wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:10 PM JST

PDB ID	:	6JLO / pdb_00006jlo
Title	:	XFEL structure of cyanobacterial photosystem II (2F state, dataset2)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2019-03-06
Resolution	:	2.40 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:

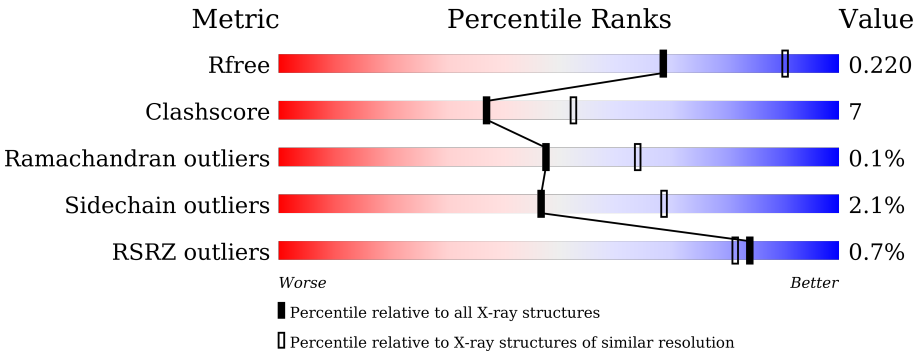
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	85% 12% ·
1	a	344	86% 11% ·
2	B	505	82% 18%
2	b	505	% 89% 11%
3	C	455	87% 11% ·
3	c	455	84% 15%

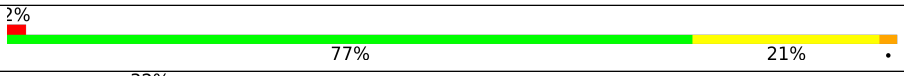
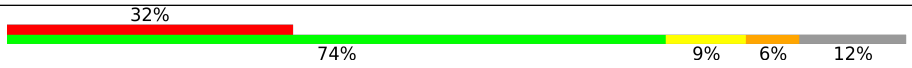
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	85% 15%
4	d	342	86% 13%
5	E	84	79% 18%
5	e	84	2% 76% 20%
6	F	44	55% 23% 23%
6	f	44	2% 50% 23% 27%
7	H	65	3% 88% 11%
7	h	65	2% 92% 8%
8	I	38	95% 5%
8	i	38	3% 84% 16%
9	J	39	3% 87% 10%
9	j	39	3% 79% 21%
10	K	37	78% 19%
10	k	37	78% 22%
11	L	37	78% 16% 5%
11	l	37	89% 11%
12	M	36	64% 28% 6%
12	m	36	75% 14% 6% 6%
13	O	244	87% 12%
13	o	244	85% 14%
14	T	32	75% 16% 6%
14	t	32	3% 84% 9% 6%
15	U	104	82% 12% 7%
15	u	104	80% 12% 7%
16	V	137	90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
41	HEC	V	205	X	-	-	-
41	HEC	v	206	X	-	-	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 55695 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
1	A	334	Total	C	N	O	S	0	54	0
			3024	1969	499	538	18			
1	a	334	Total	C	N	O	S	0	56	0
			3020	1970	497	535	18			

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
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

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

Continued on next page...

Continued from previous page...

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
4	D	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

Continued on next page...

Continued from previous page...

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

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
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

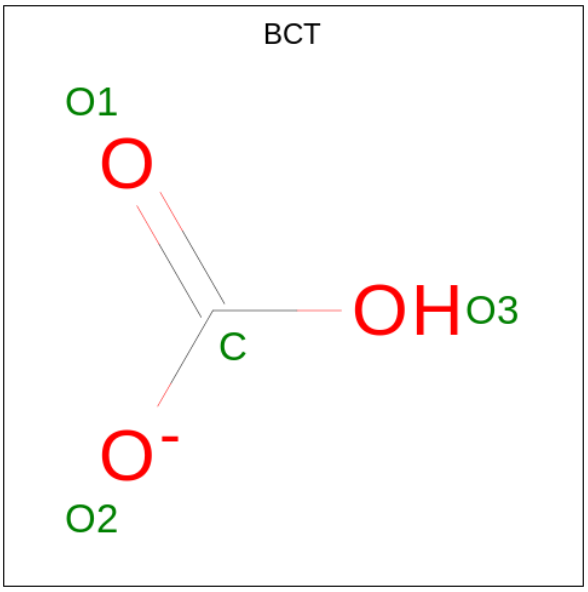
- Molecule 20 is a protein called Photosystem II protein Y.

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

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

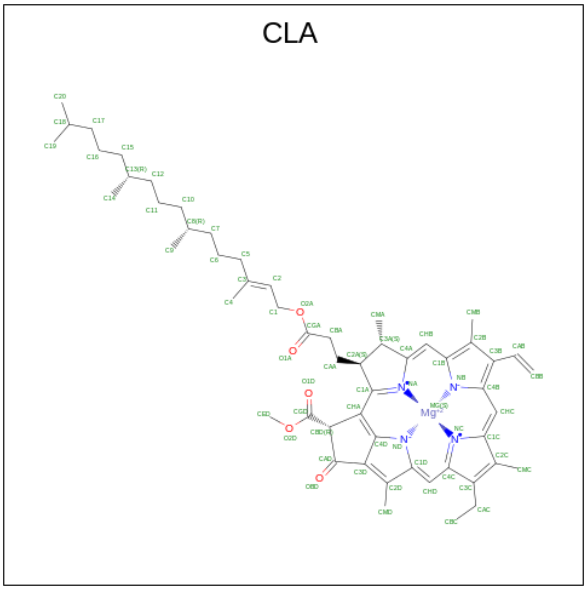
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	2
			4	4		
21	U	1	Total	Cl	0	0
			1	1		
21	a	2	Total	Cl	0	2
			4	4		
21	v	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 8 2 6	0	1
22	d	1	Total C O 8 2 6	0	1

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

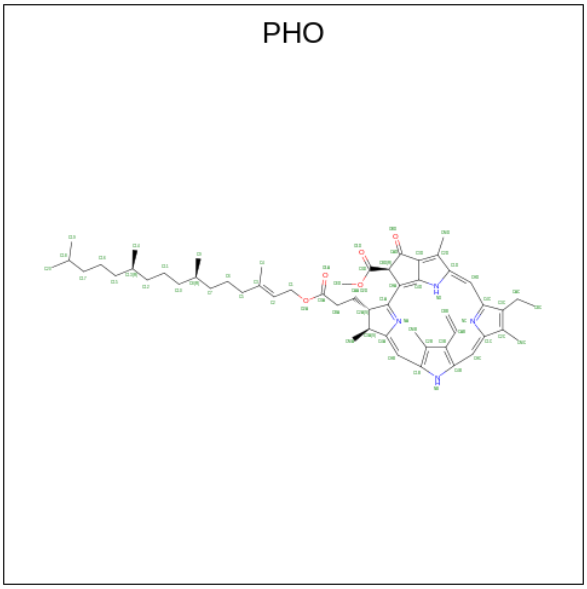
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

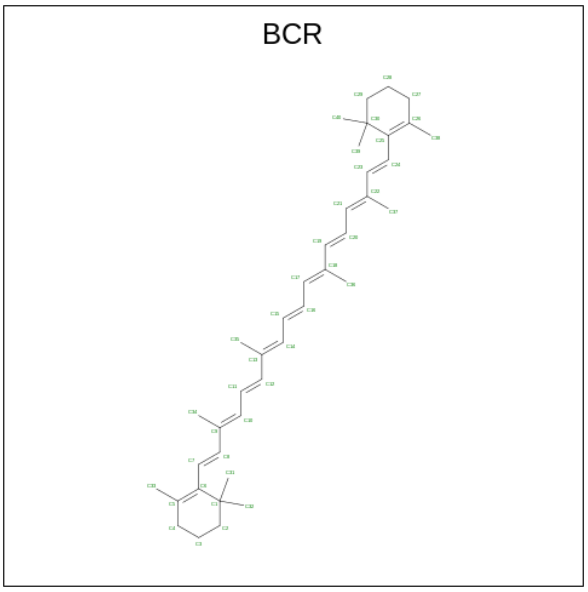
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



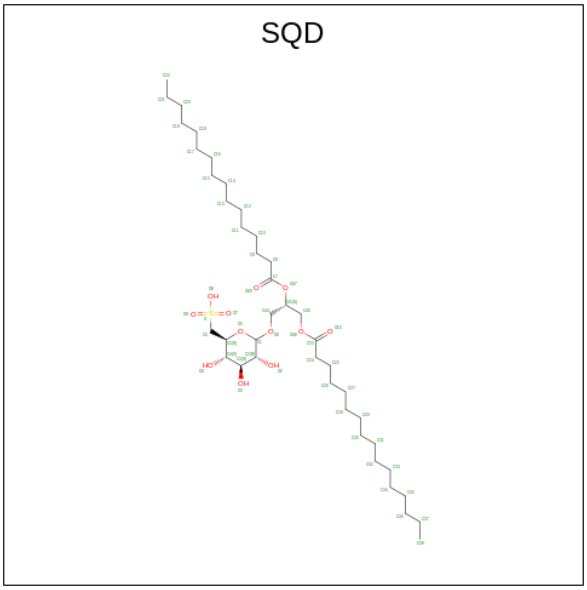
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



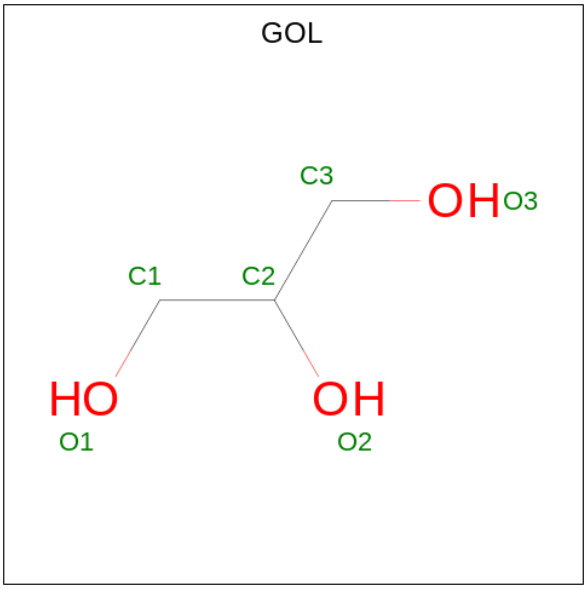
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

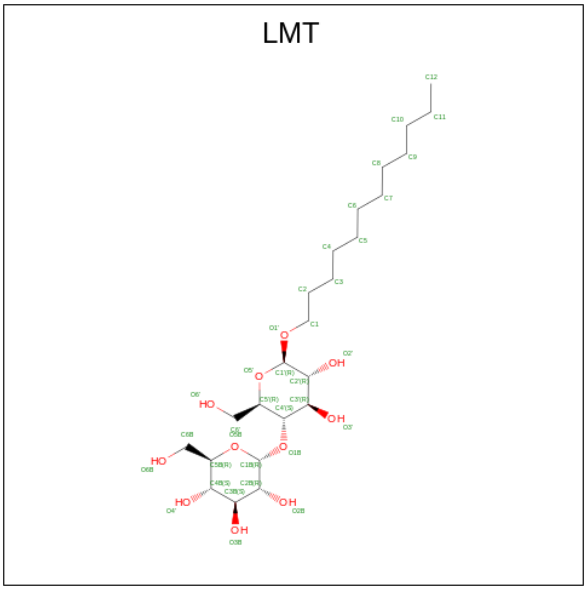
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	D	1	Total	C	O	0	0
			6	3	3		
27	F	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	T	1	Total	C	O	0	0
			6	3	3		
27	T	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 6 3 3	0	0
27	f	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	t	1	Total C O 6 3 3	0	0
27	v	1	Total C O 6 3 3	0	0
27	v	1	Total C O 6 3 3	0	0
27	v	1	Total C O 6 3 3	0	0
27	v	1	Total C O 6 3 3	0	0

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



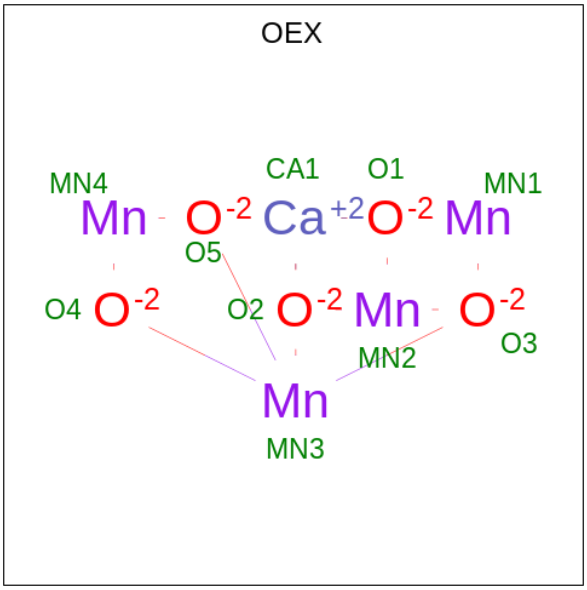
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 35 24 11	0	0
28	B	1	Total C O 25 19 6	0	0
28	C	1	Total C O 35 24 11	0	0

Continued on next page...

Continued from previous page...

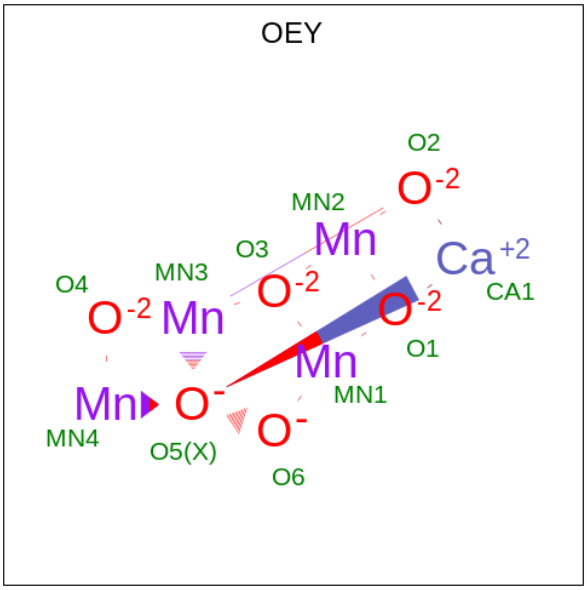
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	1	Total C O 35 24 11	0	0
28	F	1	Total C O 35 24 11	0	0
28	M	1	Total C O 35 24 11	0	0
28	M	1	Total C O 35 24 11	0	0
28	M	1	Total C O 35 24 11	0	0
28	T	1	Total C O 25 19 6	0	0
28	a	1	Total C O 35 24 11	0	0
28	a	1	Total C O 35 24 11	0	0
28	b	1	Total C O 25 19 6	0	0
28	e	1	Total C O 35 24 11	0	0
28	m	1	Total C O 35 24 11	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



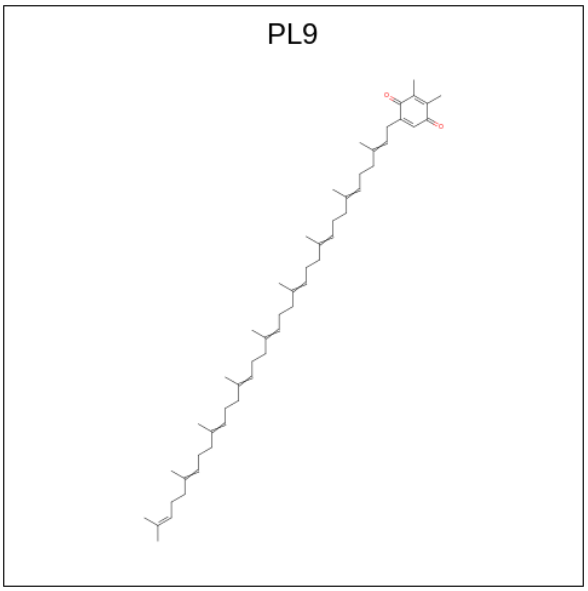
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: $CaMn_4O_6$).



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

- Molecule 31 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

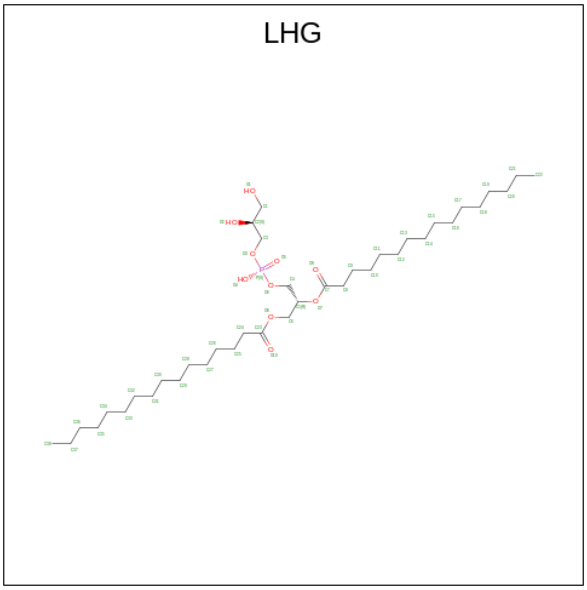
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	I	1	Total C O 40 35 5	0	0
32	J	1	Total C 10 10	0	0
32	K	1	Total C O 34 29 5	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O P 42 31 10 1	0	0
33	D	1	Total C O P 49 38 10 1	0	0
33	D	1	Total C O P 49 38 10 1	0	0
33	D	1	Total C O P 49 38 10 1	0	0

Continued on next page...

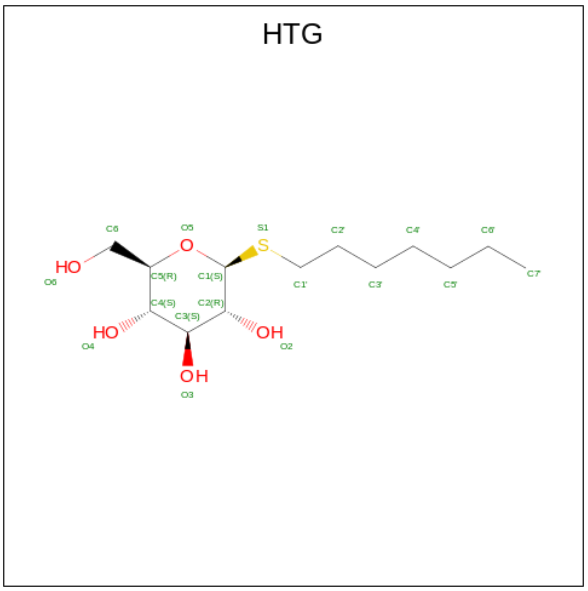
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	L	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			42	31	10	1		
33	b	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



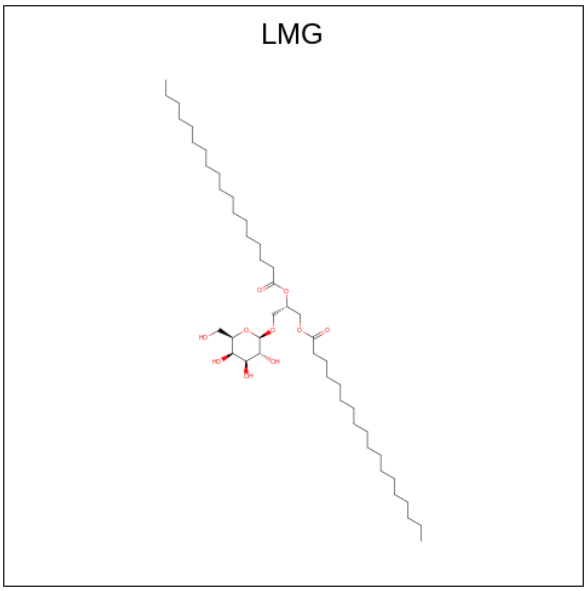
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



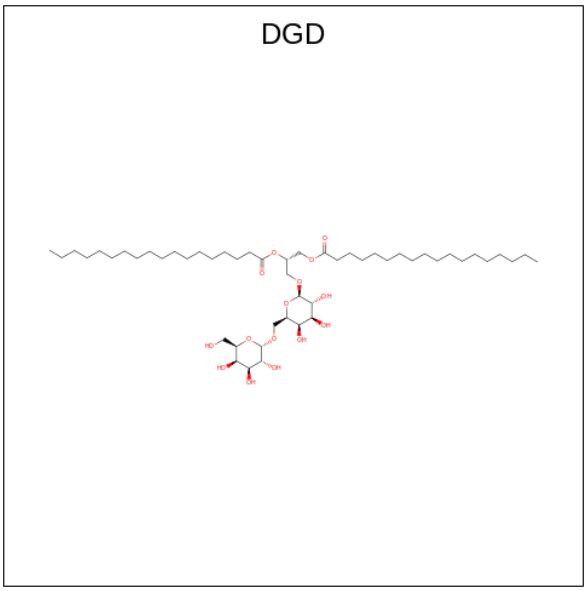
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 51 41 10	0	0
36	C	1	Total C O 51 41 10	0	0
36	C	1	Total C O 51 41 10	0	0
36	D	1	Total C O 51 41 10	0	0
36	M	1	Total C O 51 41 10	0	0
36	Z	1	Total C O 37 27 10	0	0
36	a	1	Total C O 51 41 10	0	0
36	b	1	Total C O 51 41 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	c	1	Total C O 51 41 10	0	0
36	d	1	Total C O 51 41 10	0	0
36	k	1	Total C O 51 41 10	0	0
36	z	1	Total C O 39 29 10	0	0

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



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

Continued on next page...

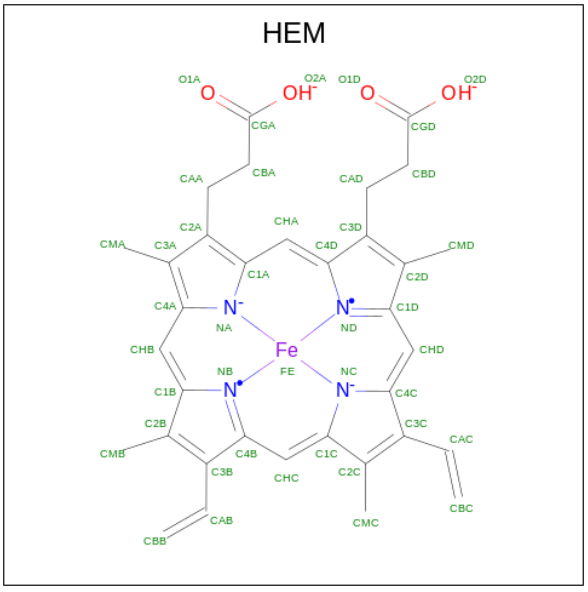
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	c	1	Total C O 62 47 15	0	0
37	d	1	Total C O 62 47 15	0	0
37	h	1	Total C O 62 47 15	0	0

- Molecule 38 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total Fe 2 2	0	1
38	a	1	Total Fe 1 1	0	1

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

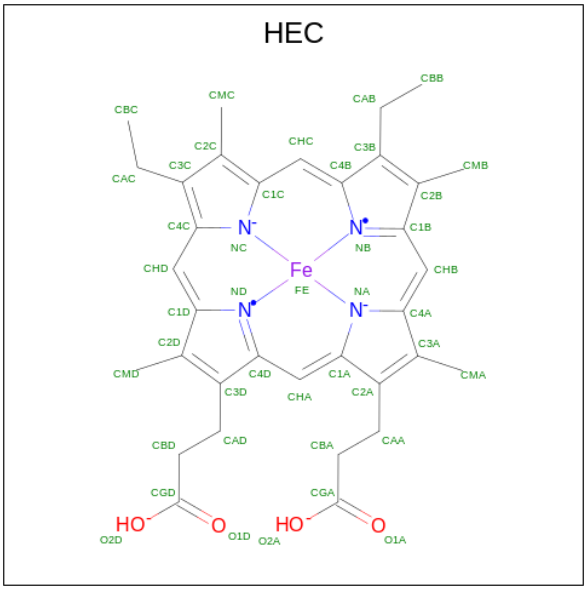


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	F	1	Total C Fe N O 43 34 1 4 4	0	0
39	e	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 41 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	A	157	Total O 169 169	0	14
42	B	287	Total O 291 291	0	4
42	C	231	Total O 235 235	0	4
42	D	143	Total O 147 147	0	5
42	E	32	Total O 33 33	0	1
42	F	11	Total O 11 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	H	44	Total O 44 44	0	0
42	I	5	Total O 5 5	0	0
42	J	10	Total O 10 10	0	0
42	K	10	Total O 10 10	0	0
42	L	11	Total O 12 12	0	1
42	M	25	Total O 25 25	0	0
42	O	178	Total O 180 180	0	2
42	T	16	Total O 17 17	0	1
42	U	80	Total O 80 80	0	0
42	V	114	Total O 116 116	0	2
42	Y	4	Total O 4 4	0	0
42	X	8	Total O 8 8	0	0
42	Z	1	Total O 1 1	0	0
42	a	151	Total O 160 160	0	11
42	b	260	Total O 263 263	0	3
42	c	194	Total O 199 199	0	5
42	d	138	Total O 141 141	0	4
42	e	20	Total O 20 20	0	0
42	f	7	Total O 7 7	0	0
42	h	43	Total O 43 43	0	0
42	i	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

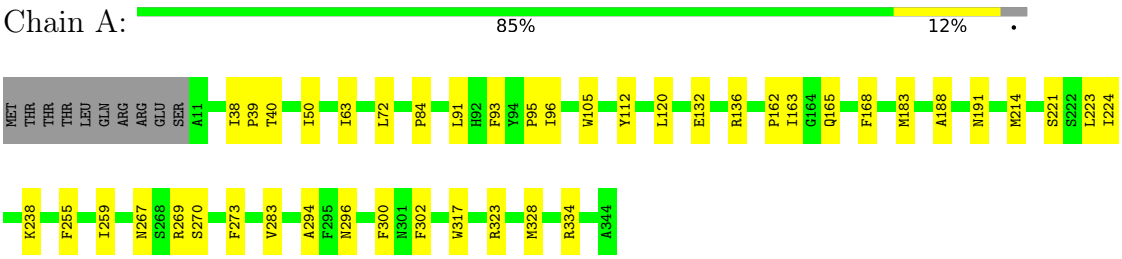
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	j	6	Total O 6 6	0	0
42	k	8	Total O 8 8	0	0
42	l	8	Total O 8 8	0	0
42	m	15	Total O 15 15	0	0
42	o	155	Total O 155 155	0	0
42	t	14	Total O 14 14	0	0
42	u	94	Total O 94 94	0	0
42	v	86	Total O 87 87	0	1
42	y	1	Total O 1 1	0	0
42	x	7	Total O 7 7	0	0

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.

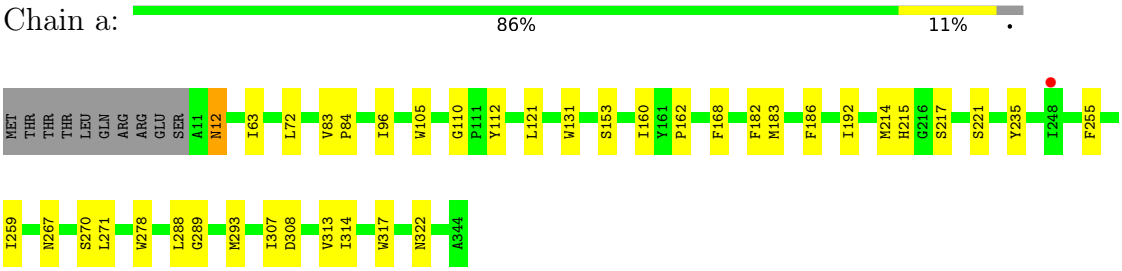
• Molecule 1: Photosystem II protein D1

Chain A:



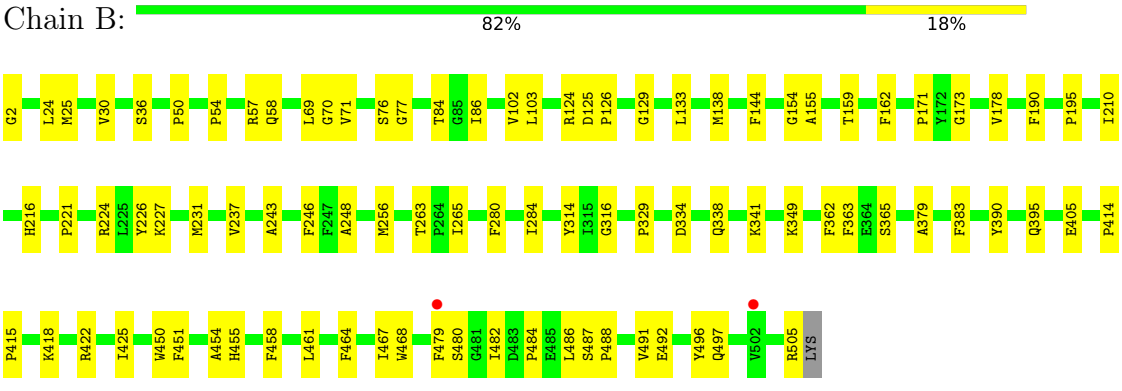
• Molecule 1: Photosystem II protein D1

Chain a:



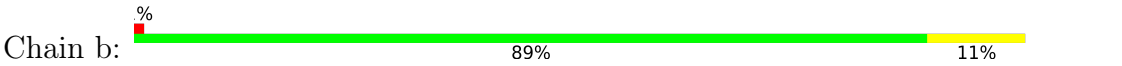
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

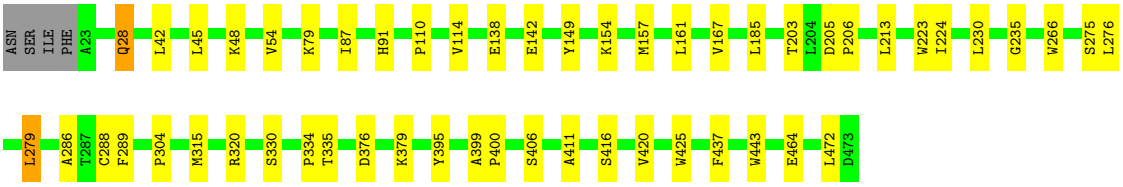




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

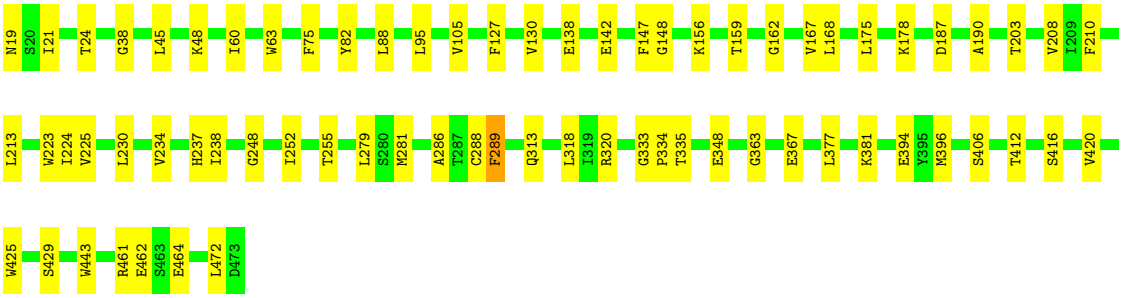




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

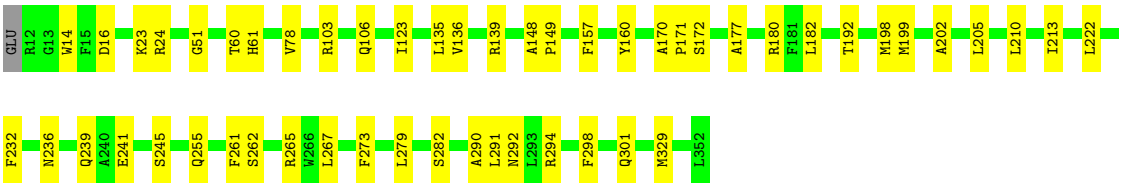




• Molecule 4: Photosystem II D2 protein

Chain D:

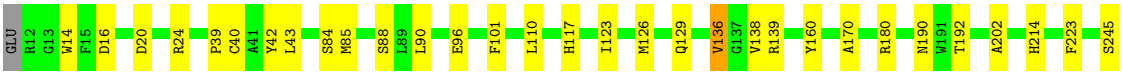




• Molecule 4: Photosystem II D2 protein

Chain d:



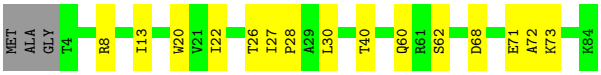




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

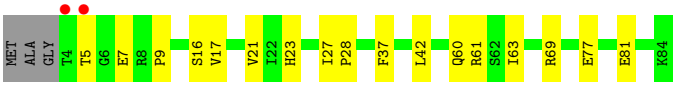




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

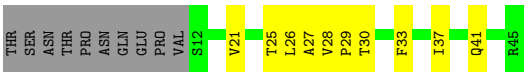




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

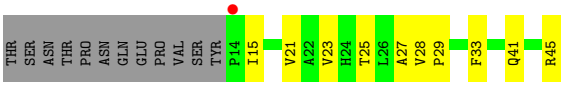




• Molecule 6: Cytochrome b559 subunit beta

Chain f:





• Molecule 7: Photosystem II reaction center protein H

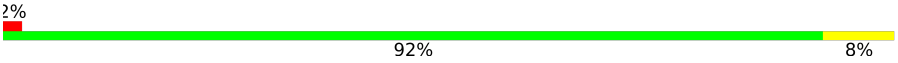
Chain H:

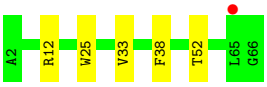




• Molecule 7: Photosystem II reaction center protein H

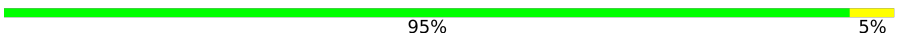
Chain h:

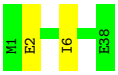




• Molecule 8: Photosystem II reaction center protein I

Chain I:

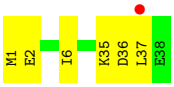




• Molecule 8: Photosystem II reaction center protein I

Chain i:

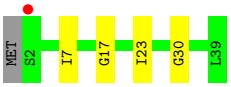




• Molecule 9: Photosystem II reaction center protein J

Chain J:

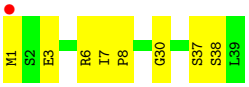




• Molecule 9: Photosystem II reaction center protein J

Chain j:

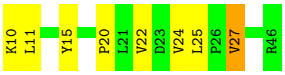




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

Chain k:

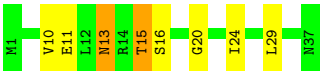




• Molecule 11: Photosystem II reaction center protein L

Chain L:

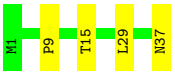




• Molecule 11: Photosystem II reaction center protein L

Chain l:

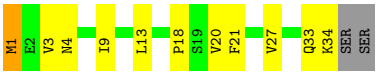




• Molecule 12: Photosystem II reaction center protein M

Chain M:

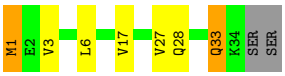




• Molecule 12: Photosystem II reaction center protein M

Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

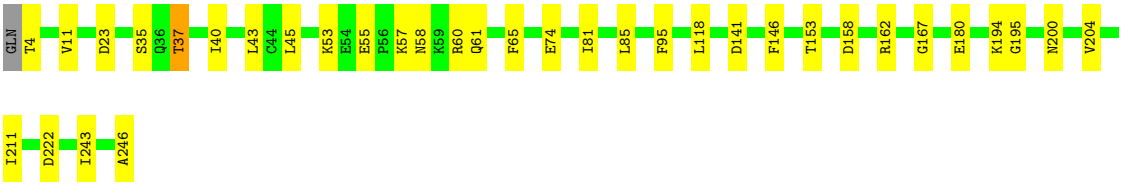




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:





• Molecule 14: Photosystem II reaction center protein T

Chain T:

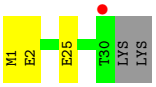




• Molecule 14: Photosystem II reaction center protein T

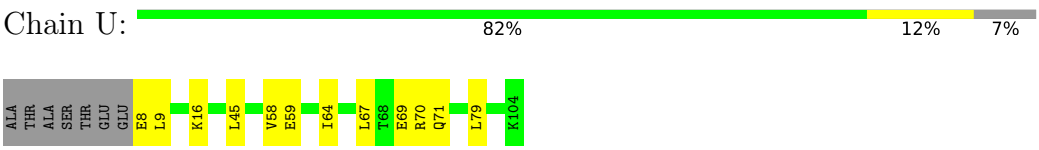
Chain t:





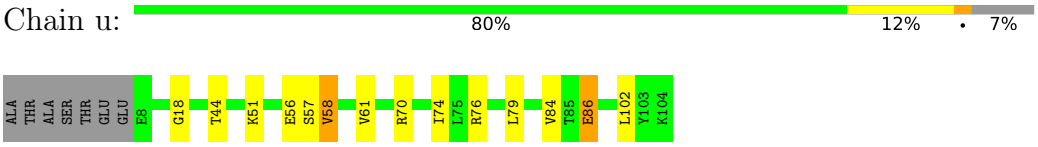
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



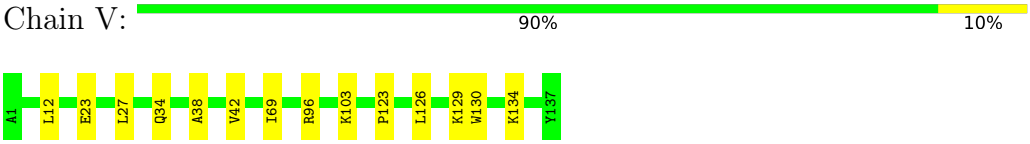
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



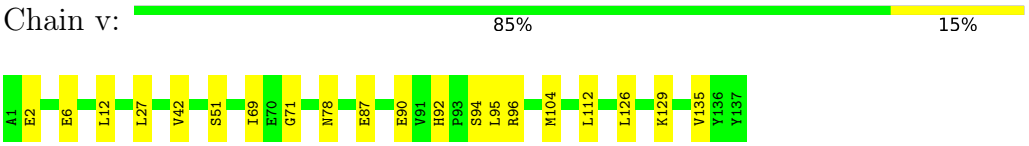
• Molecule 16: Cytochrome c-550

Chain V:



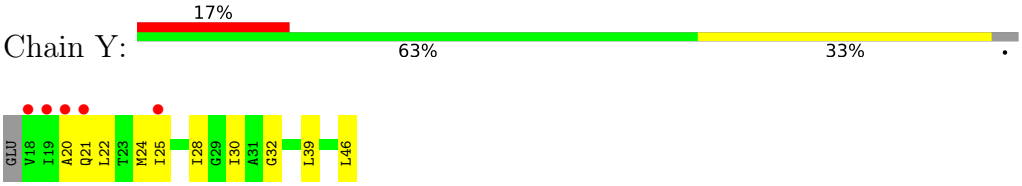
• Molecule 16: Cytochrome c-550

Chain v:



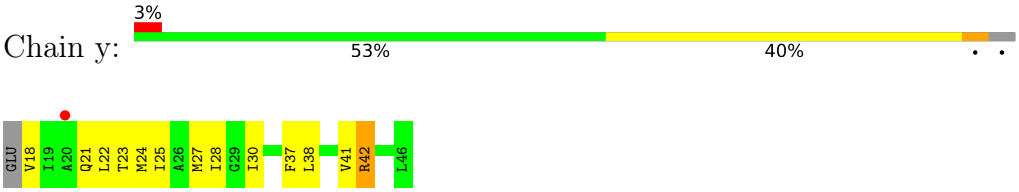
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



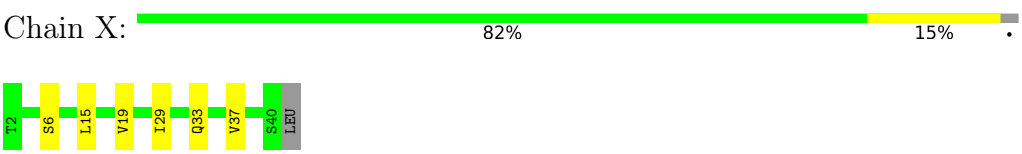
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



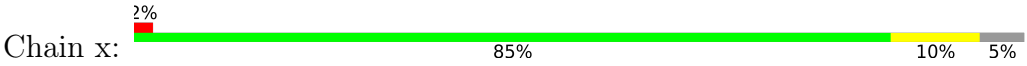
• Molecule 18: Photosystem II reaction center protein X

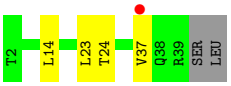
Chain X:



• Molecule 18: Photosystem II reaction center protein X

Chain x:

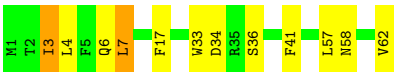




• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

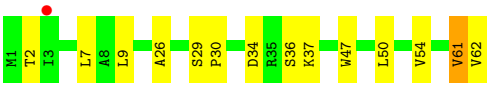




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

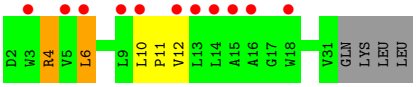




• Molecule 20: Photosystem II protein Y

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	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.40) 99.8 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.207 0.169 , 0.220	Depositor DCC
R_{free} test set	17886 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 90.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55695	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HTG, HEM, OEY, CA, LHG, LMT, CL, OEX, GOL, LMG, CLA, FME, SQD, MG, DGD, PHO, HEC, BCR, FE2, UNL, PL9, BCT

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	0.51	0/3126	0.80	1/4257 (0.0%)
1	a	0.52	0/3128	0.81	1/4260 (0.0%)
2	B	0.52	0/4191	0.82	1/5709 (0.0%)
2	b	0.52	0/4198	0.83	2/5720 (0.0%)
3	C	0.45	0/3678	0.82	0/5007
3	c	0.46	0/3774	0.80	2/5135 (0.0%)
4	D	0.55	0/2952	0.81	3/4021 (0.1%)
4	d	0.53	0/2952	0.81	3/4021 (0.1%)
5	E	0.45	0/693	0.78	0/944
5	e	0.44	0/695	0.81	0/948
6	F	0.52	0/284	0.85	0/387
6	f	0.52	0/265	0.80	0/360
7	H	0.47	0/535	0.84	0/728
7	h	0.42	0/524	0.88	1/713 (0.1%)
8	I	0.42	0/311	0.77	0/419
8	i	0.47	0/311	0.79	0/419
9	J	0.45	0/278	0.77	0/376
9	j	0.45	0/286	0.83	0/386
10	K	0.49	0/303	0.81	0/416
10	k	0.51	0/303	0.83	0/416
11	L	0.55	0/319	0.72	0/433
11	l	0.51	0/319	0.72	0/433
12	M	0.60	0/270	0.89	0/368
12	m	0.56	0/262	0.96	2/357 (0.6%)
13	O	0.47	0/1958	0.79	0/2654
13	o	0.46	0/1937	0.80	2/2625 (0.1%)
14	T	0.52	0/266	0.75	0/362
14	t	0.57	0/266	0.74	0/362
15	U	0.47	0/785	0.76	0/1064
15	u	0.47	0/785	0.73	0/1064
16	V	0.48	0/1109	0.76	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.44	0/1098	0.84	2/1488 (0.1%)
17	Y	0.46	0/216	0.81	0/289
17	y	0.46	0/216	0.78	0/289
18	X	0.43	0/290	0.75	0/392
18	x	0.45	0/284	0.72	0/384
19	Z	0.39	0/490	0.78	0/669
19	z	0.41	0/490	0.84	0/669
20	R	0.35	0/245	0.69	0/338
All	All	0.49	0/44392	0.81	20/60384 (0.0%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	170	ALA	CA-C-N	-7.22	112.54	119.76
4	D	170	ALA	C-N-CA	-7.22	112.54	119.76
4	d	170	ALA	CA-C-N	-6.25	113.50	119.76
4	d	170	ALA	C-N-CA	-6.25	113.50	119.76
1	a	83	VAL	N-CA-C	6.04	113.83	108.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	2877	33	0
1	a	3020	0	2883	37	0
2	B	4021	0	3898	66	0
2	b	4022	0	3908	42	0
3	C	3553	0	3474	42	0
3	c	3641	0	3569	48	0
4	D	2849	0	2741	38	0
4	d	2849	0	2741	41	0
5	E	668	0	658	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	670	0	664	13	0
6	F	275	0	282	9	0
6	f	257	0	269	7	0
7	H	519	0	545	11	0
7	h	511	0	532	7	0
8	I	314	0	328	1	0
8	i	314	0	328	2	0
9	J	272	0	279	4	0
9	j	280	0	291	6	0
10	K	293	0	305	8	0
10	k	293	0	305	5	0
11	L	309	0	327	8	0
11	l	309	0	327	5	0
12	M	274	0	299	8	0
12	m	269	0	288	7	0
13	O	1903	0	1886	18	0
13	o	1891	0	1870	23	0
14	T	264	0	267	4	0
14	t	264	0	267	1	0
15	U	774	0	773	5	1
15	u	774	0	773	9	0
16	V	1085	0	1095	8	0
16	v	1077	0	1082	11	0
17	Y	215	0	246	8	0
17	y	215	0	246	8	0
18	X	287	0	317	5	0
18	x	281	0	312	4	0
19	Z	479	0	516	7	0
19	z	479	0	516	9	0
20	R	239	0	262	4	0
21	A	4	0	0	0	0
21	U	1	0	0	0	0
21	a	4	0	0	0	0
21	v	1	0	0	0	0
22	A	8	0	0	0	0
22	d	8	0	0	0	0
23	A	260	0	288	16	0
23	B	1040	0	1152	53	0
23	C	845	0	936	43	0
23	D	130	0	144	3	0
23	a	195	0	216	10	0
23	b	1040	0	1152	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	c	845	0	936	38	0
23	d	195	0	216	8	0
24	A	64	0	74	2	0
24	D	128	0	148	4	0
24	a	64	0	74	1	0
24	d	128	0	148	5	0
25	A	40	0	56	1	0
25	B	120	0	168	11	0
25	C	40	0	56	3	0
25	D	40	0	56	5	0
25	H	40	0	56	4	0
25	K	80	0	112	9	0
25	T	40	0	56	5	0
25	Y	40	0	56	6	0
25	a	40	0	56	1	0
25	b	120	0	168	9	0
25	c	80	0	112	6	0
25	d	40	0	56	3	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	108	0	156	5	0
26	B	108	0	156	2	0
26	F	43	0	53	3	0
26	a	54	0	78	2	0
26	b	54	0	78	2	0
26	f	43	0	53	3	1
27	A	12	0	16	0	0
27	B	42	0	56	1	0
27	C	12	0	16	3	0
27	D	6	0	8	1	0
27	F	6	0	8	0	0
27	O	6	0	8	0	0
27	T	12	0	16	4	0
27	V	24	0	32	1	0
27	a	12	0	16	2	0
27	b	24	0	32	0	0
27	c	12	0	16	1	0
27	f	6	0	7	1	0
27	o	6	0	8	0	0
27	t	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	v	24	0	32	2	0
28	A	35	0	46	4	0
28	B	25	0	35	0	0
28	C	35	0	46	3	0
28	D	35	0	46	0	0
28	F	35	0	46	1	0
28	M	105	0	138	7	0
28	T	25	0	35	0	0
28	a	70	0	92	3	0
28	b	25	0	35	0	0
28	e	35	0	46	1	0
28	m	35	0	46	2	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	11	0	0	1	0
30	a	11	0	0	1	0
31	A	110	0	160	8	0
31	D	110	0	160	4	0
31	a	110	0	160	17	0
31	d	110	0	160	4	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	A	42	0	57	3	0
33	D	147	0	222	14	0
33	L	49	0	74	3	0
33	a	42	0	57	6	0
33	b	49	0	74	5	0
33	d	147	0	222	6	0
34	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	F	1	0	0	0	0
34	O	1	0	0	0	0
34	b	1	0	0	0	0
34	c	2	0	0	0	0
34	f	1	0	0	0	0
34	o	1	0	0	0	0
35	B	95	0	130	2	0
35	C	38	0	52	1	0
35	D	16	0	17	4	0
35	V	19	0	26	1	0
35	b	95	0	130	1	0
35	c	38	0	52	1	0
35	d	16	0	17	3	0
36	C	153	0	216	8	0
36	D	51	0	72	1	0
36	M	51	0	72	4	0
36	Z	37	0	44	1	0
36	a	51	0	72	3	0
36	b	51	0	72	5	0
36	c	51	0	72	3	0
36	d	51	0	72	5	0
36	k	51	0	72	1	0
36	z	39	0	48	6	0
37	C	186	0	246	8	0
37	D	52	0	71	6	0
37	H	62	0	82	0	0
37	c	186	0	246	8	0
37	d	62	0	82	5	0
37	h	62	0	82	1	0
38	D	2	0	0	0	0
38	a	1	0	0	0	0
39	F	43	0	30	2	0
39	e	43	0	30	2	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	169	0	0	2	0
42	B	291	0	0	1	0
42	C	235	0	0	3	0
42	D	147	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	E	33	0	0	0	0
42	F	11	0	0	0	0
42	H	44	0	0	0	0
42	I	5	0	0	0	0
42	J	10	0	0	0	0
42	K	10	0	0	1	0
42	L	12	0	0	0	0
42	M	25	0	0	1	0
42	O	180	0	0	4	0
42	T	17	0	0	2	0
42	U	80	0	0	1	0
42	V	116	0	0	0	0
42	X	8	0	0	1	0
42	Y	4	0	0	0	0
42	Z	1	0	0	0	0
42	a	160	0	0	1	0
42	b	263	0	0	2	0
42	c	199	0	0	1	0
42	d	141	0	0	3	0
42	e	20	0	0	1	0
42	f	7	0	0	2	0
42	h	43	0	0	0	0
42	i	3	0	0	0	0
42	j	6	0	0	0	0
42	k	8	0	0	1	0
42	l	8	0	0	0	0
42	m	15	0	0	0	0
42	o	155	0	0	5	0
42	t	14	0	0	0	0
42	u	94	0	0	2	0
42	v	87	0	0	0	0
42	x	7	0	0	0	0
42	y	1	0	0	0	0
All	All	55695	0	54237	756	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 756 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[A]:MET:HG2	31:A:417[A]:PL9:H102	1.48	0.93
30:a:417[B]:OEY:O6	30:a:417[B]:OEY:O5	1.90	0.89
30:A:416[B]:OEY:O6	30:A:416[B]:OEY:O5	1.90	0.88
36:a:414:LMG:H221	37:c:519:DGD:HA82	1.61	0.81
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.64	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:69:GLU:OE1	26:f:102:SQD:O3[2_554]	2.16	0.04

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	385/344 (112%)	378 (98%)	6 (2%)	1 (0%)	36	50
1	a	385/344 (112%)	381 (99%)	3 (1%)	1 (0%)	36	50
2	B	512/505 (101%)	503 (98%)	9 (2%)	0	100	100
2	b	513/505 (102%)	503 (98%)	9 (2%)	1 (0%)	43	58
3	C	461/455 (101%)	448 (97%)	11 (2%)	2 (0%)	30	43
3	c	473/455 (104%)	455 (96%)	16 (3%)	2 (0%)	30	43
4	D	355/342 (104%)	344 (97%)	11 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	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%)	58 (91%)	6 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	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%)	240 (96%)	9 (4%)	0	100	100
13	o	246/244 (101%)	238 (97%)	8 (3%)	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%)	92 (97%)	3 (3%)	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%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	3	2
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5431/5384 (101%)	5280 (97%)	142 (3%)	9 (0%)	48	58

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	416[A]	SER
3	c	416[B]	SER
19	z	30	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	312/279 (112%)	312 (100%)	0	100 100
1	a	312/279 (112%)	311 (100%)	1 (0%)	86 93
2	B	412/403 (102%)	405 (98%)	7 (2%)	53 74
2	b	413/403 (102%)	406 (98%)	7 (2%)	53 74
3	C	361/356 (101%)	356 (99%)	5 (1%)	59 79
3	c	371/356 (104%)	363 (98%)	8 (2%)	45 67
4	D	290/277 (105%)	288 (99%)	2 (1%)	76 88
4	d	290/277 (105%)	285 (98%)	5 (2%)	53 74
5	E	74/73 (101%)	73 (99%)	1 (1%)	59 79
5	e	74/73 (101%)	73 (99%)	1 (1%)	59 79
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	24 (92%)	2 (8%)	12 20
7	H	55/54 (102%)	54 (98%)	1 (2%)	51 73
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 60
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30 51
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 55
10	k	30/30 (100%)	28 (93%)	2 (7%)	15 26
11	L	36/35 (103%)	34 (94%)	2 (6%)	19 33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 60
12	M	31/32 (97%)	29 (94%)	2 (6%)	15 27
12	m	30/32 (94%)	29 (97%)	1 (3%)	33 55
13	O	214/207 (103%)	209 (98%)	5 (2%)	44 66
13	o	211/207 (102%)	203 (96%)	8 (4%)	29 49
14	T	27/28 (96%)	25 (93%)	2 (7%)	13 22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13 22
15	U	84/89 (94%)	81 (96%)	3 (4%)	31 52
15	u	84/89 (94%)	79 (94%)	5 (6%)	17 31
16	V	119/117 (102%)	118 (99%)	1 (1%)	73 86
16	v	118/117 (101%)	115 (98%)	3 (2%)	42 64
17	Y	22/23 (96%)	20 (91%)	2 (9%)	9 14
17	y	22/23 (96%)	18 (82%)	4 (18%)	2 2
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%)	47 (90%)	5 (10%)	8 12
19	z	52/52 (100%)	49 (94%)	3 (6%)	18 32
20	R	25/29 (86%)	23 (92%)	2 (8%)	11 19
All	All	4506/4403 (102%)	4410 (98%)	96 (2%)	47 69

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	90	LEU
13	o	4	THR
4	d	293	LEU
8	i	36	ASP
13	o	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
12	m	5	GLN
16	v	86	GLN
13	o	124	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	o	200	ASN
19	z	58	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	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.68	0	7,9,11	1.15	1 (14%)
12	FME	m	1	12	8,9,10	0.66	0	7,9,11	1.25	1 (14%)
14	FME	T	1	14	8,9,10	0.67	0	7,9,11	1.64	3 (42%)
8	FME	I	1	8	8,9,10	0.71	0	7,9,11	1.16	0
12	FME	M	1	12	8,9,10	0.67	0	7,9,11	1.37	2 (28%)
14	FME	t	1	14	8,9,10	0.87	0	7,9,11	2.06	3 (42%)

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

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

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	-2.89	118.38	122.82
14	t	1	FME	O-C-CA	-2.72	117.64	124.78
14	T	1	FME	O-C-CA	-2.65	117.83	124.78
12	M	1	FME	CA-N-CN	-2.32	119.26	122.82
14	T	1	FME	C-CA-N	2.30	113.87	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	1	0
12	M	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\|>2$
25	BCR	K	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	9 (16%)
24	PHO	d	402[A]	-	58,69,69	2.77	14 (24%)	56,99,99	2.90	15 (26%)
27	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.44	0
28	LMT	M	105	-	36,36,36	0.48	0	47,47,47	0.85	0
24	PHO	A	407	-	58,69,69	2.83	13 (22%)	56,99,99	2.93	16 (28%)
23	CLA	c	512	3	69,73,73	2.01	19 (27%)	83,113,113	2.76	29 (34%)
23	CLA	B	608	42	69,73,73	2.02	20 (28%)	83,113,113	2.73	31 (37%)
33	LHG	D	412	-	48,48,48	0.97	2 (4%)	51,54,54	1.11	3 (5%)
23	CLA	A	405	42	69,73,73	2.03	20 (28%)	83,113,113	2.90	29 (34%)
23	CLA	B	606	2	69,73,73	2.04	20 (28%)	83,113,113	2.86	29 (34%)
27	GOL	v	204	-	5,5,5	0.34	0	5,5,5	0.36	0
23	CLA	c	508	42	69,73,73	2.01	20 (28%)	83,113,113	2.89	34 (40%)
33	LHG	L	101	-	48,48,48	0.86	2 (4%)	51,54,54	1.11	6 (11%)
36	LMG	M	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.02	3 (5%)
37	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.03	7 (9%)
23	CLA	B	603	2	69,73,73	2.08	21 (30%)	83,113,113	2.86	34 (40%)
37	DGD	D	409	-	52,52,67	1.03	3 (5%)	60,60,81	1.12	5 (8%)
36	LMG	a	414	-	51,51,55	0.90	2 (3%)	59,59,63	1.20	6 (10%)
26	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.34	7 (11%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	c	509	3	69,73,73	2.03	19 (27%)	83,113,113	2.62	30 (36%)
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	7 (9%)
37	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	4 (5%)
23	CLA	d	404	4	69,73,73	1.97	20 (28%)	83,113,113	2.82	31 (37%)
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.91	2 (4%)
33	LHG	A	419	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
26	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.46	8 (15%)
33	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	1.05	3 (5%)
35	HTG	b	607	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	4 (17%)
24	PHO	D	402[A]	-	58,69,69	2.77	15 (25%)	56,99,99	2.86	14 (25%)
36	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	b	621	2	69,73,73	2.05	19 (27%)	83,113,113	2.84	32 (38%)
23	CLA	b	610	42	69,73,73	2.11	20 (28%)	83,113,113	2.74	27 (32%)
23	CLA	c	511	42	69,73,73	2.05	20 (28%)	83,113,113	2.77	28 (33%)
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.40	0
27	GOL	c	502	-	5,5,5	0.39	0	5,5,5	0.42	0
23	CLA	b	616	42	69,73,73	2.04	18 (26%)	83,113,113	2.69	30 (36%)
23	CLA	C	512	3	69,73,73	2.07	20 (28%)	83,113,113	2.78	32 (38%)
35	HTG	c	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.50	3 (13%)
23	CLA	c	513	3	69,73,73	2.09	20 (28%)	83,113,113	2.82	30 (36%)
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.18	0
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.58	3 (13%)
24	PHO	D	402[B]	-	58,69,69	2.82	13 (22%)	56,99,99	2.70	13 (23%)
23	CLA	c	505	3	69,73,73	1.98	20 (28%)	83,113,113	2.79	29 (34%)
31	PL9	D	408[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.74	20 (29%)
23	CLA	C	508	42	69,73,73	2.03	20 (28%)	83,113,113	2.75	26 (31%)
35	HTG	b	631	-	19,19,19	0.87	1 (5%)	23,24,24	1.42	1 (4%)
26	SQD	b	601	-	53,54,54	1.04	3 (5%)	62,65,65	1.58	12 (19%)
25	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	10 (17%)
30	OEY	a	417[B]	1,3,42	0,16,16	-	-	-		
23	CLA	d	405	4	69,73,73	2.07	19 (27%)	83,113,113	2.90	33 (39%)
23	CLA	b	622	2	69,73,73	2.01	20 (28%)	83,113,113	2.71	33 (39%)
27	GOL	v	202	-	5,5,5	0.41	0	5,5,5	0.24	0
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	8 (14%)
28	LMT	M	104	-	36,36,36	0.55	1 (2%)	47,47,47	1.00	3 (6%)
28	LMT	e	102	-	36,36,36	0.49	0	47,47,47	0.82	0
23	CLA	B	607	2	69,73,73	2.05	20 (28%)	83,113,113	2.90	29 (34%)
31	PL9	A	417[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.77	22 (32%)
28	LMT	B	634	-	25,25,36	0.52	0	30,30,47	0.79	1 (3%)
23	CLA	B	615	2	69,73,73	2.02	19 (27%)	83,113,113	2.84	31 (37%)
28	LMT	A	414	-	36,36,36	0.59	1 (2%)	47,47,47	1.37	5 (10%)
23	CLA	b	624	2	69,73,73	2.06	21 (30%)	83,113,113	2.76	30 (36%)
23	CLA	b	613	2	69,73,73	2.03	20 (28%)	83,113,113	2.77	30 (36%)
23	CLA	B	604	2	69,73,73	2.05	18 (26%)	83,113,113	2.77	28 (33%)
23	CLA	C	511	3	69,73,73	2.11	20 (28%)	83,113,113	2.77	32 (38%)
39	HEM	F	102	6,5	50,50,50	1.47	6 (12%)	66,82,82	1.80	17 (25%)
25	BCR	D	407	-	41,41,41	1.05	1 (2%)	56,56,56	1.73	12 (21%)
26	SQD	A	410	-	53,54,54	0.99	3 (5%)	62,65,65	1.44	10 (16%)
37	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	3 (3%)
25	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.43	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	O	301	-	5,5,5	0.38	0	5,5,5	0.36	0
23	CLA	B	613	2	69,73,73	1.98	19 (27%)	83,113,113	2.76	27 (32%)
27	GOL	D	403	-	5,5,5	0.44	0	5,5,5	0.29	0
35	HTG	d	414	-	16,16,19	1.19	2 (12%)	20,21,24	1.82	3 (15%)
23	CLA	c	514	3	69,73,73	2.10	20 (28%)	83,113,113	2.72	29 (34%)
37	DGD	d	408	-	63,63,67	0.93	2 (3%)	77,77,81	1.29	7 (9%)
31	PL9	a	415[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.82	21 (30%)
25	BCR	T	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.72	15 (26%)
27	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.39	0
27	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.76	0
27	GOL	v	201	-	5,5,5	0.34	0	5,5,5	0.20	0
23	CLA	b	614	2	69,73,73	2.00	19 (27%)	83,113,113	2.88	29 (34%)
25	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	12 (21%)
36	LMG	b	629	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	3 (5%)
23	CLA	C	507	3	69,73,73	2.02	17 (24%)	83,113,113	2.69	28 (33%)
23	CLA	C	502	3	69,73,73	2.05	20 (28%)	83,113,113	2.78	29 (34%)
23	CLA	A	408	1	69,73,73	2.04	20 (28%)	83,113,113	2.82	30 (36%)
23	CLA	b	617	2	69,73,73	2.10	19 (27%)	83,113,113	2.72	31 (37%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	7 (9%)
33	LHG	b	634	-	48,48,48	0.97	2 (4%)	51,54,54	1.08	2 (3%)
31	PL9	D	408[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.65	20 (29%)
23	CLA	b	619	42	69,73,73	2.03	20 (28%)	83,113,113	2.78	30 (36%)
23	CLA	B	617	2	69,73,73	2.01	19 (27%)	83,113,113	2.85	28 (33%)
23	CLA	B	605	2	69,73,73	1.93	18 (26%)	83,113,113	2.77	31 (37%)
23	CLA	b	623	2	69,73,73	2.00	19 (27%)	83,113,113	2.90	30 (36%)
25	BCR	c	526	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	10 (17%)
27	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.53	0
23	CLA	B	616	2	69,73,73	2.03	18 (26%)	83,113,113	2.80	31 (37%)
27	GOL	B	626	-	5,5,5	0.35	0	5,5,5	0.51	0
27	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
27	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.14	0
41	HEC	V	205	16	50,50,50	1.69	9 (18%)	68,82,82	1.83	22 (32%)
31	PL9	A	417[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
27	GOL	v	203	-	5,5,5	0.38	0	5,5,5	0.40	0
28	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.94	1 (2%)
23	CLA	a	408	1	69,73,73	2.01	20 (28%)	83,113,113	2.83	32 (38%)
27	GOL	A	412	-	5,5,5	0.43	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SQD	a	413	-	53,54,54	0.96	3 (5%)	62,65,65	1.56	12 (19%)
23	CLA	B	611	42	69,73,73	2.08	20 (28%)	83,113,113	2.89	29 (34%)
28	LMT	b	630	-	25,25,36	0.49	0	30,30,47	0.56	0
23	CLA	A	404	1	69,73,73	2.01	20 (28%)	83,113,113	2.80	34 (40%)
23	CLA	B	614	2	69,73,73	2.03	19 (27%)	83,113,113	2.74	29 (34%)
23	CLA	c	506	3	69,73,73	2.07	19 (27%)	83,113,113	2.75	29 (34%)
36	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	5 (8%)
23	CLA	c	510	3	69,73,73	2.03	20 (28%)	83,113,113	2.74	30 (36%)
35	HTG	B	632	-	19,19,19	1.00	2 (10%)	23,24,24	1.31	1 (4%)
23	CLA	C	513	3	69,73,73	2.08	19 (27%)	83,113,113	2.82	30 (36%)
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.55	1 (4%)
29	OEX	A	415[A]	1,3,42	0,14,14	-	-	-		
28	LMT	T	104	-	25,25,36	0.57	1 (4%)	30,30,47	0.98	1 (3%)
36	LMG	k	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.05	4 (6%)
25	BCR	b	626	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	12 (21%)
41	HEC	v	206	16	50,50,50	1.66	9 (18%)	68,82,82	1.84	19 (27%)
23	CLA	C	505	42	69,73,73	2.08	20 (28%)	83,113,113	2.82	27 (32%)
25	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	7 (12%)
22	BCT	A	403[A]	38	2,3,3	0.63	0	2,3,3	1.10	0
23	CLA	b	618	2	69,73,73	2.03	19 (27%)	83,113,113	2.85	30 (36%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.42	2 (8%)
31	PL9	a	415[A]	-	55,55,55	0.61	2 (3%)	68,69,69	1.91	20 (29%)
23	CLA	C	506	3	69,73,73	2.03	20 (28%)	83,113,113	2.70	28 (33%)
36	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	4 (6%)
35	HTG	b	602	-	19,19,19	1.02	1 (5%)	23,24,24	1.11	2 (8%)
22	BCT	A	403[B]	38	2,3,3	0.68	0	2,3,3	0.90	0
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.86	30 (36%)
26	SQD	B	636	-	53,54,54	1.06	3 (5%)	62,65,65	1.21	4 (6%)
25	BCR	d	406	-	41,41,41	1.07	1 (2%)	56,56,56	1.72	15 (26%)
23	CLA	D	405	4	69,73,73	1.92	20 (28%)	83,113,113	2.97	31 (37%)
23	CLA	B	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.81	31 (37%)
33	LHG	D	410	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	4 (7%)
31	PL9	d	407[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.55	14 (20%)
27	GOL	o	301	-	5,5,5	0.41	0	5,5,5	0.32	0
39	HEM	e	101	6,5	50,50,50	1.53	8 (16%)	66,82,82	1.73	12 (18%)
27	GOL	F	103	34	5,5,5	0.38	0	5,5,5	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	OEY	A	416[B]	1,3,42	0,16,16	-	-	-		
35	HTG	b	632	-	19,19,19	1.16	2 (10%)	23,24,24	1.70	3 (13%)
36	LMG	c	522	-	51,51,55	0.94	2 (3%)	59,59,63	1.17	7 (11%)
22	BCT	d	401[A]	-	2,3,3	0.65	0	2,3,3	0.83	0
36	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.34	6 (13%)
23	CLA	c	517	3	69,73,73	2.08	20 (28%)	83,113,113	2.83	32 (38%)
23	CLA	C	510	3	69,73,73	2.11	20 (28%)	83,113,113	2.73	31 (37%)
35	HTG	C	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.81	4 (17%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.41	9 (16%)
25	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.69	14 (25%)
27	GOL	b	603	-	5,5,5	0.37	0	5,5,5	0.50	0
23	CLA	B	609	2	69,73,73	2.01	20 (28%)	83,113,113	2.77	30 (36%)
28	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.06	3 (6%)
23	CLA	c	516	3	69,73,73	2.07	20 (28%)	83,113,113	2.93	32 (38%)
27	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.36	0
31	PL9	d	407[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.66	17 (25%)
33	LHG	a	419	-	41,41,48	1.03	2 (4%)	44,47,54	0.97	2 (4%)
26	SQD	A	413	-	53,54,54	1.04	3 (5%)	62,65,65	1.14	6 (9%)
28	LMT	a	404	-	36,36,36	0.57	1 (2%)	47,47,47	1.15	3 (6%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	7 (12%)
33	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.03	4 (7%)
22	BCT	d	401[B]	38	2,3,3	0.62	0	2,3,3	0.88	0
37	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	3 (3%)
36	LMG	D	416	40	51,51,55	0.90	2 (3%)	59,59,63	0.96	3 (5%)
27	GOL	V	202	-	5,5,5	0.36	0	5,5,5	0.41	0
23	CLA	B	602	42	69,73,73	2.09	22 (31%)	83,113,113	2.82	29 (34%)
28	LMT	a	418	-	36,36,36	0.43	0	47,47,47	0.76	0
37	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	4 (5%)
36	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.12	4 (8%)
23	CLA	C	503	3	69,73,73	2.03	20 (28%)	83,113,113	2.74	29 (34%)
23	CLA	b	620	2	69,73,73	1.95	19 (27%)	83,113,113	2.77	29 (34%)
36	LMG	d	416	40	51,51,55	0.91	2 (3%)	59,59,63	1.10	4 (6%)
24	PHO	d	402[B]	-	58,69,69	2.78	14 (24%)	56,99,99	2.86	15 (26%)
25	BCR	Y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	14 (25%)
23	CLA	C	504	3	69,73,73	2.09	20 (28%)	83,113,113	2.86	27 (32%)
27	GOL	B	629	-	5,5,5	0.42	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	625	2	69,73,73	2.01	18 (26%)	83,113,113	2.86	30 (36%)
27	GOL	b	605	-	5,5,5	0.36	0	5,5,5	0.24	0
25	BCR	A	409	-	41,41,41	1.07	1 (2%)	56,56,56	1.24	7 (12%)
23	CLA	C	509	3	69,73,73	2.04	20 (28%)	83,113,113	2.83	30 (36%)
23	CLA	a	409	42	69,73,73	2.03	19 (27%)	83,113,113	2.87	33 (39%)
23	CLA	c	507	3	69,73,73	2.02	19 (27%)	83,113,113	2.87	29 (34%)
27	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.13	0
27	GOL	f	101	34	5,5,5	0.30	0	5,5,5	0.40	0
23	CLA	a	411	1	69,73,73	2.05	19 (27%)	83,113,113	2.81	32 (38%)
25	BCR	B	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.41	6 (10%)
25	BCR	a	412	-	41,41,41	1.05	1 (2%)	56,56,56	1.30	6 (10%)
33	LHG	d	411	-	48,48,48	0.96	2 (4%)	51,54,54	1.05	2 (3%)
35	HTG	D	415	-	16,16,19	1.06	2 (12%)	20,21,24	1.47	1 (5%)
33	LHG	D	411	-	48,48,48	0.91	3 (6%)	51,54,54	0.90	3 (5%)
35	HTG	b	608	-	19,19,19	1.06	2 (10%)	23,24,24	1.08	2 (8%)
27	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.26	0
29	OEX	a	416[A]	1,3,42	0,14,14	-	-	-		
26	SQD	F	104	-	42,43,54	1.19	4 (9%)	51,54,65	1.54	9 (17%)
23	CLA	b	611	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	31 (37%)
25	BCR	b	628	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	10 (17%)
35	HTG	B	623	-	19,19,19	0.83	1 (5%)	23,24,24	1.47	3 (13%)
23	CLA	D	406	4	69,73,73	2.02	19 (27%)	83,113,113	2.85	31 (37%)
27	GOL	t	102	-	5,5,5	0.48	0	5,5,5	0.11	0
27	GOL	B	630	-	5,5,5	0.34	0	5,5,5	0.41	0
27	GOL	B	635	-	5,5,5	0.38	0	5,5,5	0.44	0
35	HTG	V	206	-	19,19,19	1.04	2 (10%)	23,24,24	1.35	4 (17%)
23	CLA	B	610	2	69,73,73	2.01	19 (27%)	83,113,113	2.79	31 (37%)
23	CLA	b	615	2	69,73,73	2.04	19 (27%)	83,113,113	2.82	30 (36%)
27	GOL	V	201	-	5,5,5	0.34	0	5,5,5	0.38	0
27	GOL	V	203	-	5,5,5	0.42	0	5,5,5	0.30	0
23	CLA	A	406	42	69,73,73	2.04	19 (27%)	83,113,113	2.84	30 (36%)
23	CLA	d	403	42	69,73,73	2.03	19 (27%)	83,113,113	2.84	31 (37%)
25	BCR	t	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.68	14 (25%)
28	LMT	m	102	-	36,36,36	0.52	0	47,47,47	1.11	4 (8%)
27	GOL	V	204	-	5,5,5	0.37	0	5,5,5	0.27	0
27	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.26	0
27	GOL	B	627	-	5,5,5	0.37	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HTG	B	624	-	19,19,19	1.03	2 (10%)	23,24,24	2.12	4 (17%)
23	CLA	c	515	3	69,73,73	1.98	19 (27%)	83,113,113	2.85	30 (36%)
25	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
24	PHO	a	410	-	58,69,69	2.75	13 (22%)	56,99,99	2.77	15 (26%)
28	LMT	D	404	-	36,36,36	0.44	0	47,47,47	0.98	1 (2%)
23	CLA	C	514	3	69,73,73	2.08	20 (28%)	83,113,113	2.76	29 (34%)
35	HTG	B	631	-	19,19,19	1.04	1 (5%)	23,24,24	1.43	2 (8%)

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
25	BCR	K	101	-	-	2/29/63/63	0/2/2/2
24	PHO	d	402[A]	-	-	1/37/103/103	0/5/6/6
27	GOL	c	501	-	-	0/4/4/4	-
28	LMT	M	105	-	-	7/21/61/61	0/2/2/2
24	PHO	A	407	-	-	4/37/103/103	0/5/6/6
23	CLA	c	512	3	-	4/39/115/115	-
23	CLA	B	608	42	-	8/39/115/115	-
33	LHG	D	412	-	-	16/53/53/53	-
23	CLA	A	405	42	-	4/39/115/115	-
23	CLA	B	606	2	-	3/39/115/115	-
27	GOL	v	204	-	-	2/4/4/4	-
23	CLA	c	508	42	-	11/39/115/115	-
33	LHG	L	101	-	-	12/53/53/53	-
36	LMG	M	101	-	-	10/46/66/70	0/1/1/1
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
23	CLA	B	603	2	-	7/39/115/115	-
37	DGD	D	409	-	-	19/47/67/95	0/1/1/2
36	LMG	a	414	-	-	14/46/66/70	0/1/1/1
26	SQD	B	621	-	-	20/49/69/69	0/1/1/1
37	DGD	H	102	-	-	11/51/91/95	0/2/2/2
23	CLA	c	509	3	-	5/39/115/115	-
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	518	-	-	12/51/91/95	0/2/2/2
23	CLA	d	404	4	-	7/39/115/115	-
28	LMT	M	102	-	-	5/21/61/61	0/2/2/2
33	LHG	A	419	-	-	21/46/46/53	-
26	SQD	f	102	-	-	14/38/58/69	0/1/1/1
33	LHG	d	410	-	-	5/53/53/53	-
35	HTG	b	607	-	-	2/10/30/30	0/1/1/1
24	PHO	D	402[A]	-	-	0/37/103/103	0/5/6/6
36	LMG	C	501	-	-	17/46/66/70	0/1/1/1
23	CLA	b	621	2	-	2/39/115/115	-
23	CLA	b	610	42	-	14/39/115/115	-
23	CLA	c	511	42	-	4/39/115/115	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
27	GOL	a	401	-	-	2/4/4/4	-
27	GOL	c	502	-	-	2/4/4/4	-
23	CLA	b	616	42	-	6/39/115/115	-
23	CLA	C	512	3	-	5/39/115/115	-
35	HTG	c	524	-	-	0/10/30/30	0/1/1/1
23	CLA	c	513	3	-	14/39/115/115	-
27	GOL	B	625	-	-	0/4/4/4	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	PHO	D	402[B]	-	-	2/37/103/103	0/5/6/6
23	CLA	c	505	3	-	7/39/115/115	-
31	PL9	D	408[B]	-	-	7/53/73/73	0/1/1/1
23	CLA	C	508	42	-	7/39/115/115	-
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
26	SQD	b	601	-	-	25/49/69/69	0/1/1/1
25	BCR	c	518	-	-	1/29/63/63	0/2/2/2
23	CLA	d	405	4	-	8/39/115/115	-
23	CLA	b	622	2	-	5/39/115/115	-
27	GOL	v	202	-	-	2/4/4/4	-
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
28	LMT	M	104	-	-	11/21/61/61	0/2/2/2
28	LMT	e	102	-	-	7/21/61/61	0/2/2/2
23	CLA	B	607	2	-	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	A	417[B]	-	-	11/53/73/73	0/1/1/1
28	LMT	B	634	-	-	6/17/37/61	0/1/1/2
23	CLA	B	615	2	-	20/39/115/115	-
28	LMT	A	414	-	-	6/21/61/61	0/2/2/2
23	CLA	b	624	2	-	3/39/115/115	-
23	CLA	b	613	2	-	4/39/115/115	-
23	CLA	B	604	2	-	9/39/115/115	-
23	CLA	C	511	3	-	11/39/115/115	-
39	HEM	F	102	6,5	-	8/14/54/54	-
25	BCR	D	407	-	-	6/29/63/63	0/2/2/2
26	SQD	A	410	-	-	9/49/69/69	0/1/1/1
37	DGD	c	520	-	-	19/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	O	301	-	-	2/4/4/4	-
23	CLA	B	613	2	-	4/39/115/115	-
27	GOL	D	403	-	-	2/4/4/4	-
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
23	CLA	c	514	3	-	10/39/115/115	-
37	DGD	d	408	-	-	28/51/91/95	0/2/2/2
31	PL9	a	415[B]	-	-	15/53/73/73	0/1/1/1
25	BCR	T	103	-	-	3/29/63/63	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
27	GOL	C	524	-	-	0/4/4/4	-
27	GOL	v	201	-	-	3/4/4/4	-
23	CLA	b	614	2	-	8/39/115/115	-
25	BCR	K	103	-	-	1/29/63/63	0/2/2/2
36	LMG	b	629	-	-	8/46/66/70	0/1/1/1
23	CLA	C	507	3	-	11/39/115/115	-
23	CLA	C	502	3	-	11/39/115/115	-
23	CLA	A	408	1	-	12/39/115/115	-
23	CLA	b	617	2	-	2/39/115/115	-
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2
33	LHG	b	634	-	-	17/53/53/53	-
31	PL9	D	408[A]	-	-	8/53/73/73	0/1/1/1
23	CLA	b	619	42	-	6/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	617	2	-	6/39/115/115	-
23	CLA	B	605	2	-	2/39/115/115	-
23	CLA	b	623	2	-	19/39/115/115	-
25	BCR	c	526	-	-	3/29/63/63	0/2/2/2
27	GOL	C	525	-	-	0/4/4/4	-
23	CLA	B	616	2	-	11/39/115/115	-
27	GOL	B	626	-	-	0/4/4/4	-
27	GOL	T	102	-	-	2/4/4/4	-
27	GOL	b	604	-	-	0/4/4/4	-
41	HEC	V	205	16	1/1/3/7	6/14/54/54	-
31	PL9	A	417[A]	-	-	10/53/73/73	0/1/1/1
27	GOL	v	203	-	-	2/4/4/4	-
28	LMT	F	101	-	-	5/21/61/61	0/2/2/2
23	CLA	a	408	1	-	6/39/115/115	-
27	GOL	A	412	-	-	2/4/4/4	-
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
23	CLA	B	611	42	-	8/39/115/115	-
28	LMT	b	630	-	-	4/17/37/61	0/1/1/2
23	CLA	A	404	1	-	4/39/115/115	-
23	CLA	B	614	2	-	9/39/115/115	-
23	CLA	c	506	3	-	5/39/115/115	-
36	LMG	C	519	-	-	11/46/66/70	0/1/1/1
23	CLA	c	510	3	-	14/39/115/115	-
35	HTG	B	632	-	-	1/10/30/30	0/1/1/1
23	CLA	C	513	3	-	9/39/115/115	-
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
28	LMT	T	104	-	-	7/17/37/61	0/1/1/2
36	LMG	k	101	-	-	17/46/66/70	0/1/1/1
25	BCR	b	626	-	-	4/29/63/63	0/2/2/2
41	HEC	v	206	16	1/1/3/7	2/14/54/54	-
23	CLA	C	505	42	-	4/39/115/115	-
25	BCR	b	627	-	-	2/29/63/63	0/2/2/2
23	CLA	b	618	2	-	3/39/115/115	-
35	HTG	B	622	-	-	4/10/30/30	0/1/1/1
31	PL9	a	415[A]	-	-	14/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	506	3	-	8/39/115/115	-
36	LMG	C	520	-	-	13/46/66/70	0/1/1/1
35	HTG	b	602	-	-	3/10/30/30	0/1/1/1
23	CLA	b	612	2	-	10/39/115/115	-
26	SQD	B	636	-	-	15/49/69/69	0/1/1/1
25	BCR	d	406	-	-	5/29/63/63	0/2/2/2
23	CLA	D	405	4	-	4/39/115/115	-
23	CLA	B	612	2	-	5/39/115/115	-
33	LHG	D	410	-	-	14/53/53/53	-
31	PL9	d	407[A]	-	-	8/53/73/73	0/1/1/1
27	GOL	o	301	-	-	0/4/4/4	-
39	HEM	e	101	6,5	-	5/14/54/54	-
27	GOL	F	103	34	-	2/4/4/4	-
35	HTG	b	632	-	-	4/10/30/30	0/1/1/1
36	LMG	c	522	-	-	4/46/66/70	0/1/1/1
36	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
23	CLA	c	517	3	-	4/39/115/115	-
23	CLA	C	510	3	-	12/39/115/115	-
35	HTG	C	523	-	-	3/10/30/30	0/1/1/1
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
27	GOL	b	603	-	-	0/4/4/4	-
23	CLA	B	609	2	-	1/39/115/115	-
28	LMT	C	521	-	-	10/21/61/61	0/2/2/2
23	CLA	c	516	3	-	10/39/115/115	-
27	GOL	a	402	-	-	2/4/4/4	-
31	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
33	LHG	a	419	-	-	17/46/46/53	-
26	SQD	A	413	-	-	14/49/69/69	0/1/1/1
28	LMT	a	404	-	-	5/21/61/61	0/2/2/2
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
33	LHG	d	409	-	-	5/53/53/53	-
37	DGD	h	102	-	-	13/51/91/95	0/2/2/2
36	LMG	D	416	40	-	9/46/66/70	0/1/1/1
27	GOL	V	202	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	42	-	12/39/115/115	-
28	LMT	a	418	-	-	4/21/61/61	0/2/2/2
37	DGD	c	521	-	-	12/51/91/95	0/2/2/2
36	LMG	z	101	-	-	15/34/54/70	0/1/1/1
23	CLA	C	503	3	-	7/39/115/115	-
23	CLA	b	620	2	-	5/39/115/115	-
36	LMG	d	416	40	-	10/46/66/70	0/1/1/1
24	PHO	d	402[B]	-	-	3/37/103/103	0/5/6/6
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	C	504	3	-	3/39/115/115	-
27	GOL	B	629	-	-	2/4/4/4	-
23	CLA	b	625	2	-	12/39/115/115	-
27	GOL	b	605	-	-	2/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	C	509	3	-	9/39/115/115	-
23	CLA	a	409	42	-	10/39/115/115	-
23	CLA	c	507	3	-	3/39/115/115	-
27	GOL	T	101	-	-	0/4/4/4	-
27	GOL	f	101	34	-	2/4/4/4	-
23	CLA	a	411	1	-	10/39/115/115	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	BCR	a	412	-	-	0/29/63/63	0/2/2/2
33	LHG	d	411	-	-	13/53/53/53	-
35	HTG	D	415	-	-	0/7/27/30	0/1/1/1
33	LHG	D	411	-	-	9/53/53/53	-
35	HTG	b	608	-	-	1/10/30/30	0/1/1/1
27	GOL	B	628	-	-	2/4/4/4	-
26	SQD	F	104	-	-	17/38/58/69	0/1/1/1
23	CLA	b	611	2	-	4/39/115/115	-
25	BCR	b	628	-	-	1/29/63/63	0/2/2/2
35	HTG	B	623	-	-	6/10/30/30	0/1/1/1
23	CLA	D	406	4	-	4/39/115/115	-
27	GOL	t	102	-	-	0/4/4/4	-
27	GOL	B	630	-	-	4/4/4/4	-
27	GOL	B	635	-	-	0/4/4/4	-
35	HTG	V	206	-	-	4/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	610	2	-	6/39/115/115	-
23	CLA	b	615	2	-	12/39/115/115	-
27	GOL	V	201	-	-	4/4/4/4	-
27	GOL	V	203	-	-	2/4/4/4	-
23	CLA	A	406	42	-	6/39/115/115	-
23	CLA	d	403	42	-	7/39/115/115	-
25	BCR	t	101	-	-	3/29/63/63	0/2/2/2
28	LMT	m	102	-	-	5/21/61/61	0/2/2/2
27	GOL	V	204	-	-	2/4/4/4	-
27	GOL	b	606	-	-	4/4/4/4	-
27	GOL	B	627	-	-	2/4/4/4	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
23	CLA	c	515	3	-	4/39/115/115	-
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
24	PHO	a	410	-	-	7/37/103/103	0/5/6/6
28	LMT	D	404	-	-	8/21/61/61	0/2/2/2
23	CLA	C	514	3	-	7/39/115/115	-
35	HTG	B	631	-	-	2/10/30/30	0/1/1/1

