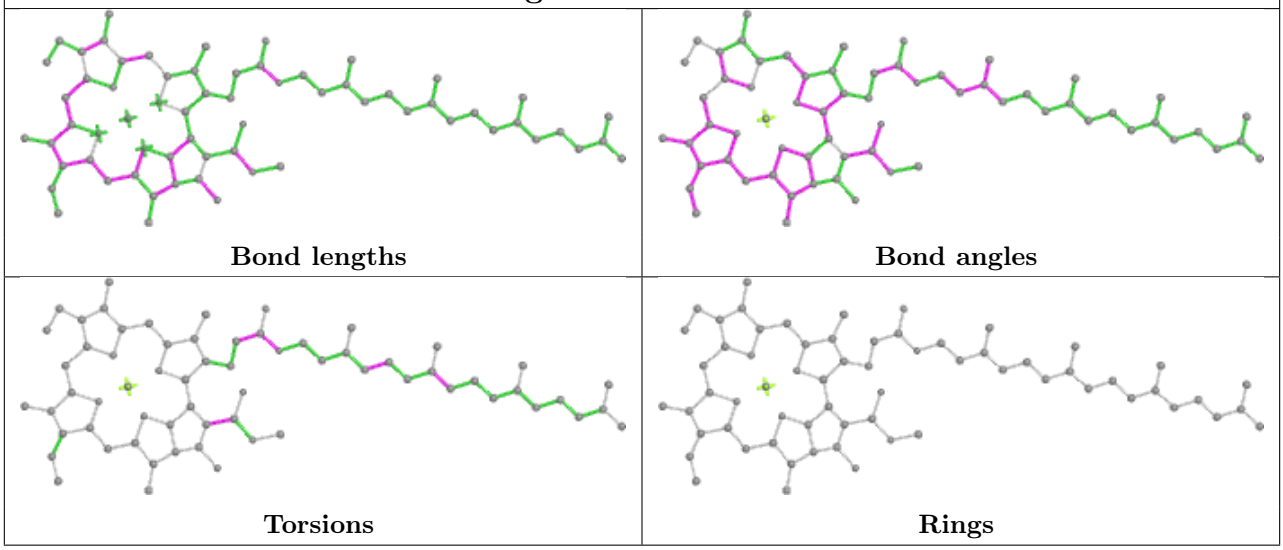


Rings

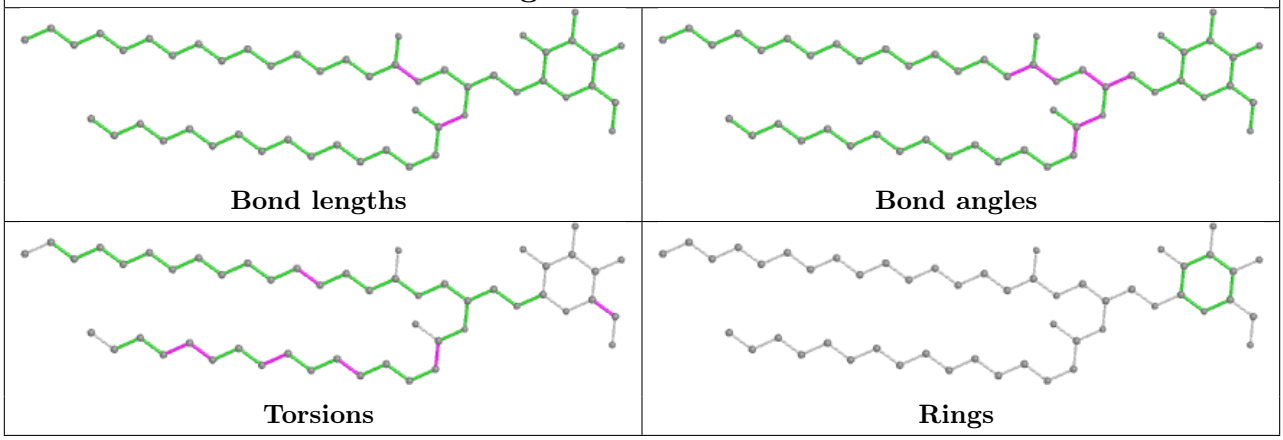
Ligand PL9 a 416 (B)



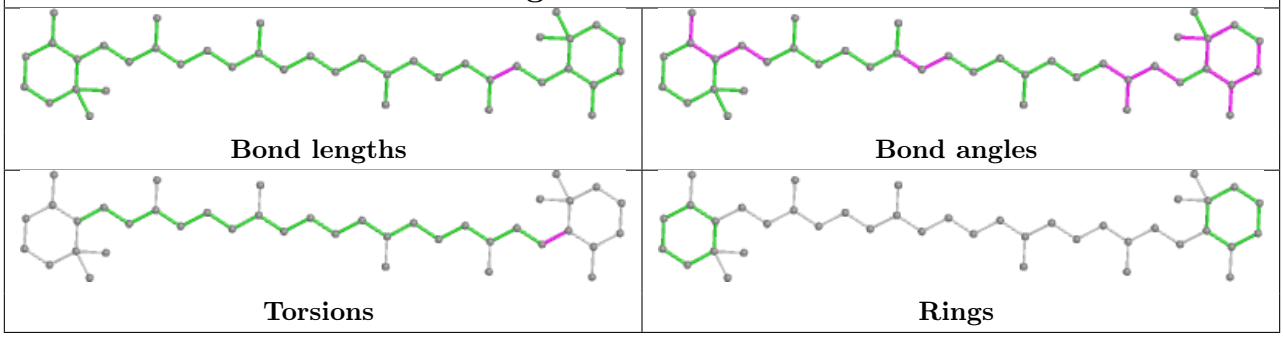
Ligand CLA C 512



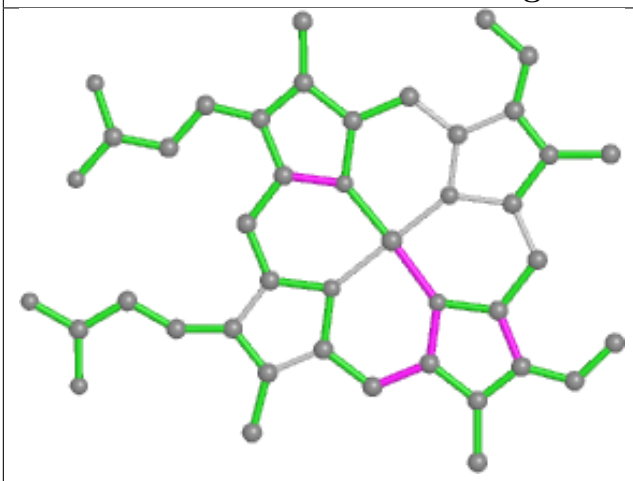
Ligand LMG D 412



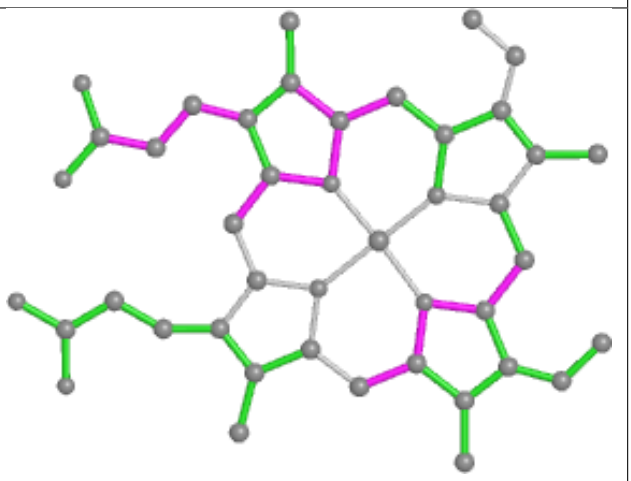
Ligand BCR b 628



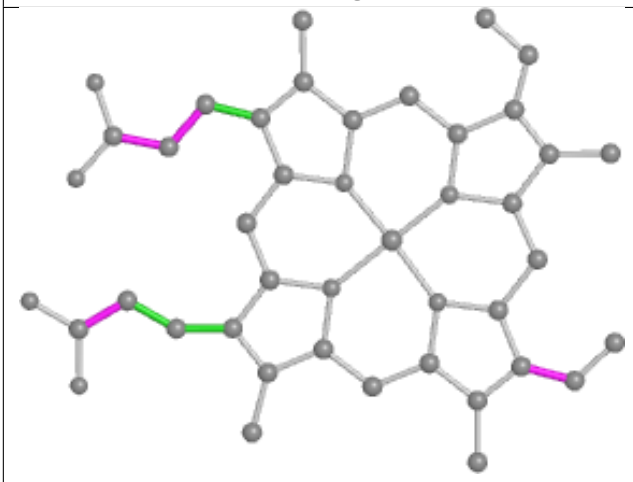
Ligand HEM e 102



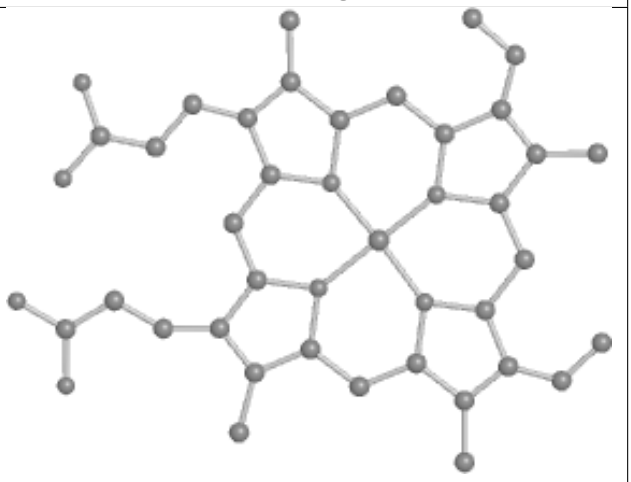
Bond lengths



Bond angles

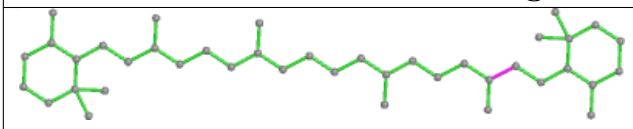


Torsions

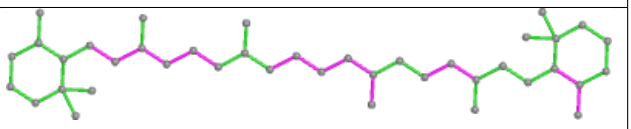


Rings

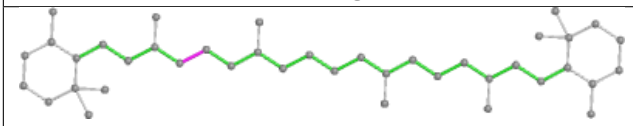
Ligand BCR h 101



Bond lengths



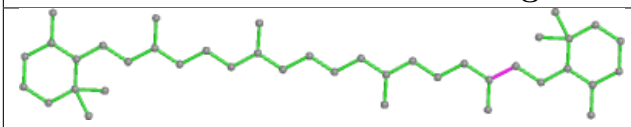
Bond angles



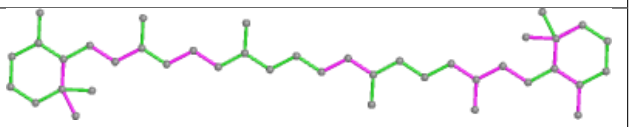
Torsions

Rings

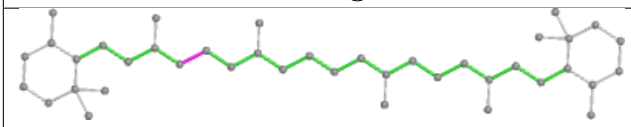
Ligand BCR H 102



Bond lengths



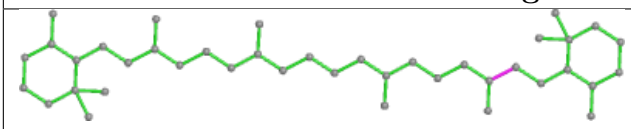
Bond angles



Torsions

Rings

Ligand BCR A 411



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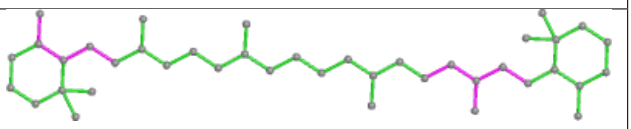

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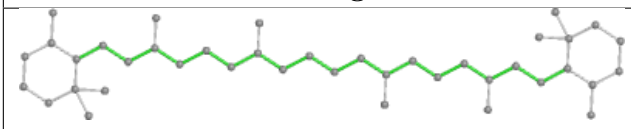
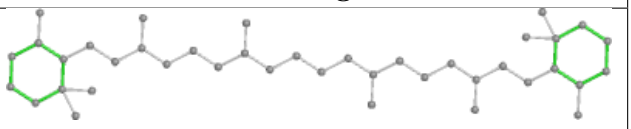
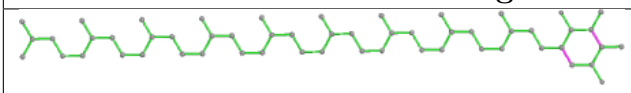


Torsions



Rings

Ligand PL9 D 405 (B)



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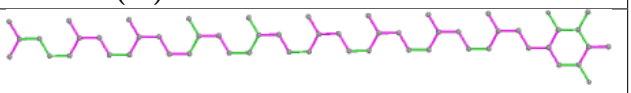

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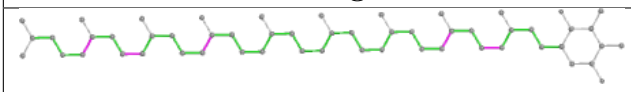

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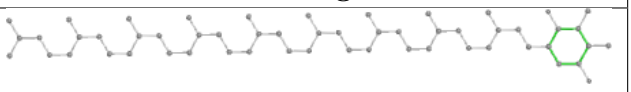
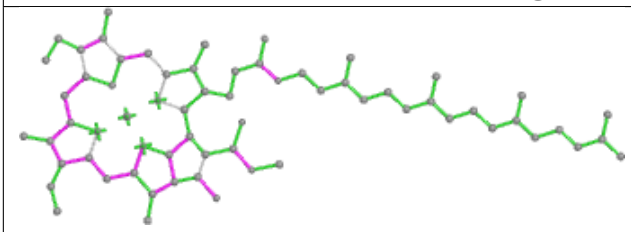


Rings

Ligand CLA c 514



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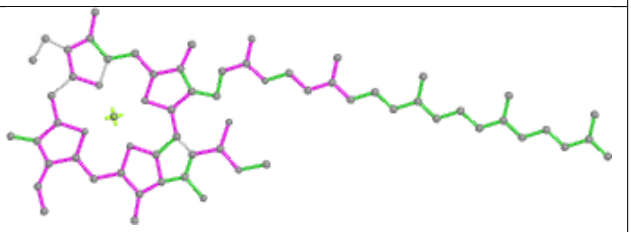
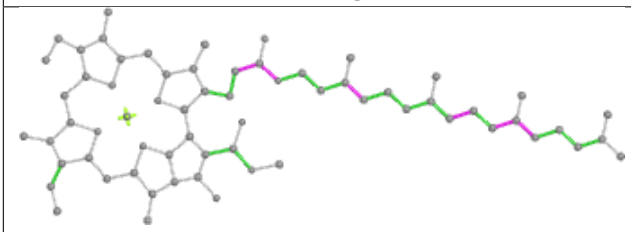


Bond angles



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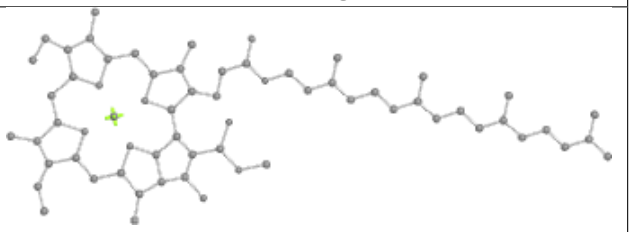
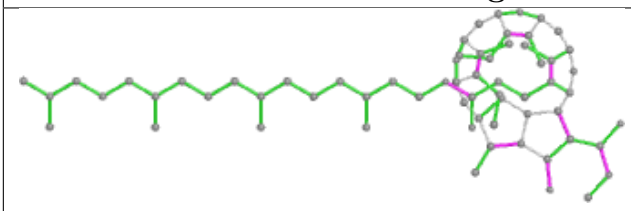


Rings

Ligand PHO A 409 (A)



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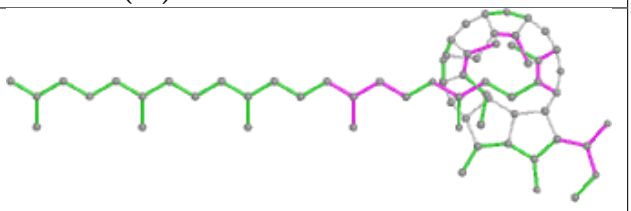
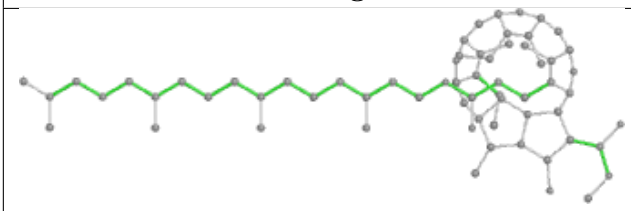


Bond angles



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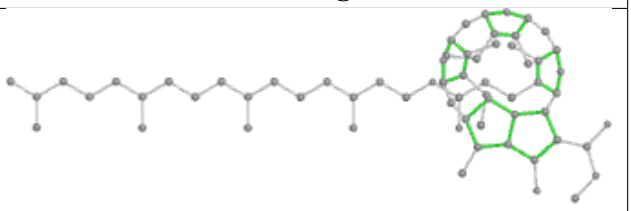
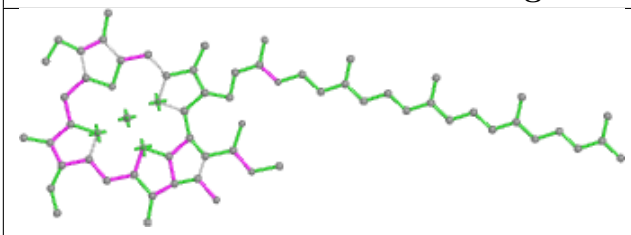


Rings

Ligand CLA C 501



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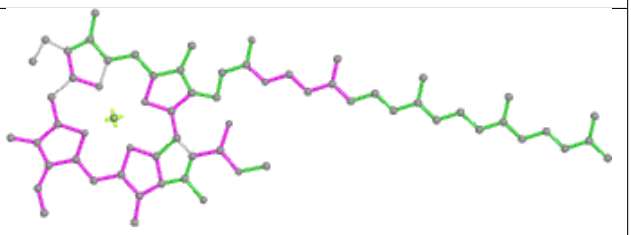

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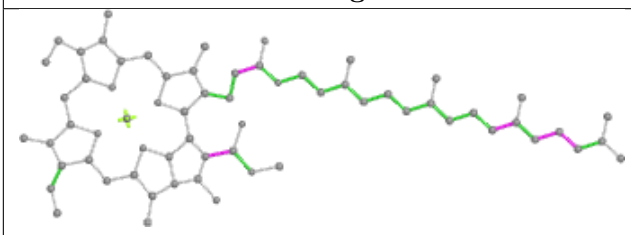

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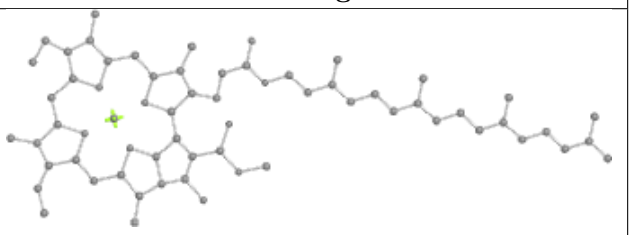
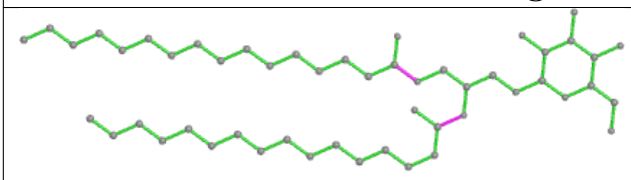


Rings

Ligand LMG j 101



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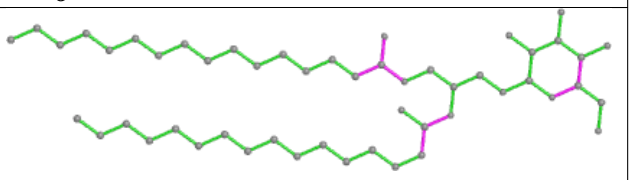
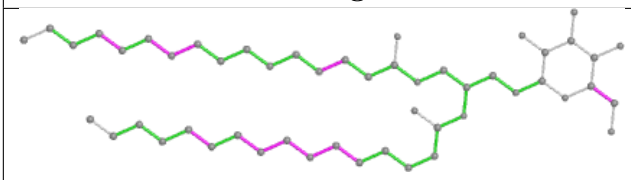


Bond angles



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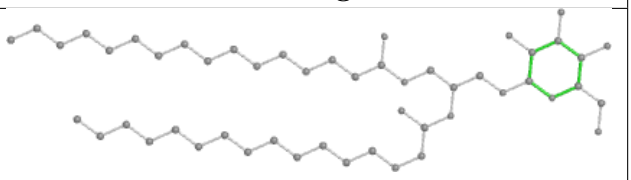
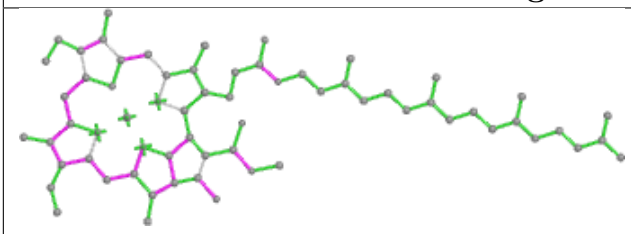
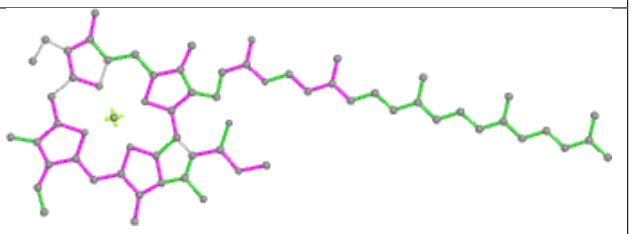
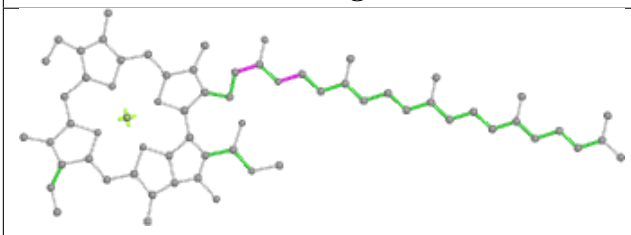
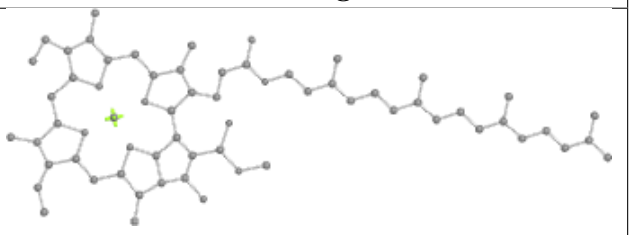
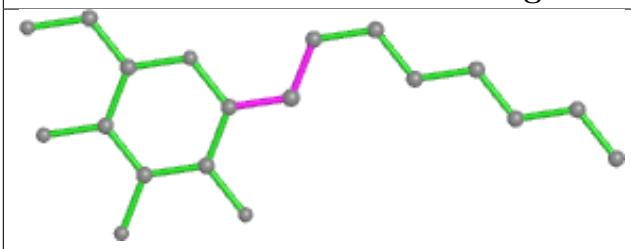
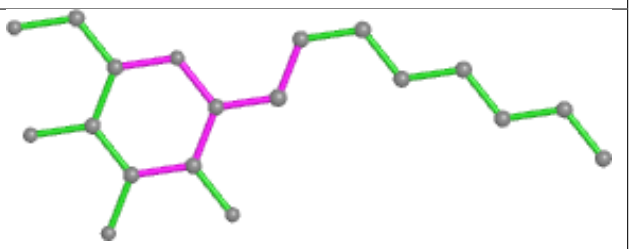
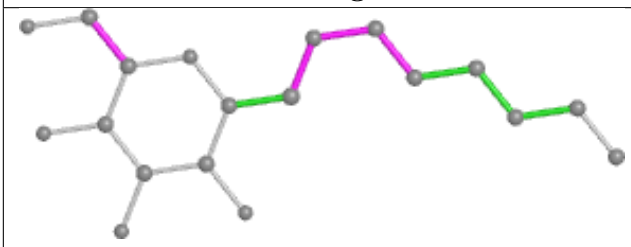
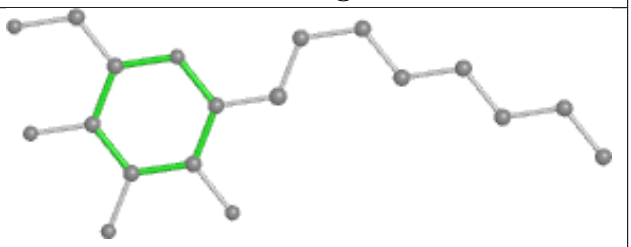
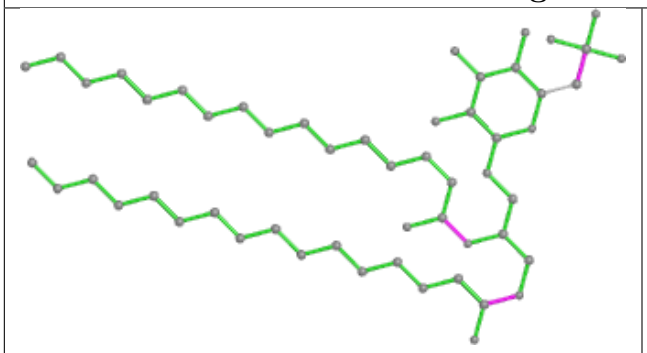


Rings

Ligand CLA b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG b 633	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 414



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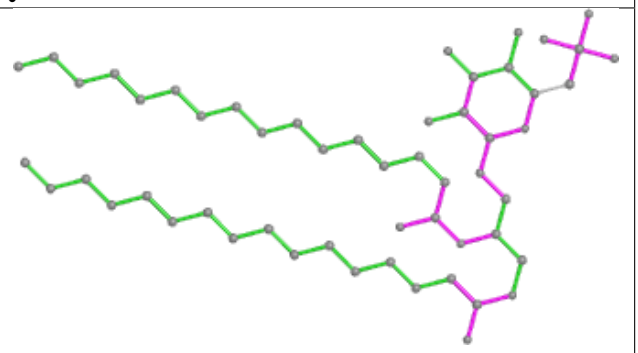
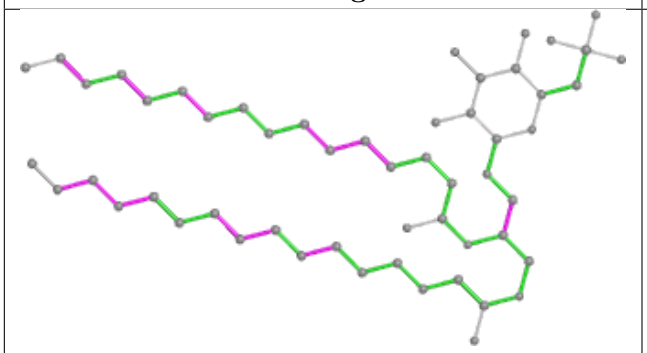


Bond angles



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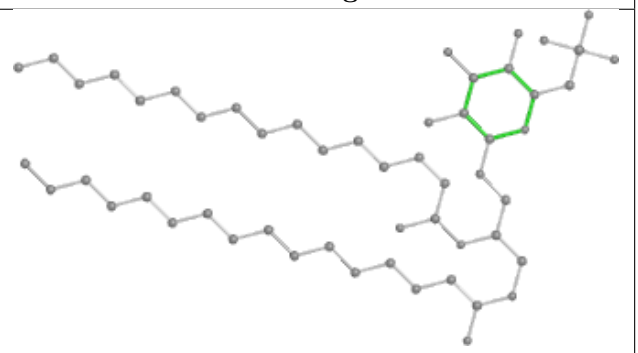
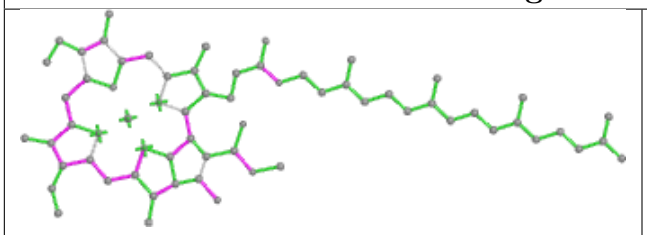


Rings

Ligand CLA B 605



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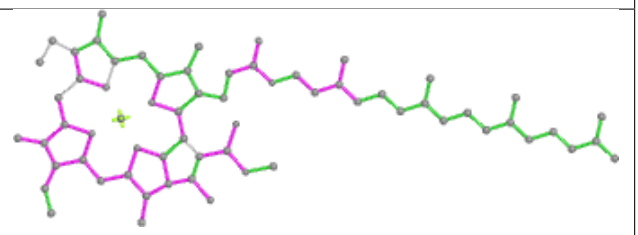
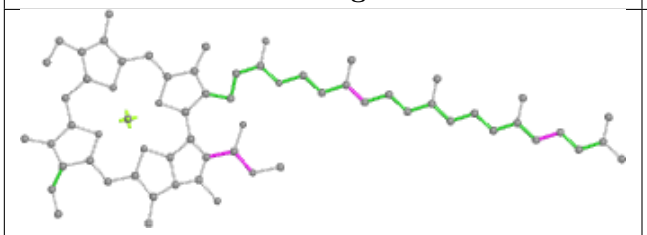


Bond angles



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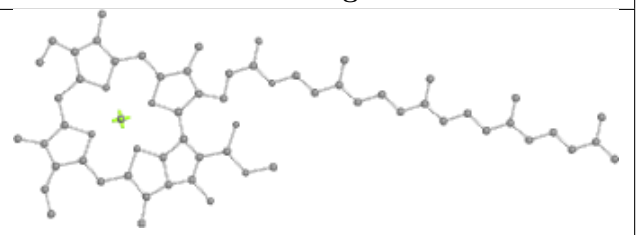

Rings

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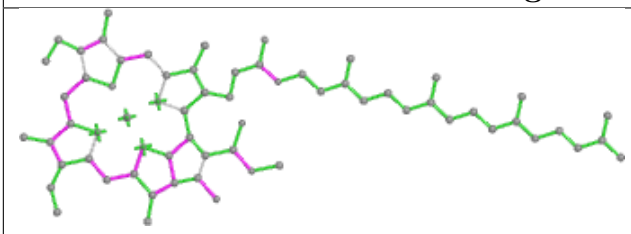

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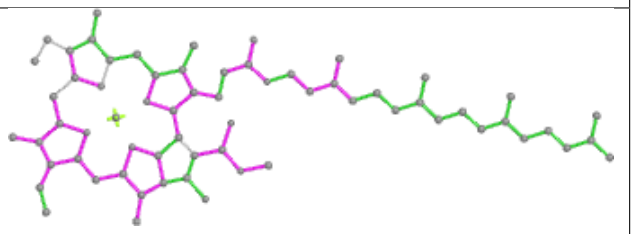
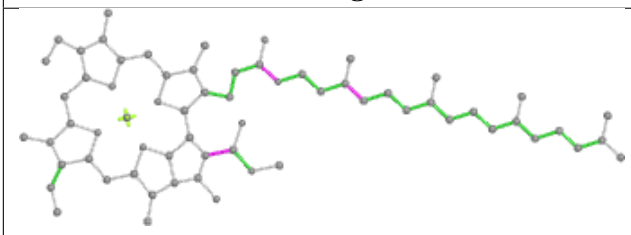


Bond angles



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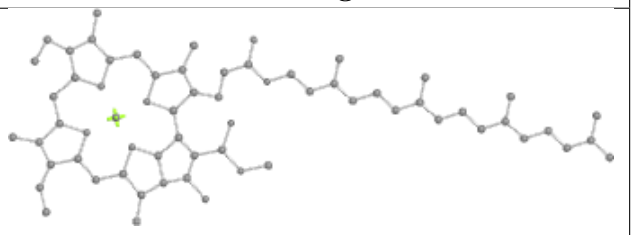
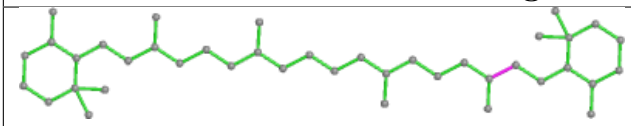


Rings

Ligand BCR B 618



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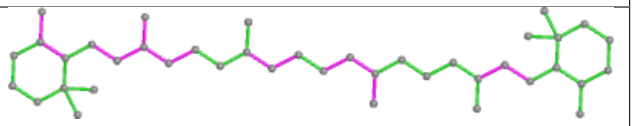
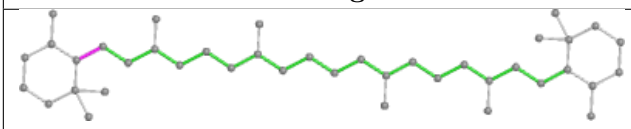


Bond angles



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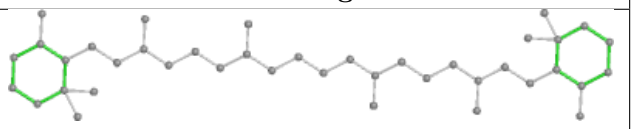
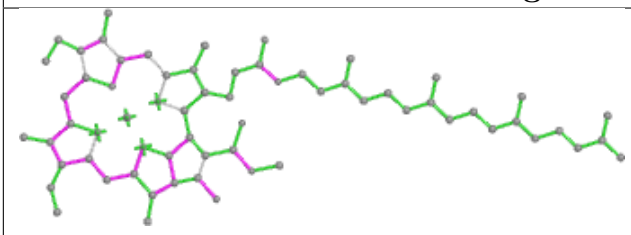
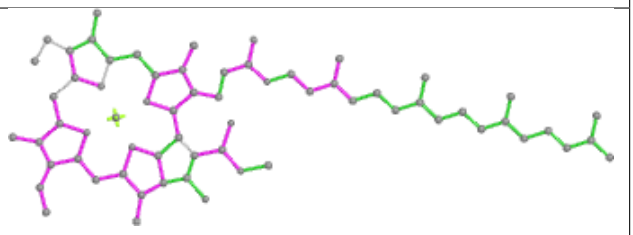


Rings

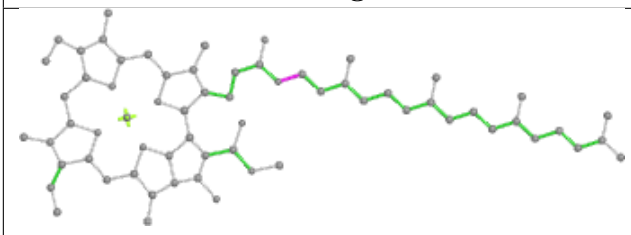
Ligand CLA D 402



Bond lengths



Bond angles



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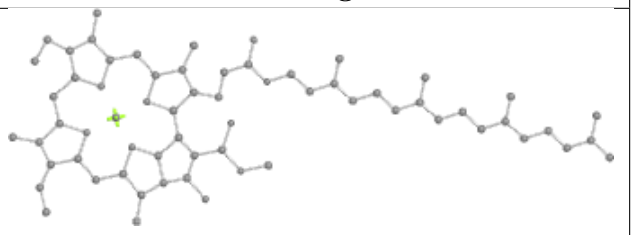
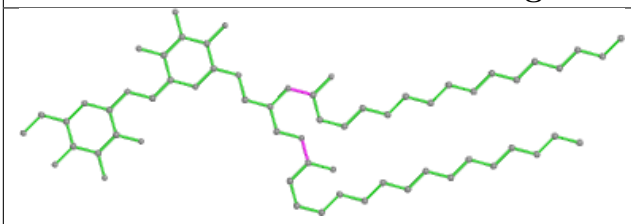
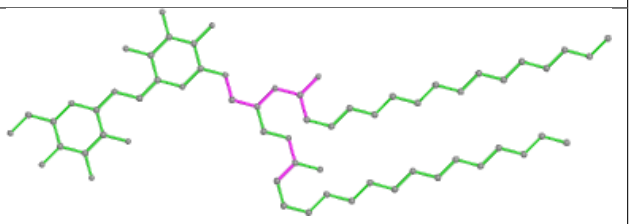


Rings

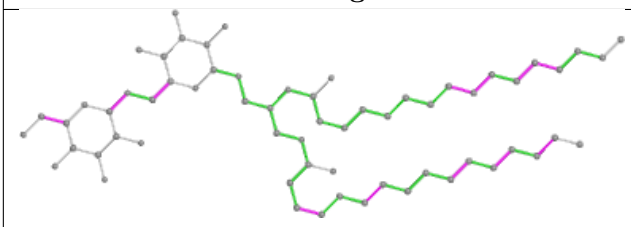
Ligand DGD c 519



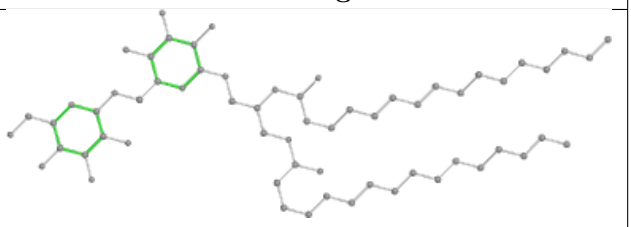
Bond lengths



Bond angles

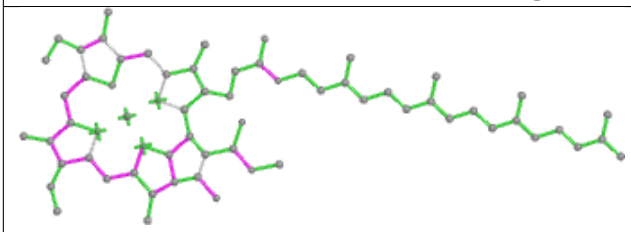


Torsions



Rings

Ligand CLA a 409



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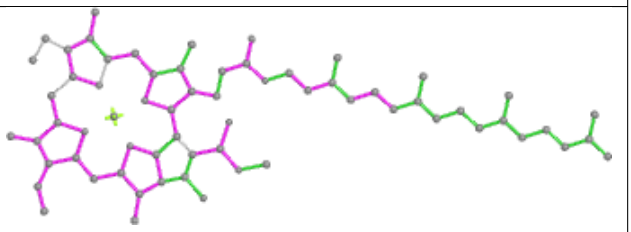

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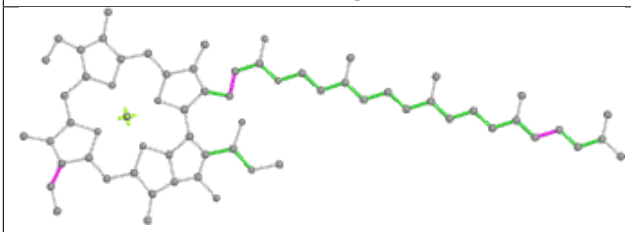

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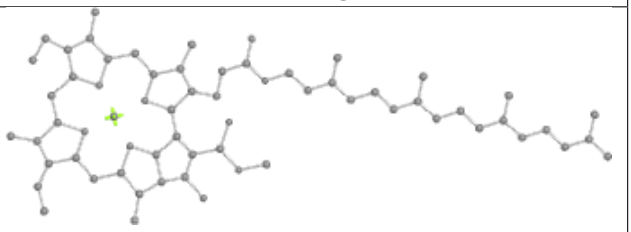
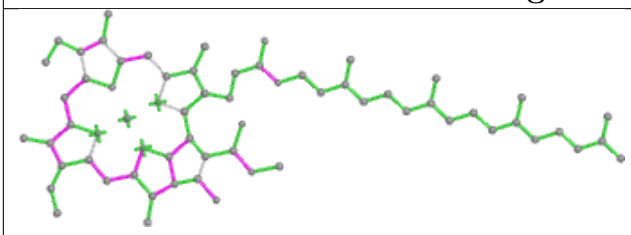


Rings

Ligand CLA b 615



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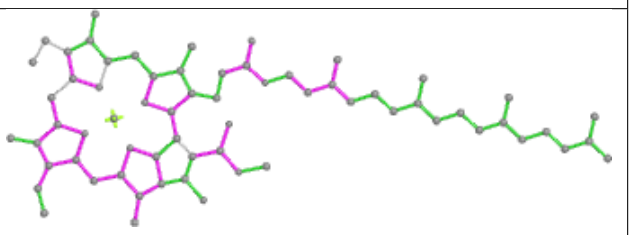
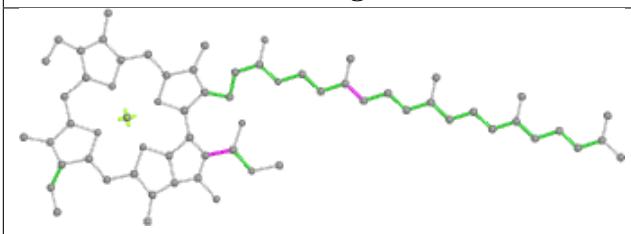


Bond angles



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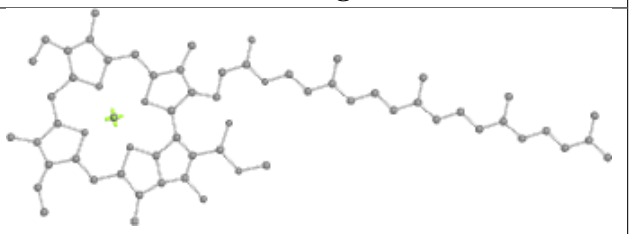
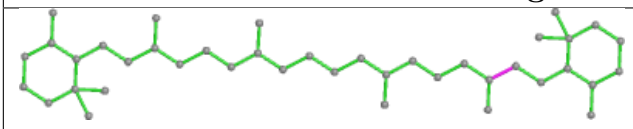


Rings

Ligand BCR c 518



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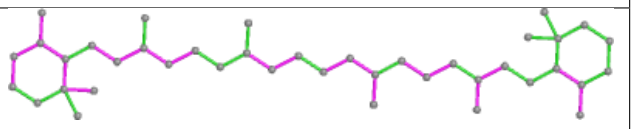
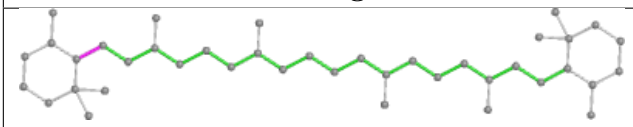


Bond angles



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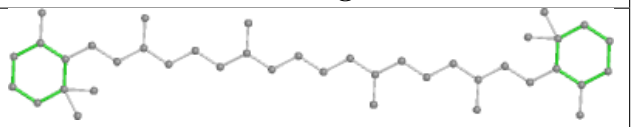
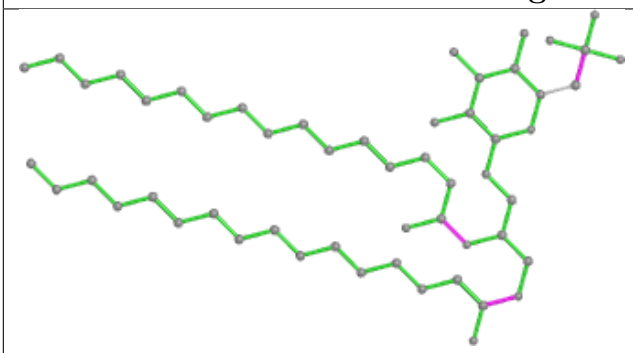


Rings

Ligand SQD a 405



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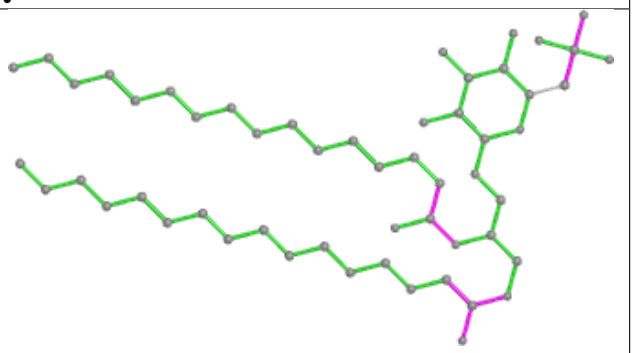
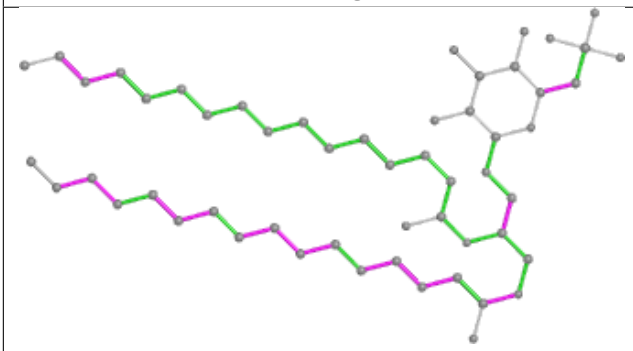


Bond angles



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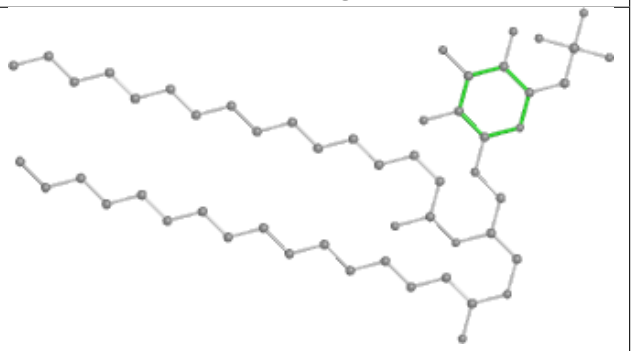
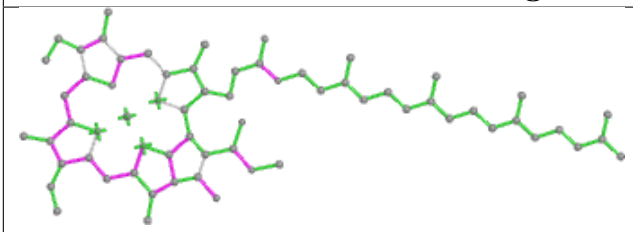


Rings

Ligand CLA B 607



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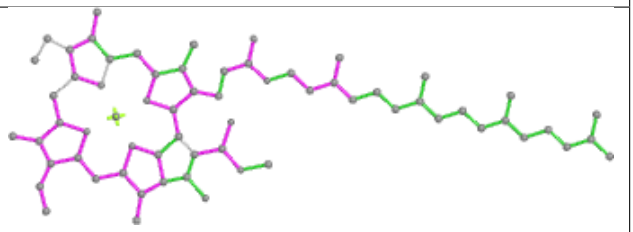
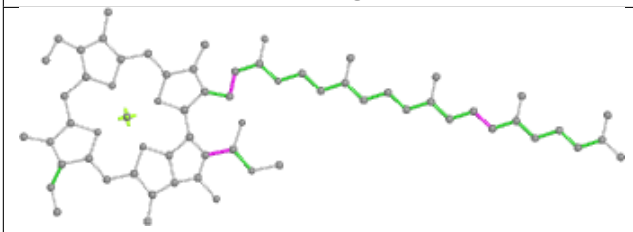


Bond angles



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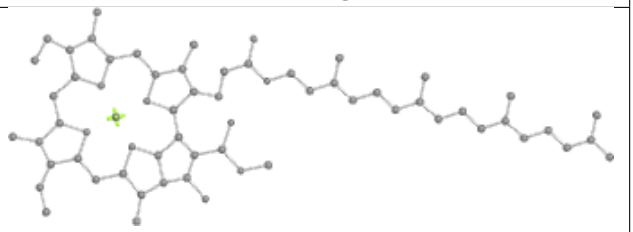
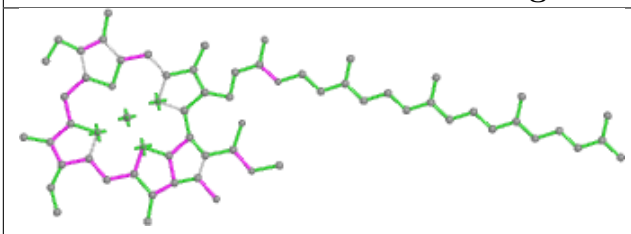


Rings

Ligand CLA c 507



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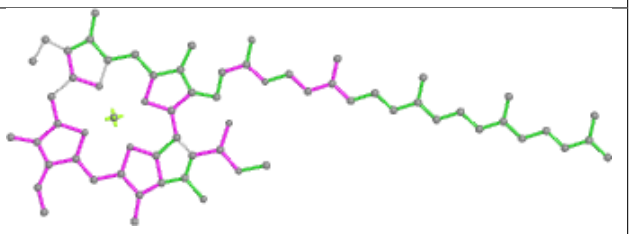
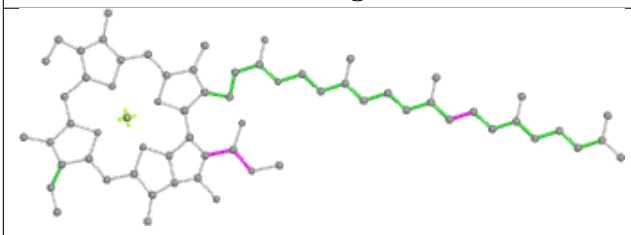


Bond angles



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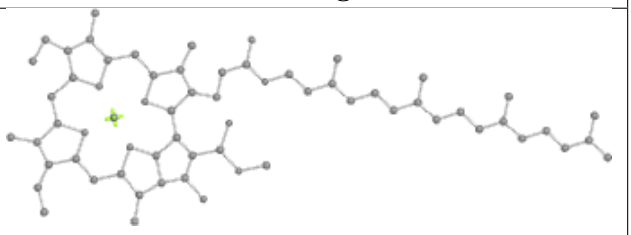
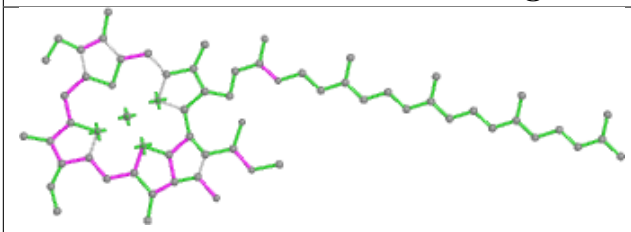


Rings

Ligand CLA C 502



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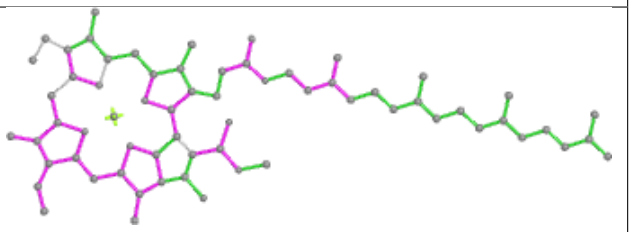
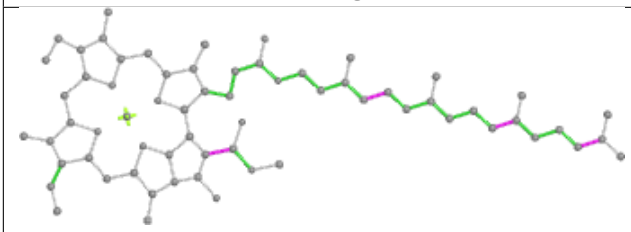
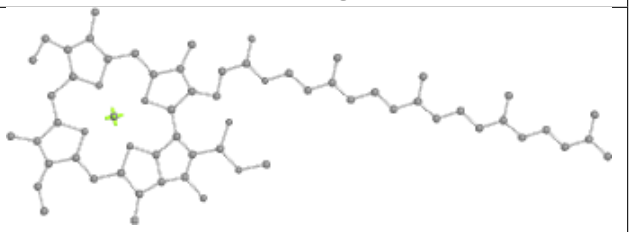


Bond angles

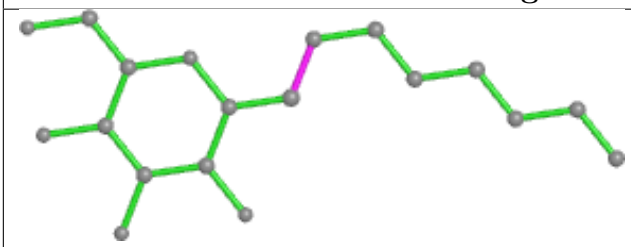


Torsions



Rings

Ligand HTG B 623



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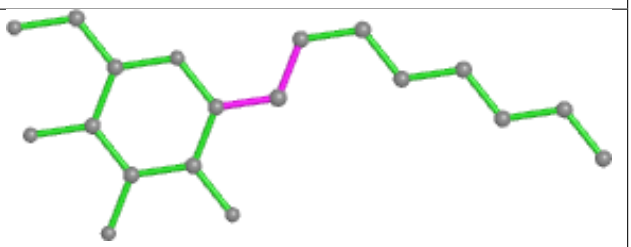
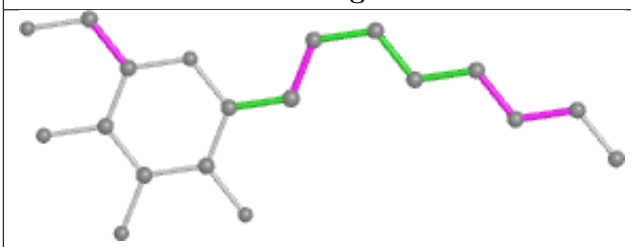


Bond angles



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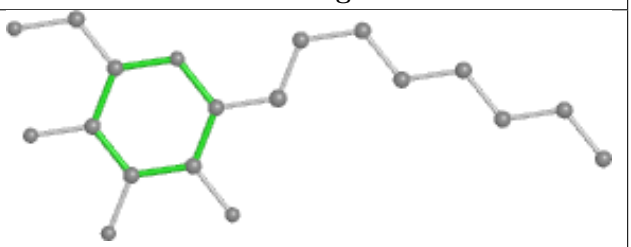
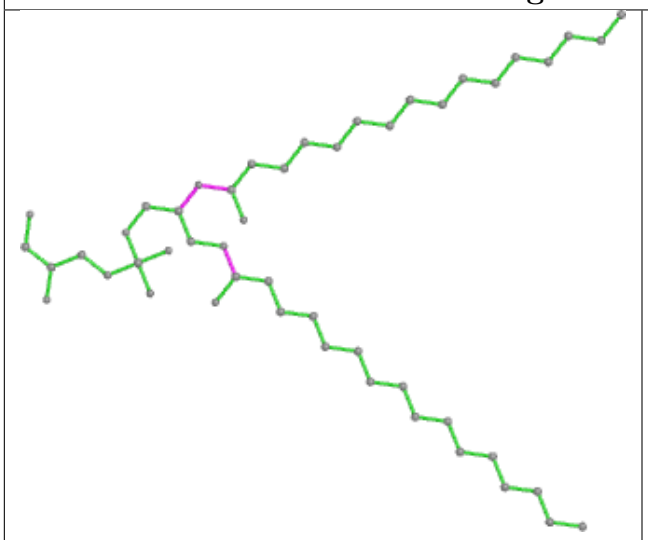


Rings

Ligand LHG d 406



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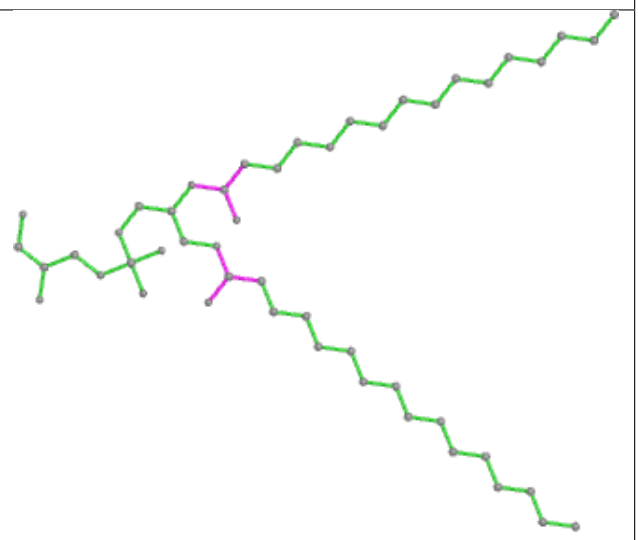

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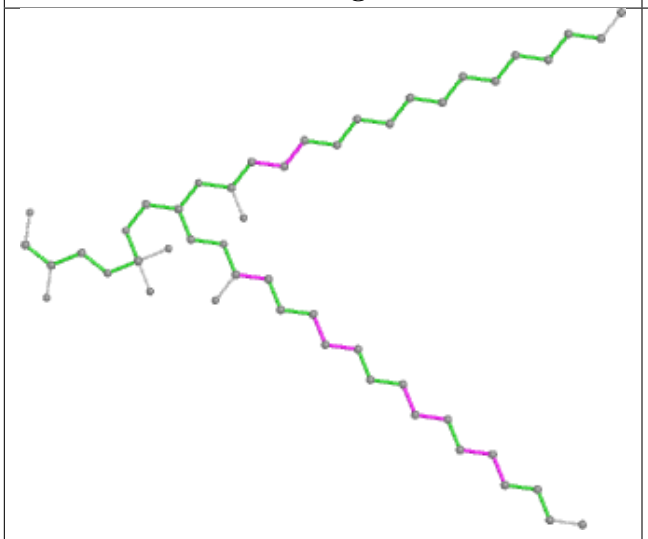

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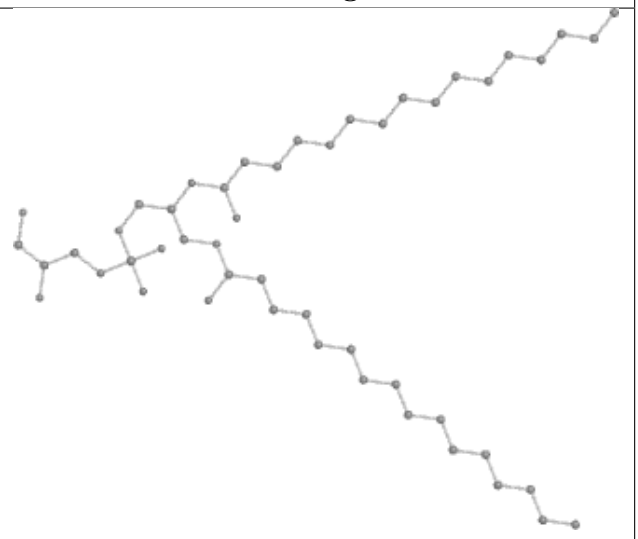
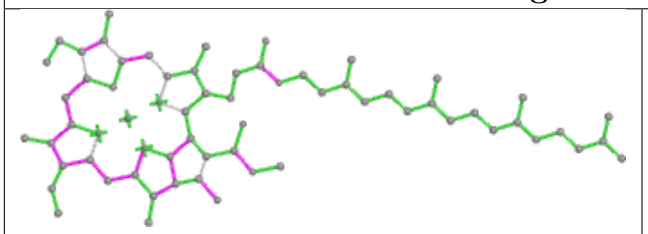


Rings

Ligand CLA c 516



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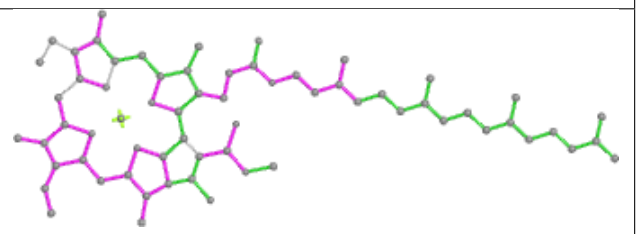
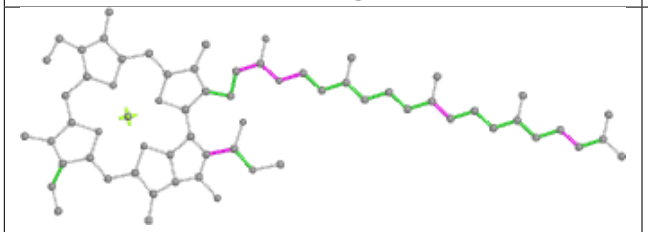


Bond angles



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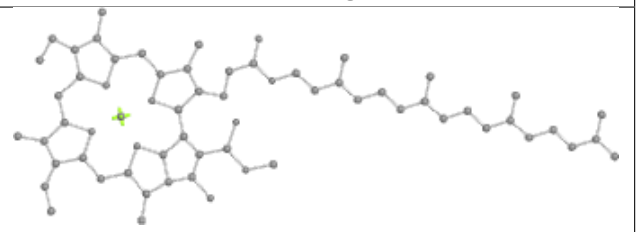
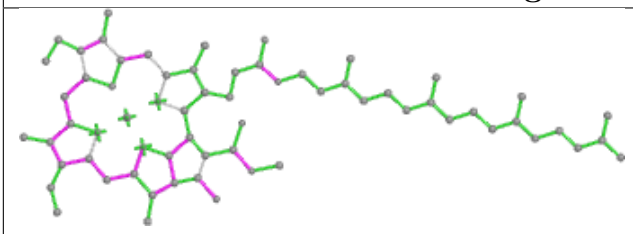


Rings

Ligand CLA B 617



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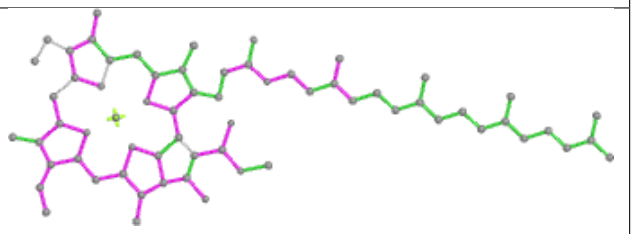
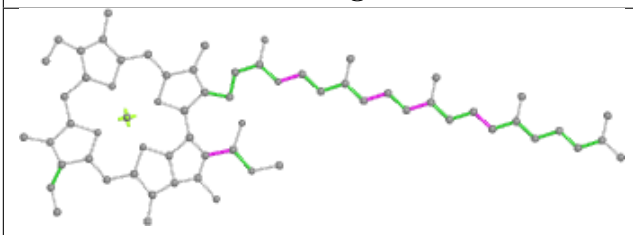


Bond angles



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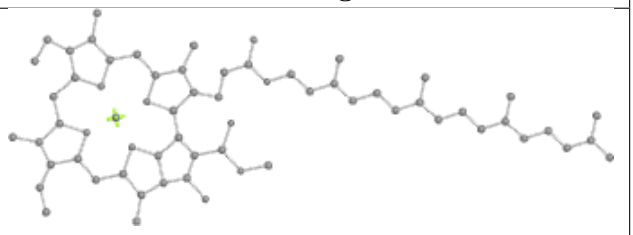

Rings

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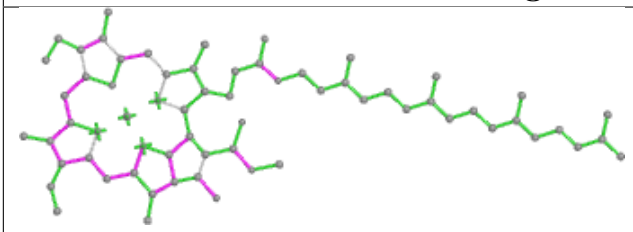

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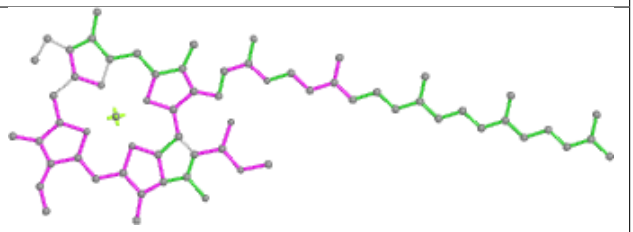
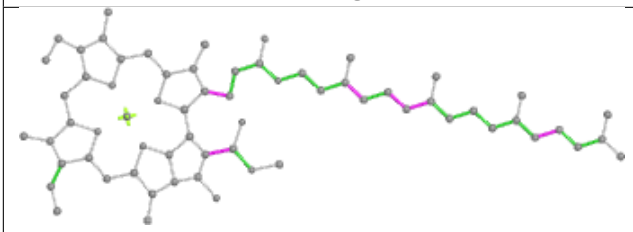


Bond angles



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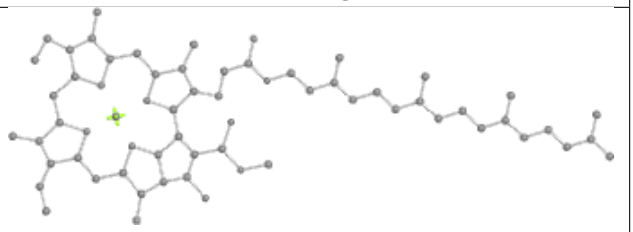
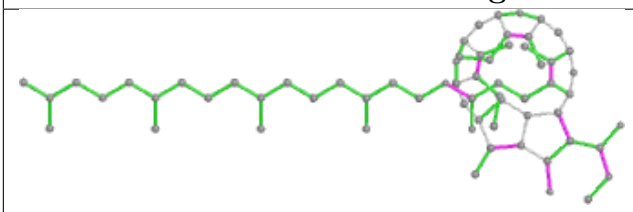


Rings

Ligand PHO A 409 (B)



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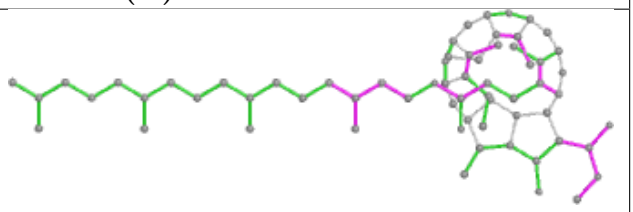
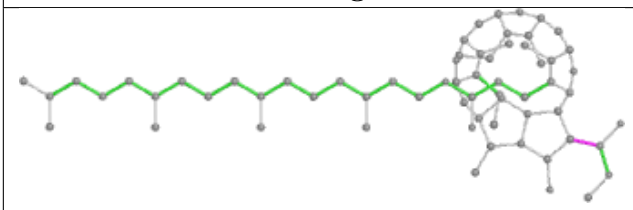
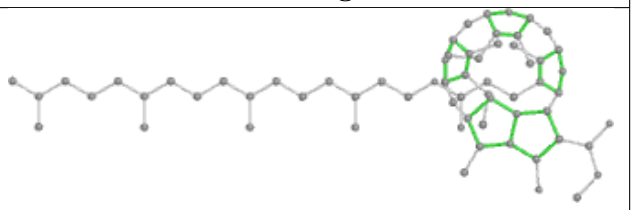


Bond angles

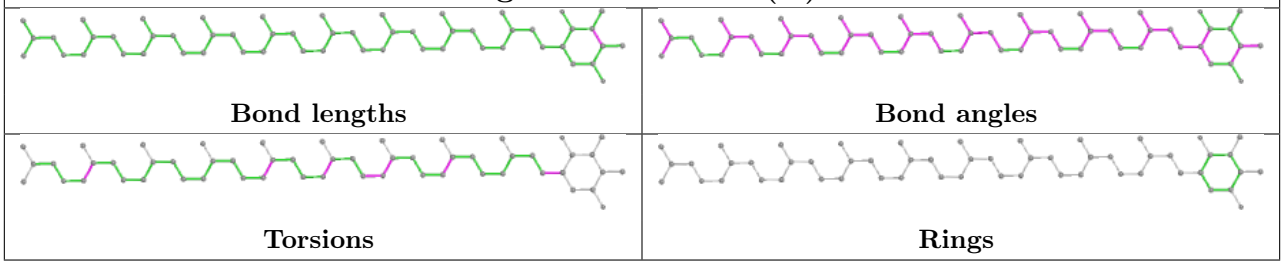


Torsions

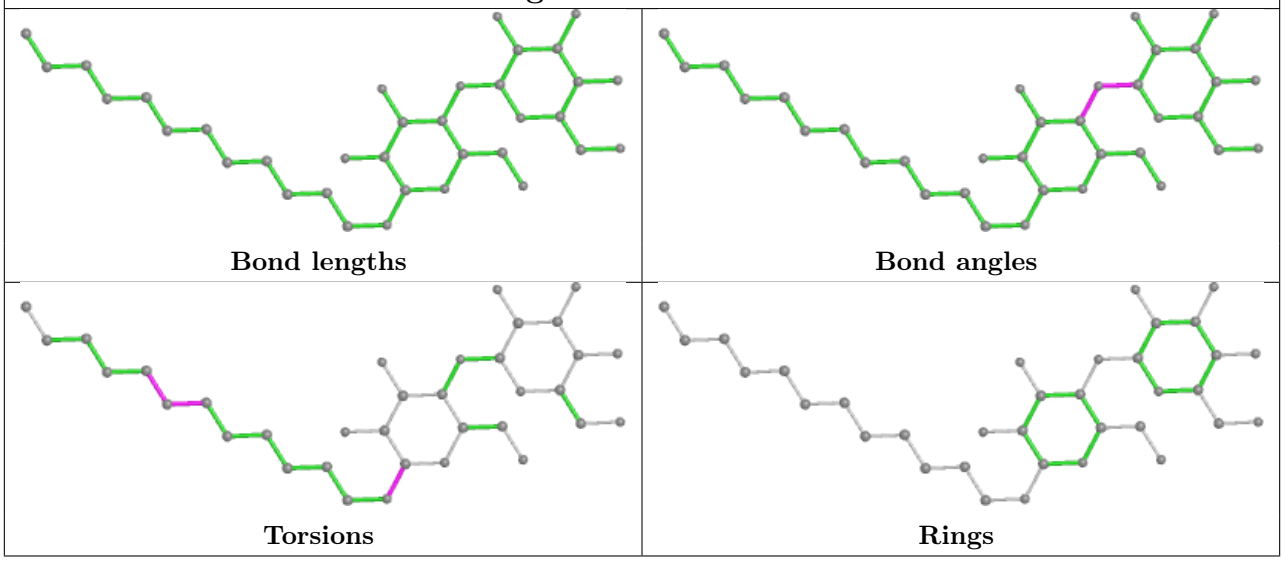


Rings

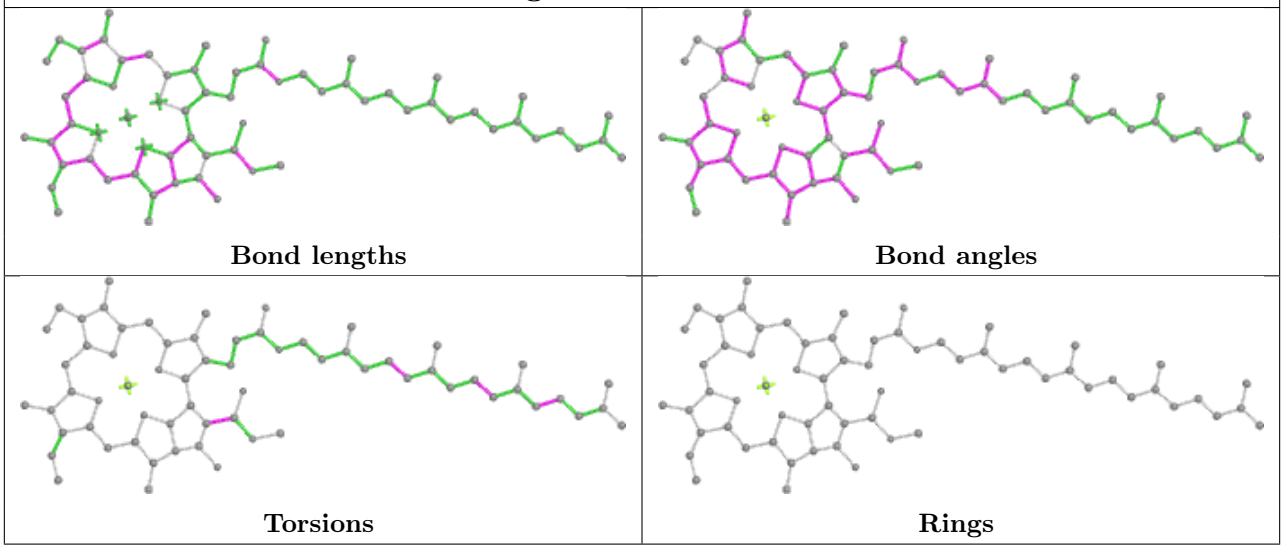
Ligand PL9 A 420 (A)