The worst 5 of 1643 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402[B]	PHO	C1B-C2B	9.34	1.49	1.39
24	A	407	PHO	C1B-C2B	9.25	1.49	1.39
24	A	407	PHO	C1D-C2D	9.02	1.49	1.39
24	a	410	PHO	C1B-C2B	8.96	1.49	1.39
24	d	402[B]	PHO	C1B-C2B	8.90	1.49	1.39

The worst 5 of 2918 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	410	PHO	C2D-C1D-ND	11.73	117.62	109.53
24	d	402[B]	PHO	C2D-C1D-ND	11.67	117.58	109.53
24	D	402[A]	PHO	C2D-C1D-ND	11.62	117.55	109.53
24	D	402[B]	PHO	C2D-C1D-ND	11.49	117.46	109.53
24	d	402[A]	PHO	C2D-C1D-ND	11.10	117.19	109.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
41	V	205	HEC	NA
41	v	206	HEC	NA

5 of 1423 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	C14-C13-C15-C16
23	B	603	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

174 monomers are involved in 429 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	101	BCR	7	0
24	d	402[A]	PHO	2	0
28	M	105	LMT	4	0
24	A	407	PHO	2	0
23	c	512	CLA	4	0
23	B	608	CLA	5	0
33	D	412	LHG	9	0
23	A	405	CLA	4	0
23	B	606	CLA	5	0
23	c	508	CLA	3	0
33	L	101	LHG	3	0
36	M	101	LMG	4	0
37	C	517	DGD	3	0
23	B	603	CLA	3	0
37	D	409	DGD	6	0
36	a	414	LMG	3	0
26	B	621	SQD	1	0
23	c	509	CLA	6	0
37	C	516	DGD	4	0
37	C	518	DGD	1	0
23	d	404	CLA	4	0
28	M	102	LMT	3	0
33	A	419	LHG	3	0
26	f	102	SQD	3	1
24	D	402[A]	PHO	2	0
36	C	501	LMG	4	0
23	b	621	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	610	CLA	4	0
23	c	511	CLA	3	0
25	y	101	BCR	1	0
27	a	401	GOL	1	0
27	c	502	GOL	1	0
23	b	616	CLA	2	0
23	C	512	CLA	4	0
35	c	524	HTG	1	0
23	c	513	CLA	4	0
35	C	522	HTG	1	0
24	D	402[B]	PHO	2	0
23	c	505	CLA	5	0
31	D	408[B]	PL9	3	0
23	C	508	CLA	5	0
26	b	601	SQD	2	0
25	c	518	BCR	3	0
30	a	417[B]	OEY	1	0
23	d	405	CLA	3	0
23	b	622	CLA	2	0
27	v	202	GOL	1	0
25	C	515	BCR	3	0
28	e	102	LMT	1	0
23	B	607	CLA	6	0
31	A	417[B]	PL9	3	0
23	B	615	CLA	7	0
28	A	414	LMT	4	0
23	b	624	CLA	3	0
23	b	613	CLA	3	0
23	B	604	CLA	3	0
23	C	511	CLA	3	0
39	F	102	HEM	2	0
25	D	407	BCR	5	0
26	A	410	SQD	3	0
37	c	520	DGD	2	0
25	B	619	BCR	4	0
23	B	613	CLA	3	0
27	D	403	GOL	1	0
35	d	414	HTG	3	0
23	c	514	CLA	2	0
37	d	408	DGD	5	0
31	a	415[B]	PL9	7	0
25	T	103	BCR	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	524	GOL	2	0
27	v	201	GOL	1	0
23	b	614	CLA	4	0
25	K	103	BCR	2	0
36	b	629	LMG	5	0
23	C	507	CLA	6	0
23	C	502	CLA	4	0
23	A	408	CLA	4	0
23	b	617	CLA	1	0
37	c	519	DGD	5	0
33	b	634	LHG	5	0
31	D	408[A]	PL9	1	0
23	B	617	CLA	7	0
23	B	605	CLA	3	0
23	b	623	CLA	4	0
25	c	526	BCR	3	0
27	C	525	GOL	1	0
23	B	616	CLA	5	0
27	T	102	GOL	2	0
31	A	417[A]	PL9	5	0
28	F	101	LMT	1	0
23	a	408	CLA	5	0
26	a	413	SQD	2	0
23	B	611	CLA	4	0
23	A	404	CLA	3	0
23	B	614	CLA	3	0
23	c	506	CLA	3	0
36	C	519	LMG	1	0
23	c	510	CLA	4	0
23	C	513	CLA	4	0
36	k	101	LMG	1	0
25	b	626	BCR	4	0
23	C	505	CLA	3	0
25	b	627	BCR	4	0
23	b	618	CLA	4	0
35	B	622	HTG	1	0
31	a	415[A]	PL9	10	0
23	C	506	CLA	4	0
36	C	520	LMG	3	0
23	b	612	CLA	4	0
26	B	636	SQD	1	0
25	d	406	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	405	CLA	3	0
23	B	612	CLA	2	0
33	D	410	LHG	4	0
31	d	407[A]	PL9	1	0
39	e	101	HEM	2	0
30	A	416[B]	OEY	1	0
35	b	632	HTG	1	0
36	c	522	LMG	3	0
36	Z	101	LMG	1	0
23	c	517	CLA	3	0
23	C	510	CLA	4	0
25	h	101	BCR	5	0
25	B	620	BCR	4	0
23	B	609	CLA	1	0
28	C	521	LMT	3	0
23	c	516	CLA	3	0
27	a	402	GOL	1	0
31	d	407[B]	PL9	3	0
33	a	419	LHG	6	0
26	A	413	SQD	2	0
28	a	404	LMT	2	0
25	H	101	BCR	4	0
37	h	102	DGD	1	0
36	D	416	LMG	1	0
27	V	202	GOL	1	0
23	B	602	CLA	1	0
28	a	418	LMT	1	0
37	c	521	DGD	1	0
36	z	101	LMG	6	0
23	C	503	CLA	2	0
23	b	620	CLA	2	0
36	d	416	LMG	5	0
24	d	402[B]	PHO	3	0
25	Y	101	BCR	6	0
23	C	504	CLA	3	0
27	B	629	GOL	1	0
23	b	625	CLA	2	0
25	A	409	BCR	1	0
23	C	509	CLA	4	0
23	a	409	CLA	5	0
23	c	507	CLA	5	0
27	T	101	GOL	2	0

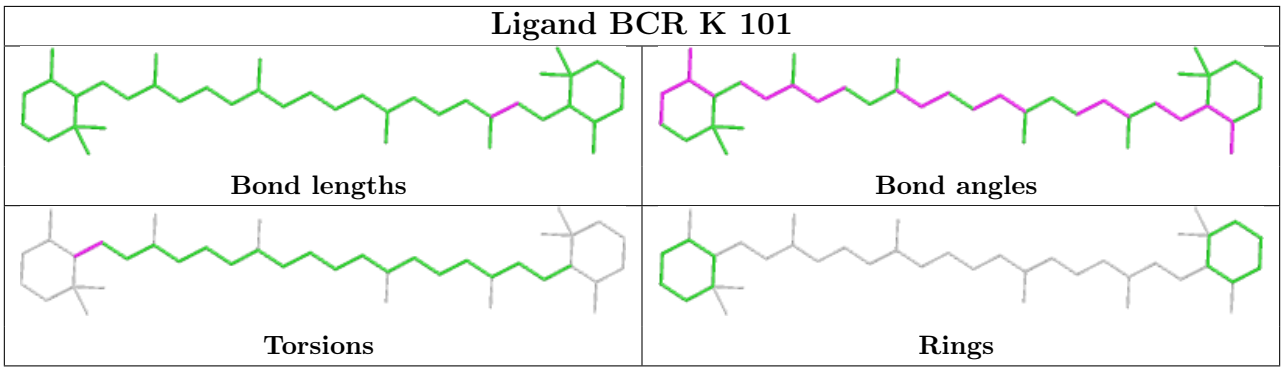
Continued on next page...

Continued from previous page...

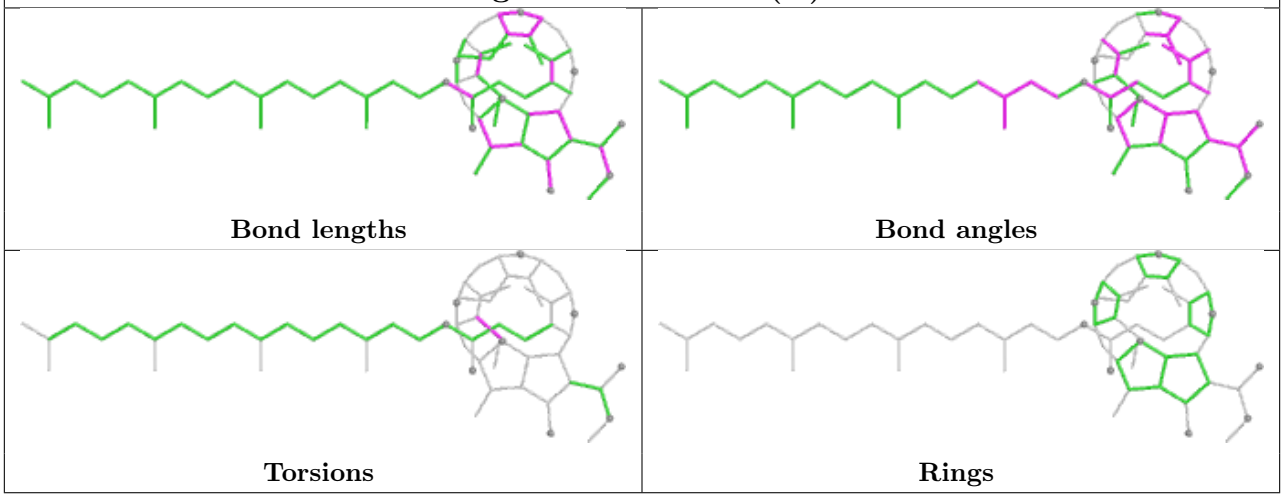
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	f	101	GOL	1	0
25	B	618	BCR	3	0
25	a	412	BCR	1	0
33	d	411	LHG	6	0
35	D	415	HTG	4	0
33	D	411	LHG	1	0
26	F	104	SQD	3	0
23	b	611	CLA	2	0
25	b	628	BCR	1	0
35	B	623	HTG	1	0
35	V	206	HTG	1	0
23	B	610	CLA	3	0
23	b	615	CLA	1	0
23	A	406	CLA	6	0
23	d	403	CLA	1	0
25	t	101	BCR	4	0
28	m	102	LMT	2	0
23	c	515	CLA	2	0
25	k	102	BCR	2	0
24	a	410	PHO	1	0
23	C	514	CLA	6	0

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.

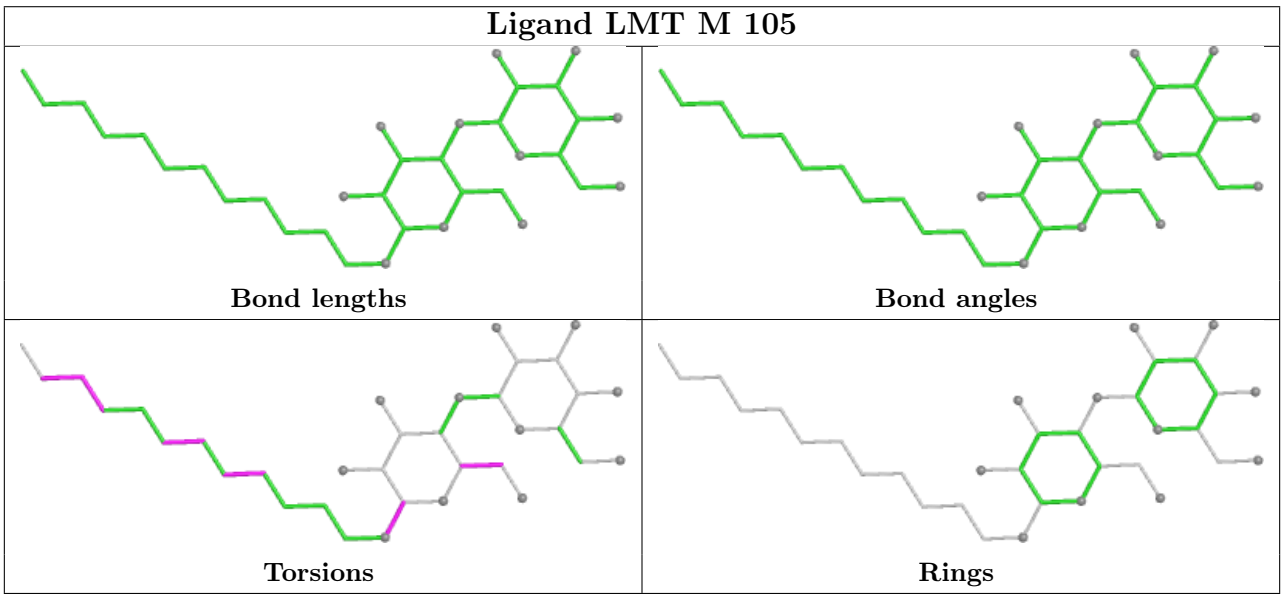
Ligand BCR K 101



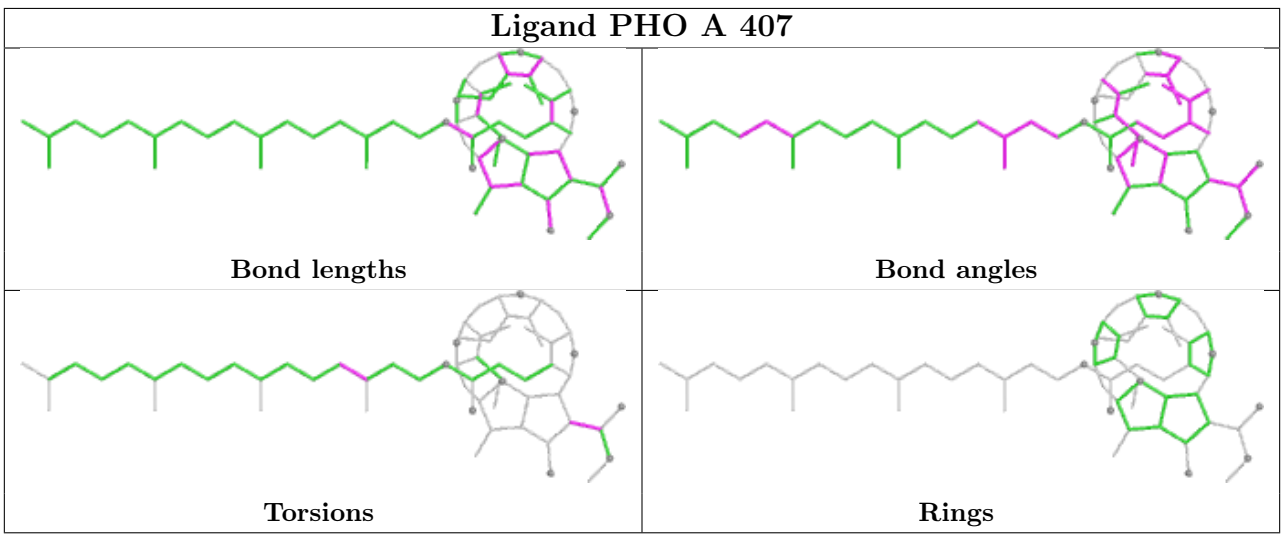
Ligand PHO d 402 (A)



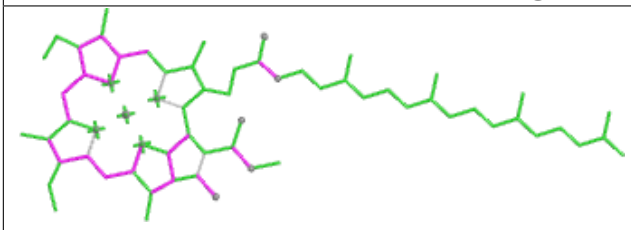
Ligand LMT M 105



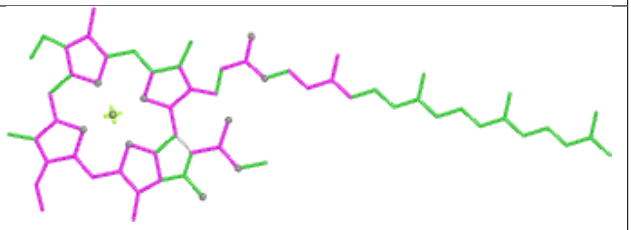
Ligand PHO A 407



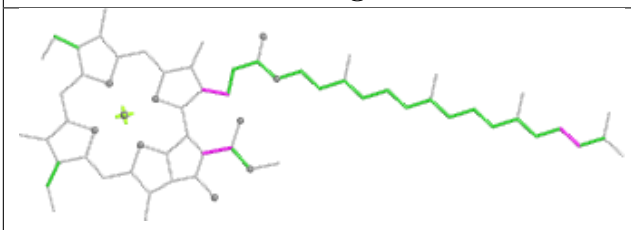
Ligand CLA c 512



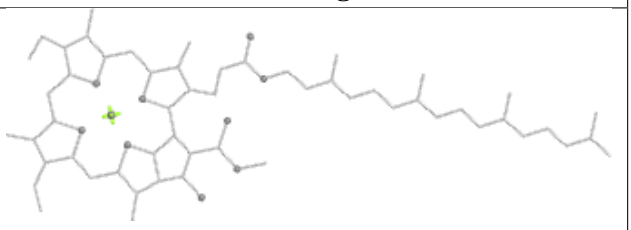
Bond lengths



Bond angles

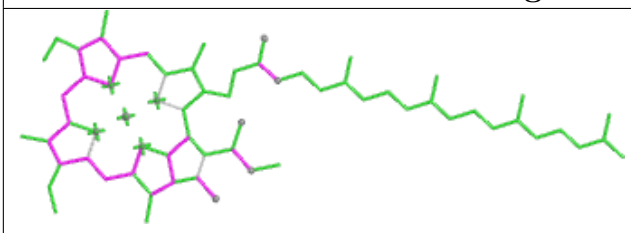


Torsions

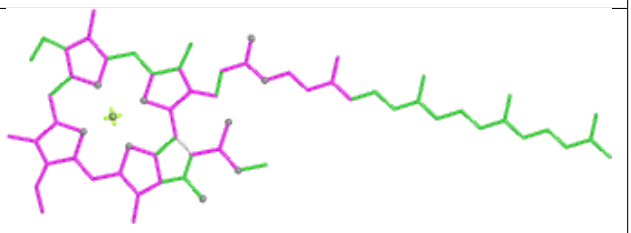


Rings

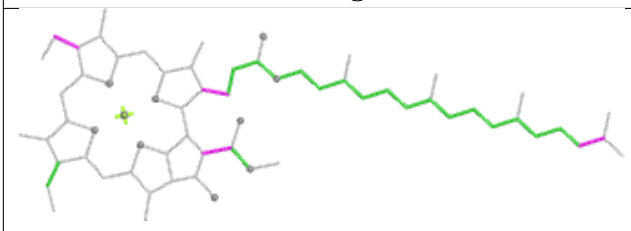
Ligand CLA B 608



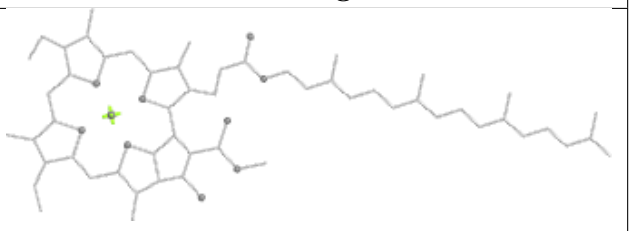
Bond lengths



Bond angles

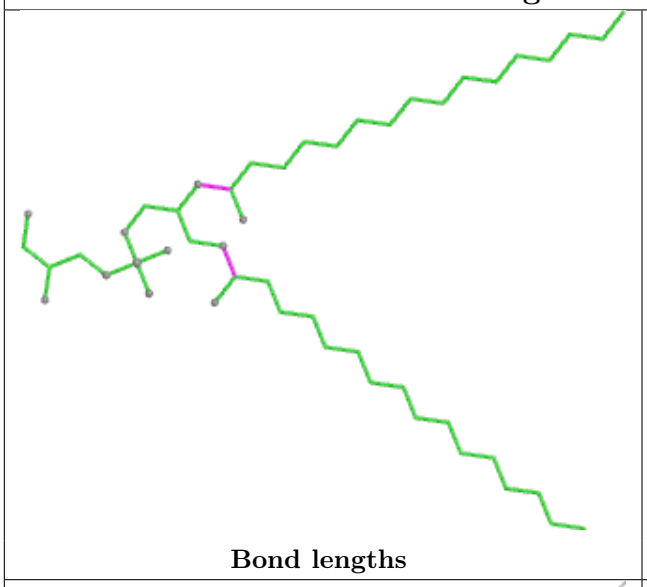


Torsions

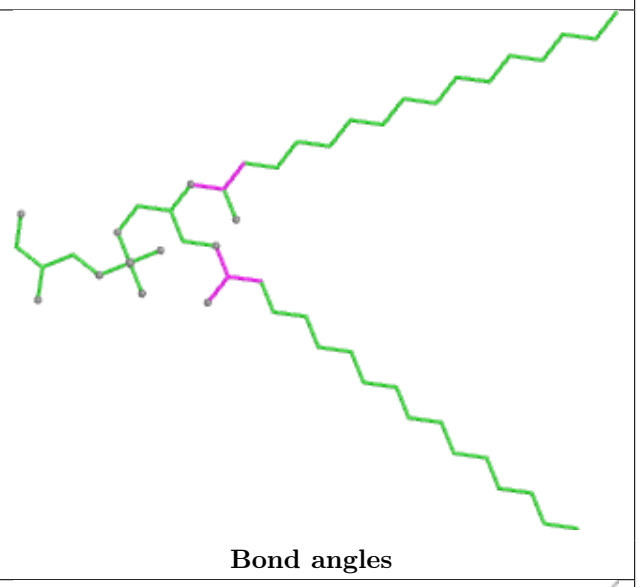


Rings

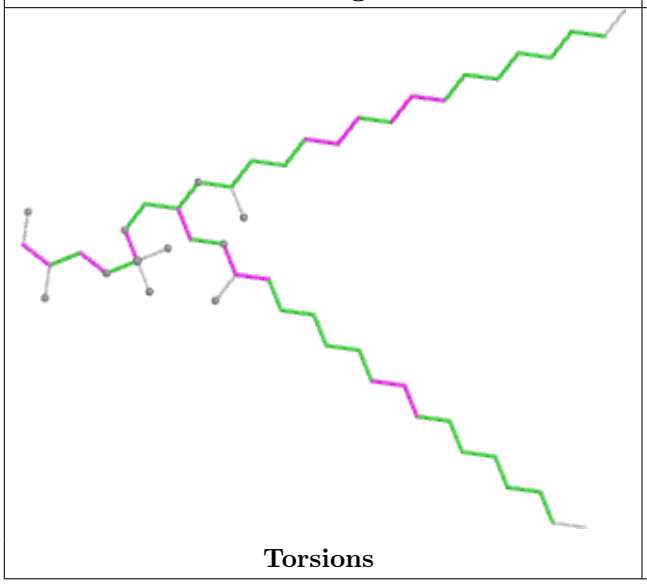
Ligand LHG D 412



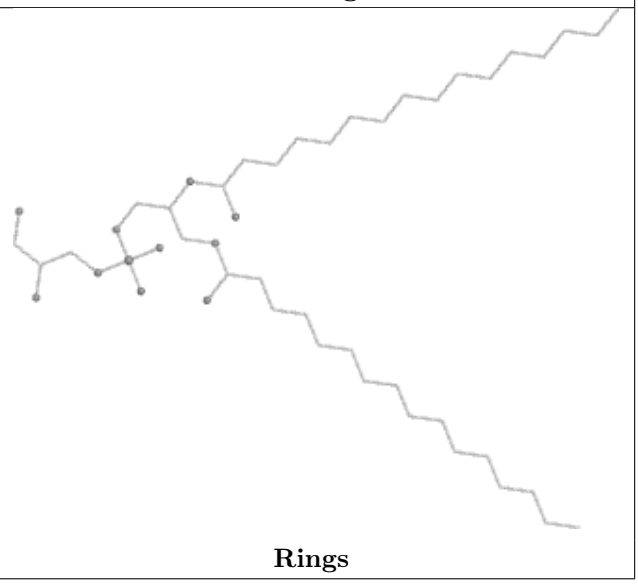
Bond lengths



Bond angles

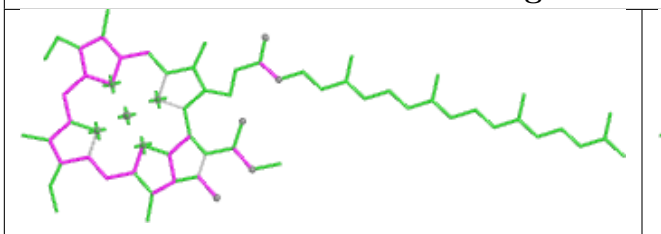


Torsions

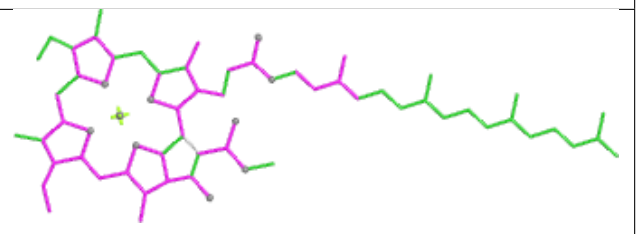


Rings

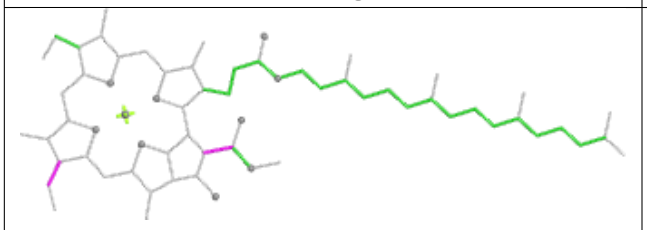
Ligand CLA A 405



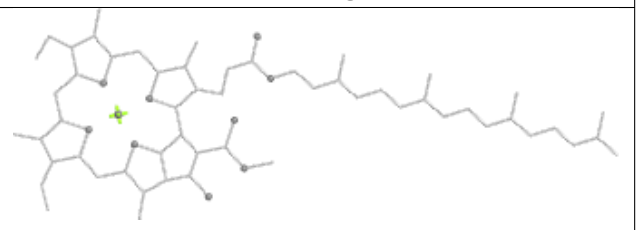
Bond lengths



Bond angles

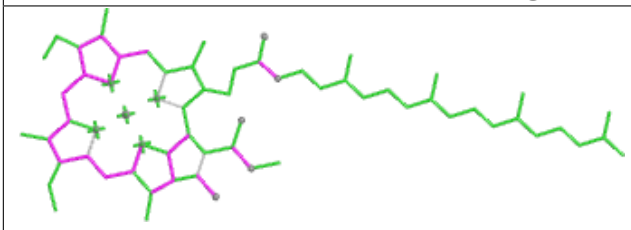


Torsions

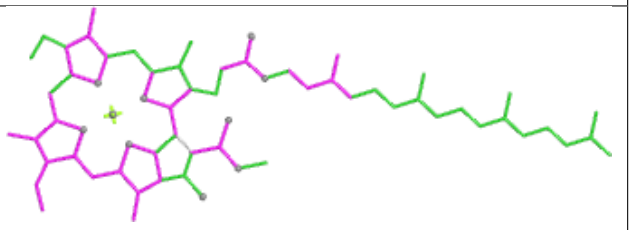


Rings

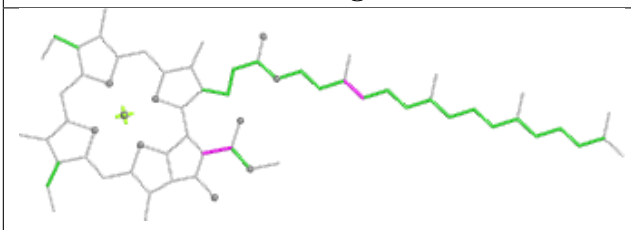
Ligand CLA B 606



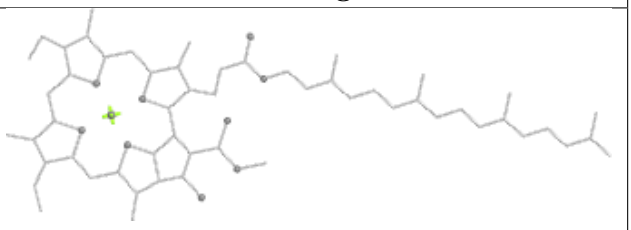
Bond lengths



Bond angles

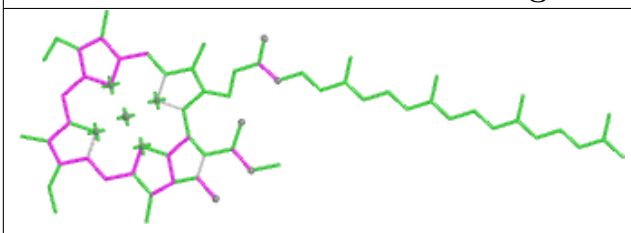


Torsions

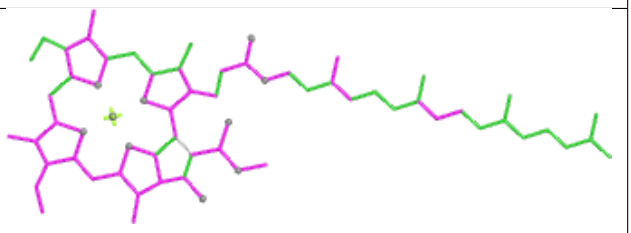


Rings

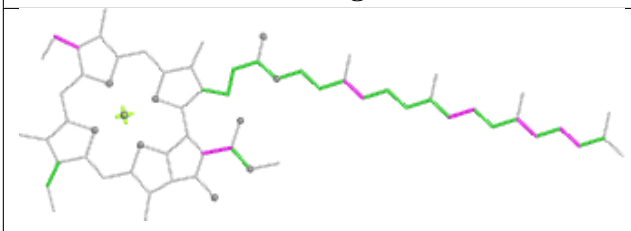
Ligand CLA c 508



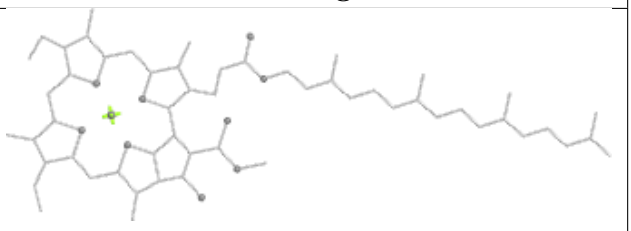
Bond lengths



Bond angles

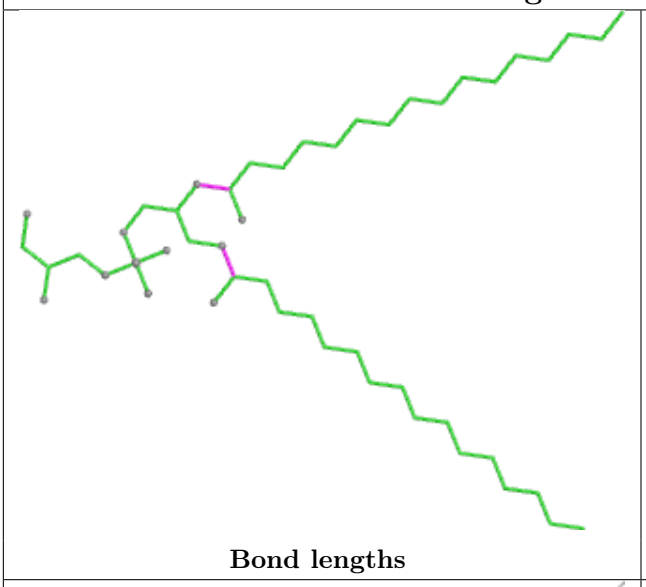


Torsions

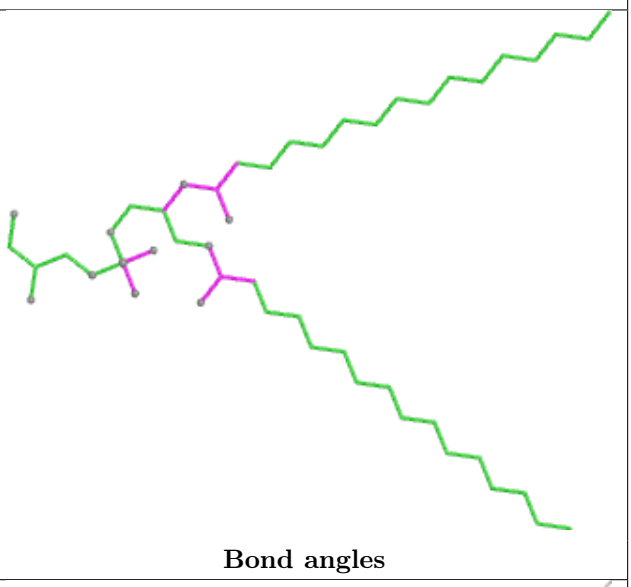


Rings

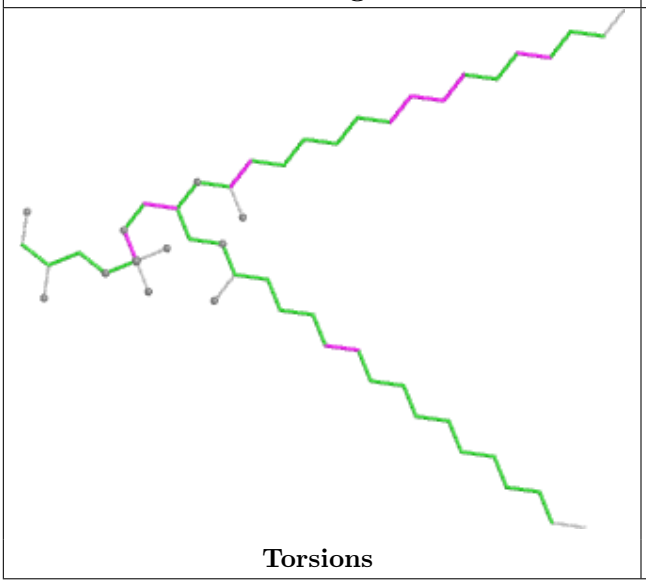
Ligand LHG L 101



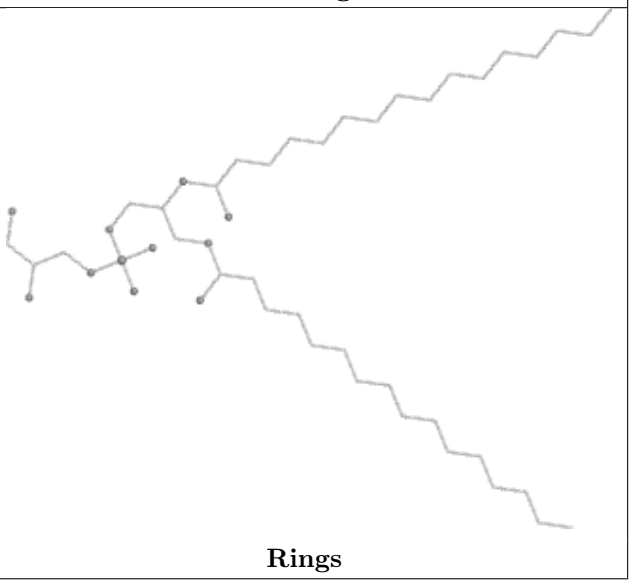
Bond lengths



Bond angles

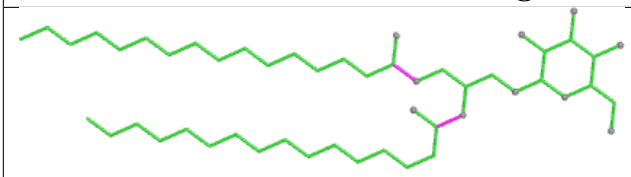


Torsions

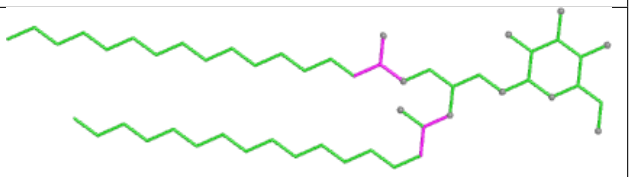


Rings

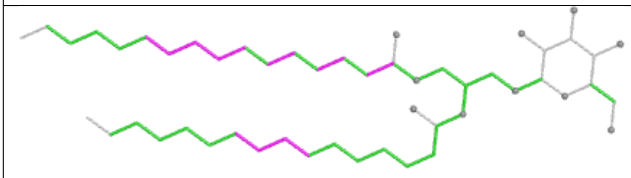
Ligand LMG M 101



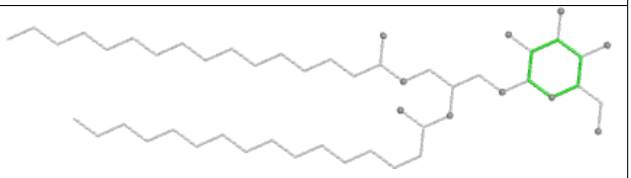
Bond lengths



Bond angles

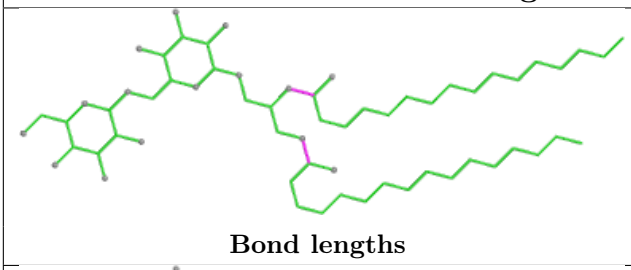


Torsions

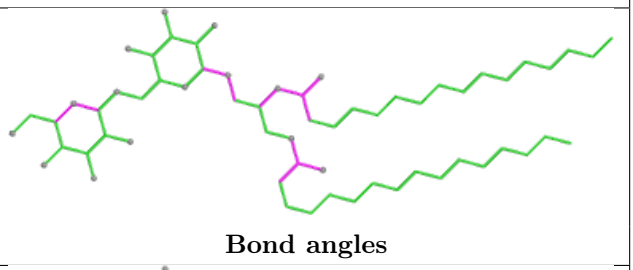


Rings

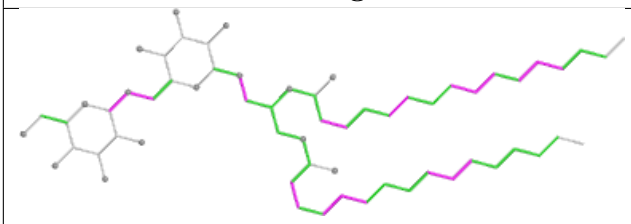
Ligand DGD C 517



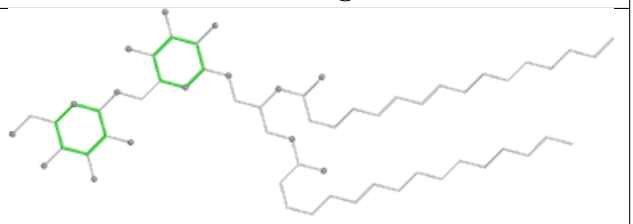
Bond lengths



Bond angles

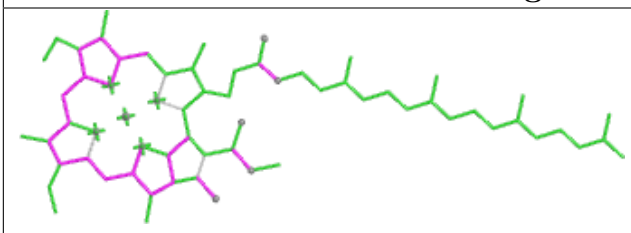


Torsions

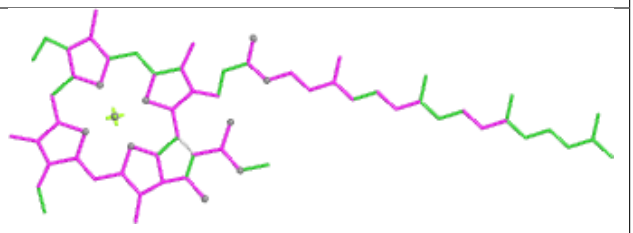


Rings

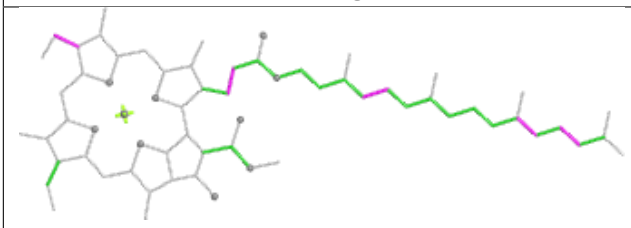
Ligand CLA B 603



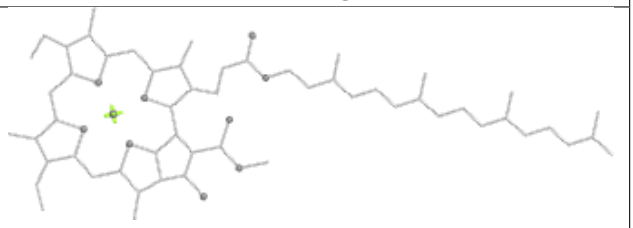
Bond lengths



Bond angles

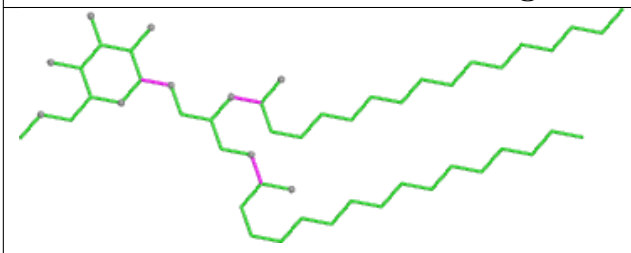


Torsions

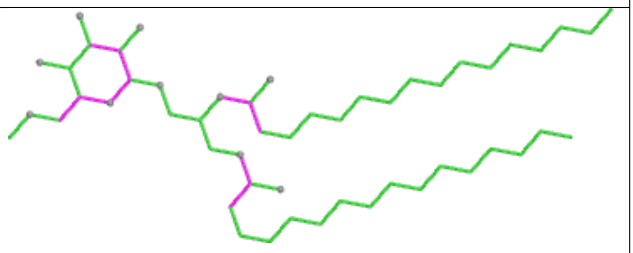


Rings

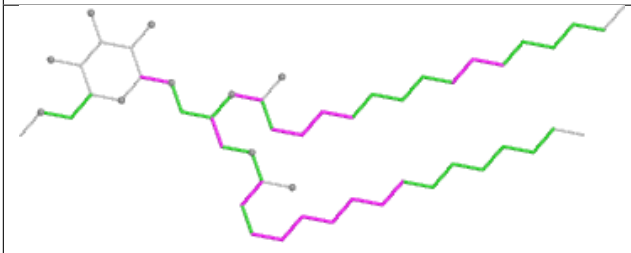
Ligand DGD D 409



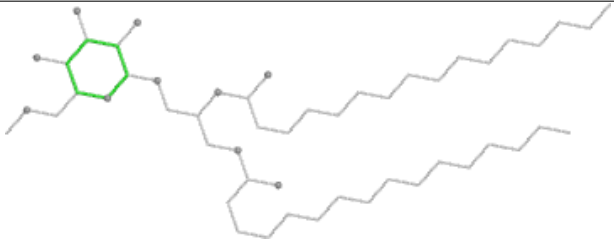
Bond lengths



Bond angles

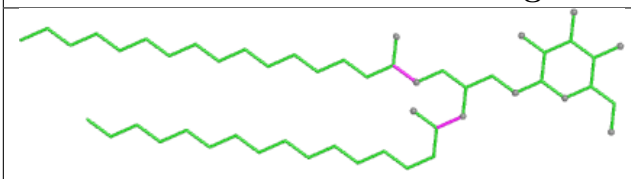


Torsions

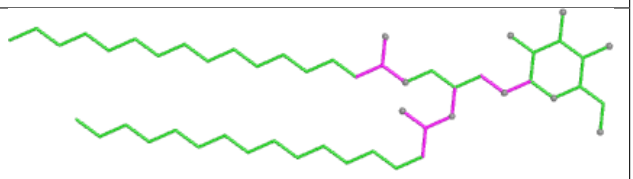


Rings

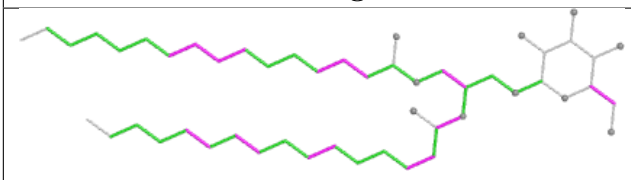
Ligand LMG a 414



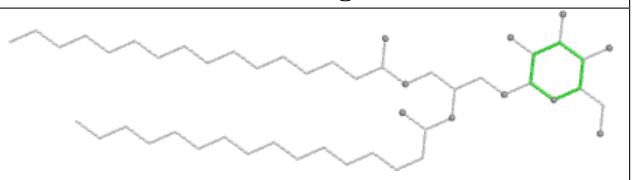
Bond lengths



Bond angles

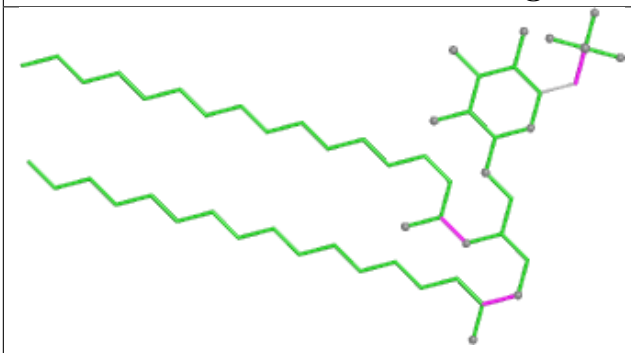


Torsions

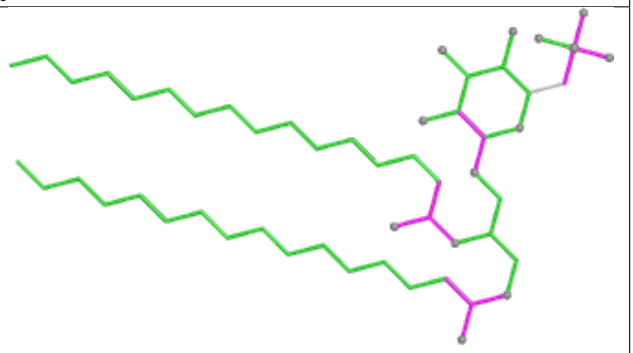


Rings

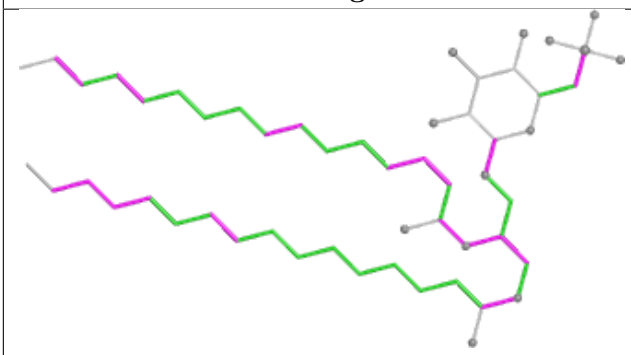
Ligand SQD B 621



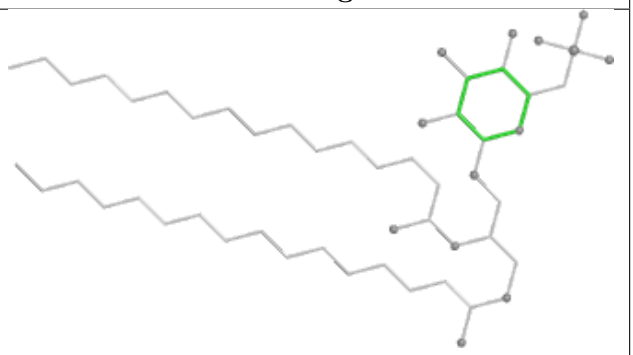
Bond lengths



Bond angles

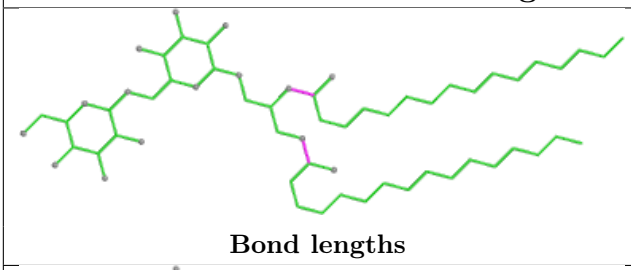


Torsions

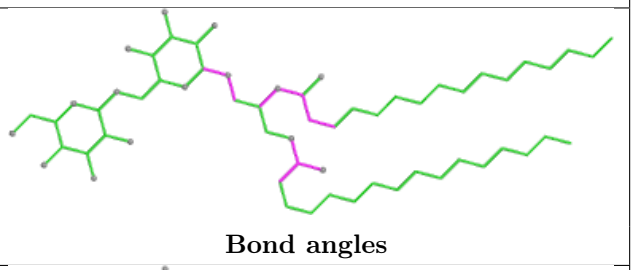


Rings

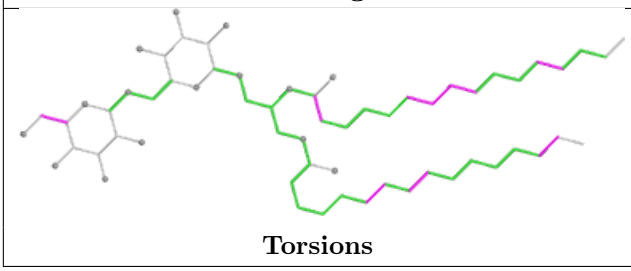
Ligand DGD H 102



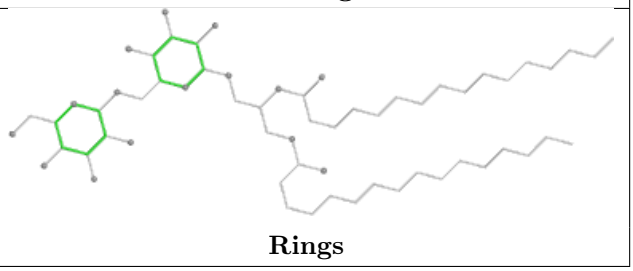
Bond lengths



Bond angles

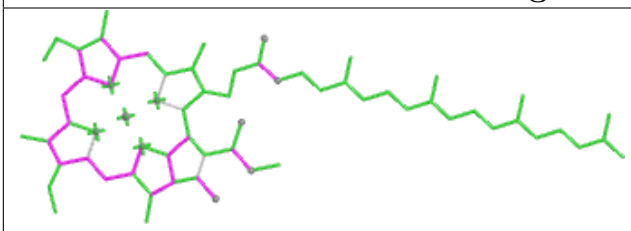


Torsions

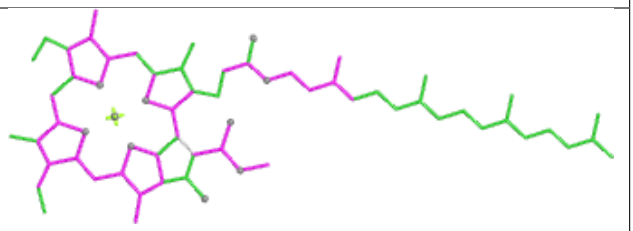


Rings

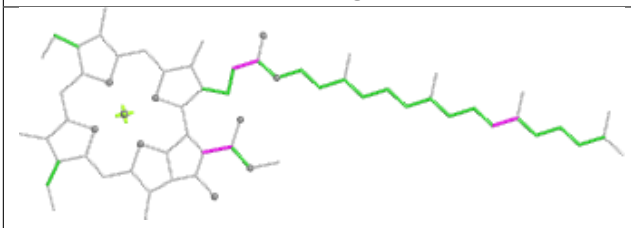
Ligand CLA c 509



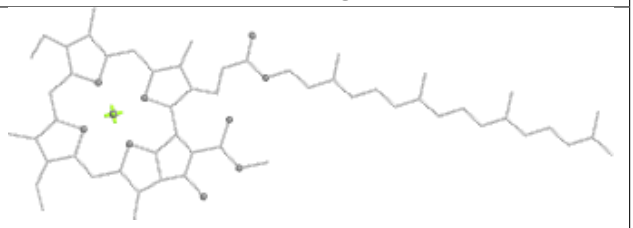
Bond lengths



Bond angles

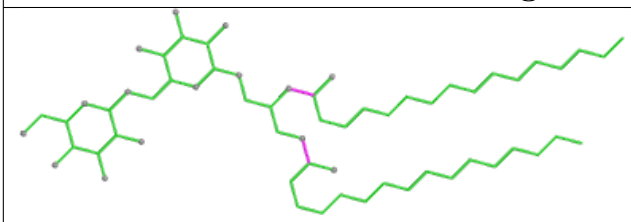


Torsions

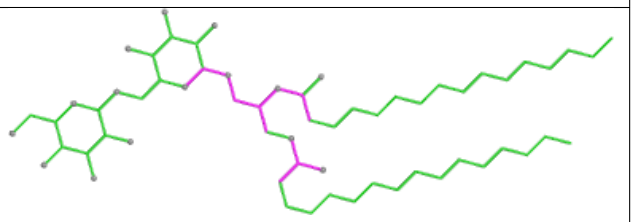


Rings

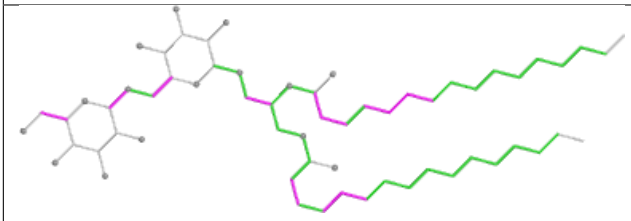
Ligand DGD C 516



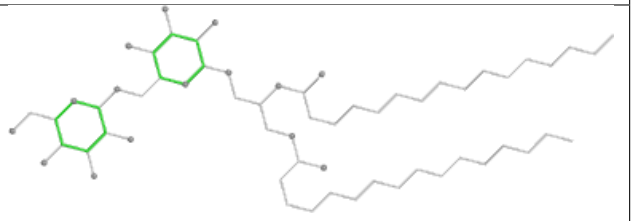
Bond lengths



Bond angles

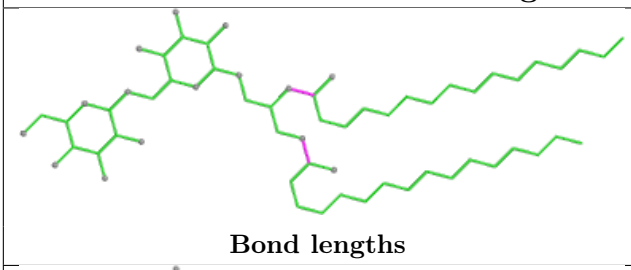


Torsions

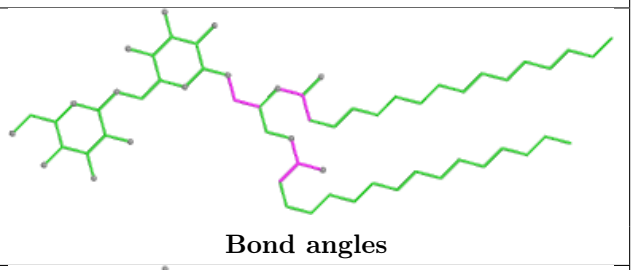


Rings

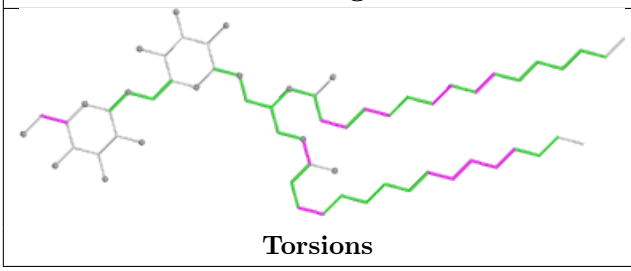
Ligand DGD C 518



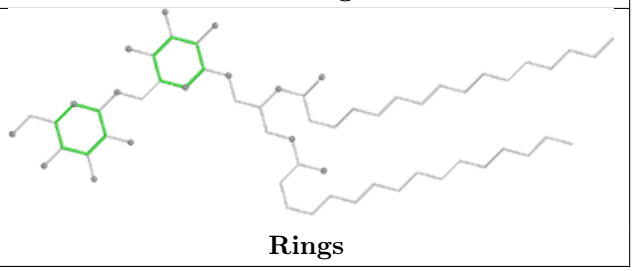
Bond lengths



Bond angles

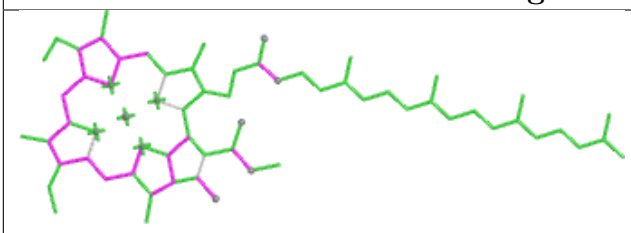


Torsions

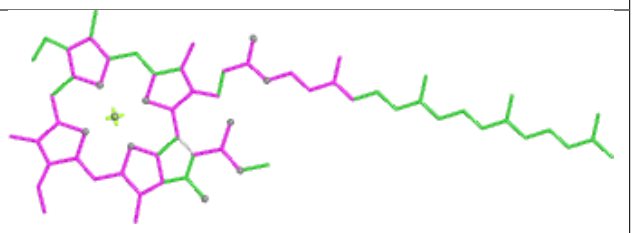


Rings

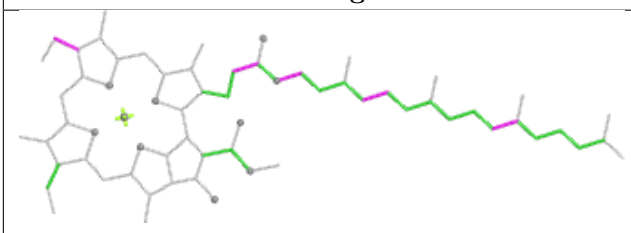
Ligand CLA d 404



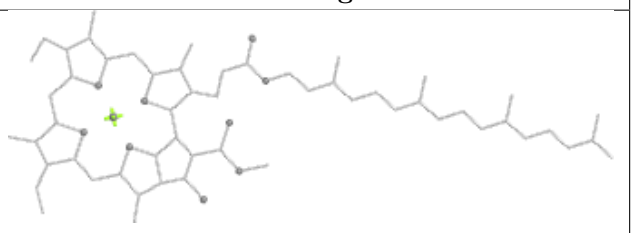
Bond lengths



Bond angles

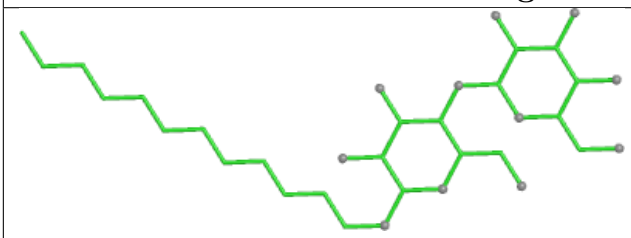


Torsions

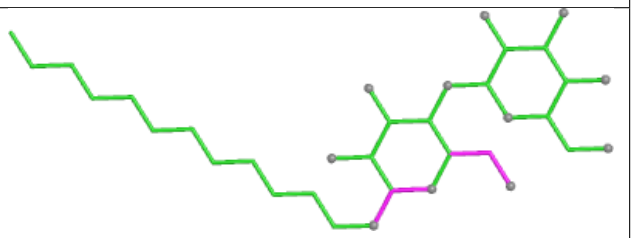


Rings

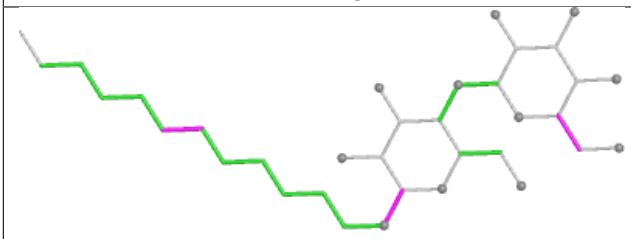
Ligand LMT M 102



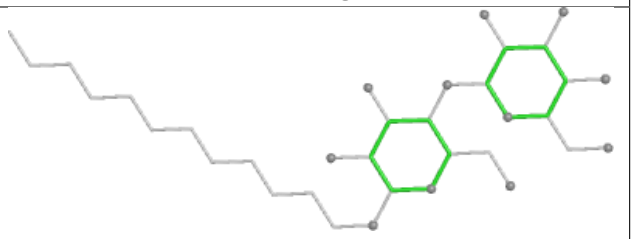
Bond lengths



Bond angles

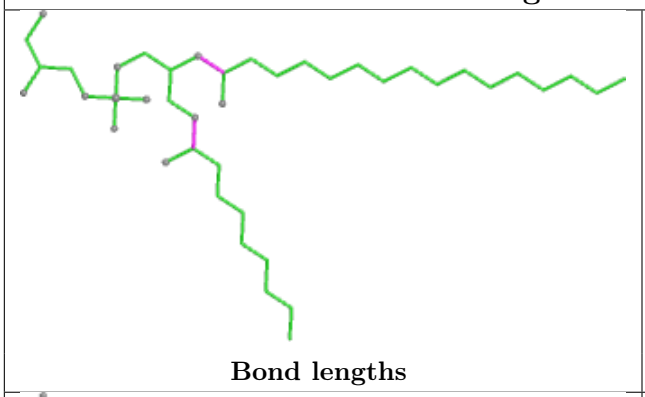


Torsions

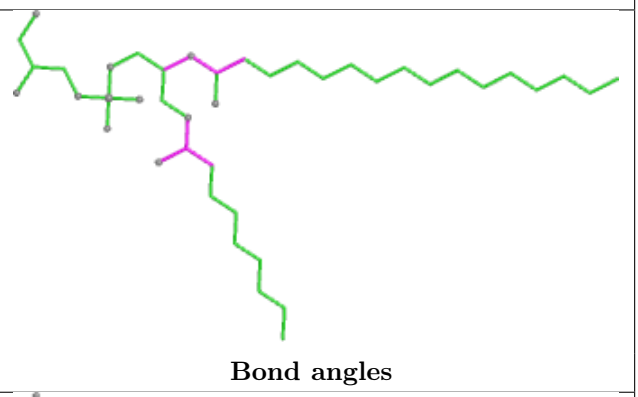


Rings

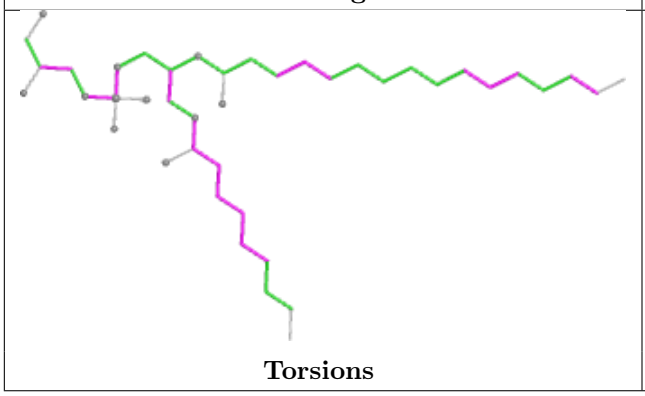
Ligand LHG A 419



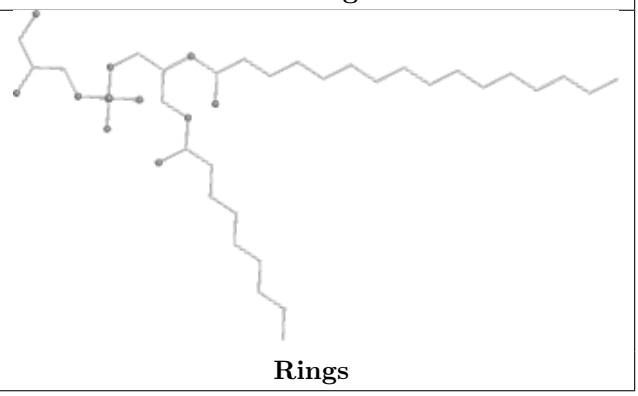
Bond lengths



Bond angles

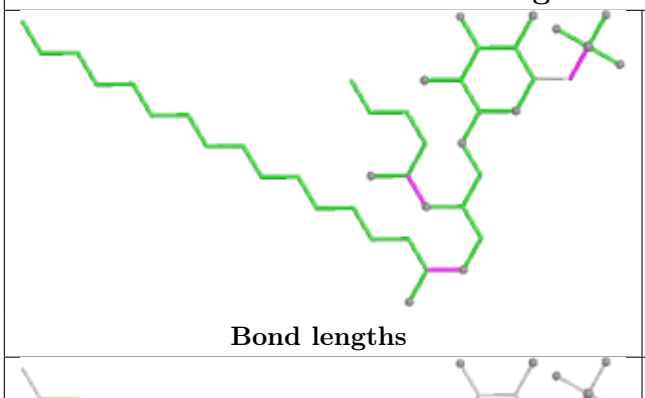


Torsions

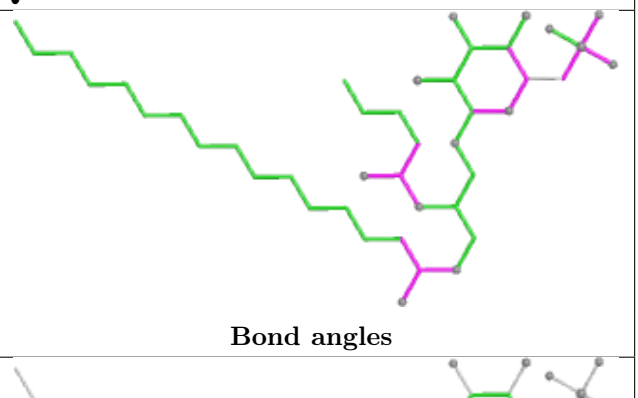


Rings

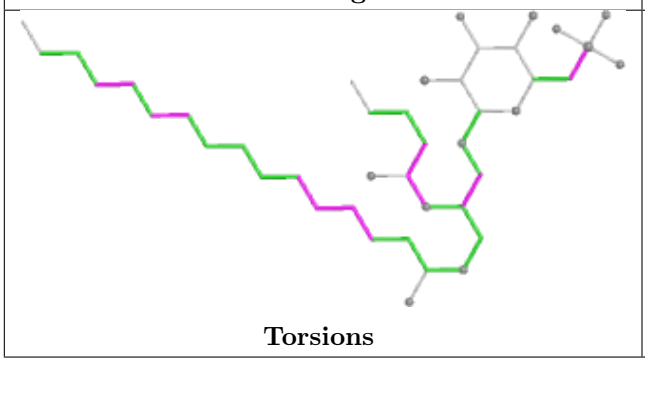
Ligand SQD f 102



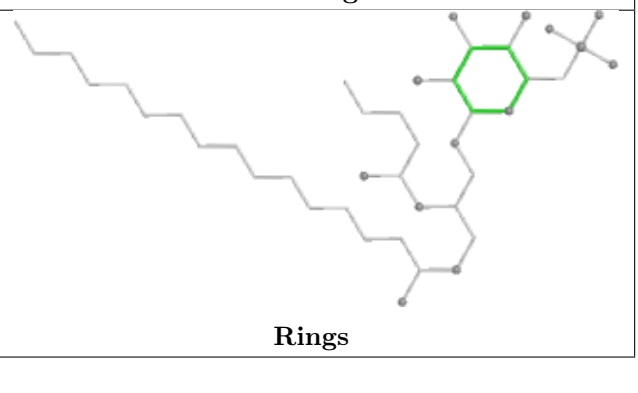
Bond lengths



Bond angles

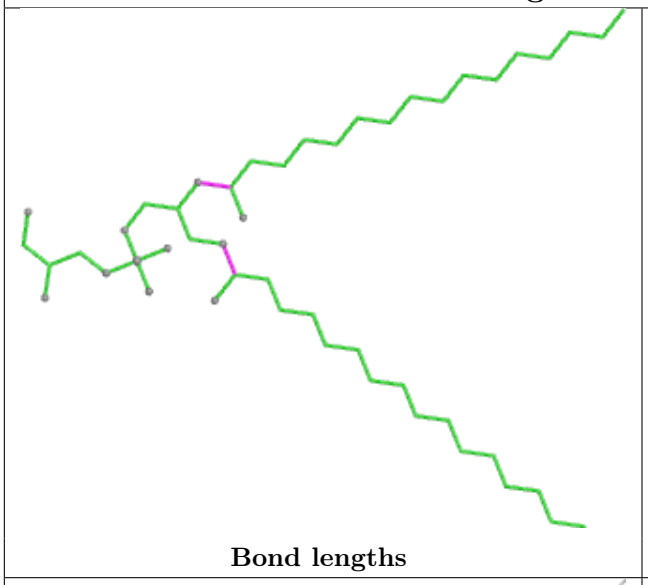


Torsions

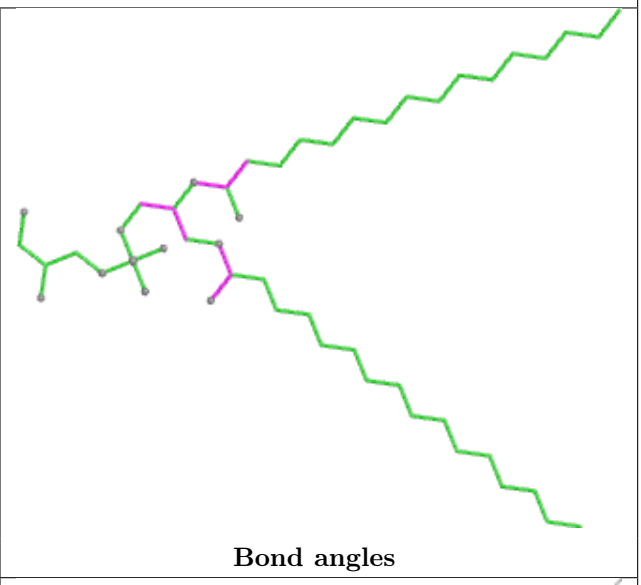


Rings

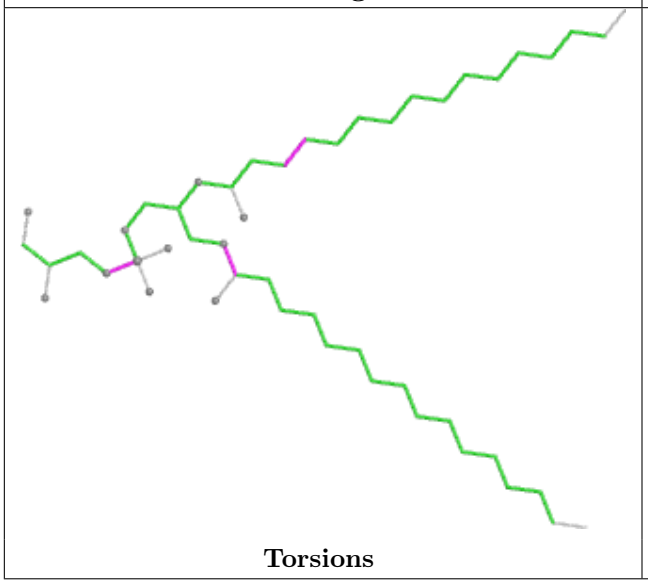
Ligand LHG d 410



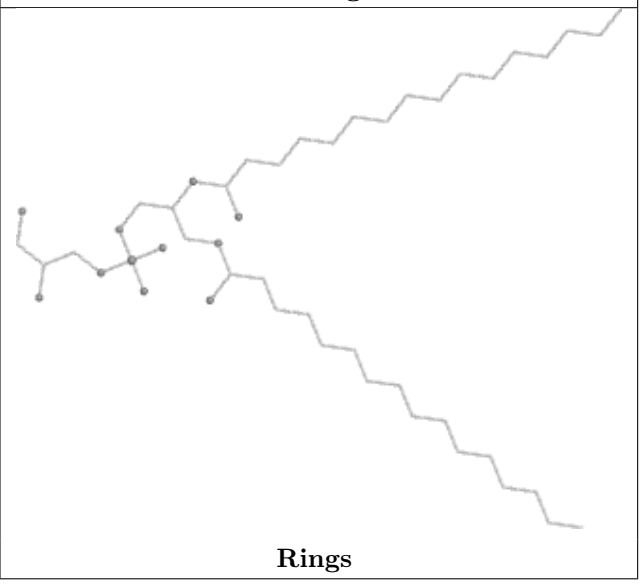
Bond lengths



Bond angles

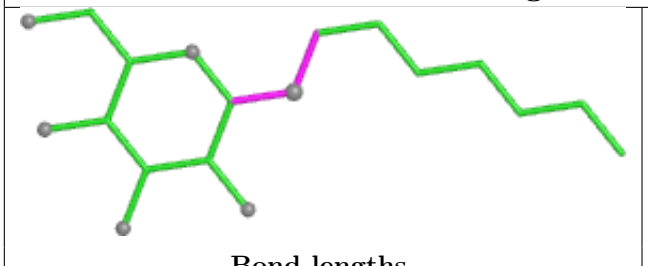


Torsions

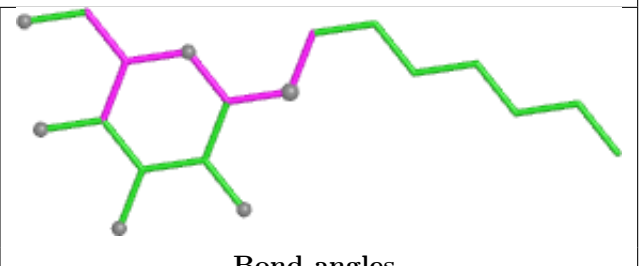


Rings

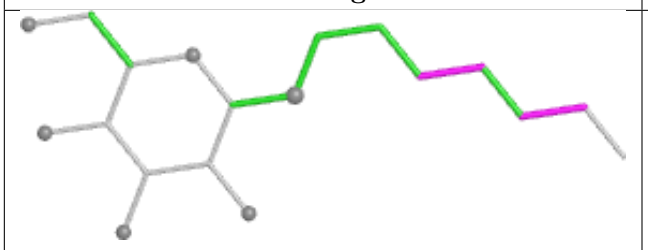
Ligand HTG b 607



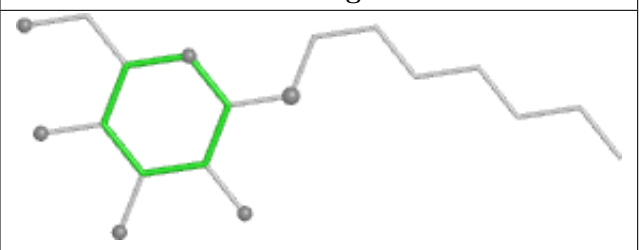
Bond lengths



Bond angles

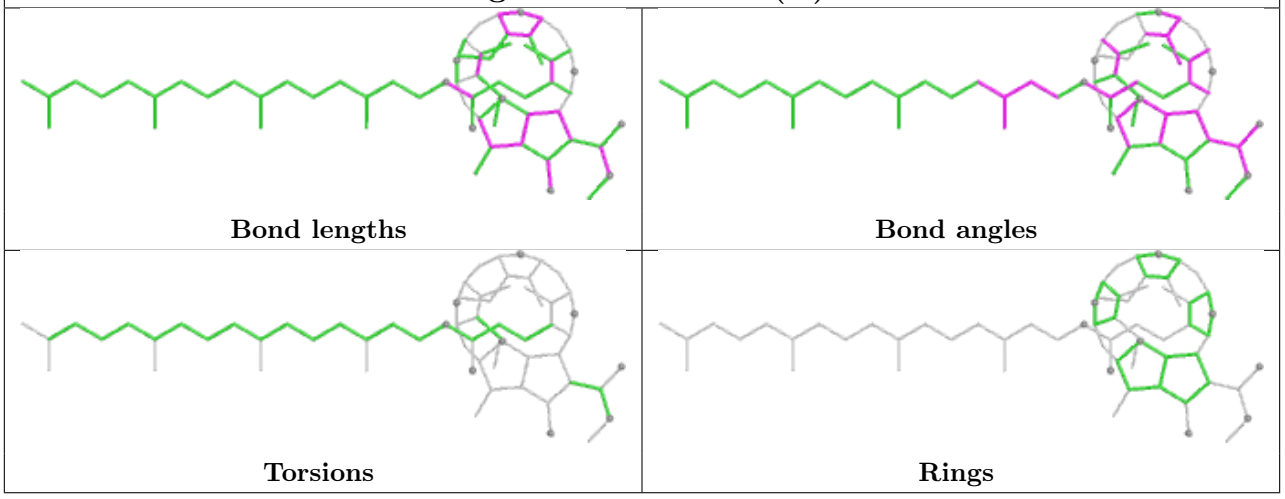


Torsions

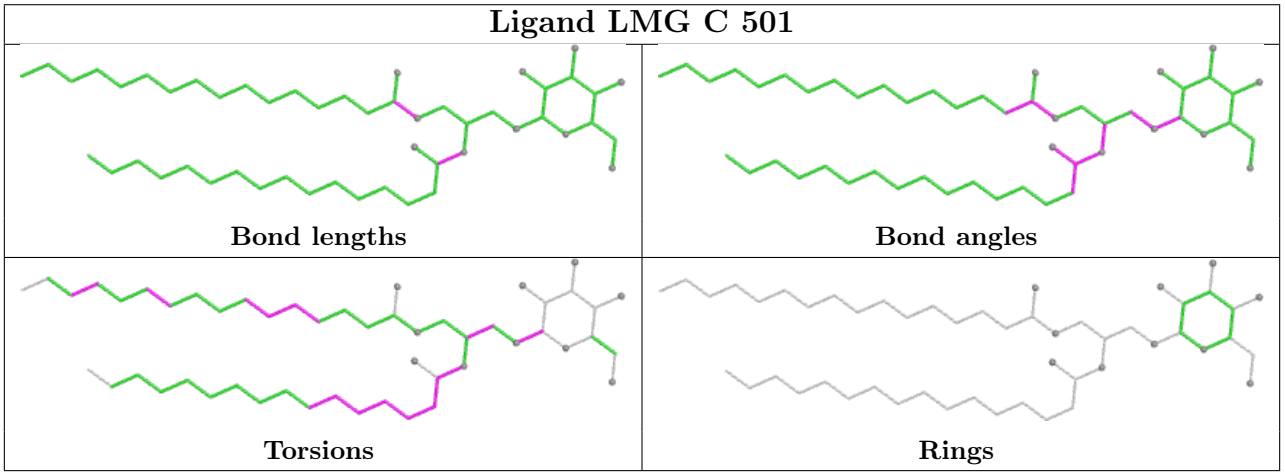


Rings

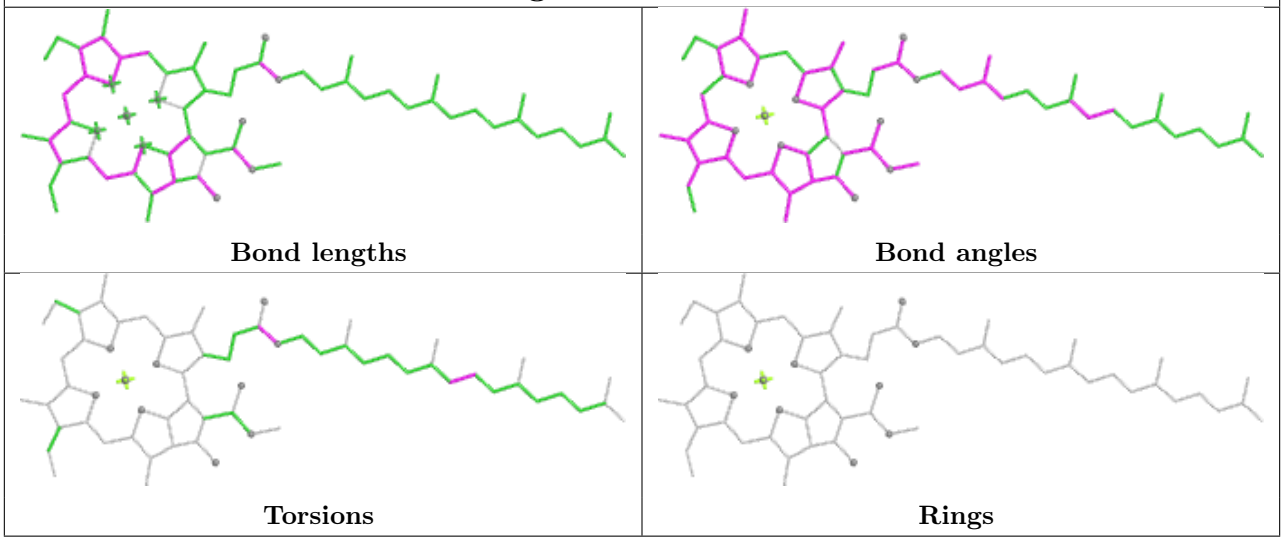
Ligand PHO D 402 (A)