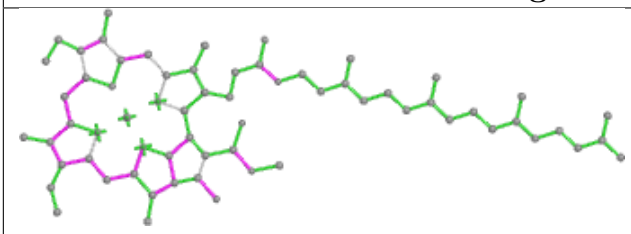
Ligand LMT a 421



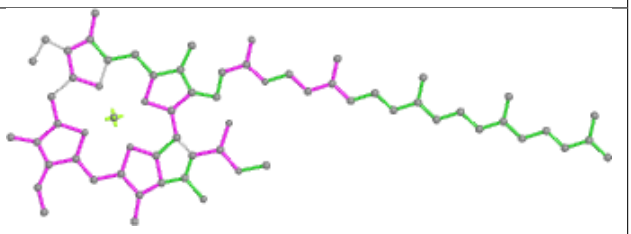
Ligand CLA C 508



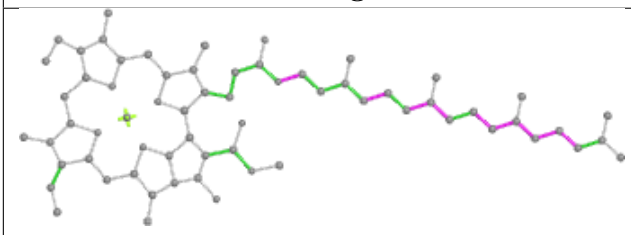
Ligand CLA c 513



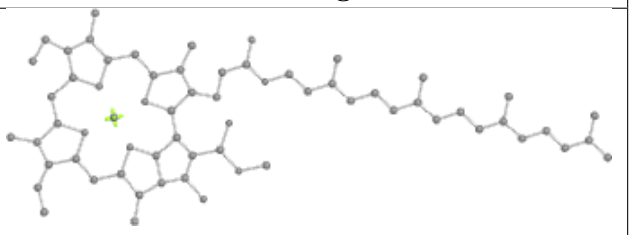
Bond lengths



Bond angles

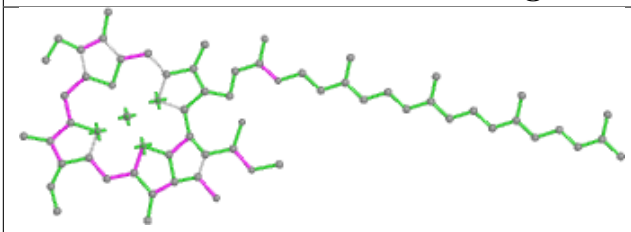


Torsions



Rings

Ligand CLA B 602



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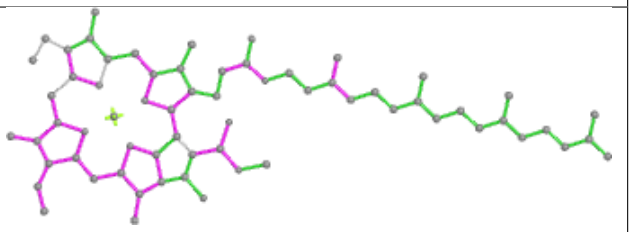
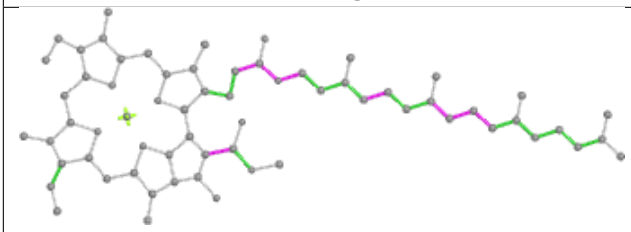


Bond angles



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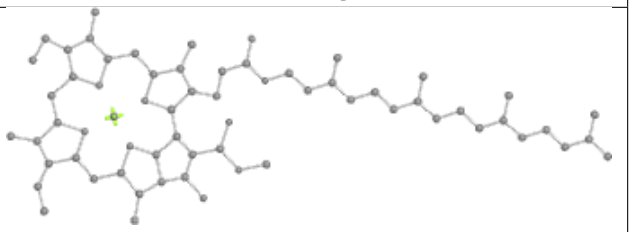
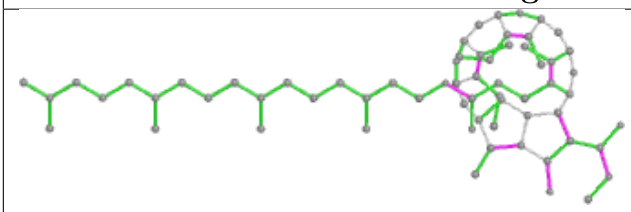


Rings

Ligand PHO A 408



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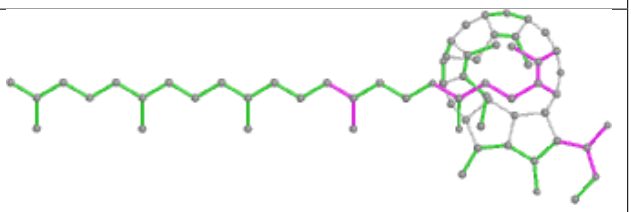
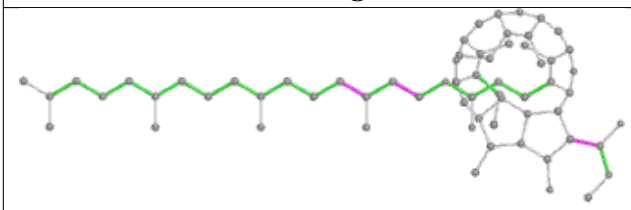


Bond angles



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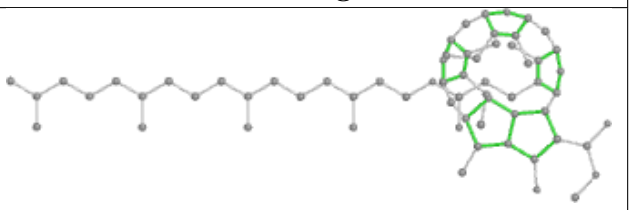
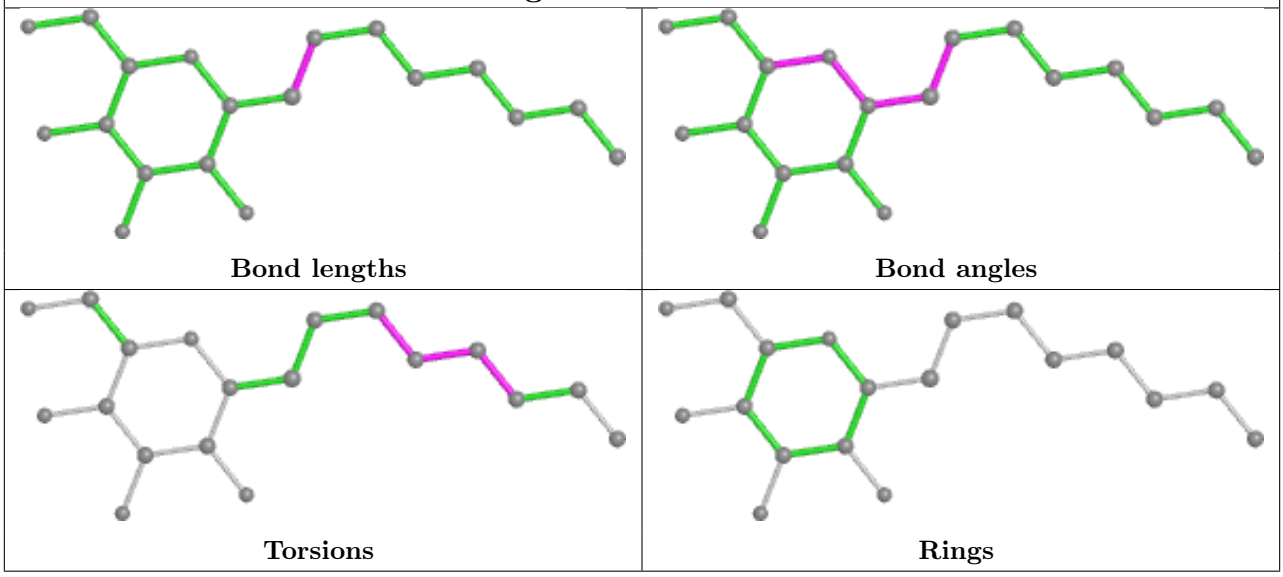
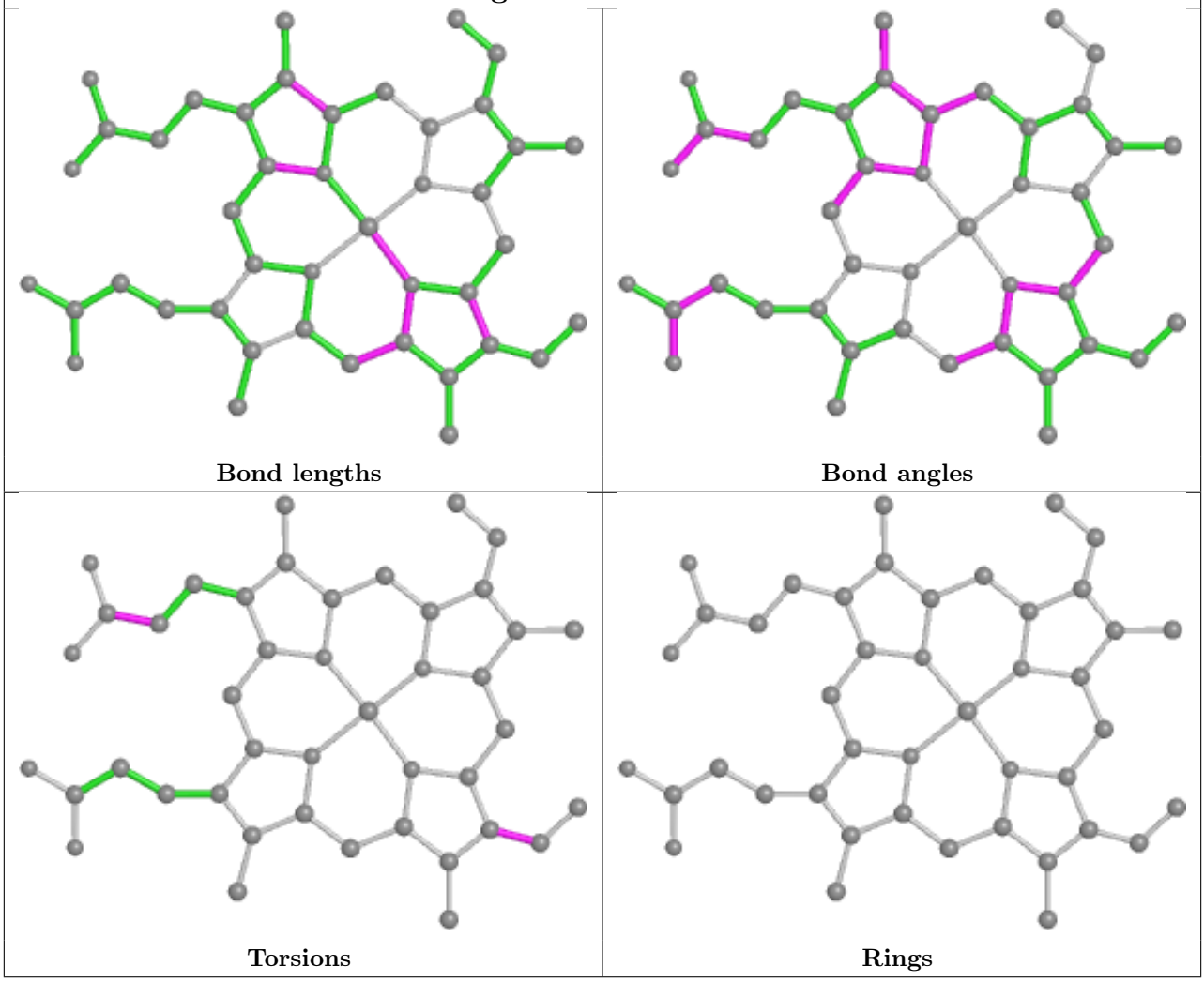


Rings

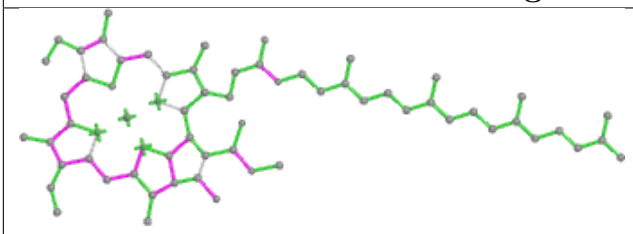
Ligand HTG b 602



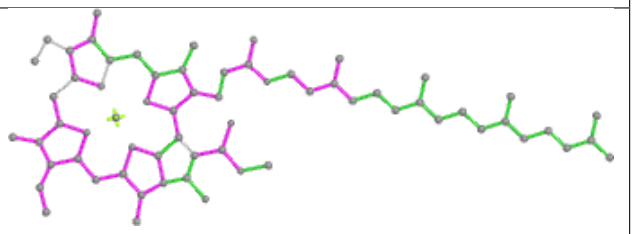
Ligand HEM v 205



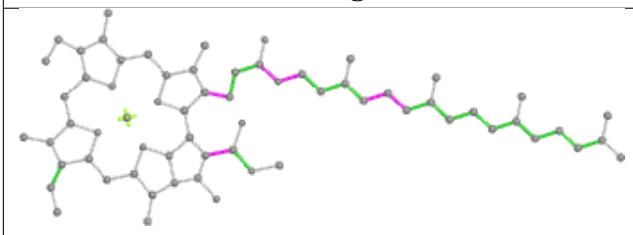
Ligand CLA C 513



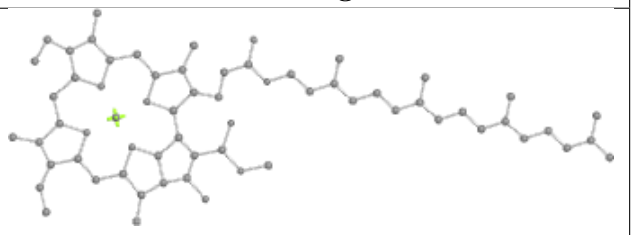
Bond lengths



Bond angles

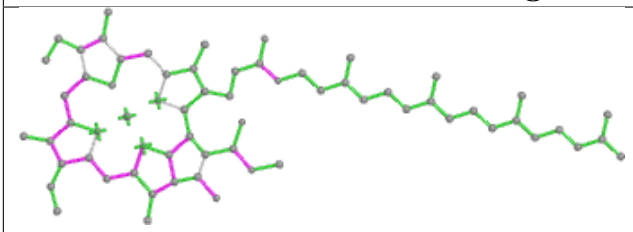


Torsions



Rings

Ligand CLA C 503



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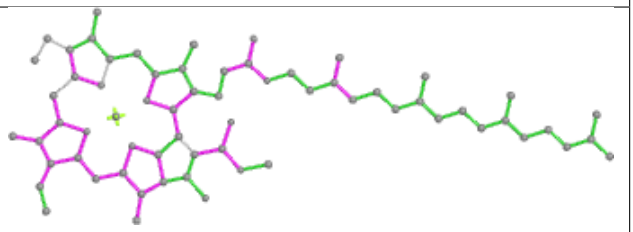
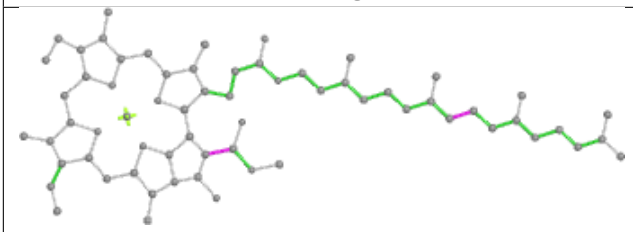


Bond angles



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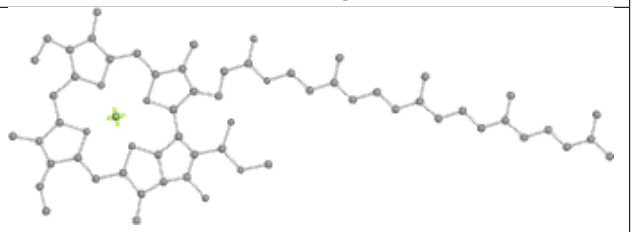
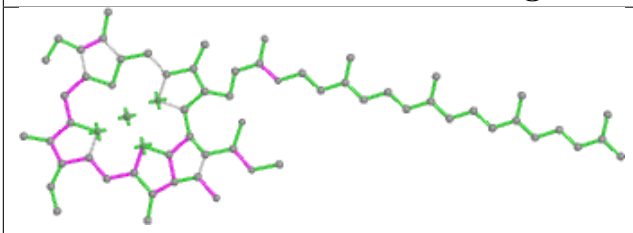


Rings

Ligand CLA A 405



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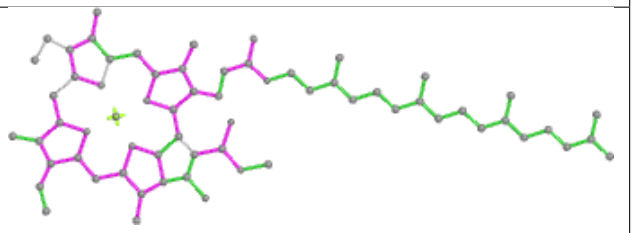
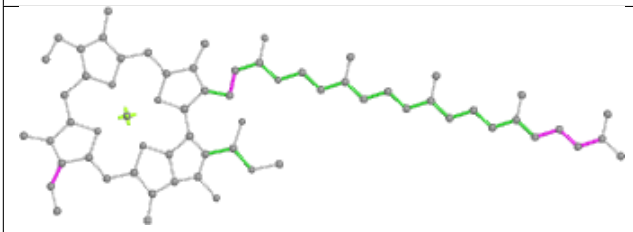


Bond angles



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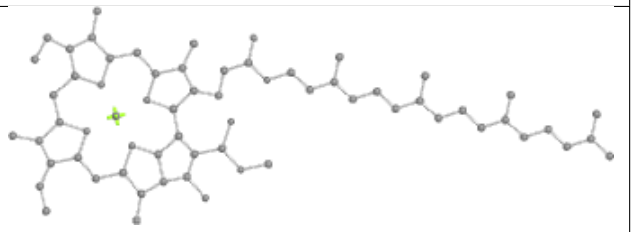
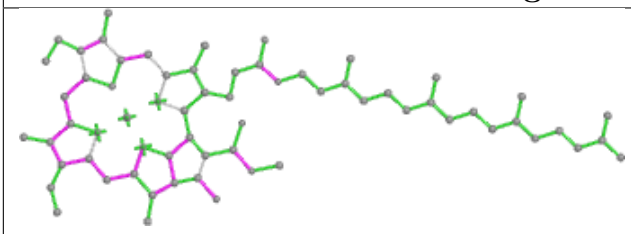


Rings

Ligand CLA A 410



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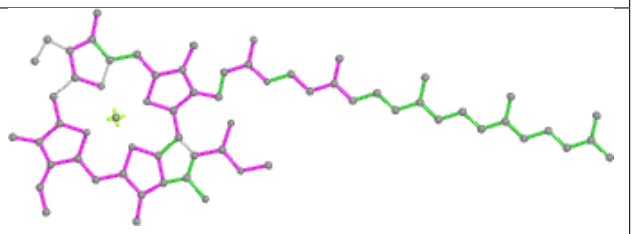
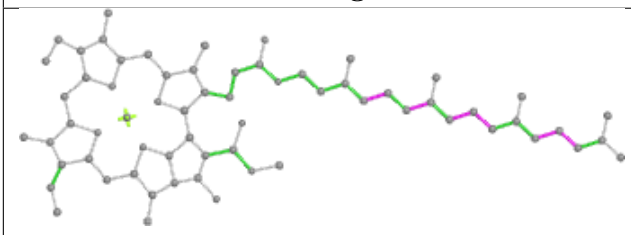


Bond angles



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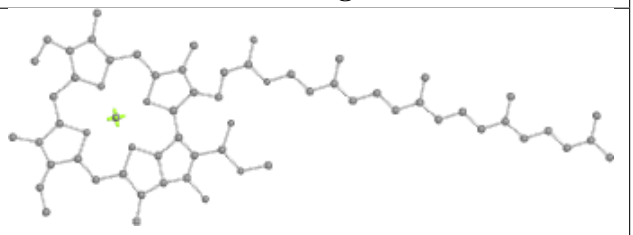
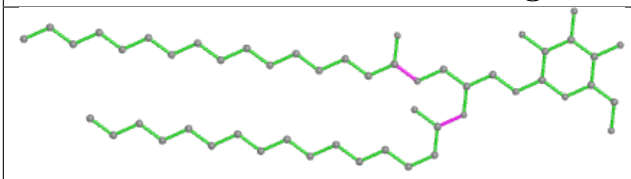


Rings

Ligand LMG a 415



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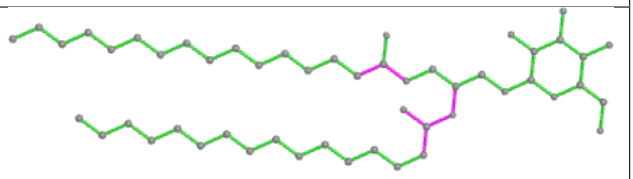
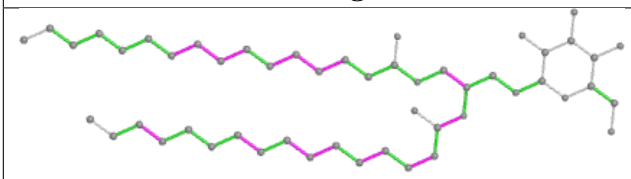


Bond angles



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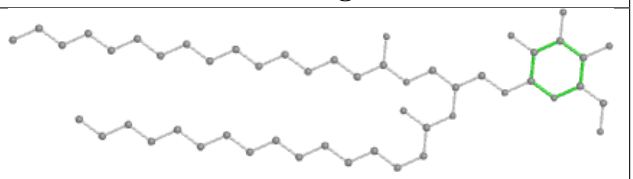
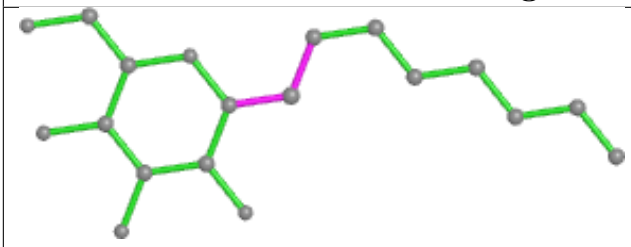


Rings

Ligand HTG V 207



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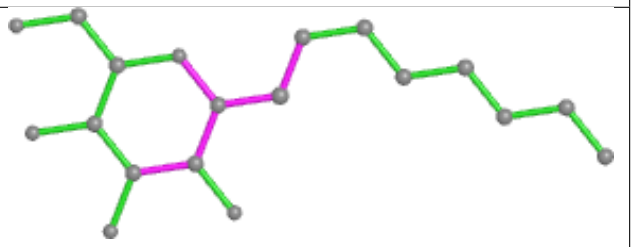
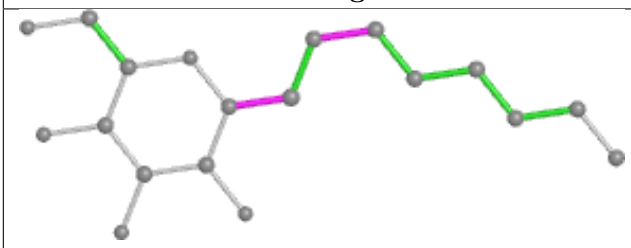


Bond angles



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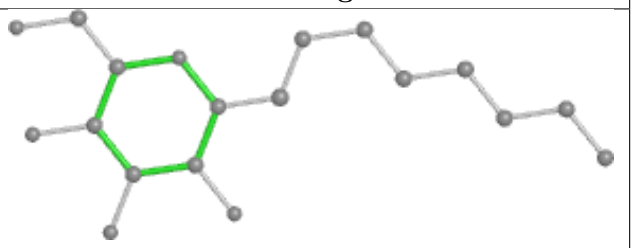
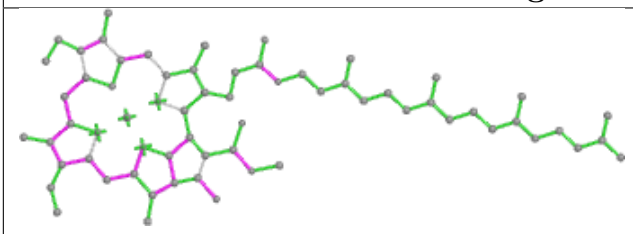


Rings

Ligand CLA b 613



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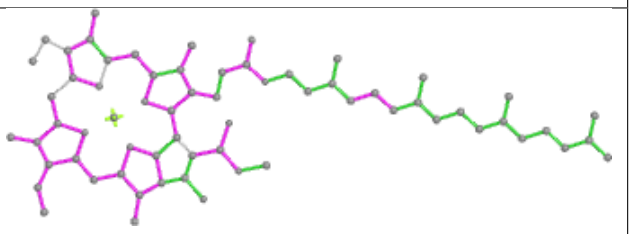
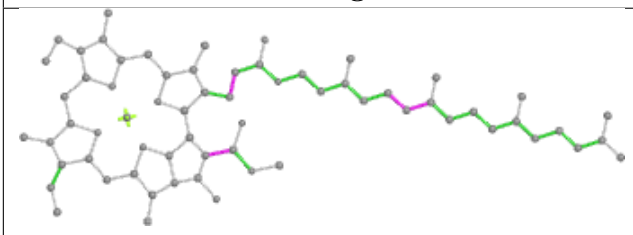
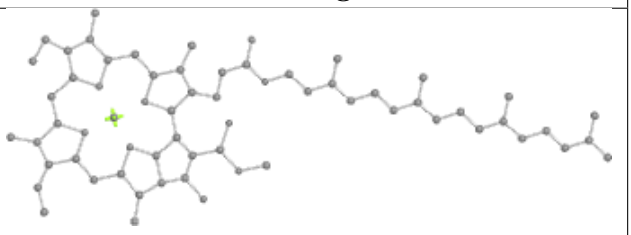


Bond angles

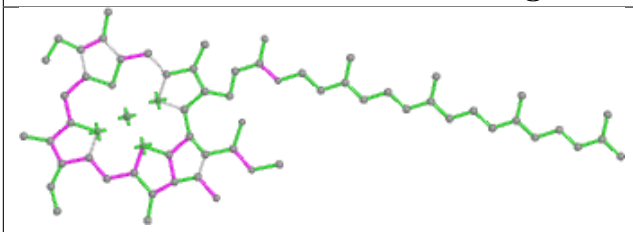


Torsions

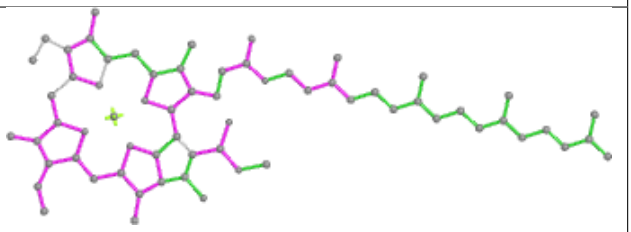


Rings

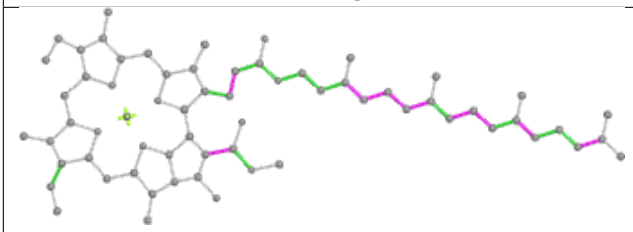
Ligand CLA B 615



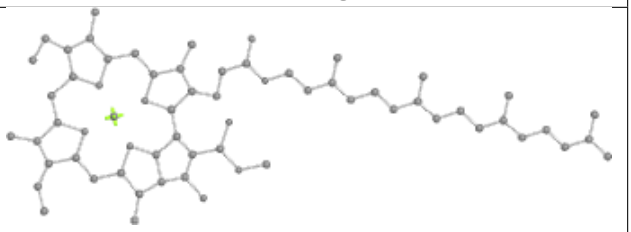
Bond lengths



Bond angles



Torsions



Rings

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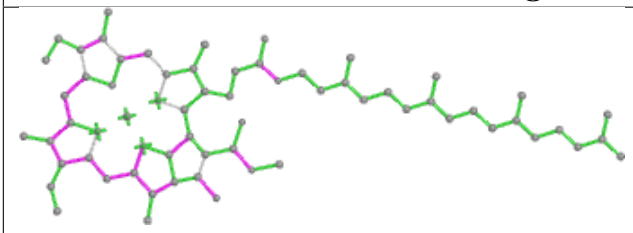
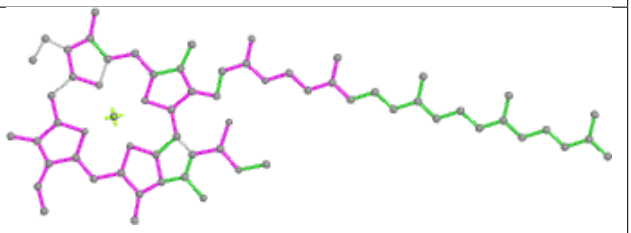
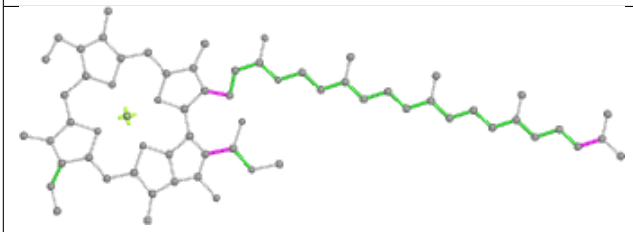


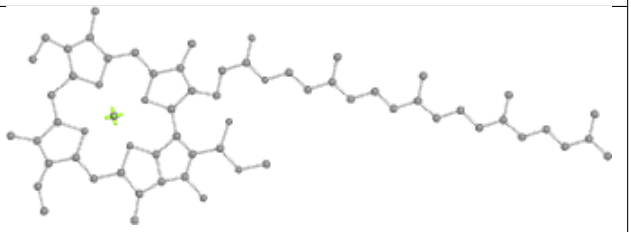
Bond lengths



Bond angles

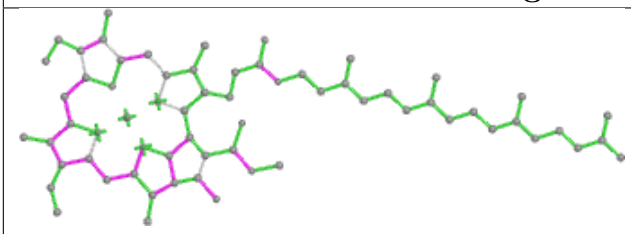


Torsions

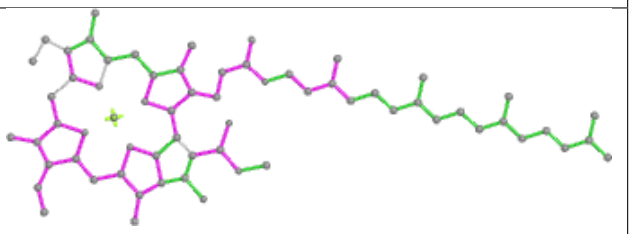


Rings

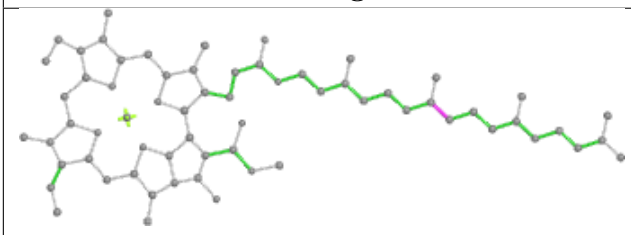
Ligand CLA A 407



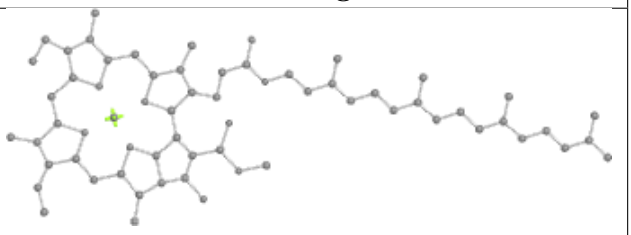
Bond lengths



Bond angles

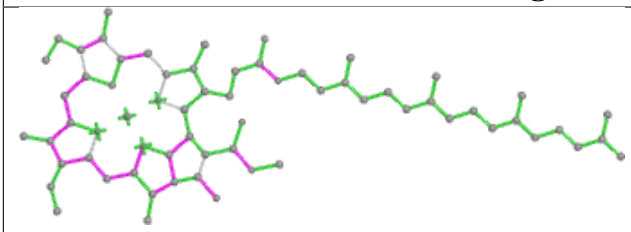


Torsions

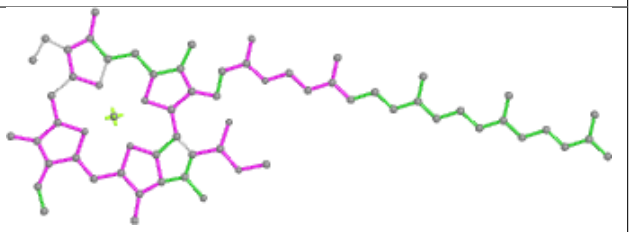


Rings

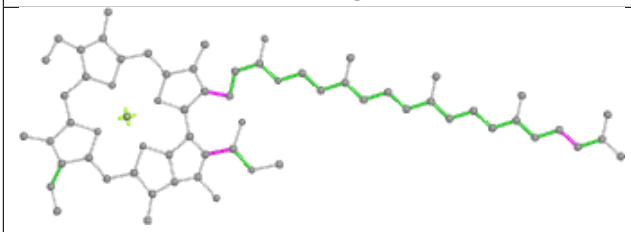
Ligand CLA c 512



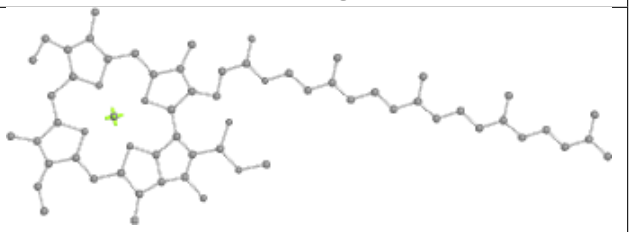
Bond lengths



Bond angles

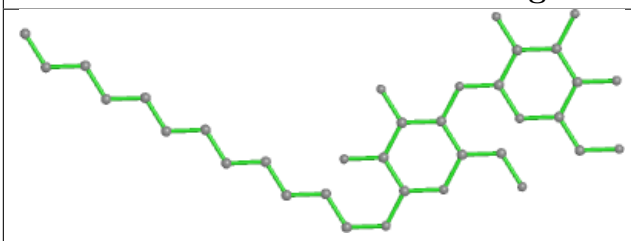


Torsions

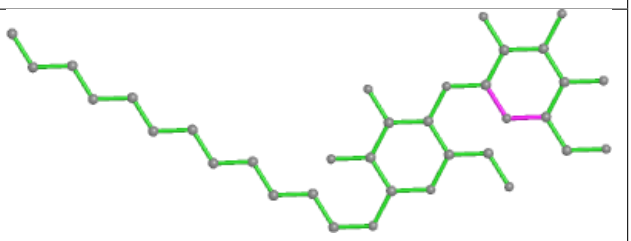


Rings

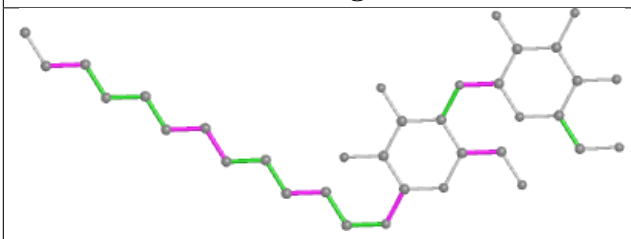
Ligand LMT f 103



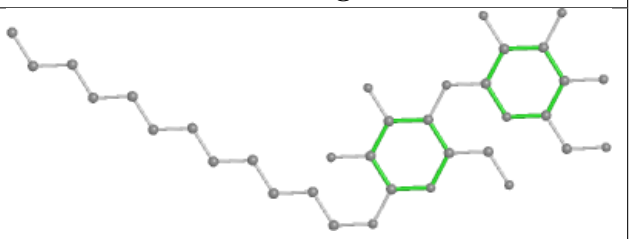
Bond lengths



Bond angles

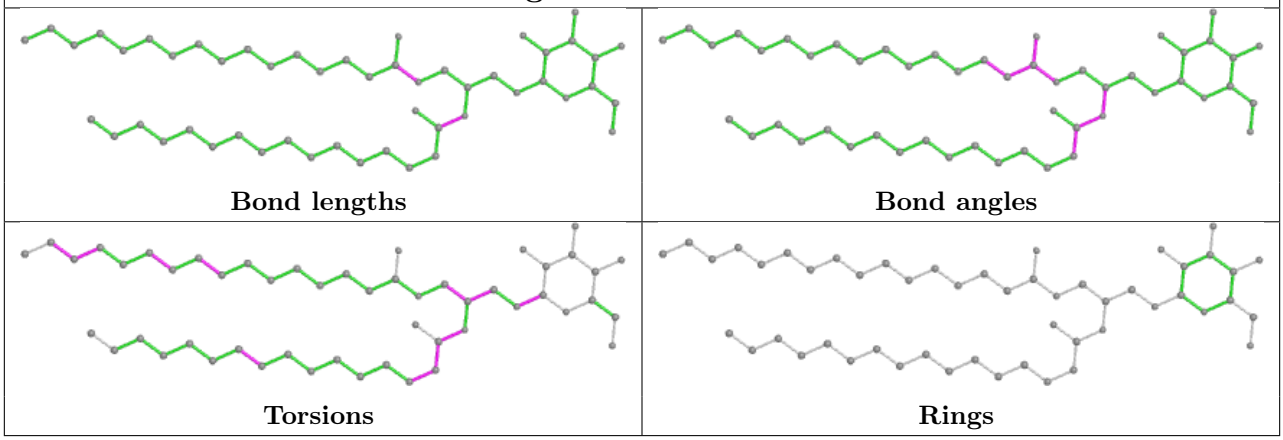


Torsions

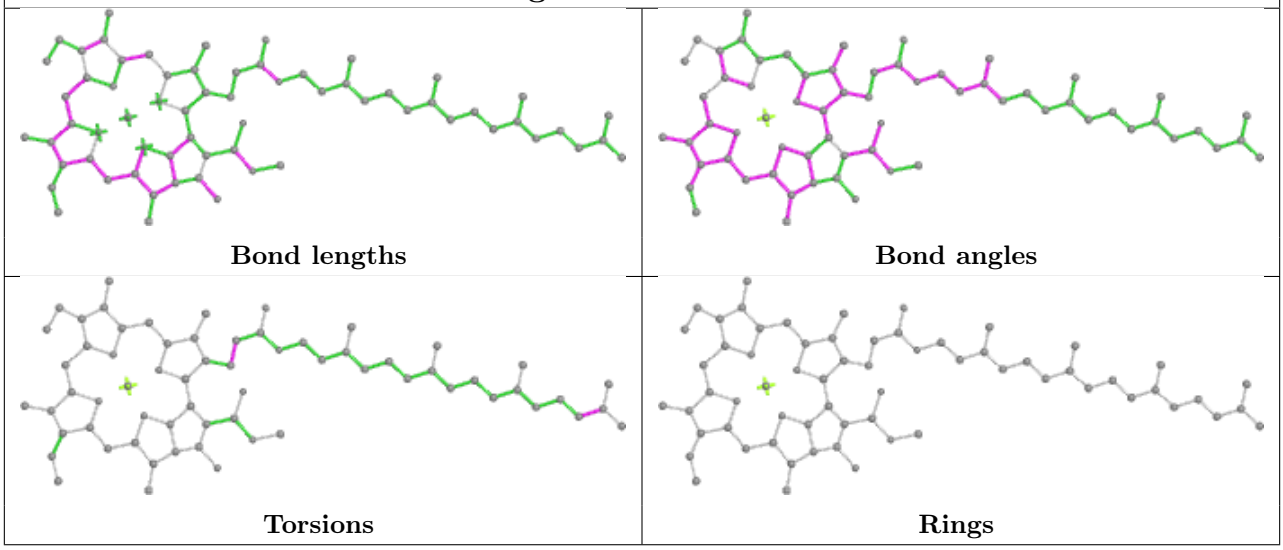


Rings

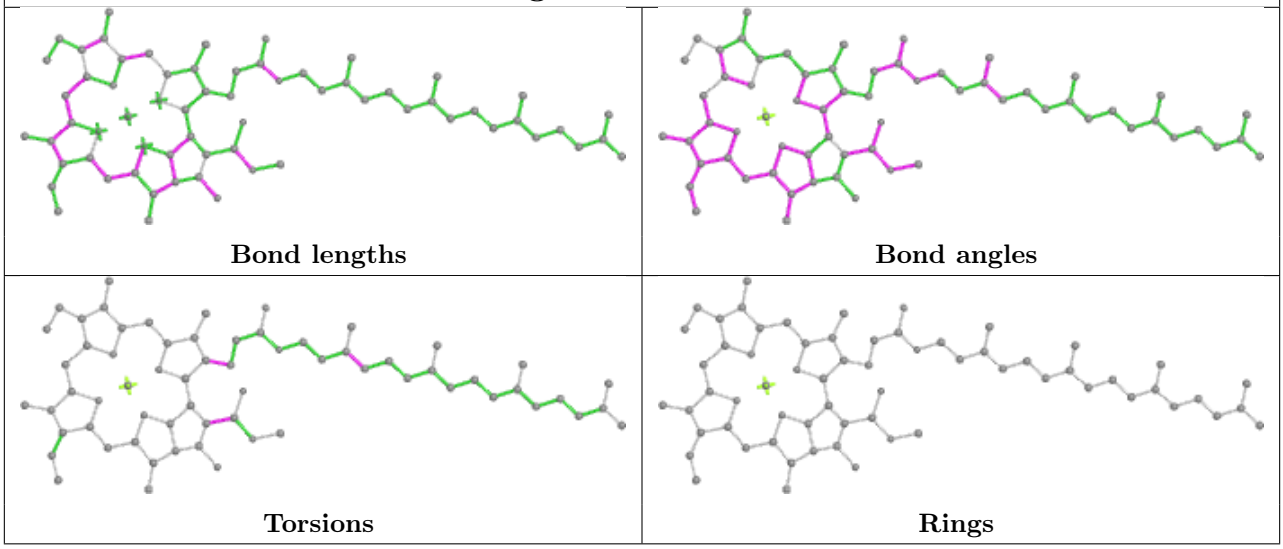
Ligand LMG c 522



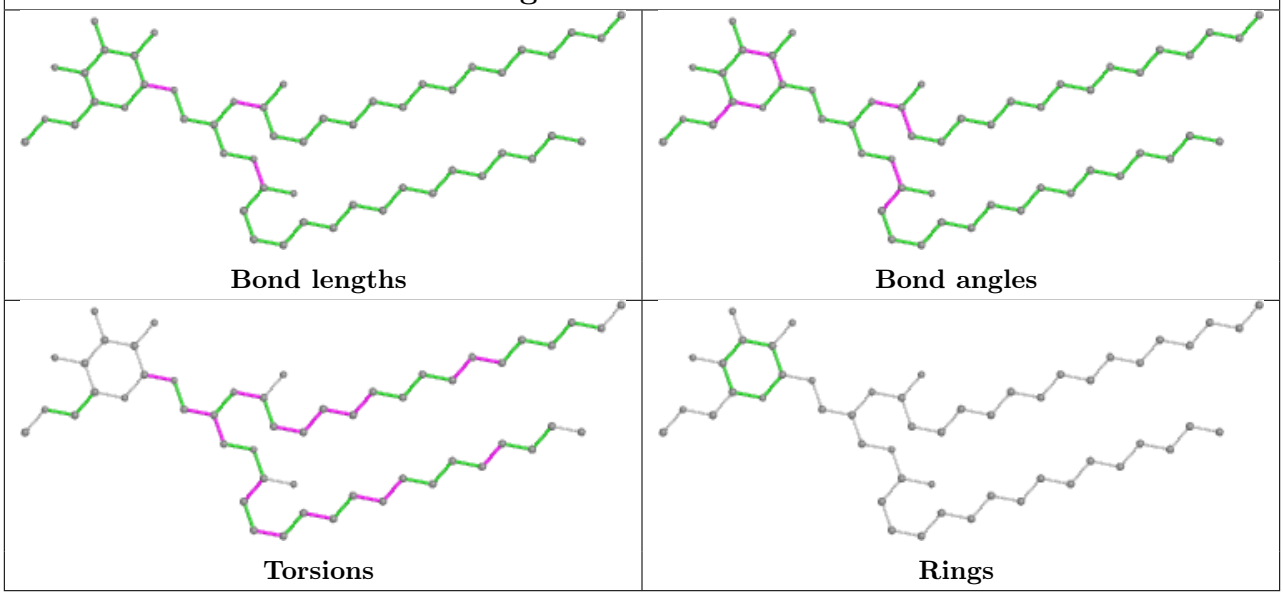
Ligand CLA b 612



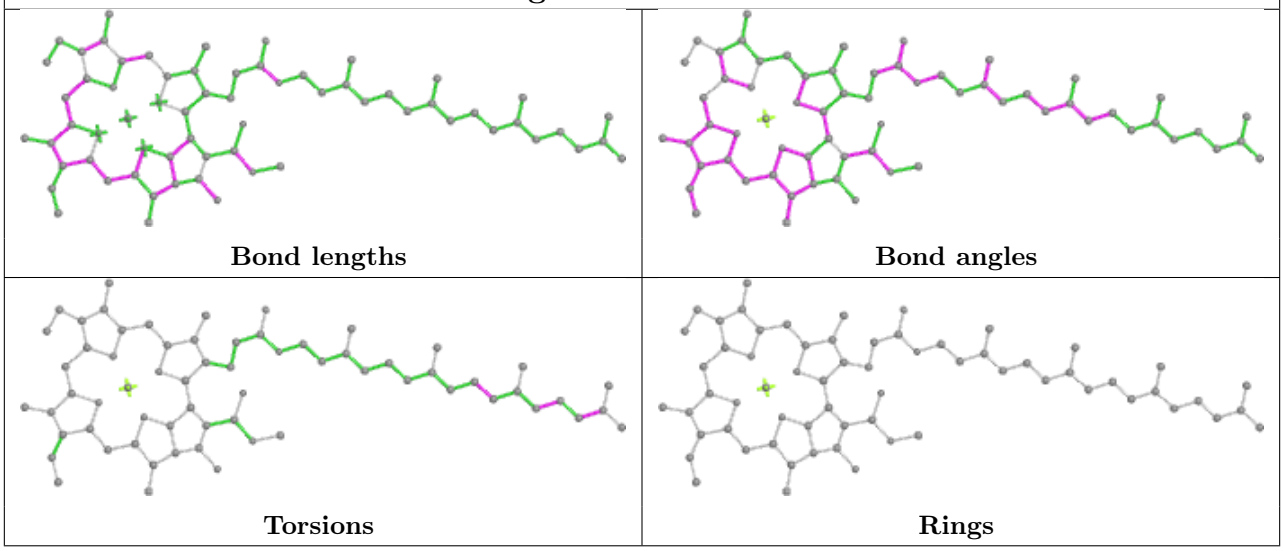
Ligand CLA b 619



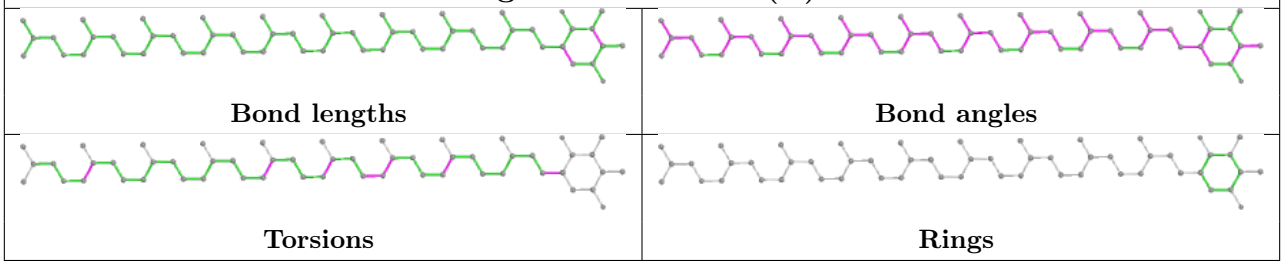
Ligand DGD D 406



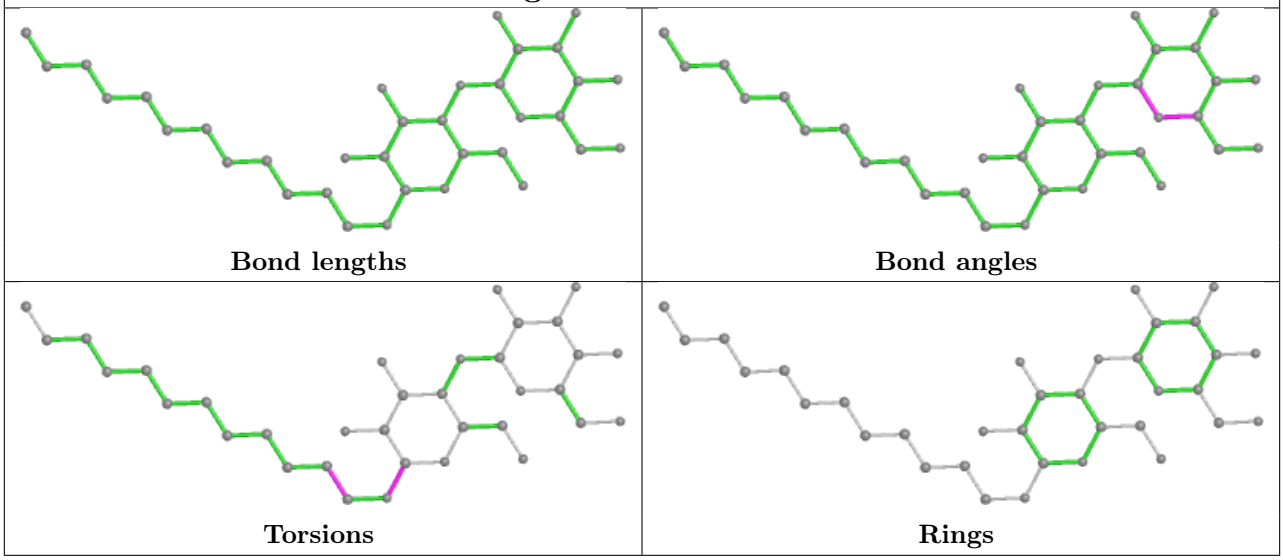
Ligand CLA b 625



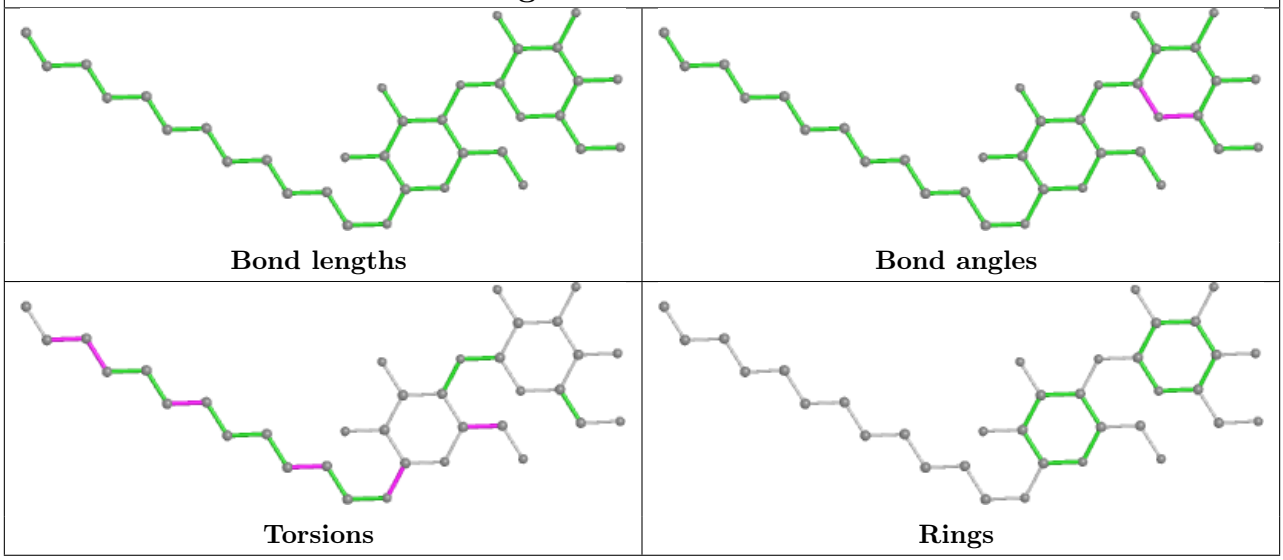
Ligand PL9 A 420 (B)



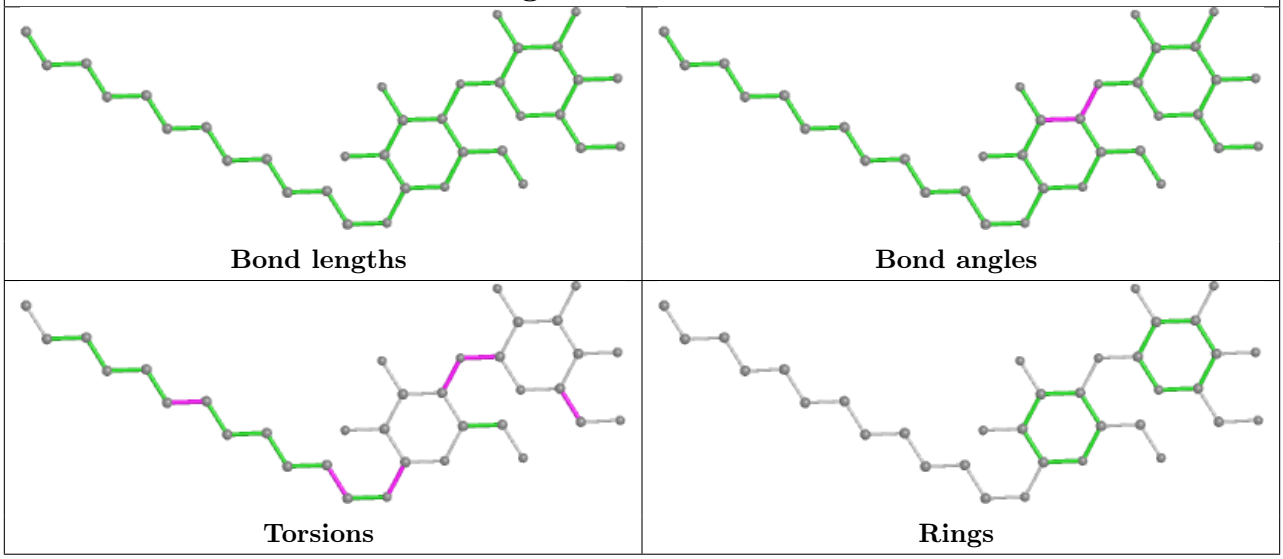
Ligand LMT F 101



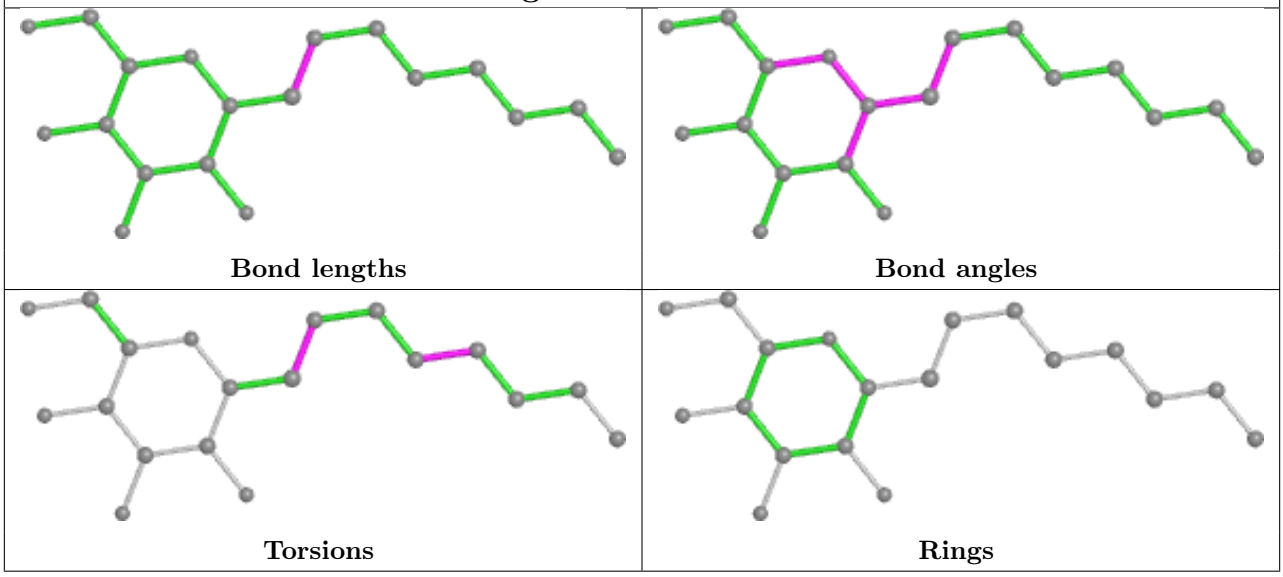
Ligand LMT M 104



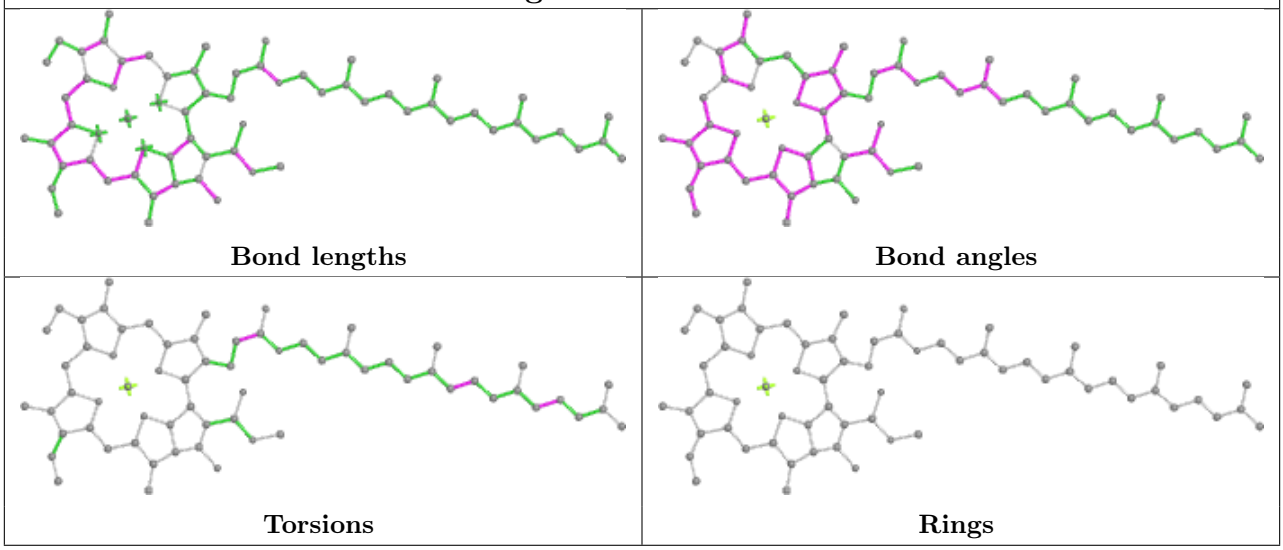
Ligand LMT D 401



Ligand HTG B 624



Ligand CLA B 613



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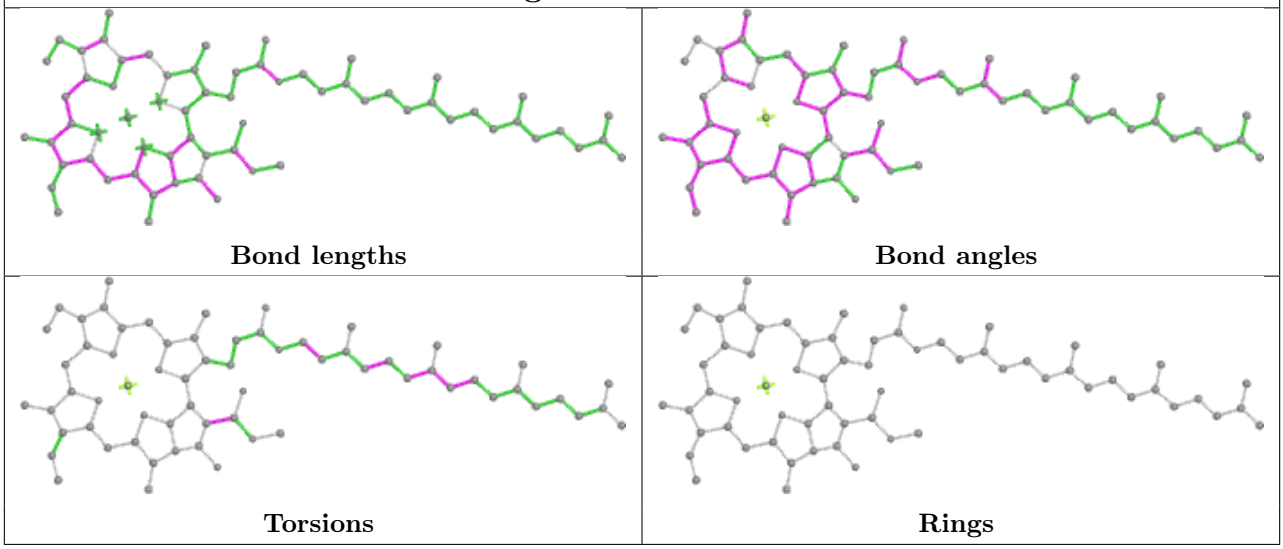

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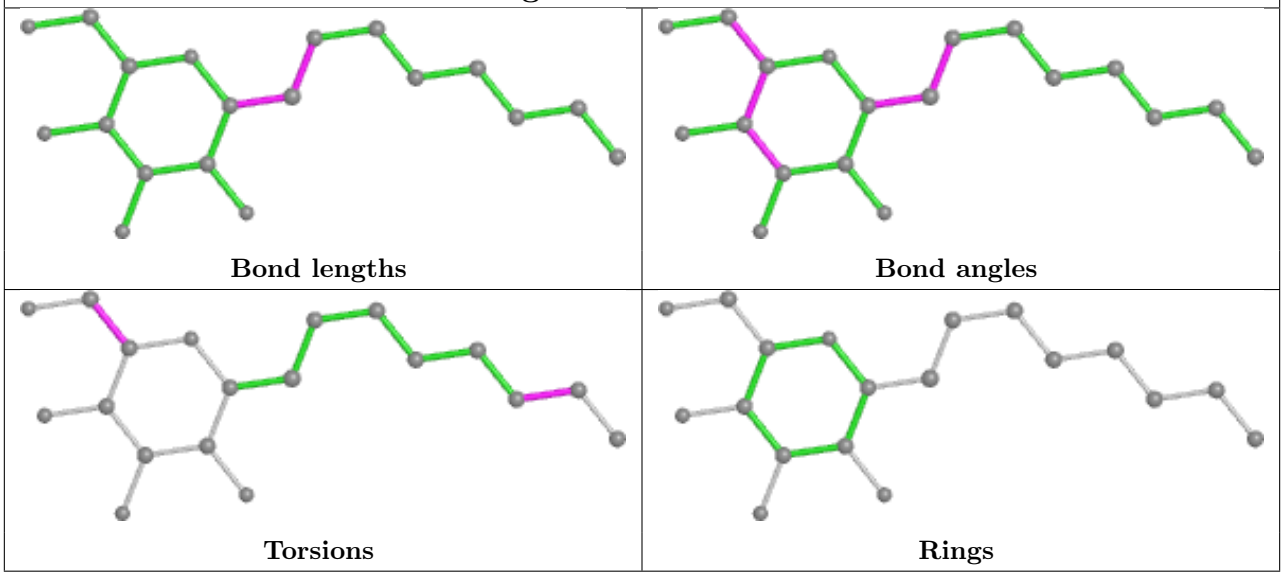
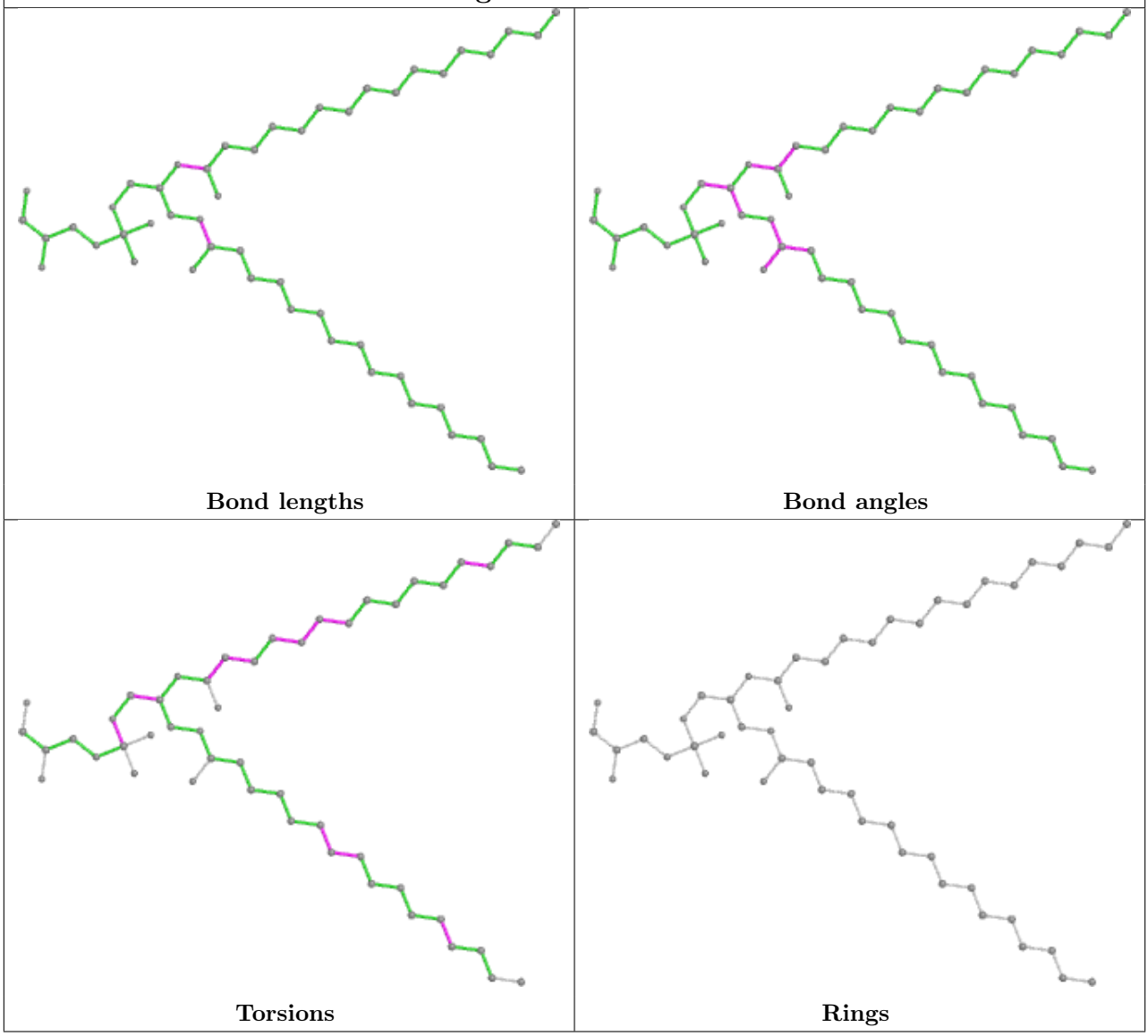
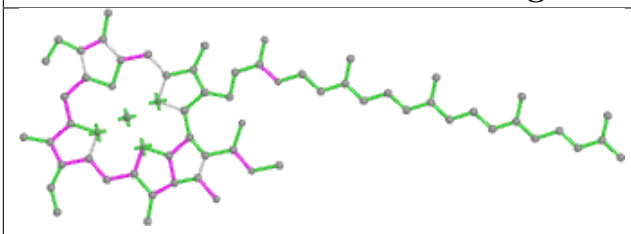