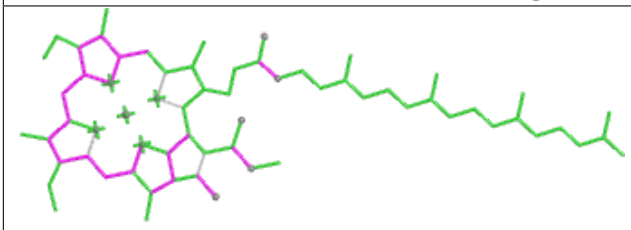
Ligand LMG C 501



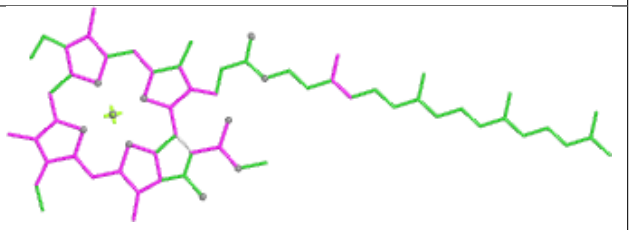
Ligand CLA b 621



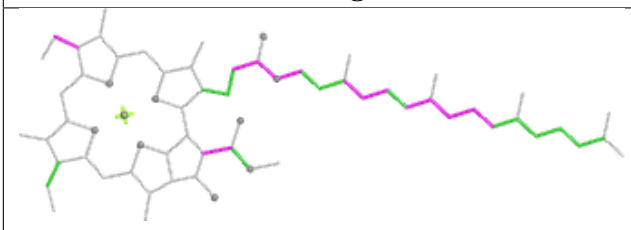
Ligand CLA b 610



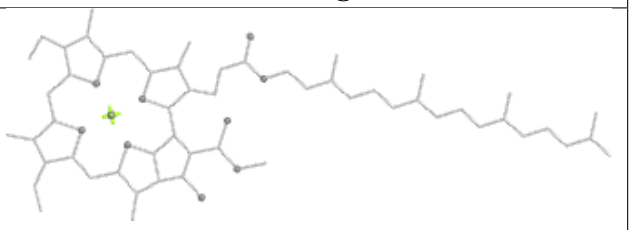
Bond lengths



Bond angles

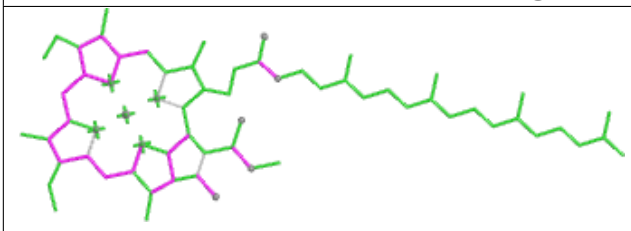


Torsions

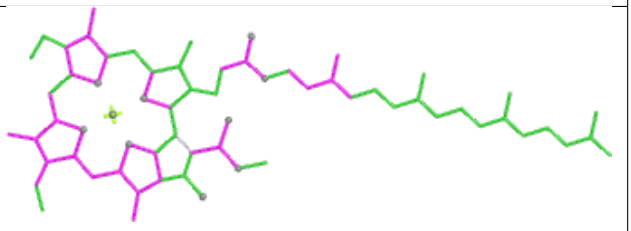


Rings

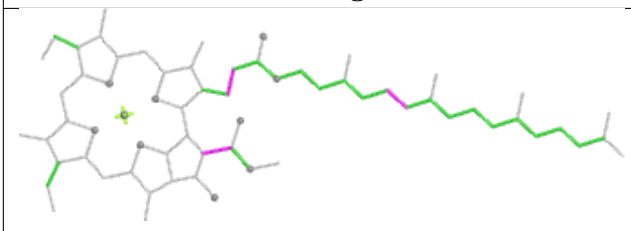
Ligand CLA c 511



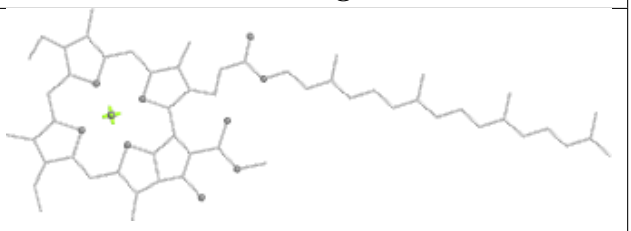
Bond lengths



Bond angles

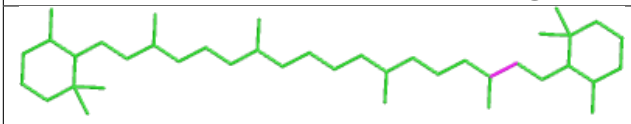


Torsions

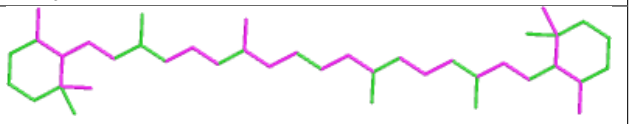


Rings

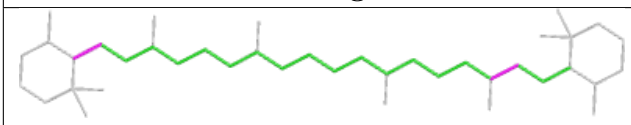
Ligand BCR y 101



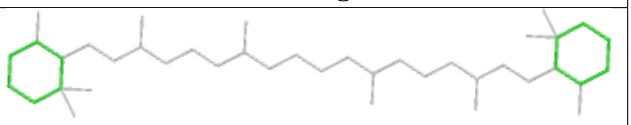
Bond lengths



Bond angles

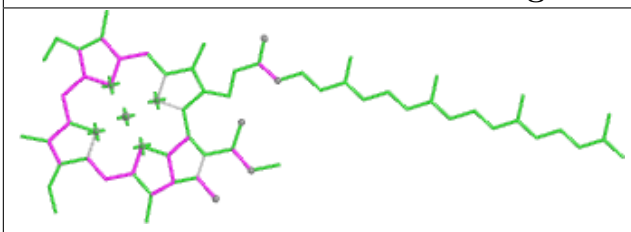


Torsions

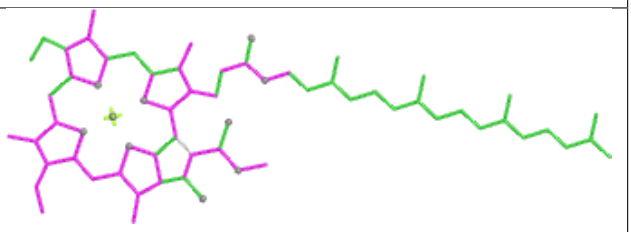


Rings

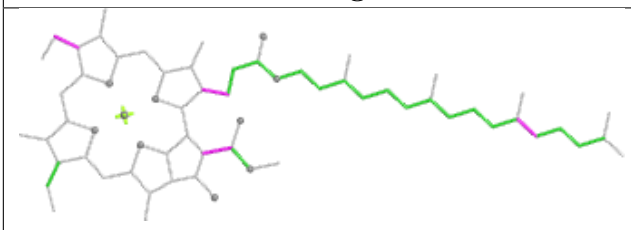
Ligand CLA b 616



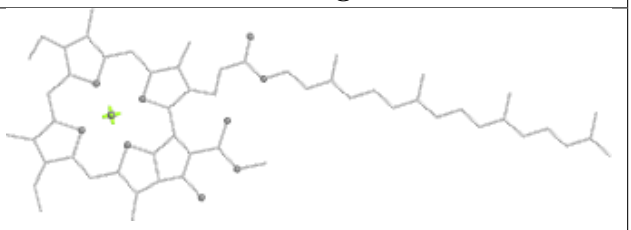
Bond lengths



Bond angles

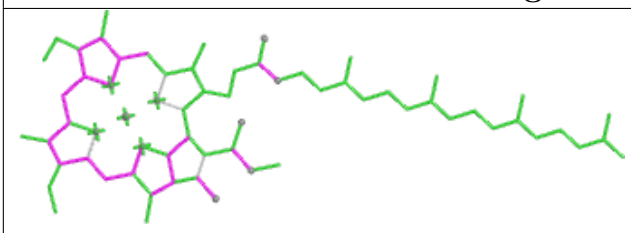


Torsions

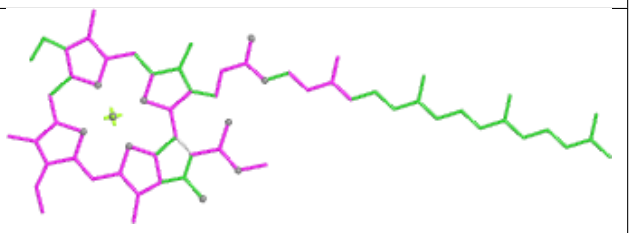


Rings

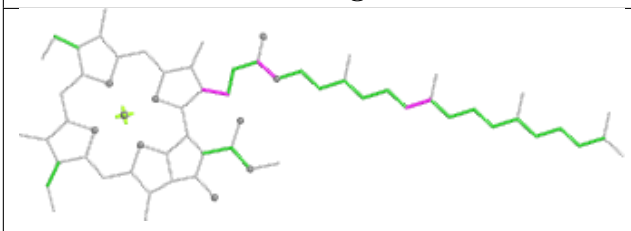
Ligand CLA C 512



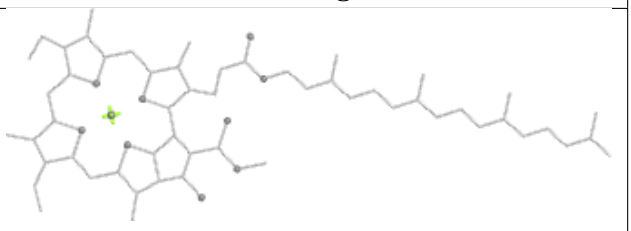
Bond lengths



Bond angles

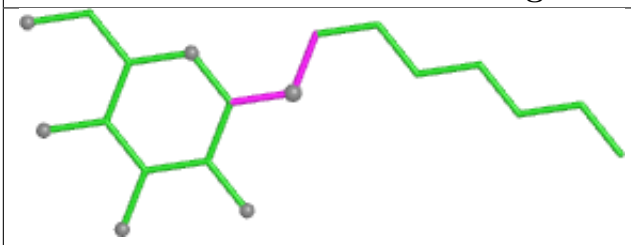


Torsions

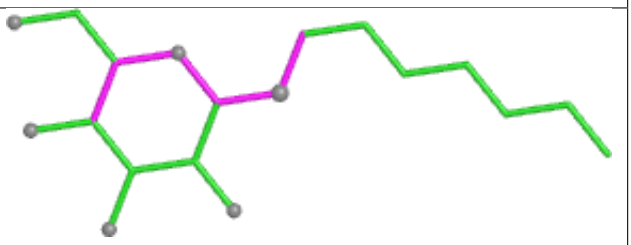


Rings

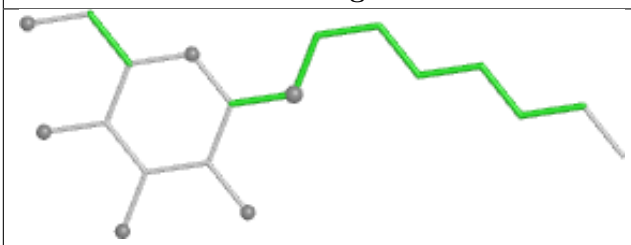
Ligand HTG c 524



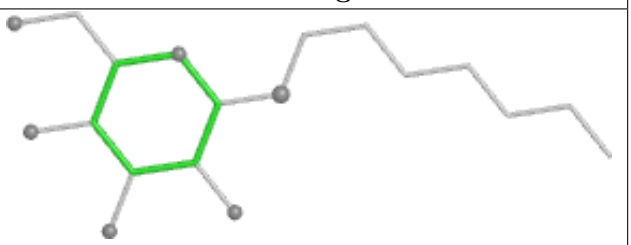
Bond lengths



Bond angles

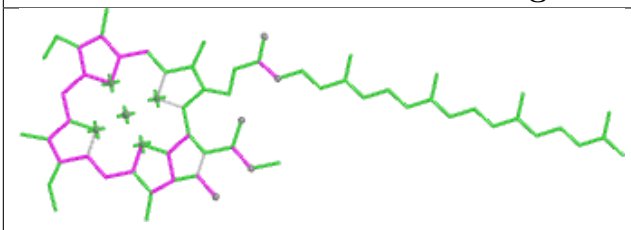


Torsions

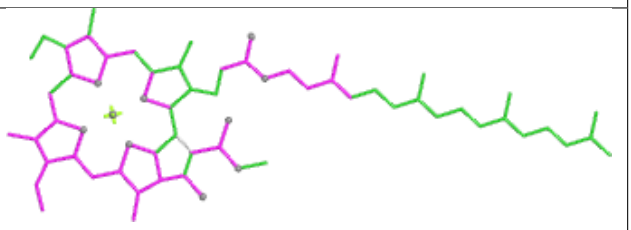


Rings

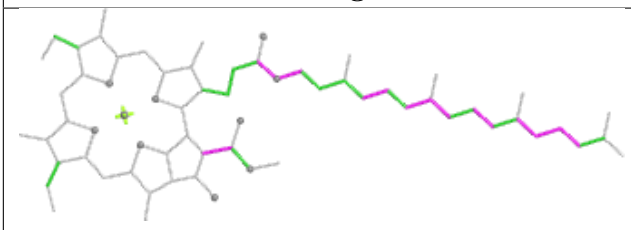
Ligand CLA c 513



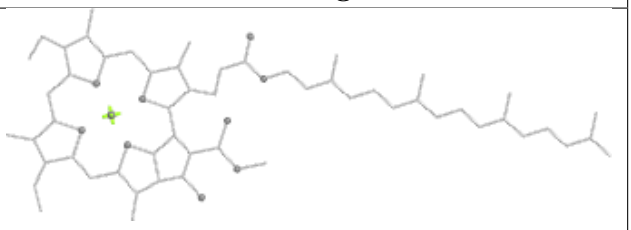
Bond lengths



Bond angles

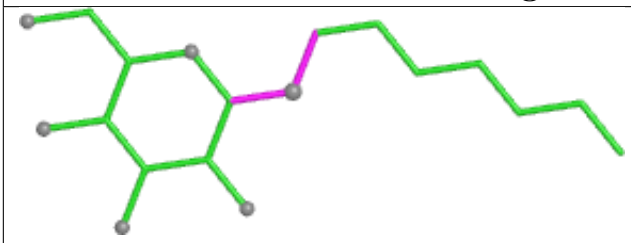


Torsions

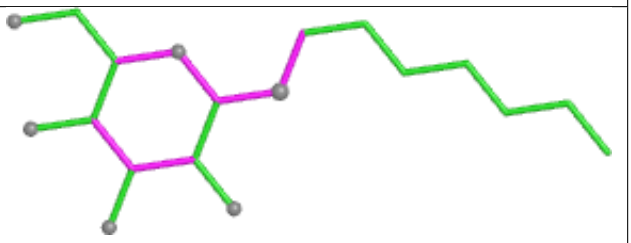


Rings

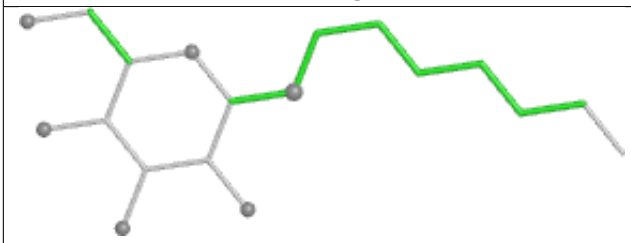
Ligand HTG C 522



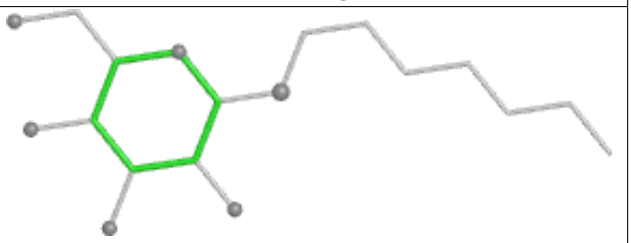
Bond lengths



Bond angles

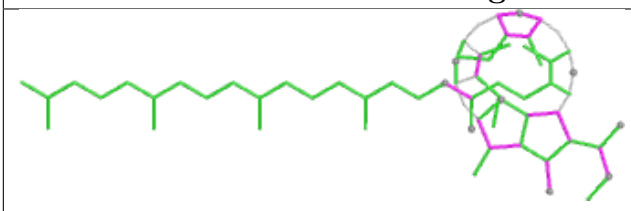


Torsions

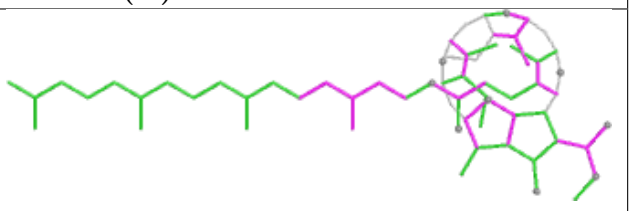


Rings

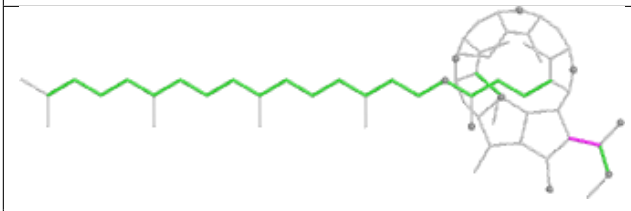
Ligand PHO D 402 (B)



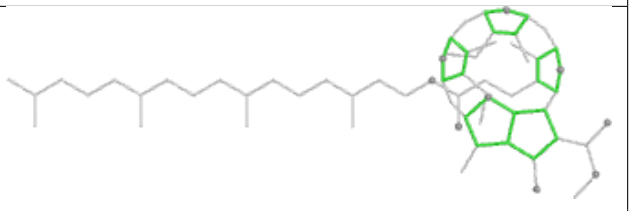
Bond lengths



Bond angles

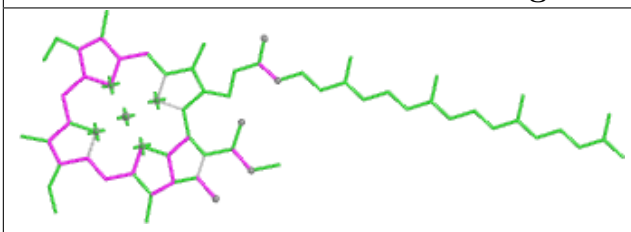


Torsions

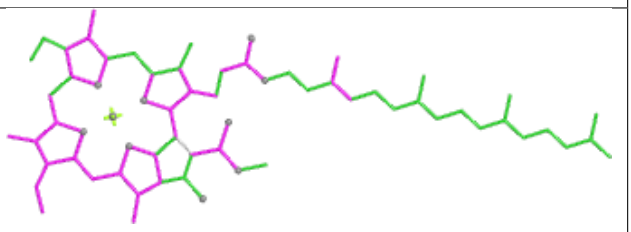


Rings

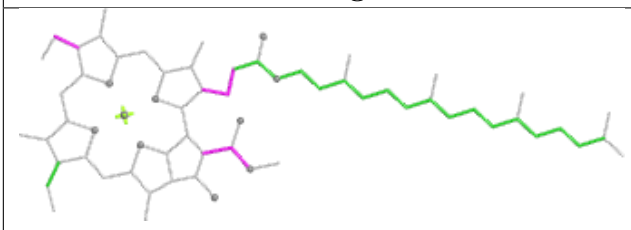
Ligand CLA c 505



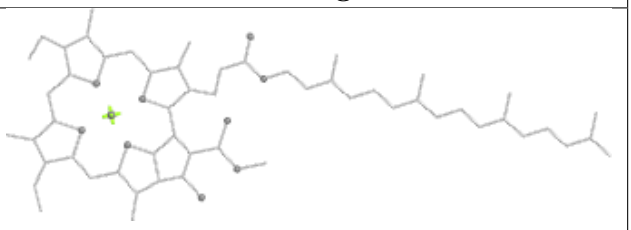
Bond lengths



Bond angles



Torsions

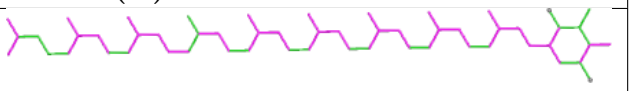


Rings

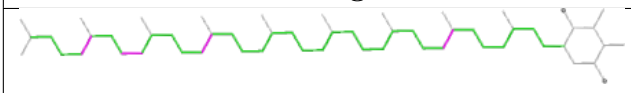
Ligand PL9 D 408 (B)



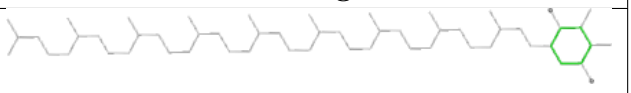
Bond lengths



Bond angles

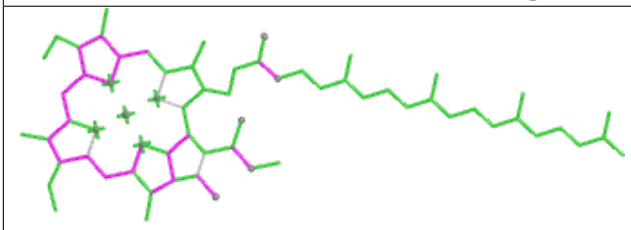


Torsions

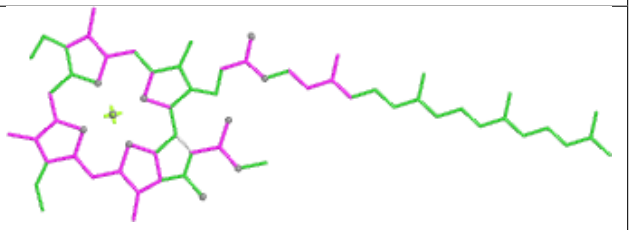


Rings

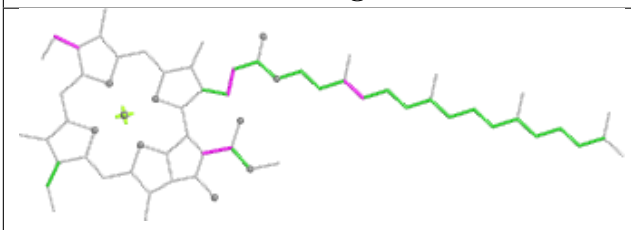
Ligand CLA C 508



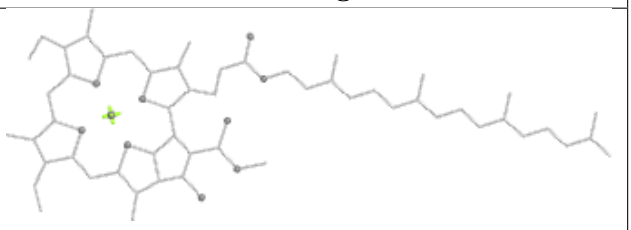
Bond lengths



Bond angles

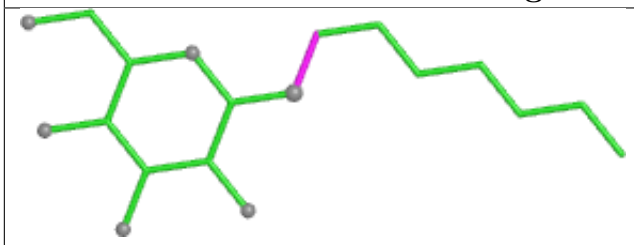


Torsions

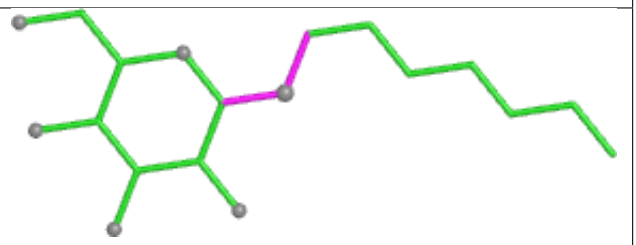


Rings

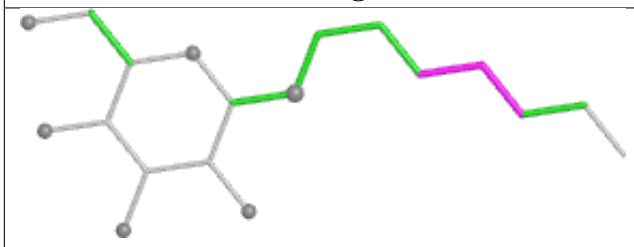
Ligand HTG b 631



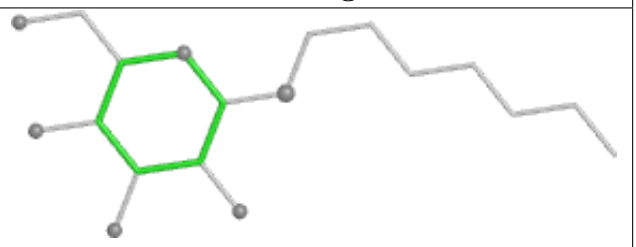
Bond lengths



Bond angles

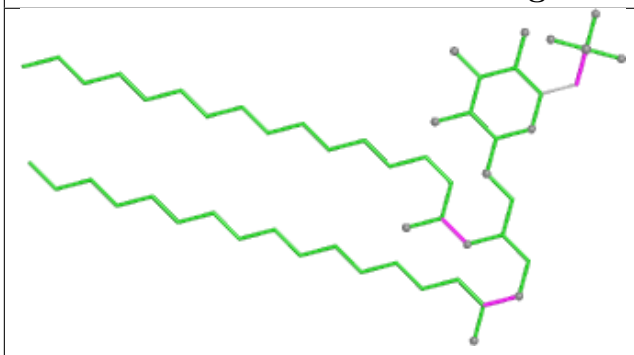


Torsions

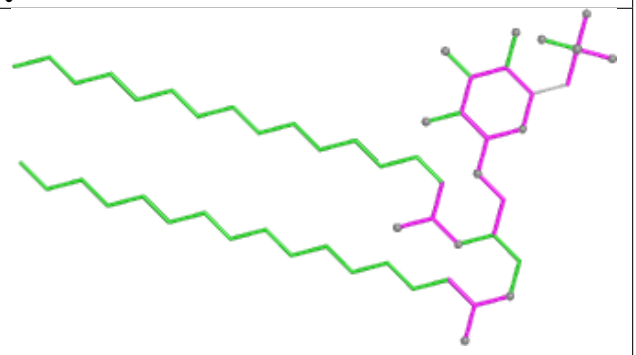


Rings

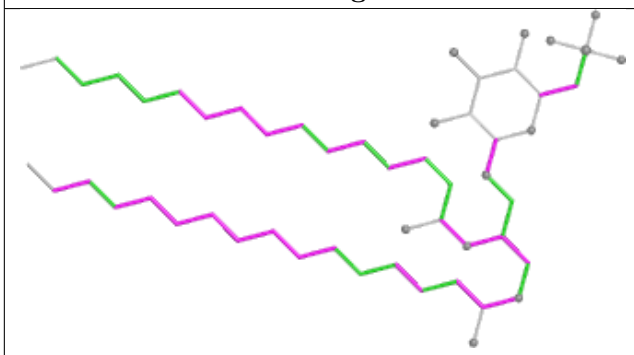
Ligand SQD b 601



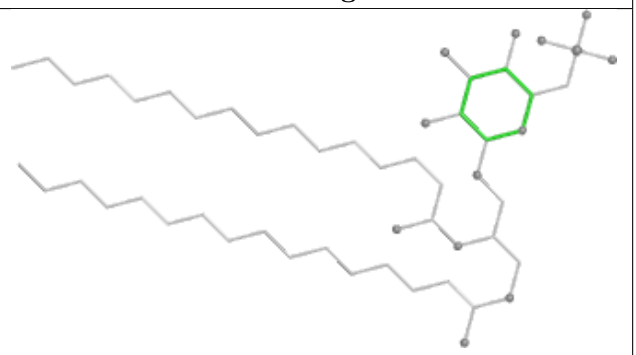
Bond lengths



Bond angles

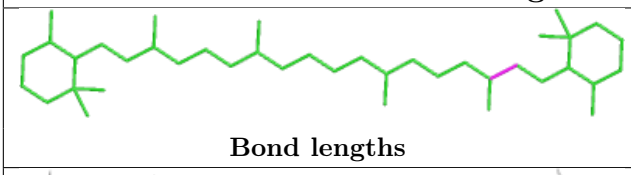


Torsions

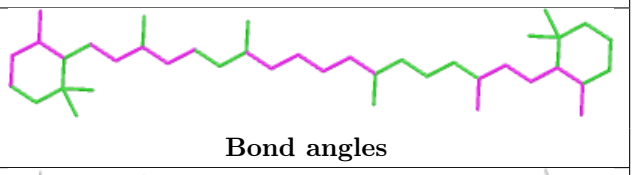


Rings

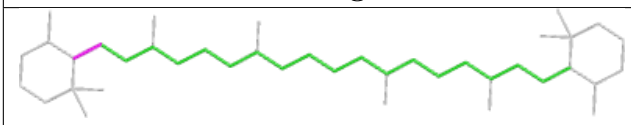
Ligand BCR c 518



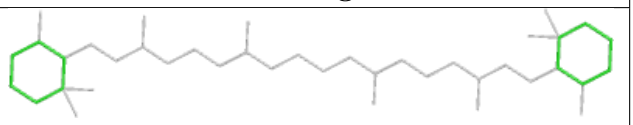
Bond lengths



Bond angles

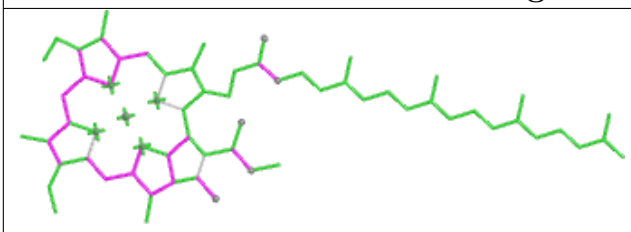


Torsions

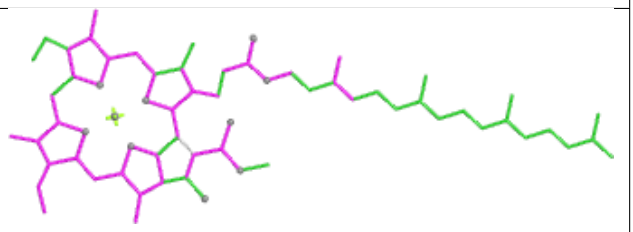


Rings

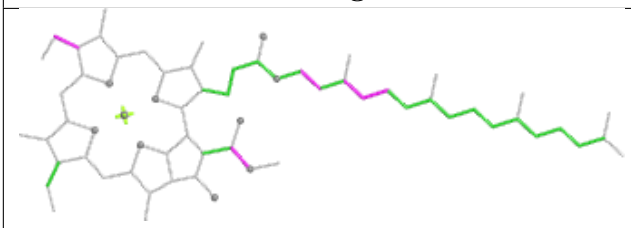
Ligand CLA d 405



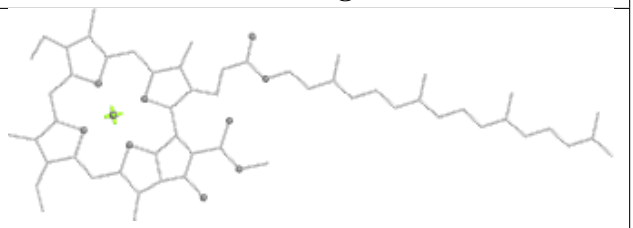
Bond lengths



Bond angles

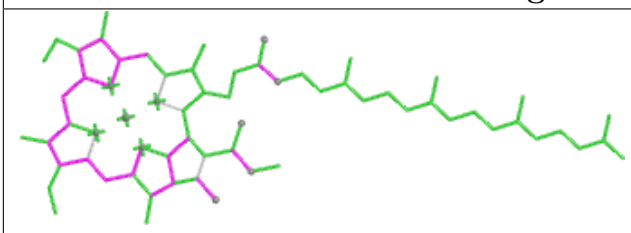


Torsions

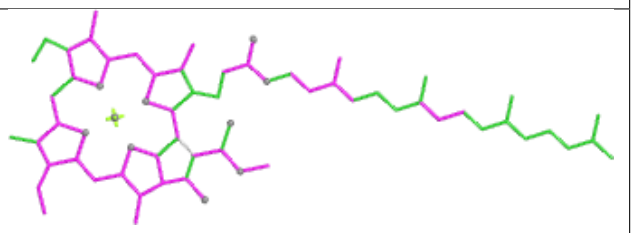


Rings

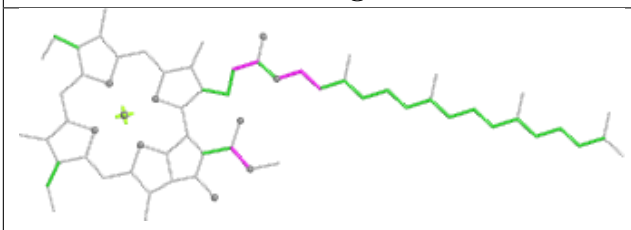
Ligand CLA b 622



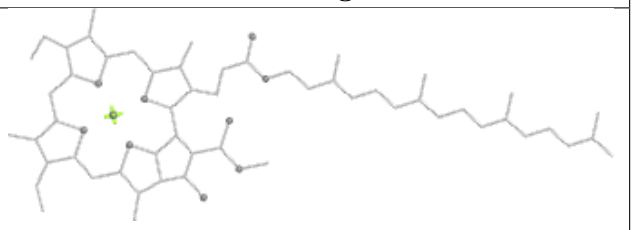
Bond lengths



Bond angles

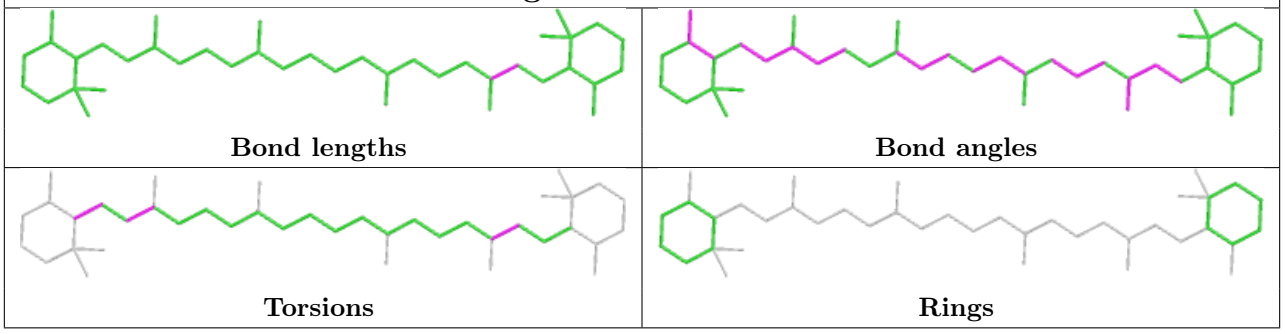


Torsions

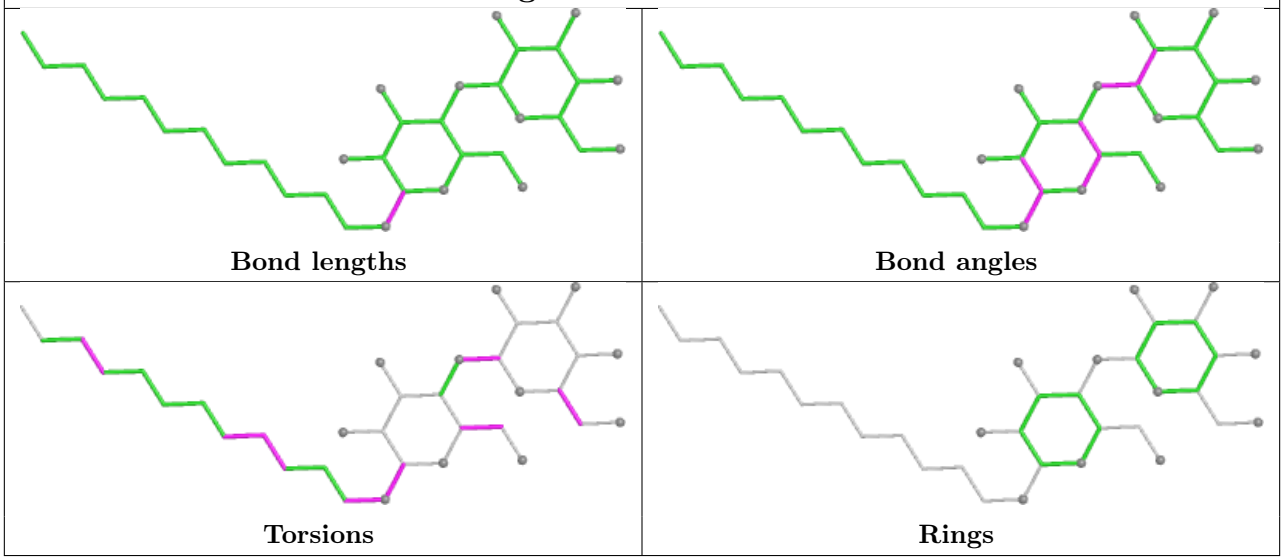


Rings

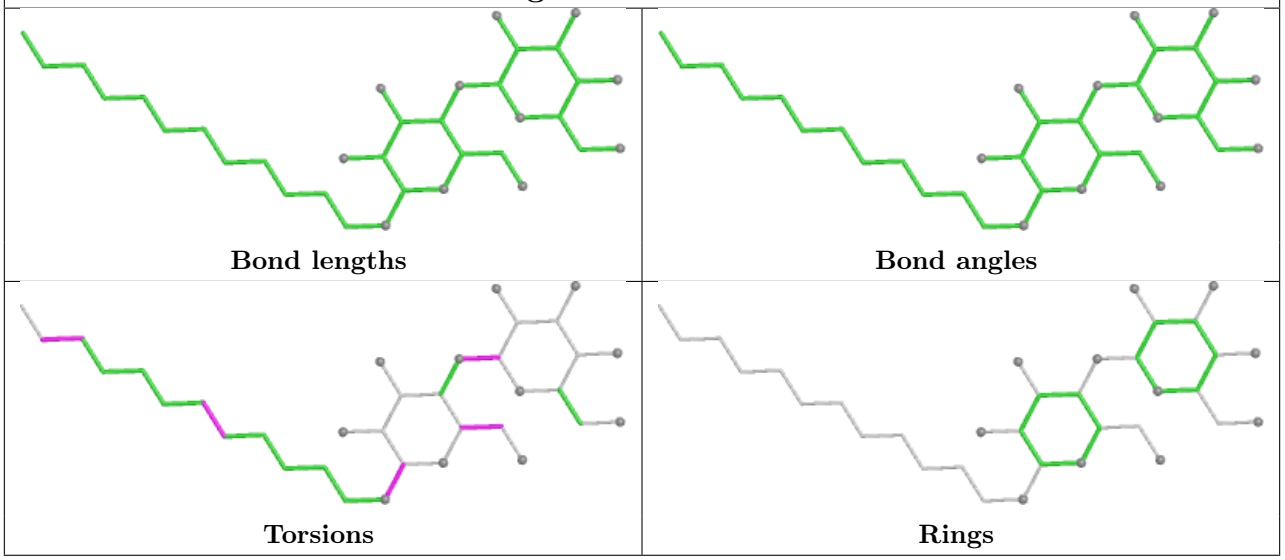
Ligand BCR C 515



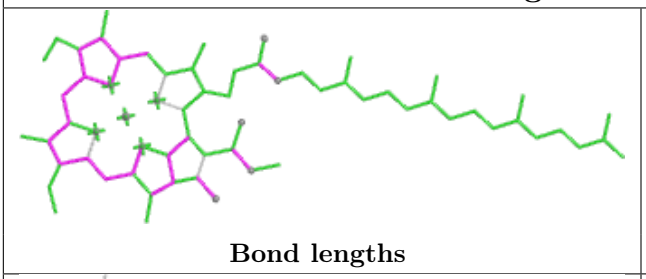
Ligand LMT M 104



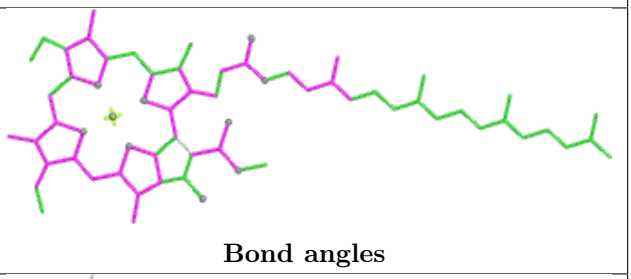
Ligand LMT e 102



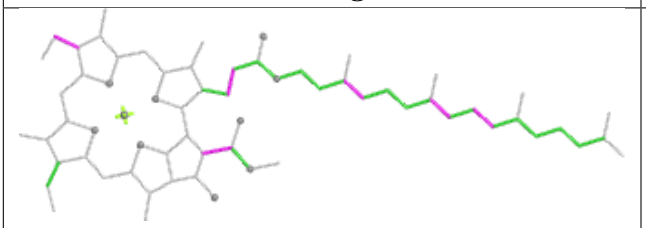
Ligand CLA B 607



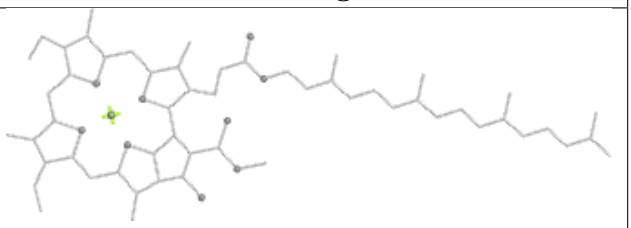
Bond lengths



Bond angles



Torsions

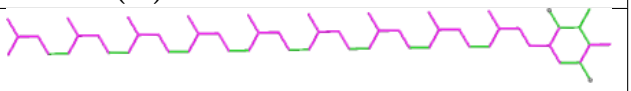


Rings

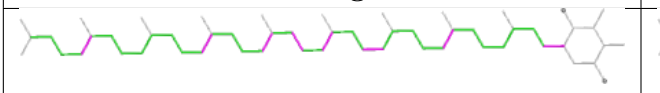
Ligand PL9 A 417 (B)



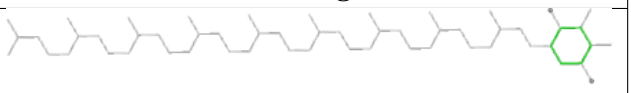
Bond lengths



Bond angles

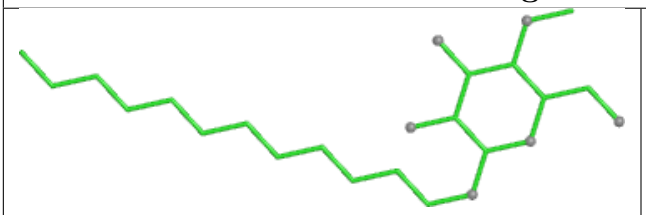


Torsions

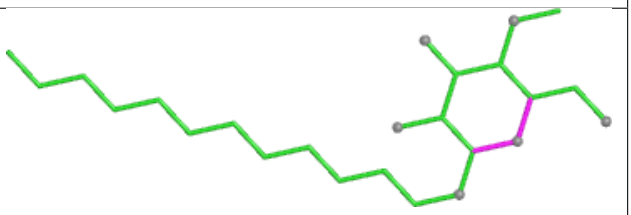


Rings

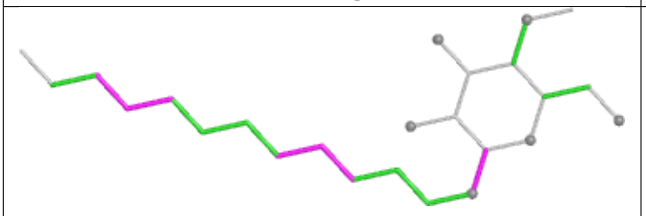
Ligand LMT B 634



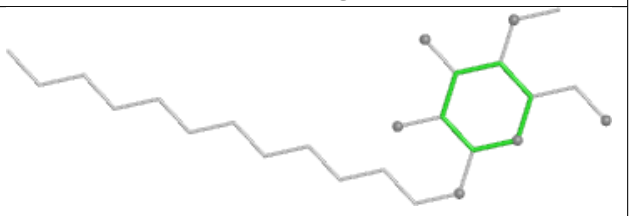
Bond lengths



Bond angles

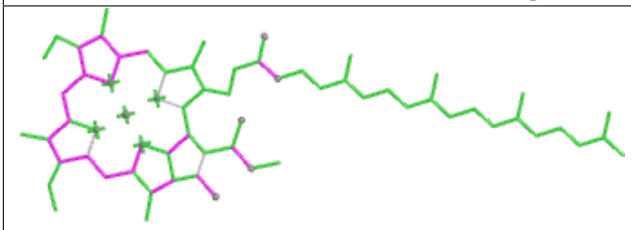


Torsions

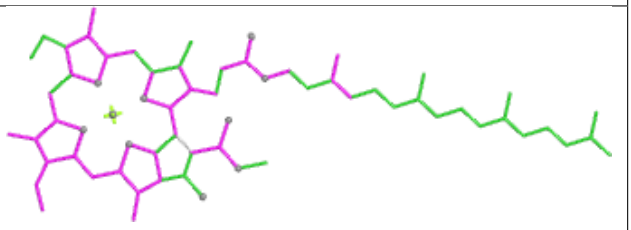


Rings

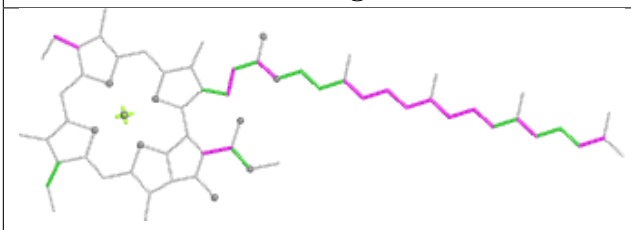
Ligand CLA B 615



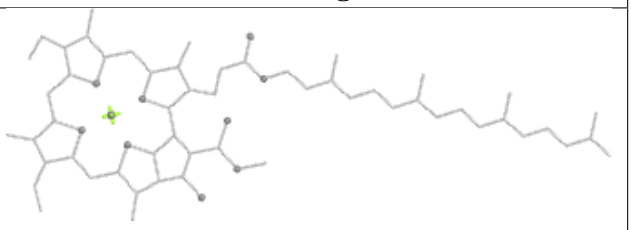
Bond lengths



Bond angles

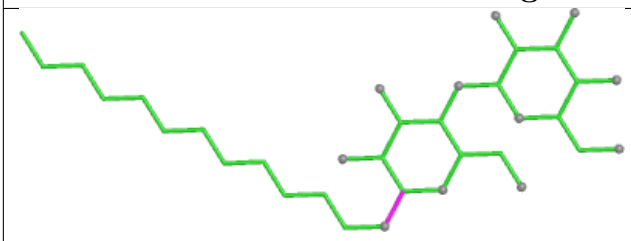


Torsions

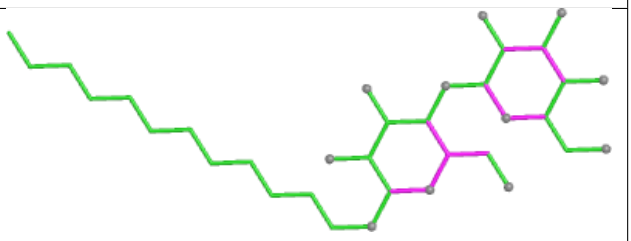


Rings

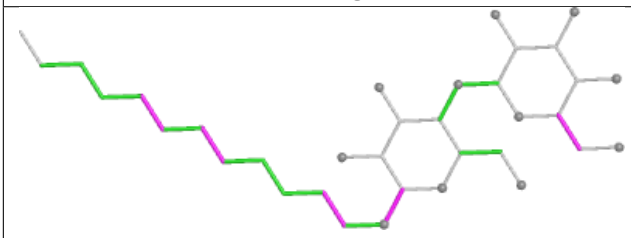
Ligand LMT A 414



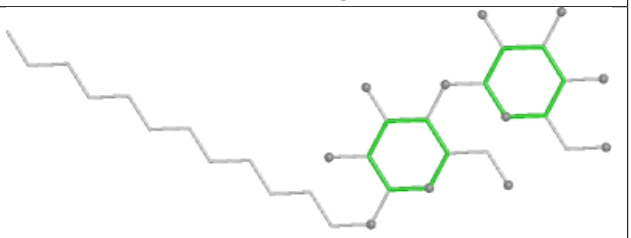
Bond lengths



Bond angles

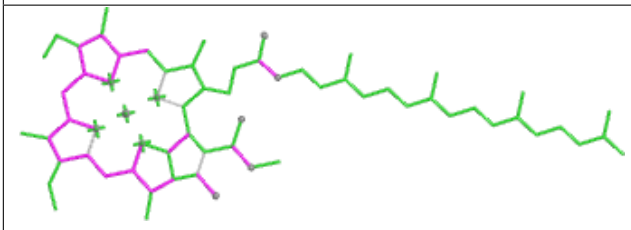


Torsions

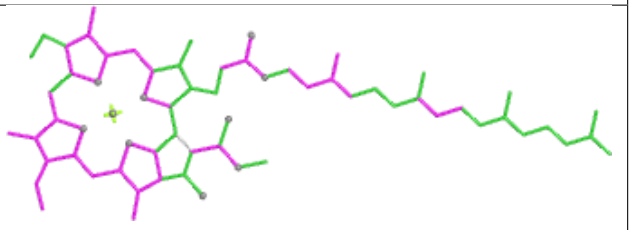


Rings

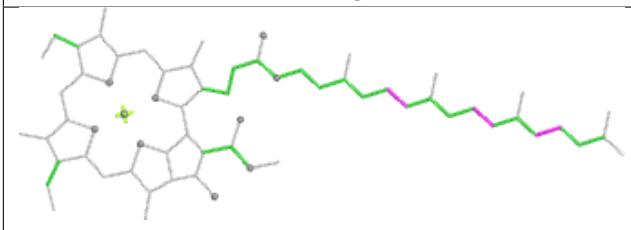
Ligand CLA b 624



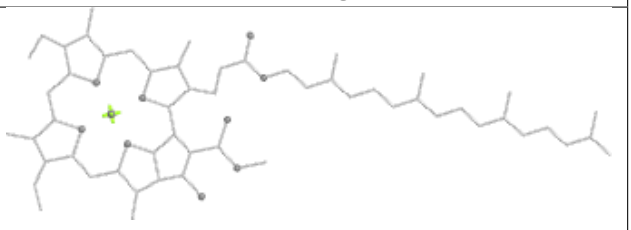
Bond lengths



Bond angles

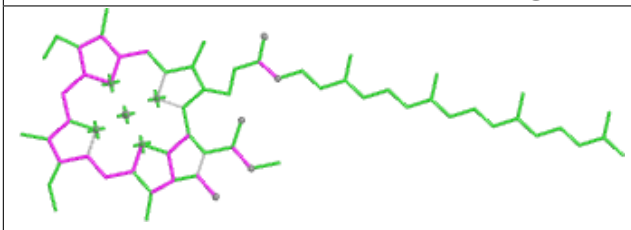


Torsions

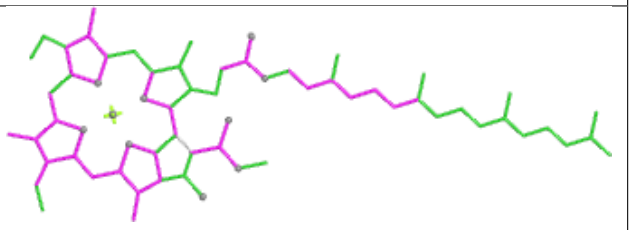


Rings

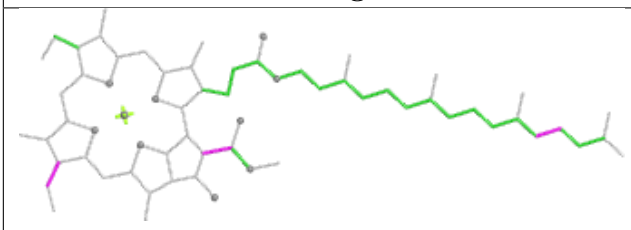
Ligand CLA b 613



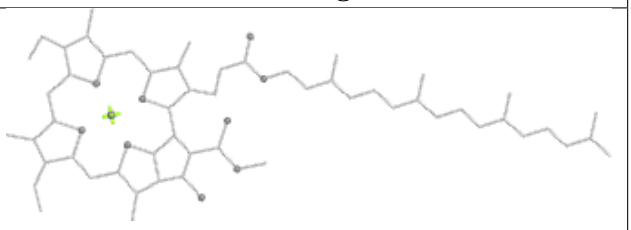
Bond lengths



Bond angles

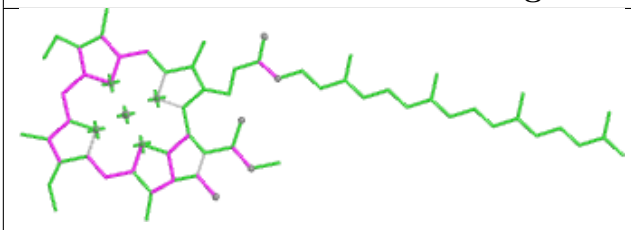


Torsions

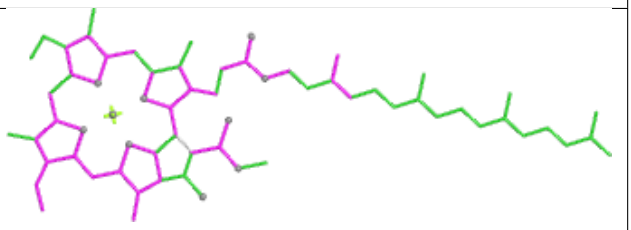


Rings

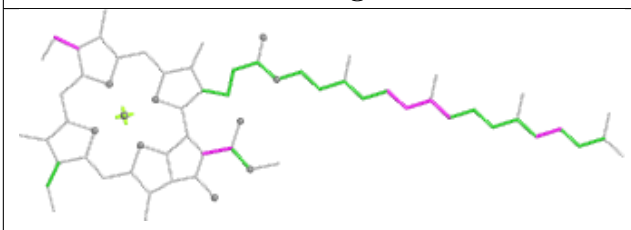
Ligand CLA B 604



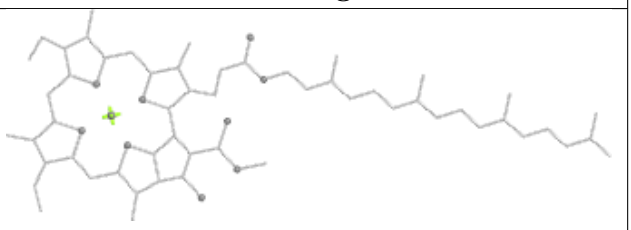
Bond lengths



Bond angles

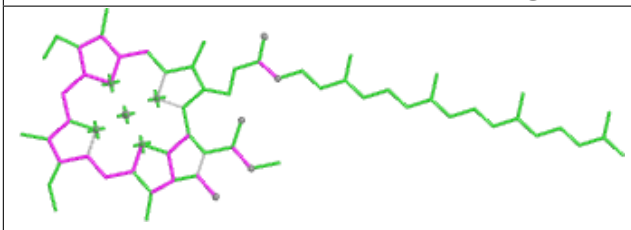


Torsions

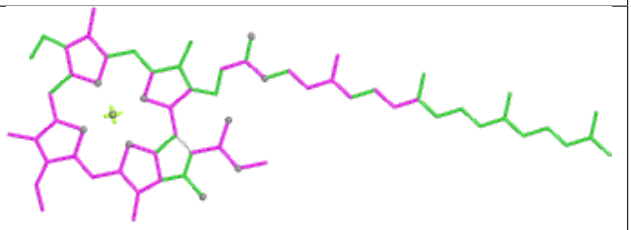


Rings

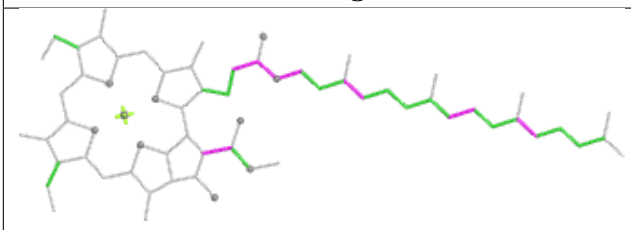
Ligand CLA C 511



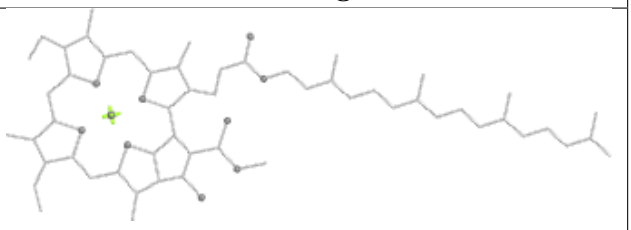
Bond lengths



Bond angles

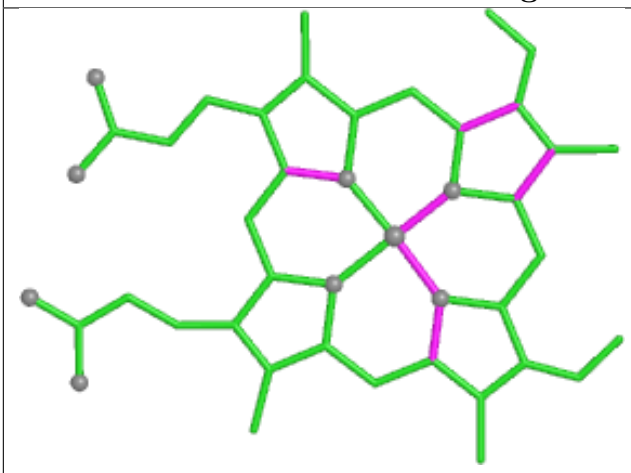


Torsions

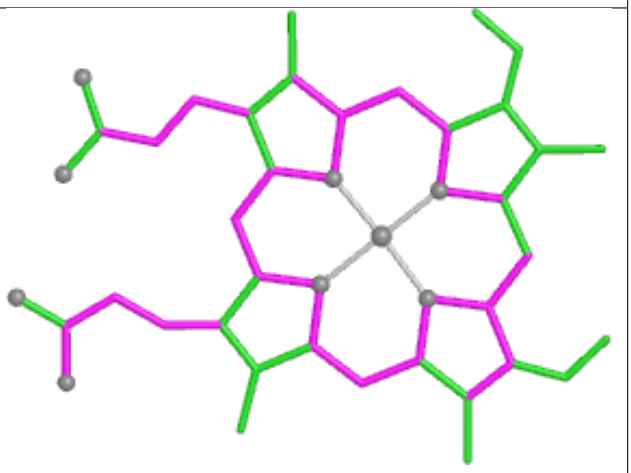


Rings

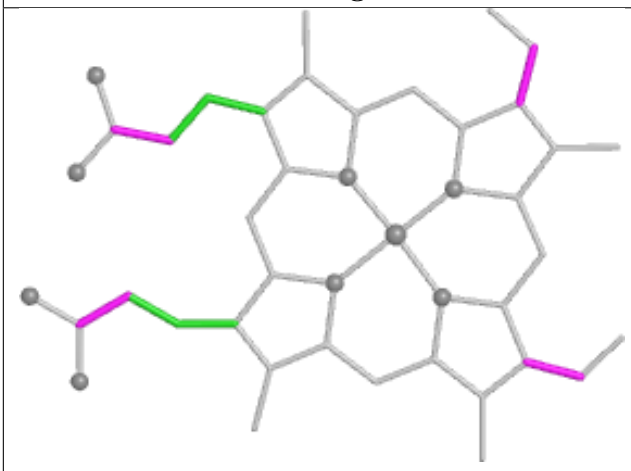
Ligand HEM F 102



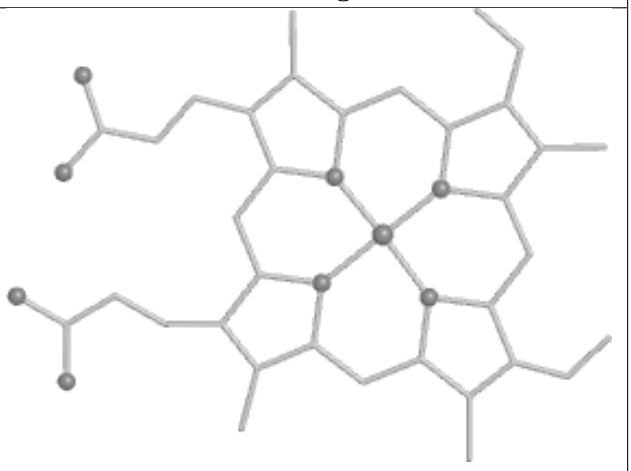
Bond lengths



Bond angles

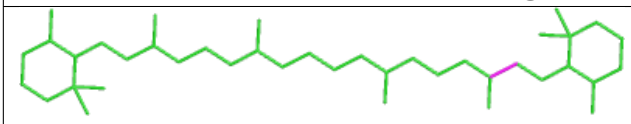


Torsions

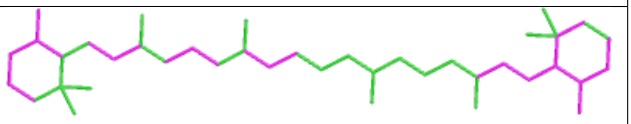


Rings

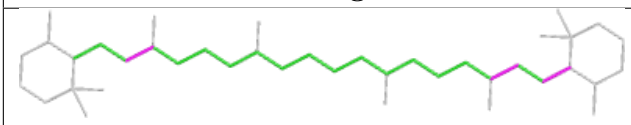
Ligand BCR D 407



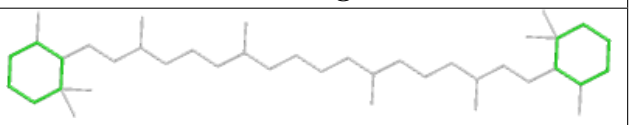
Bond lengths



Bond angles

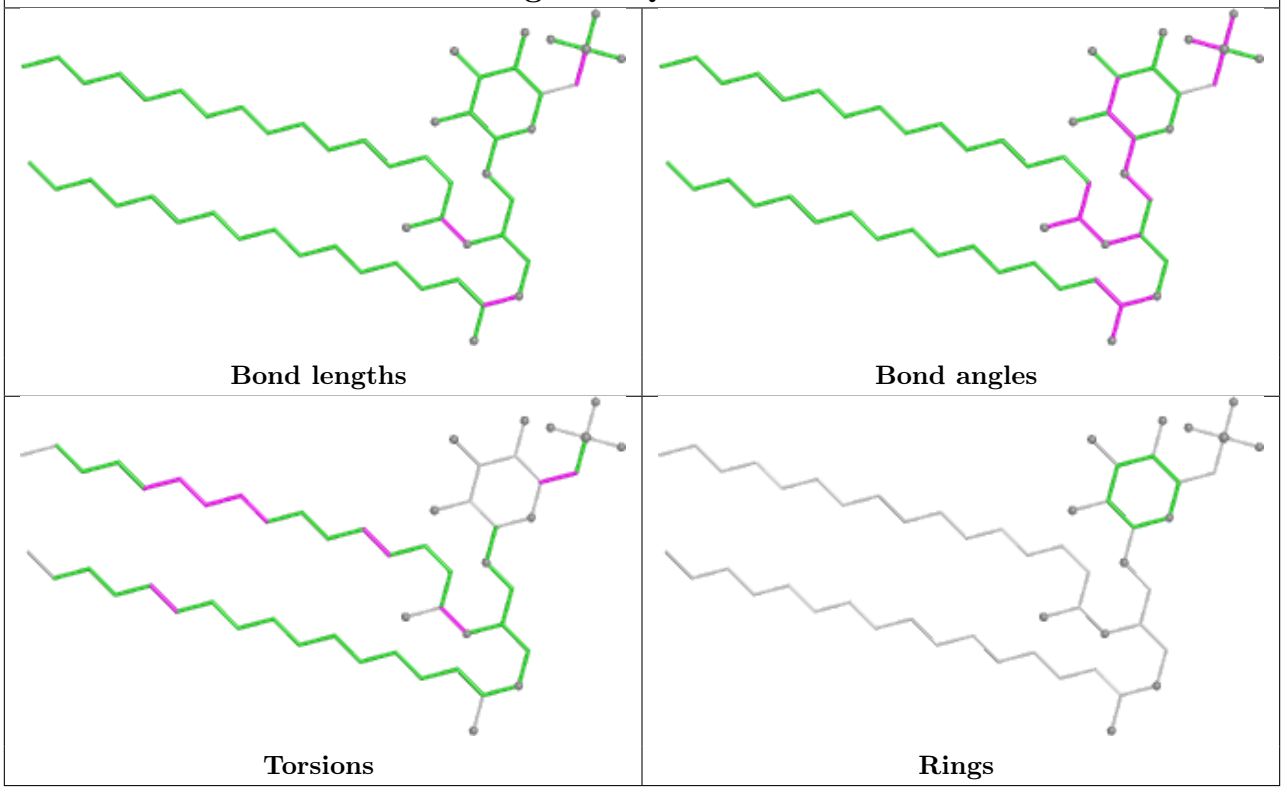


Torsions

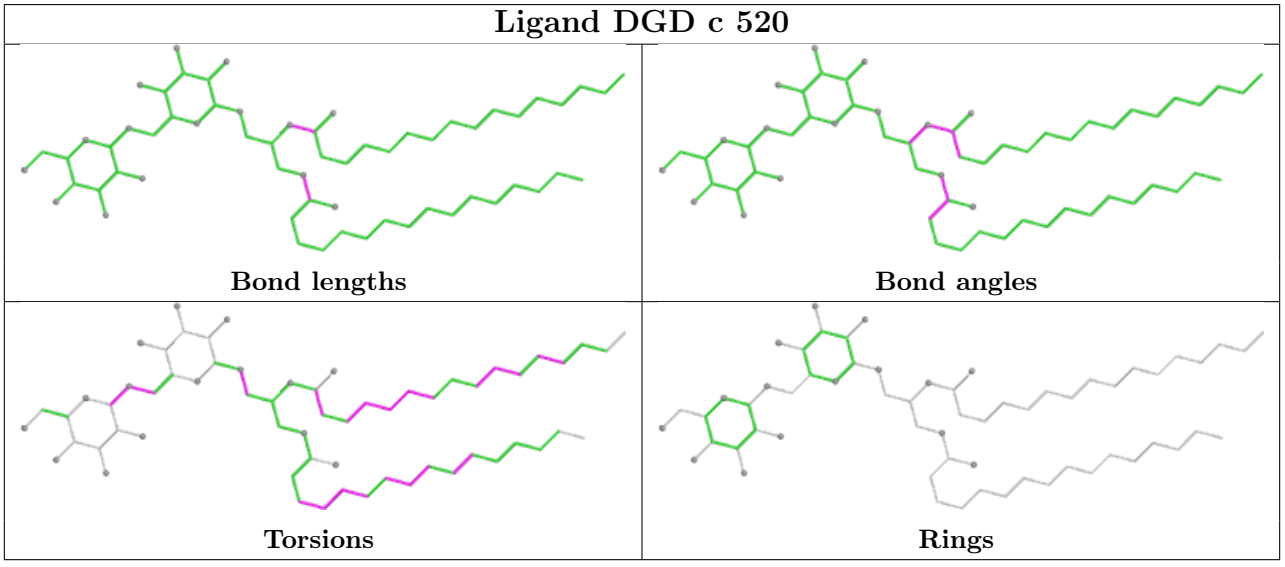


Rings

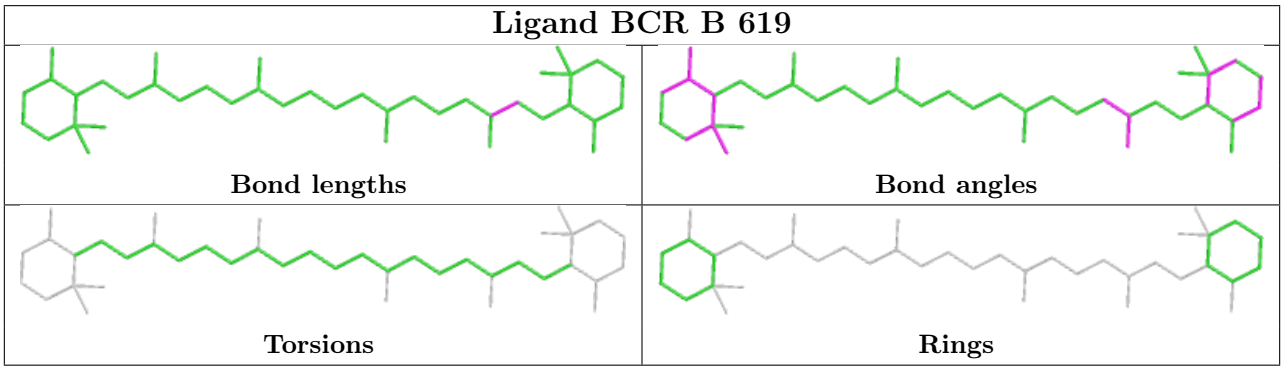
Ligand SQD A 410



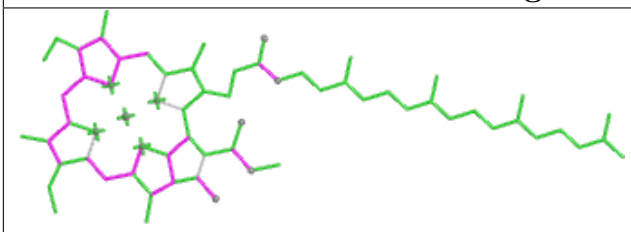
Ligand DGD c 520



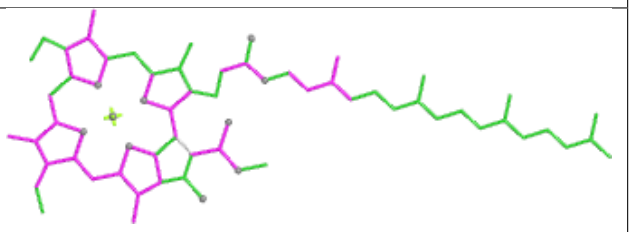
Ligand BCR B 619



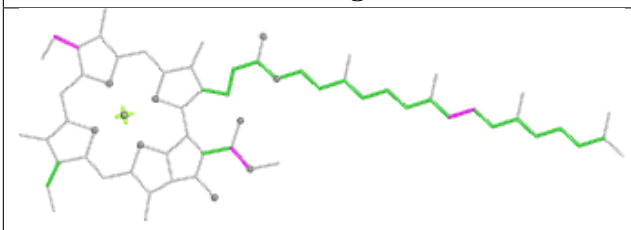
Ligand CLA B 613



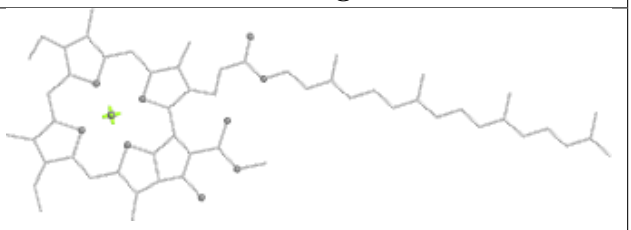
Bond lengths



Bond angles

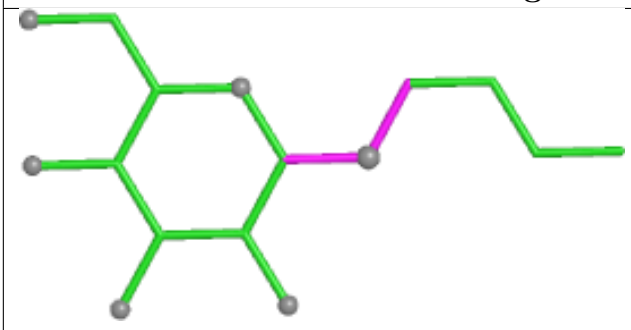


Torsions

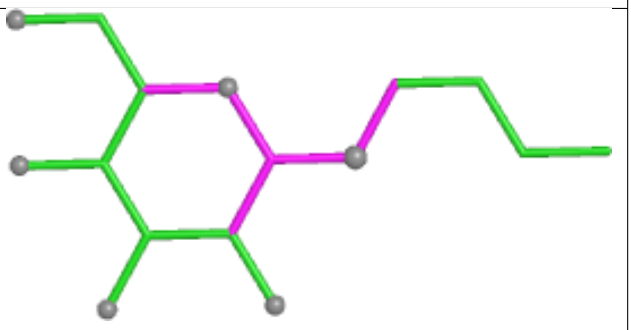


Rings

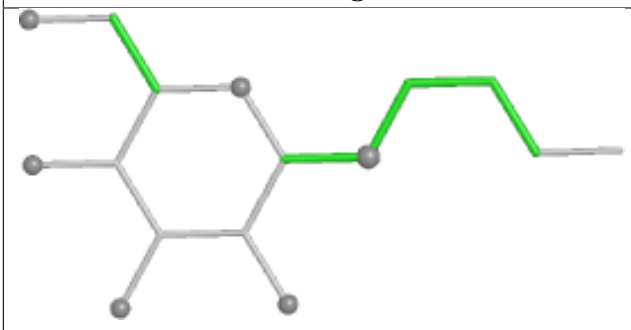
Ligand HTG d 414



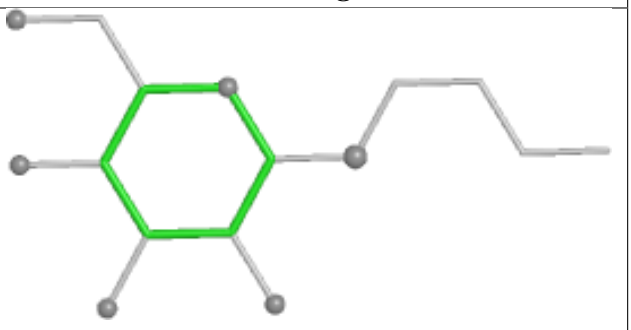
Bond lengths



Bond angles

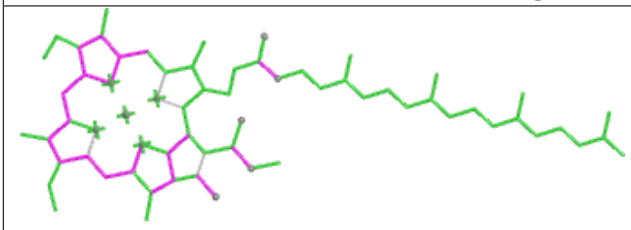


Torsions

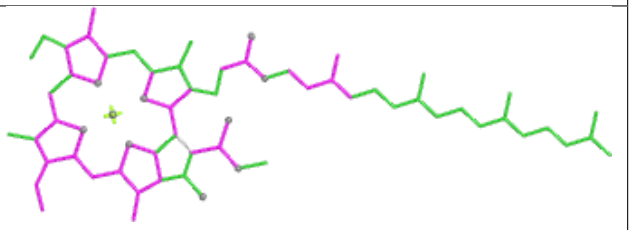


Rings

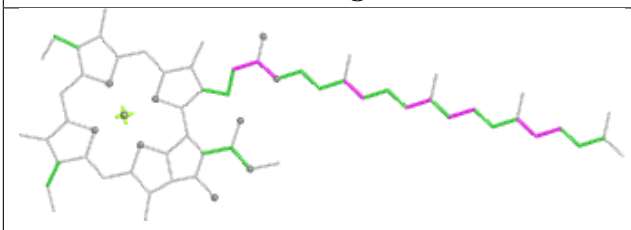
Ligand CLA c 514



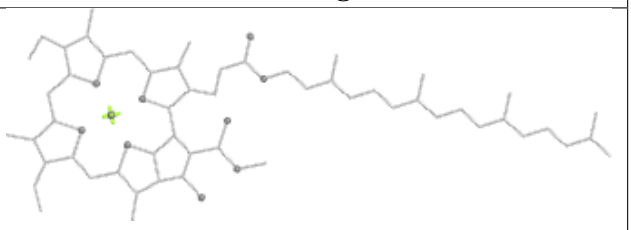
Bond lengths



Bond angles

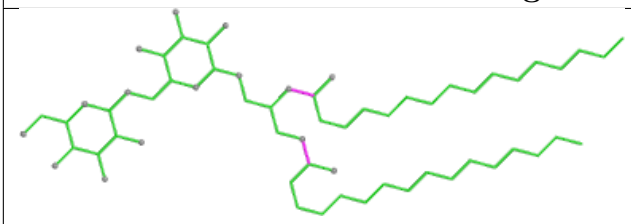


Torsions

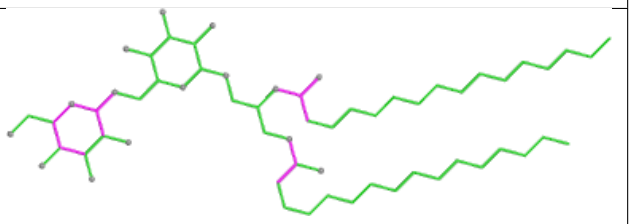


Rings

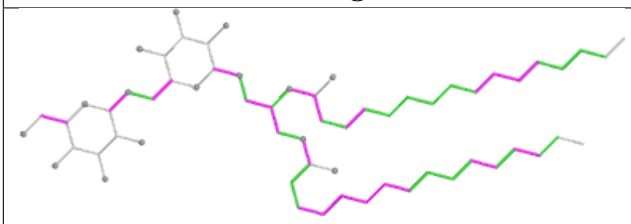
Ligand DGD d 408



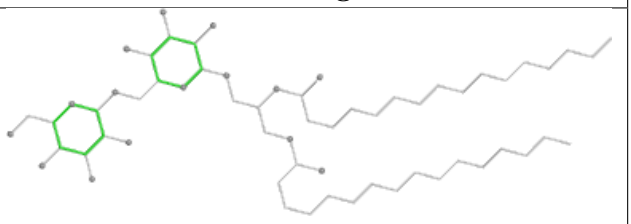
Bond lengths



Bond angles

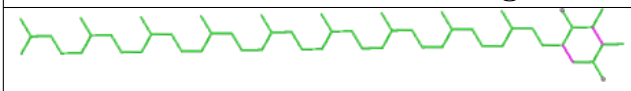


Torsions

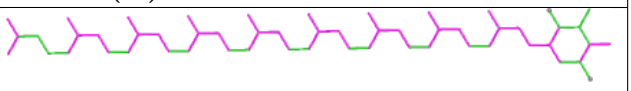


Rings

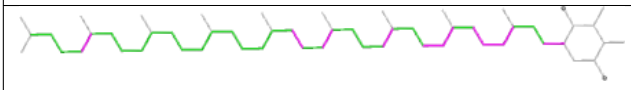
Ligand PL9 a 415 (B)