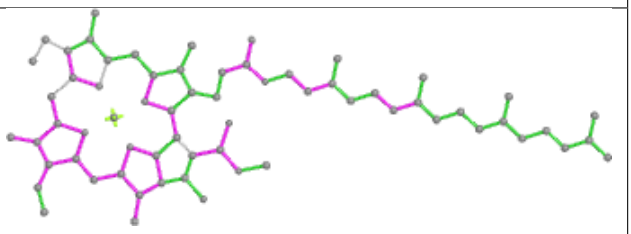
Ligand LHG l 101



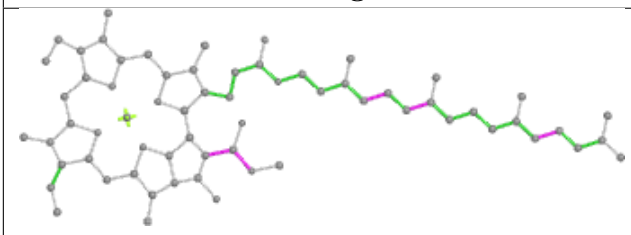
Ligand CLA b 614



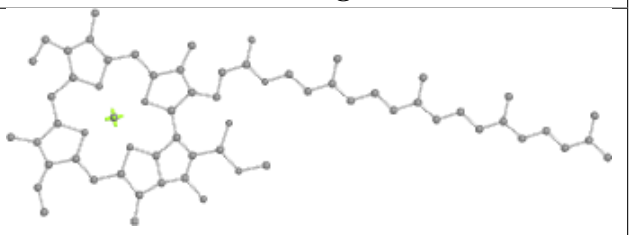
Bond lengths



Bond angles

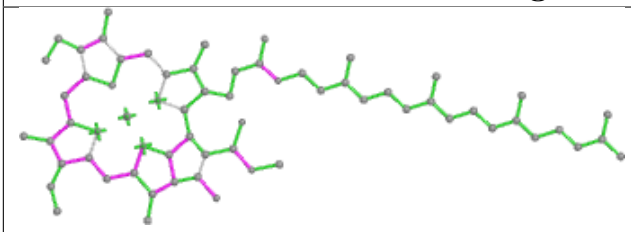


Torsions

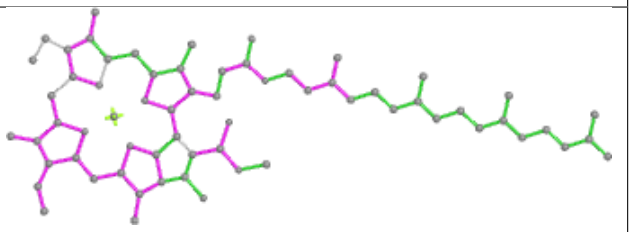


Rings

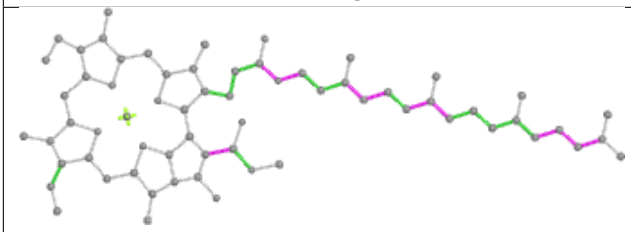
Ligand CLA c 510



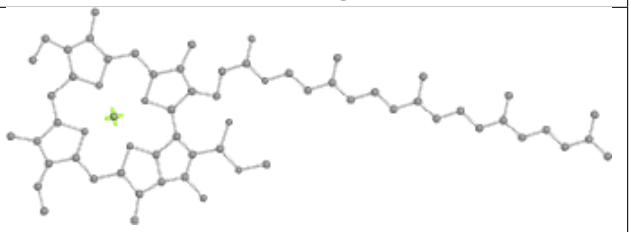
Bond lengths



Bond angles

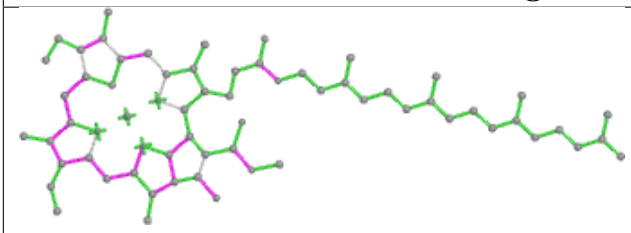


Torsions

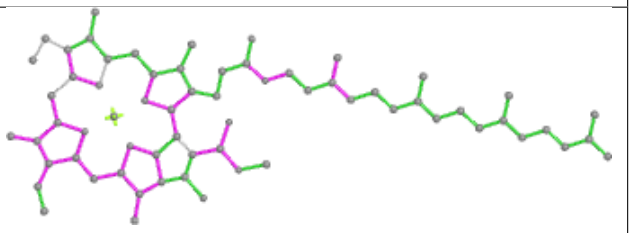


Rings

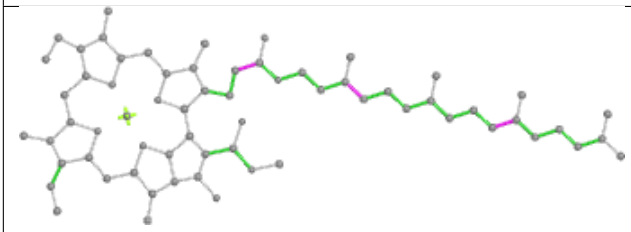
Ligand CLA C 505



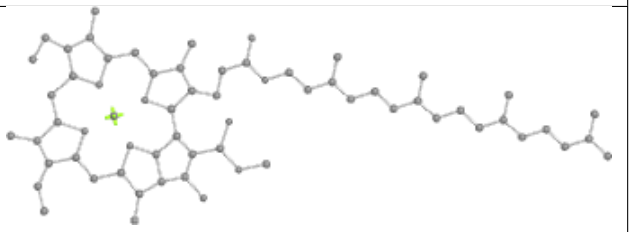
Bond lengths



Bond angles

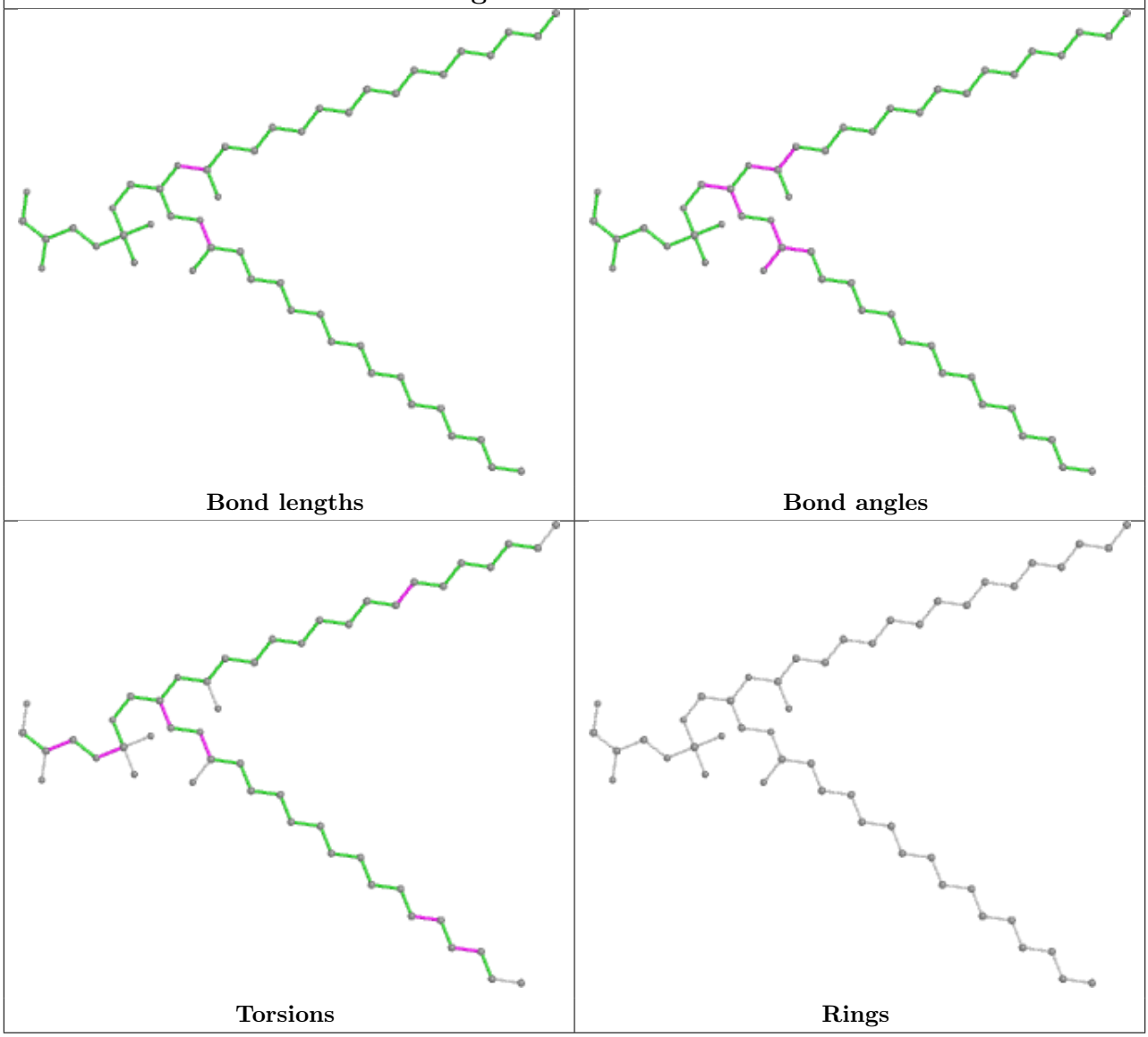


Torsions



Rings

Ligand LHG d 407



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	334/344 (97%)	0.06	2 (0%) 89 91	28, 37, 66, 107	0
1	a	334/344 (97%)	0.17	10 (2%) 50 59	29, 38, 73, 150	0
2	B	504/505 (99%)	0.08	7 (1%) 75 80	29, 42, 76, 120	0
2	b	503/505 (99%)	0.21	24 (4%) 30 39	30, 43, 83, 162	0
3	C	451/455 (99%)	0.02	3 (0%) 87 91	32, 49, 69, 110	0
3	c	455/455 (100%)	0.07	4 (0%) 84 88	36, 53, 70, 121	0
4	D	341/342 (99%)	0.02	1 (0%) 94 95	27, 38, 62, 134	0
4	d	341/342 (99%)	0.02	2 (0%) 89 91	28, 41, 65, 112	0
5	E	81/84 (96%)	0.62	8 (9%) 7 11	44, 62, 92, 139	0
5	e	81/84 (96%)	0.90	10 (12%) 4 5	47, 65, 110, 167	0
6	F	34/44 (77%)	0.31	3 (8%) 10 14	45, 54, 92, 96	0
6	f	32/44 (72%)	0.29	2 (6%) 20 27	45, 54, 112, 130	0
7	H	65/65 (100%)	0.19	3 (4%) 32 42	39, 52, 68, 144	0
7	h	65/65 (100%)	0.09	2 (3%) 49 58	40, 54, 74, 162	0
8	I	37/38 (97%)	0.21	3 (8%) 12 16	44, 52, 104, 148	0
8	i	37/38 (97%)	0.18	2 (5%) 25 34	41, 50, 97, 126	0
9	J	38/39 (97%)	0.48	3 (7%) 12 17	42, 58, 135, 165	0
9	j	39/39 (100%)	0.74	4 (10%) 6 9	46, 59, 130, 162	0
10	K	37/37 (100%)	-0.03	0 100 100	50, 58, 72, 91	0
10	k	37/37 (100%)	0.23	0 100 100	50, 63, 79, 98	0
11	L	37/37 (100%)	0.14	1 (2%) 54 63	28, 34, 94, 106	0
11	l	37/37 (100%)	0.18	1 (2%) 54 63	30, 36, 90, 121	0
12	M	33/36 (91%)	0.27	2 (6%) 21 28	28, 36, 61, 112	0
12	m	33/36 (91%)	0.27	0 100 100	30, 37, 66, 108	0

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.02	3 (1%) 79 83	29, 47, 91, 130	0
13	o	243/244 (99%)	0.10	4 (1%) 72 77	31, 49, 103, 167	0
14	T	29/32 (90%)	0.16	1 (3%) 45 53	30, 36, 62, 135	0
14	t	29/32 (90%)	0.11	0 100 100	31, 37, 64, 128	0
15	U	97/104 (93%)	-0.08	0 100 100	35, 46, 75, 109	0
15	u	97/104 (93%)	-0.03	0 100 100	37, 49, 68, 117	0
16	V	137/137 (100%)	-0.06	0 100 100	31, 45, 65, 84	0
16	v	137/137 (100%)	0.08	1 (0%) 87 91	39, 56, 82, 129	0
17	Y	29/30 (96%)	1.78	7 (24%) 0 0	60, 71, 151, 153	0
17	y	29/30 (96%)	0.80	2 (6%) 16 23	68, 80, 106, 124	0
18	X	39/40 (97%)	0.48	4 (10%) 6 9	47, 60, 112, 132	0
18	x	38/40 (95%)	0.53	4 (10%) 6 9	52, 61, 113, 134	0
19	Z	62/62 (100%)	0.54	7 (11%) 5 7	56, 72, 108, 126	0
19	z	62/62 (100%)	1.11	10 (16%) 1 2	70, 83, 128, 175	0
20	R	18/34 (52%)	7.53	18 (100%) 0 0	111, 142, 168, 174	0
All	All	5275/5384 (97%)	0.17	158 (2%) 50 59	27, 47, 89, 175	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	16.6
20	R	18	TRP	14.5
20	R	15	ALA	13.8
5	e	5	THR	13.8
2	b	496	TYR	10.6

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
14	FME	T	1	10/11	0.94	0.11	37,40,54,78	0
12	FME	M	1	10/11	0.97	0.13	26,45,71,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.97	0.13	39,48,57,57	0
12	FME	m	1	10/11	0.97	0.16	34,45,87,98	0
8	FME	I	1	10/11	0.98	0.11	36,46,51,55	0
14	FME	t	1	10/11	0.98	0.12	28,35,39,84	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	DGD	e	101	62/66	0.44	0.39	66,114,163,166	0
29	LMT	F	101	35/35	0.54	0.33	97,128,145,146	0
29	LMT	C	521	35/35	0.57	0.32	94,119,146,148	0
29	LMT	b	631	25/35	0.58	0.32	72,95,139,144	0
33	UNL	C	527	34/-	0.59	0.22	76,103,111,117	0
38	LHG	a	422	42/49	0.59	0.30	78,125,159,162	0
33	UNL	a	403	30/-	0.62	0.24	77,91,116,118	0
37	DGD	D	406	52/66	0.63	0.28	67,101,132,138	0
29	LMT	a	421	35/35	0.64	0.37	94,110,132,135	0
33	UNL	A	421	28/-	0.66	0.22	68,84,98,99	0
33	UNL	c	526	32/-	0.66	0.23	77,98,122,128	0
33	UNL	j	102	10/-	0.66	0.21	70,80,90,91	0
29	LMT	M	103	35/35	0.67	0.25	45,92,128,137	0
36	HTG	c	525	19/19	0.67	0.34	68,104,113,143	0
36	HTG	d	411	16/19	0.67	0.19	70,111,121,126	0
29	LMT	D	401	35/35	0.68	0.28	75,118,137,137	0
29	LMT	f	103	35/35	0.70	0.29	72,117,137,137	0
36	HTG	H	101	16/19	0.71	0.27	70,131,138,139	0
33	UNL	B	634	33/-	0.72	0.24	54,88,123,126	0
27	SQD	f	102	43/54	0.72	0.27	97,116,146,147	0
33	UNL	J	101	10/-	0.72	0.22	46,70,80,85	0
29	LMT	a	404	35/35	0.73	0.24	47,86,111,123	0
34	LMG	Z	101	37/55	0.73	0.27	57,108,124,127	0
35	CA	b	610	1/1	0.73	0.17	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	HTG	b	609	19/19	0.74	0.21	62,113,140,141	0
33	UNL	m	101	10/-	0.74	0.22	50,57,79,81	0
29	LMT	m	102	35/35	0.75	0.23	47,95,121,125	0
36	HTG	B	633	19/19	0.76	0.21	53,110,132,175	0
32	PL9	a	416[A]	55/55	0.76	0.25	83,102,111,114	55
32	PL9	a	416[B]	55/55	0.76	0.25	84,102,111,114	55
36	HTG	B	625	19/19	0.76	0.26	64,120,133,158	0
29	LMT	A	417	35/35	0.77	0.21	41,79,99,112	0
38	LHG	E	101	42/49	0.77	0.22	69,98,119,122	0
29	LMT	M	104	35/35	0.77	0.22	46,79,89,95	0
33	UNL	b	634	33/-	0.78	0.25	48,98,141,142	0
27	SQD	b	601	54/54	0.78	0.18	52,72,120,129	0
28	GOL	V	202	6/6	0.79	0.38	62,77,81,82	0
33	UNL	d	410	36/-	0.80	0.20	53,77,122,126	0
27	SQD	A	416	54/54	0.80	0.19	47,73,104,112	0
33	UNL	I	101	40/-	0.80	0.25	43,83,129,135	0
32	PL9	A	420[A]	55/55	0.81	0.23	70,87,101,101	55
33	UNL	i	101	40/-	0.81	0.23	50,74,125,128	0
32	PL9	A	420[B]	55/55	0.81	0.23	71,87,101,101	55
29	LMT	T	104	25/35	0.81	0.23	38,71,116,121	0
28	GOL	v	201	6/6	0.81	0.34	78,85,89,90	0
36	HTG	b	633	19/19	0.81	0.22	70,120,135,135	0
27	SQD	B	621	54/54	0.82	0.19	48,81,143,146	0
34	LMG	C	519	51/55	0.82	0.19	50,78,102,103	0
29	LMT	B	635	25/35	0.82	0.24	38,73,124,127	0
34	LMG	z	101	39/55	0.83	0.24	69,112,127,136	0
29	LMT	M	101	35/35	0.83	0.20	39,82,98,103	0
28	GOL	T	102	6/6	0.83	0.28	103,114,116,120	0
34	LMG	C	520	51/55	0.83	0.20	53,105,116,119	0
36	HTG	C	523	19/19	0.83	0.22	75,95,121,124	0
27	SQD	a	405	54/54	0.83	0.16	45,76,111,114	0
34	LMG	c	523	51/55	0.83	0.23	49,106,118,120	0
33	UNL	M	102	10/-	0.84	0.19	50,64,69,73	0
34	LMG	a	415	51/55	0.85	0.18	58,75,96,97	0
33	UNL	D	411	40/-	0.85	0.18	57,79,113,123	0
34	LMG	A	422	51/55	0.86	0.17	56,79,99,104	0
37	DGD	C	517	62/66	0.86	0.15	37,52,86,94	0
34	LMG	b	630	51/55	0.86	0.17	39,48,68,82	0
27	SQD	F	103	43/54	0.87	0.21	74,97,116,118	0
34	LMG	c	522	51/55	0.87	0.18	52,86,107,110	0
28	GOL	b	607	6/6	0.87	0.16	64,77,80,80	0
33	UNL	X	101	18/-	0.87	0.16	58,70,93,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	c	502	6/6	0.87	0.43	70,79,91,98	0
28	GOL	t	102	6/6	0.87	0.42	49,76,86,89	0
36	HTG	B	624	19/19	0.88	0.17	54,64,74,81	0
33	UNL	d	412	18/-	0.88	0.20	61,68,102,107	0
37	DGD	h	102	62/66	0.88	0.15	35,48,63,73	0
28	GOL	A	415	6/6	0.88	0.17	54,73,76,79	0
36	HTG	b	632	19/19	0.88	0.24	51,67,77,78	0
28	GOL	a	402	6/6	0.89	0.22	76,90,92,92	0
37	DGD	c	520	62/66	0.89	0.16	38,51,100,112	0
28	GOL	O	301	6/6	0.89	0.10	68,76,77,77	0
24	CLA	C	513	65/65	0.89	0.17	50,64,93,98	0
28	GOL	C	524	6/6	0.89	0.28	63,65,79,82	0
34	LMG	B	622	51/55	0.89	0.16	32,49,69,85	0
28	GOL	A	413	6/6	0.90	0.12	43,44,56,59	0
37	DGD	H	103	62/66	0.90	0.16	32,47,70,74	0
28	GOL	A	414	6/6	0.90	0.25	52,54,57,60	0
36	HTG	c	524	19/19	0.90	0.14	81,89,96,118	0
27	SQD	A	412	54/54	0.90	0.17	43,76,91,94	0
36	HTG	b	608	19/19	0.90	0.13	48,68,78,79	0
28	GOL	B	636	6/6	0.90	0.12	48,51,55,55	0
24	CLA	c	517	65/65	0.91	0.15	61,77,92,94	0
24	CLA	c	511	65/65	0.91	0.14	43,54,62,67	0
36	HTG	V	207	19/19	0.91	0.24	63,87,104,205	0
28	GOL	T	101	6/6	0.91	0.34	55,69,88,96	0
28	GOL	B	630	6/6	0.91	0.24	50,66,68,71	0
37	DGD	c	521	62/66	0.91	0.15	39,51,82,89	0
27	SQD	a	414	54/54	0.91	0.15	54,77,98,101	0
36	HTG	B	632	19/19	0.91	0.13	41,75,91,92	0
38	LHG	D	407	49/49	0.91	0.17	35,47,59,64	0
28	GOL	v	202	6/6	0.91	0.19	72,79,89,99	0
36	HTG	C	522	19/19	0.91	0.15	72,80,91,95	0
34	LMG	j	101	51/55	0.92	0.15	46,56,92,106	0
28	GOL	b	606	6/6	0.92	0.19	75,79,94,95	0
24	CLA	c	515	65/65	0.92	0.15	43,55,73,80	0
35	CA	f	104	1/1	0.92	0.09	97,97,97,97	0
24	CLA	b	619	65/65	0.92	0.15	35,49,56,65	0
28	GOL	f	101	6/6	0.92	0.20	74,84,86,89	0
38	LHG	D	409	49/49	0.92	0.19	37,54,105,113	0
37	DGD	C	518	62/66	0.92	0.14	37,47,75,87	0
24	CLA	C	506	65/65	0.92	0.14	44,60,101,105	0
24	CLA	C	511	65/65	0.93	0.12	42,56,67,78	0
36	HTG	b	602	19/19	0.93	0.12	35,49,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	602	65/65	0.93	0.16	44,61,94,111	0
34	LMG	D	412	51/55	0.93	0.16	35,55,100,106	0
24	CLA	b	611	65/65	0.93	0.15	46,69,101,116	0
24	CLA	b	612	65/65	0.93	0.15	33,44,51,57	0
28	GOL	V	203	6/6	0.93	0.15	39,50,64,67	0
28	GOL	a	401	6/6	0.93	0.27	50,61,66,76	0
24	CLA	b	616	65/65	0.93	0.14	30,43,84,96	0
24	CLA	b	617	65/65	0.93	0.14	26,34,42,50	0
24	CLA	B	614	65/65	0.93	0.14	25,35,63,75	0
24	CLA	b	626	65/65	0.93	0.13	35,50,97,100	0
33	UNL	d	409	17/-	0.93	0.18	46,63,91,92	0
36	HTG	B	623	19/19	0.93	0.14	37,51,65,70	0
24	CLA	c	507	65/65	0.93	0.13	41,51,60,77	0
24	CLA	C	501	65/65	0.93	0.14	38,47,69,78	0
28	GOL	B	628	6/6	0.93	0.16	52,70,78,85	0
24	CLA	C	504	65/65	0.93	0.15	35,46,77,83	0
28	GOL	v	203	6/6	0.93	0.17	46,50,57,61	0
22	CL	v	204	1/1	0.93	0.11	88,88,88,88	0
24	CLA	C	507	65/65	0.93	0.14	40,52,67,72	0
24	CLA	b	621	65/65	0.94	0.13	26,38,48,55	0
24	CLA	C	508	65/65	0.94	0.13	35,48,107,117	0
28	GOL	V	205	6/6	0.94	0.20	71,75,81,91	0
24	CLA	c	505	65/65	0.94	0.13	40,54,62,66	0
24	CLA	C	509	65/65	0.94	0.14	41,52,73,76	0
24	CLA	c	508	65/65	0.94	0.12	38,50,71,75	0
24	CLA	c	509	65/65	0.94	0.12	34,45,64,72	0
24	CLA	c	510	65/65	0.94	0.12	44,62,87,95	0
24	CLA	B	607	65/65	0.94	0.14	31,43,85,91	0
28	GOL	o	301	6/6	0.94	0.17	64,70,80,88	0
24	CLA	c	512	65/65	0.94	0.13	36,46,109,121	0
24	CLA	c	514	65/65	0.94	0.12	38,50,60,68	0
24	CLA	C	512	65/65	0.94	0.12	46,64,76,80	0
33	UNL	D	410	17/-	0.94	0.16	39,67,83,87	0
28	GOL	B	626	6/6	0.94	0.14	39,52,57,71	0
24	CLA	c	516	65/65	0.94	0.13	51,62,77,83	0
24	CLA	B	603	65/65	0.94	0.13	33,42,47,53	0
37	DGD	c	519	62/66	0.94	0.13	37,46,91,95	0
35	CA	B	601	1/1	0.94	0.07	118,118,118,118	0
35	CA	F	104	1/1	0.94	0.07	82,82,82,82	0
26	BCR	b	628	40/40	0.94	0.14	31,43,54,61	0
26	BCR	c	527	40/40	0.94	0.12	56,72,78,81	0
26	BCR	h	101	40/40	0.94	0.12	39,54,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	k	101	40/40	0.94	0.14	44,60,70,74	0
26	BCR	y	101	40/40	0.94	0.14	43,60,68,76	0
28	GOL	V	201	6/6	0.94	0.21	68,75,76,79	0
38	LHG	d	406	49/49	0.94	0.16	41,49,58,63	0
38	LHG	d	407	49/49	0.94	0.16	30,39,57,75	0
38	LHG	l	101	49/49	0.94	0.16	33,44,53,59	0
32	PL9	D	405[B]	55/55	0.95	0.15	27,35,43,47	55
26	BCR	D	404	40/40	0.95	0.14	36,49,79,88	0
26	BCR	H	102	40/40	0.95	0.13	36,52,65,68	0
26	BCR	K	101	40/40	0.95	0.14	43,55,62,63	0
26	BCR	T	103	40/40	0.95	0.12	28,45,55,58	0
26	BCR	Y	101	40/40	0.95	0.11	48,59,67,72	0
24	CLA	C	510	65/65	0.95	0.12	39,51,60,69	0
26	BCR	c	518	40/40	0.95	0.14	39,55,64,64	0
28	GOL	b	603	6/6	0.95	0.20	53,57,64,80	0
24	CLA	b	622	65/65	0.95	0.13	29,39,47,49	0
26	BCR	d	404	40/40	0.95	0.14	38,50,73,79	0
24	CLA	b	624	65/65	0.95	0.14	27,39,83,97	0
24	CLA	b	625	65/65	0.95	0.12	34,44,62,67	0
24	CLA	B	608	65/65	0.95	0.13	24,33,44,53	0
24	CLA	C	503	65/65	0.95	0.13	39,50,59,65	0
24	CLA	B	610	65/65	0.95	0.13	35,46,55,71	0
24	CLA	D	403	65/65	0.95	0.13	39,49,99,104	0
24	CLA	a	409	65/65	0.95	0.14	27,32,48,57	0
24	CLA	C	505	65/65	0.95	0.13	32,47,66,74	0
37	DGD	C	516	62/66	0.95	0.14	33,44,85,86	0
24	CLA	B	604	65/65	0.95	0.13	33,43,50,53	0
24	CLA	b	613	65/65	0.95	0.13	34,43,52,58	0
24	CLA	c	513	65/65	0.95	0.13	43,54,67,82	0
24	CLA	B	615	65/65	0.95	0.14	27,38,82,86	0
24	CLA	B	616	65/65	0.95	0.13	33,44,60,68	0
24	CLA	b	618	65/65	0.95	0.12	32,42,51,56	0
24	CLA	B	617	65/65	0.95	0.15	31,50,107,110	0
28	GOL	B	627	6/6	0.95	0.22	56,65,80,92	0
24	CLA	d	401	65/65	0.95	0.13	26,32,41,51	0
24	CLA	d	403	65/65	0.95	0.13	39,49,98,106	0
38	LHG	D	408	49/49	0.95	0.16	30,41,62,74	0
28	GOL	B	631	6/6	0.95	0.32	48,62,69,70	0
25	PHO	a	420[A]	64/64	0.95	0.14	31,41,46,49	64
38	LHG	L	101	49/49	0.95	0.15	31,43,54,61	0
25	PHO	a	420[B]	64/64	0.95	0.14	31,40,46,50	64
26	BCR	B	620	40/40	0.95	0.14	31,43,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	C	514	40/40	0.95	0.13	49,65,73,78	0
38	LHG	d	408	49/49	0.95	0.17	34,52,103,105	0
32	PL9	D	405[A]	55/55	0.95	0.15	28,35,45,49	55
25	PHO	A	409[B]	64/64	0.96	0.14	30,39,44,49	64
24	CLA	B	609	65/65	0.96	0.14	32,42,52,54	0
23	BCT	a	419[A]	4/4	0.96	0.13	53,54,57,63	4
26	BCR	A	411	40/40	0.96	0.15	29,37,44,45	0
26	BCR	B	619	40/40	0.96	0.14	26,36,55,58	0
24	CLA	a	410	65/65	0.96	0.14	29,40,99,105	0
24	CLA	a	412	65/65	0.96	0.15	32,45,111,115	0
26	BCR	C	515	40/40	0.96	0.15	39,53,60,63	0
24	CLA	c	506	65/65	0.96	0.13	38,50,63,69	0
28	GOL	B	629	6/6	0.96	0.13	43,47,50,52	0
24	CLA	B	611	65/65	0.96	0.13	35,44,50,57	0
24	CLA	B	612	65/65	0.96	0.14	26,35,47,53	0
23	BCT	a	419[B]	4/4	0.96	0.13	53,53,57,64	4
24	CLA	b	614	65/65	0.96	0.13	26,39,70,74	0
28	GOL	C	525	6/6	0.96	0.12	39,48,50,51	0
24	CLA	b	615	65/65	0.96	0.13	28,38,50,52	0
24	CLA	A	405	65/65	0.96	0.14	25,32,41,57	0
24	CLA	B	605	65/65	0.96	0.13	25,35,67,69	0
24	CLA	B	606	65/65	0.96	0.13	28,37,50,52	0
24	CLA	A	406	65/65	0.96	0.14	24,32,38,45	0
24	CLA	b	620	65/65	0.96	0.13	33,44,51,57	0
28	GOL	V	204	6/6	0.96	0.12	55,61,65,65	0
26	BCR	t	101	40/40	0.96	0.13	30,43,60,68	0
24	CLA	A	410	65/65	0.96	0.13	29,47,108,113	0
24	CLA	D	402	65/65	0.96	0.14	24,33,52,57	0
24	CLA	d	402	65/65	0.96	0.13	26,35,54,64	0
32	PL9	d	405[A]	55/55	0.96	0.16	25,35,44,49	55
32	PL9	d	405[B]	55/55	0.96	0.16	25,35,43,49	55
28	GOL	b	604	6/6	0.96	0.16	41,56,70,75	0
28	GOL	b	605	6/6	0.96	0.21	53,64,74,84	0
24	CLA	b	623	65/65	0.96	0.14	28,39,55,57	0
25	PHO	A	408	64/64	0.96	0.13	26,32,38,43	0
25	PHO	A	409[A]	64/64	0.96	0.14	29,40,44,47	64
39	HEM	e	102	43/43	0.96	0.17	53,76,114,130	0
40	MG	j	103	1/1	0.96	0.17	55,55,55,55	0
25	PHO	a	411	64/64	0.97	0.14	26,34,40,45	0
24	CLA	B	613	65/65	0.97	0.12	27,36,45,47	0
24	CLA	A	407	65/65	0.97	0.12	27,37,90,96	0
24	CLA	C	502	65/65	0.97	0.12	36,44,55,70	0

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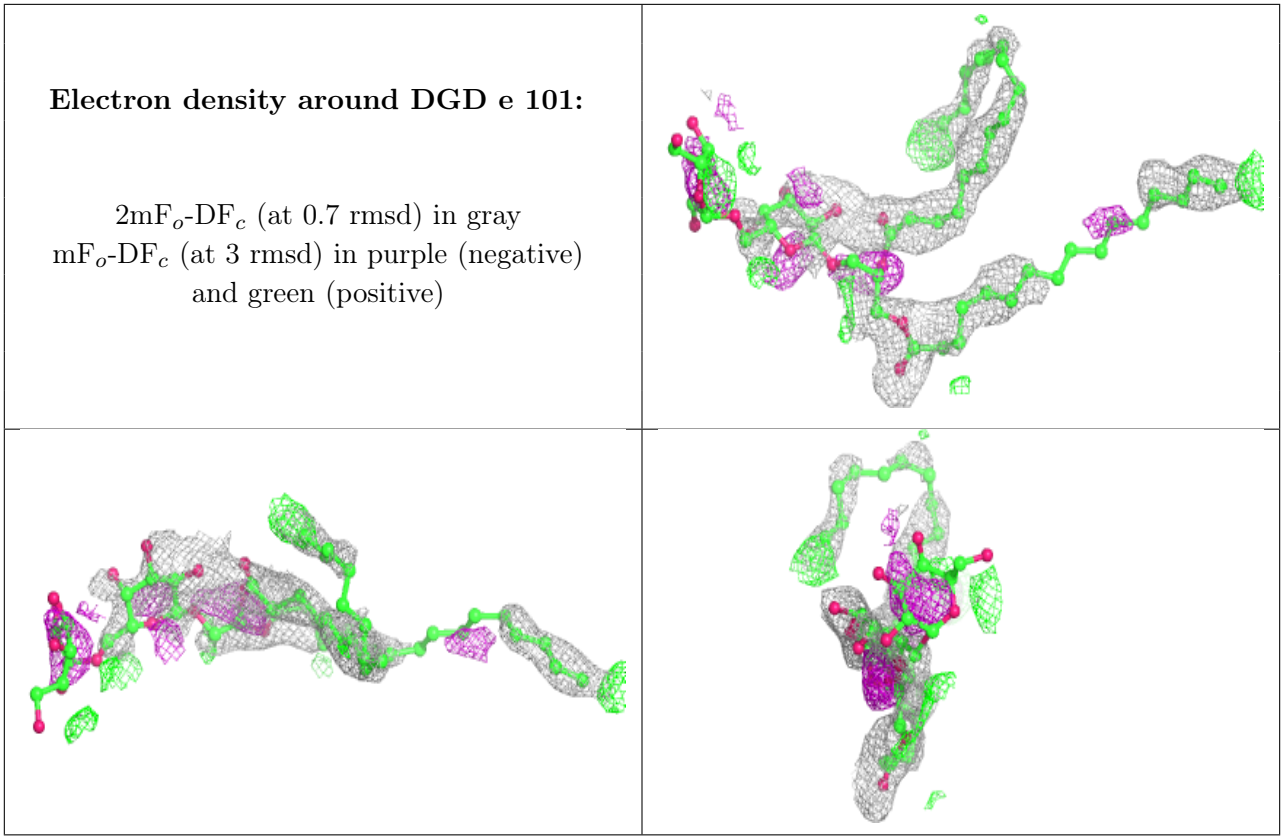
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	a	413	40/40	0.97	0.12	28,38,46,47	0
26	BCR	b	627	40/40	0.97	0.14	30,39,47,47	0
26	BCR	B	618	40/40	0.97	0.14	28,37,45,45	0
40	MG	J	102	1/1	0.97	0.09	50,50,50,50	0
26	BCR	b	629	40/40	0.97	0.14	37,48,60,64	0
23	BCT	A	404[A]	4/4	0.98	0.12	51,52,57,63	4
23	BCT	A	404[B]	4/4	0.98	0.12	51,52,57,63	4
28	GOL	c	501	6/6	0.98	0.14	43,46,52,53	0
35	CA	C	526	1/1	0.98	0.07	67,67,67,67	0
22	CL	A	403[B]	1/1	0.98	0.12	33,33,33,33	1
22	CL	U	201	1/1	0.98	0.17	93,93,93,93	0
35	CA	c	503	1/1	0.98	0.08	63,63,63,63	0
39	HEM	F	102	43/43	0.98	0.13	46,64,75,83	0
39	HEM	V	206	43/43	0.98	0.12	34,39,47,50	0
35	CA	c	504	1/1	0.98	0.06	73,73,73,73	0
39	HEM	v	205	43/43	0.98	0.11	41,49,55,57	0
22	CL	A	403[A]	1/1	0.98	0.12	33,33,33,33	1
35	CA	o	302	1/1	0.98	0.06	86,86,86,86	0
30	OEX	a	417[A]	10/10	0.99	0.12	31,37,39,45	10
31	OEY	A	419[B]	11/11	0.99	0.14	31,36,42,47	11
31	OEY	a	418[B]	11/11	0.99	0.13	32,37,44,57	11
22	CL	a	408[B]	1/1	0.99	0.10	38,38,38,38	1
21	FE2	a	406[B]	1/1	0.99	0.13	46,46,46,46	0
22	CL	A	402[A]	1/1	0.99	0.12	30,30,30,30	1
22	CL	A	402[B]	1/1	0.99	0.12	31,31,31,31	1
22	CL	a	407[A]	1/1	0.99	0.09	34,34,34,34	1
22	CL	a	407[B]	1/1	0.99	0.09	33,33,33,33	1
22	CL	a	408[A]	1/1	0.99	0.10	40,40,40,40	1
30	OEX	A	418[A]	10/10	0.99	0.13	31,35,38,46	10
35	CA	O	302	1/1	0.99	0.05	80,80,80,80	0
21	FE2	A	401[A]	1/1	1.00	0.11	45,45,45,45	1
21	FE2	A	401[B]	1/1	1.00	0.11	47,47,47,47	1

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.

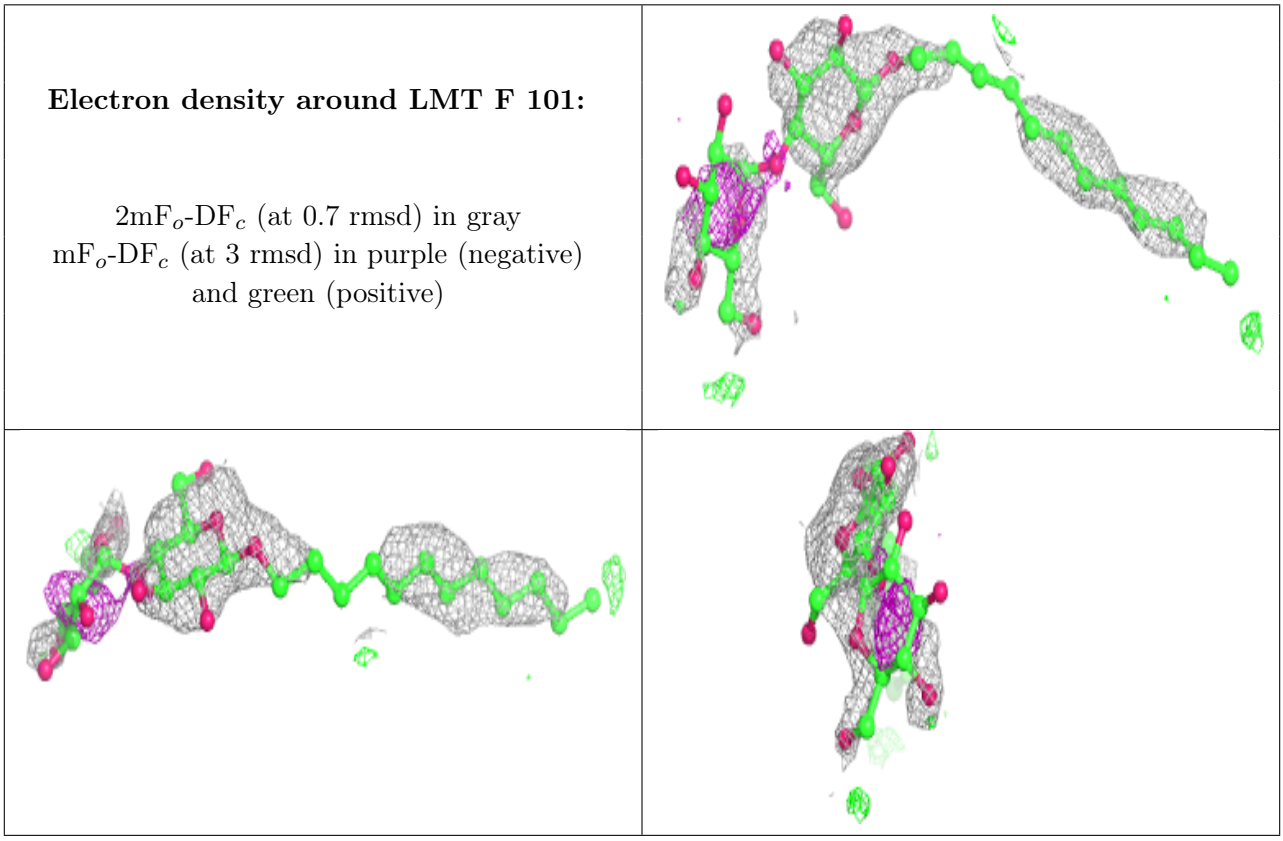
Electron density around DGD e 101:

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



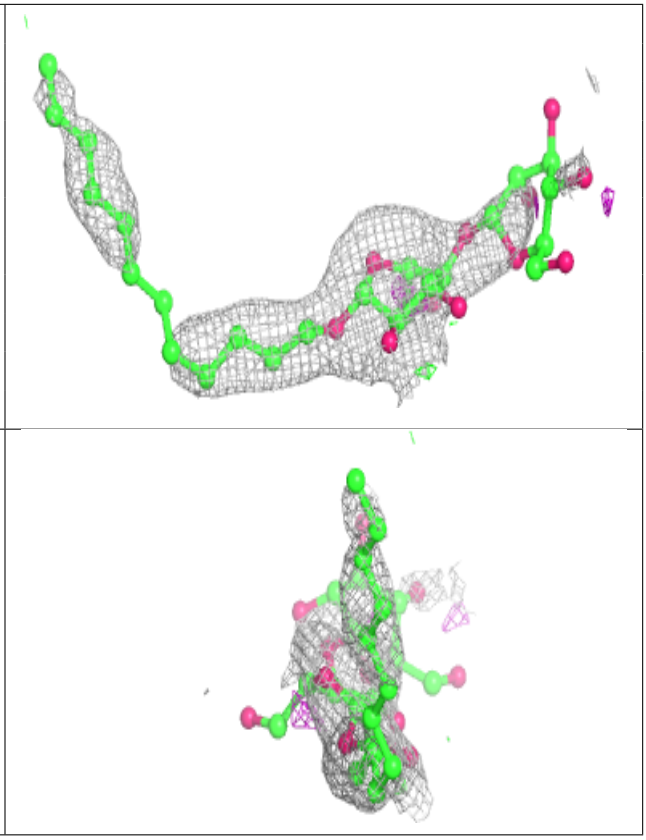
Electron density around LMT F 101:

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



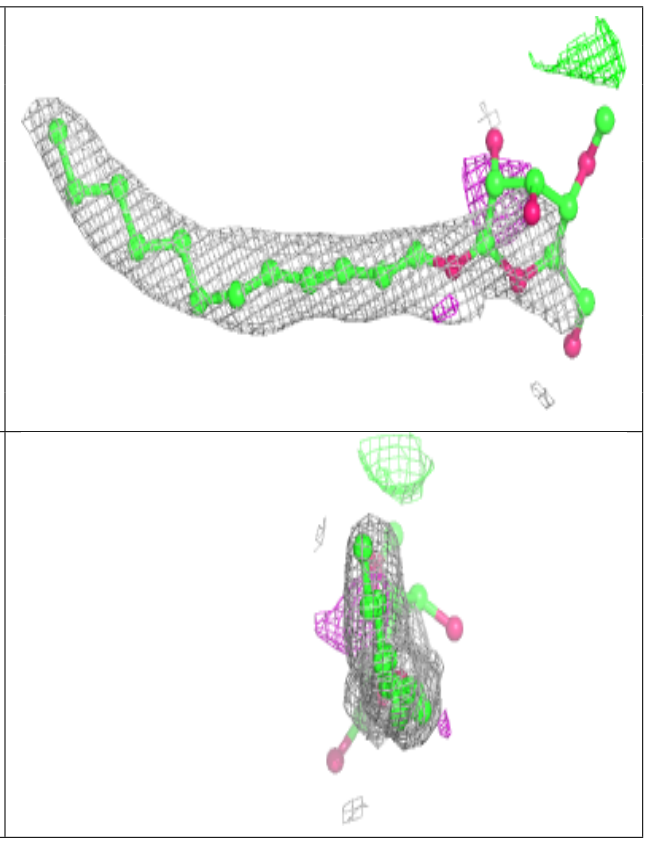
Electron density around LMT C 521:

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



Electron density around LMT b 631:

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



Electron density around LHG a 422:

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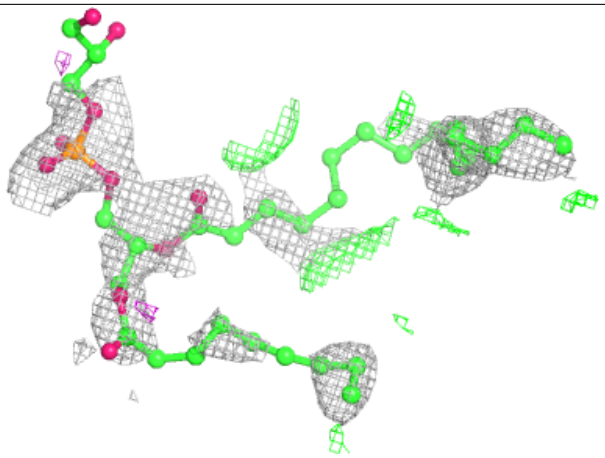
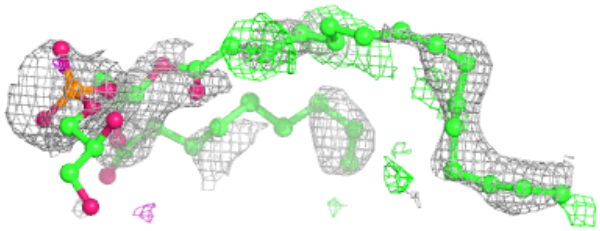
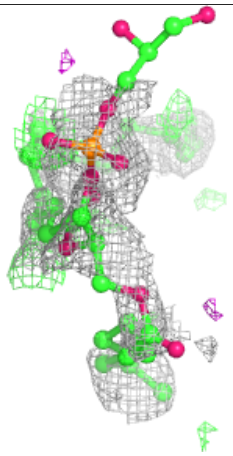
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

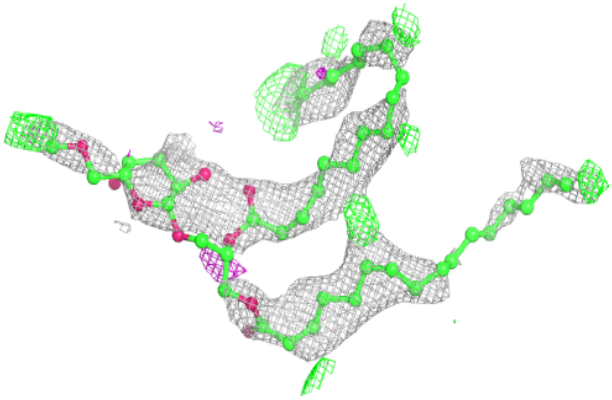


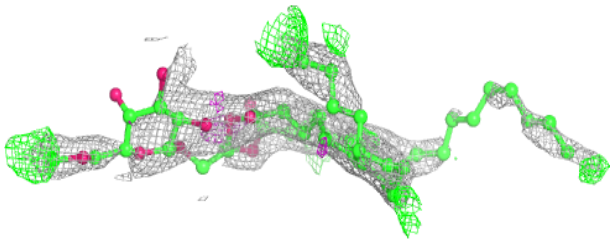


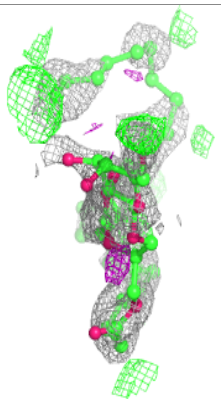


Electron density around DGD D 406:

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

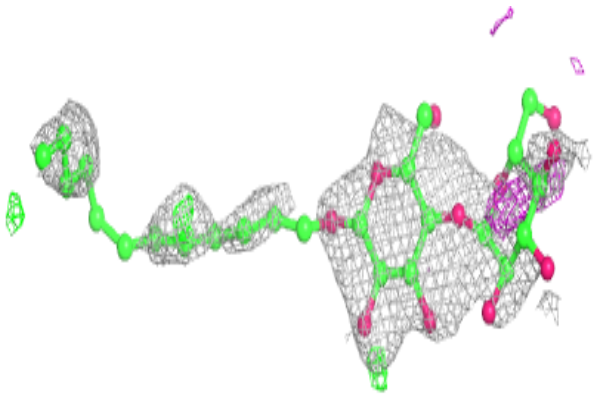


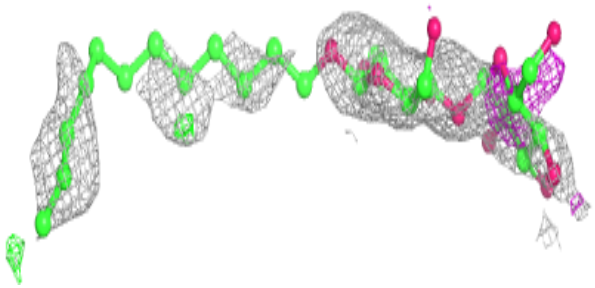


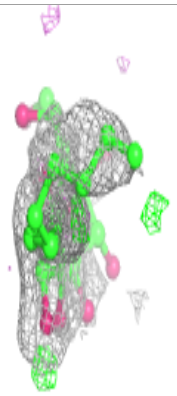


Electron density around LMT a 421:

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

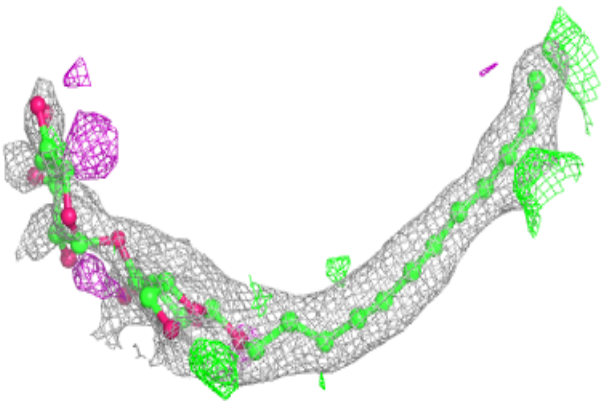


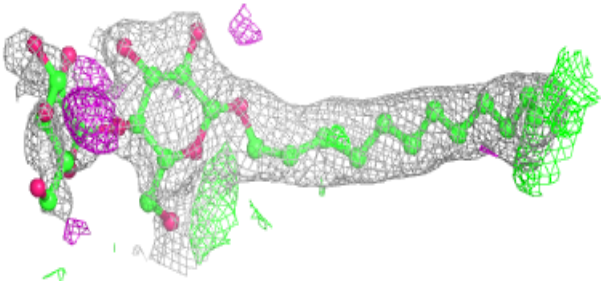


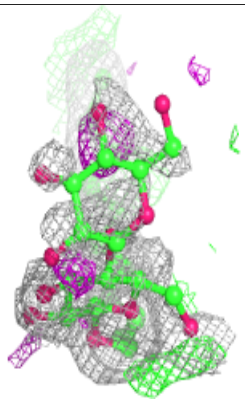


Electron density around LMT M 103:

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

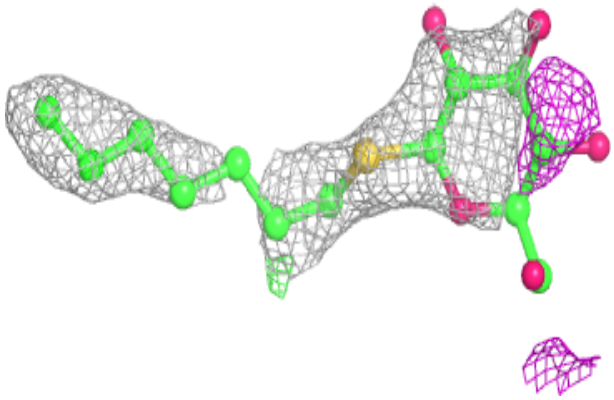


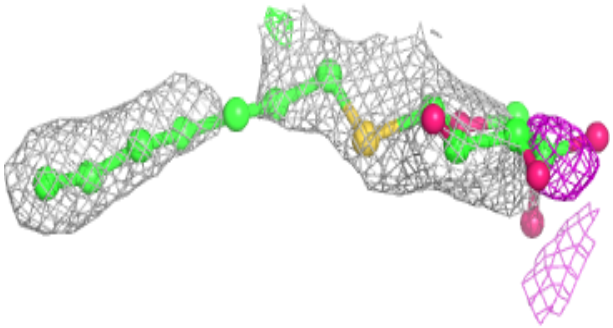


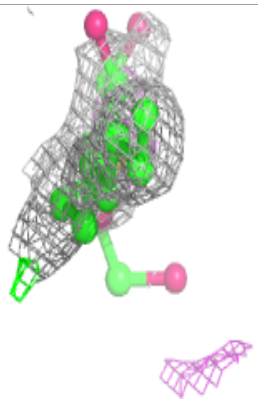


Electron density around HTG c 525:

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

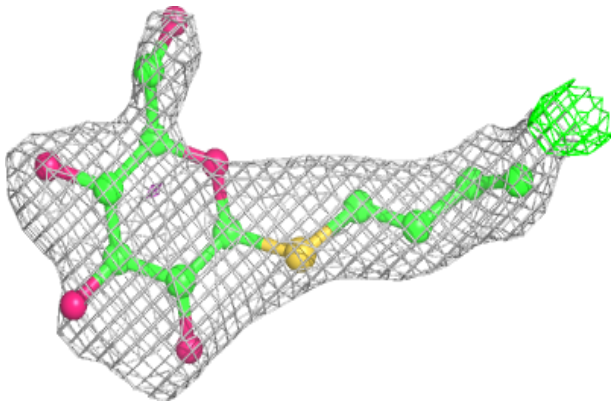


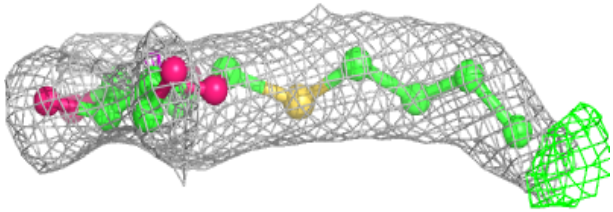


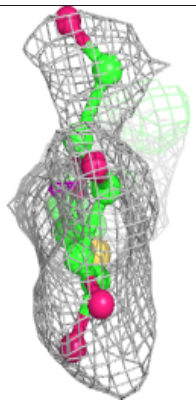


Electron density around HTG d 411:

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

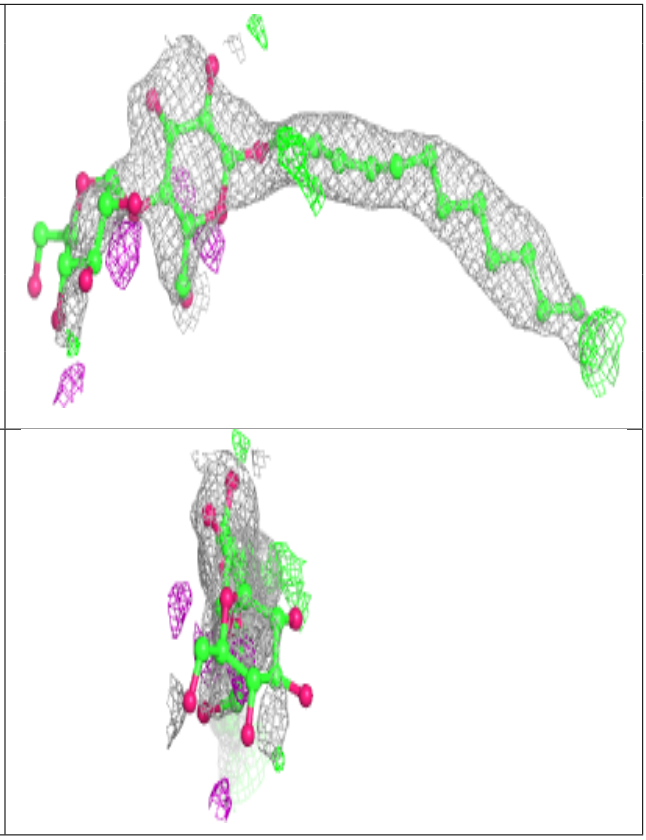






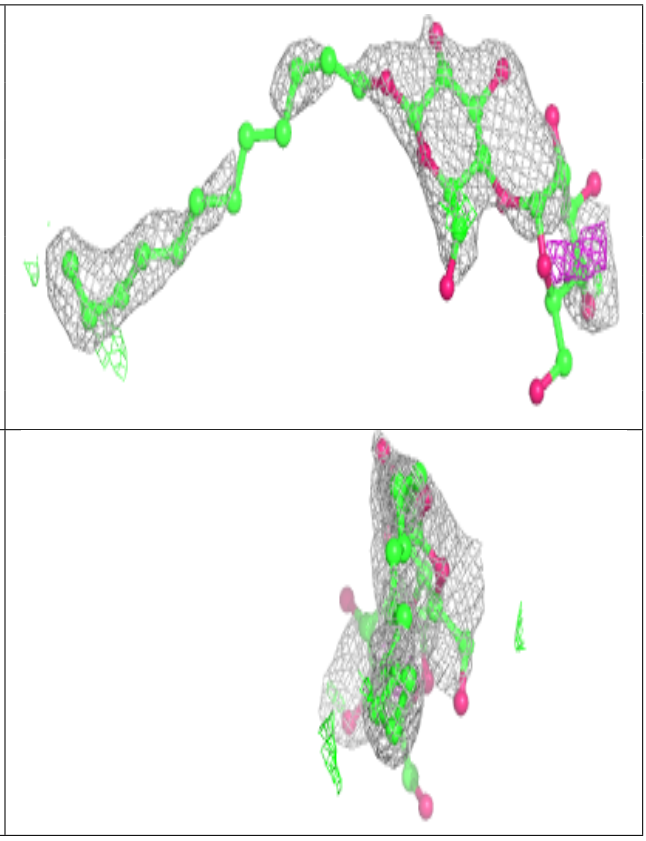
Electron density around LMT D 401:

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



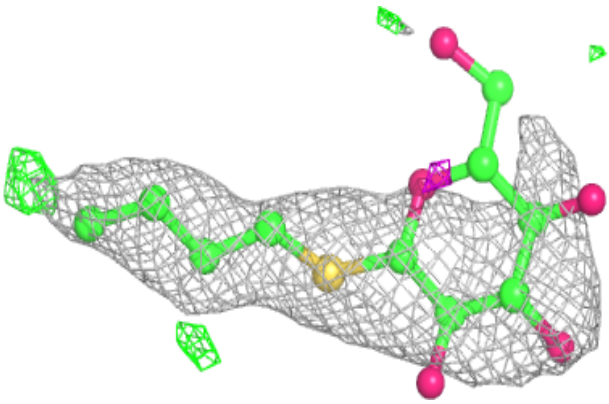
Electron density around LMT f 103:

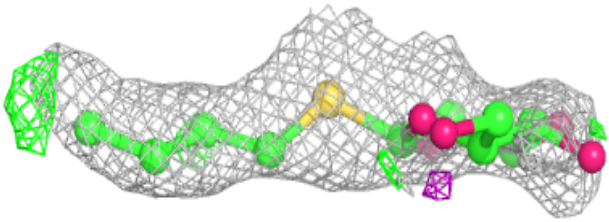
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

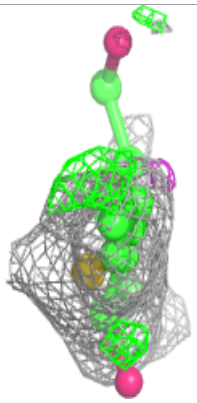


Electron density around HTG H 101:

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

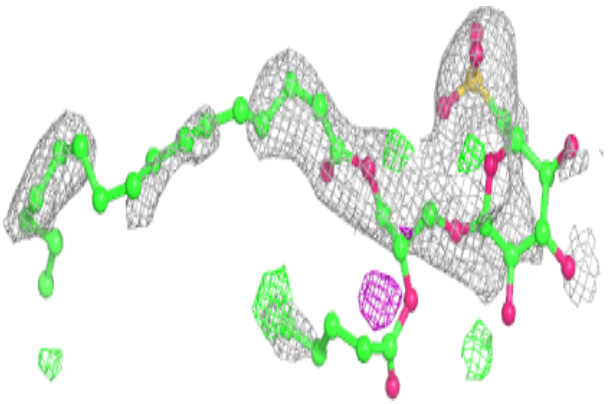


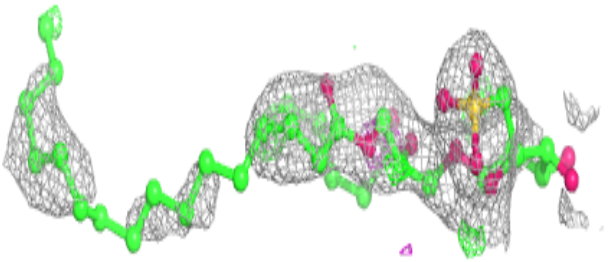


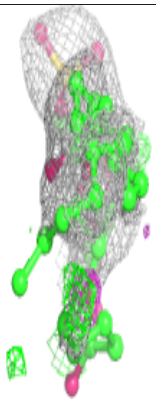


Electron density around SQD f 102:

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

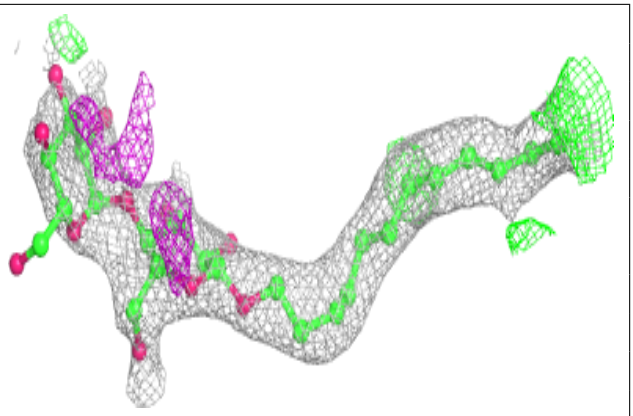


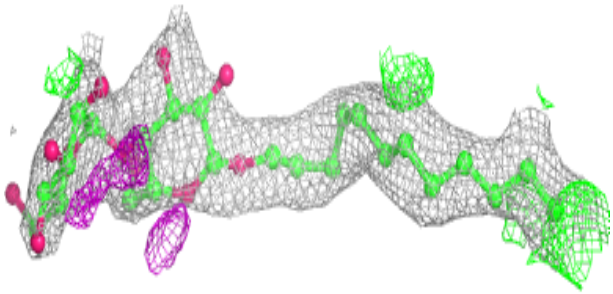


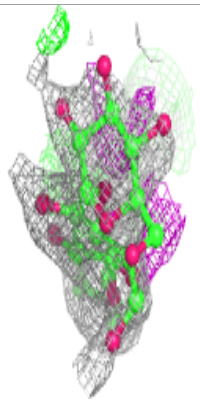


Electron density around LMT a 404:

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

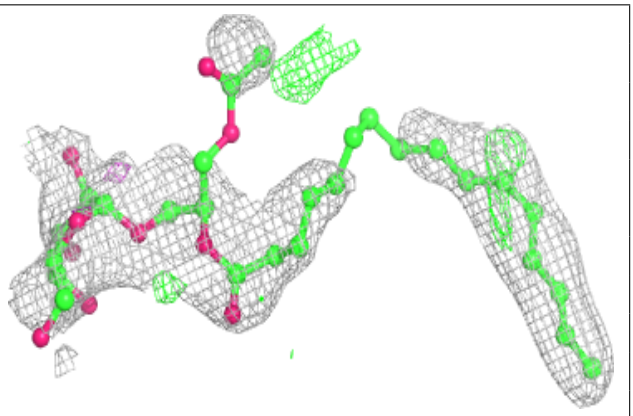


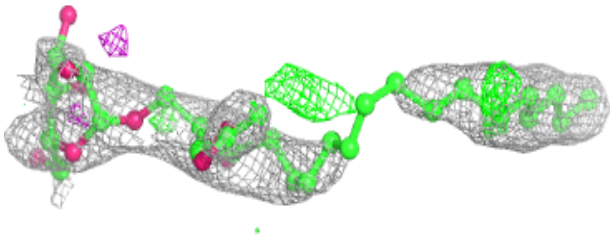


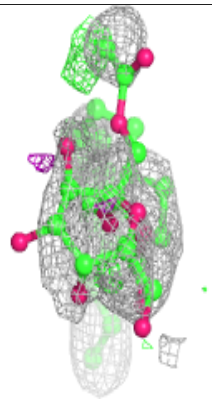


Electron density around LMG Z 101:

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

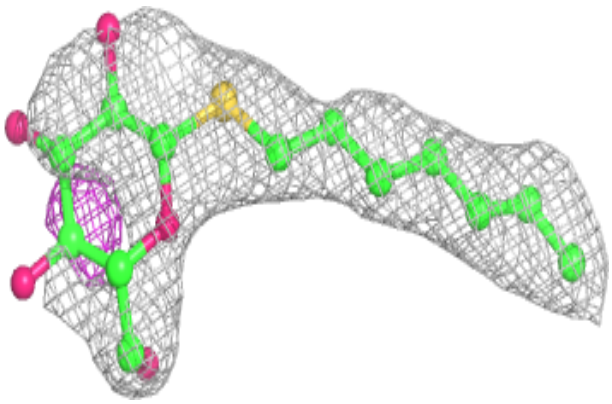


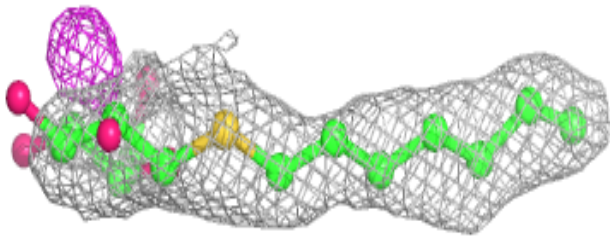


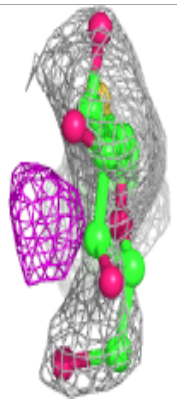


Electron density around HTG b 609:

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

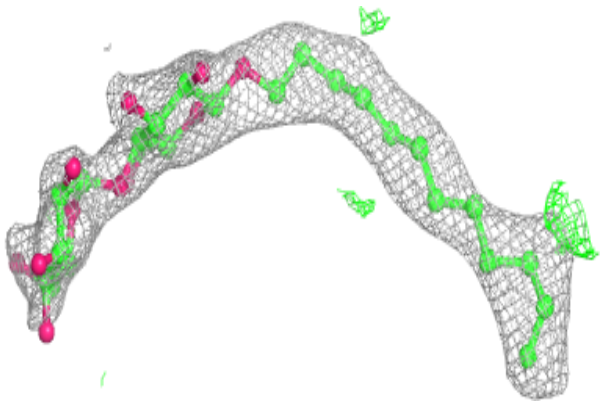


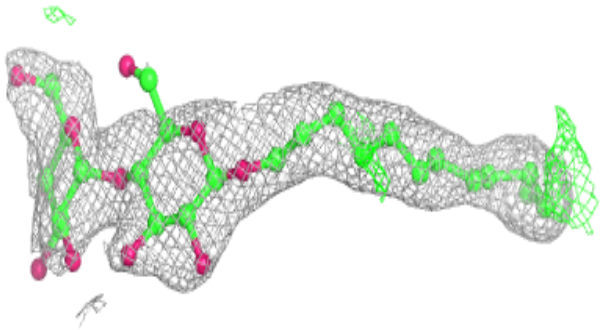


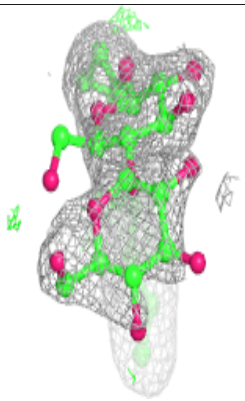


Electron density around LMT m 102:

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

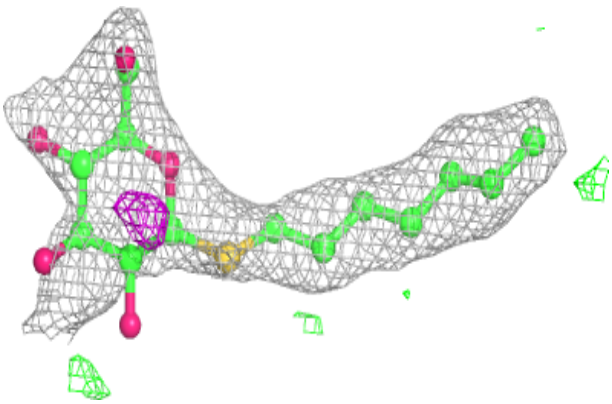


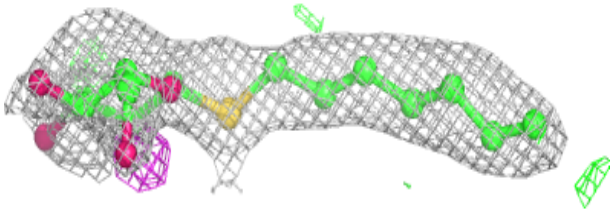


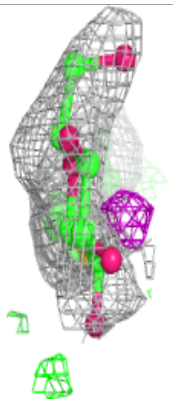


Electron density around HTG B 633:

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

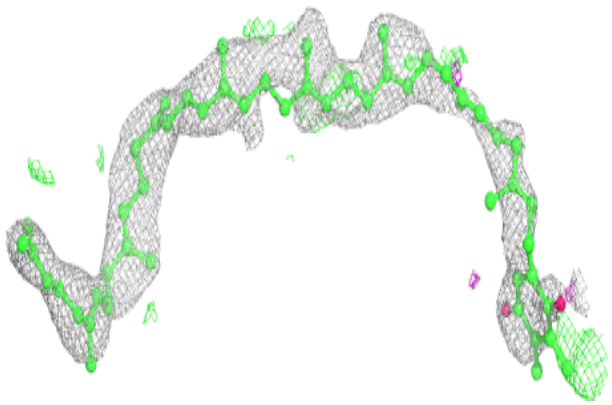


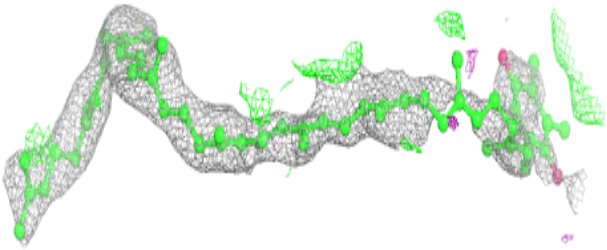


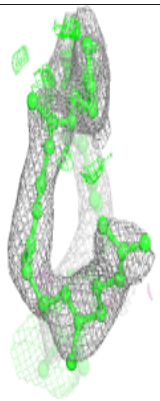


Electron density around PL9 a 416 (A):

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

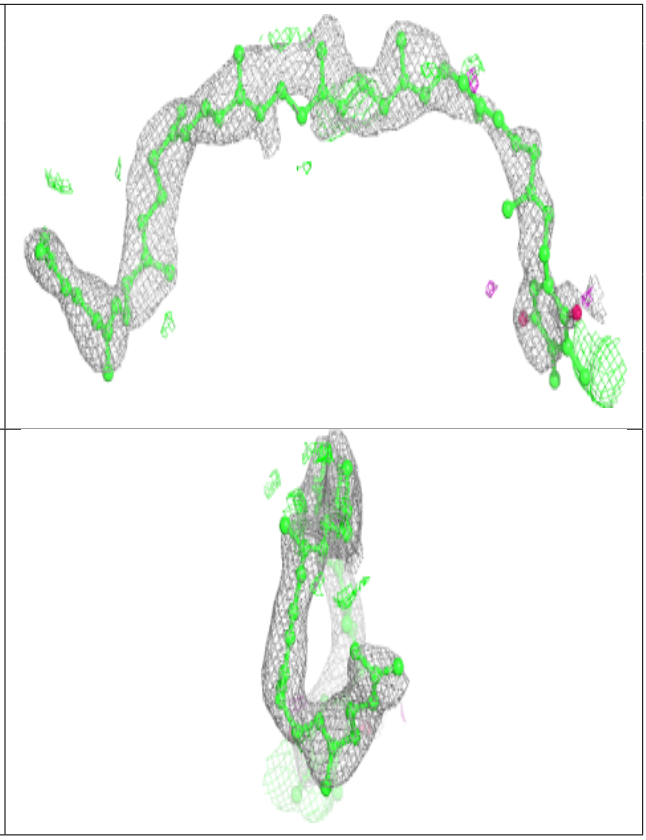






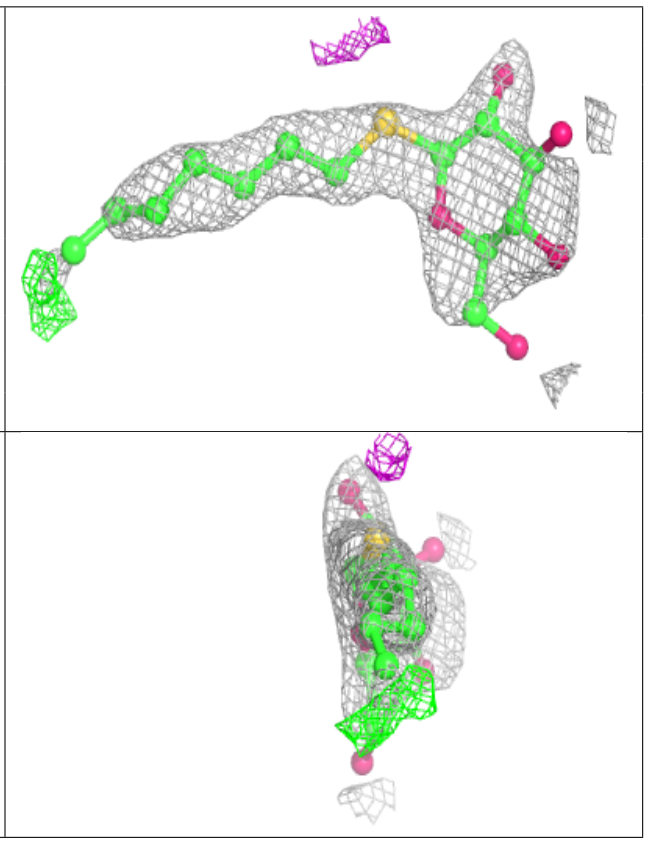
Electron density around PL9 a 416 (B):

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



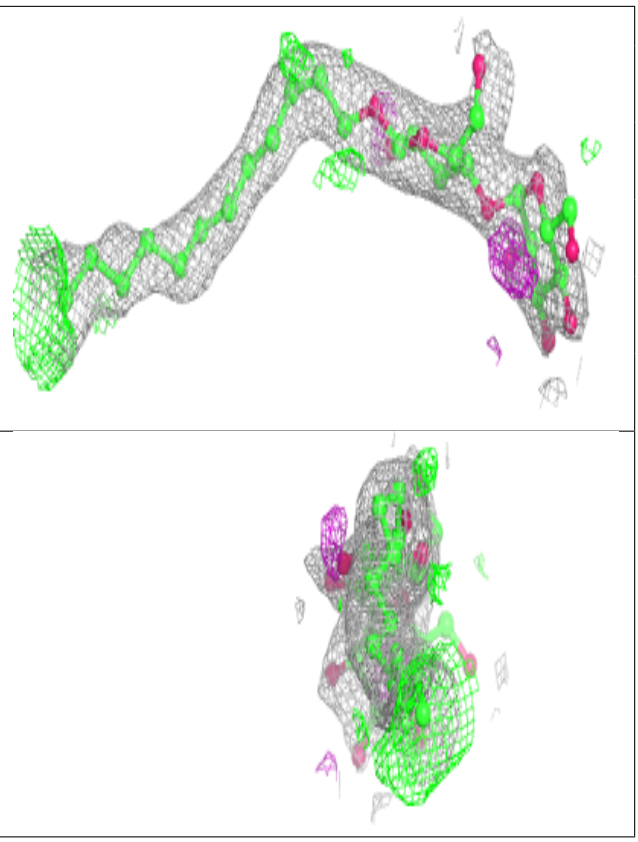
Electron density around HTG B 625:

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



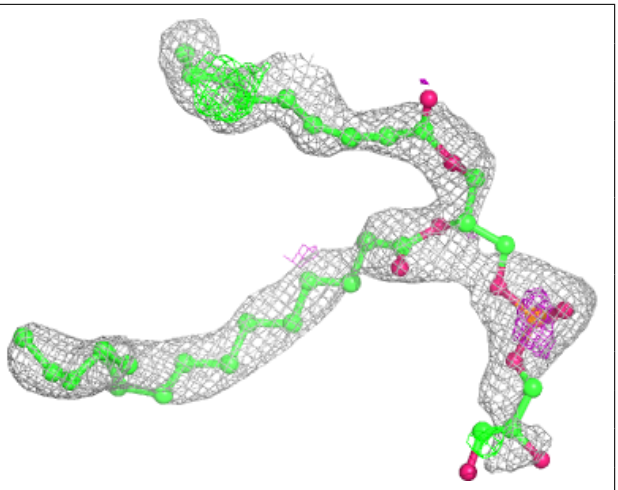
Electron density around LMT A 417:

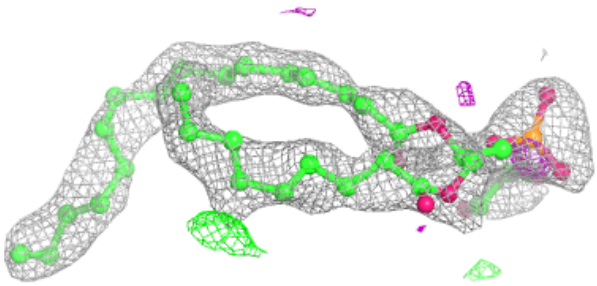
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

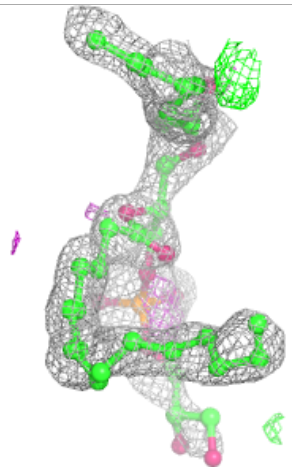


Electron density around LHG E 101:

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

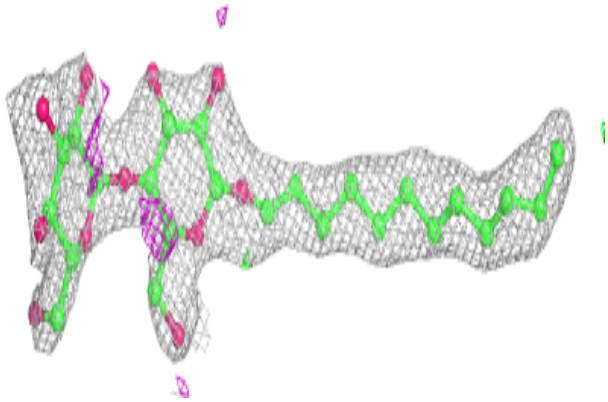


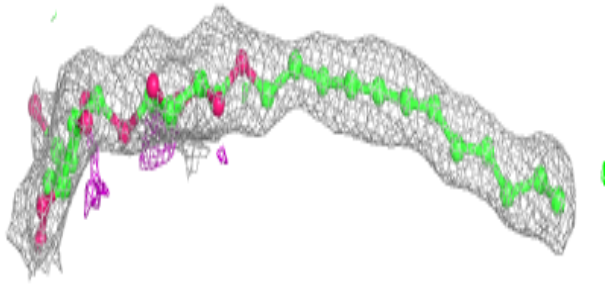


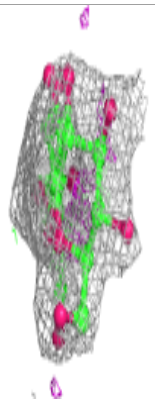


Electron density around LMT M 104:

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

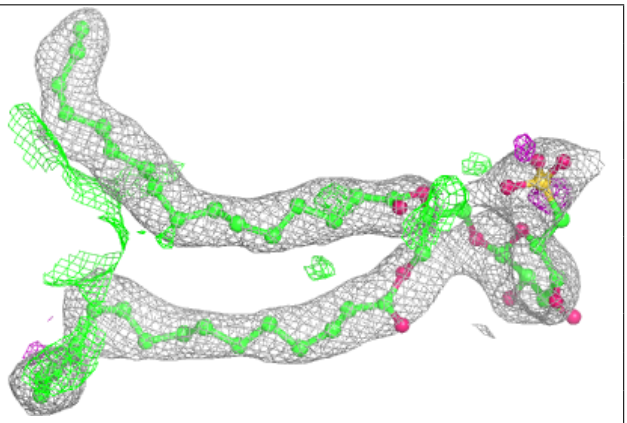


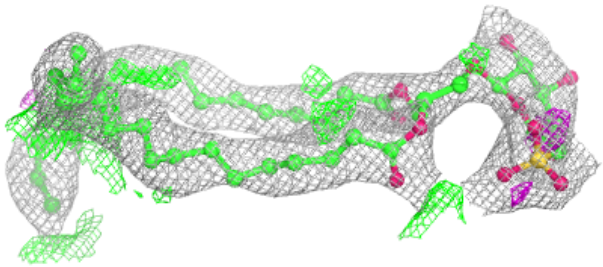


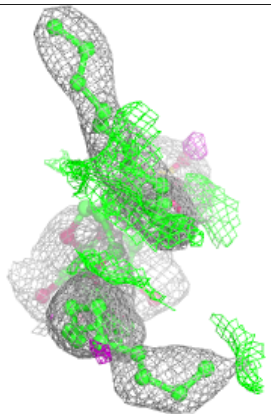


Electron density around SQD b 601:

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

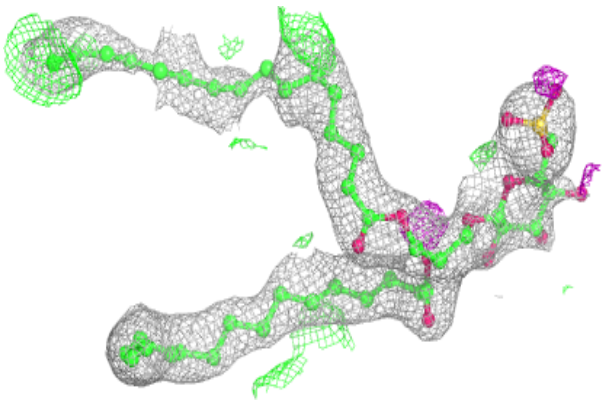


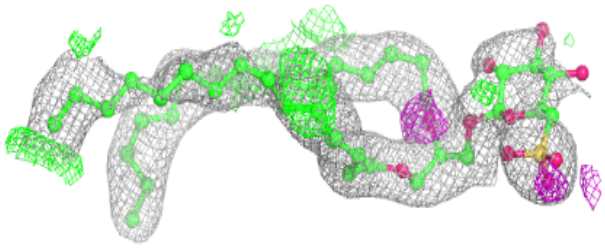


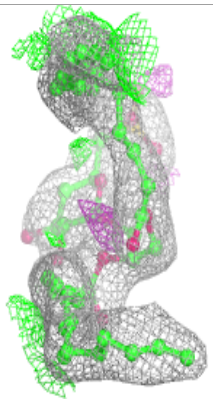


Electron density around SQD A 416:

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

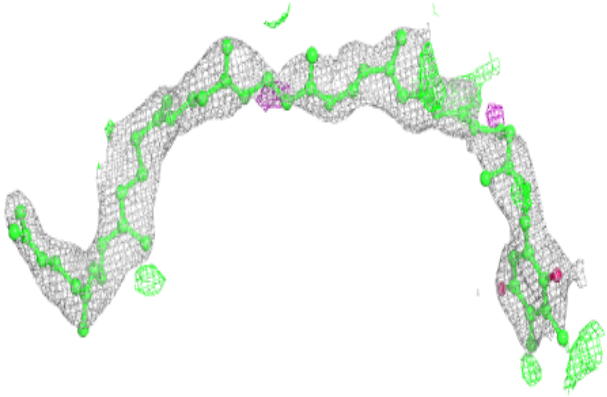


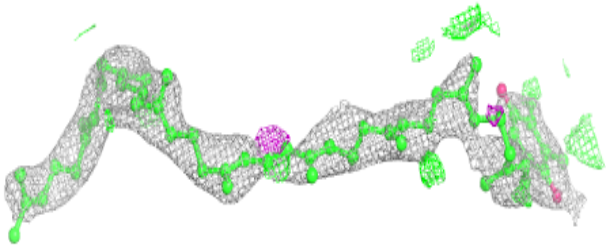


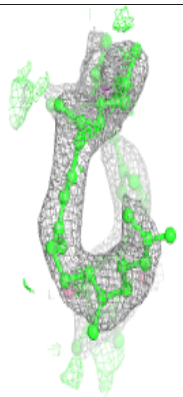


Electron density around PL9 A 420 (A):

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

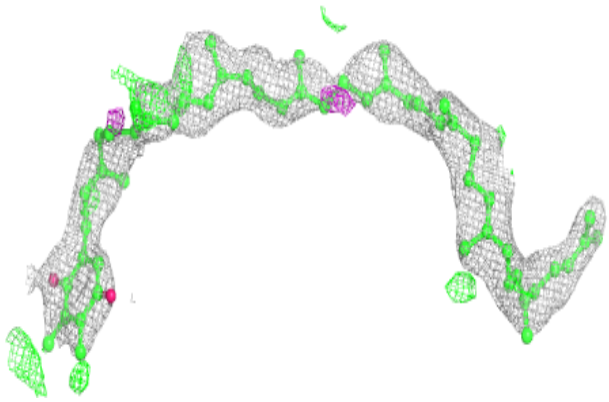


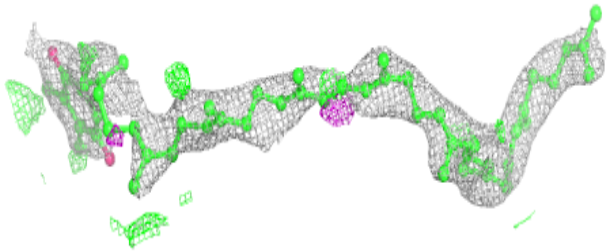


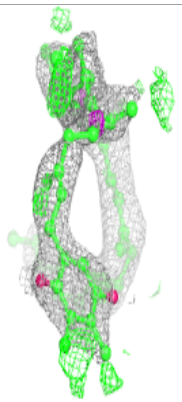


Electron density around PL9 A 420 (B):

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

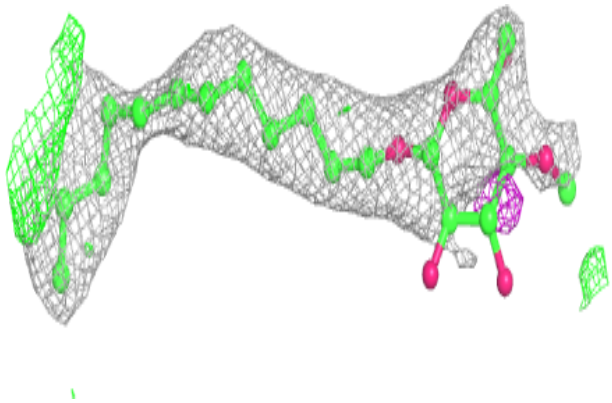


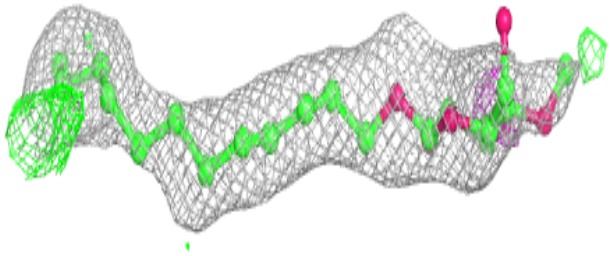


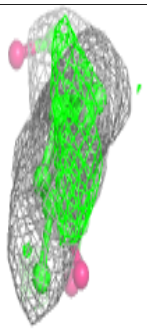


Electron density around LMT T 104:

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

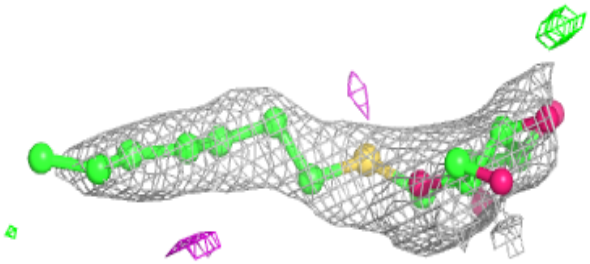


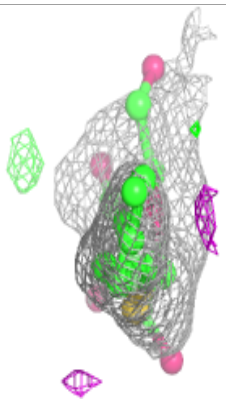




Electron density around HTG b 633:

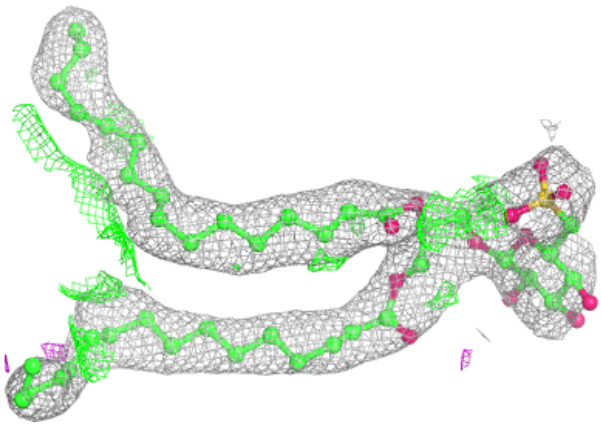
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

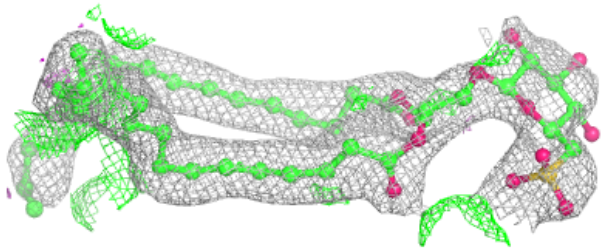


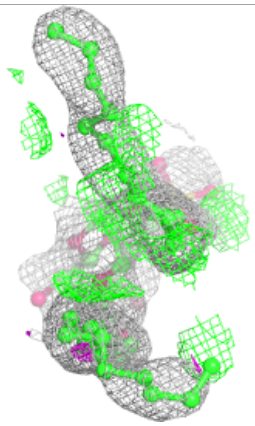


Electron density around SQD B 621:

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

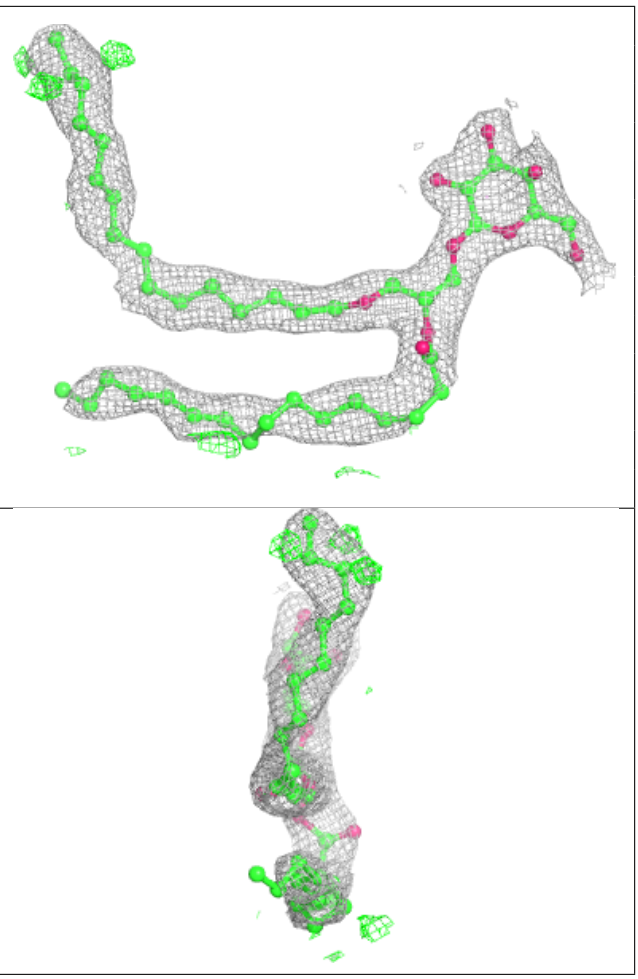






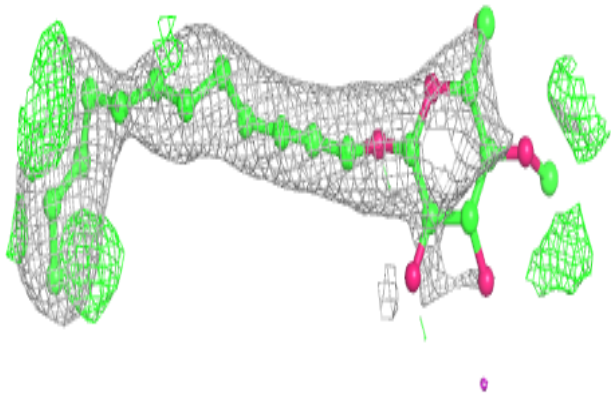
Electron density around LMG C 519:

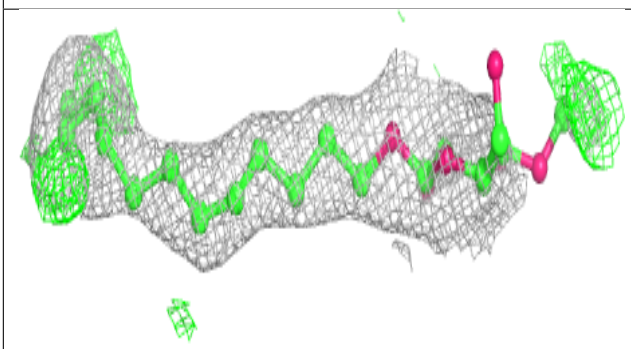
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

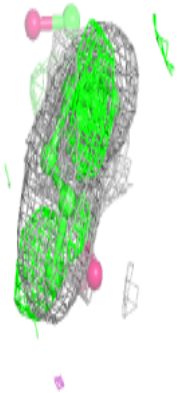


Electron density around LMT B 635:

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

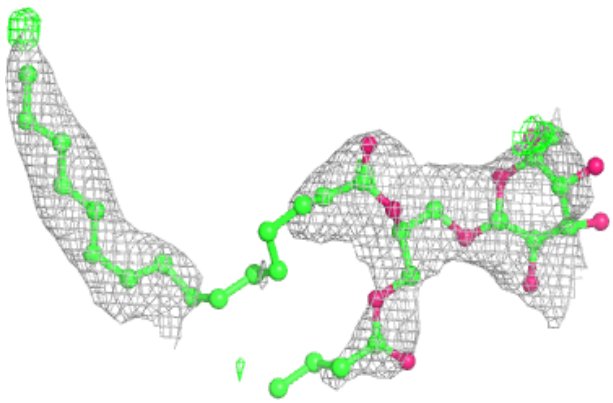


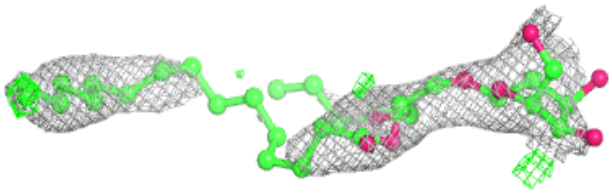


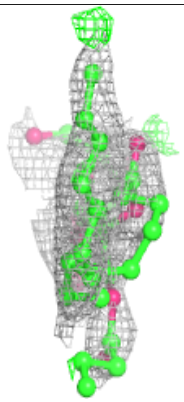


Electron density around LMG z 101:

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

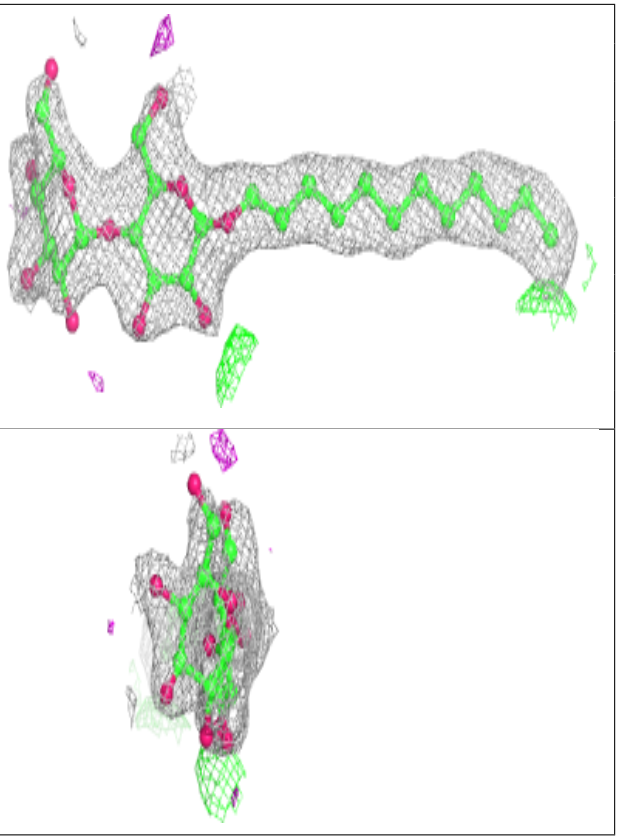


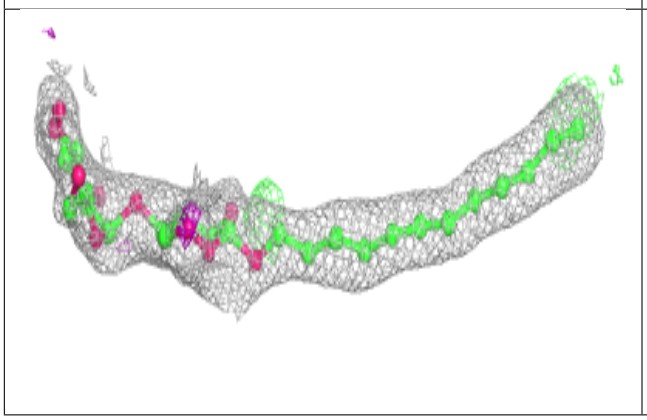




Electron density around LMT M 101:

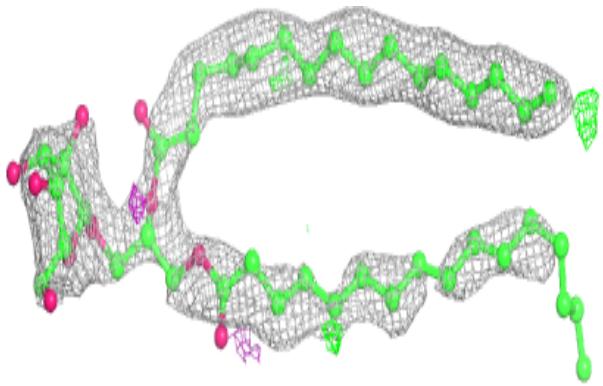
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

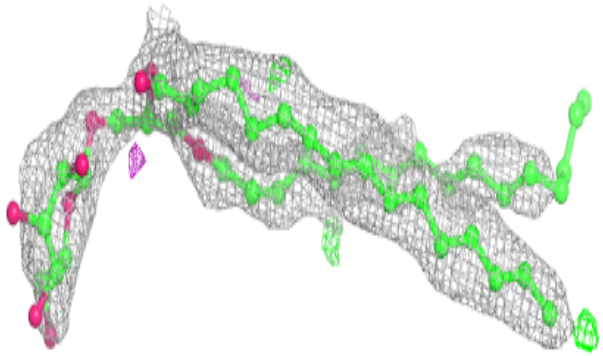


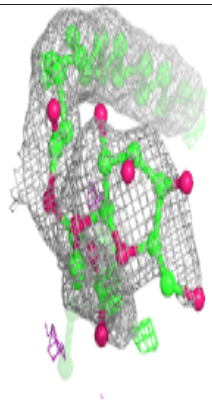


Electron density around LMG C 520:

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

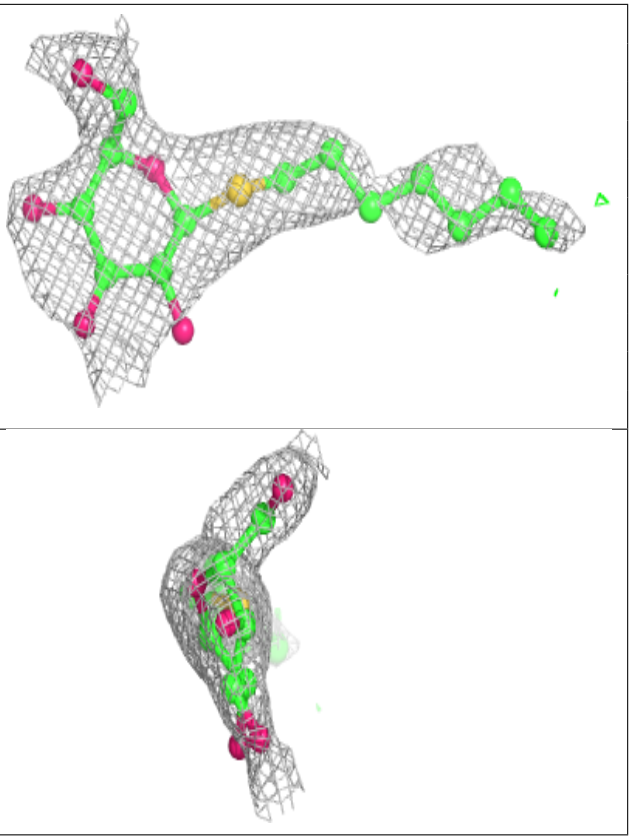


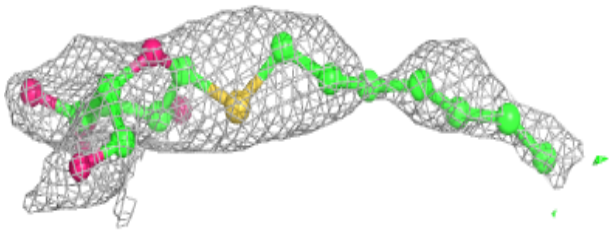




Electron density around HTG C 523:

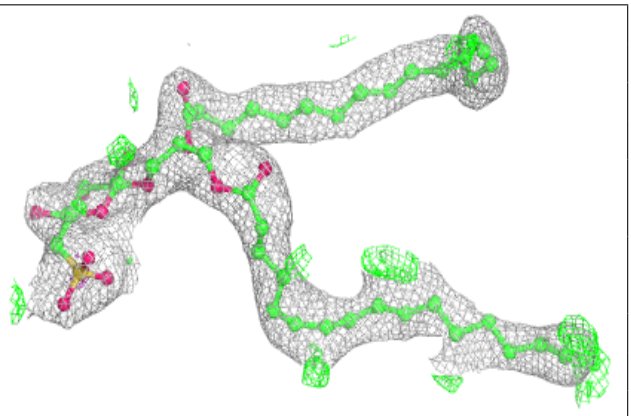
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

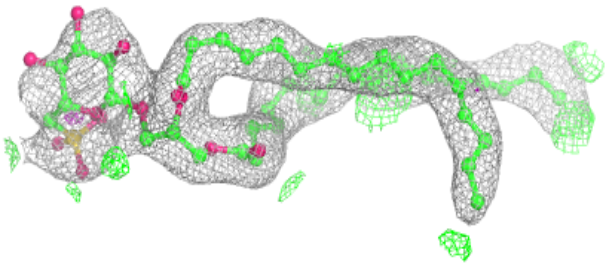


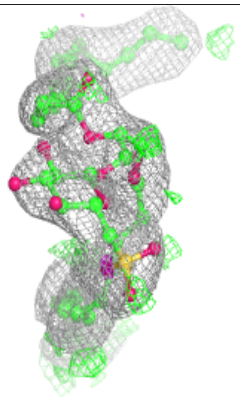


Electron density around SQD a 405:

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

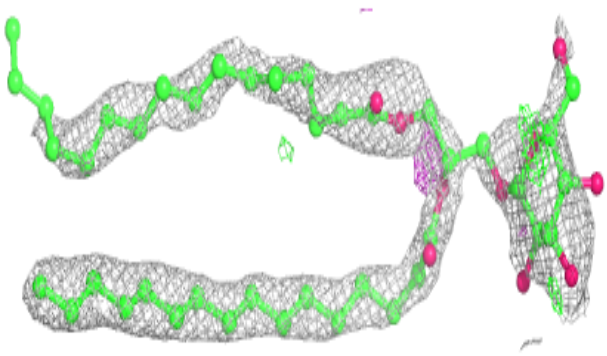


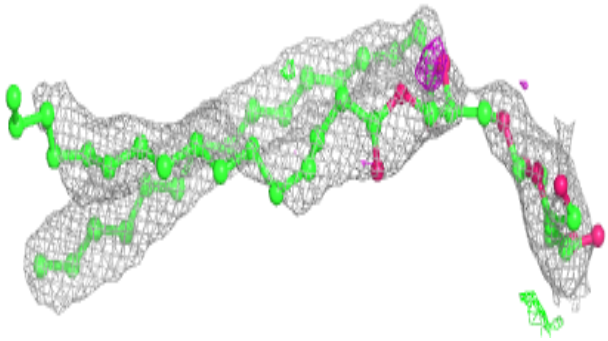


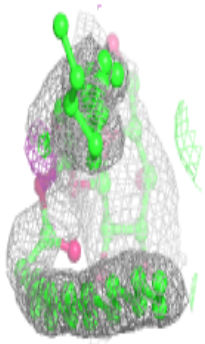


Electron density around LMG c 523:

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

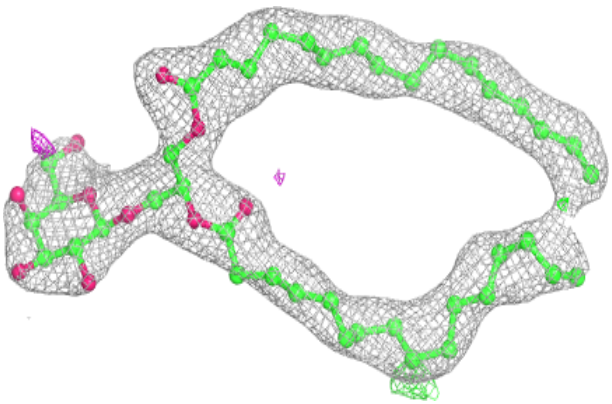


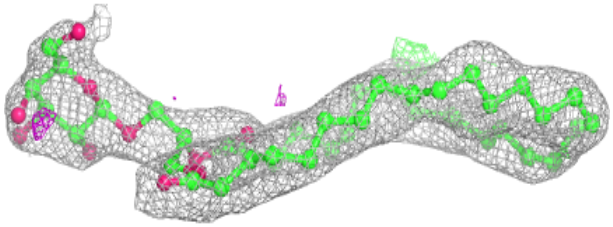


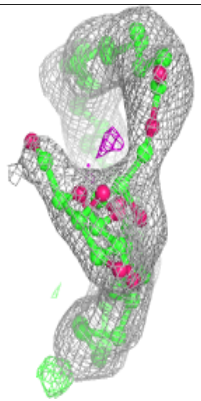


Electron density around LMG a 415:

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

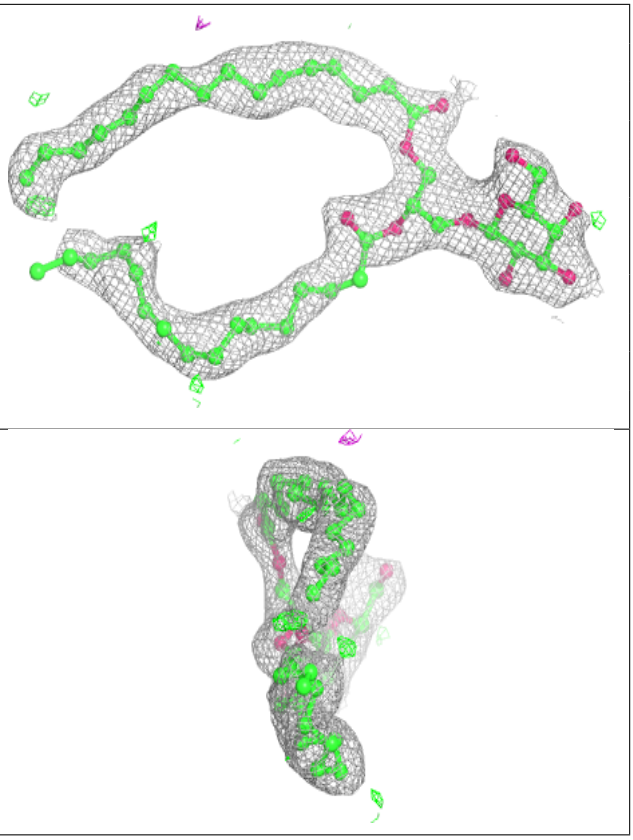






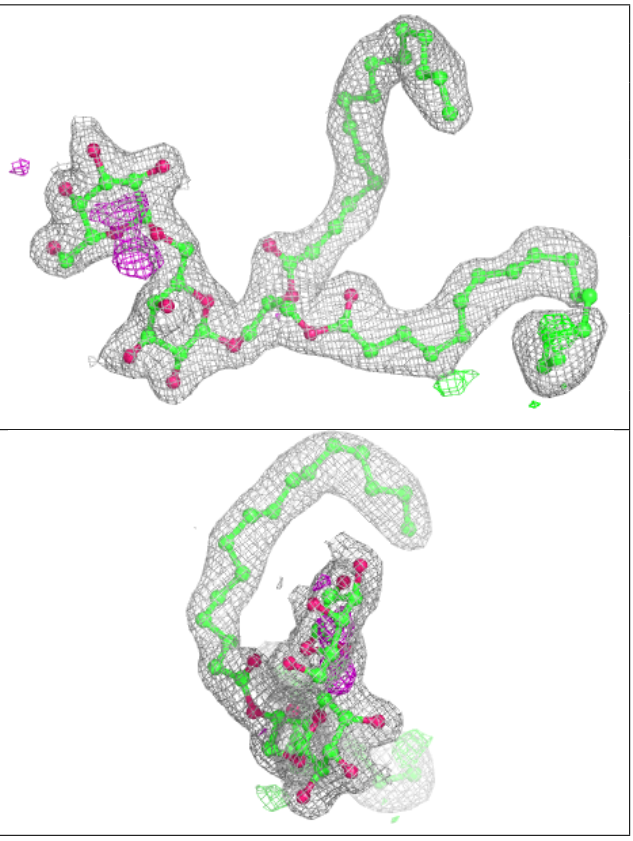
Electron density around LMG A 422:

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



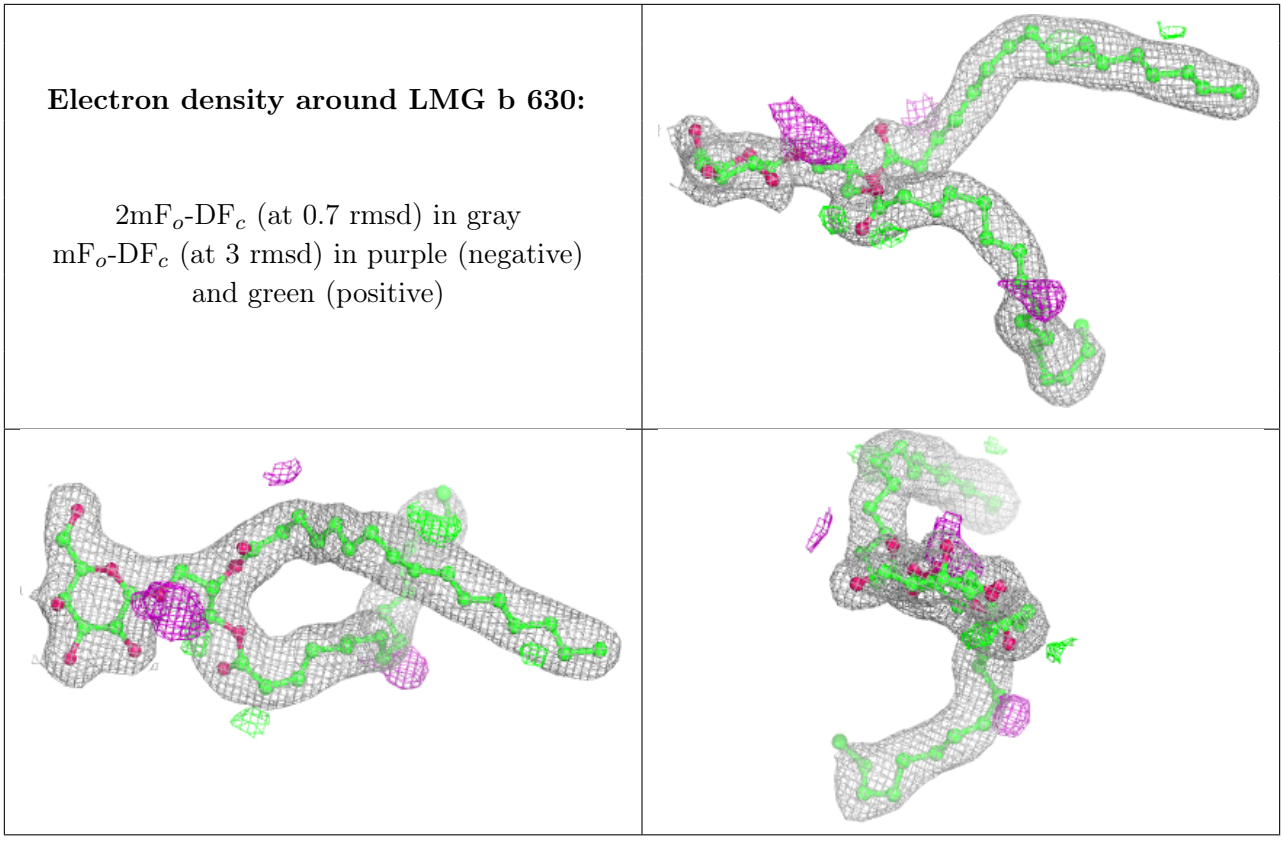
Electron density around DGD C 517:

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



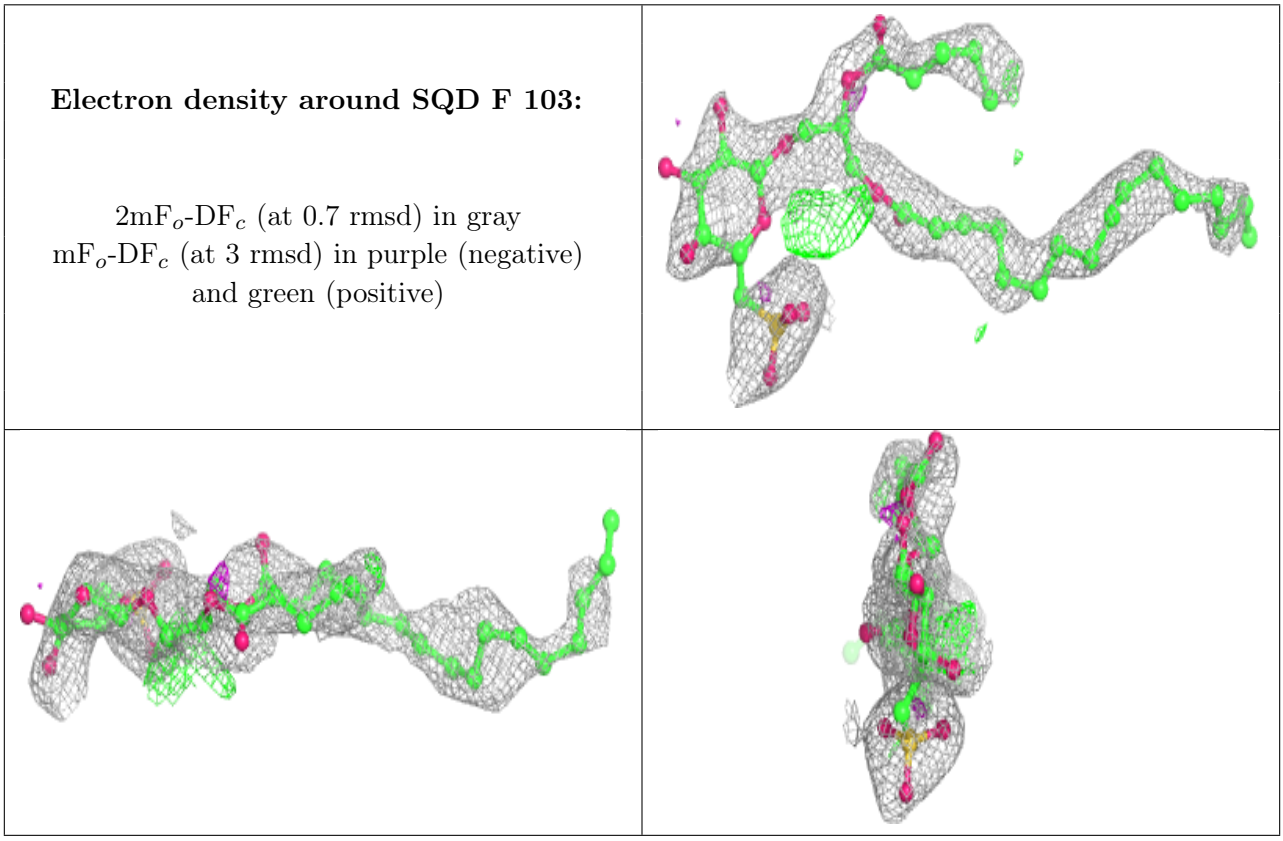
Electron density around LMG b 630:

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



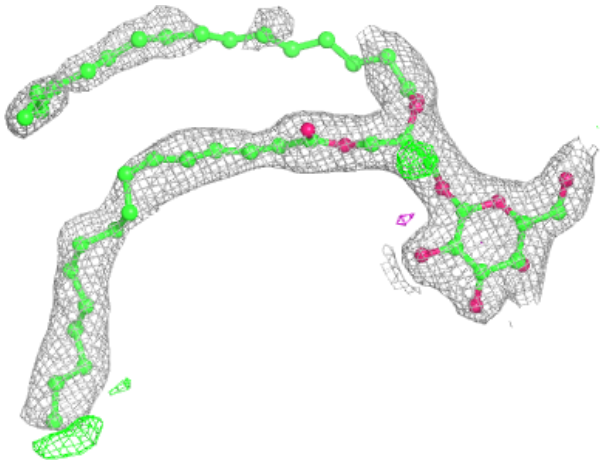
Electron density around SQD F 103:

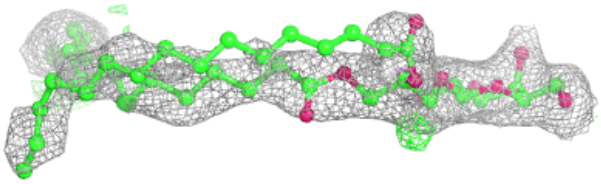
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

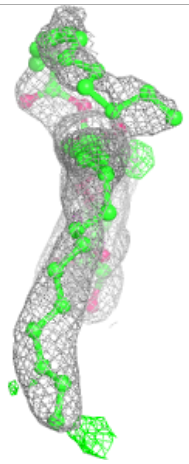


Electron density around LMG c 522:

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

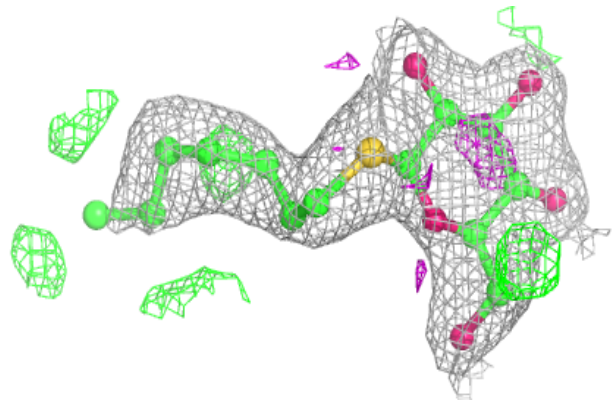


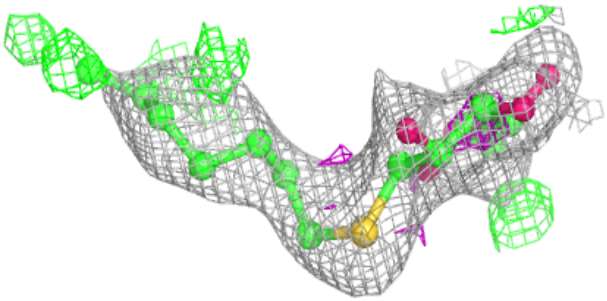




Electron density around HTG B 624:

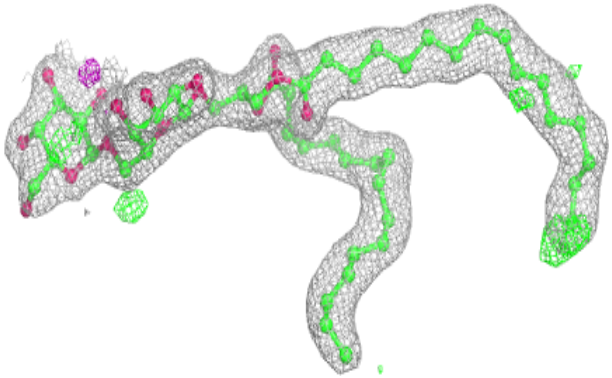
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

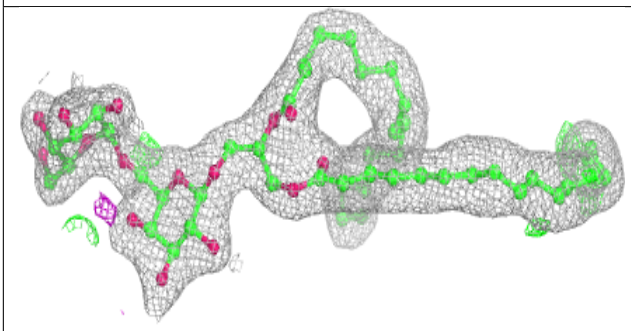


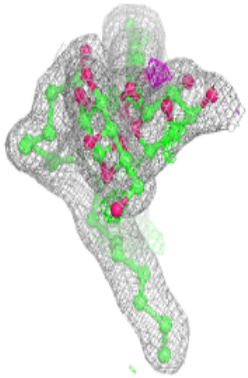


Electron density around DGD h 102:

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

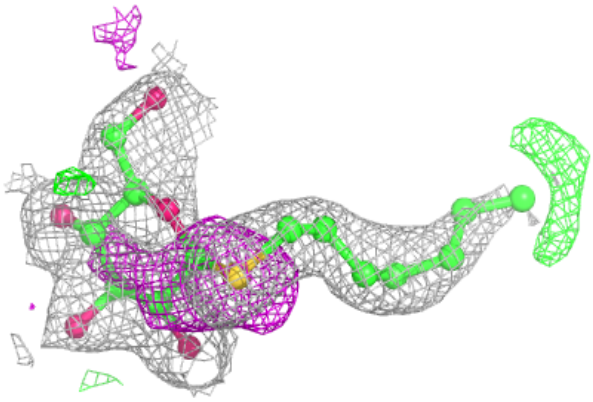


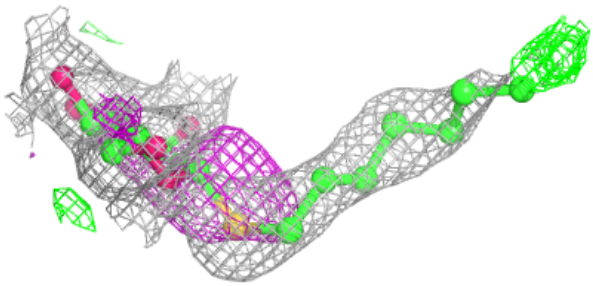


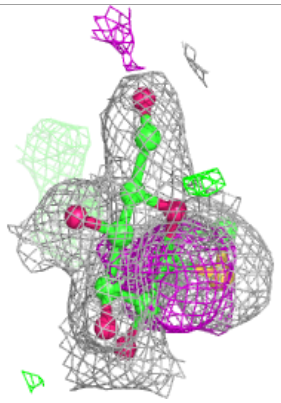


Electron density around HTG b 632:

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

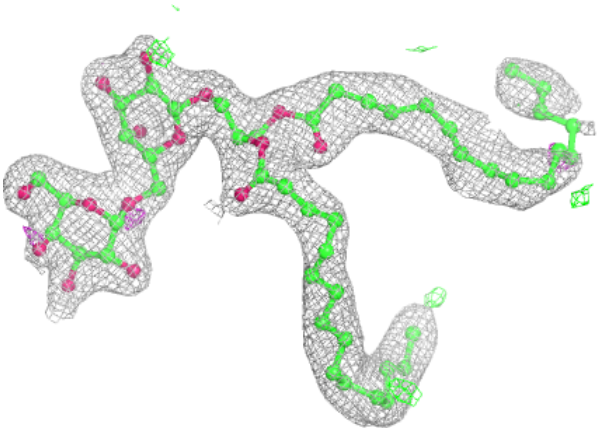


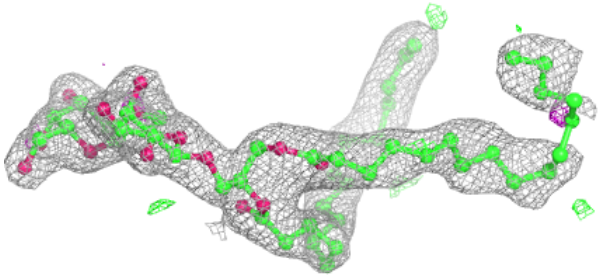


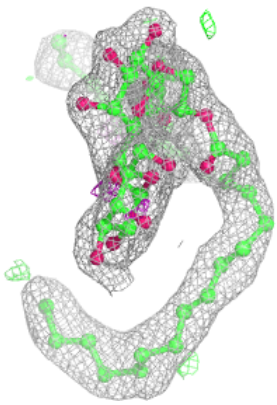


Electron density around DGD c 520:

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

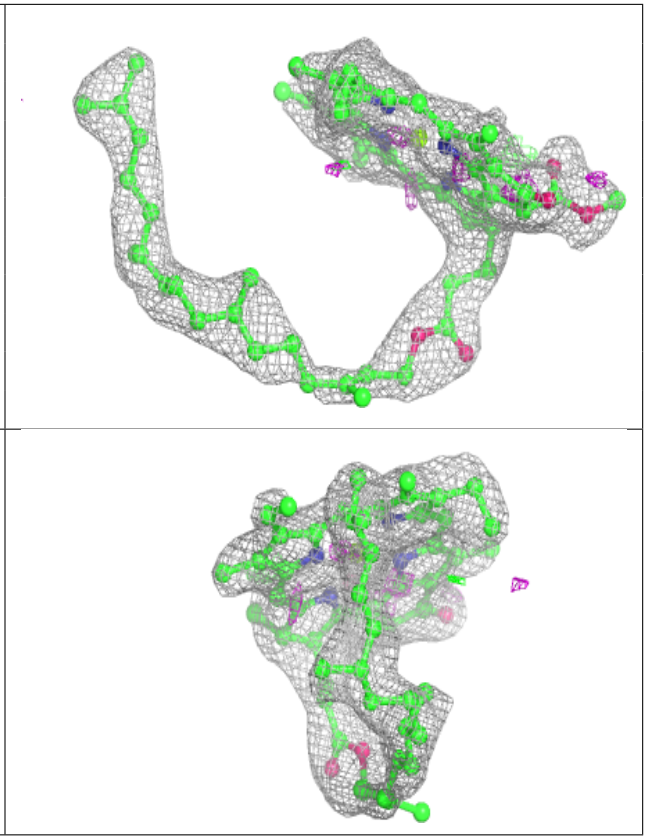






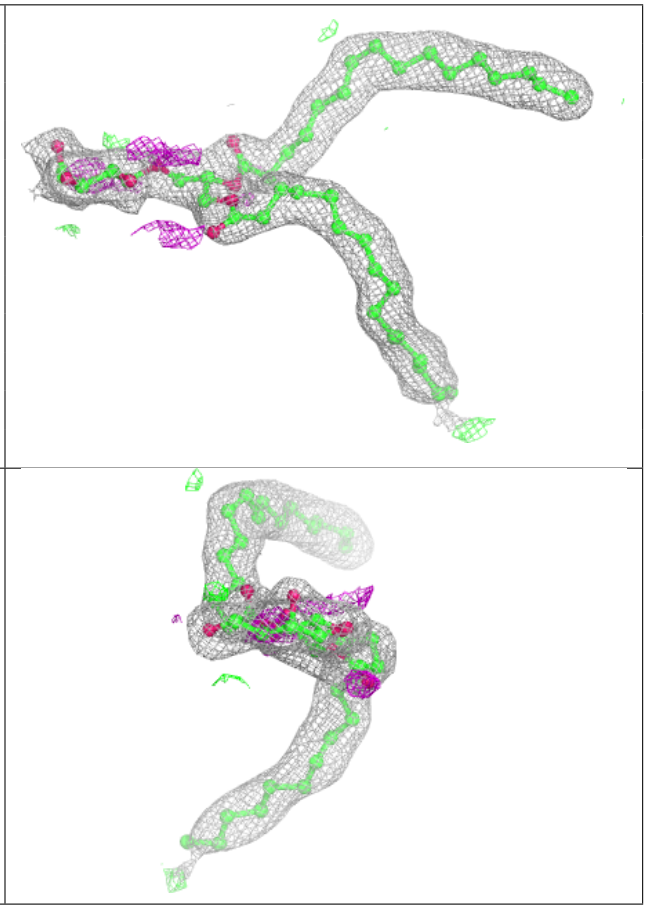
Electron density around CLA C 513:

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



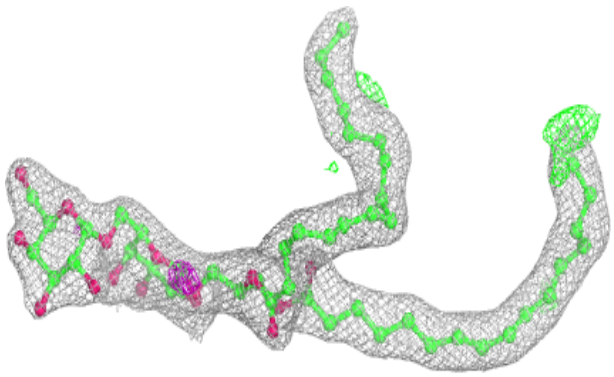
Electron density around LMG B 622:

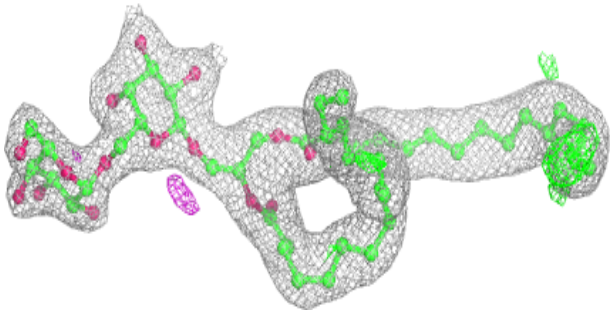
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

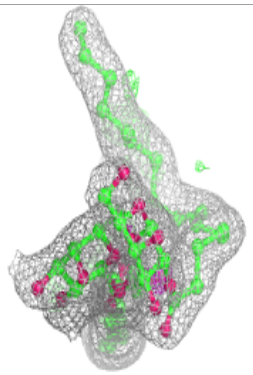


Electron density around DGD H 103:

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

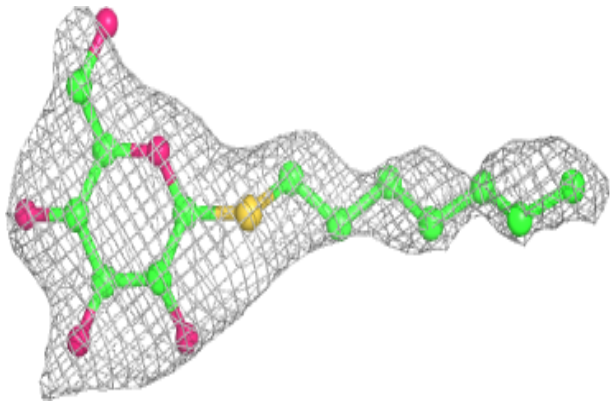


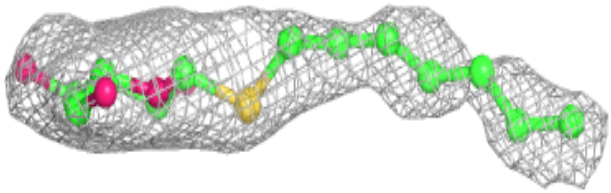


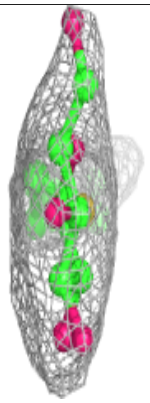


Electron density around HTG c 524:

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

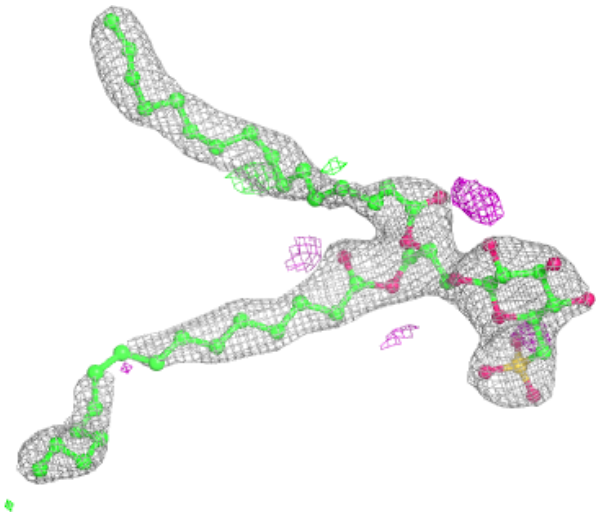


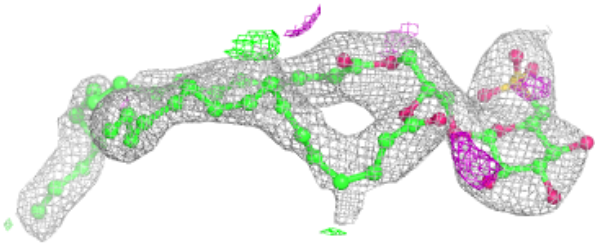


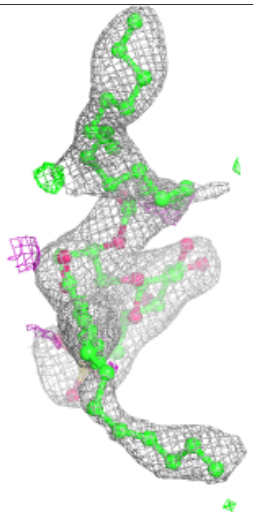


Electron density around SQD A 412:

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

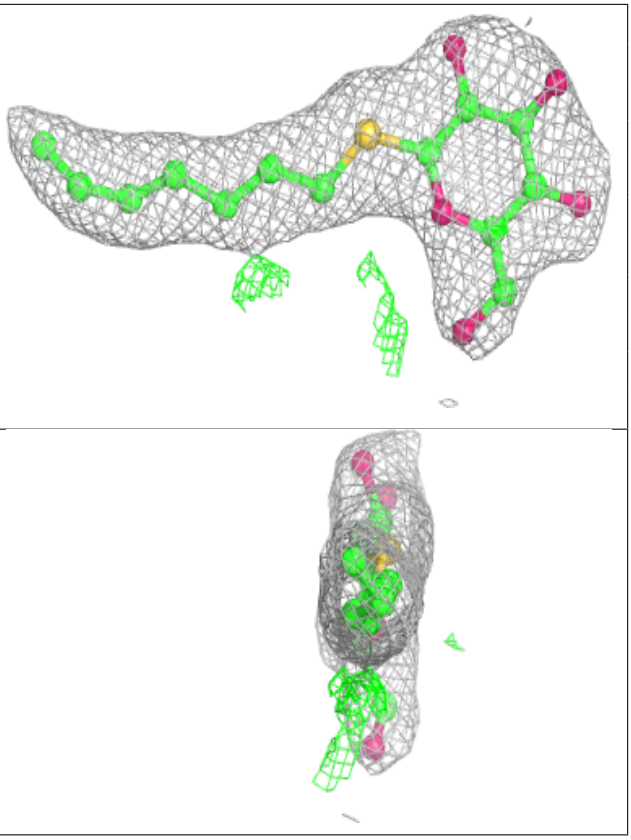


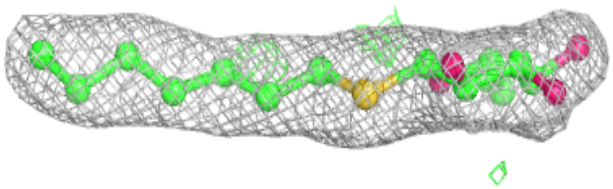




Electron density around HTG b 608:

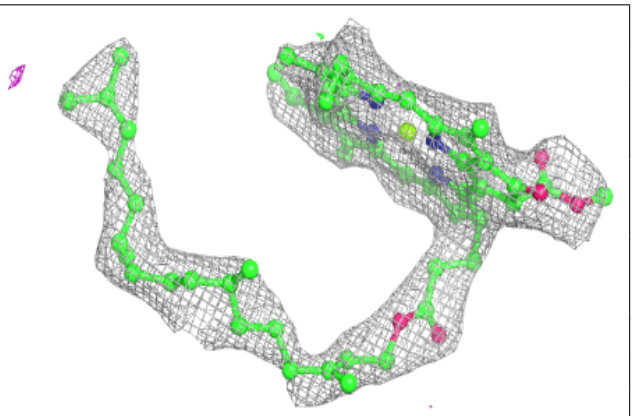
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

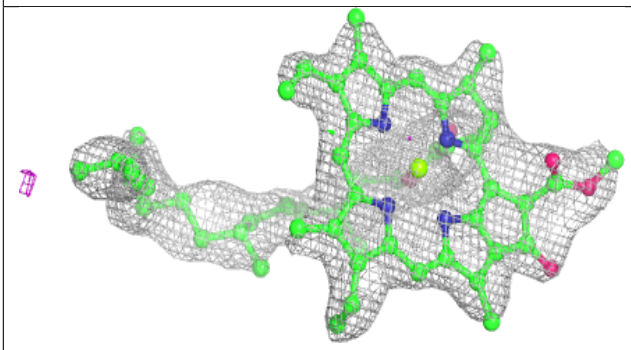


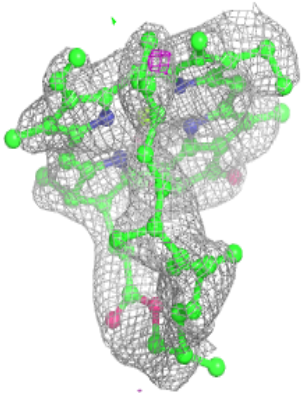


Electron density around CLA c 517:

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

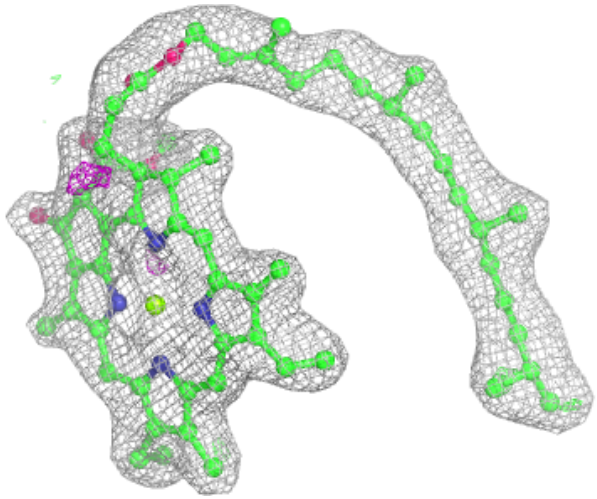


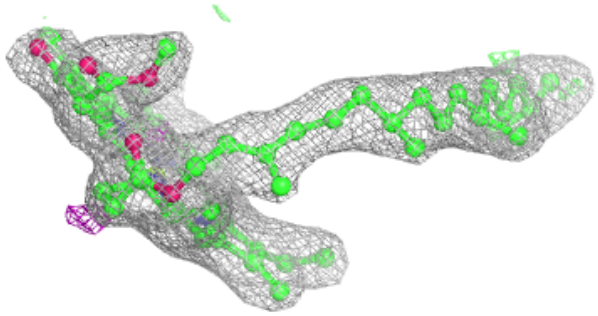


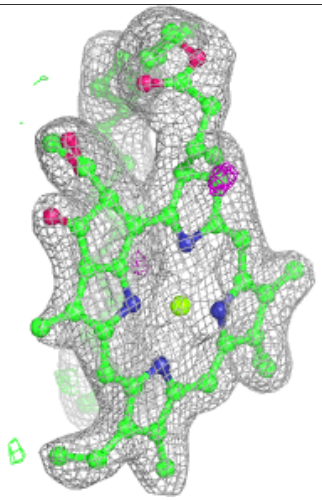


Electron density around CLA c 511:

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

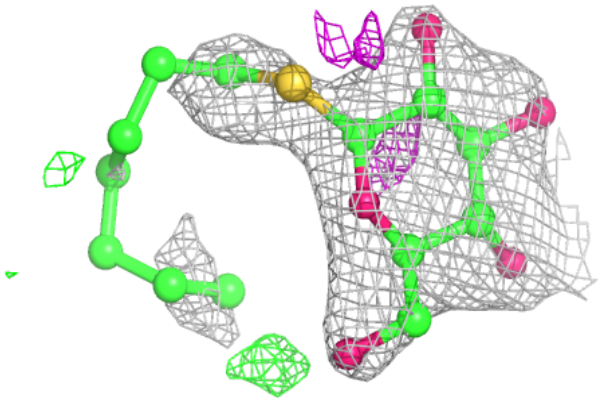


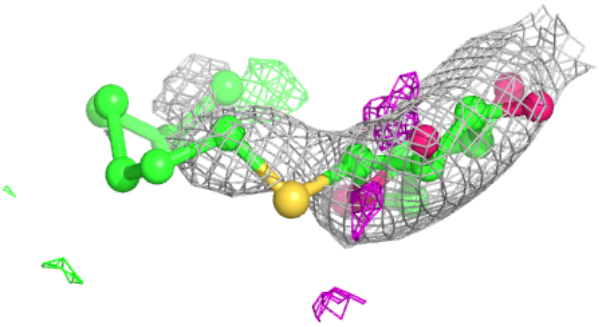


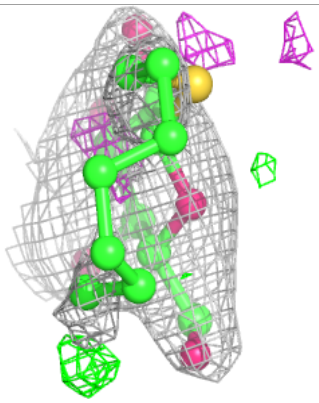


Electron density around HTG V 207:

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

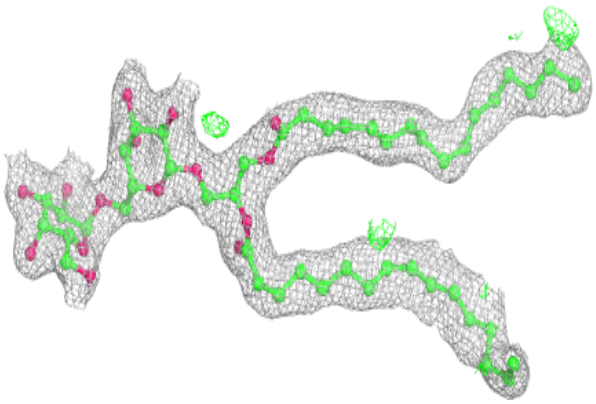


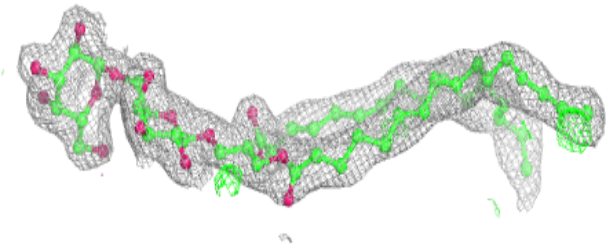


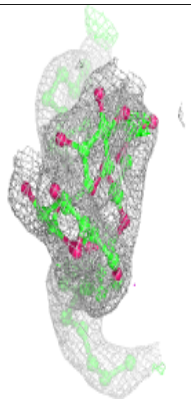


Electron density around DGD c 521:

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

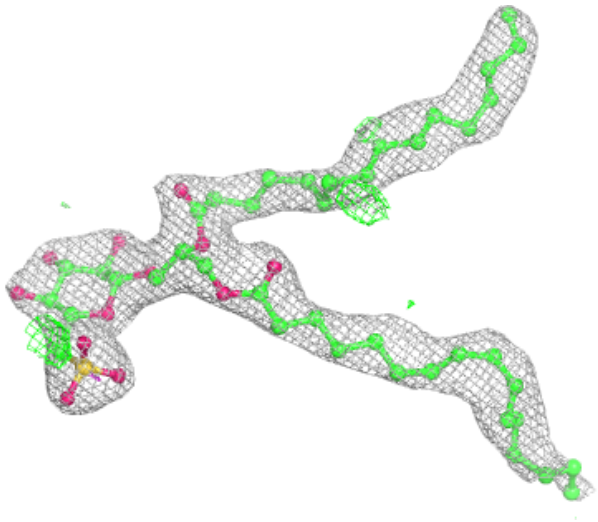


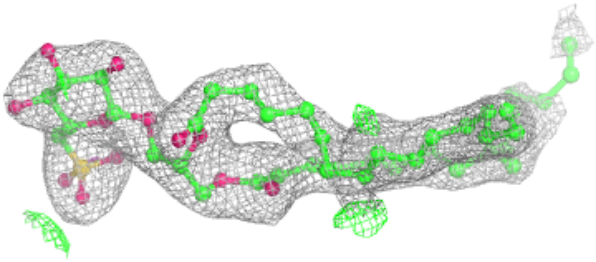


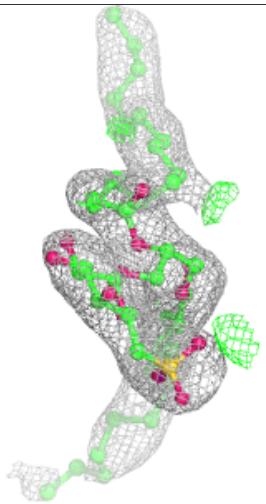


Electron density around SQD a 414:

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

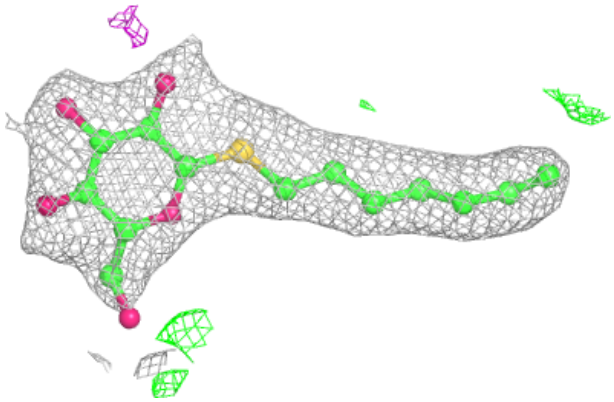


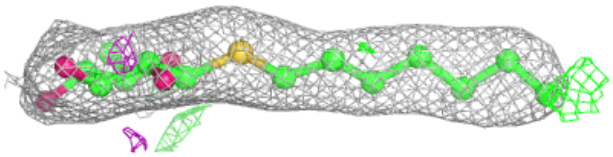


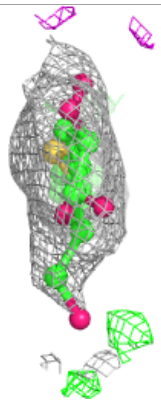


Electron density around HTG B 632:

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

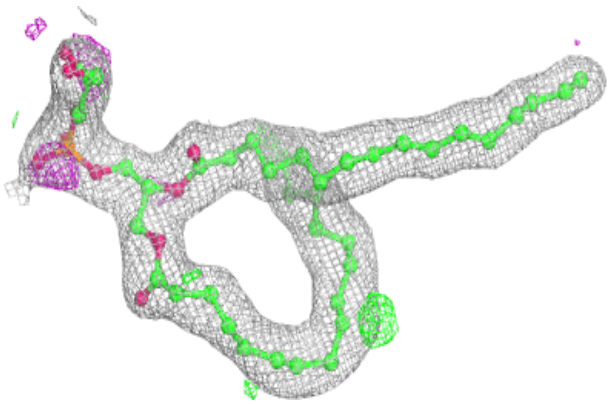


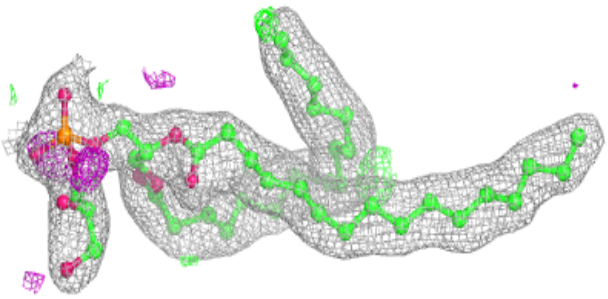




Electron density around LHG D 407:

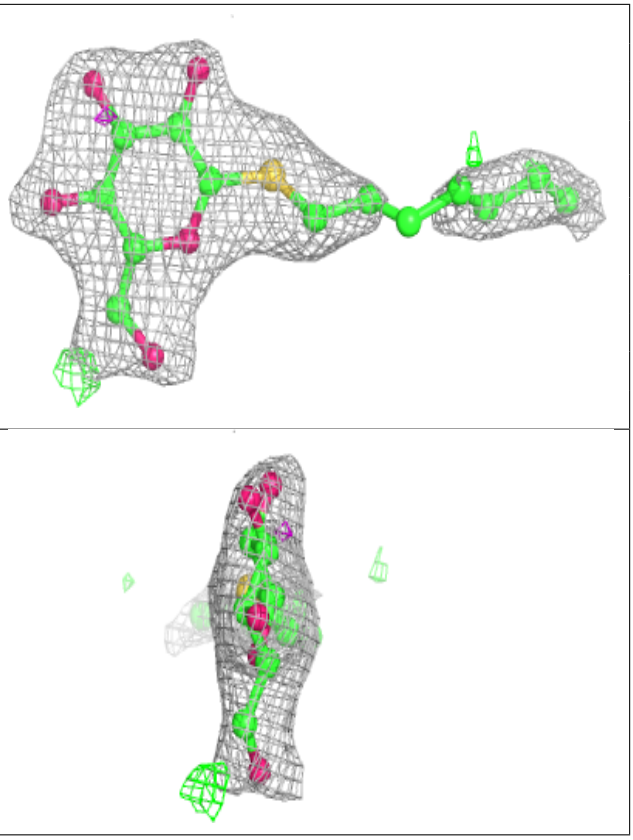
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





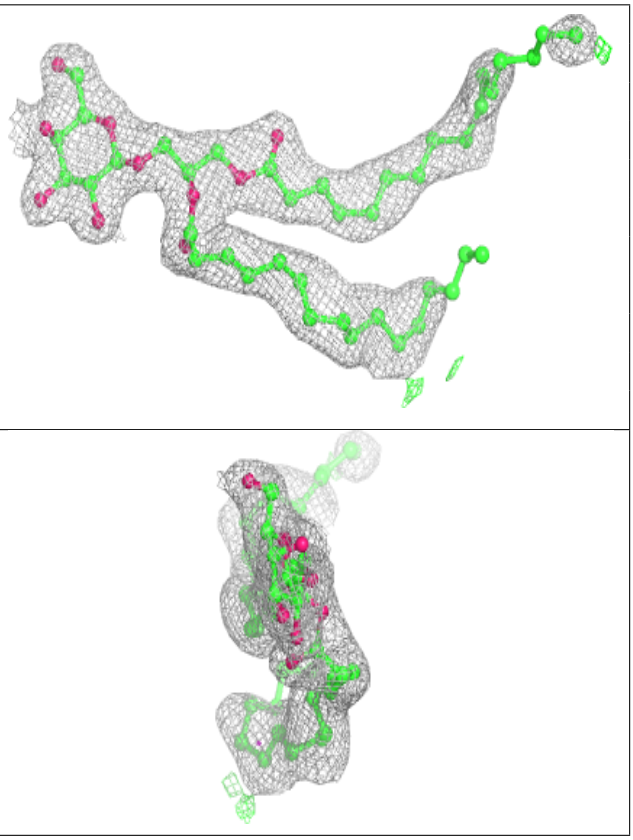
Electron density around HTG C 522:

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



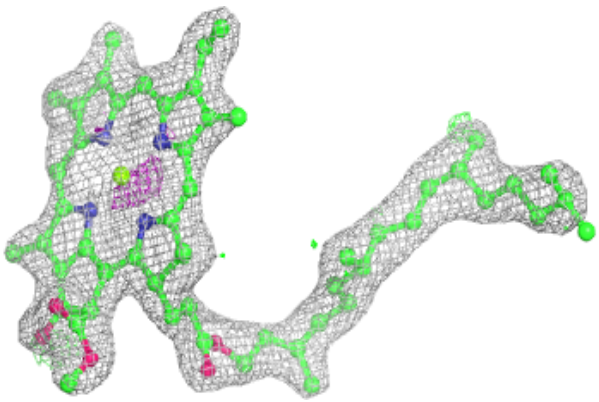
Electron density around LMG j 101:

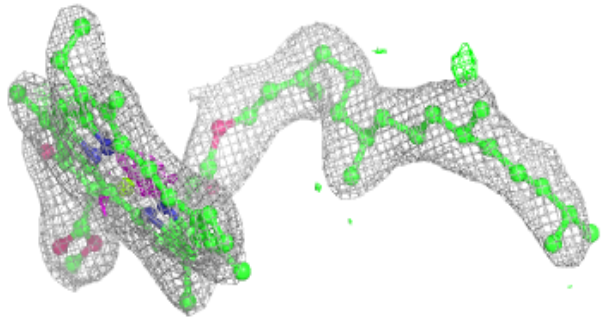
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

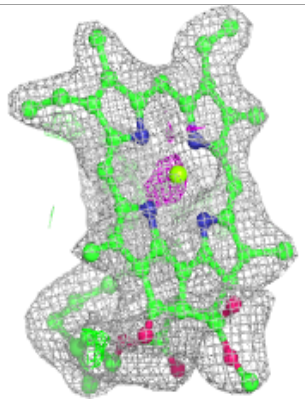


Electron density around CLA c 515:

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

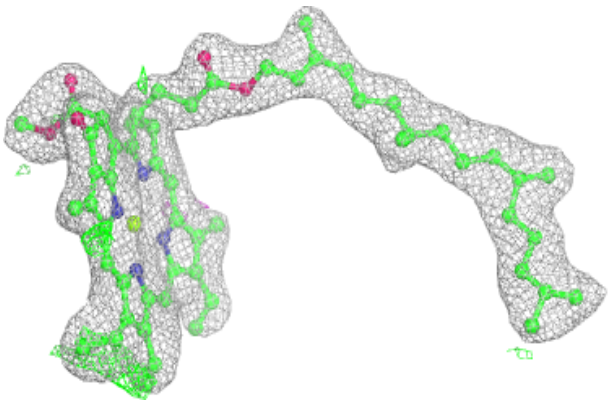


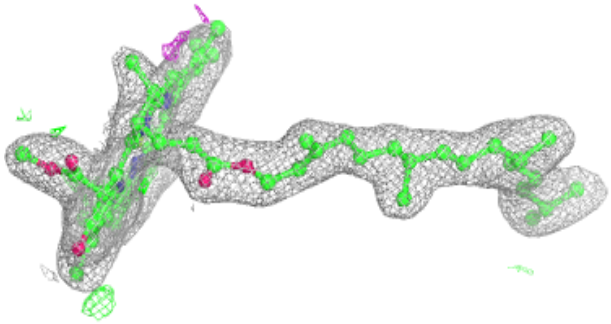


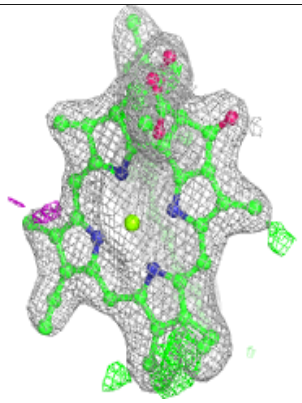


Electron density around CLA b 619:

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

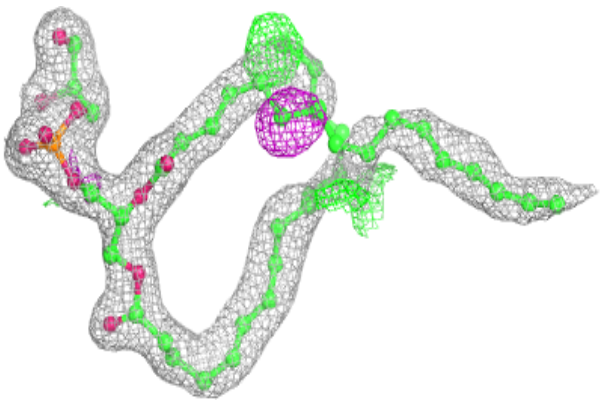


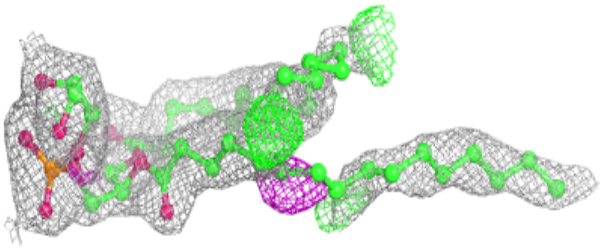


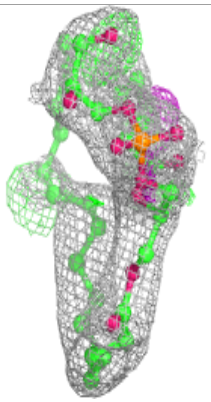


Electron density around LHG D 409:

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

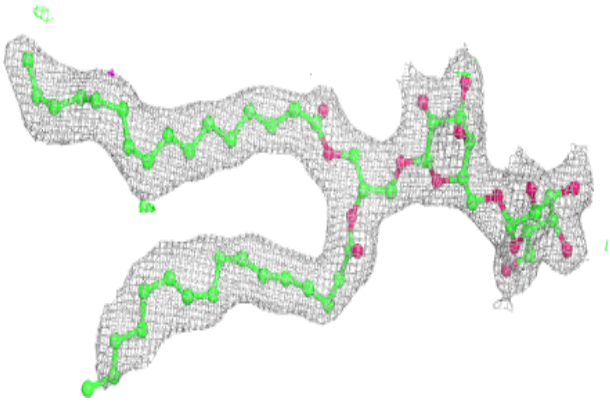


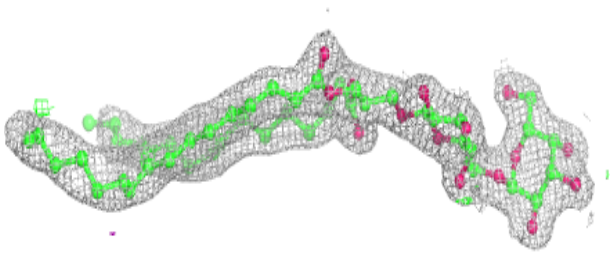


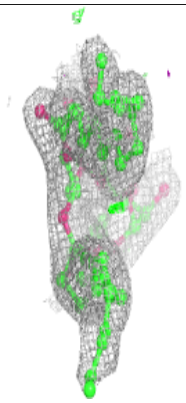


Electron density around DGD C 518:

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

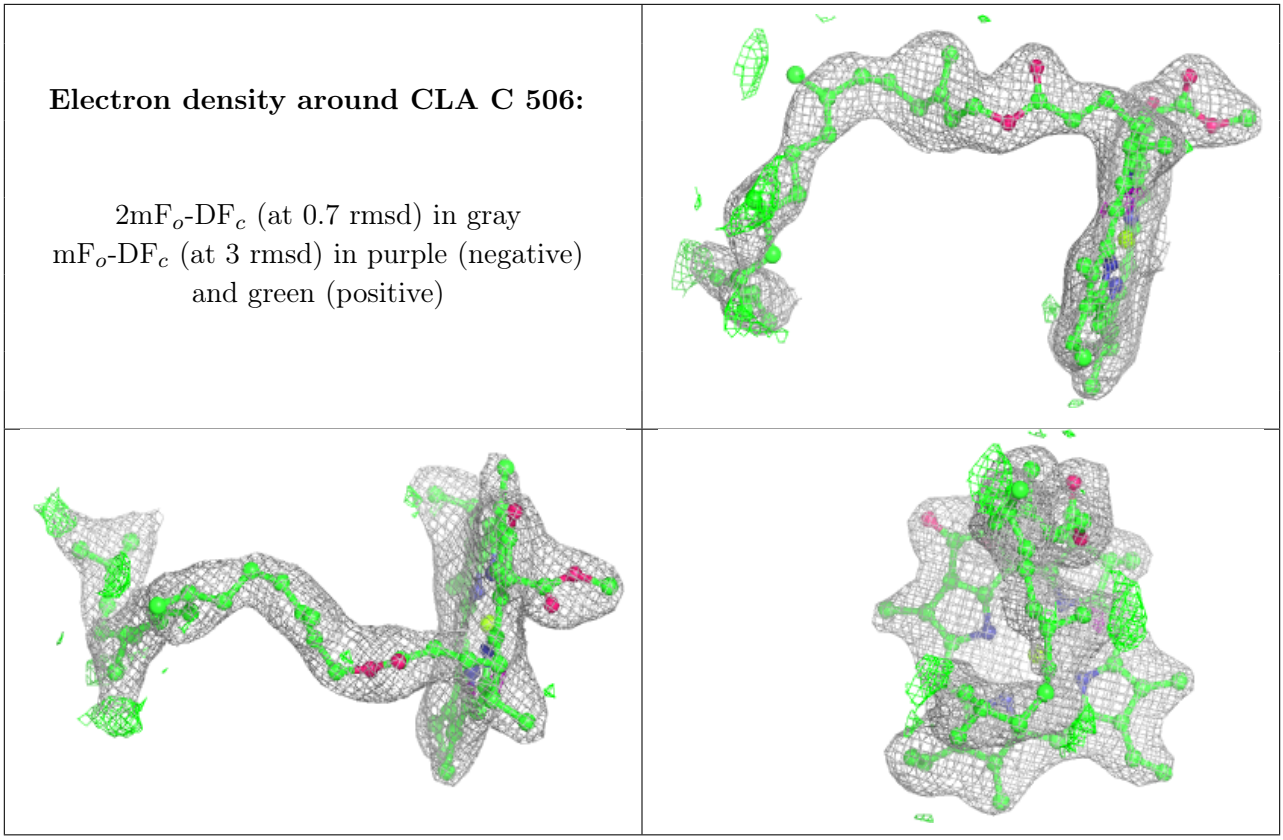






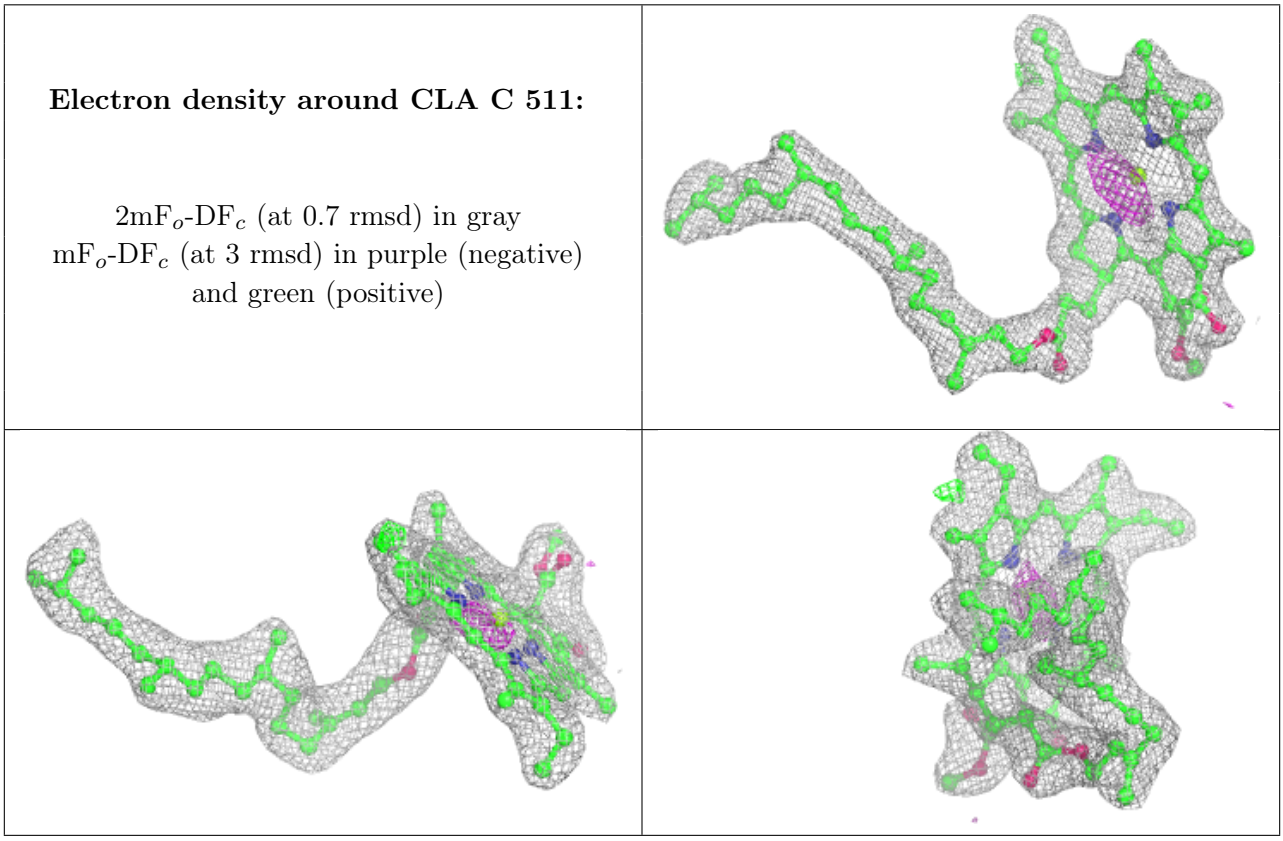
Electron density around CLA C 506:

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



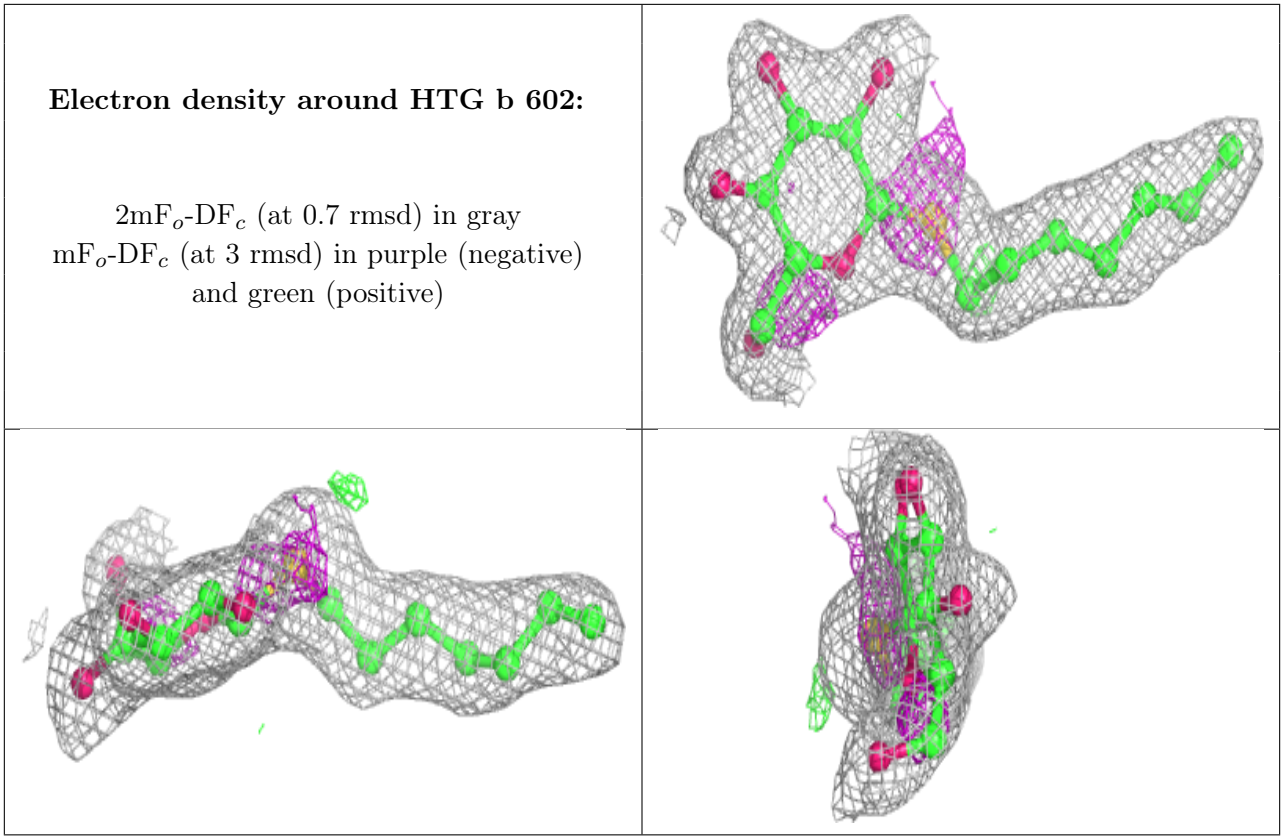
Electron density around CLA C 511:

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



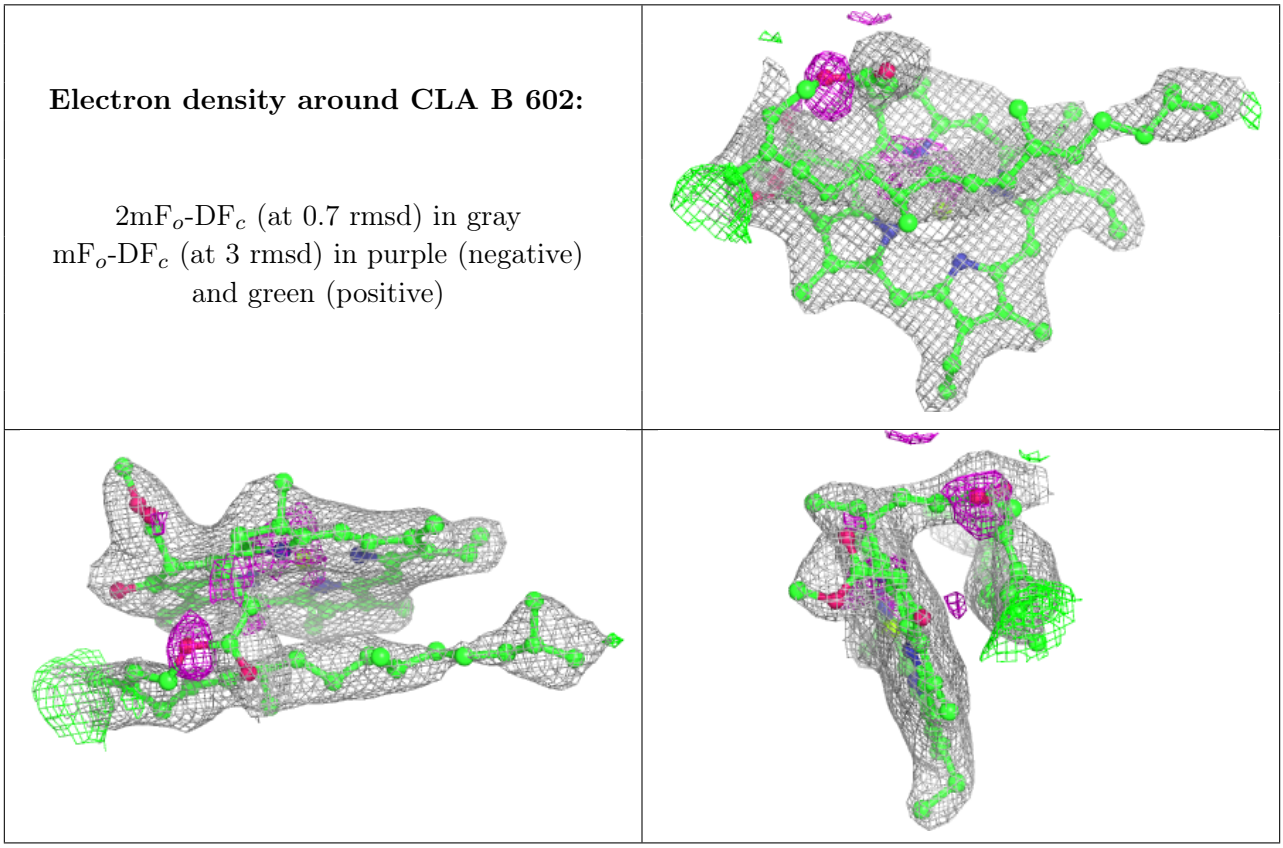
Electron density around HTG b 602:

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



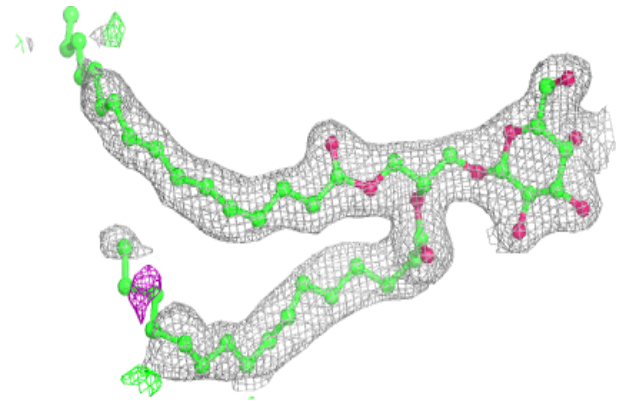
Electron density around CLA B 602:

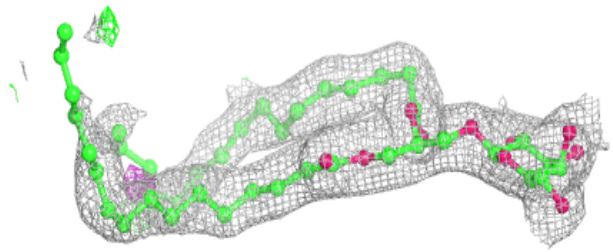
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

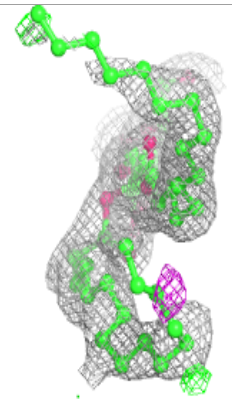


Electron density around LMG D 412:

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

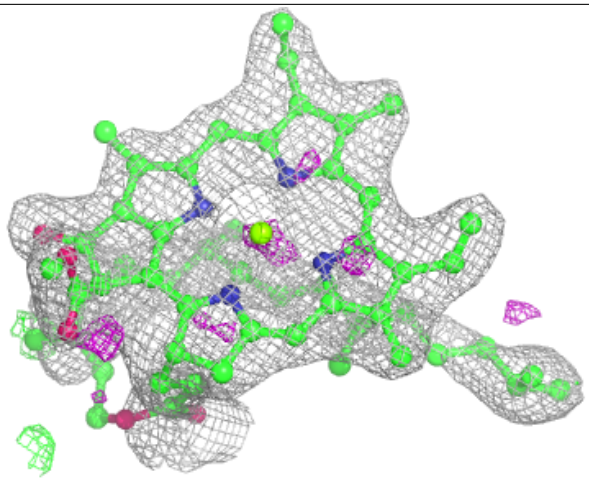


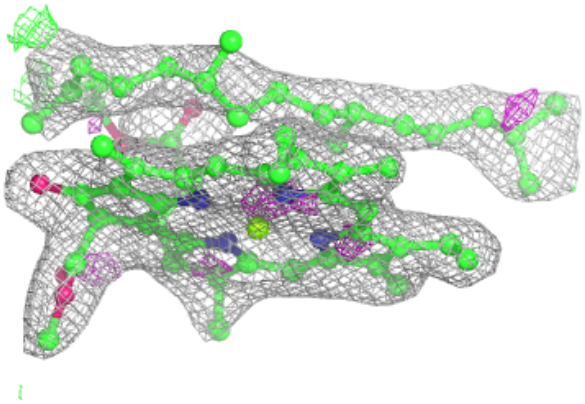


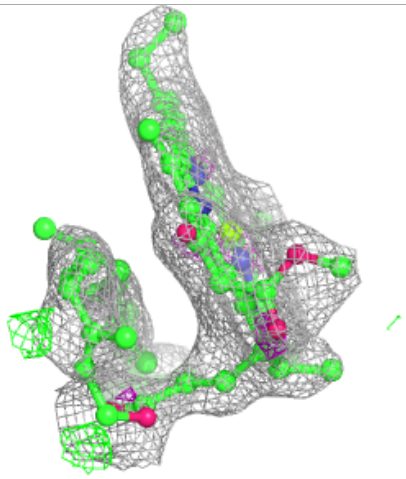


Electron density around CLA b 611:

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

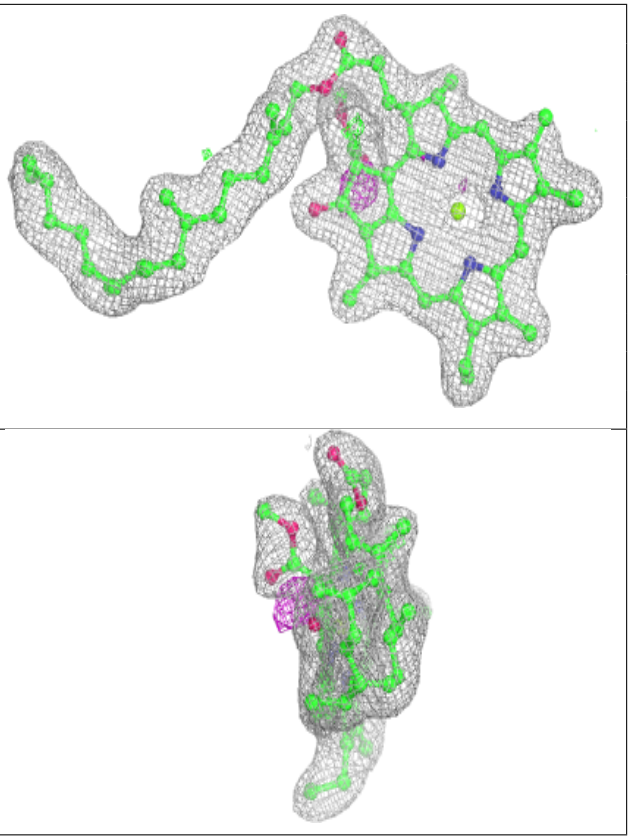






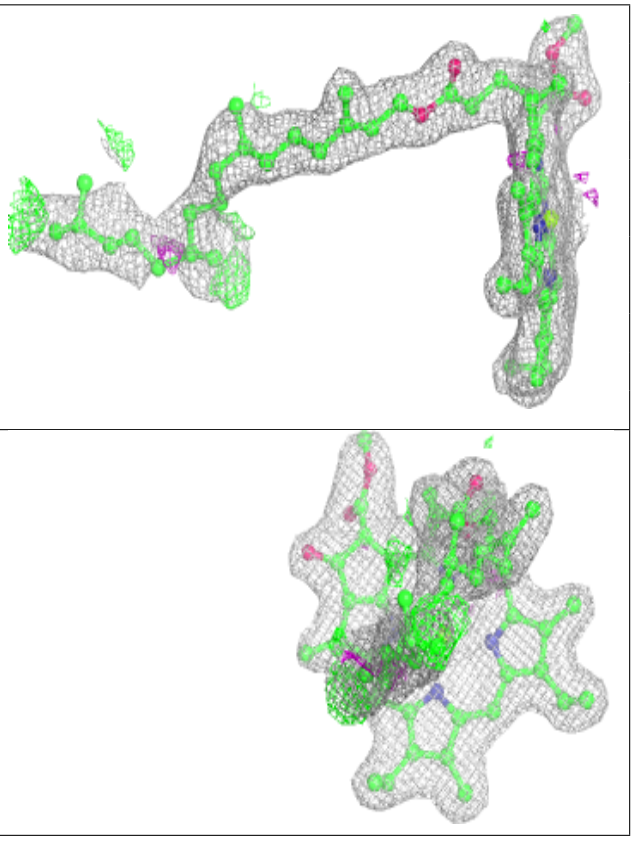
Electron density around CLA b 612:

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



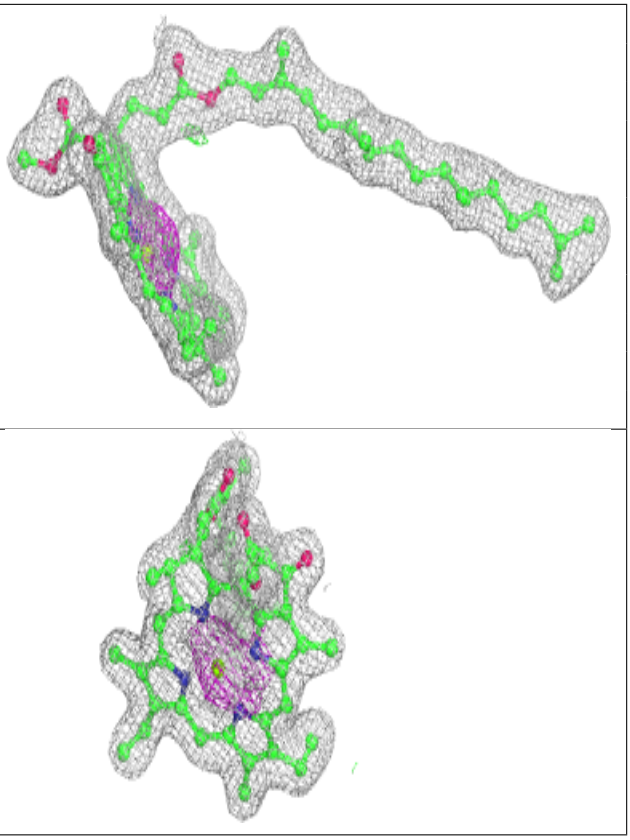
Electron density around CLA b 616:

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



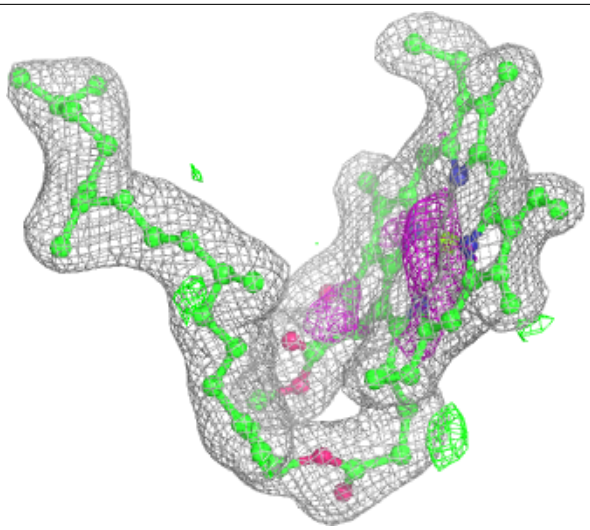
Electron density around CLA b 617:

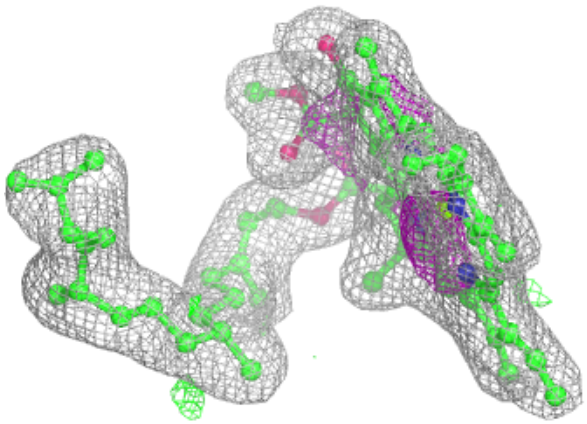
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

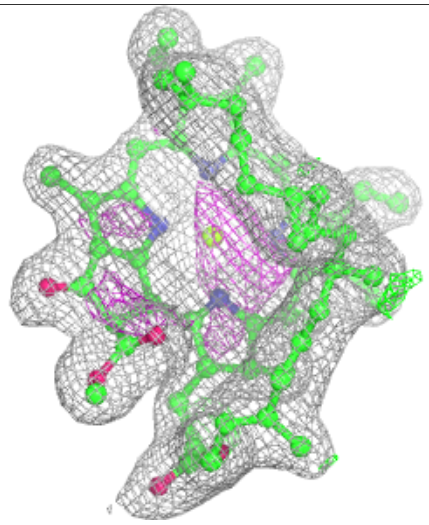


Electron density around CLA B 614:

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

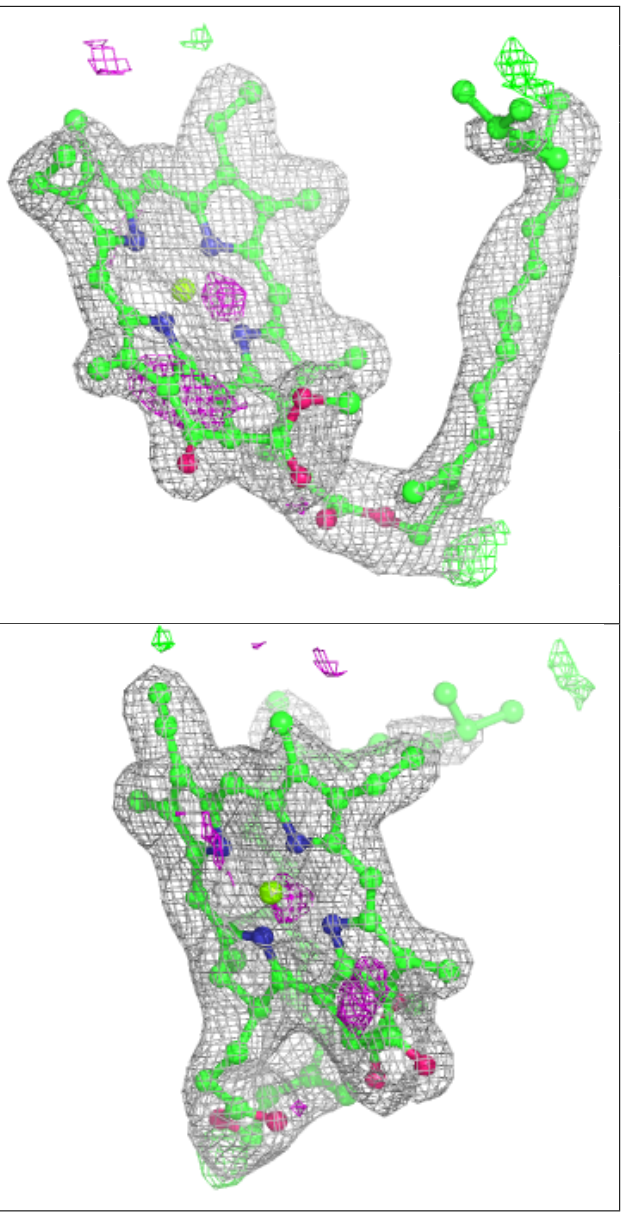






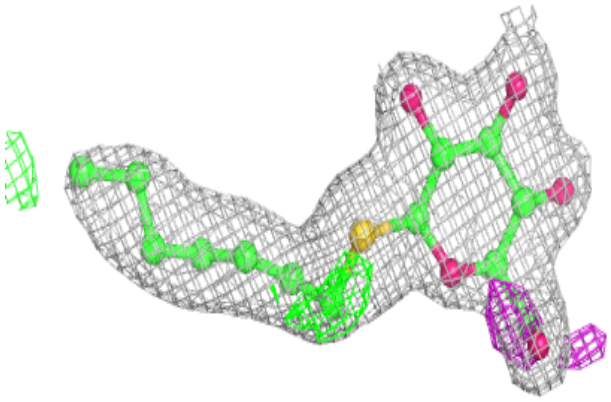
Electron density around CLA b 626:

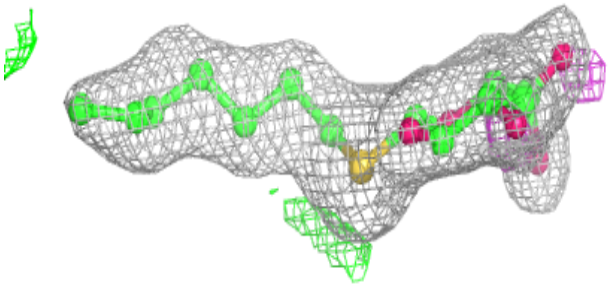
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

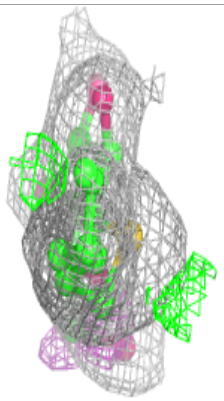


Electron density around HTG B 623:

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

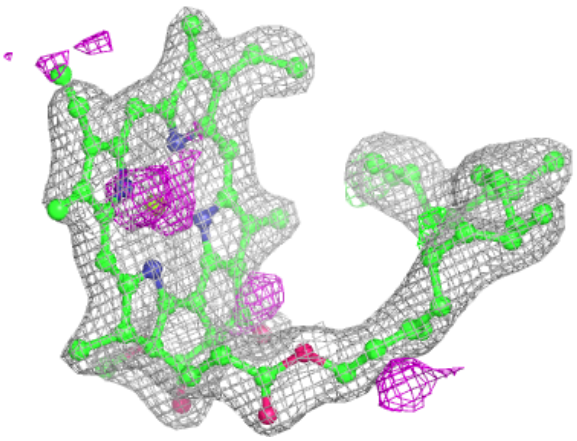


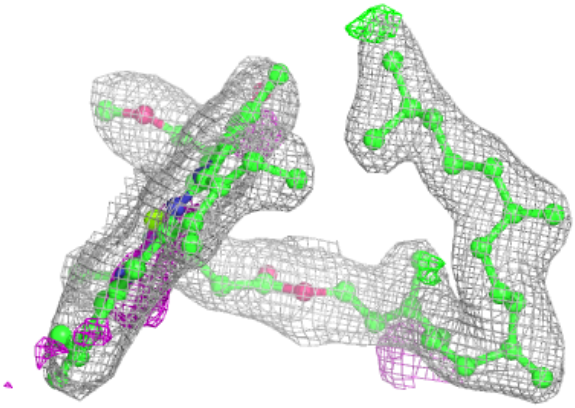


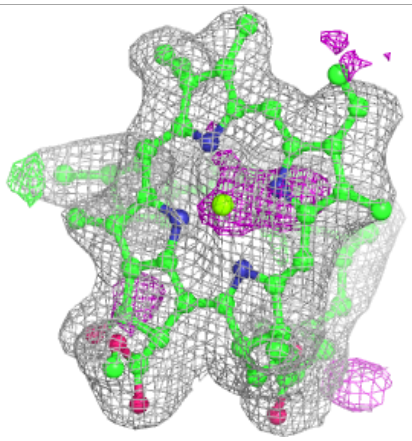


Electron density around CLA c 507:

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

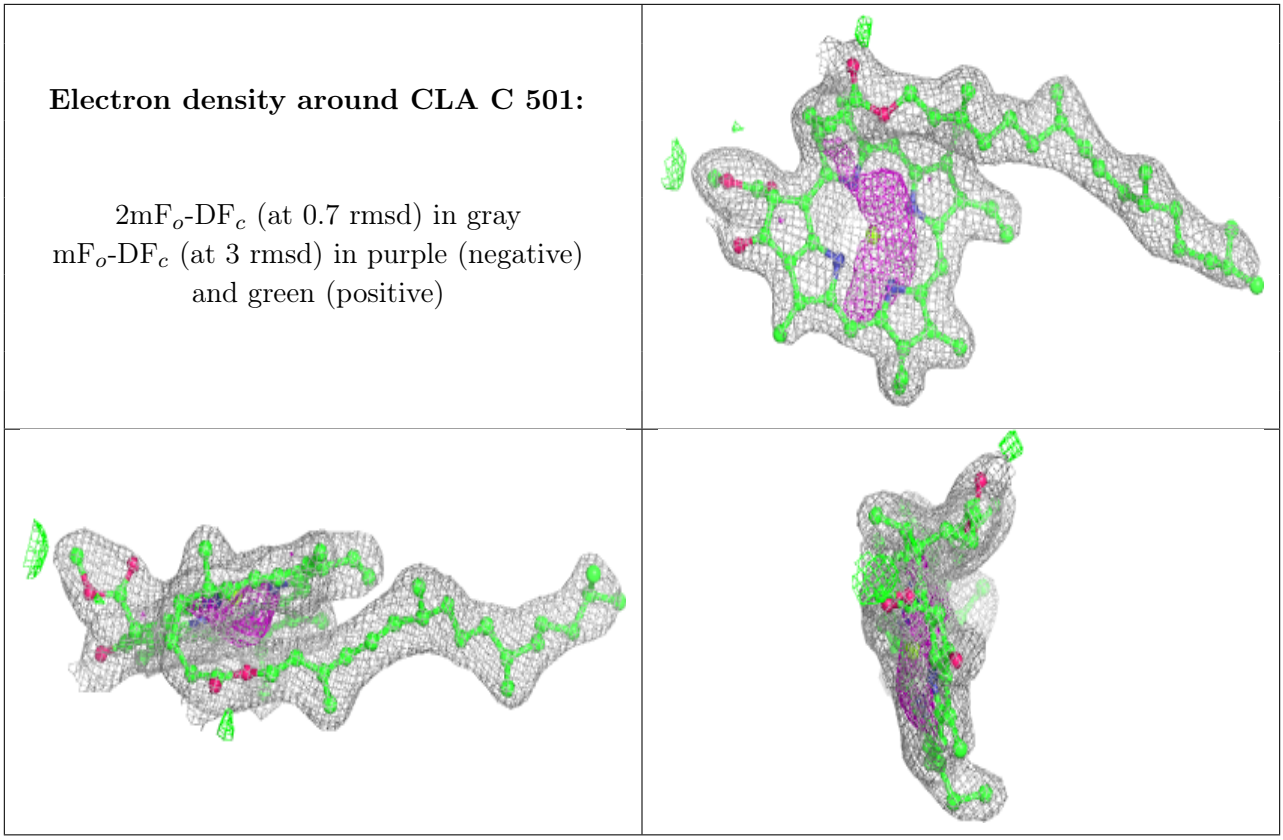






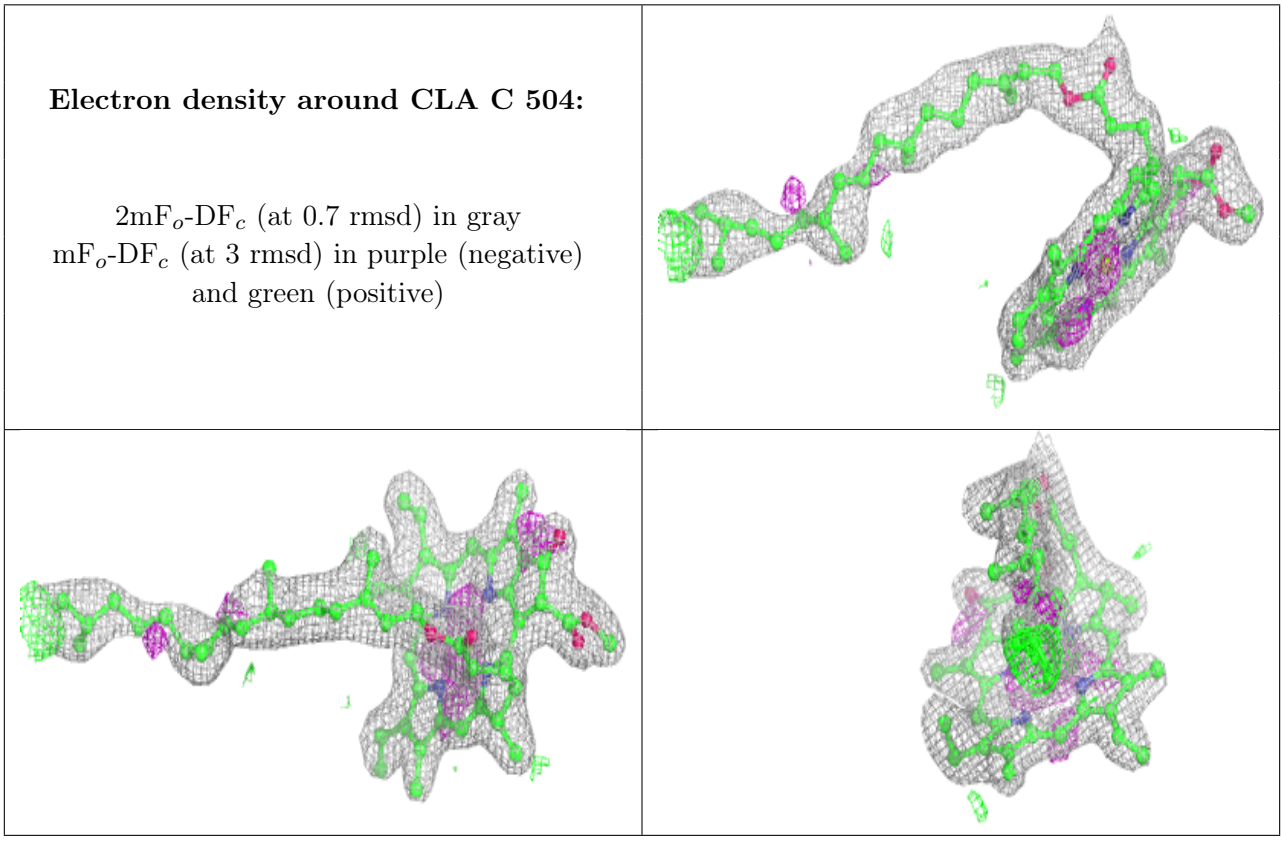
Electron density around CLA C 501:

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



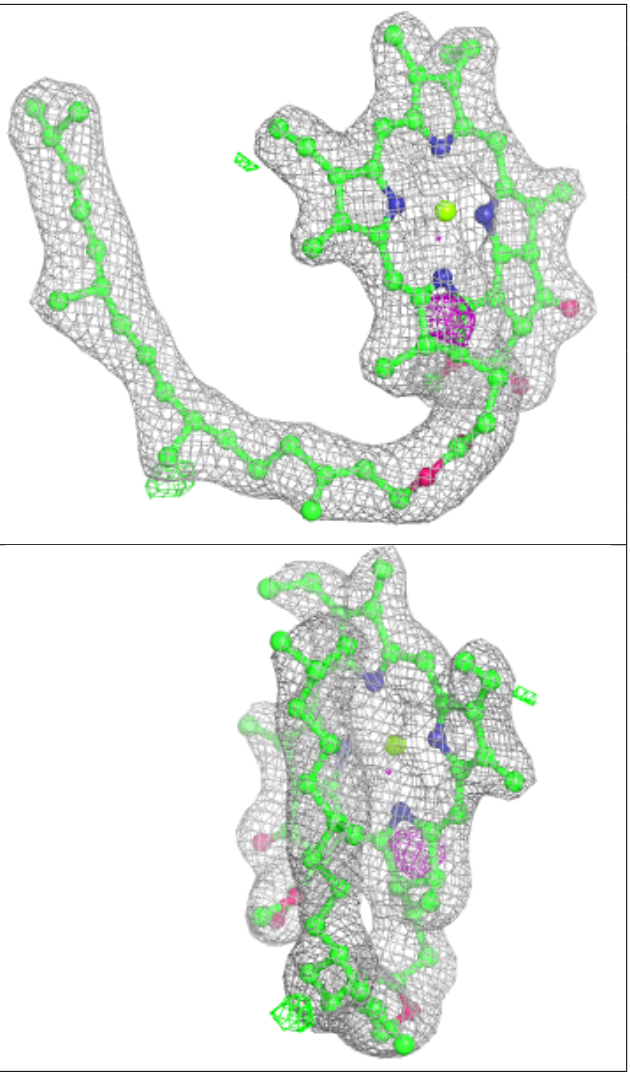
Electron density around CLA C 504:

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



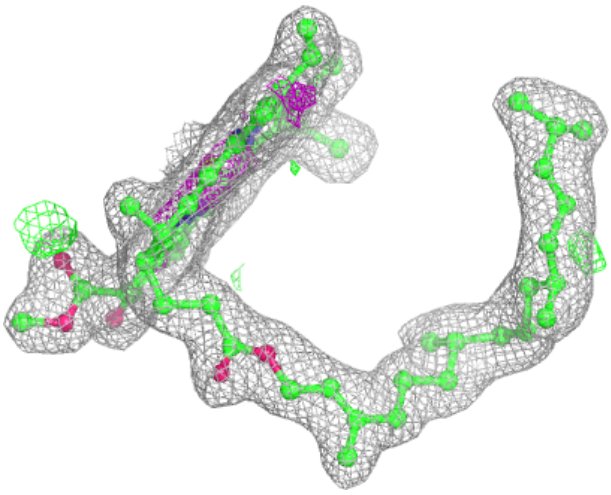
Electron density around CLA C 507:

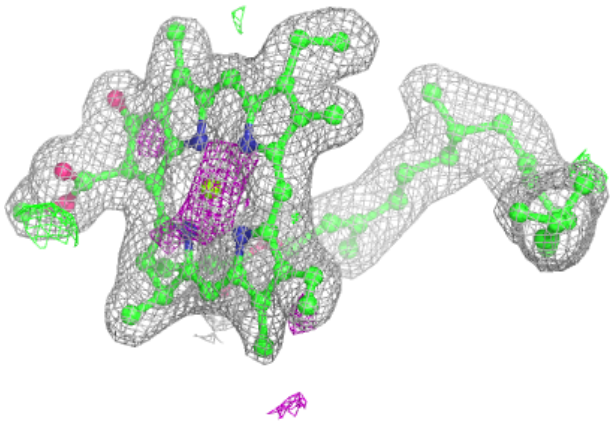
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

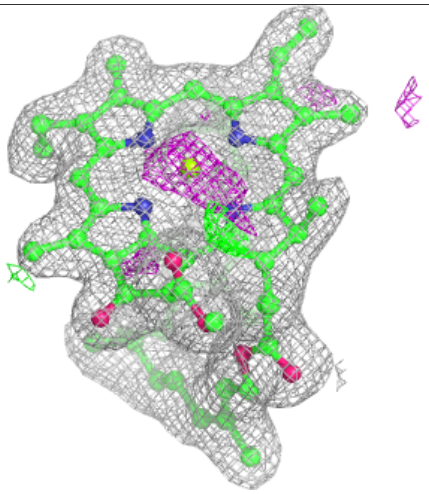


Electron density around CLA b 621:

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

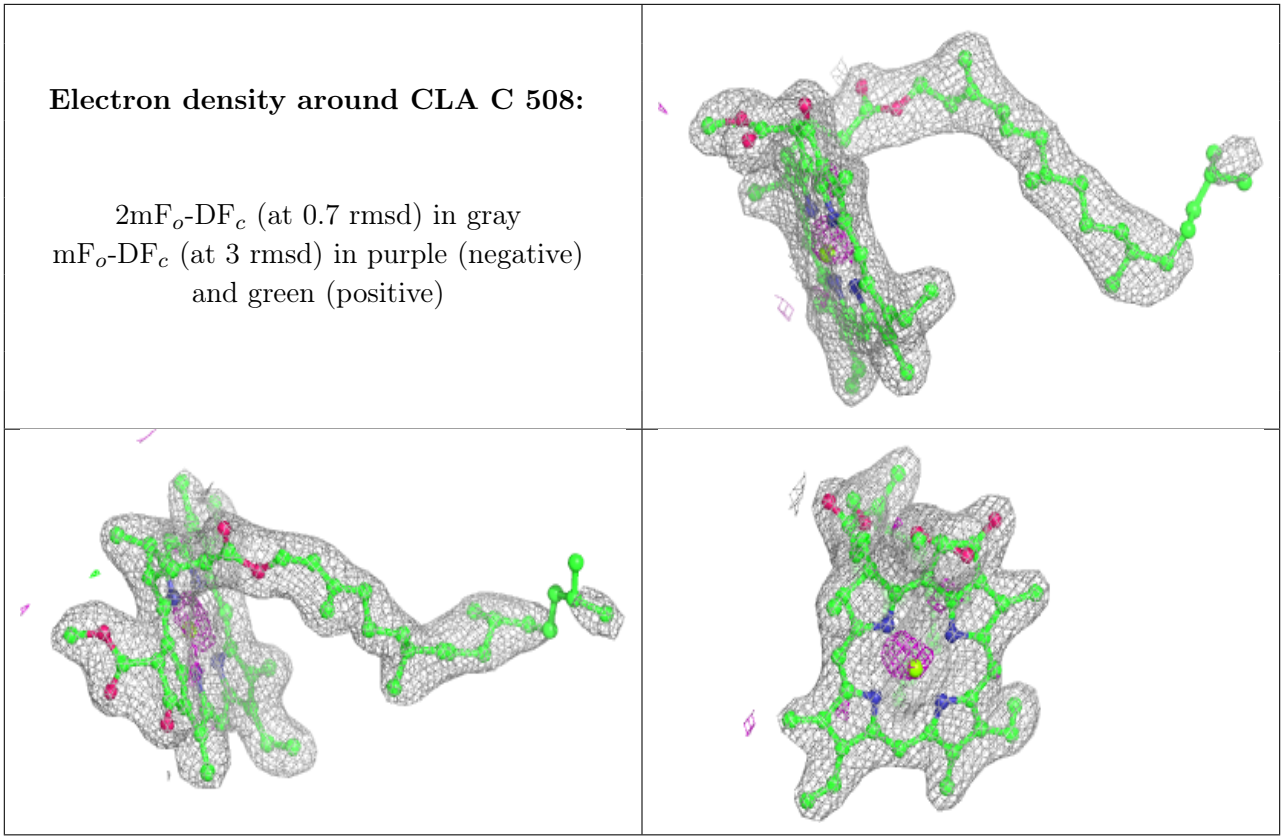






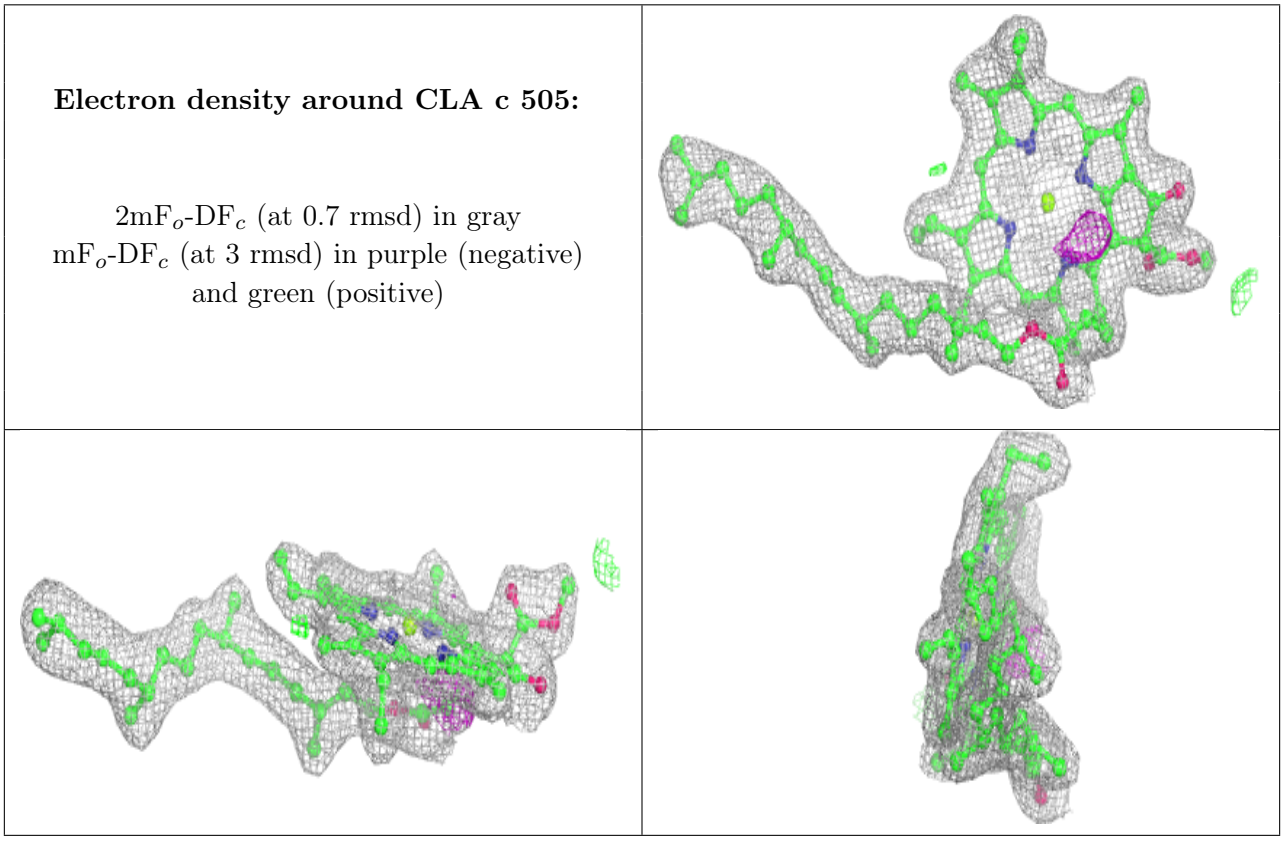
Electron density around CLA C 508:

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



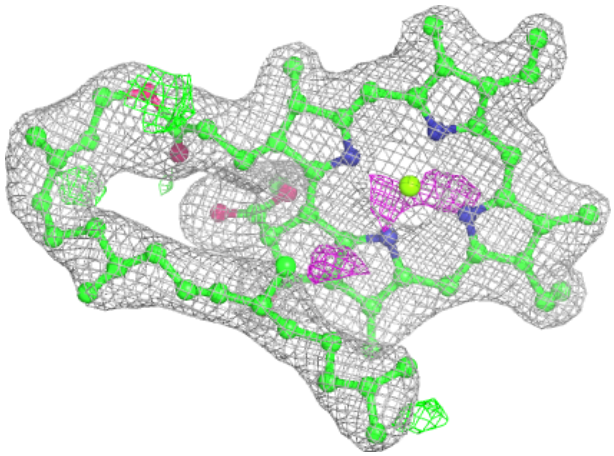
Electron density around CLA c 505:

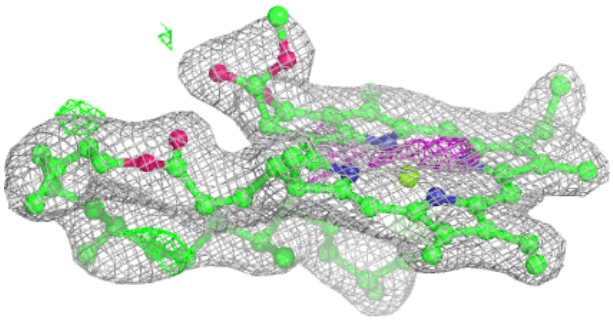
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

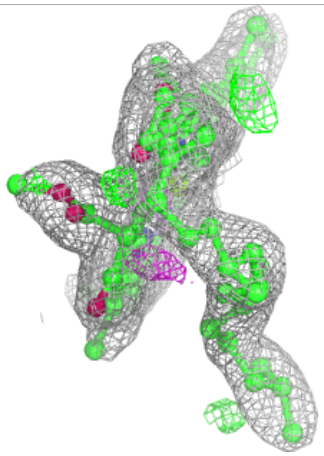


Electron density around CLA C 509:

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

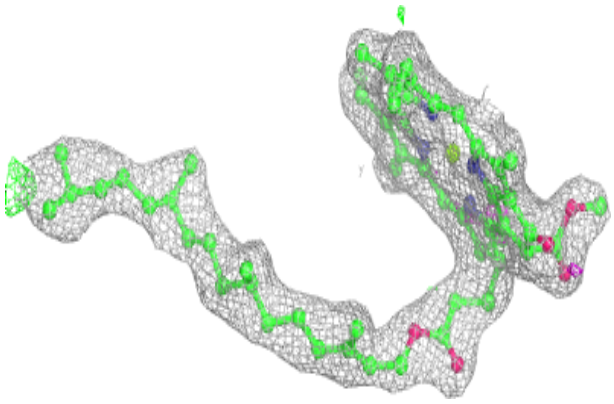


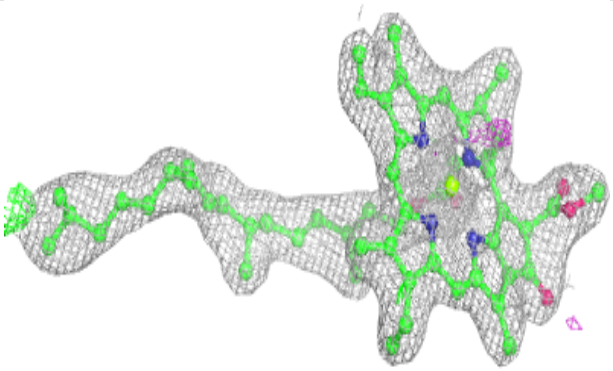


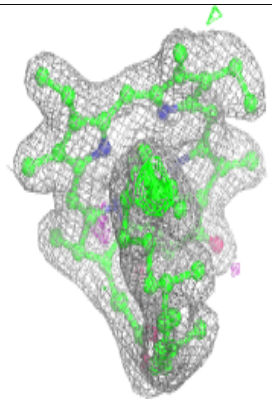


Electron density around CLA c 508:

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

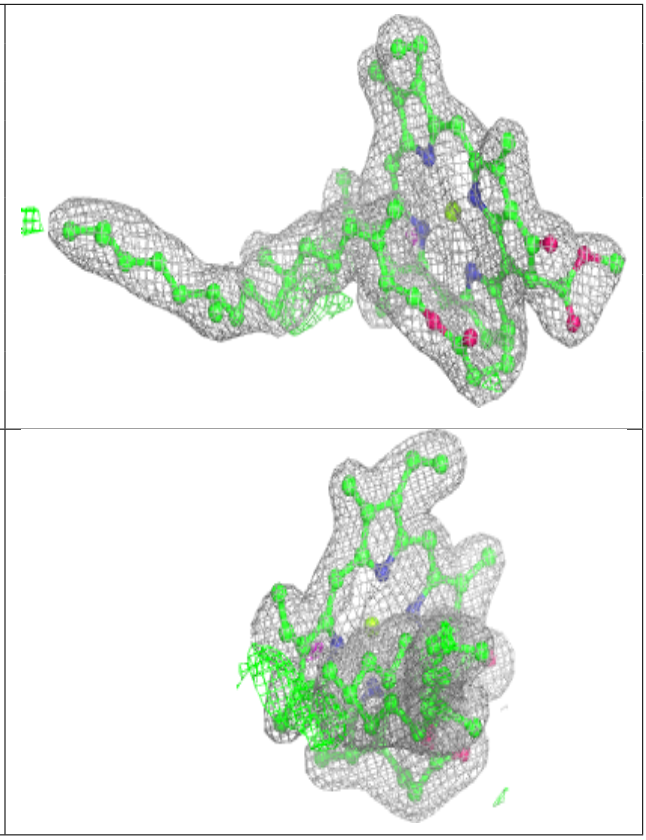






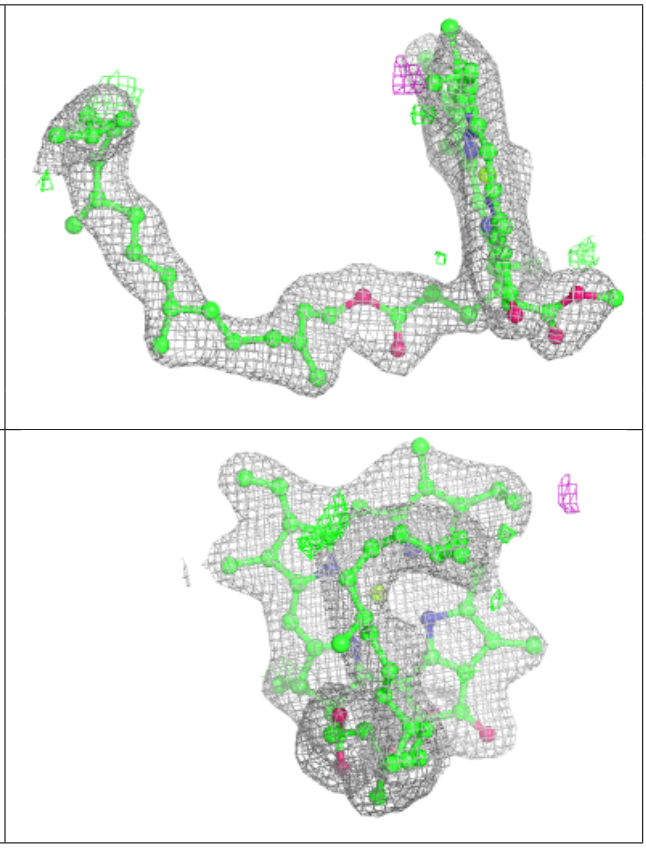
Electron density around CLA c 509:

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



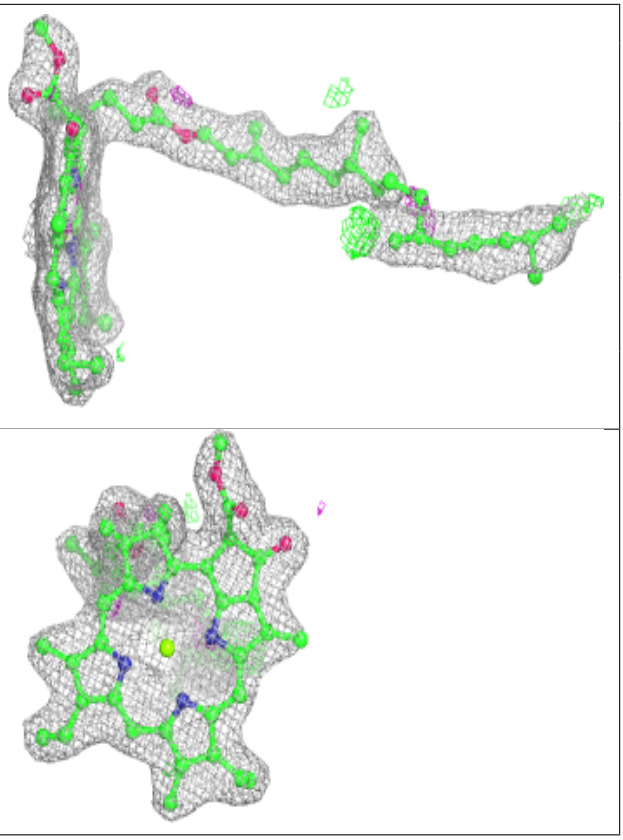
Electron density around CLA c 510:

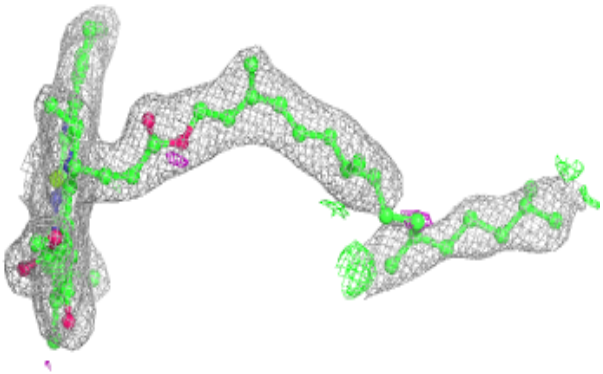
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 607:

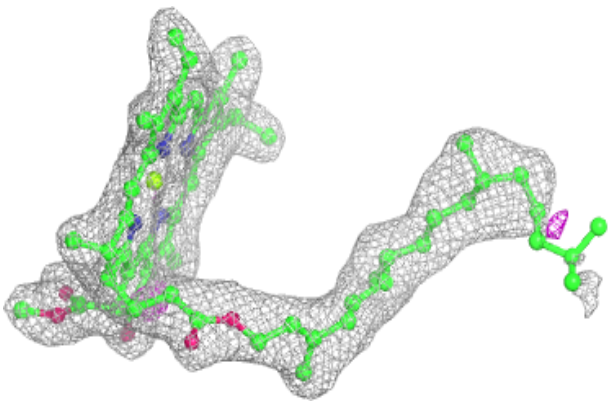
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

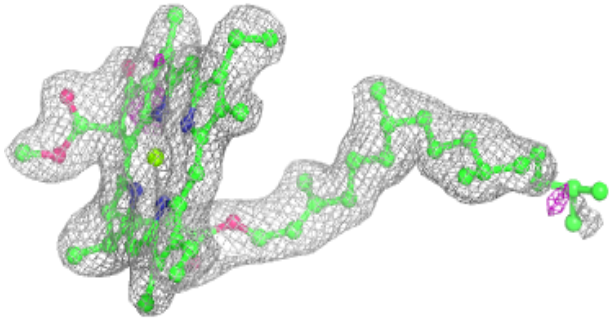


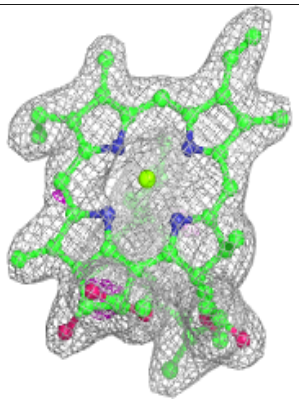


Electron density around CLA c 512:

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

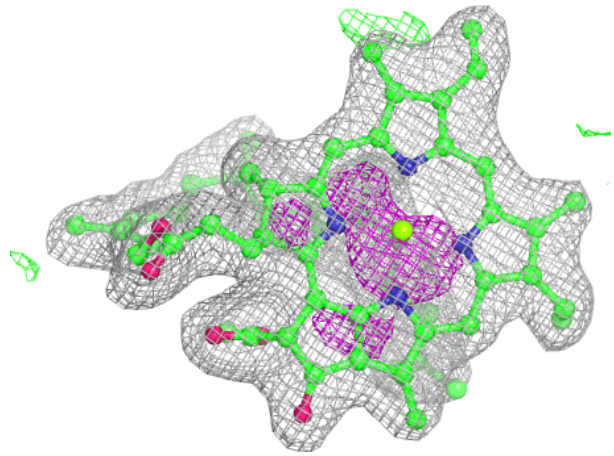


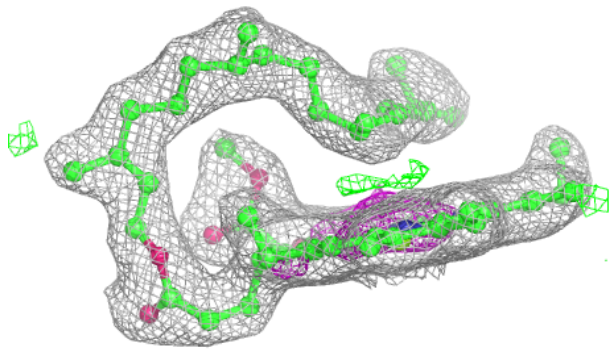


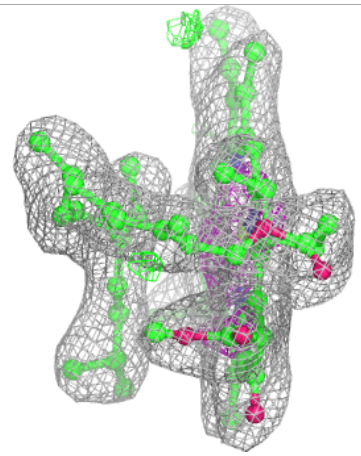


Electron density around CLA c 514:

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

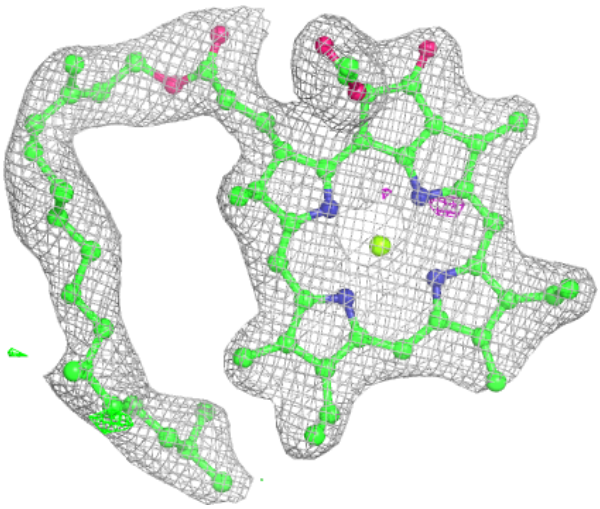


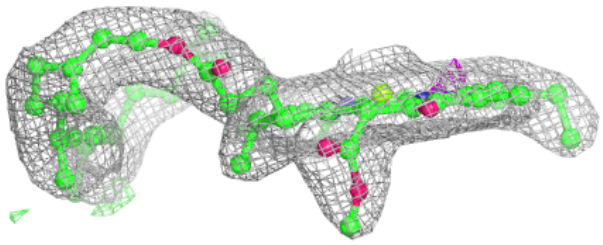


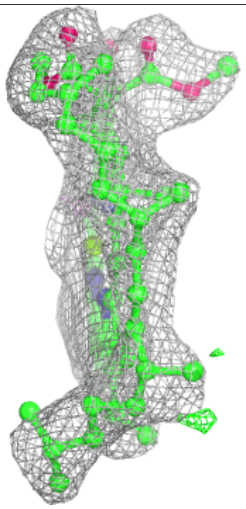


Electron density around CLA C 512:

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

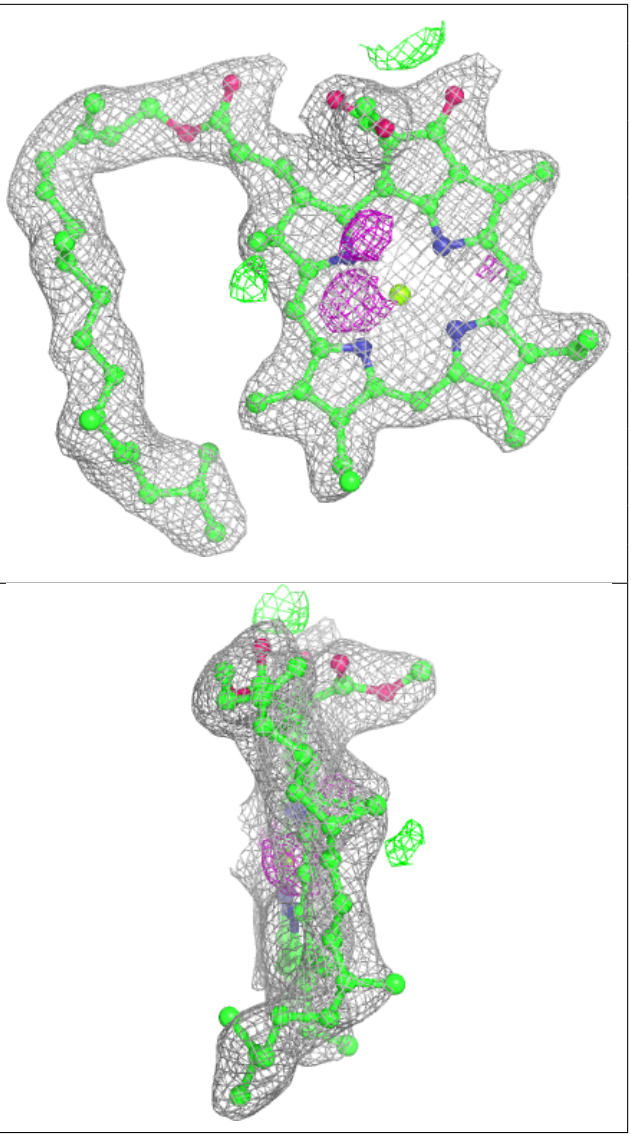






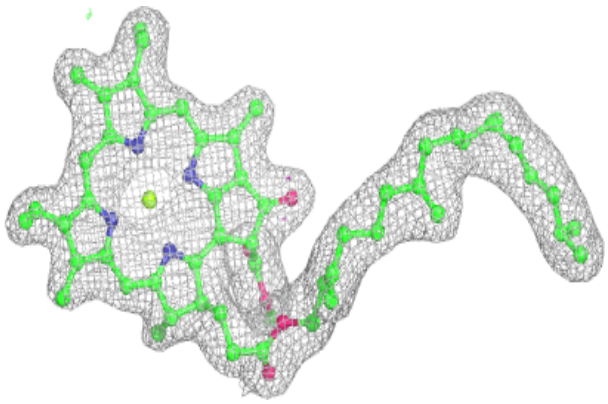
Electron density around CLA c 516:

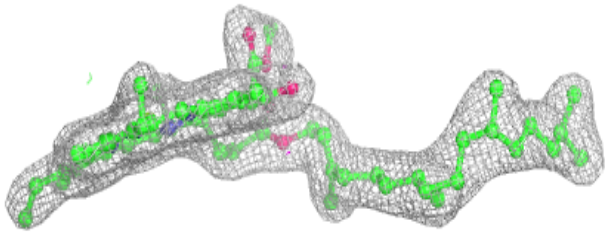
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

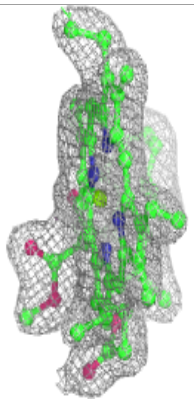


Electron density around CLA B 603:

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

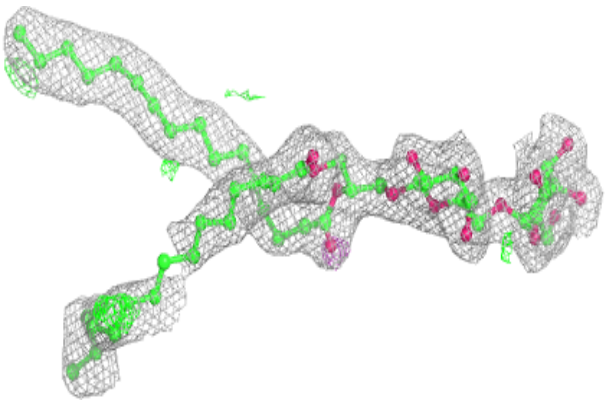


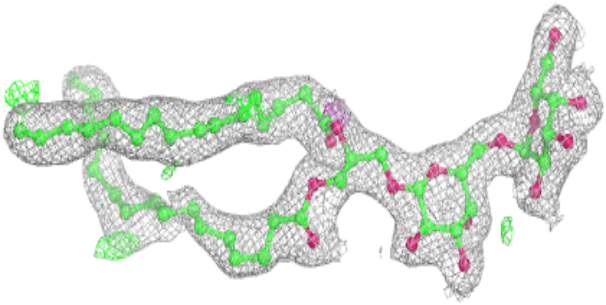


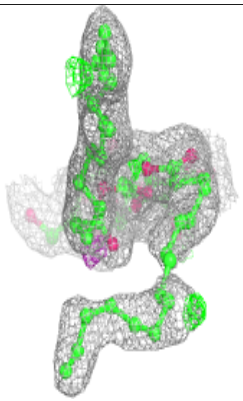


Electron density around DGD c 519:

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

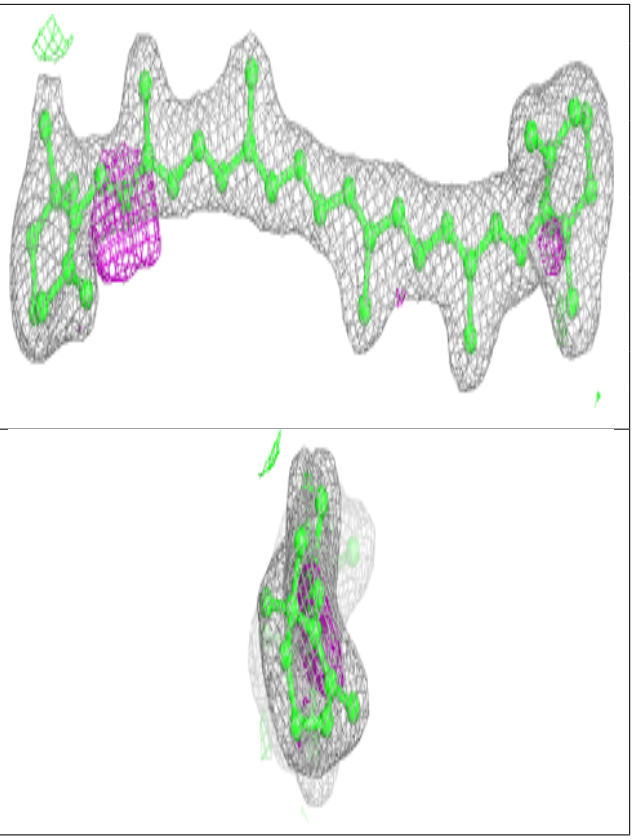






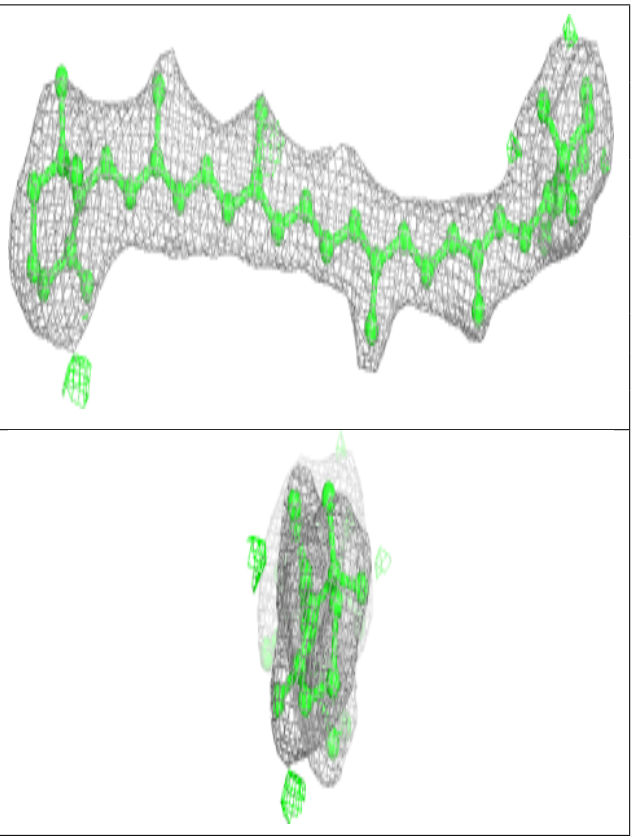
Electron density around BCR b 628:

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



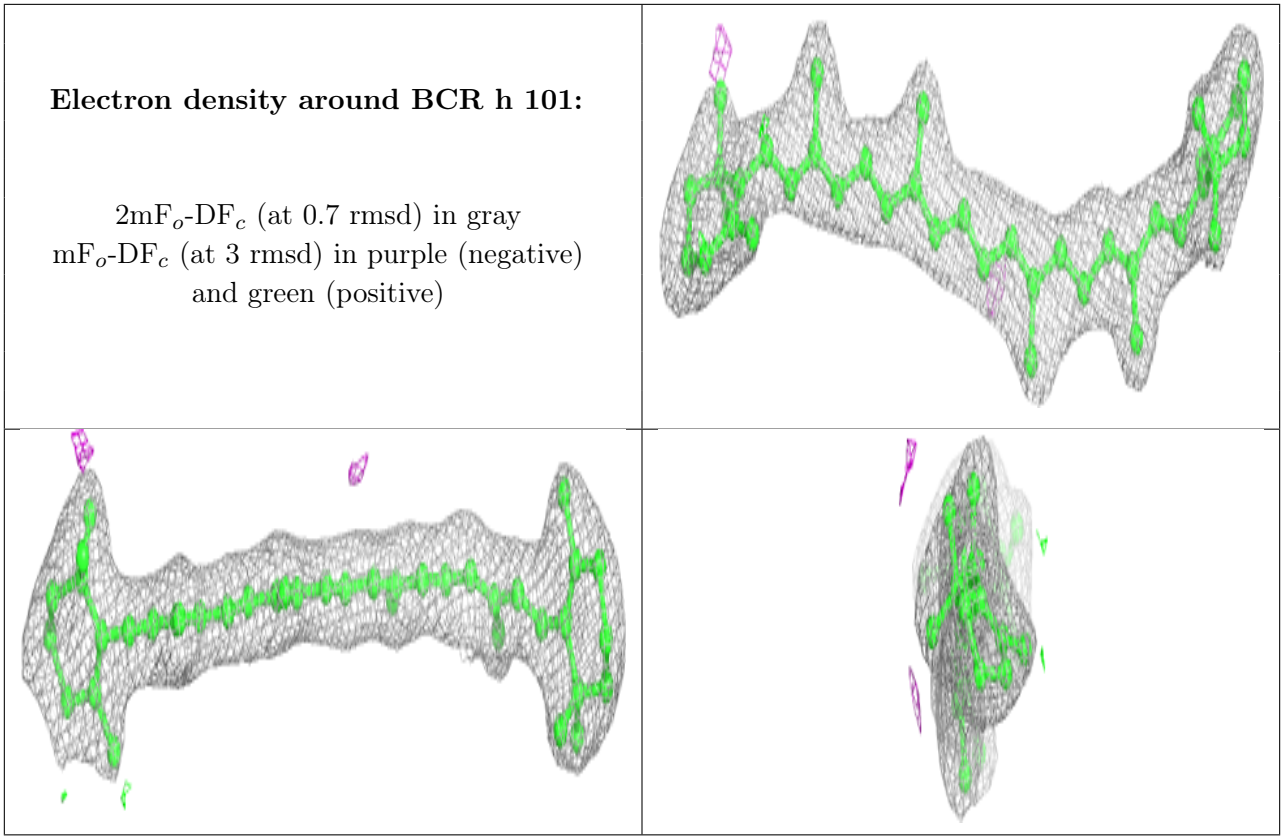
Electron density around BCR c 527:

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



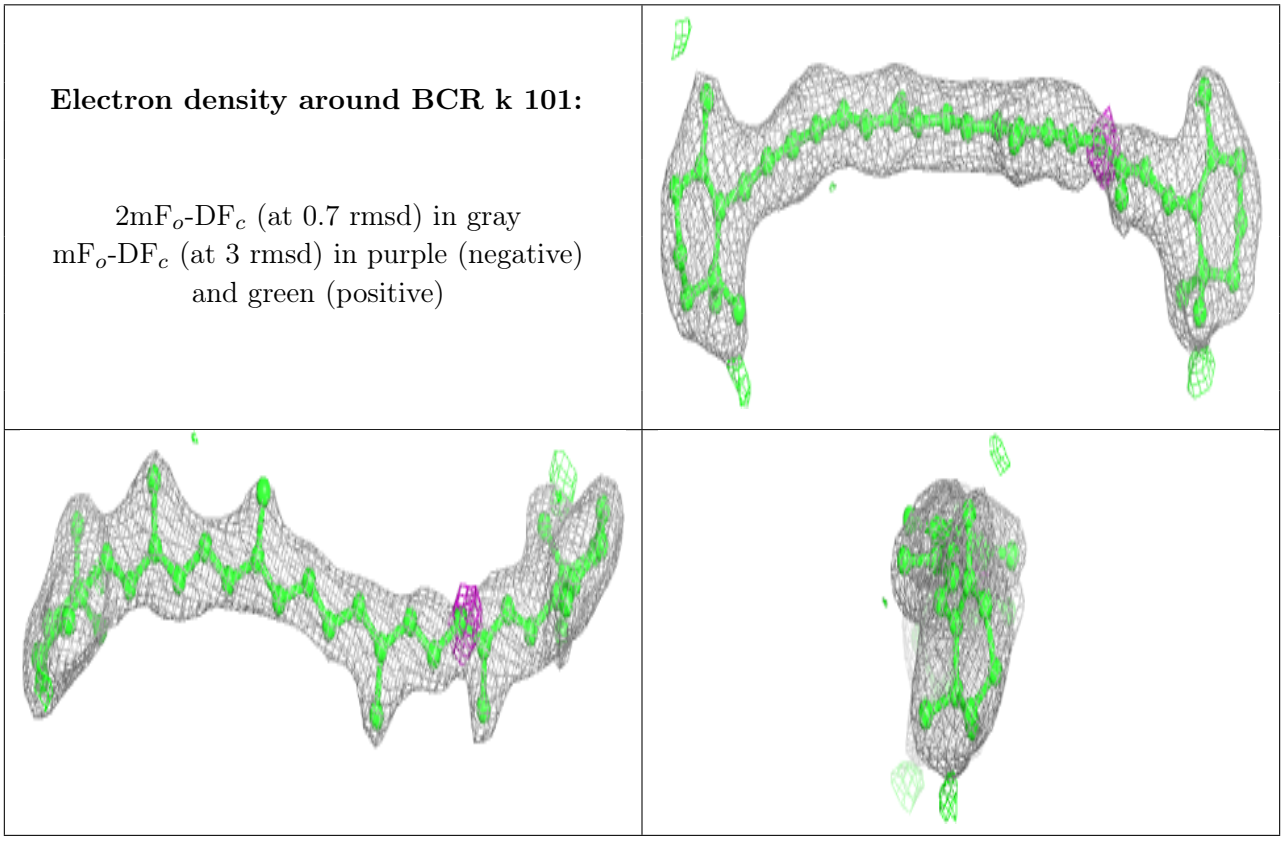
Electron density around BCR h 101:

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



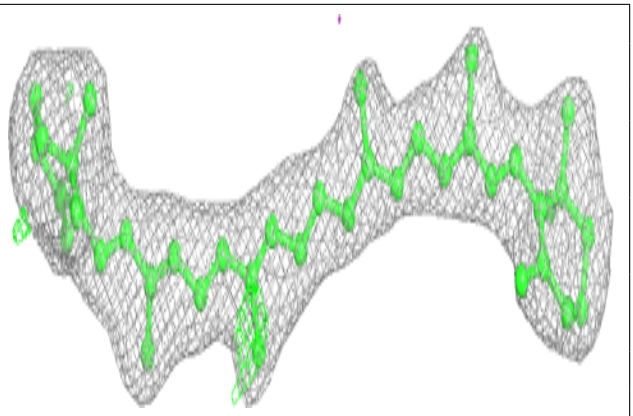
Electron density around BCR k 101:

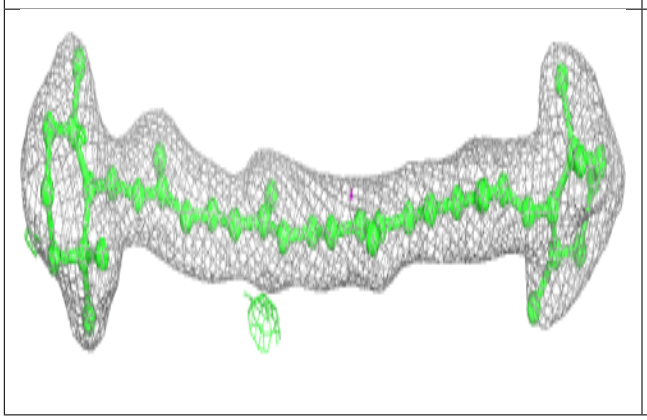
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

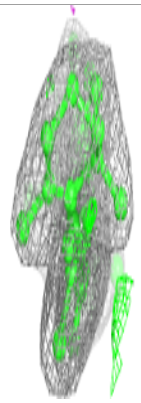


Electron density around BCR y 101:

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

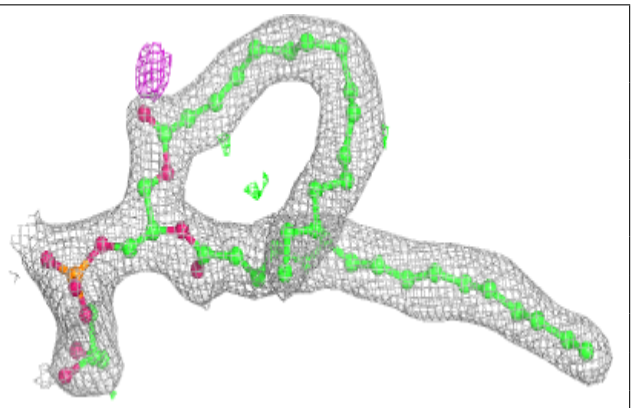


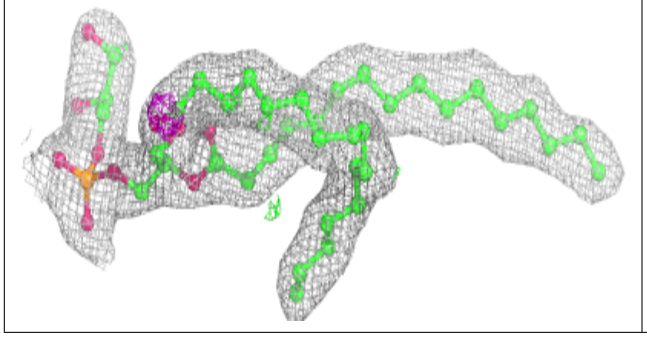


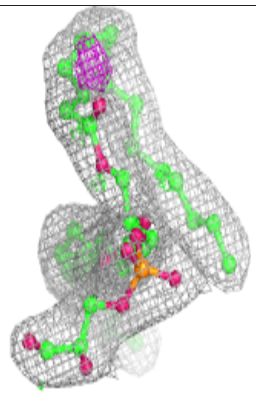


Electron density around LHG d 406:

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

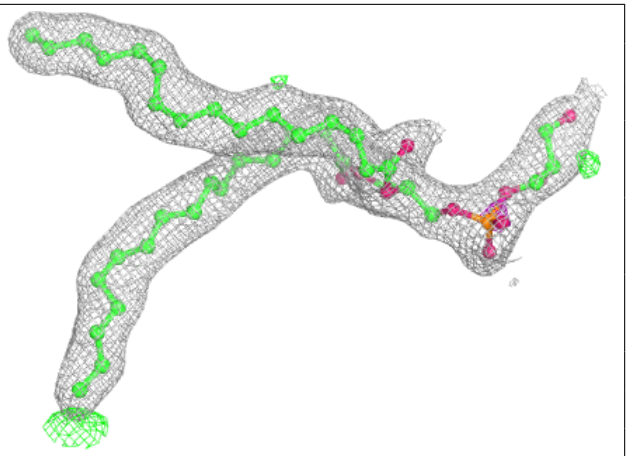


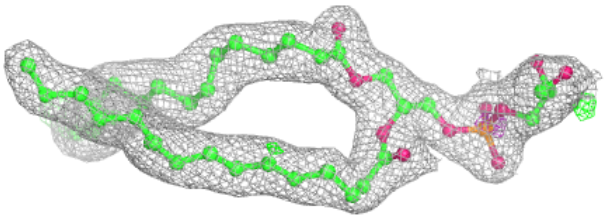


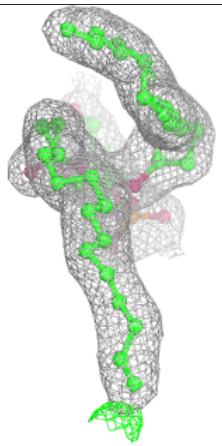


Electron density around LHG d 407:

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

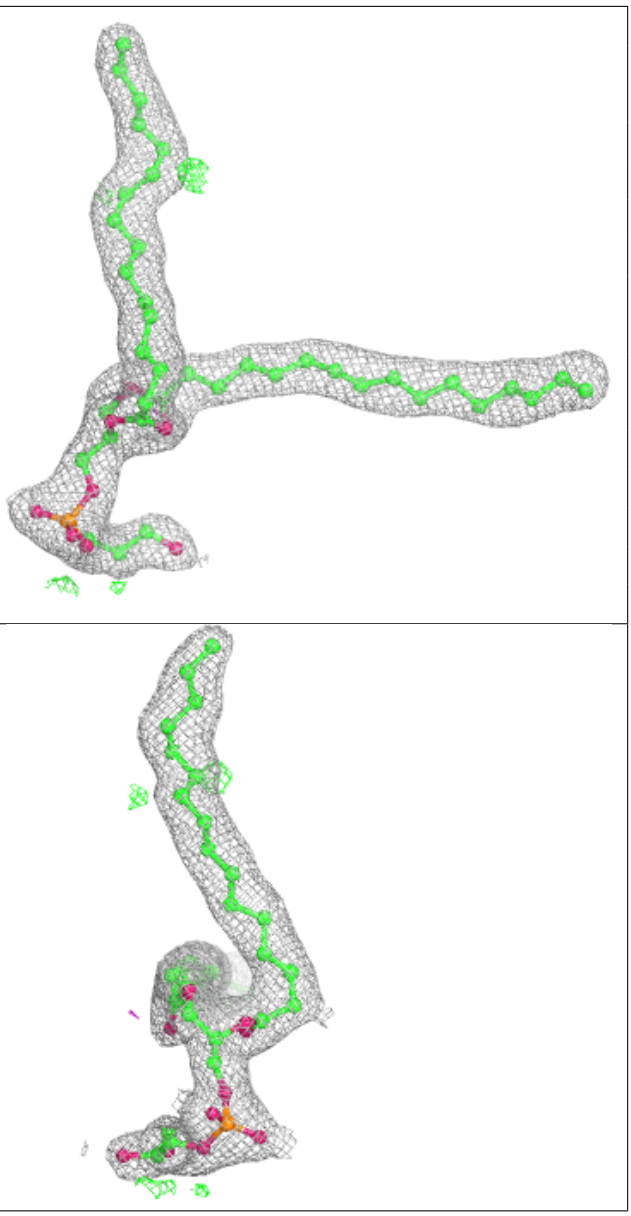






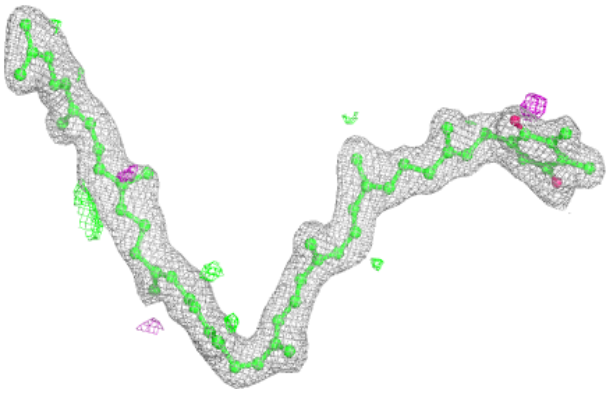
Electron density around LHG l 101:

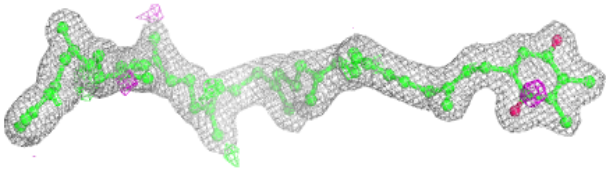
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

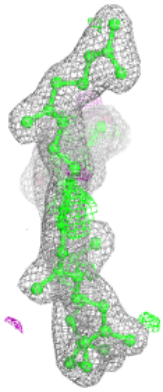


Electron density around PL9 D 405 (B):

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

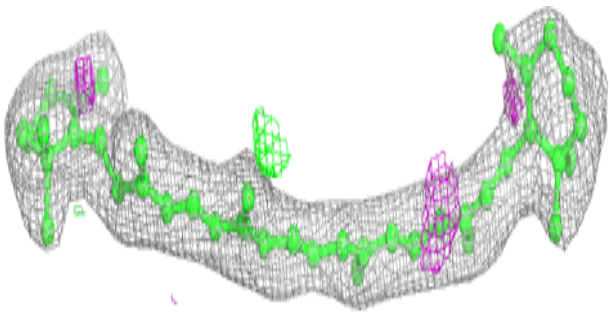


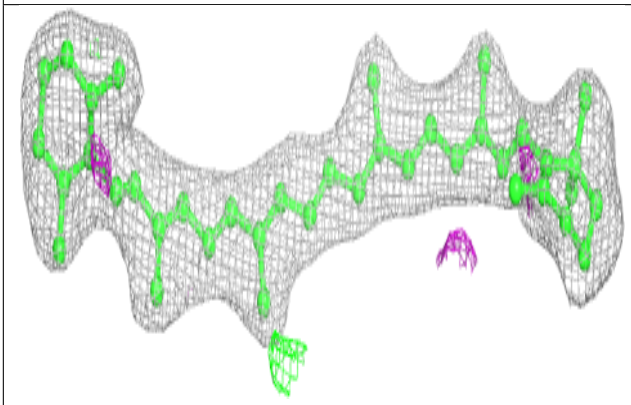


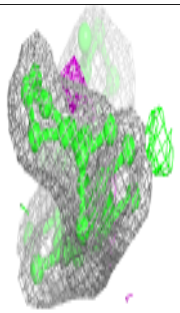


Electron density around BCR D 404:

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

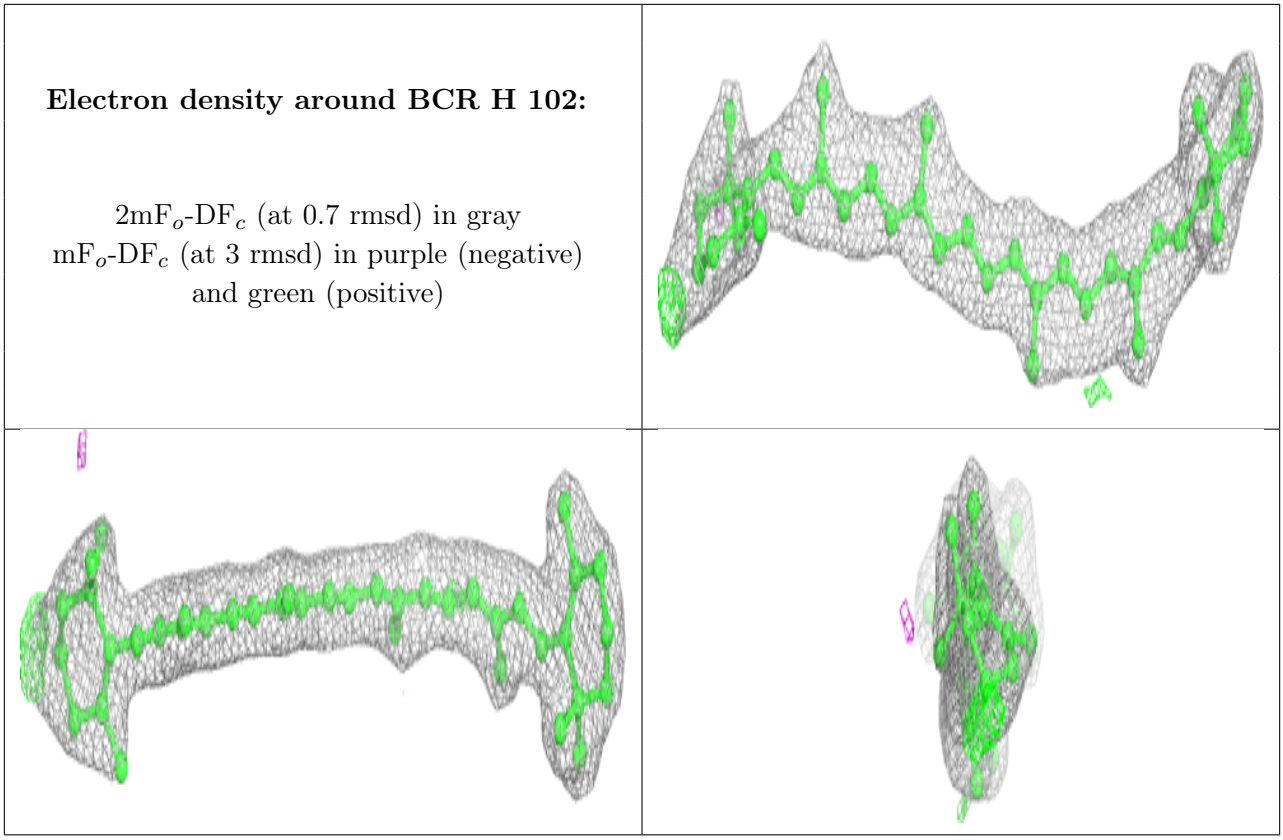






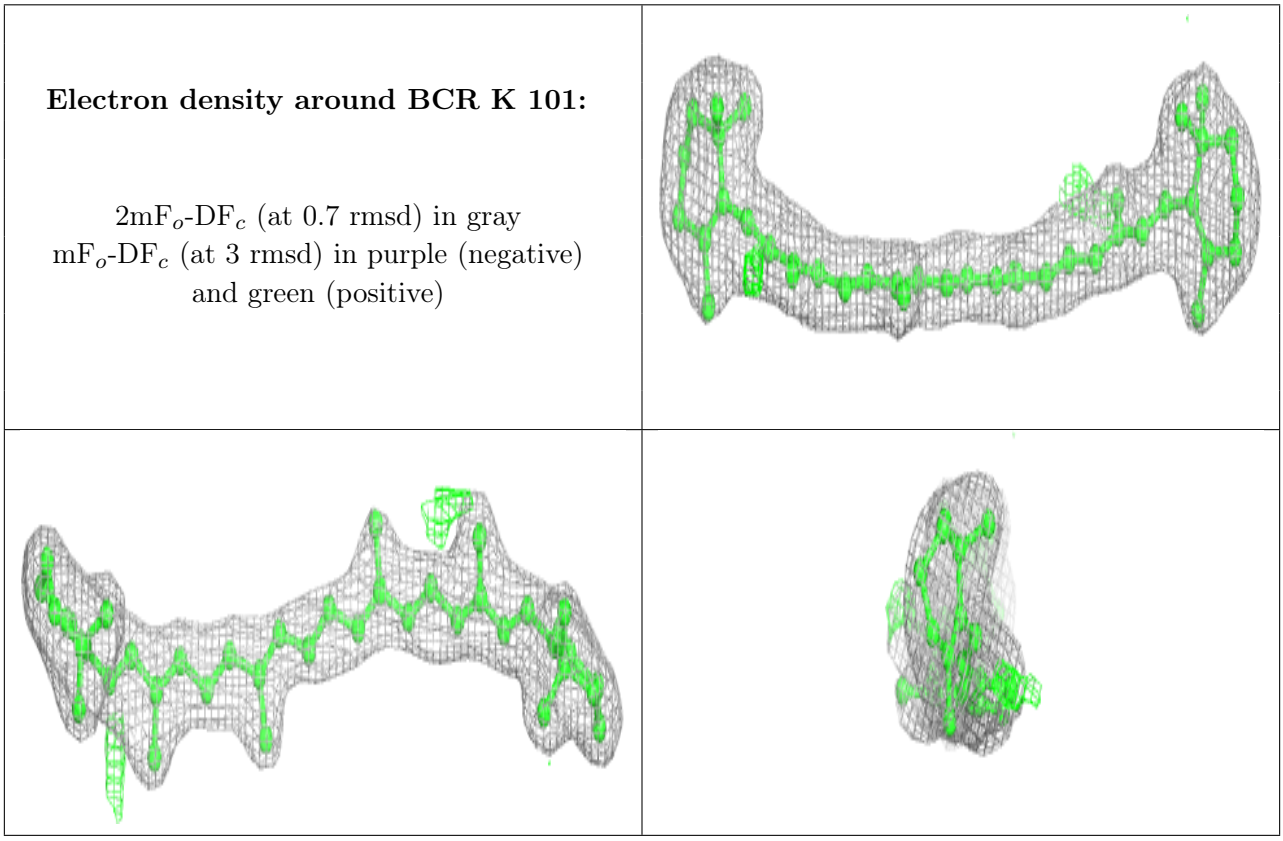
Electron density around BCR H 102:

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



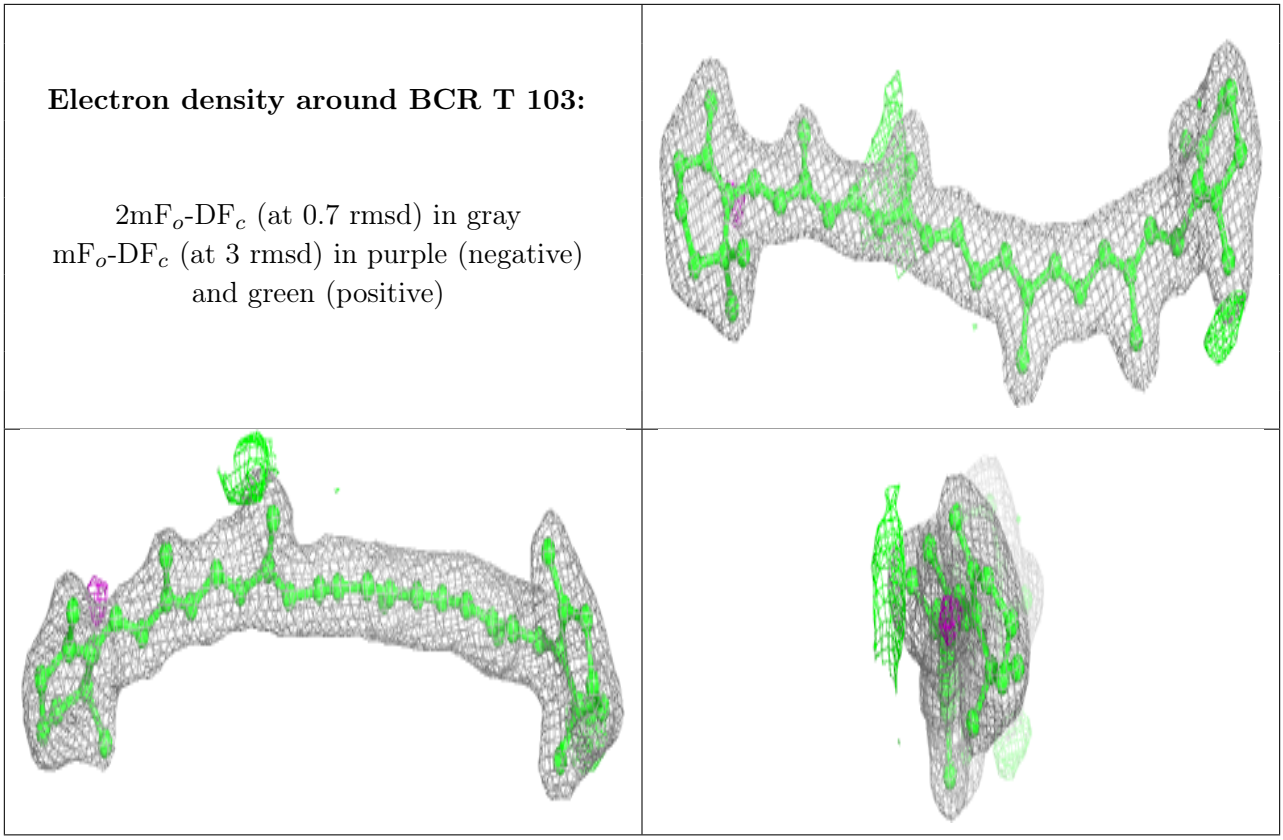
Electron density around BCR K 101:

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



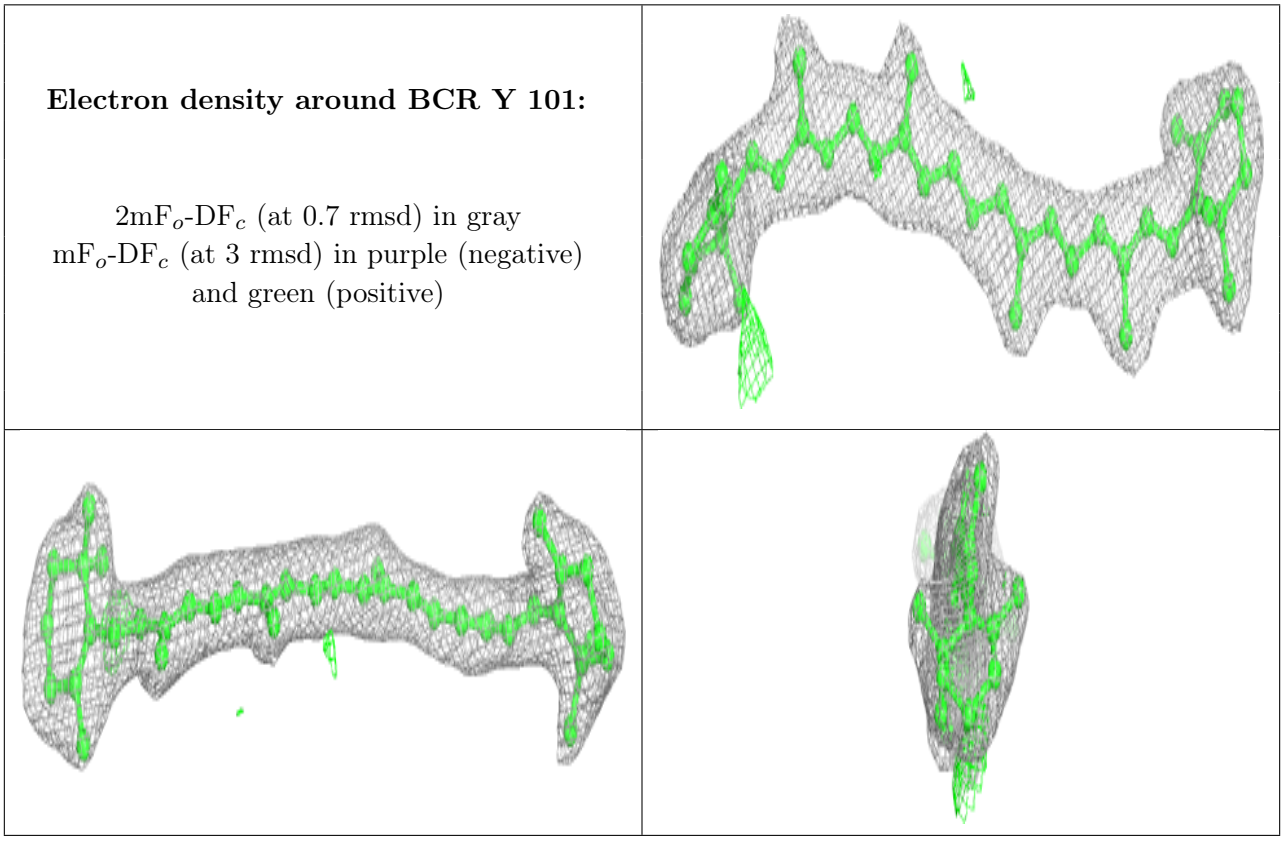
Electron density around BCR T 103:

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



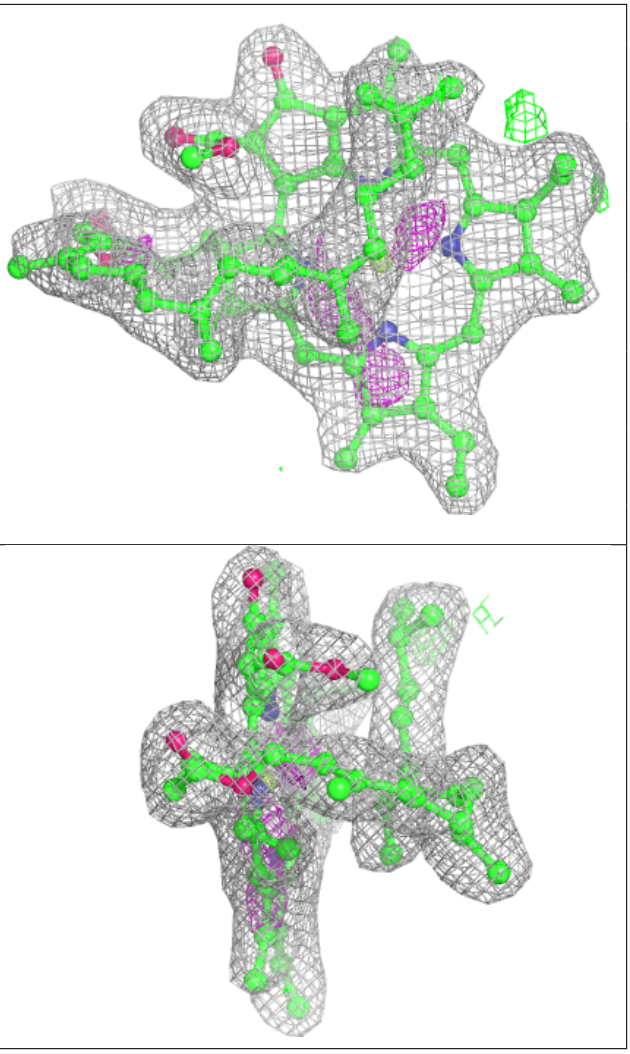
Electron density around BCR Y 101:

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



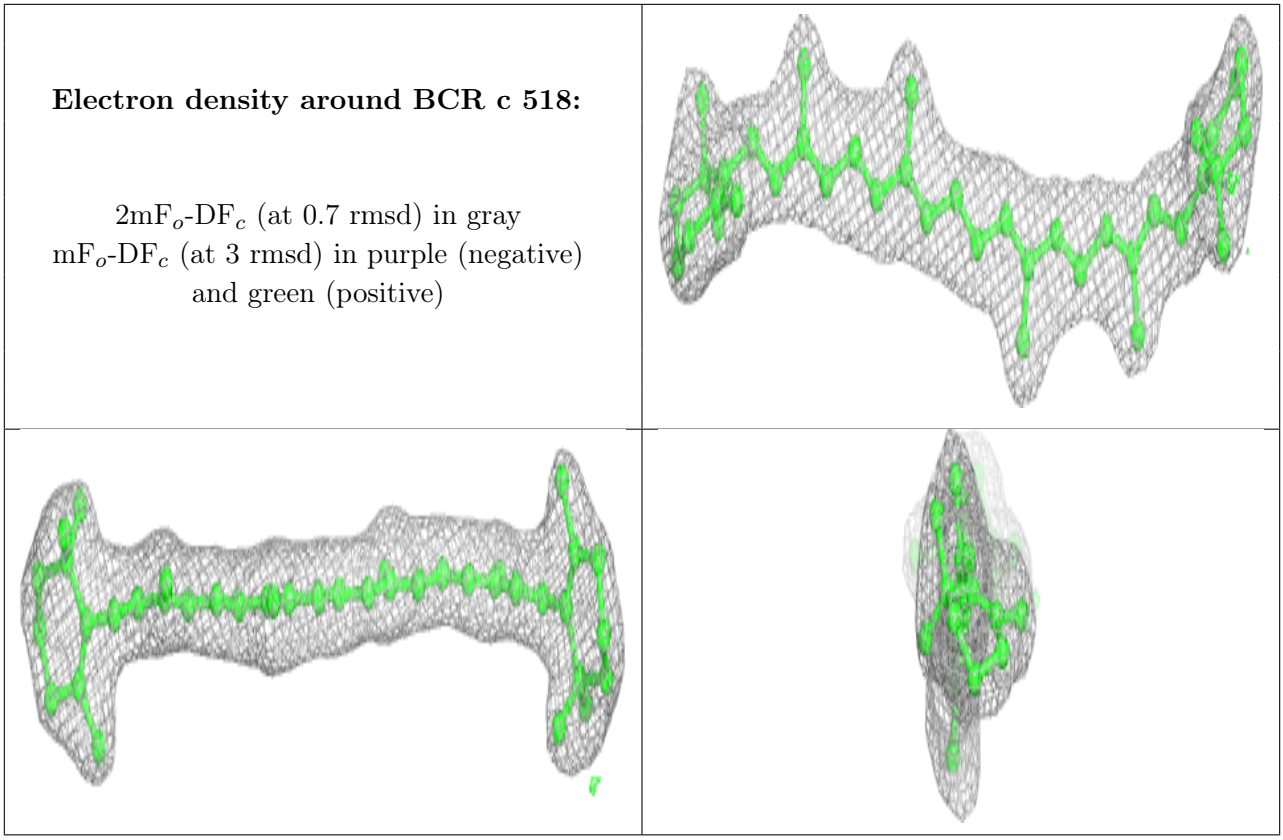
Electron density around CLA C 510:

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



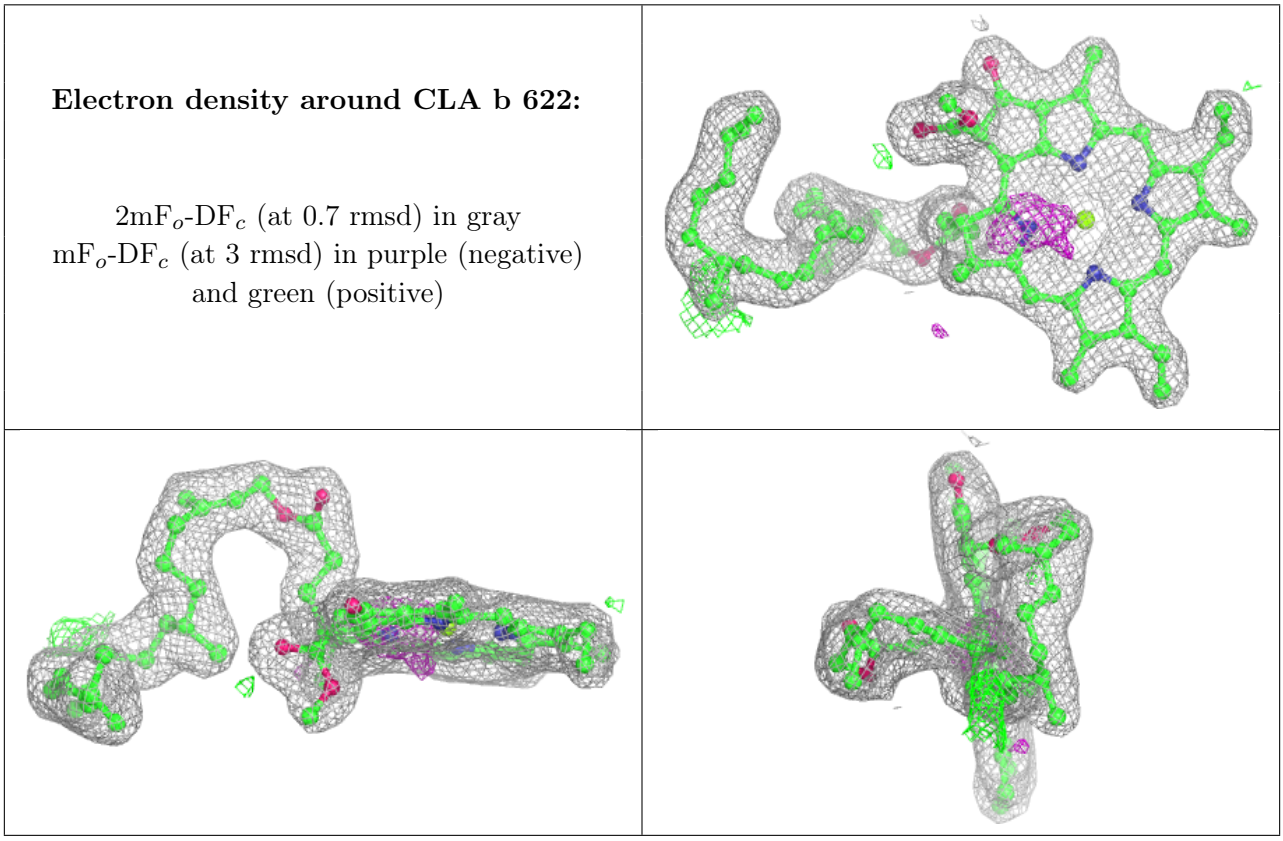
Electron density around BCR c 518:

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



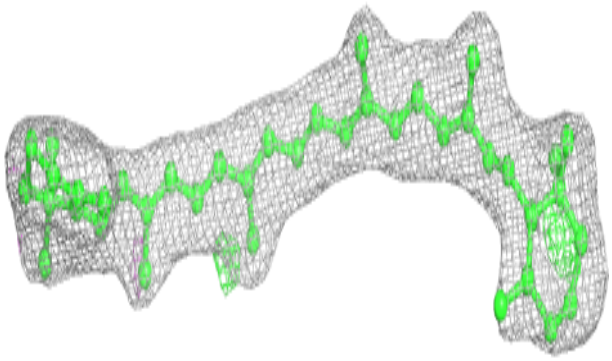
Electron density around CLA b 622:

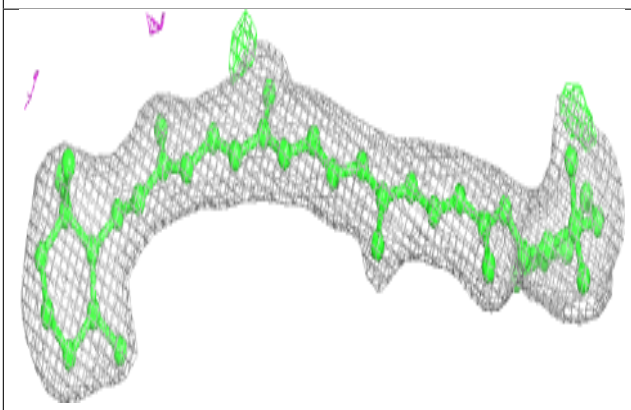
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

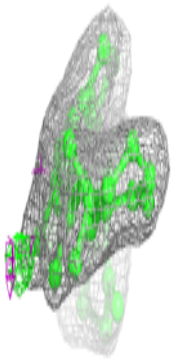


Electron density around BCR d 404:

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

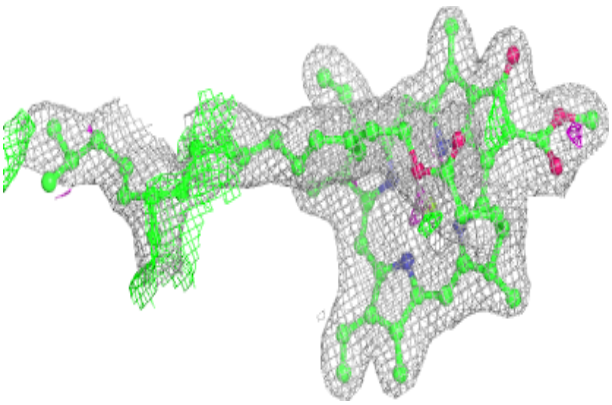


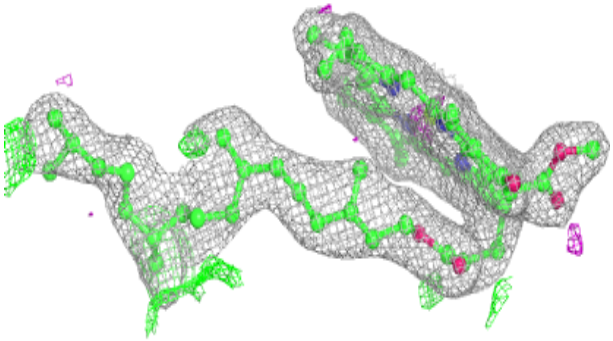


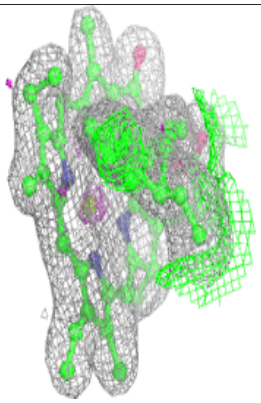


Electron density around CLA b 624:

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

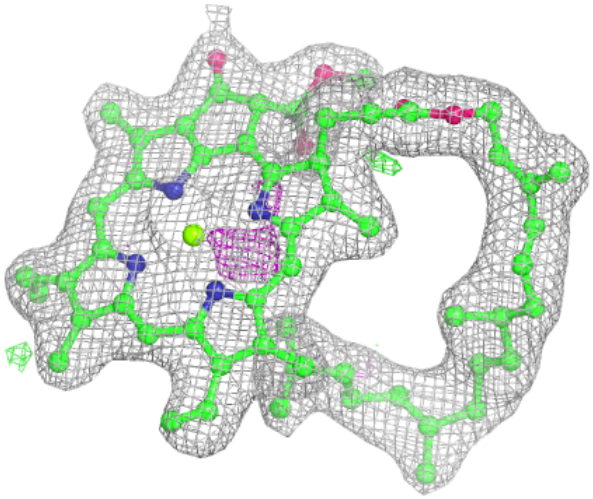


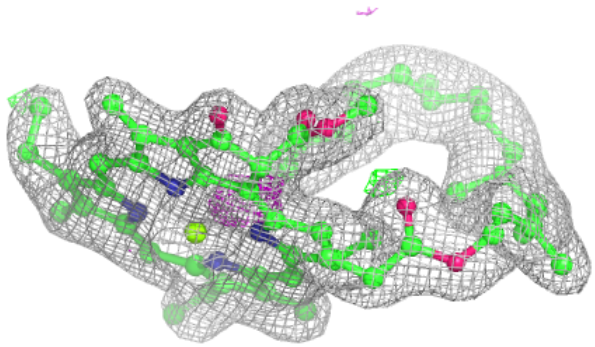


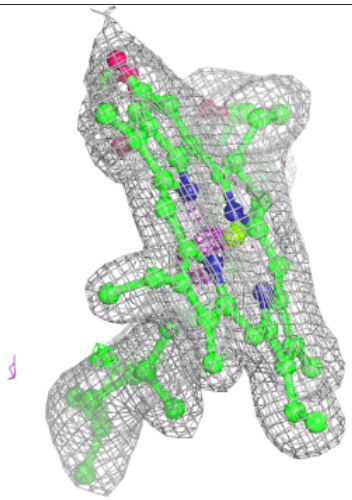


Electron density around CLA b 625:

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

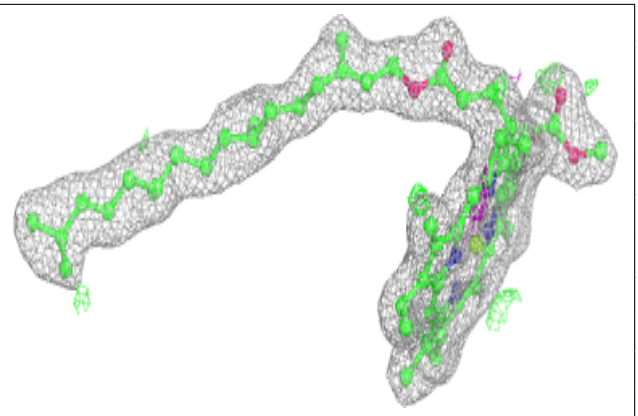


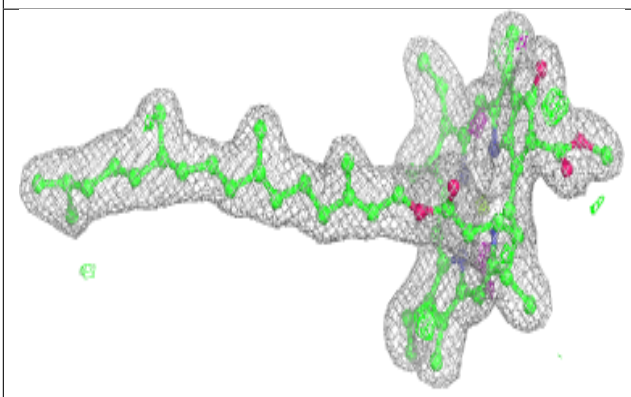


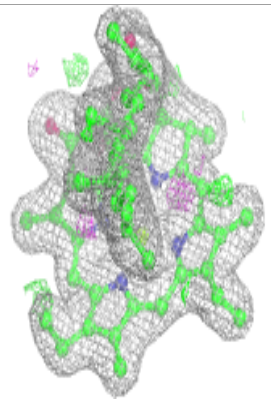


Electron density around CLA B 608:

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

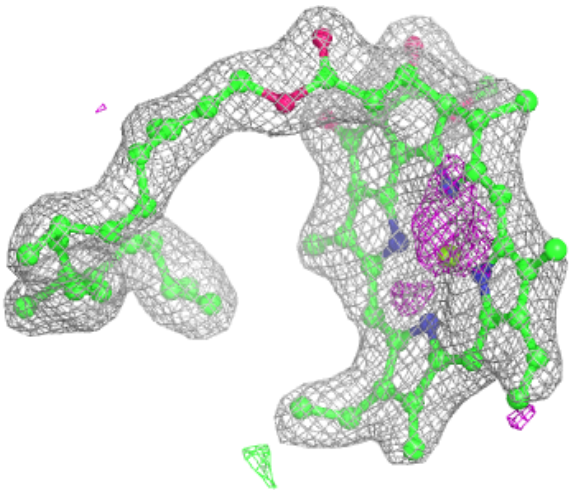


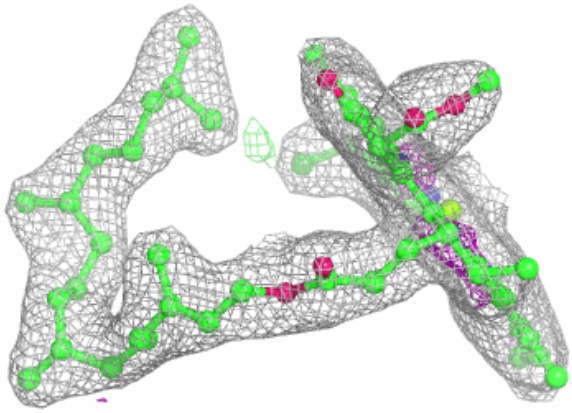


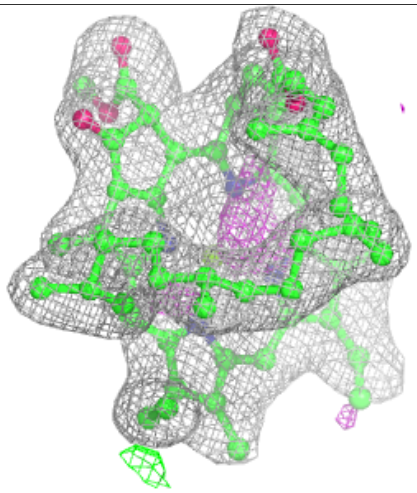


Electron density around CLA C 503:

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

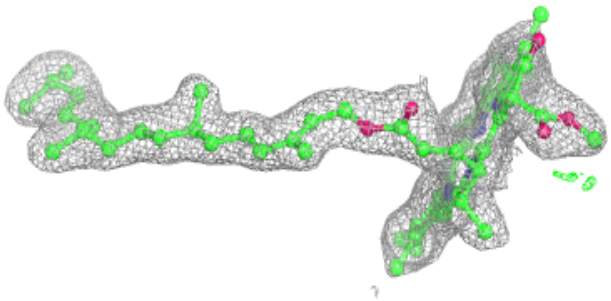






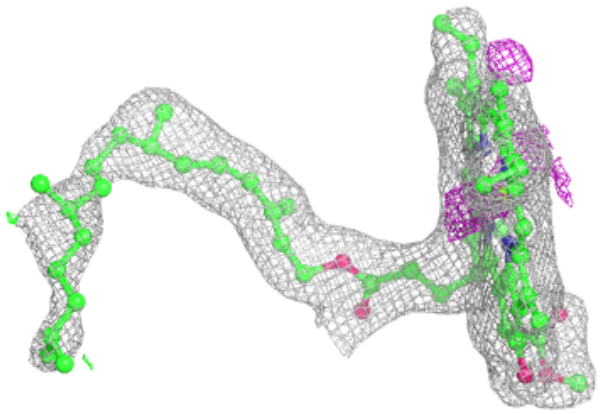
Electron density around CLA B 610:

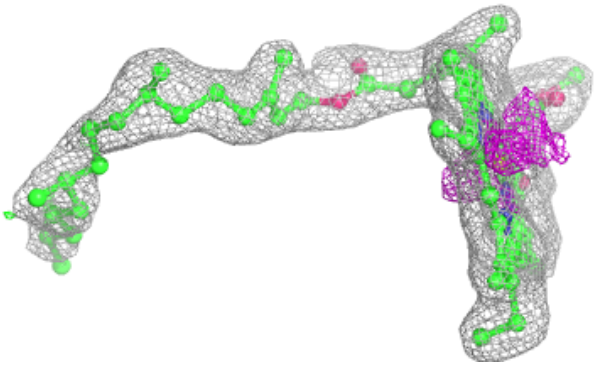
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

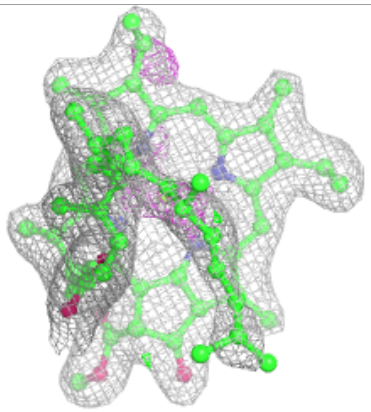


Electron density around CLA D 403:

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

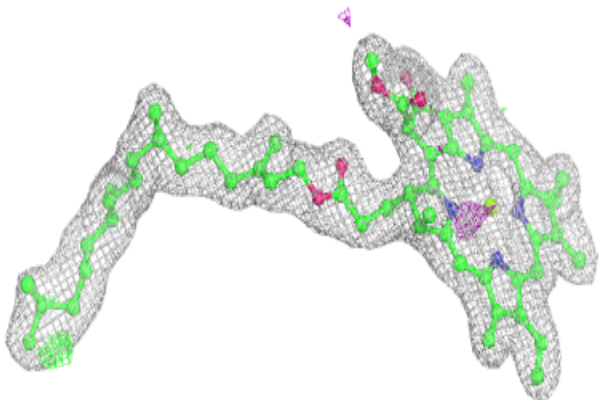


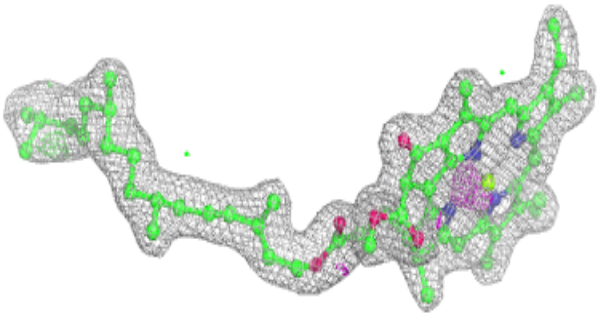


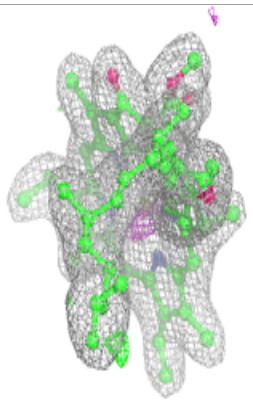


Electron density around CLA a 409:

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

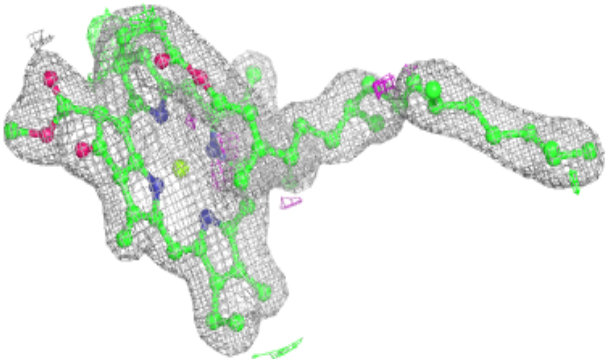


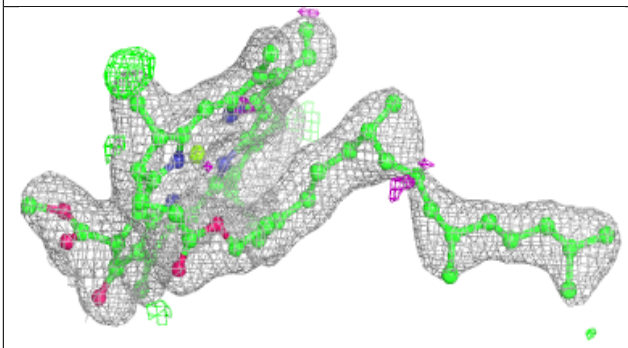


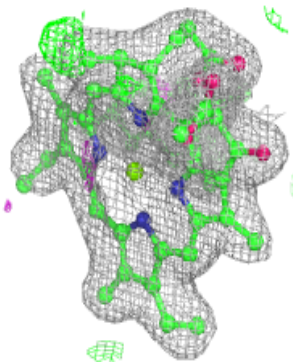


Electron density around CLA C 505:

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

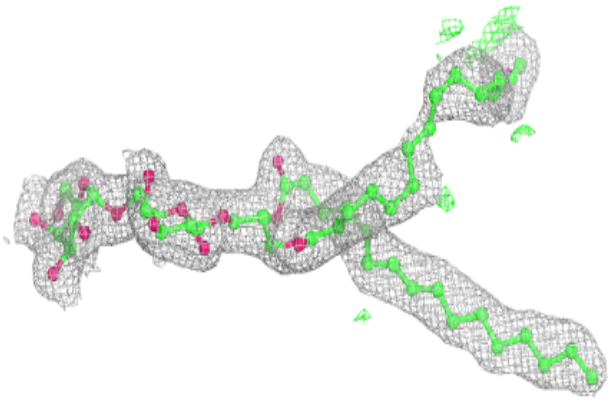


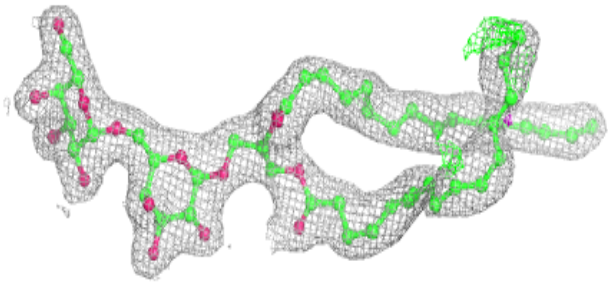


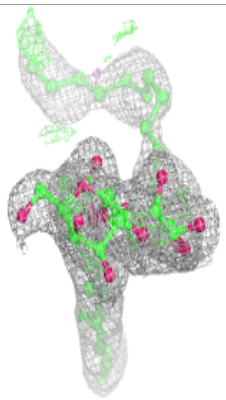


Electron density around DGD C 516:

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

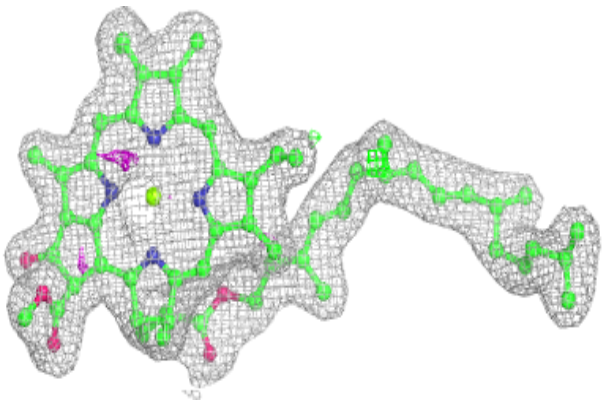


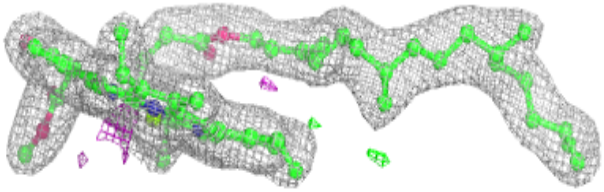


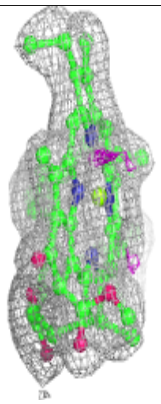


Electron density around CLA B 604:

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

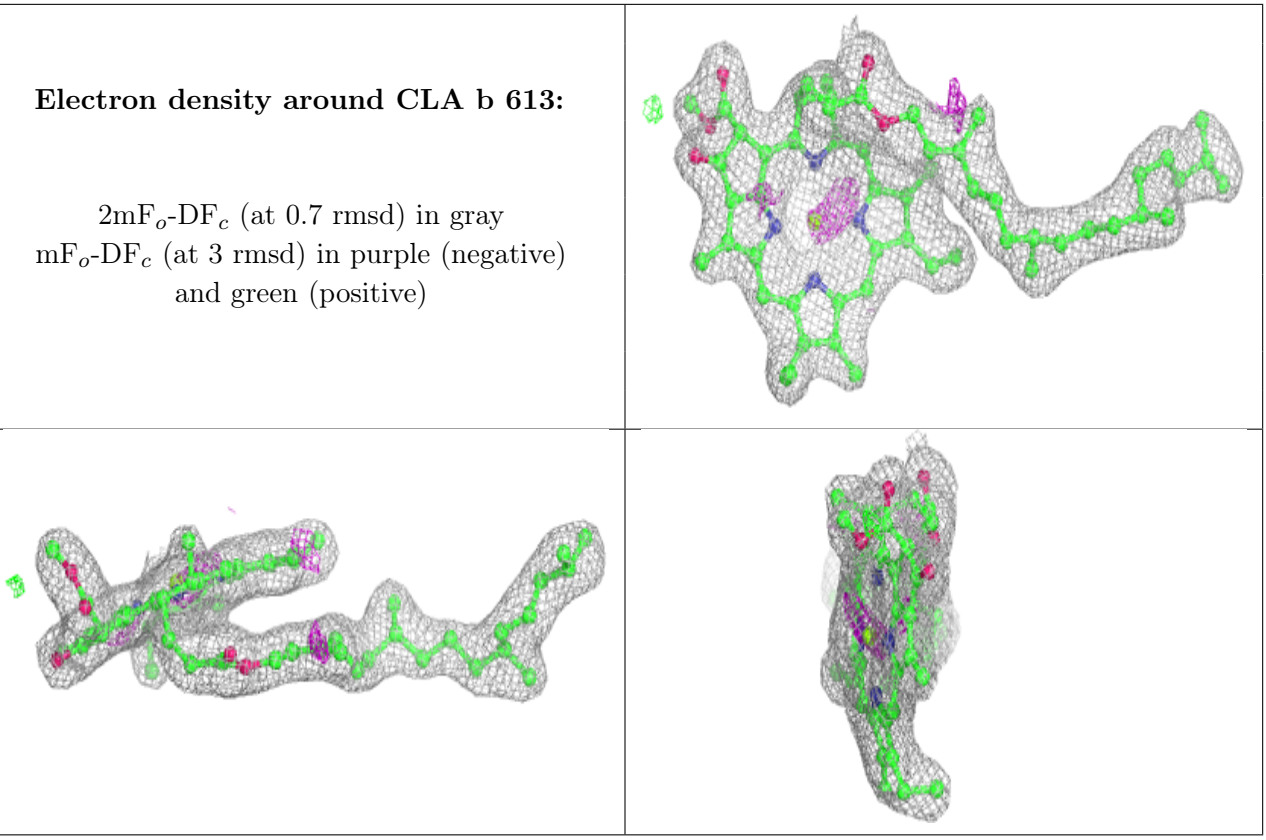






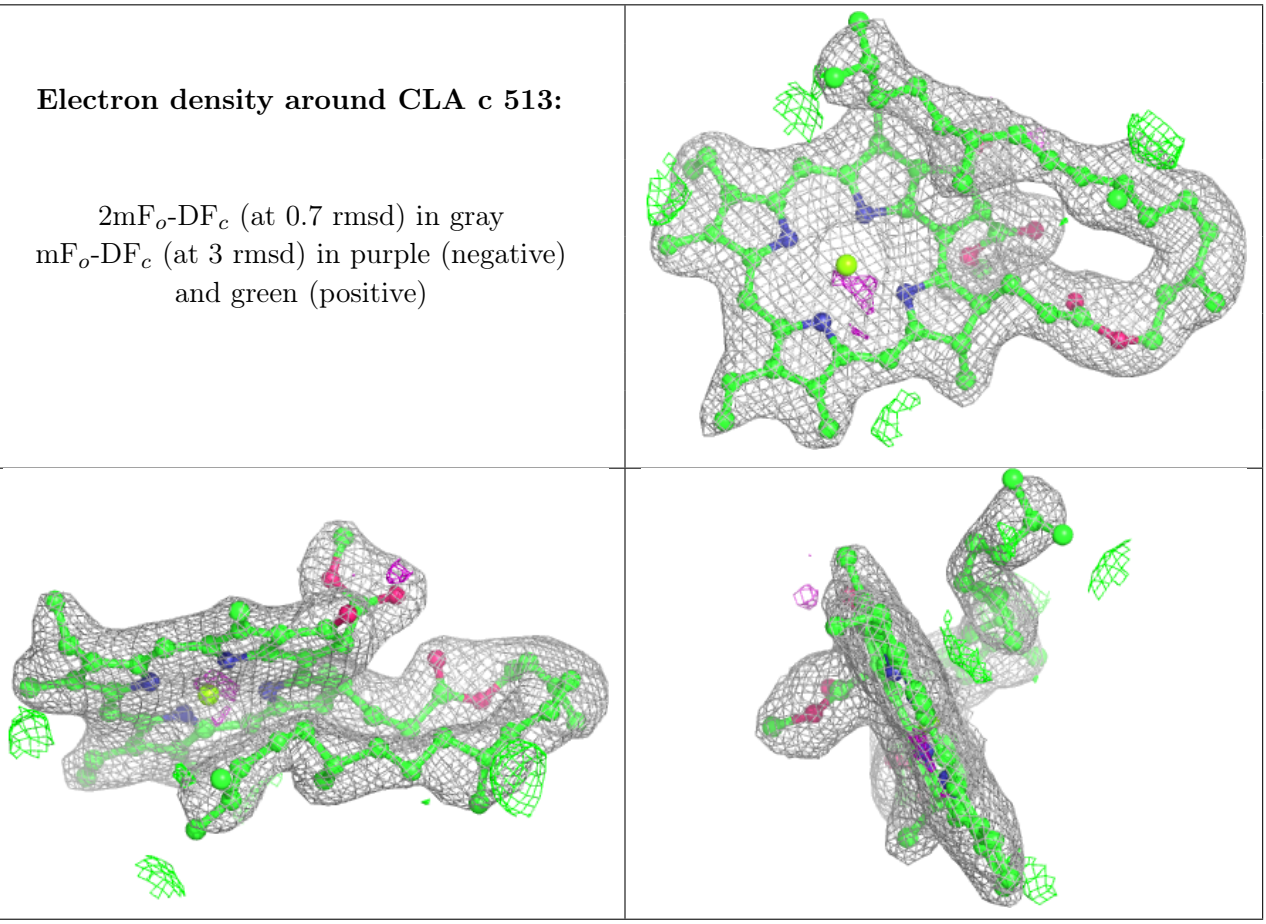
Electron density around CLA b 613:

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



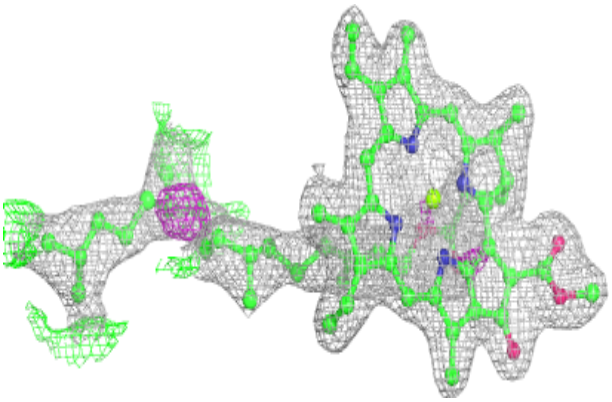
Electron density around CLA c 513:

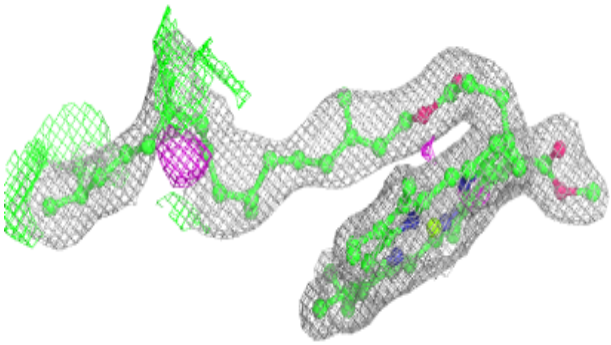
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

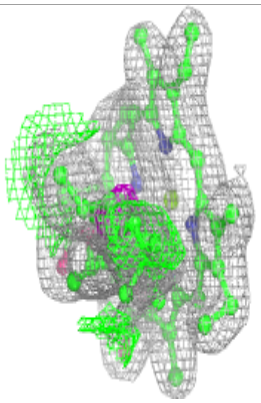


Electron density around CLA B 615:

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

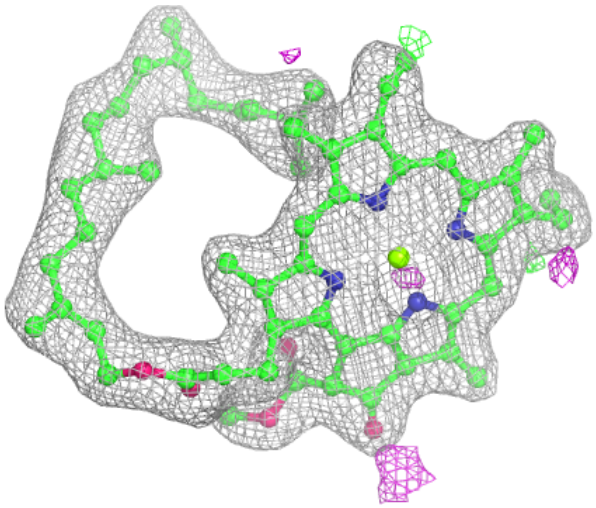


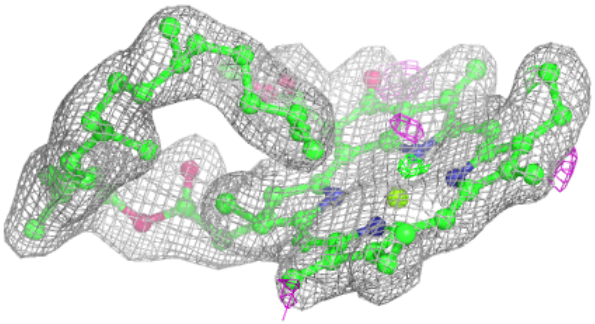


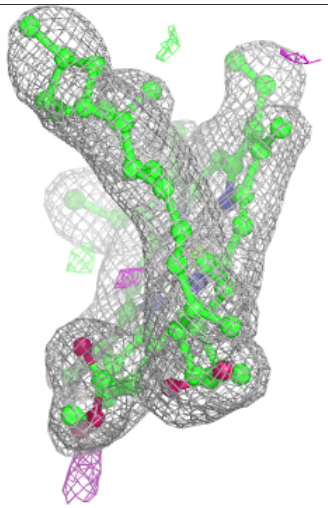


Electron density around CLA B 616:

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

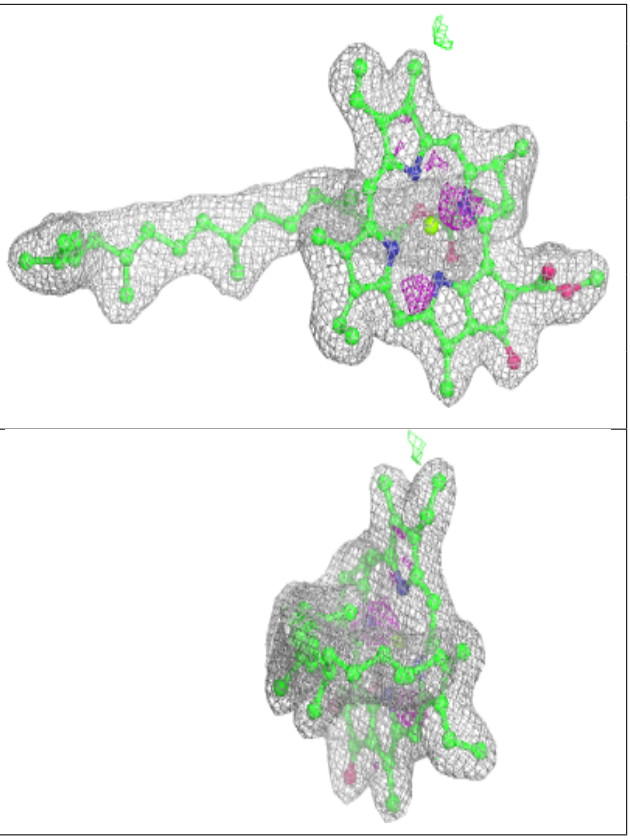


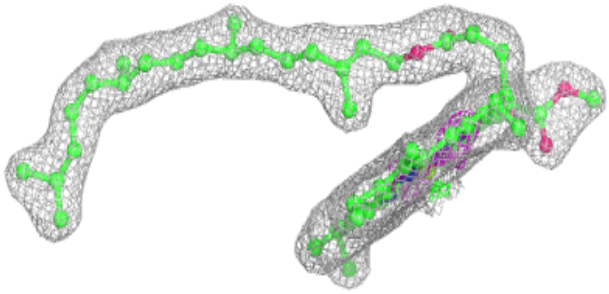




Electron density around CLA b 618:

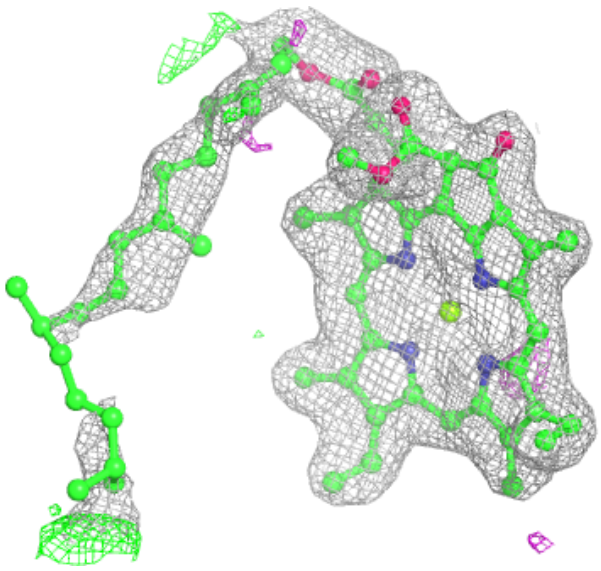
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

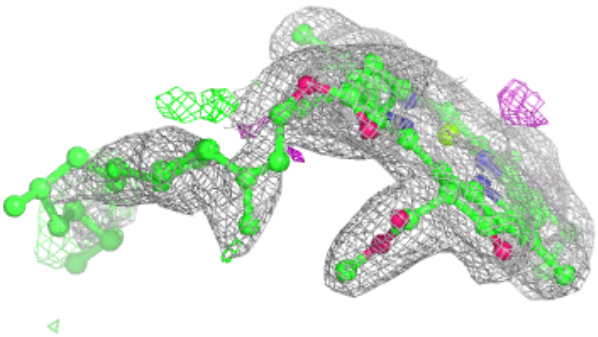


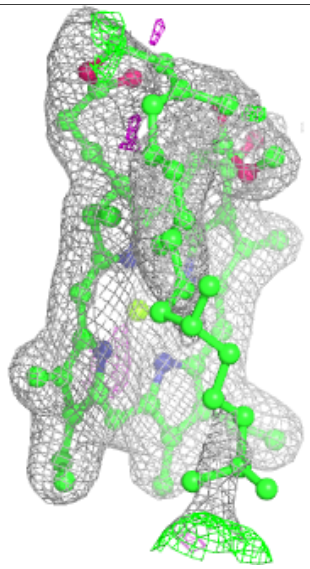


Electron density around CLA B 617:

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

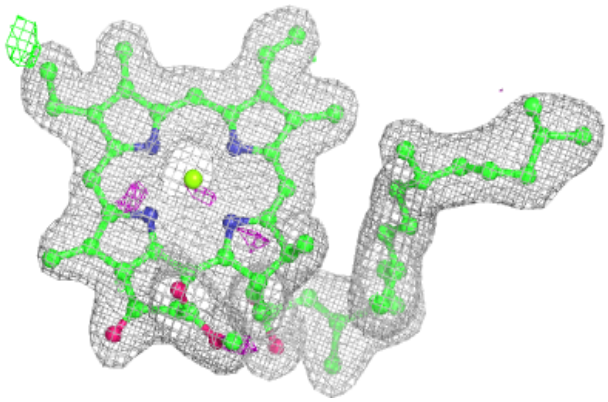


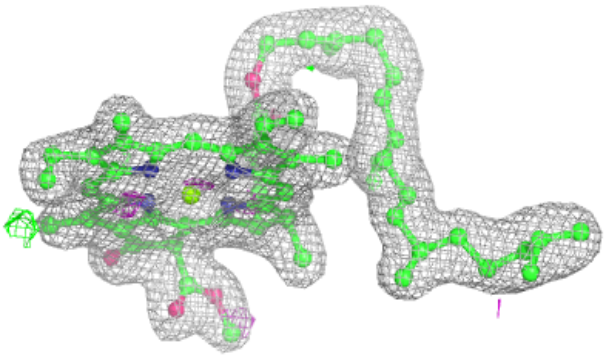


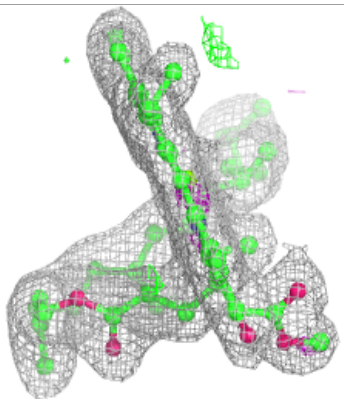


Electron density around CLA d 401:

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

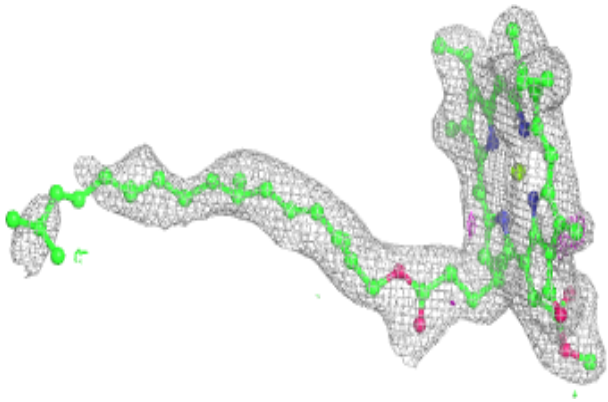


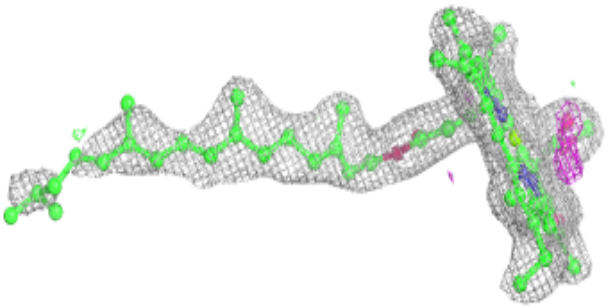


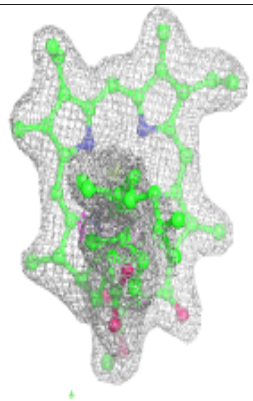


Electron density around CLA d 403:

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

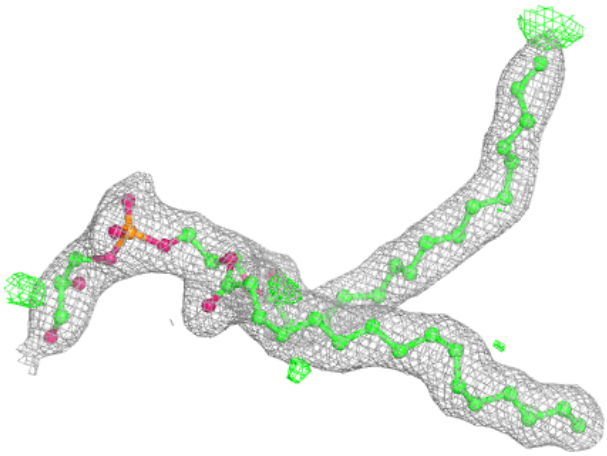


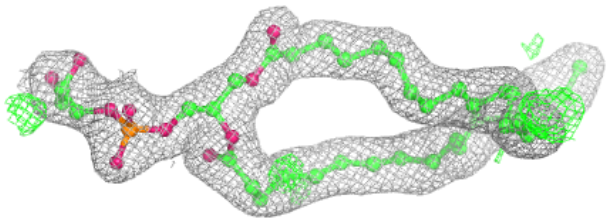


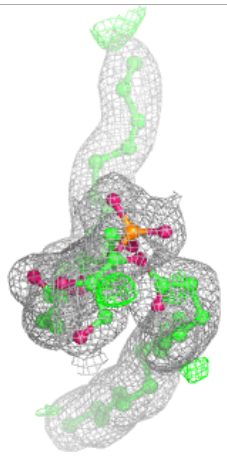


Electron density around LHG D 408:

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

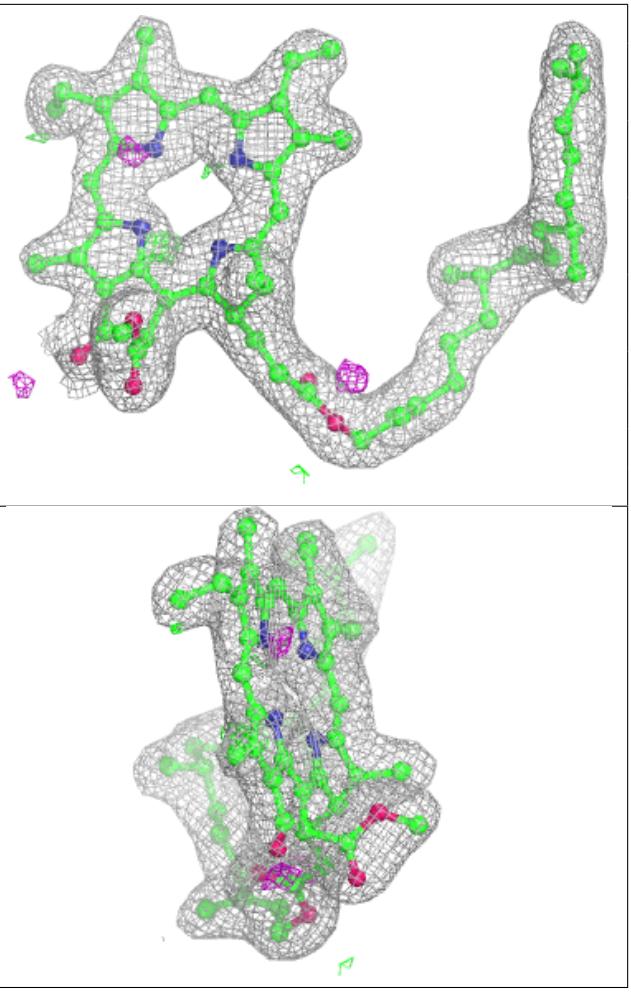






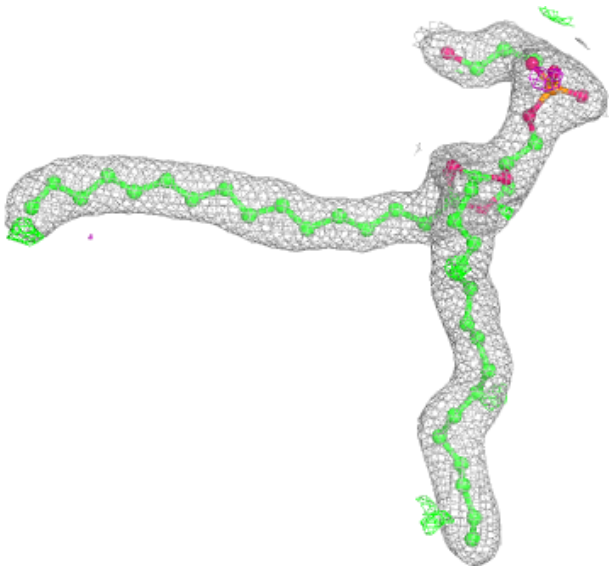
Electron density around PHO a 420 (A):

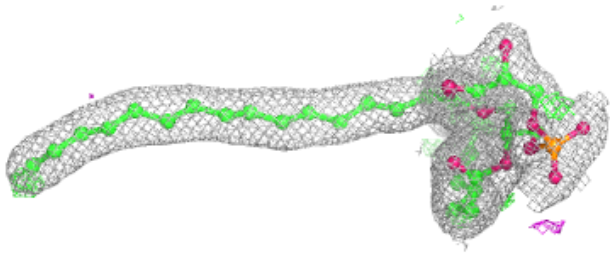
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

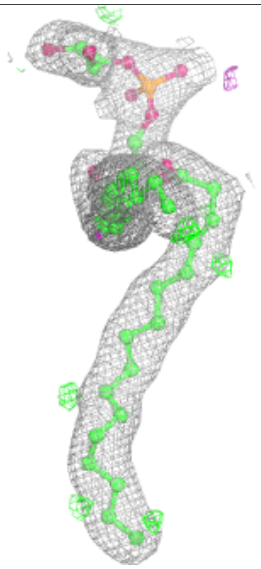


Electron density around LHG L 101:

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

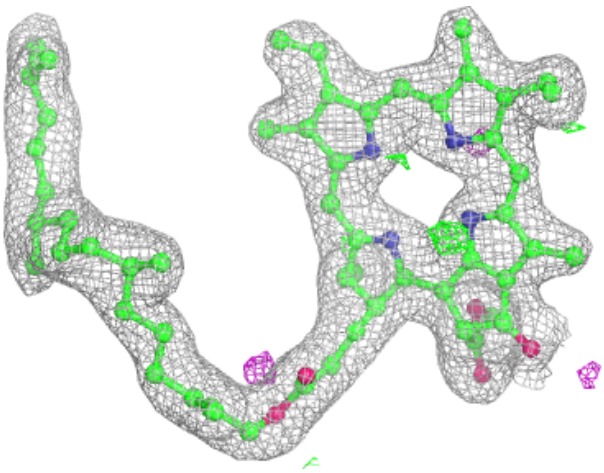


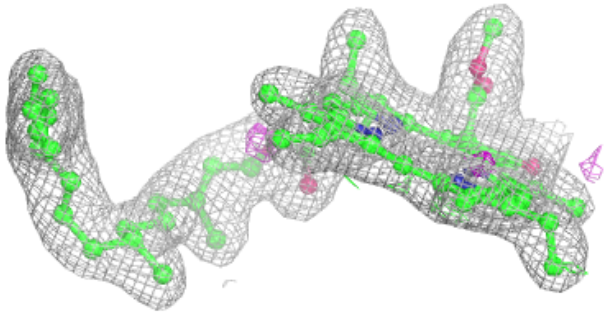


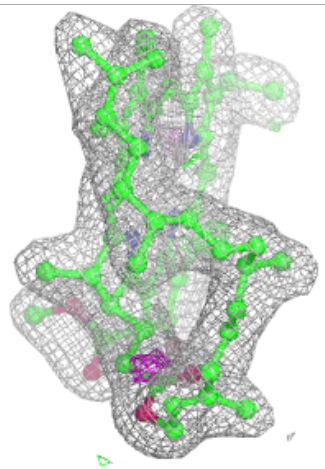


Electron density around PHO a 420 (B):

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

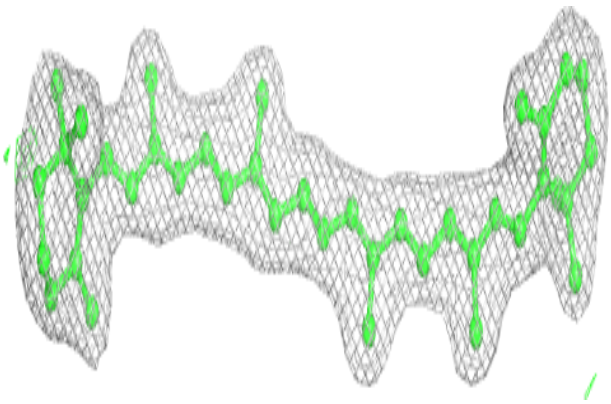


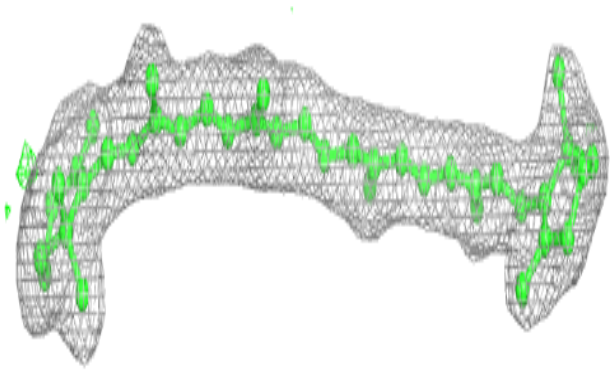


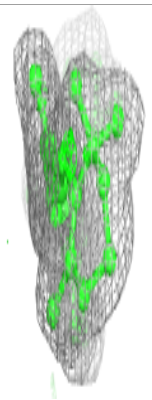


Electron density around BCR B 620:

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

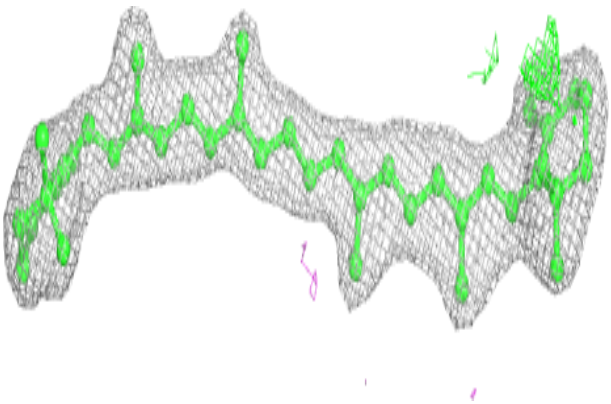


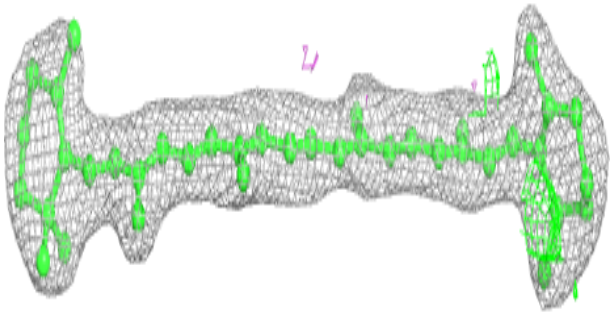


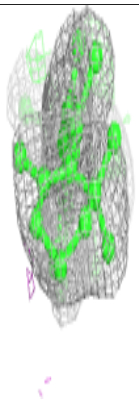


Electron density around BCR C 514:

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

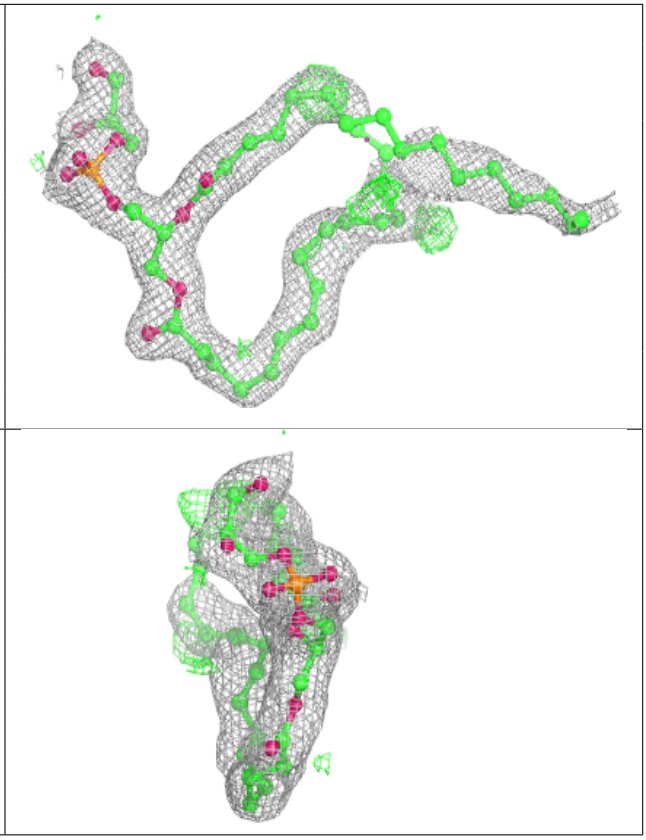


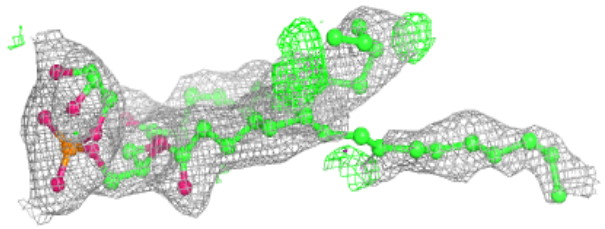




Electron density around LHG d 408:

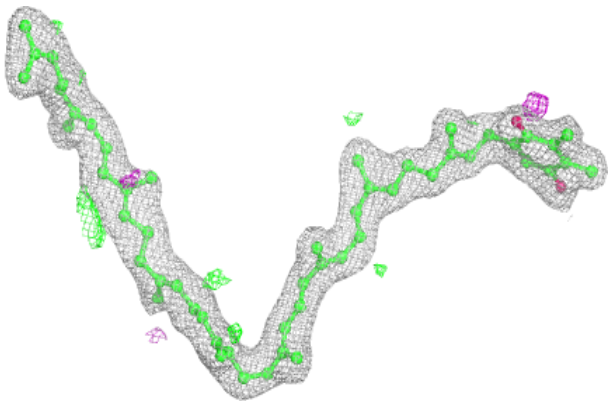
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

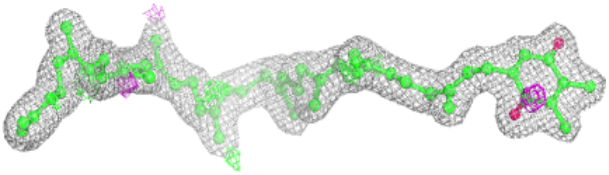


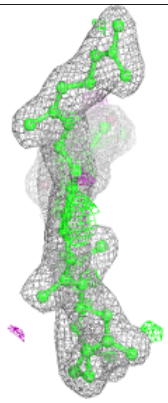


Electron density around PL9 D 405 (A):

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

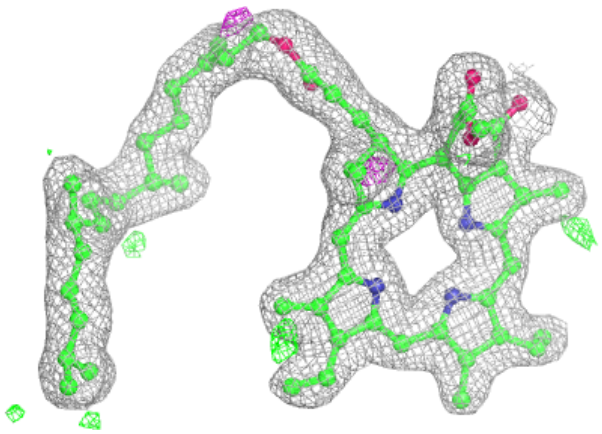


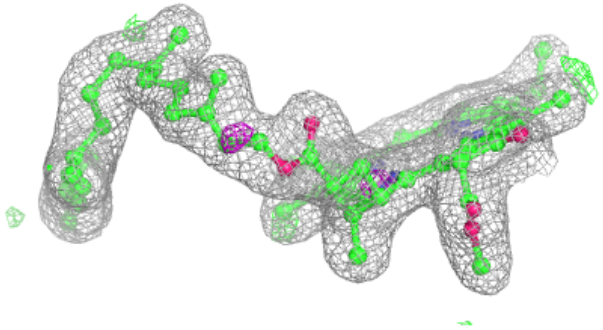


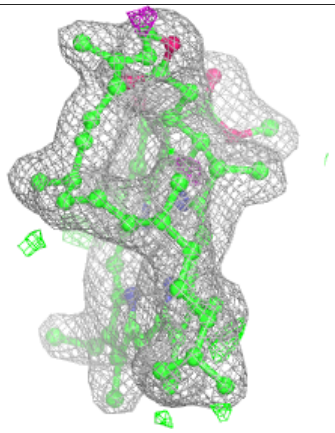


Electron density around PHO A 409 (B):

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

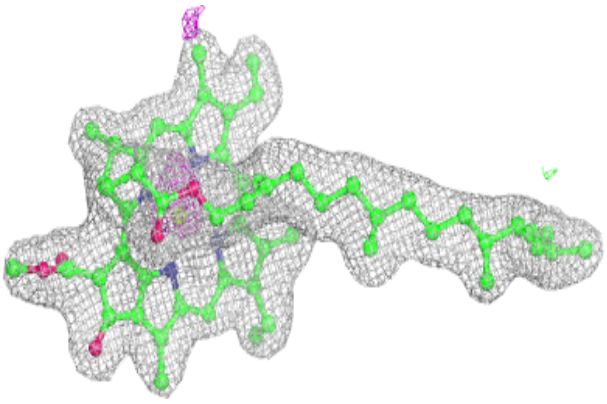


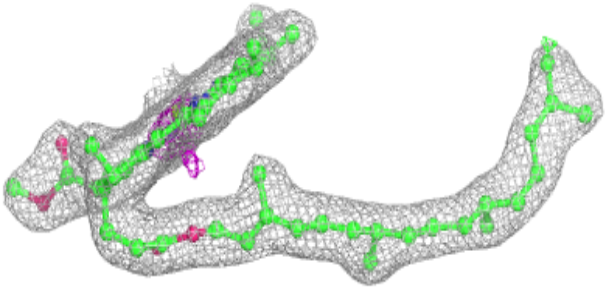


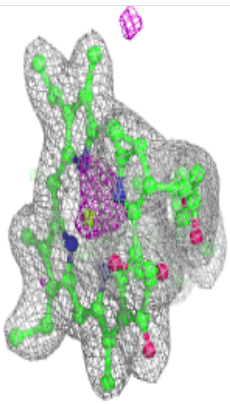


Electron density around CLA B 609:

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

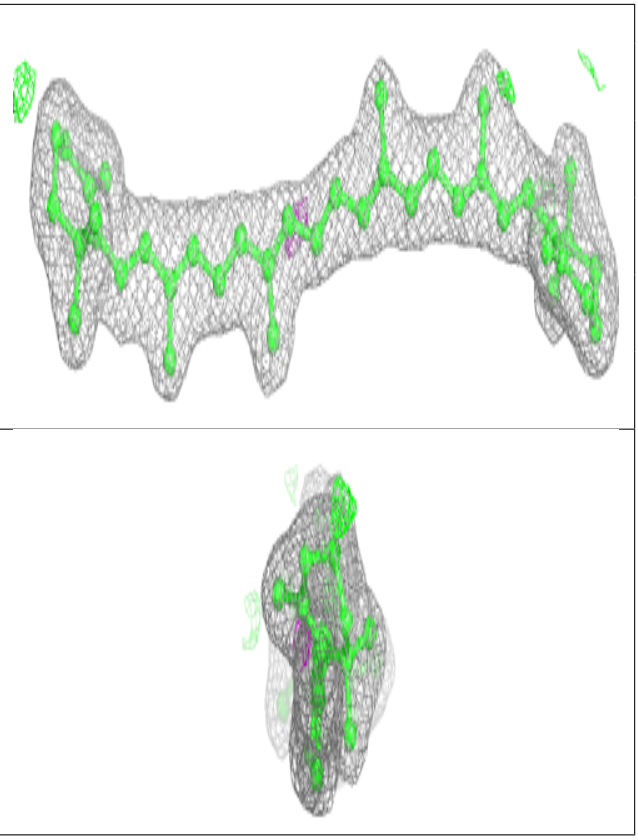






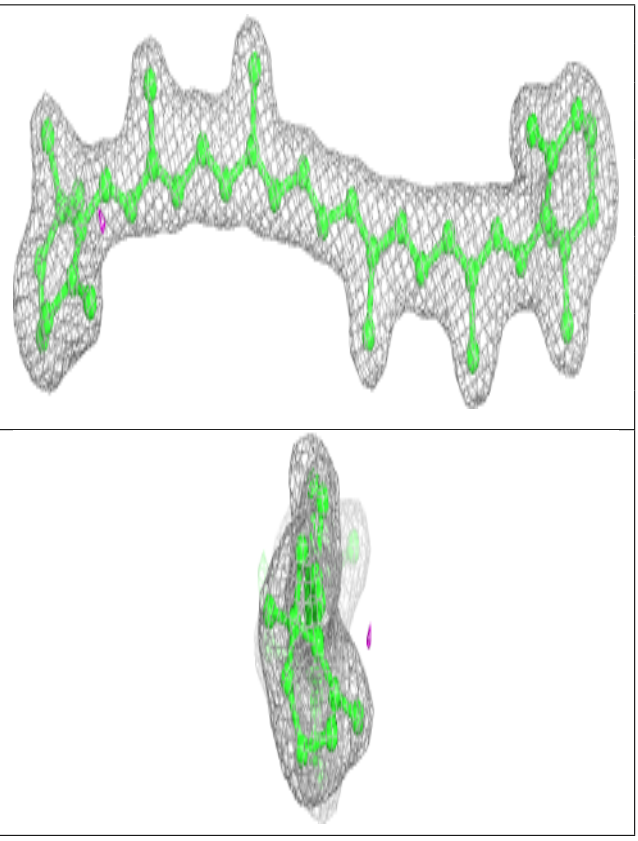
Electron density around BCR A 411:

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



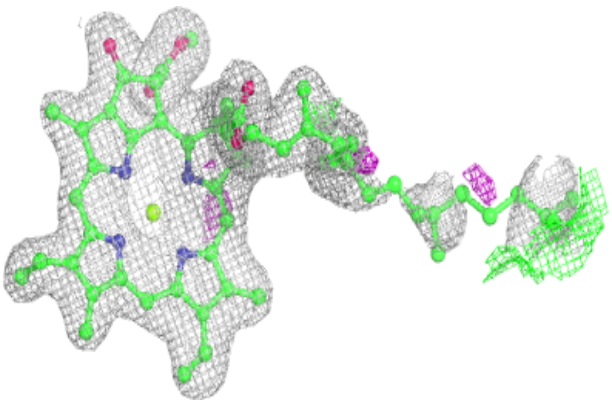
Electron density around BCR B 619:

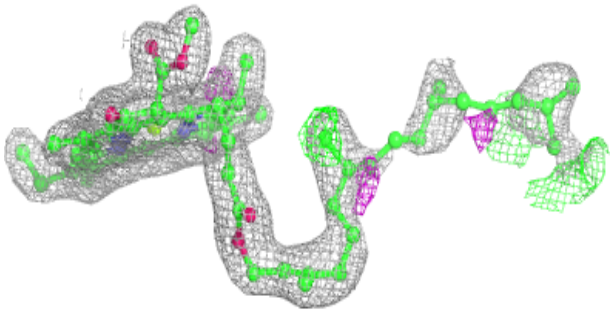
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

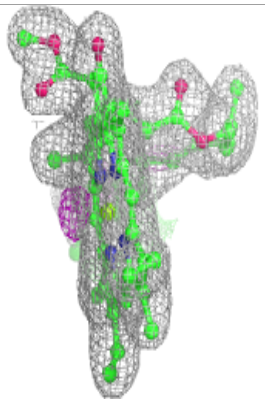


Electron density around CLA a 410:

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

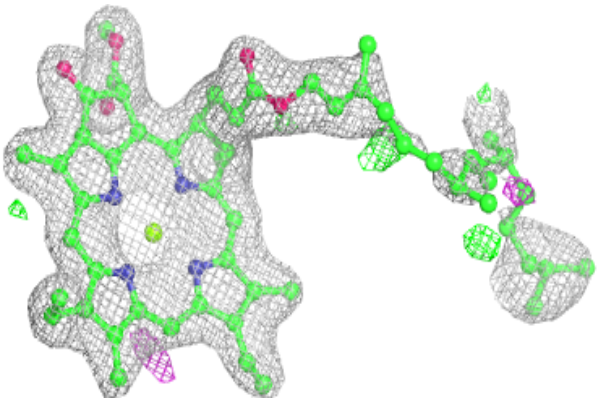


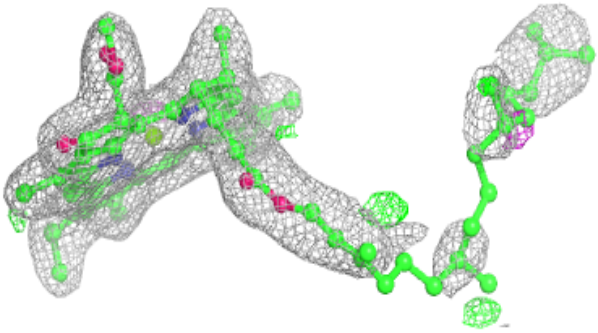


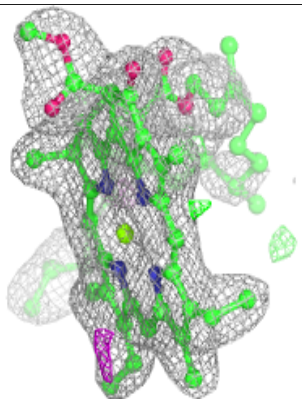


Electron density around CLA a 412:

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

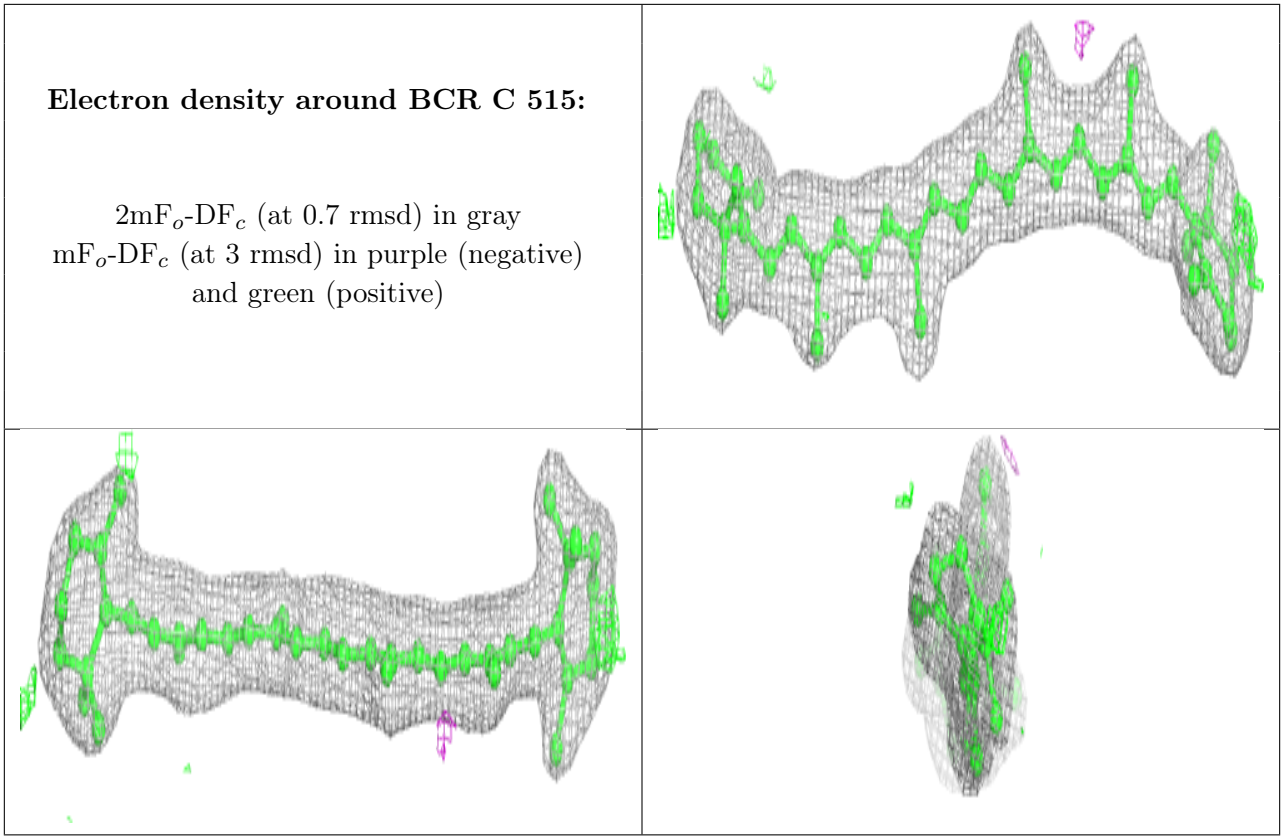






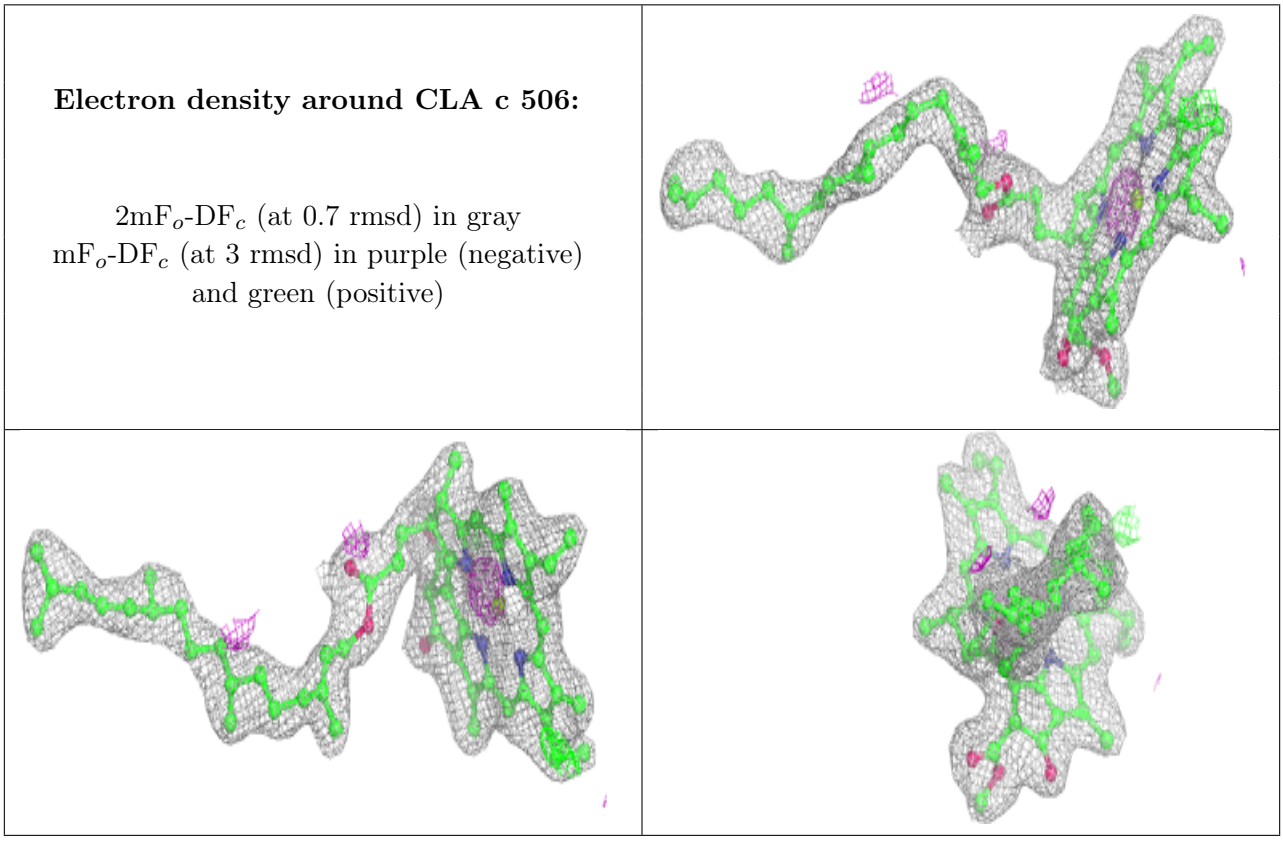
Electron density around BCR C 515:

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



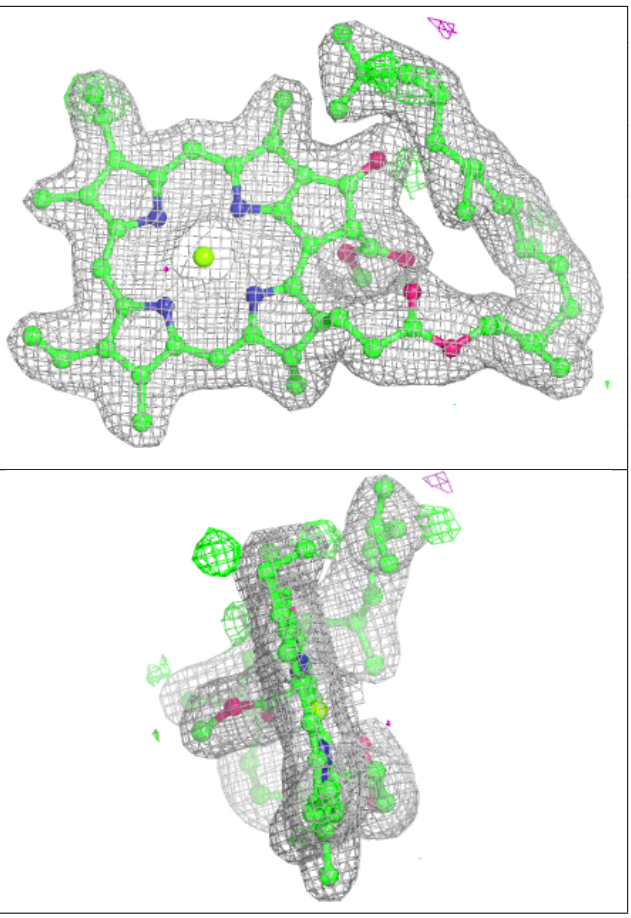
Electron density around CLA c 506:

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



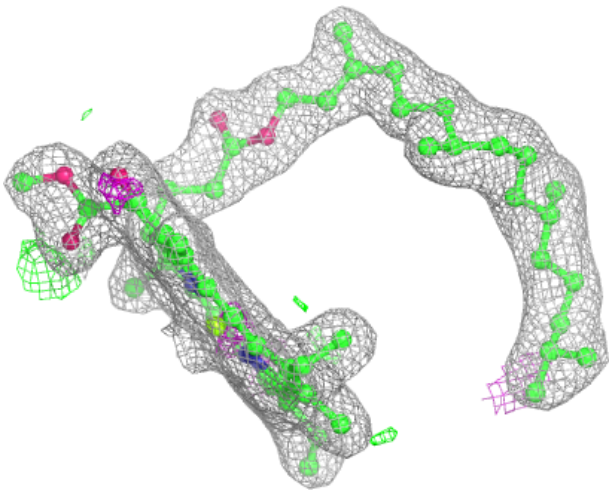
Electron density around CLA B 611:

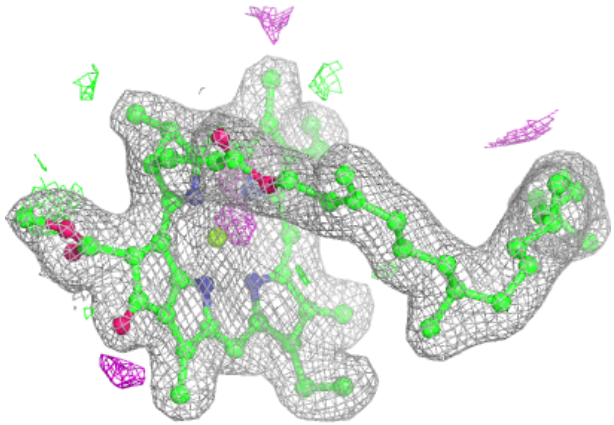
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

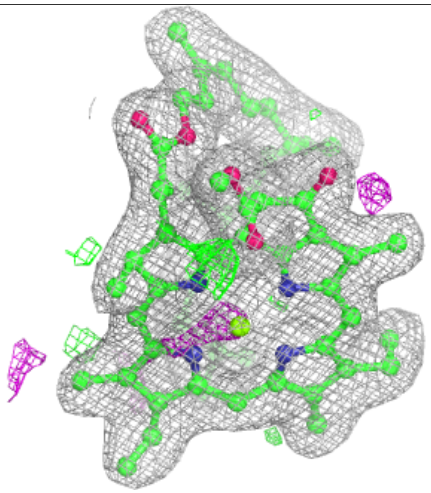


Electron density around CLA B 612:

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

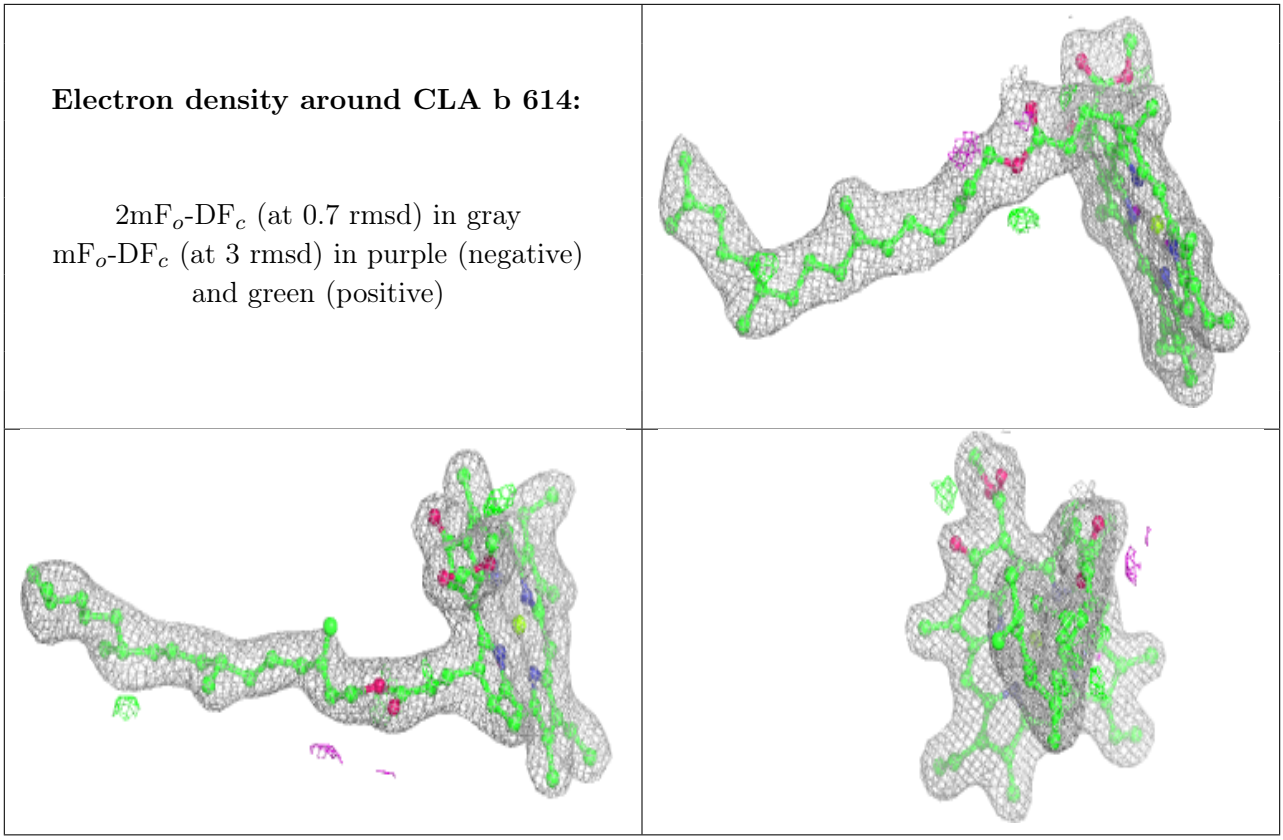






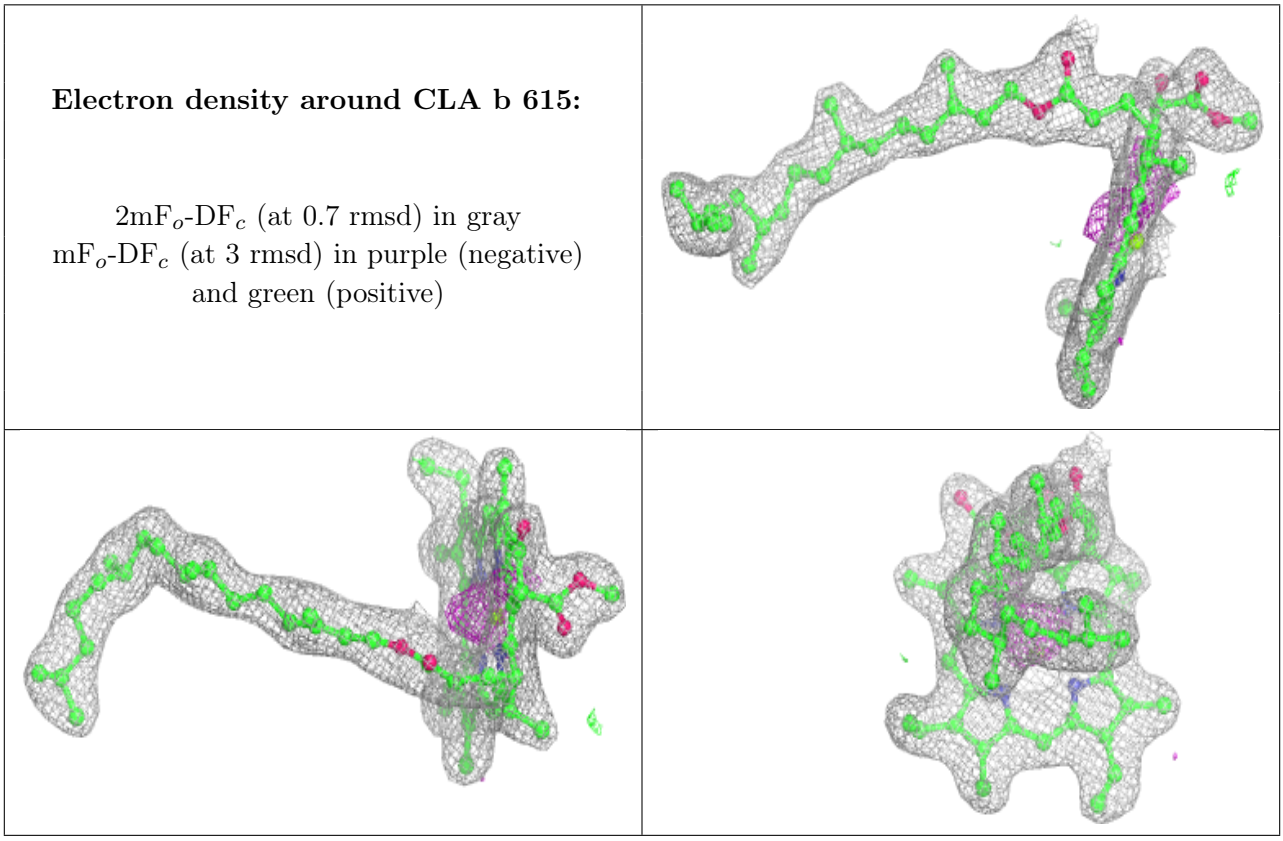
Electron density around CLA b 614:

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



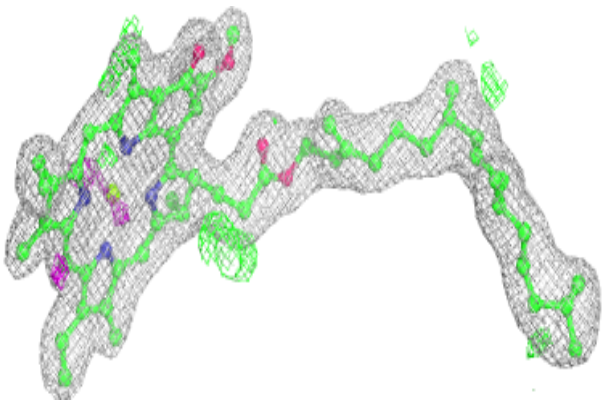
Electron density around CLA b 615:

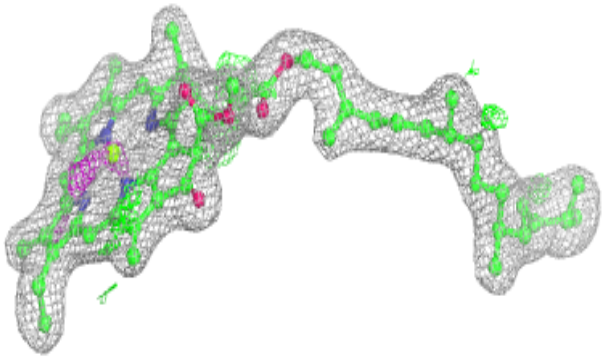
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

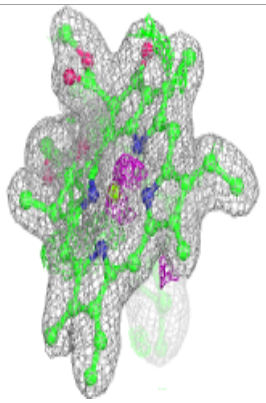


Electron density around CLA A 405:

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

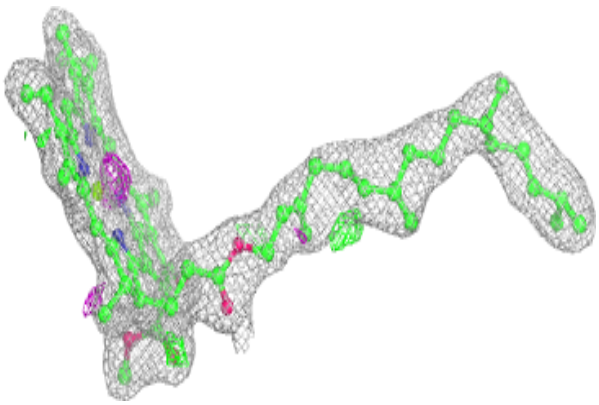


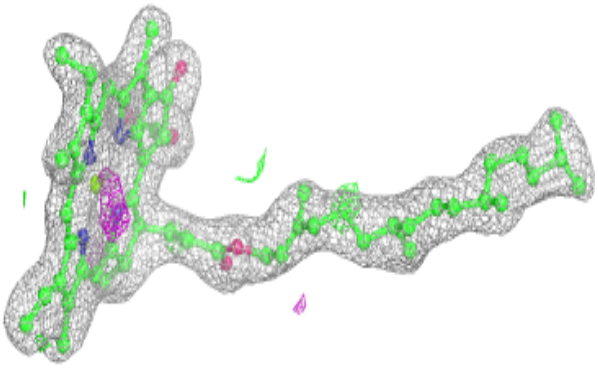


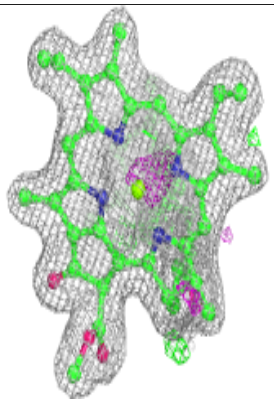


Electron density around CLA B 605:

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

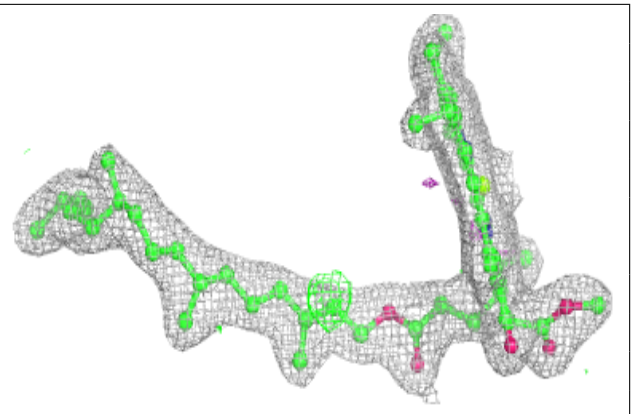


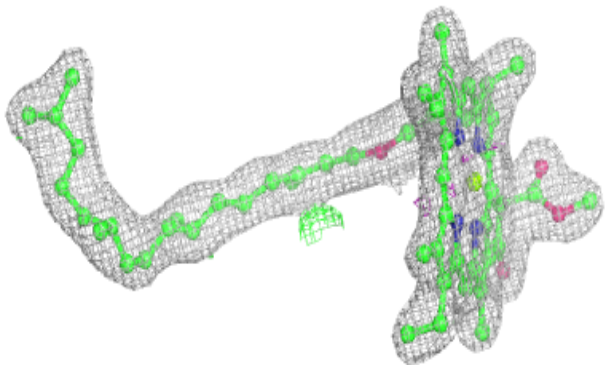


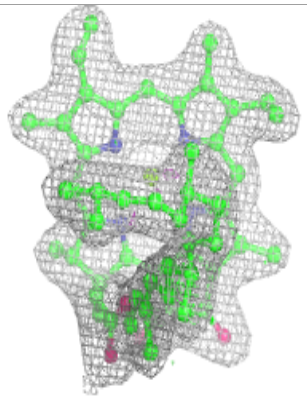


Electron density around CLA B 606:

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

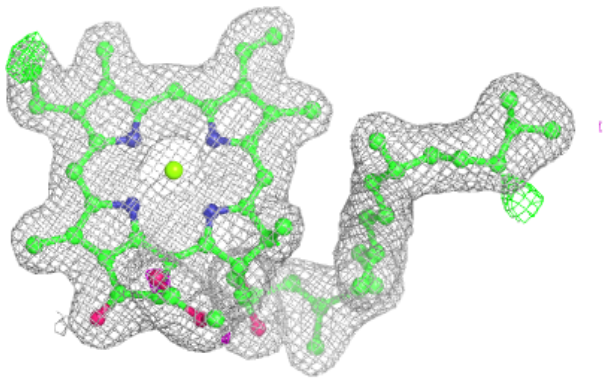


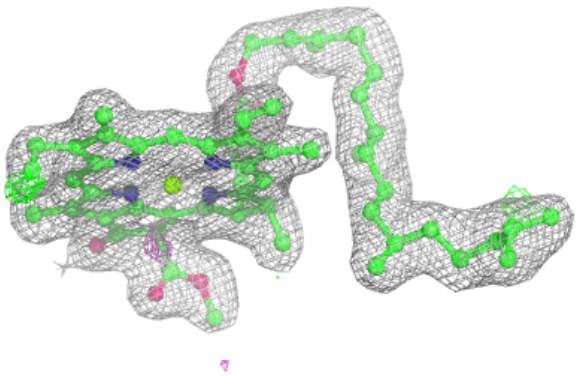


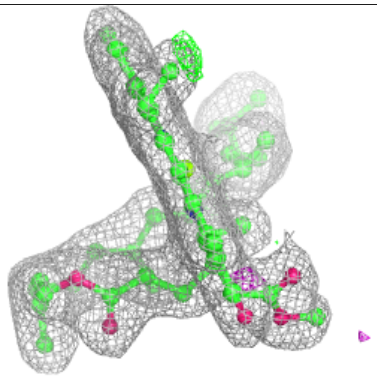


Electron density around CLA A 406:

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

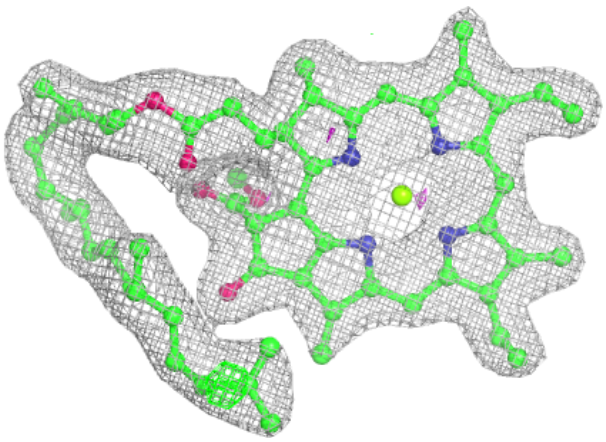


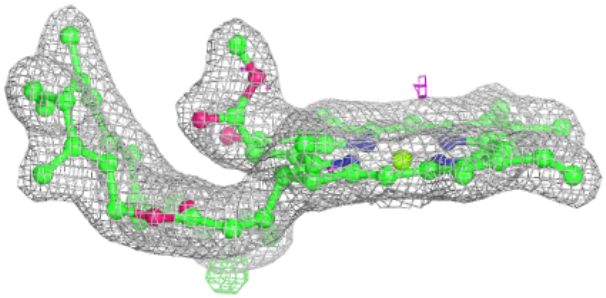


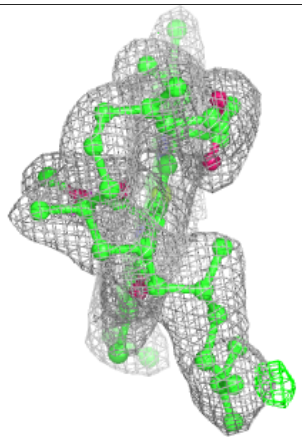


Electron density around CLA b 620:

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

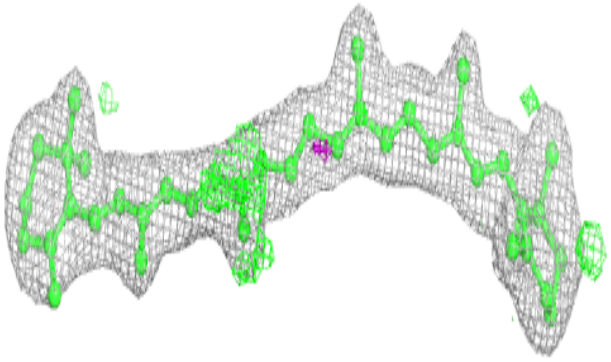


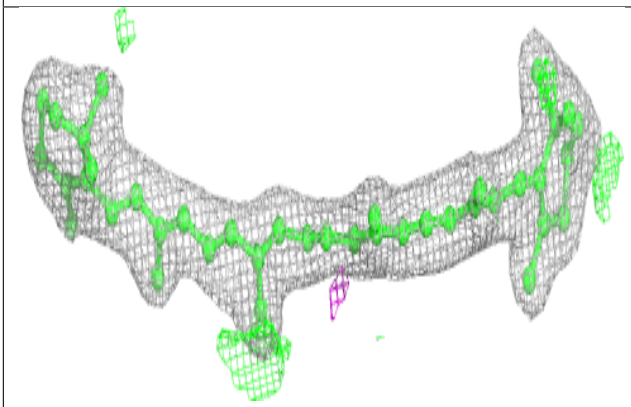


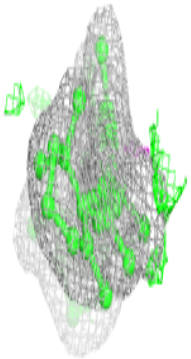


Electron density around BCR t 101:

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

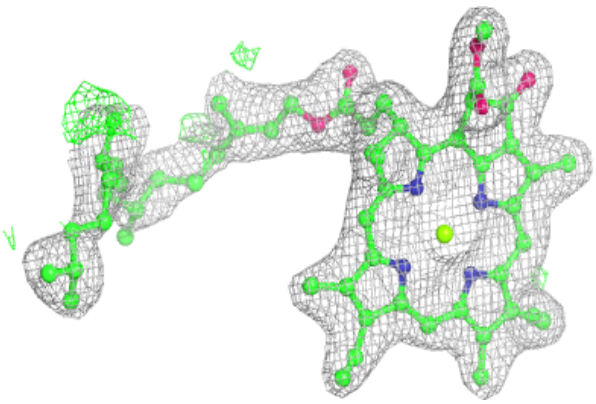


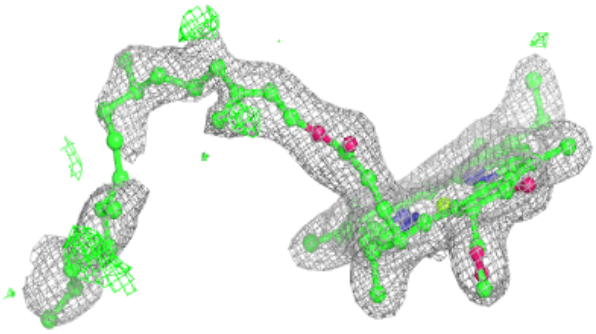


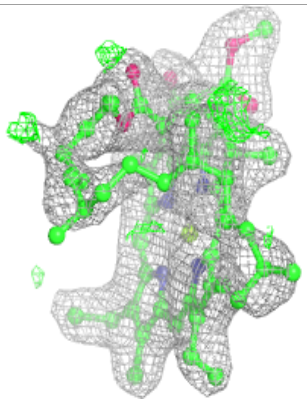


Electron density around CLA A 410:

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

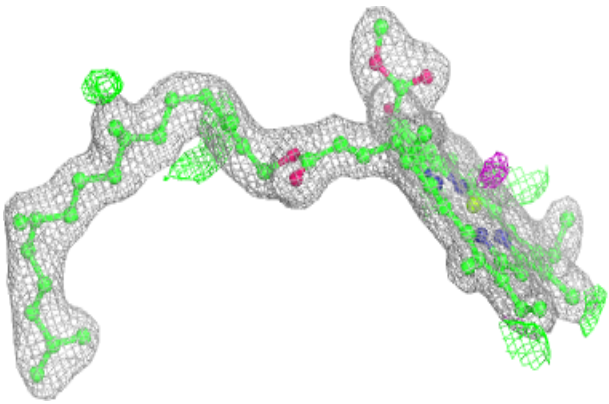


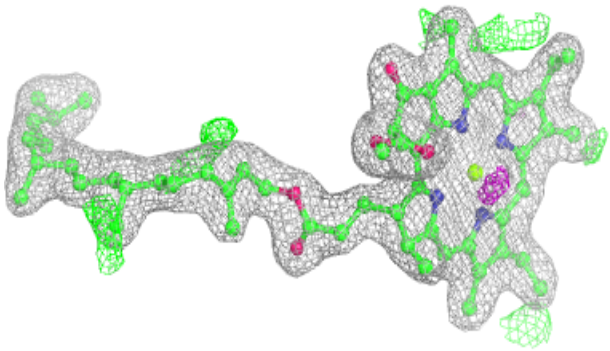




Electron density around CLA D 402:

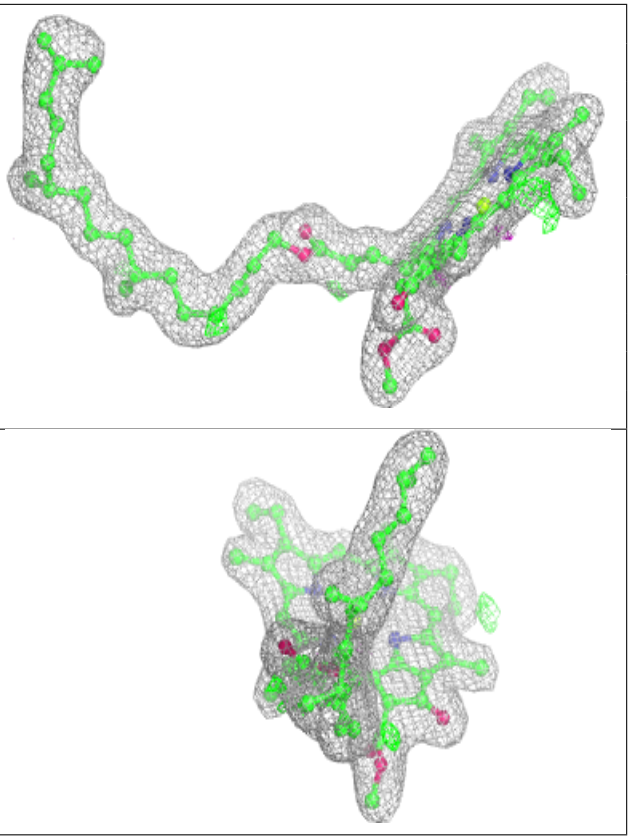
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

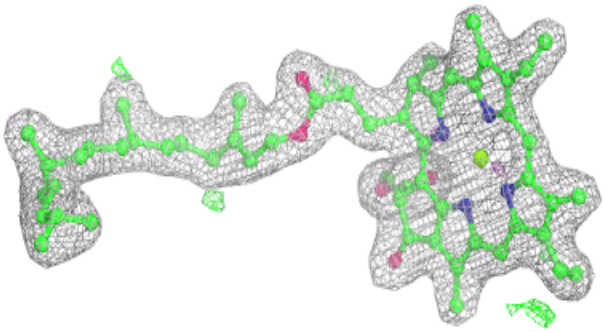




Electron density around CLA d 402:

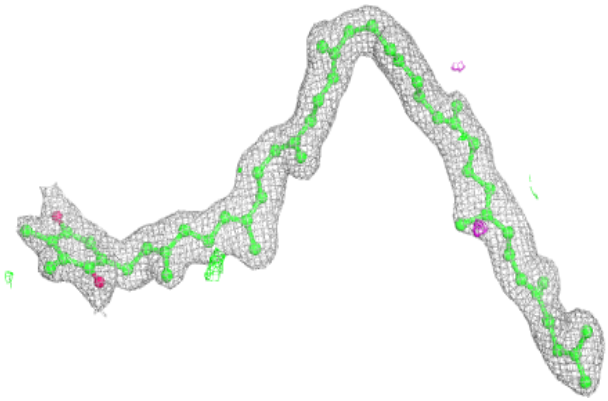
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

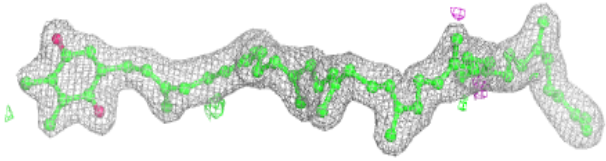


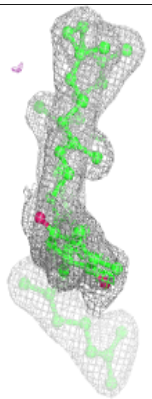


Electron density around PL9 d 405 (A):

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

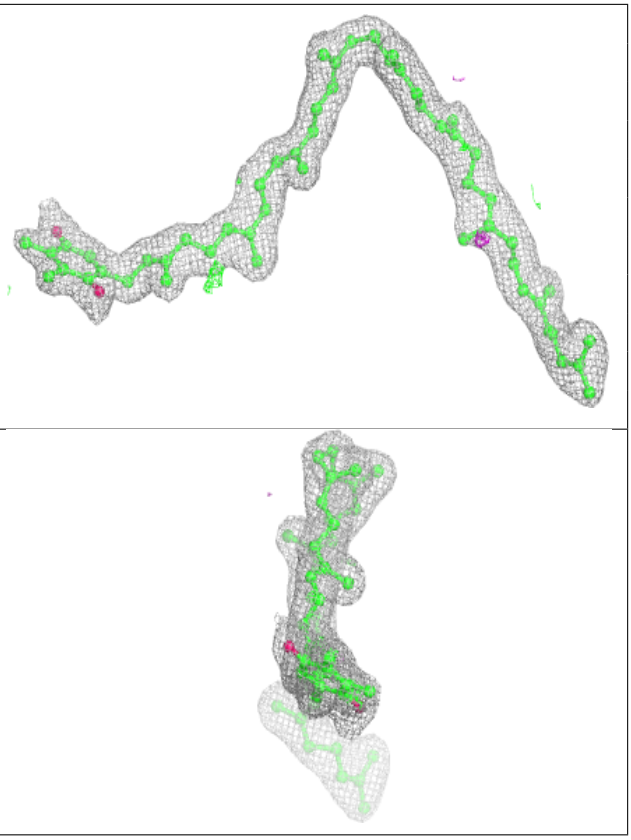






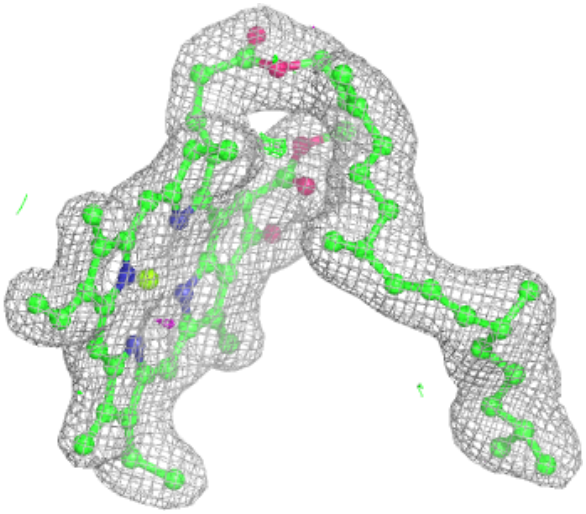
Electron density around PL9 d 405 (B):

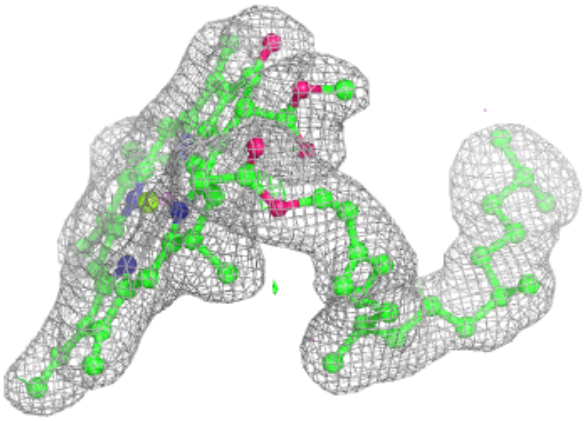
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

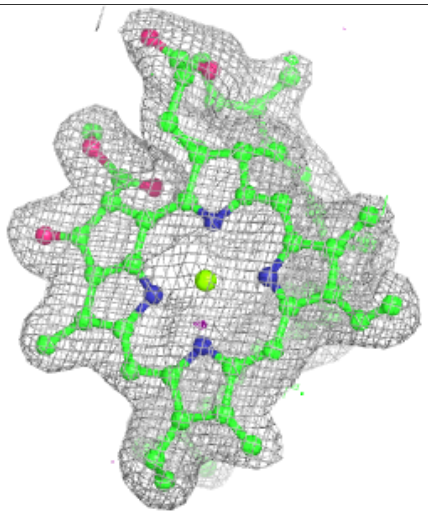


Electron density around CLA b 623:

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

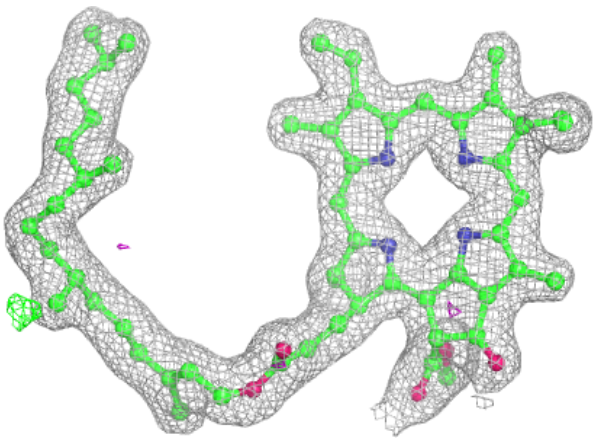


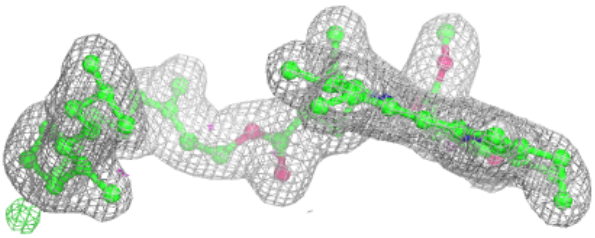


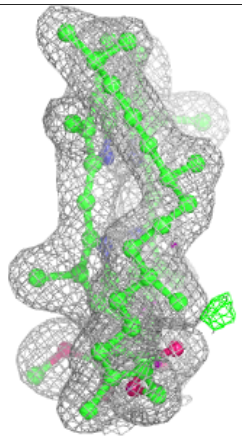


Electron density around PHO A 408:

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

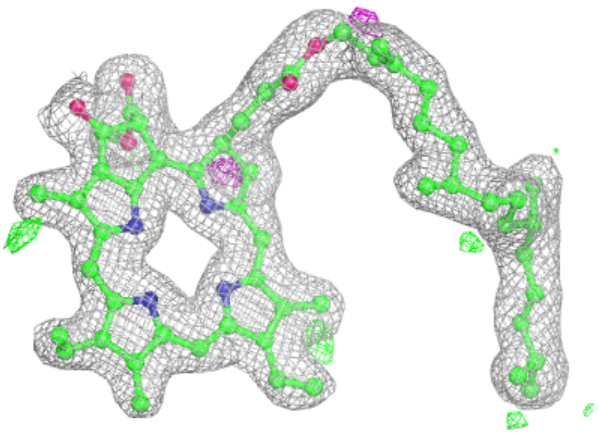


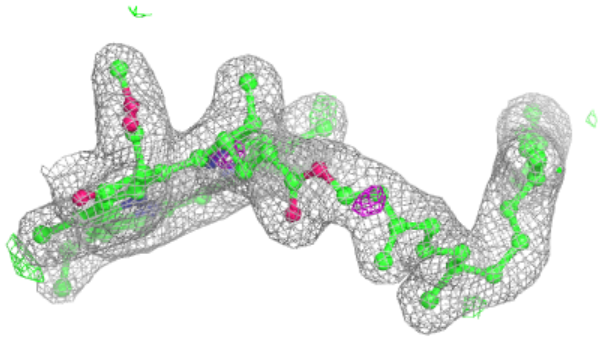


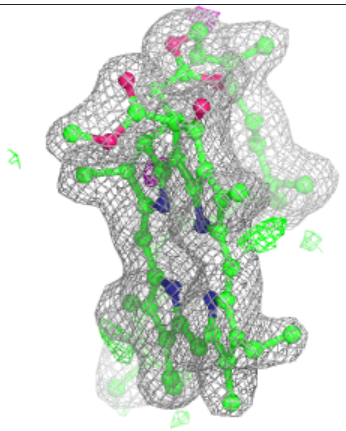


Electron density around PHO A 409 (A):

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

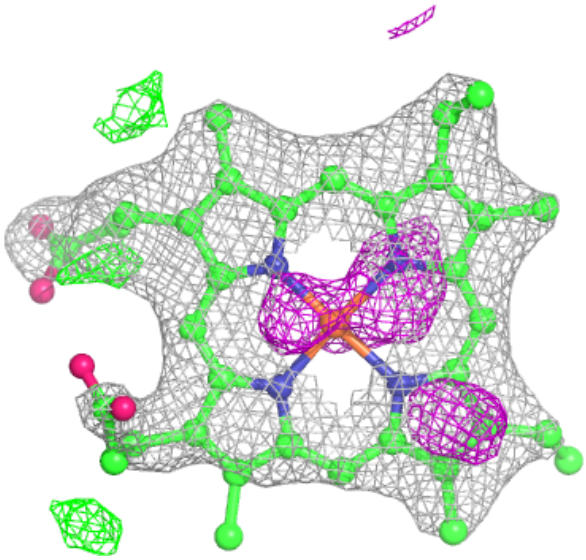


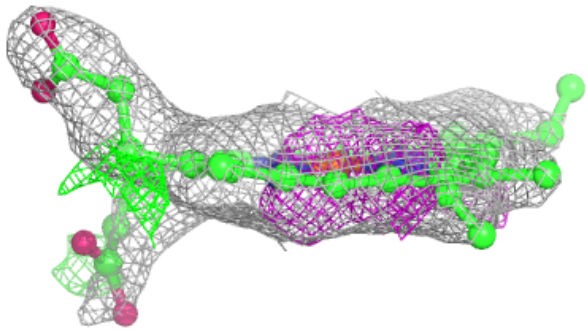


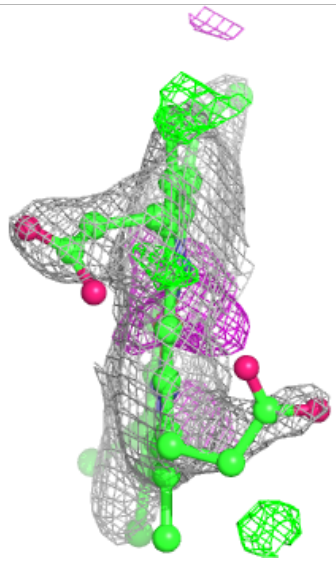


Electron density around HEM e 102:

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

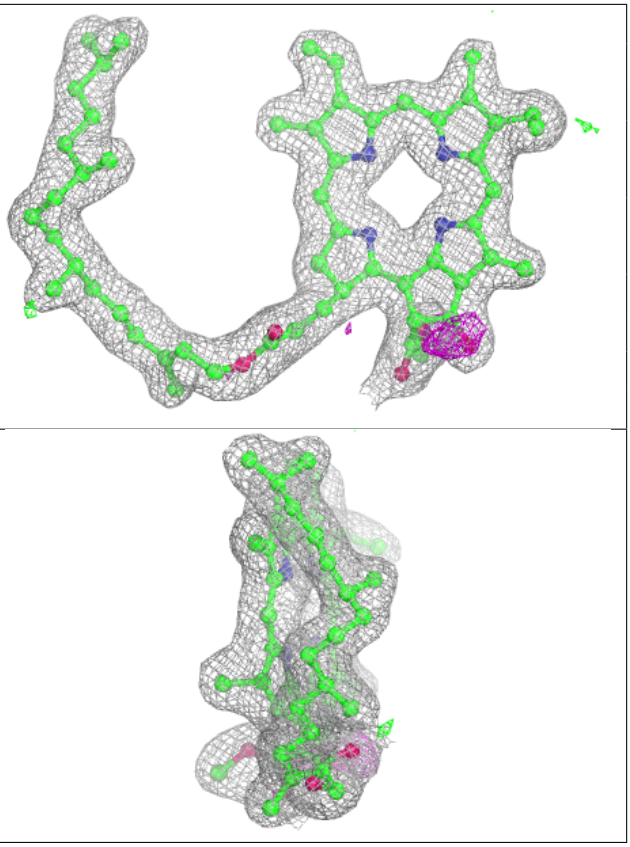






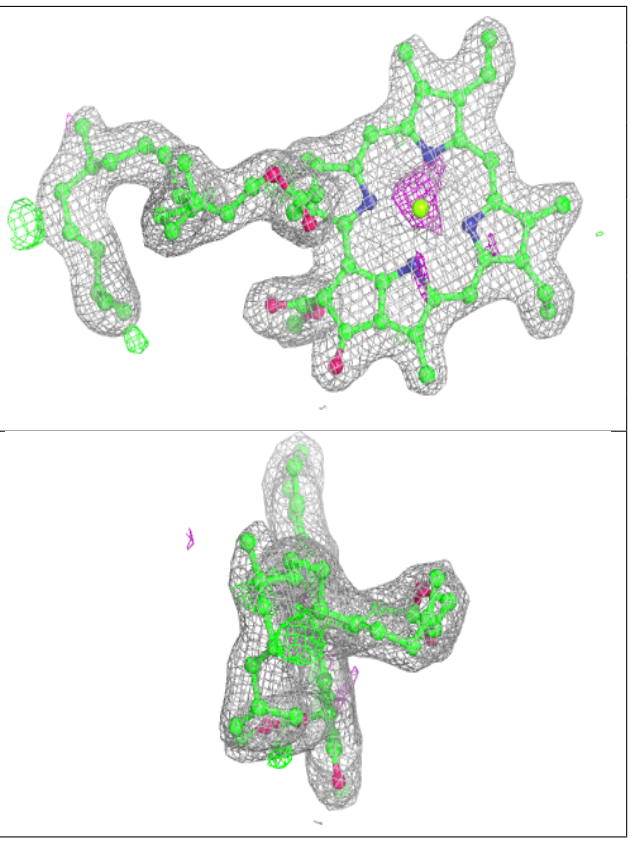
Electron density around PHO a 411:

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



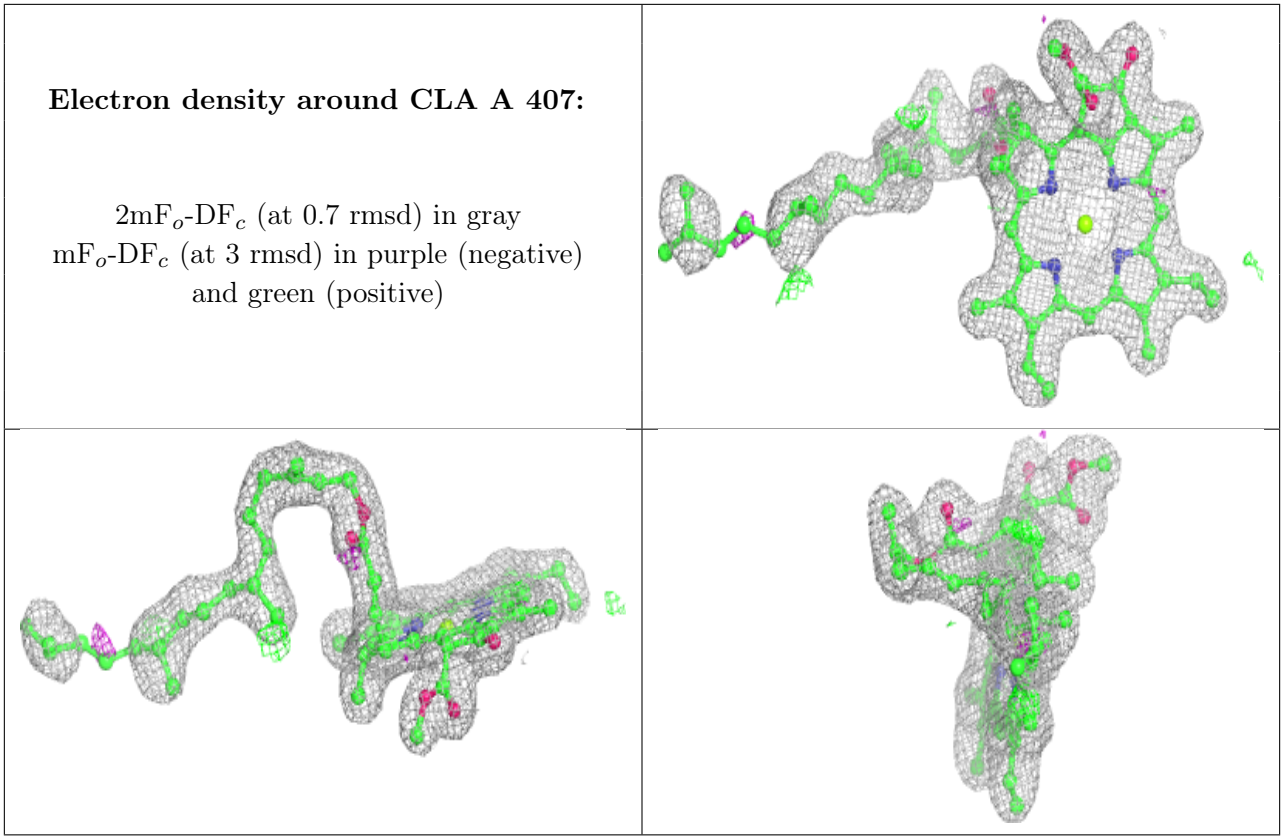
Electron density around CLA B 613:

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



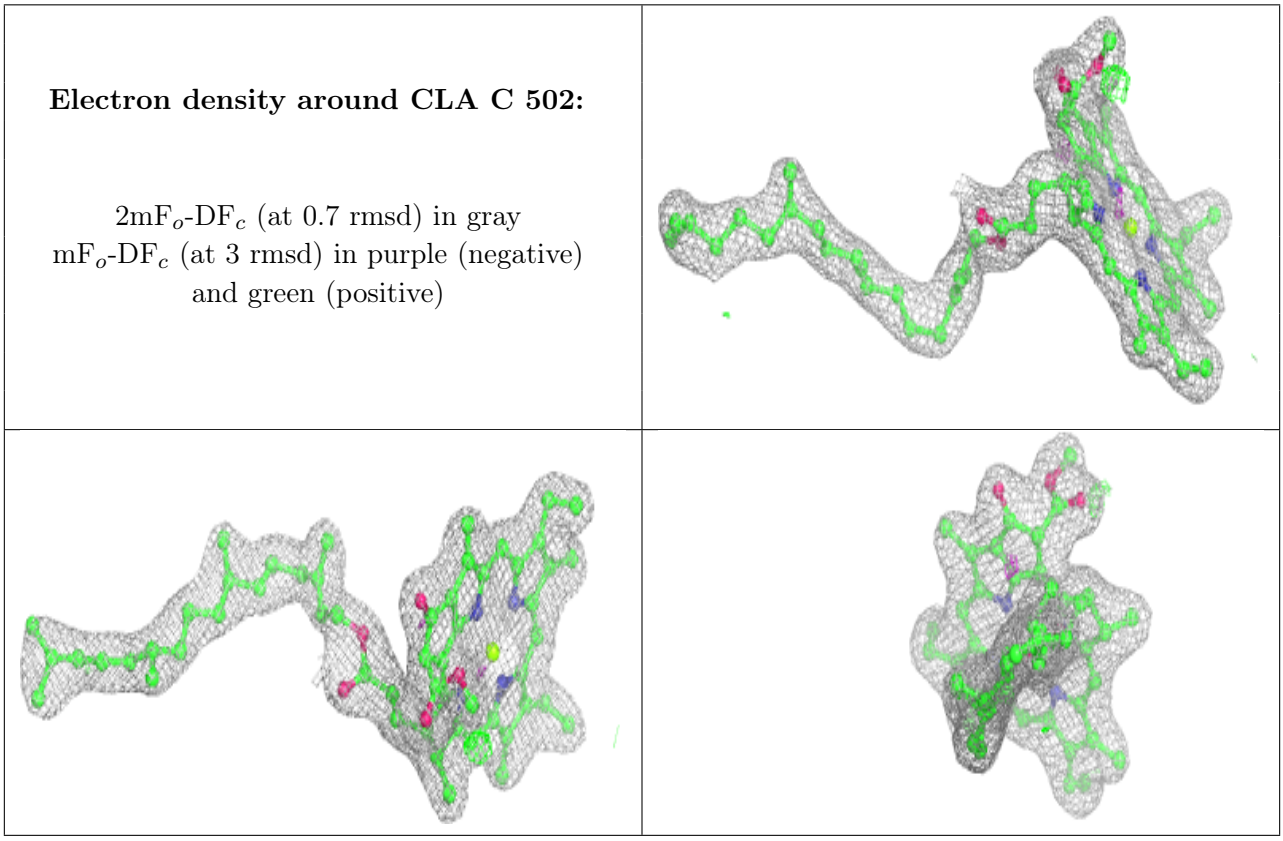
Electron density around CLA A 407:

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



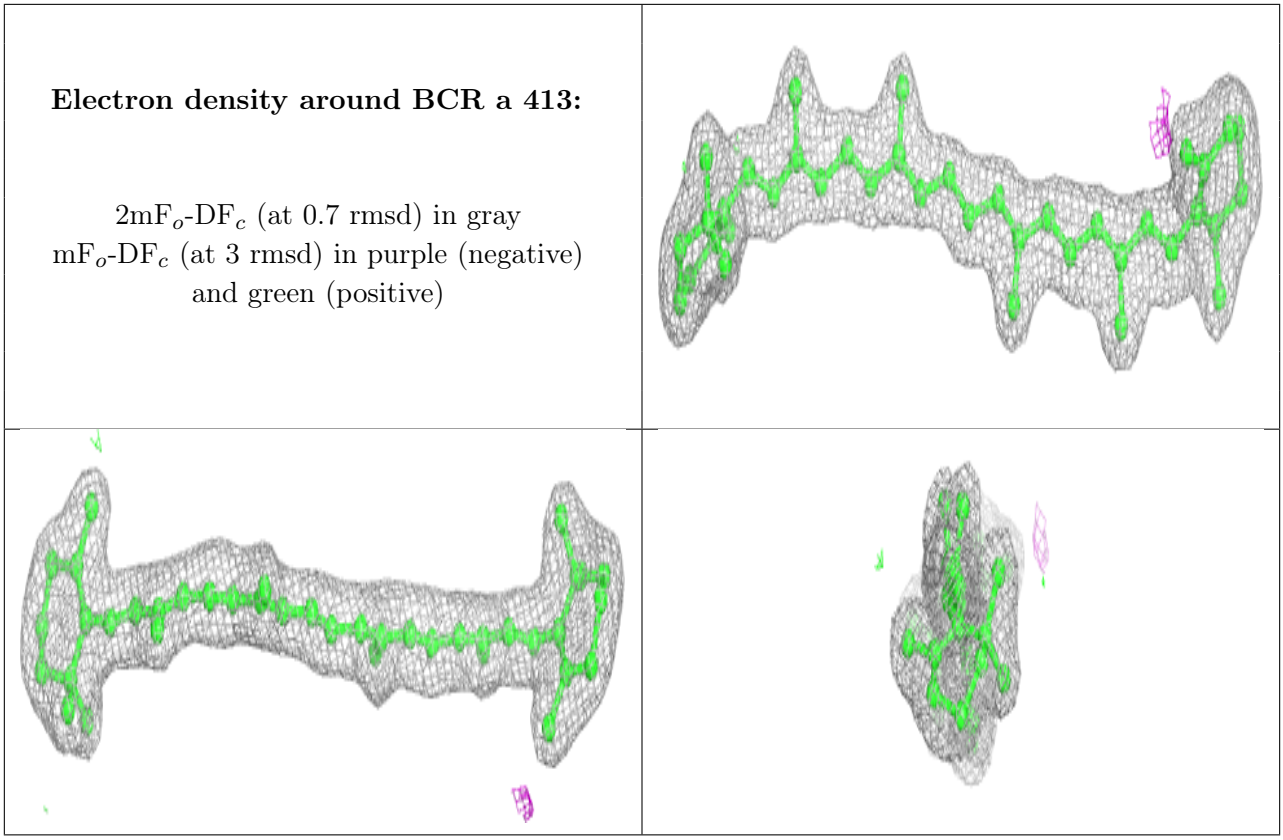
Electron density around CLA C 502:

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



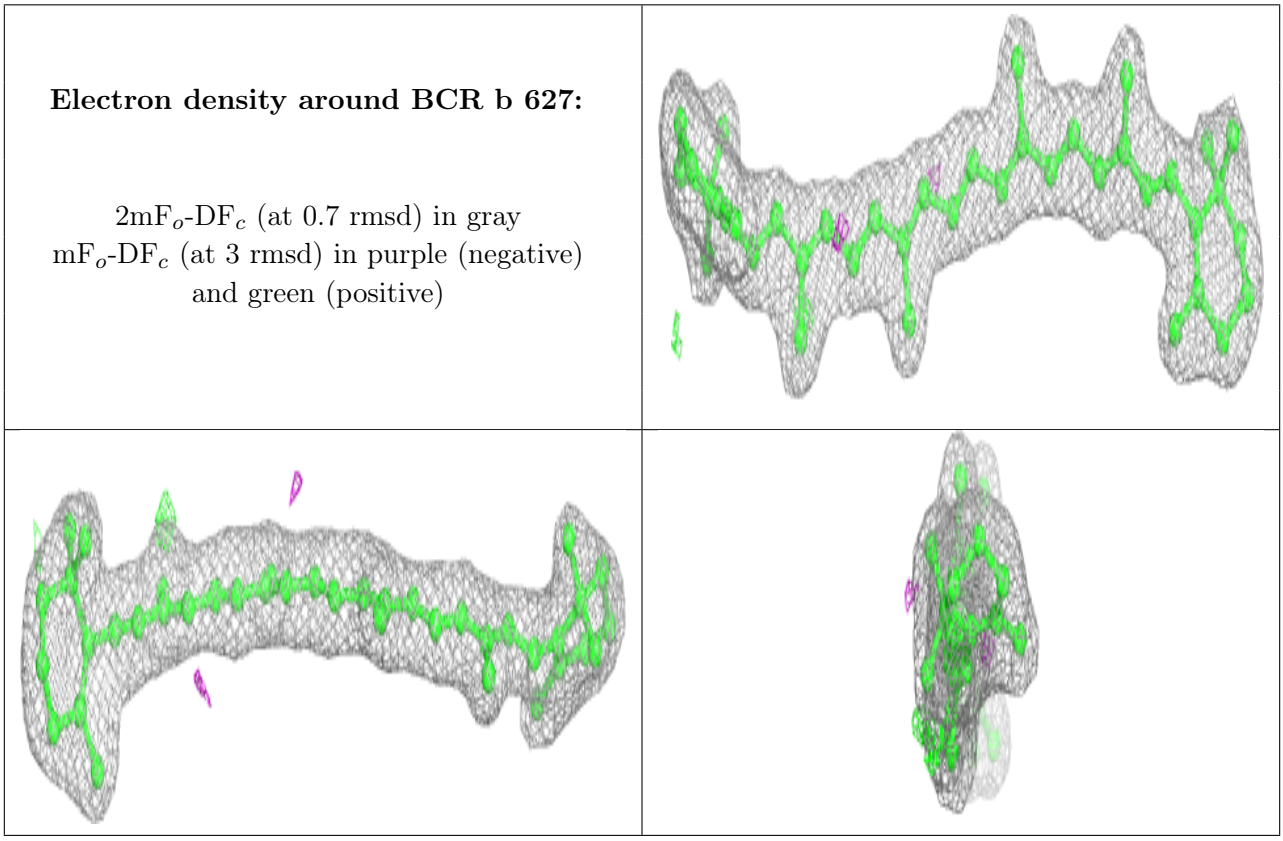
Electron density around BCR a 413:

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



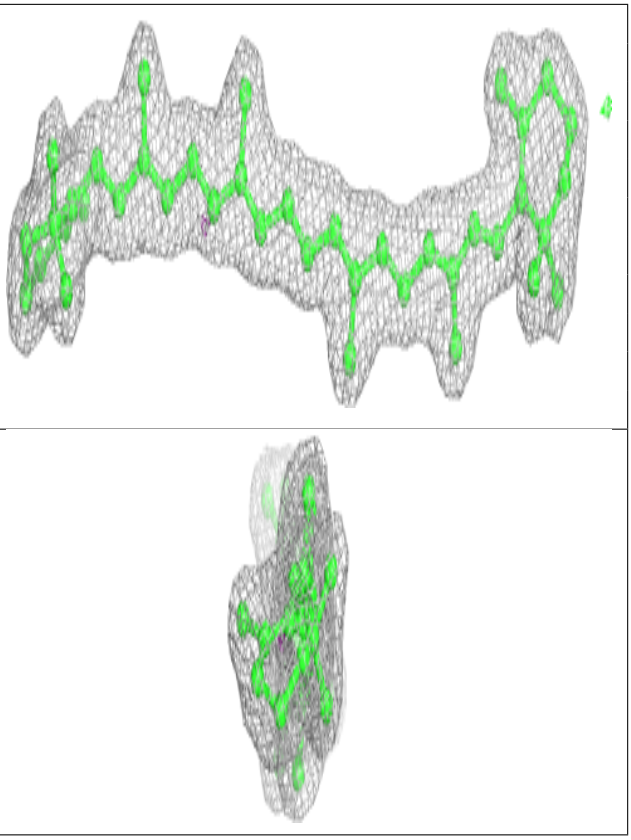
Electron density around BCR b 627:

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



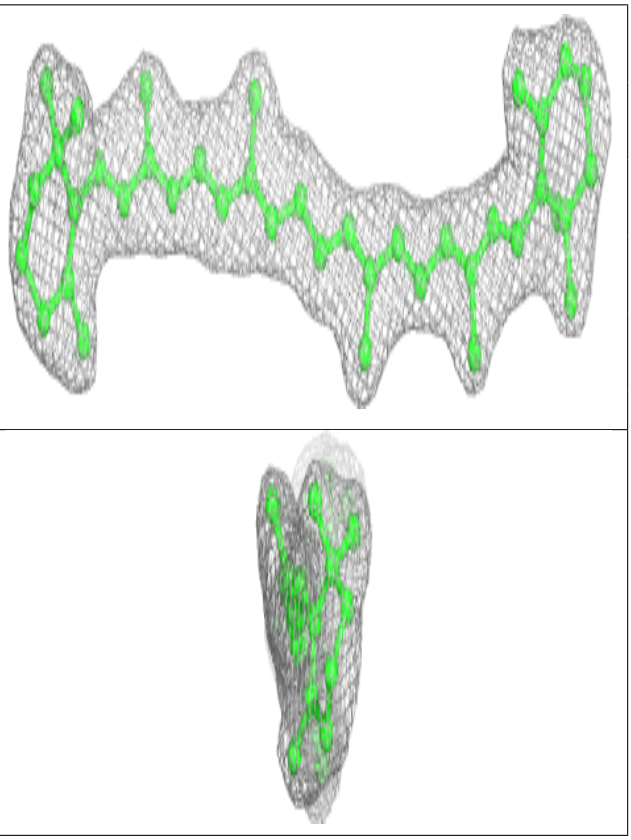
Electron density around BCR B 618:

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



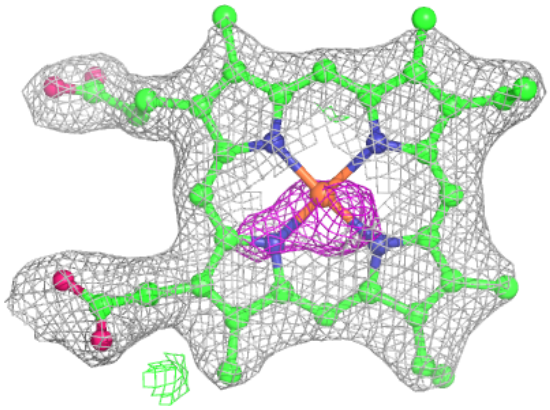
Electron density around BCR b 629:

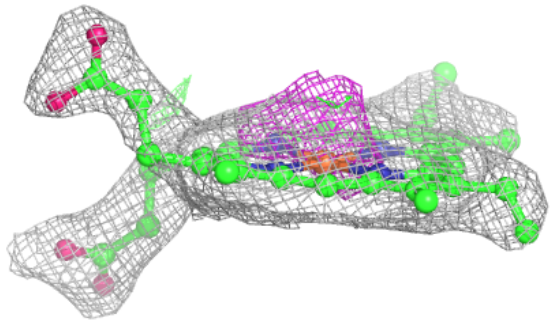
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

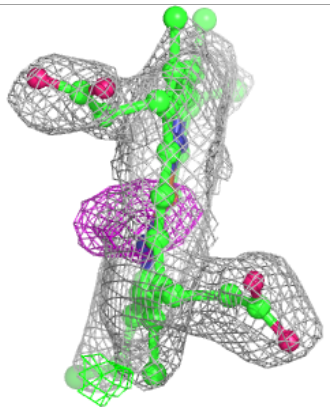


Electron density around HEM F 102:

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

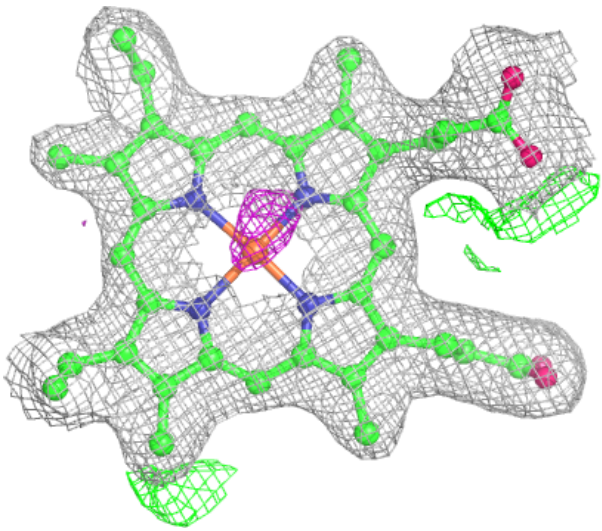


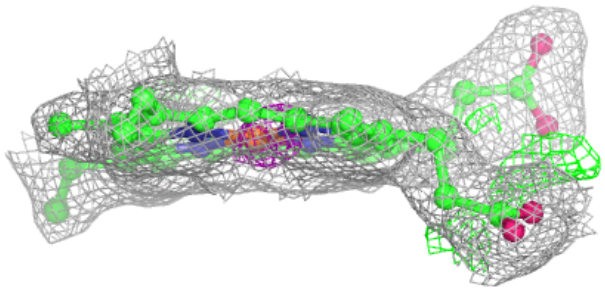


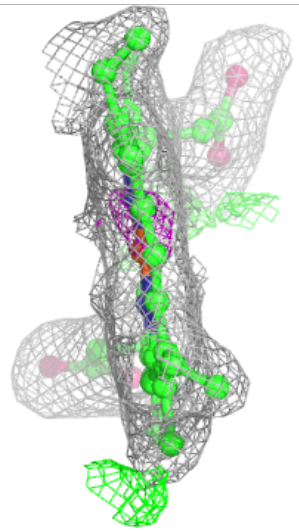


Electron density around HEM V 206:

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

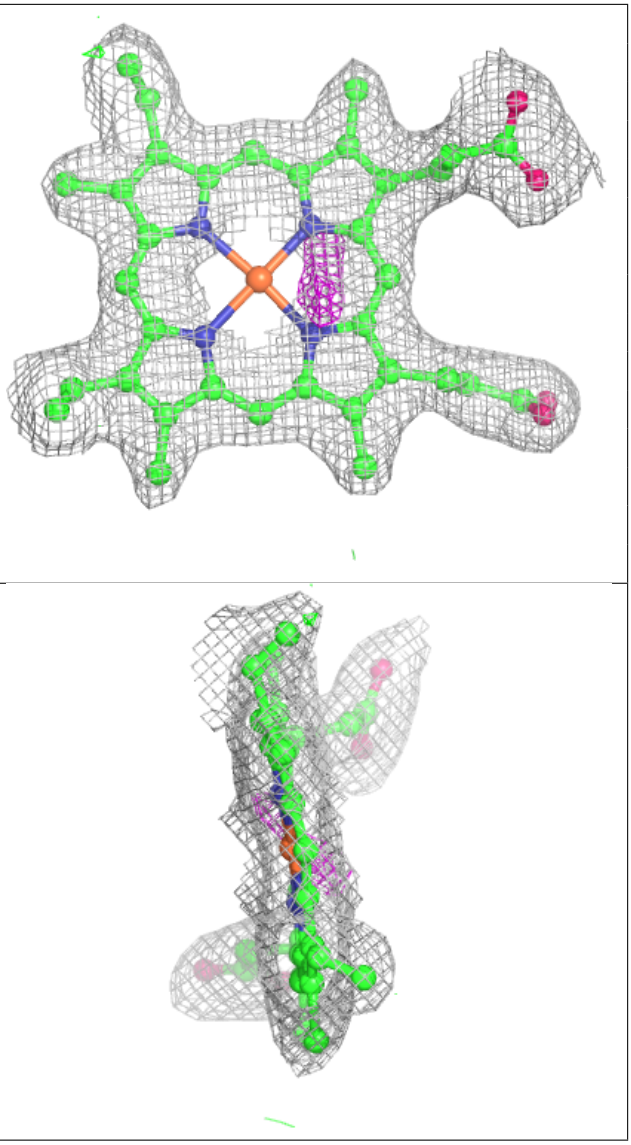






Electron density around HEM v 205:

$2mF_o$-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.