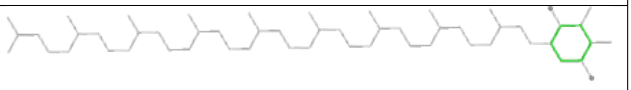
Bond lengths



Bond angles

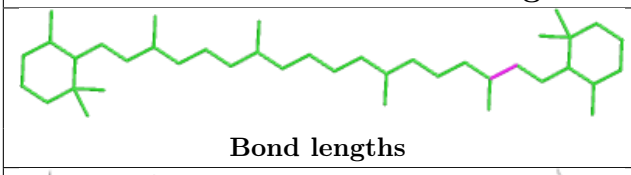


Torsions

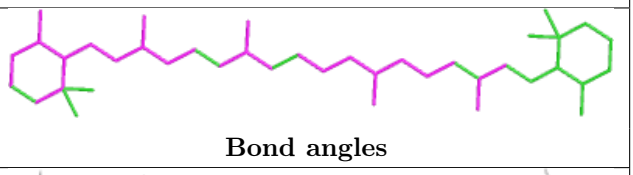


Rings

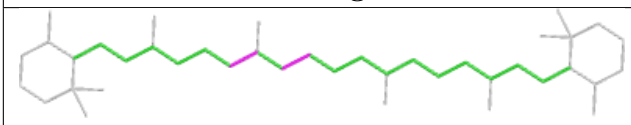
Ligand BCR T 103



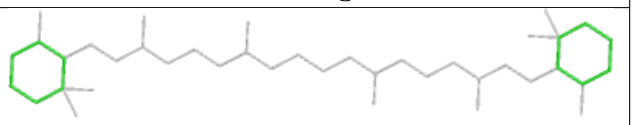
Bond lengths



Bond angles

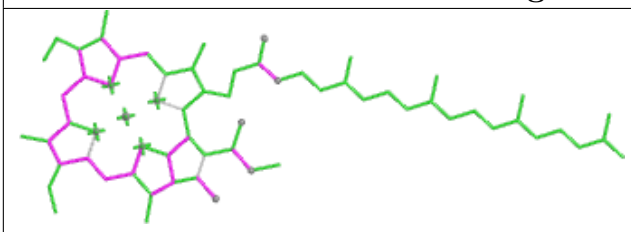


Torsions

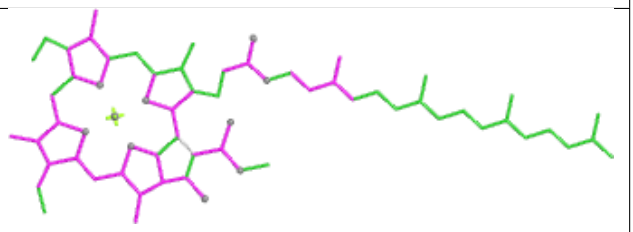


Rings

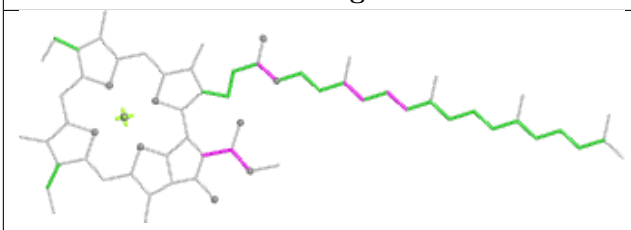
Ligand CLA b 614



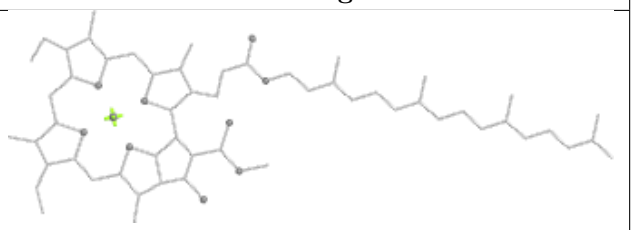
Bond lengths



Bond angles

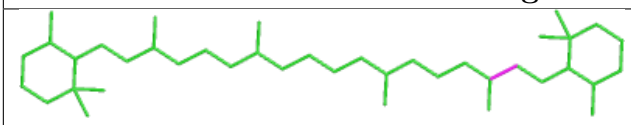


Torsions

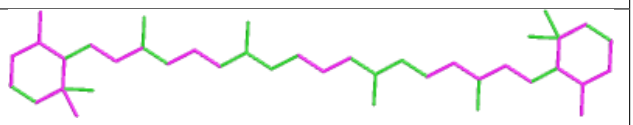


Rings

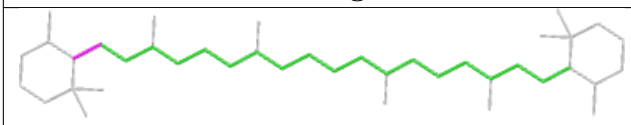
Ligand BCR K 103



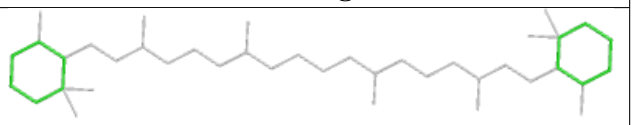
Bond lengths



Bond angles

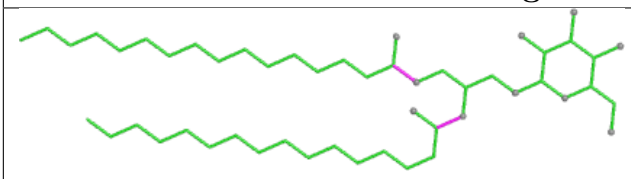


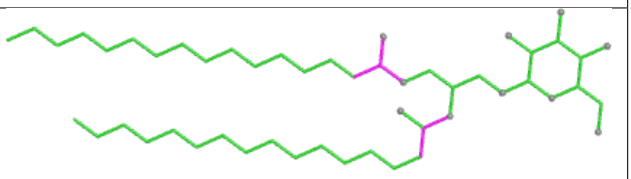
Torsions

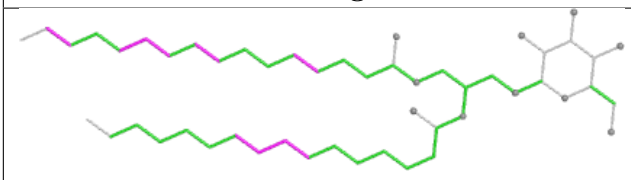


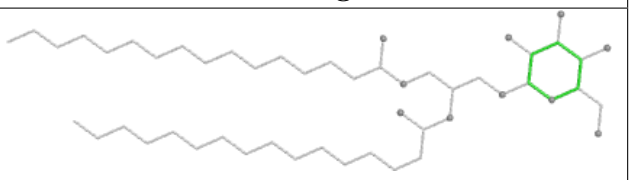
Rings

Ligand LMG b 629

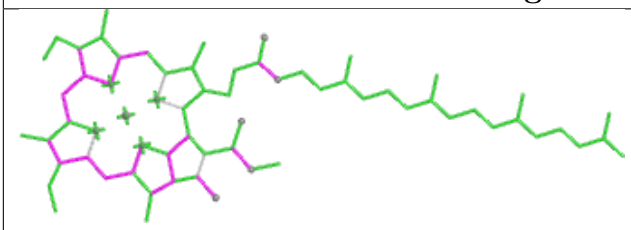

Bond lengths

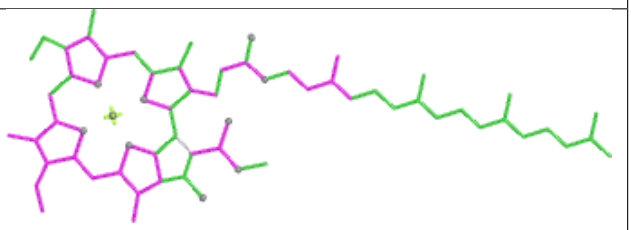

Bond angles

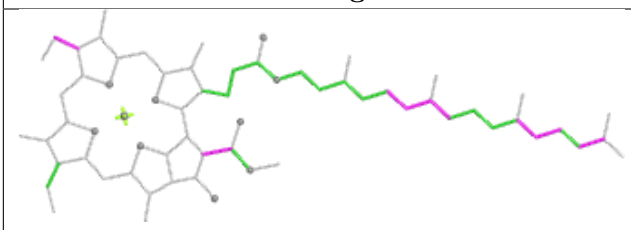

Torsions

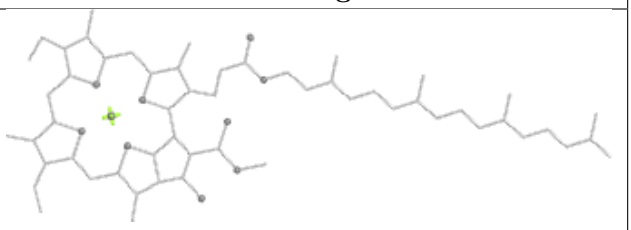

Rings

Ligand CLA C 507

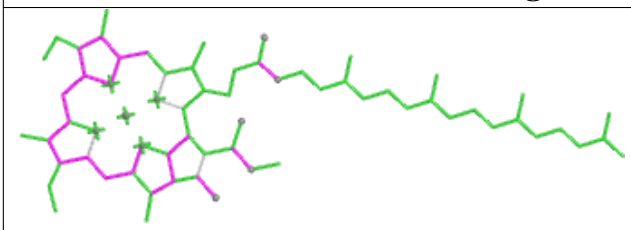

Bond lengths

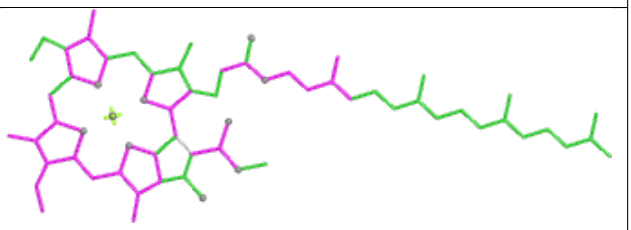

Bond angles

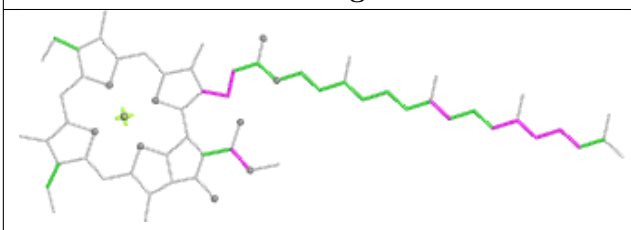

Torsions

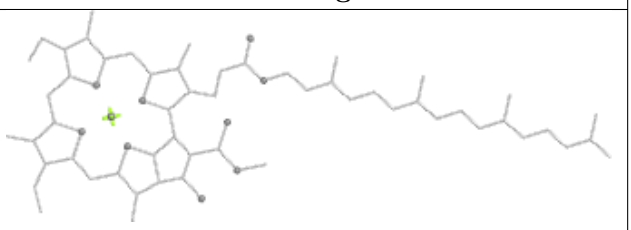

Rings

Ligand CLA C 502

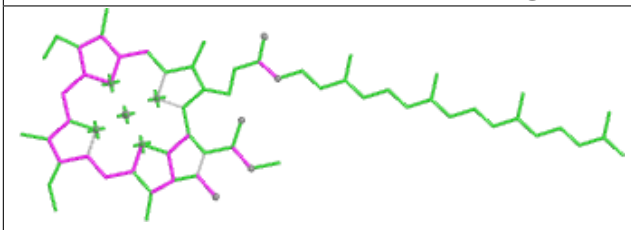

Bond lengths


Bond angles

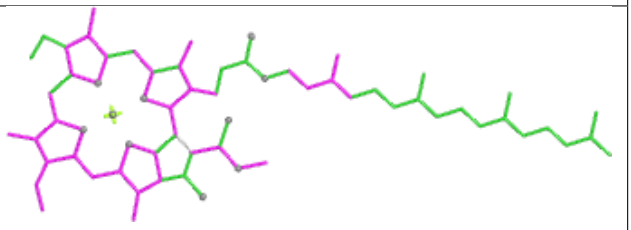

Torsions


Rings

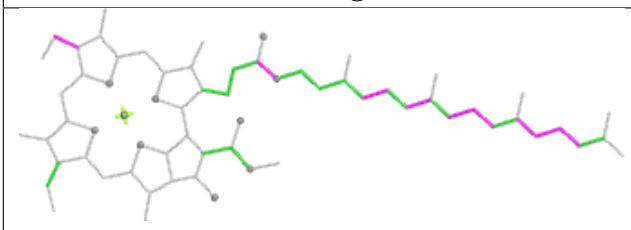
Ligand CLA A 408



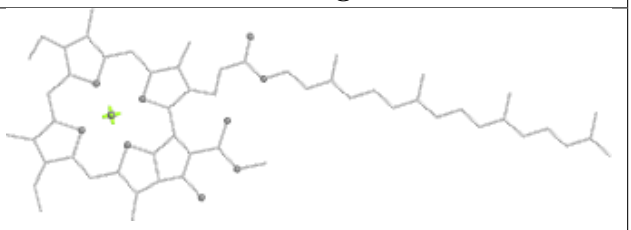
Bond lengths



Bond angles

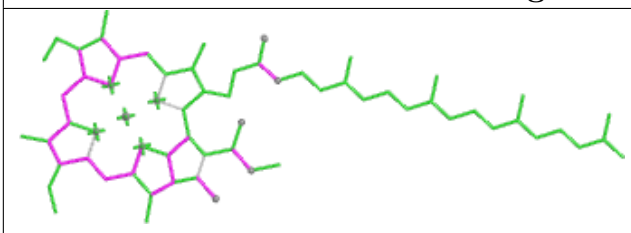


Torsions

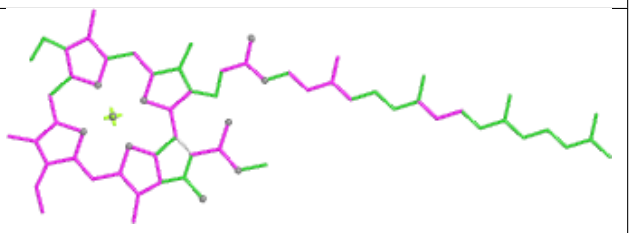


Rings

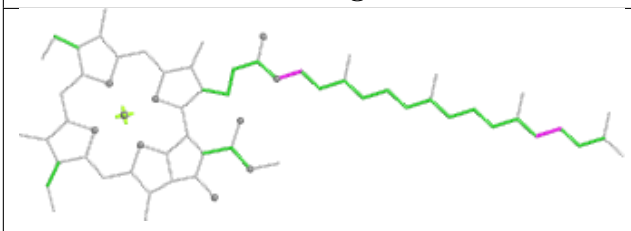
Ligand CLA b 617



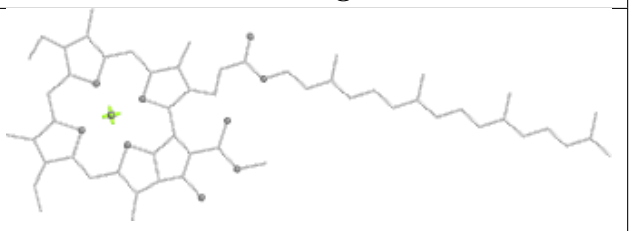
Bond lengths



Bond angles

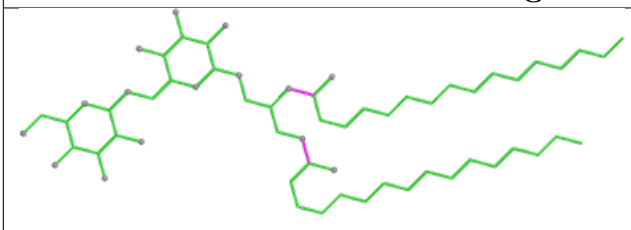


Torsions

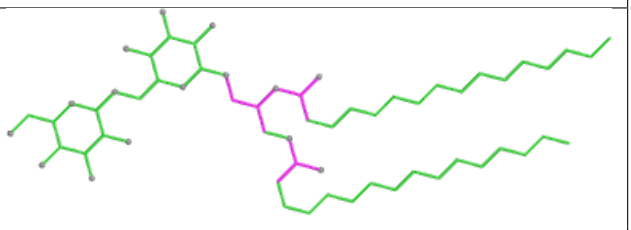


Rings

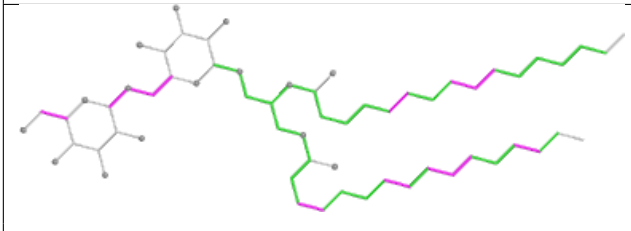
Ligand DGD c 519



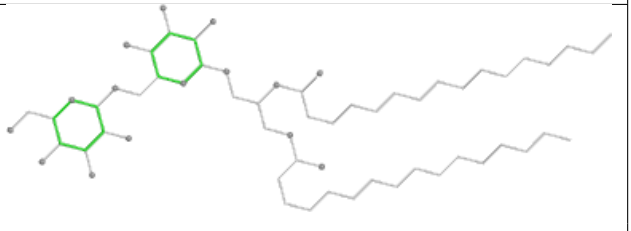
Bond lengths



Bond angles

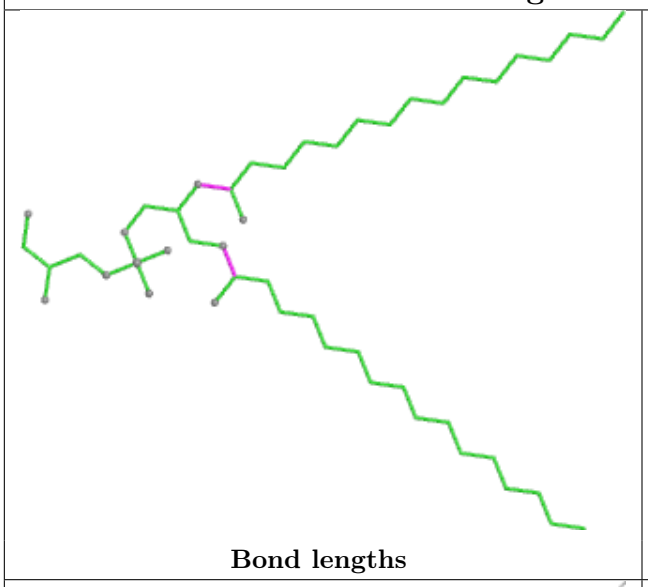


Torsions

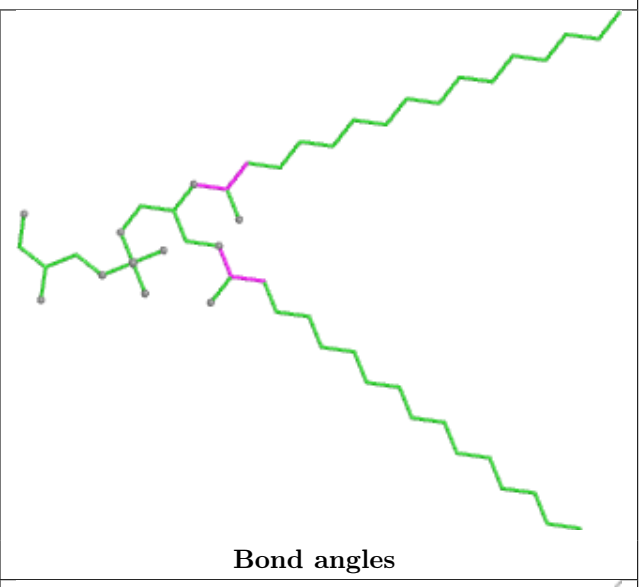


Rings

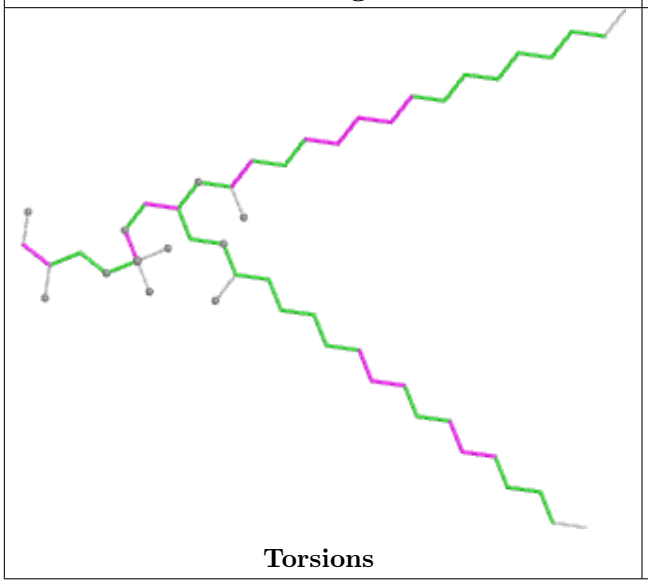
Ligand LHG b 634



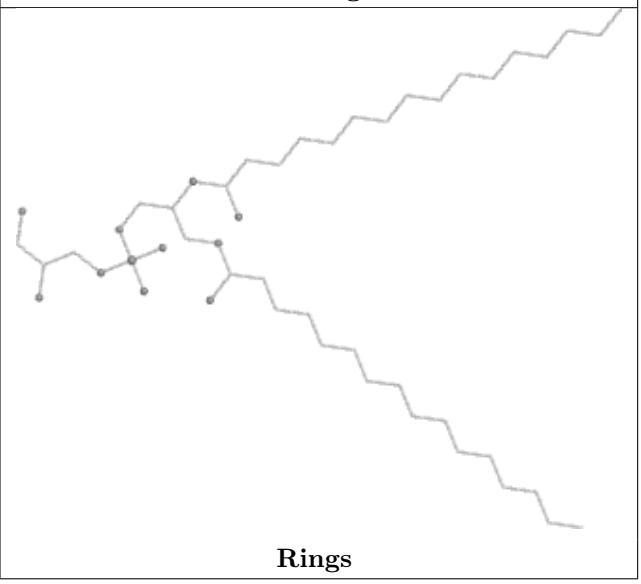
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 D 408 (A)



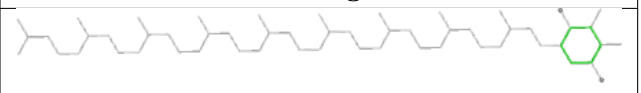
Bond lengths



Bond angles

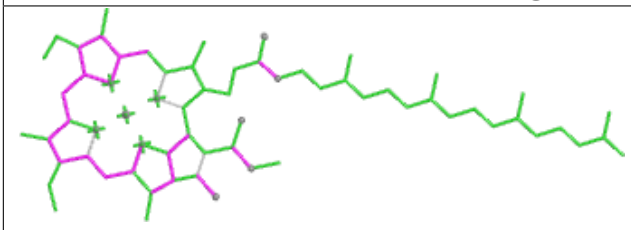


Torsions

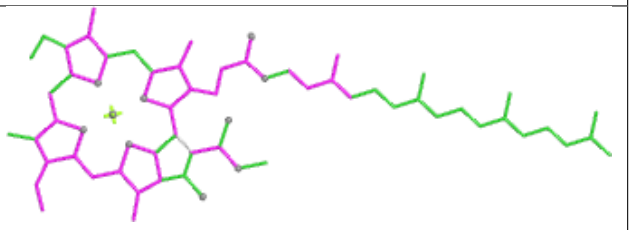


Rings

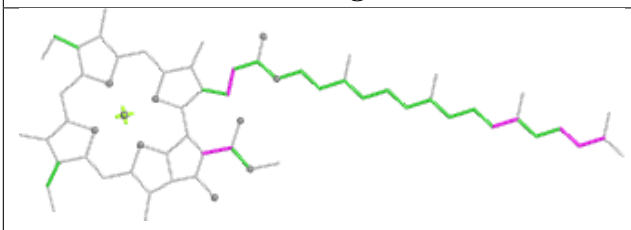
Ligand CLA b 619



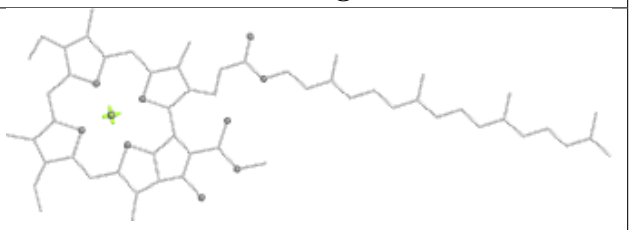
Bond lengths



Bond angles

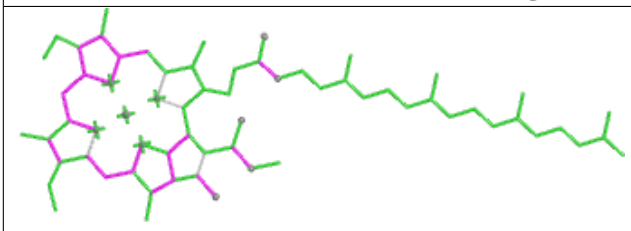


Torsions

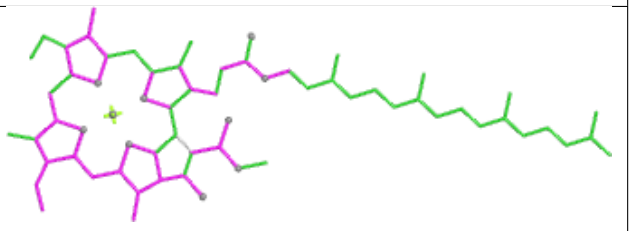


Rings

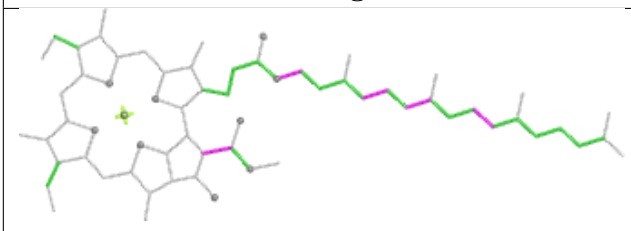
Ligand CLA B 617



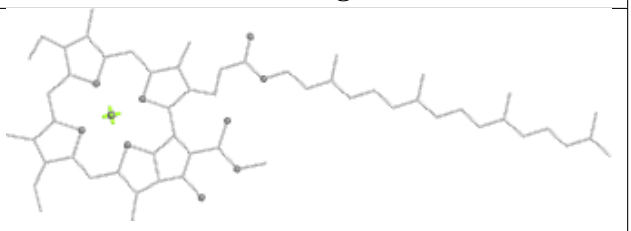
Bond lengths



Bond angles

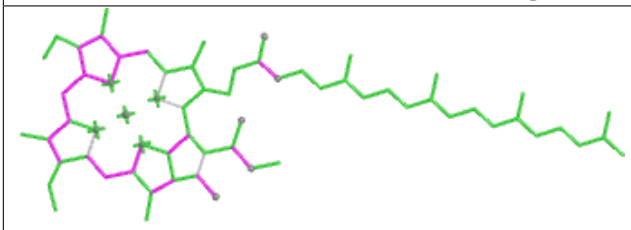


Torsions

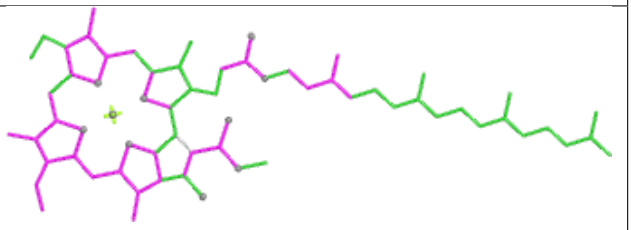


Rings

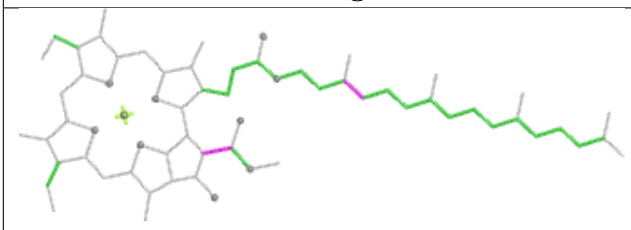
Ligand CLA B 605



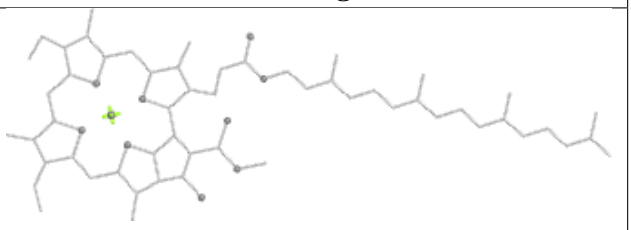
Bond lengths



Bond angles

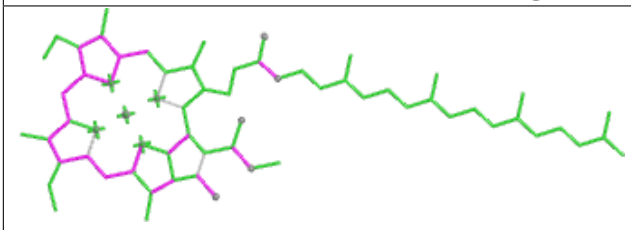


Torsions

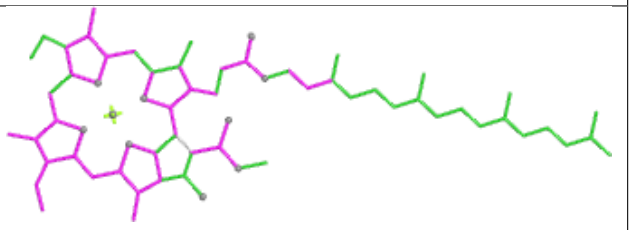


Rings

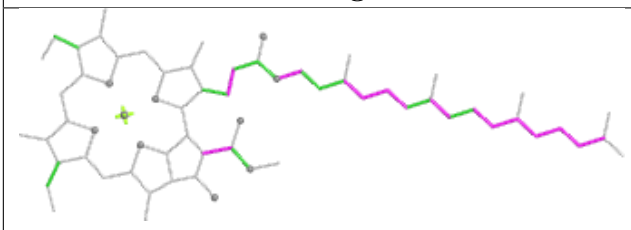
Ligand CLA b 623



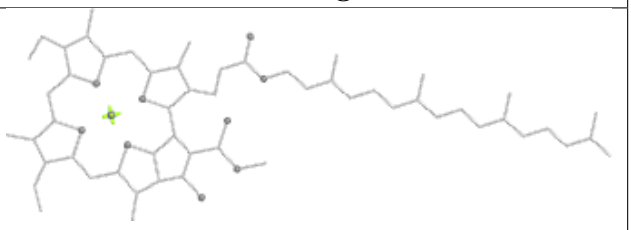
Bond lengths



Bond angles



Torsions

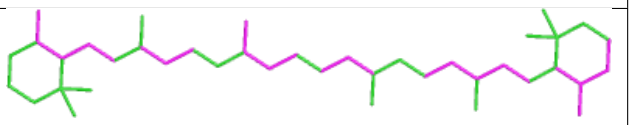


Rings

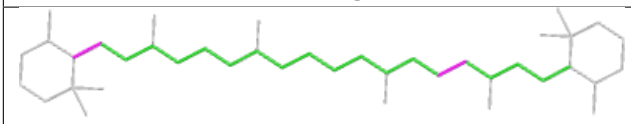
Ligand BCR c 526



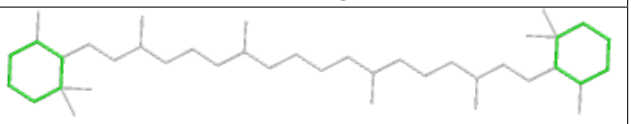
Bond lengths



Bond angles

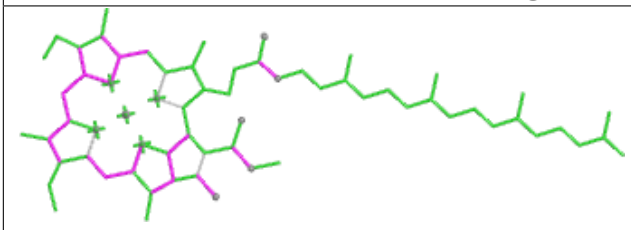


Torsions

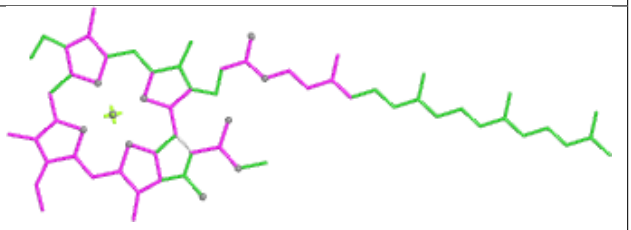


Rings

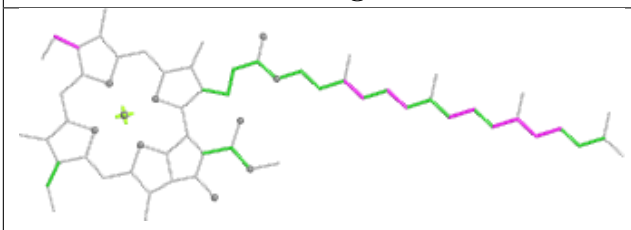
Ligand CLA B 616



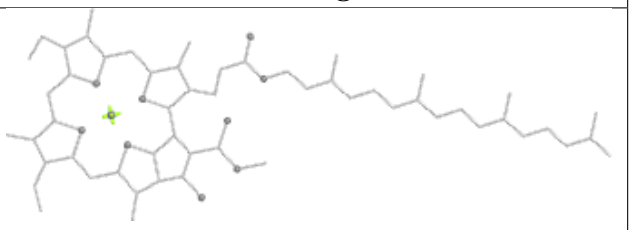
Bond lengths



Bond angles

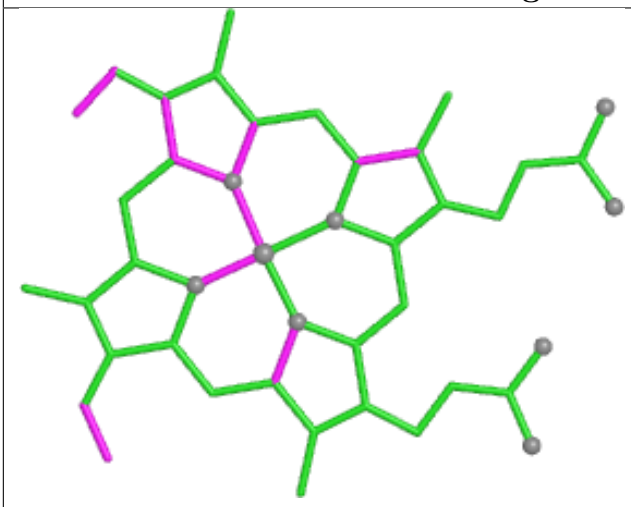


Torsions

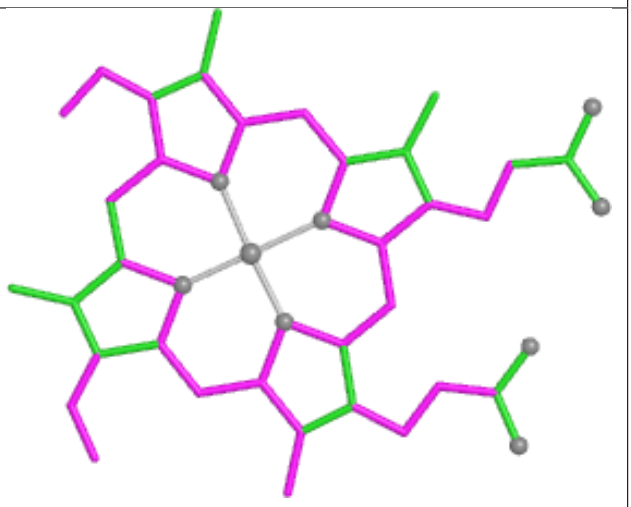


Rings

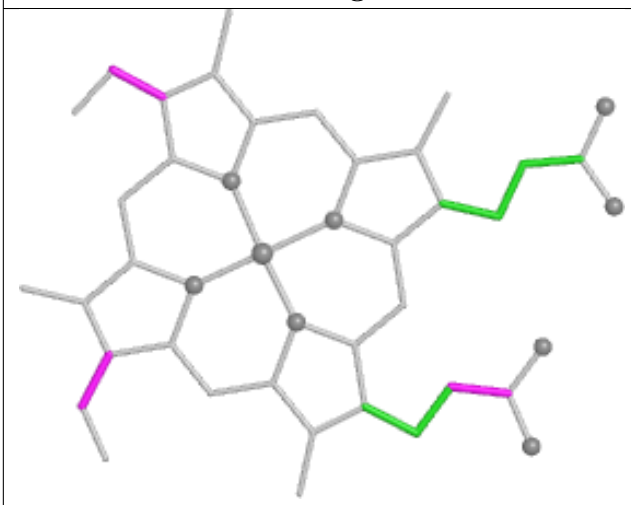
Ligand HEC V 205



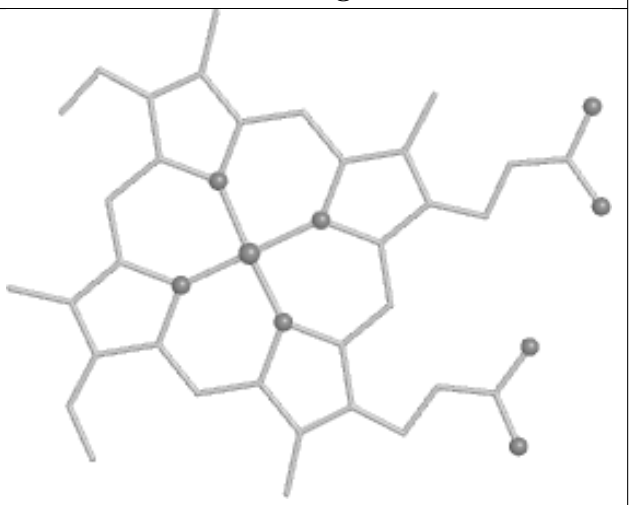
Bond lengths



Bond angles



Torsions

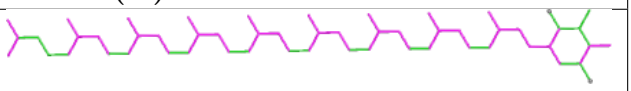


Rings

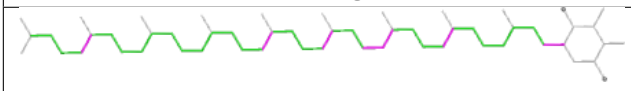
Ligand PL9 A 417 (A)



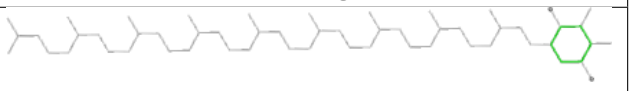
Bond lengths



Bond angles

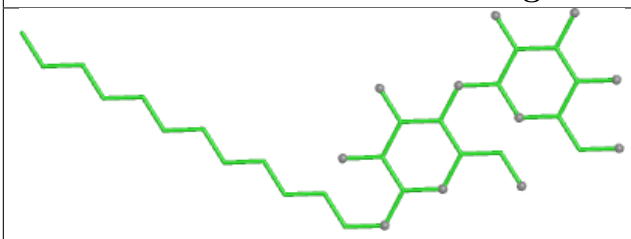


Torsions

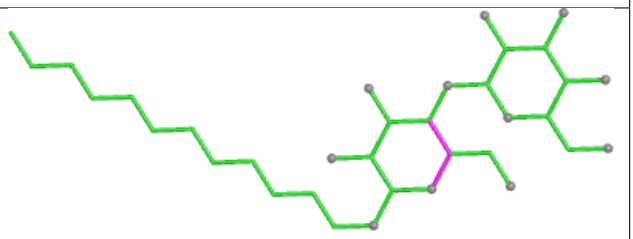


Rings

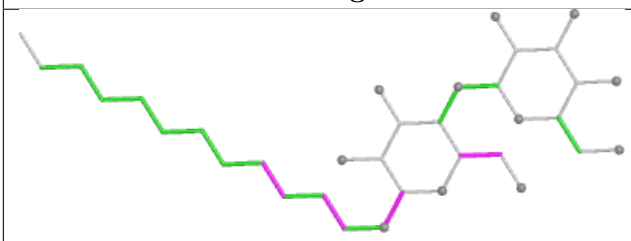
Ligand LMT F 101



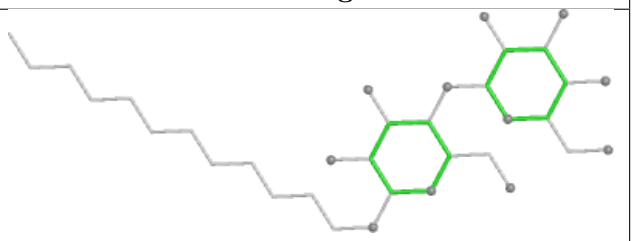
Bond lengths



Bond angles

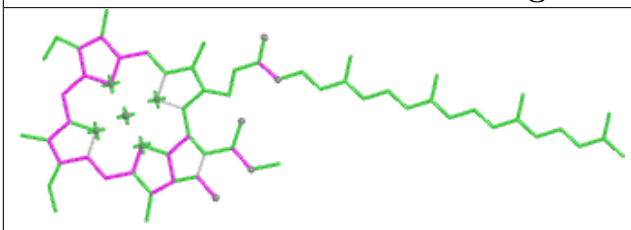


Torsions

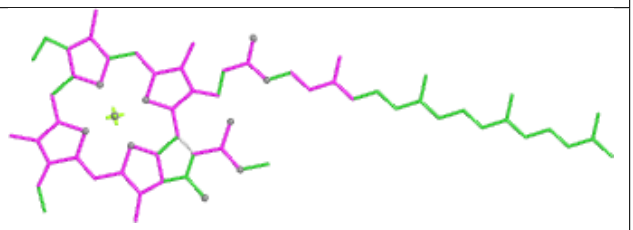


Rings

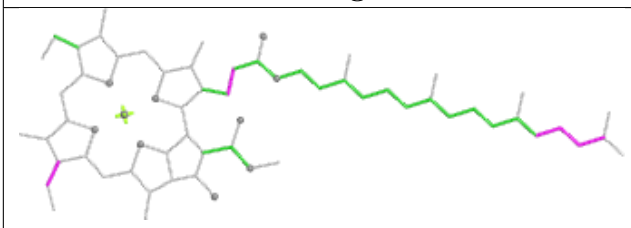
Ligand CLA a 408



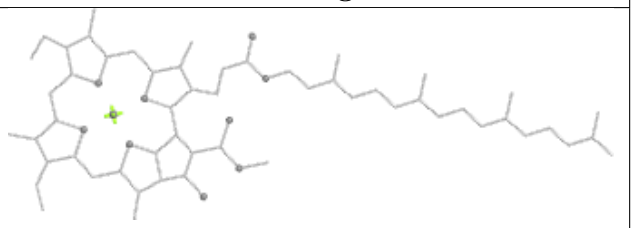
Bond lengths



Bond angles

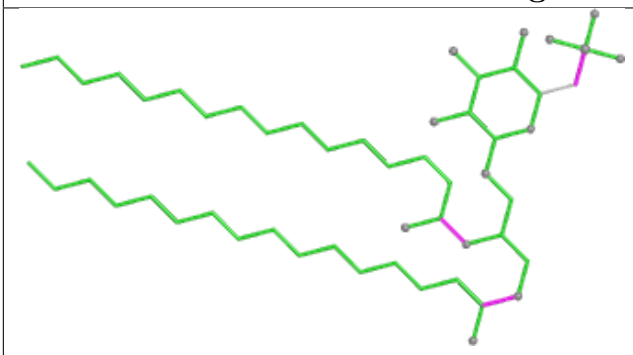


Torsions

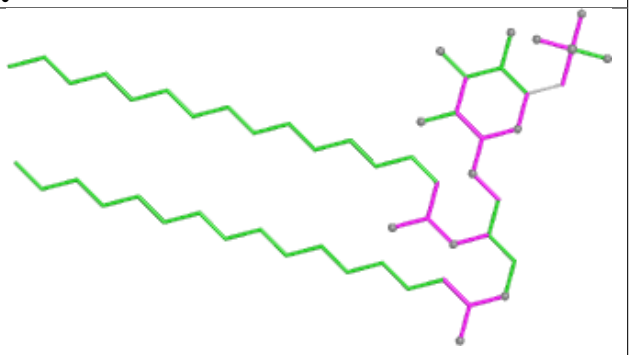


Rings

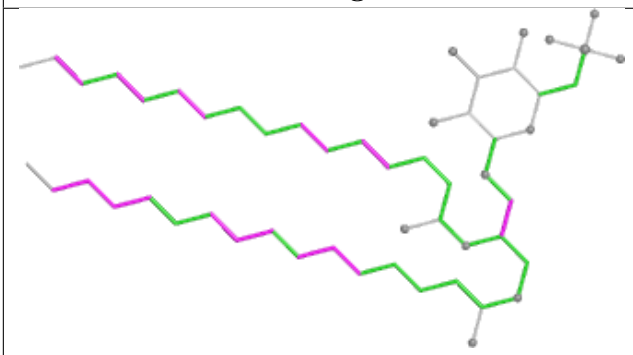
Ligand SQD a 413



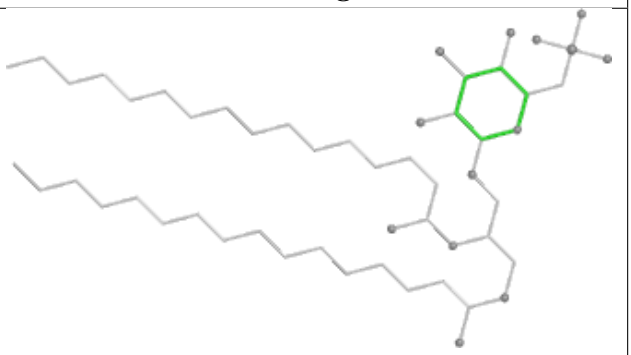
Bond lengths



Bond angles

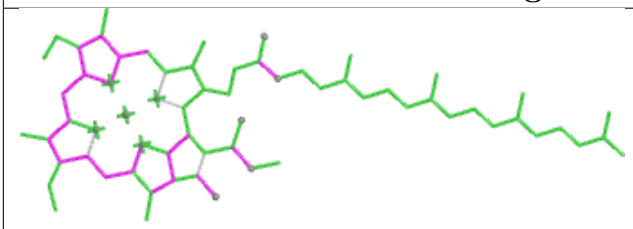


Torsions

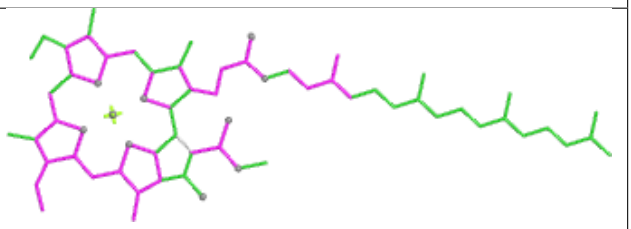


Rings

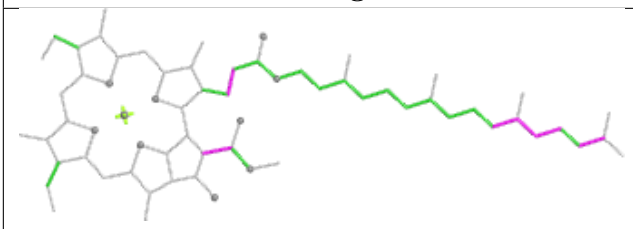
Ligand CLA B 611



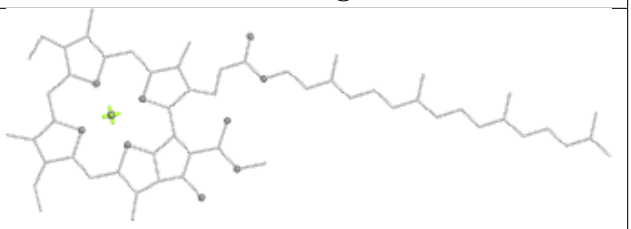
Bond lengths



Bond angles

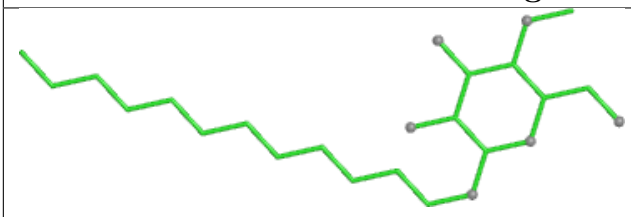


Torsions

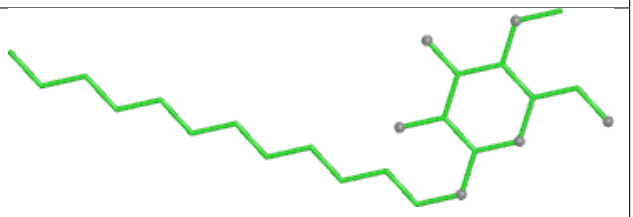


Rings

Ligand LMT b 630



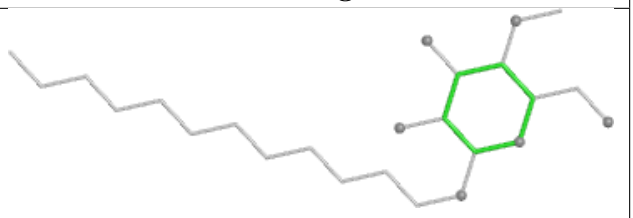
Bond lengths



Bond angles

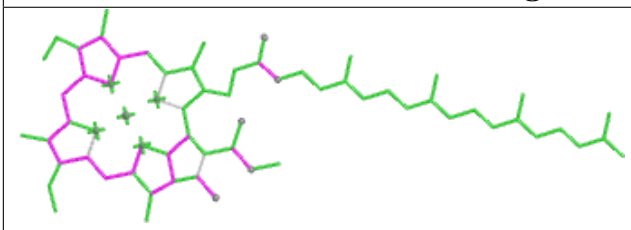


Torsions

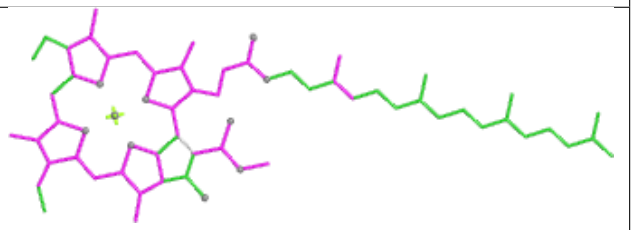


Rings

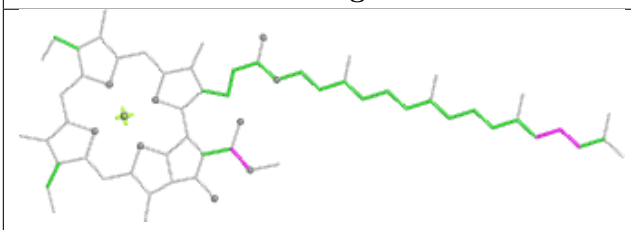
Ligand CLA A 404



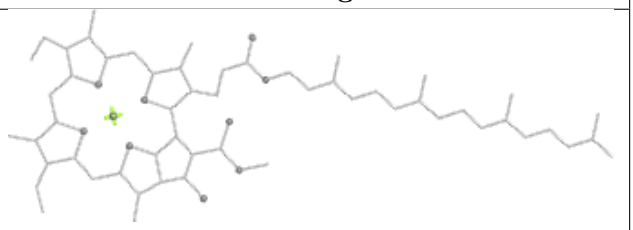
Bond lengths



Bond angles

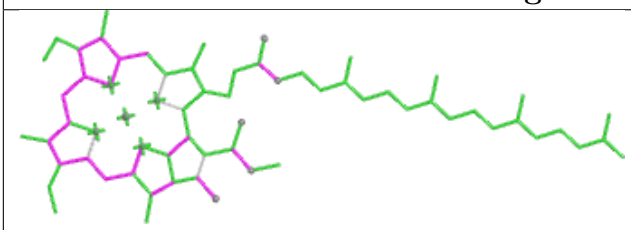


Torsions

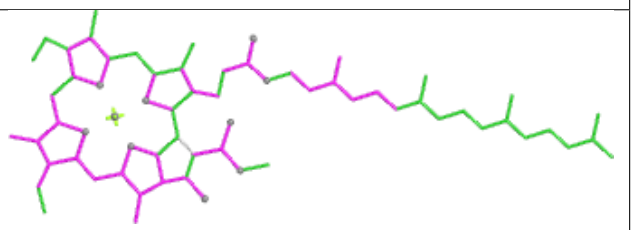


Rings

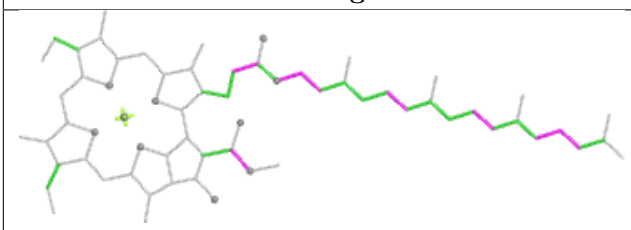
Ligand CLA B 614



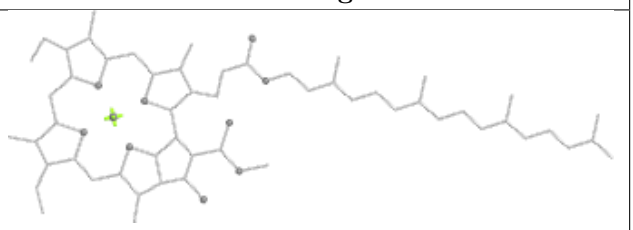
Bond lengths



Bond angles

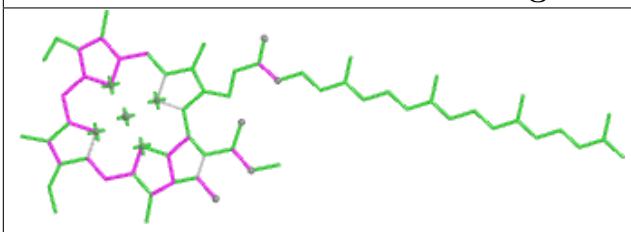


Torsions

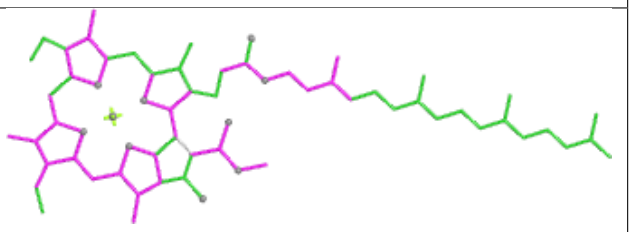


Rings

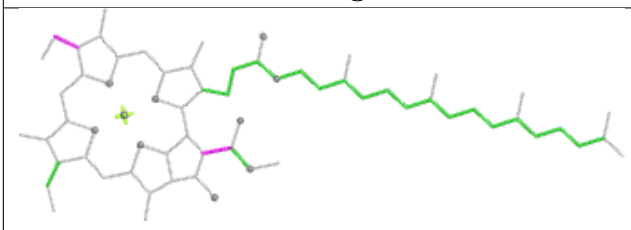
Ligand CLA c 506



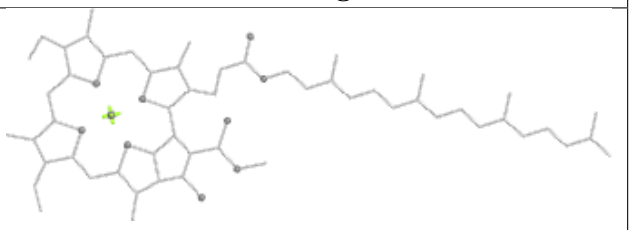
Bond lengths



Bond angles

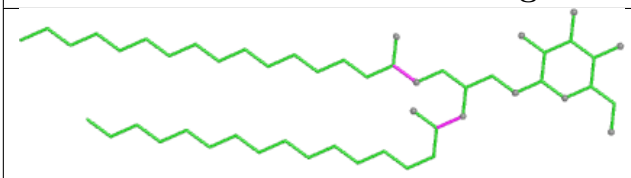


Torsions

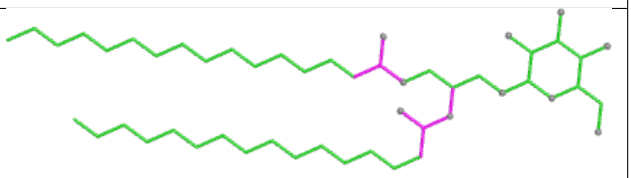


Rings

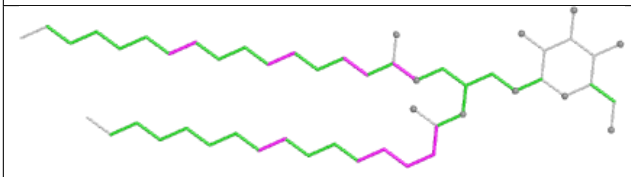
Ligand LMG C 519



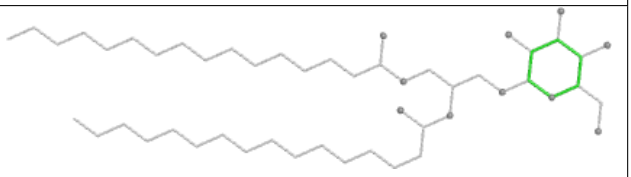
Bond lengths



Bond angles

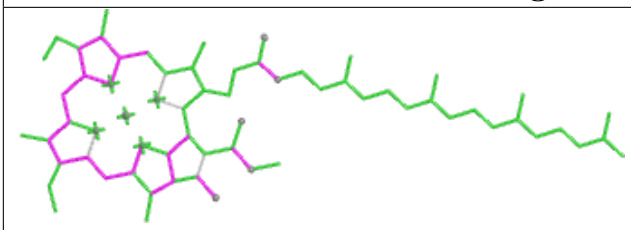


Torsions

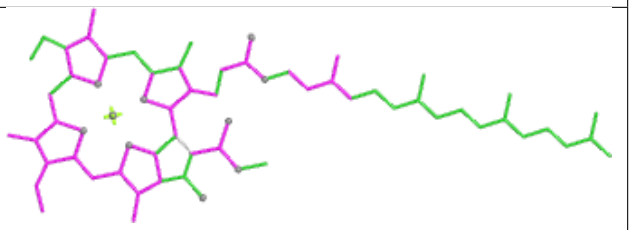


Rings

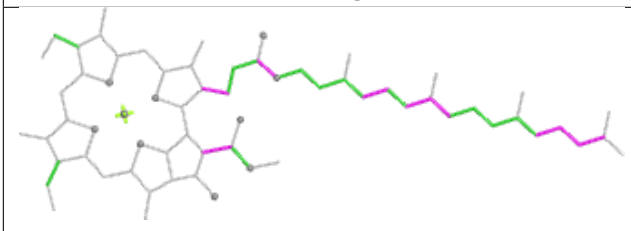
Ligand CLA c 510



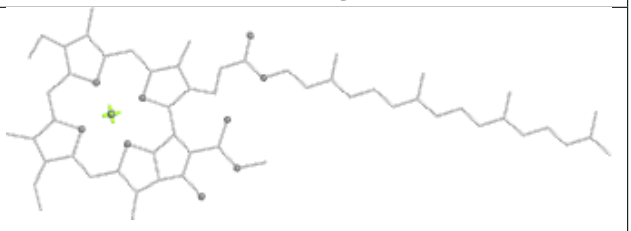
Bond lengths



Bond angles

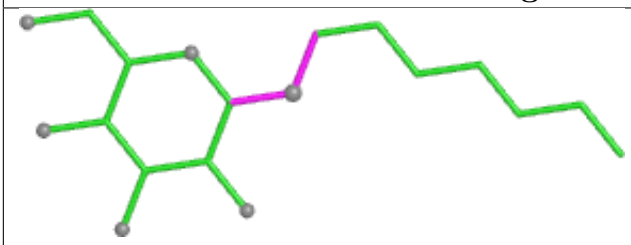


Torsions

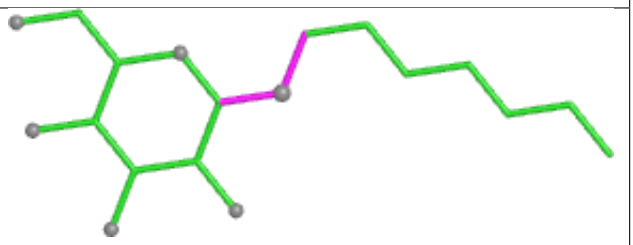


Rings

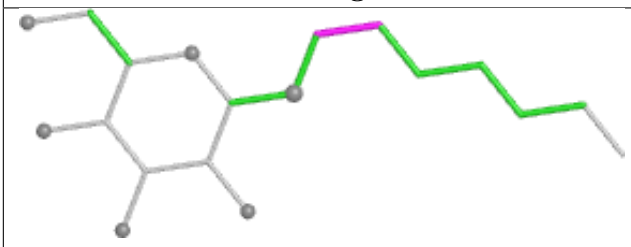
Ligand HTG B 632



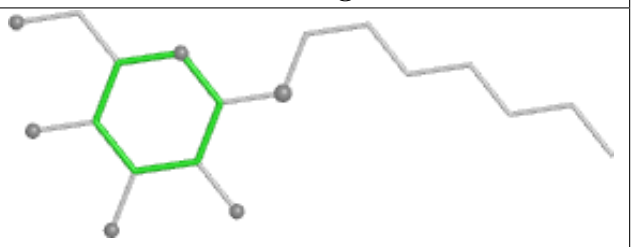
Bond lengths



Bond angles

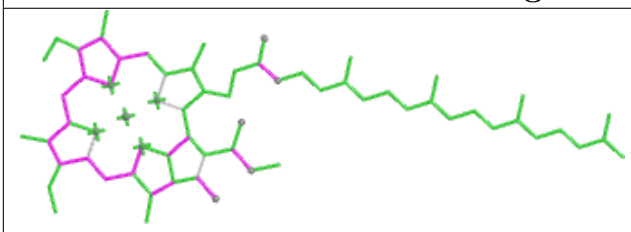


Torsions

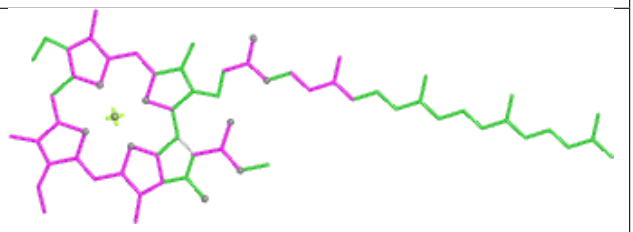


Rings

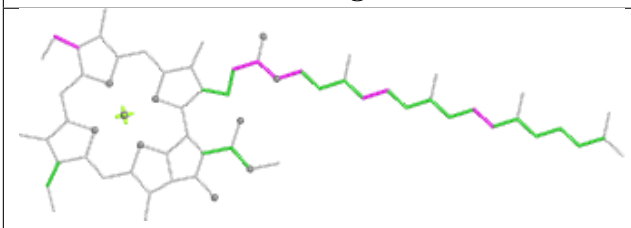
Ligand CLA C 513



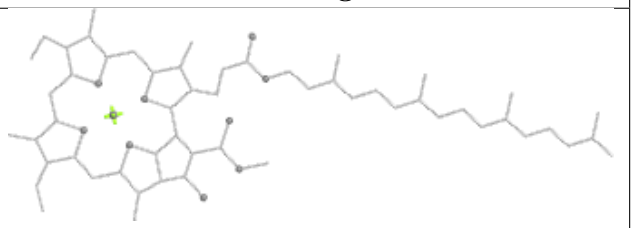
Bond lengths



Bond angles

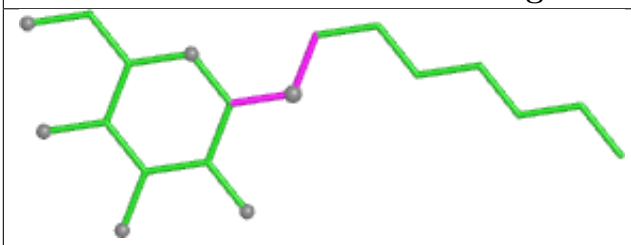


Torsions

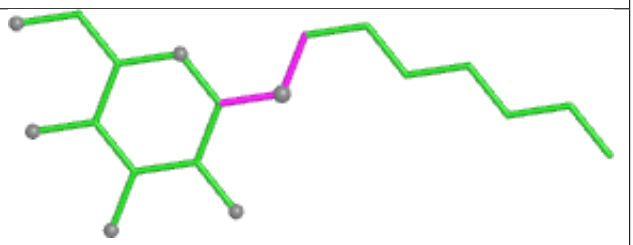


Rings

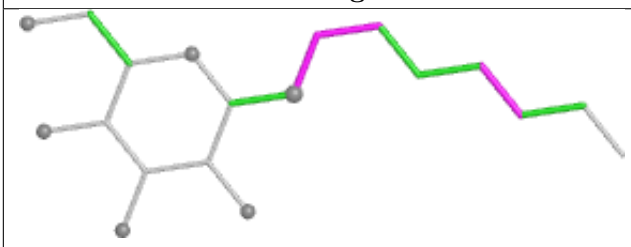
Ligand HTG c 523



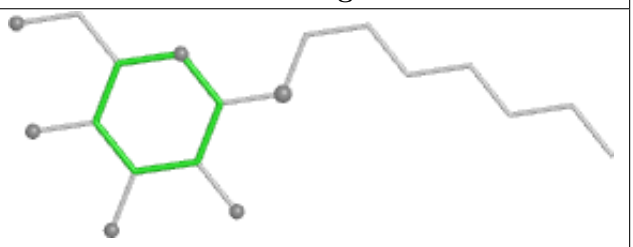
Bond lengths



Bond angles

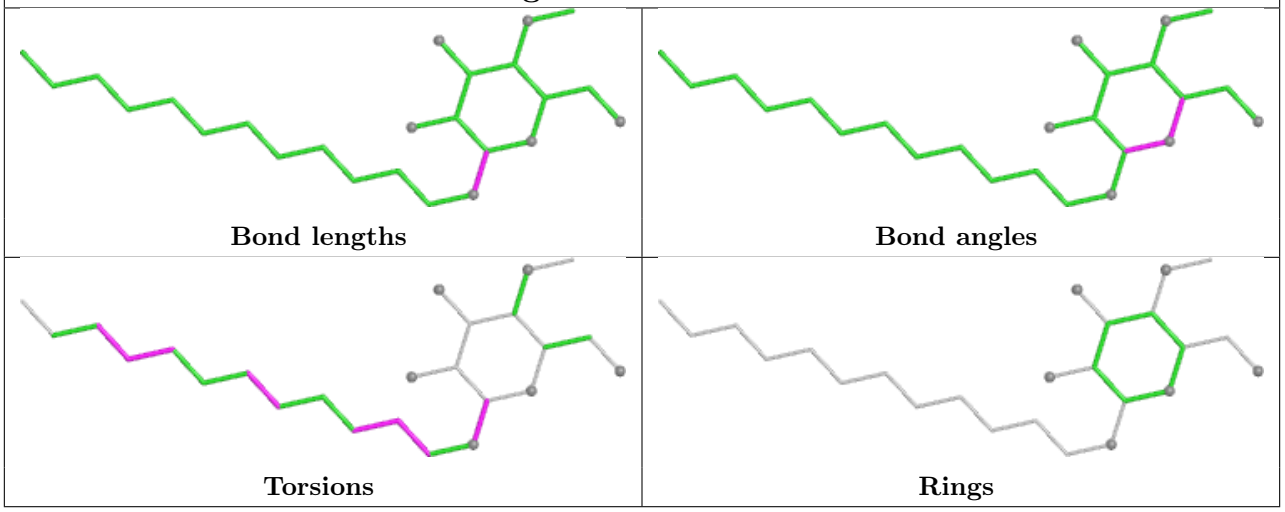


Torsions

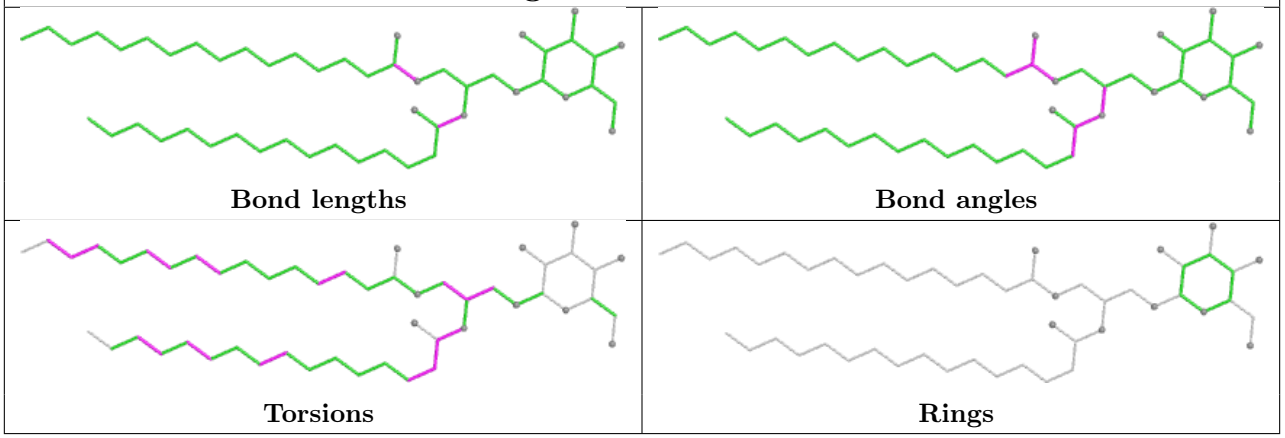


Rings

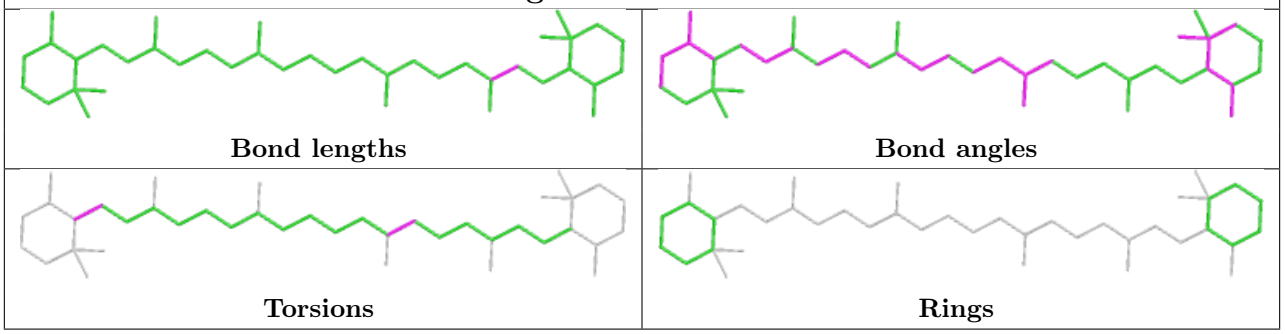
Ligand LMT T 104



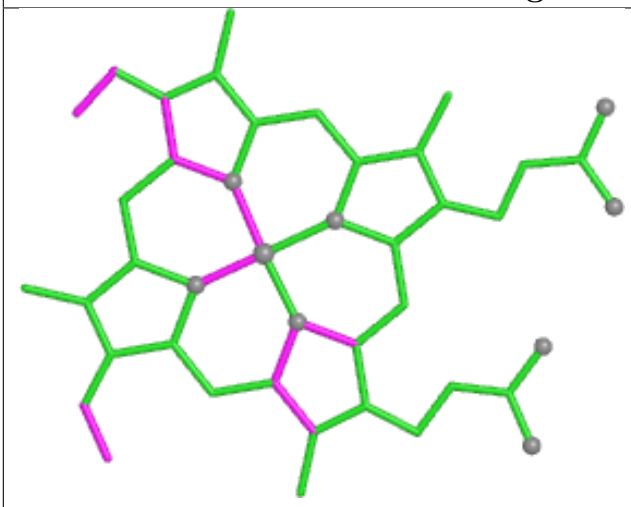
Ligand LMG k 101



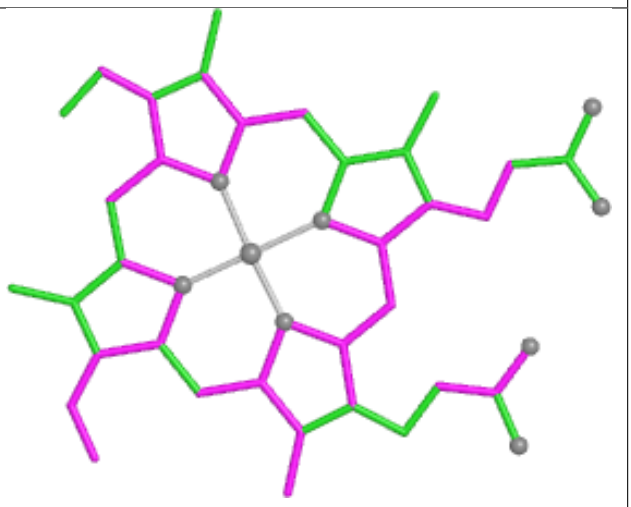
Ligand BCR b 626



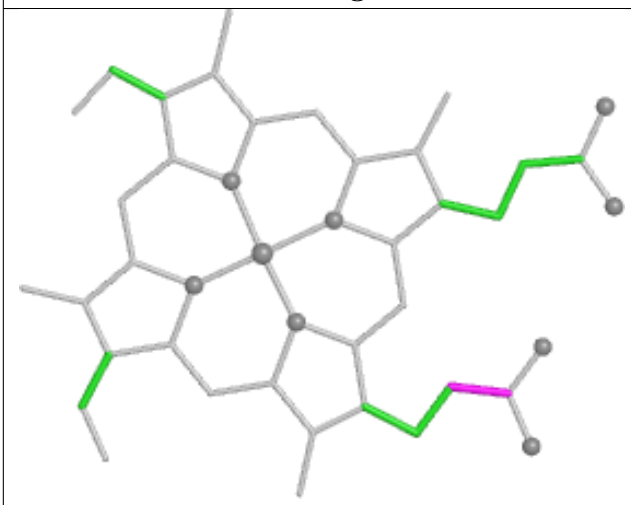
Ligand HEC v 206



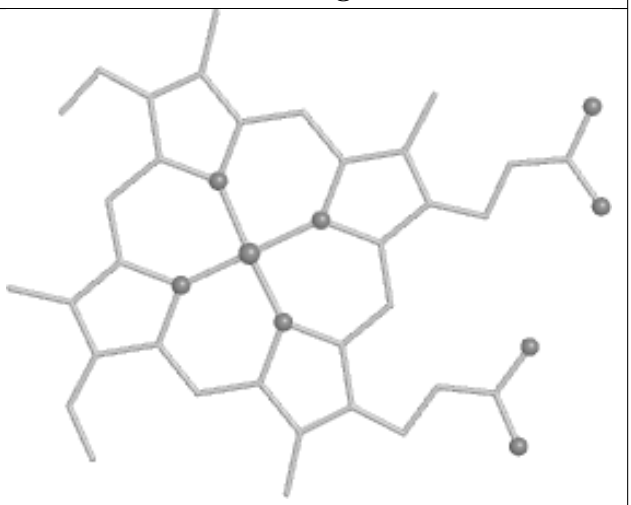
Bond lengths



Bond angles

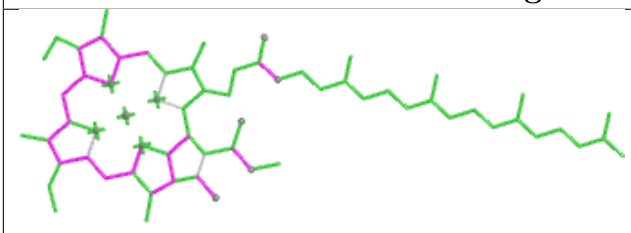


Torsions

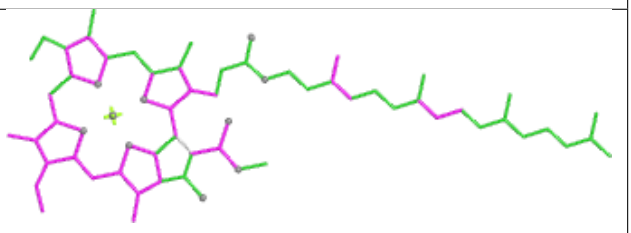


Rings

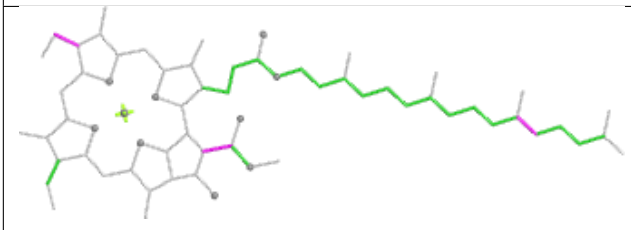
Ligand CLA C 505



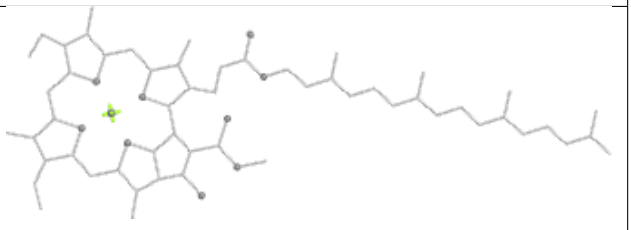
Bond lengths



Bond angles

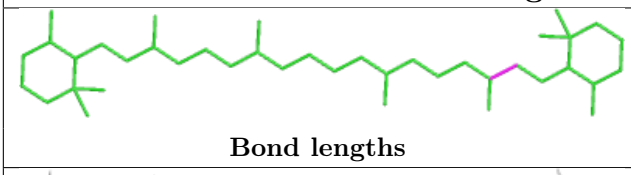


Torsions

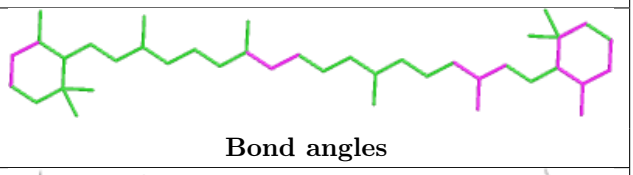


Rings

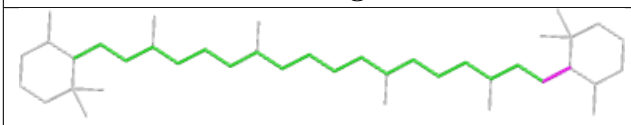
Ligand BCR b 627



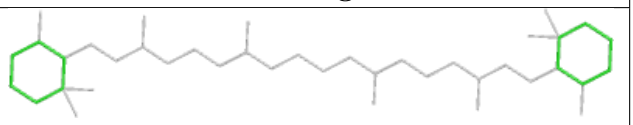
Bond lengths



Bond angles

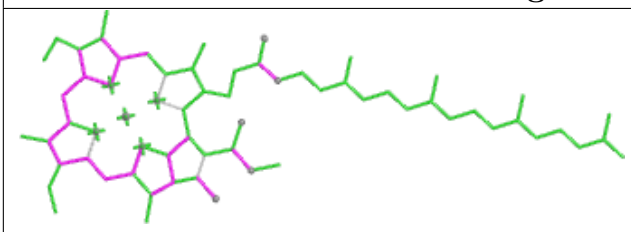


Torsions

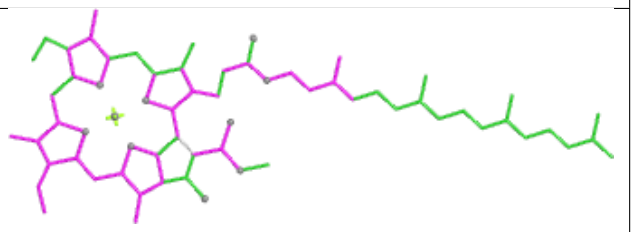


Rings

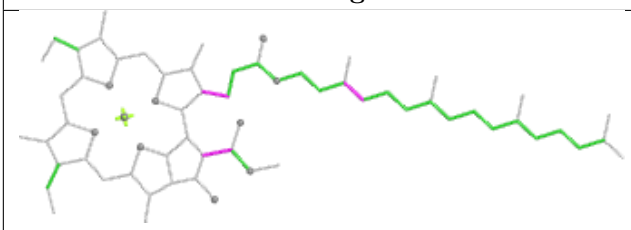
Ligand CLA b 618



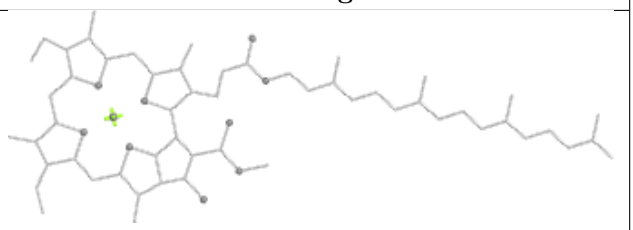
Bond lengths



Bond angles

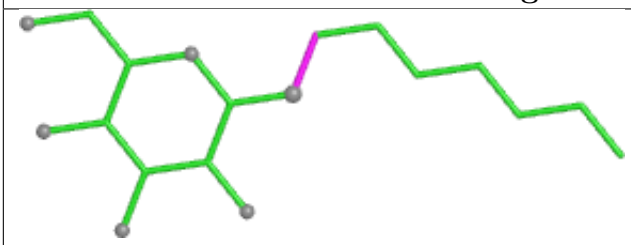


Torsions

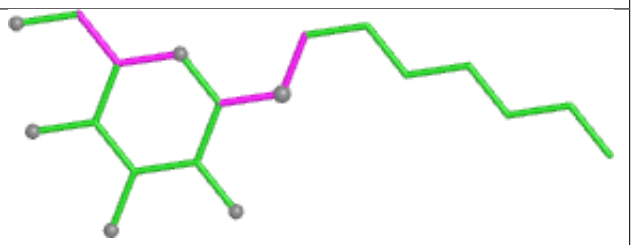


Rings

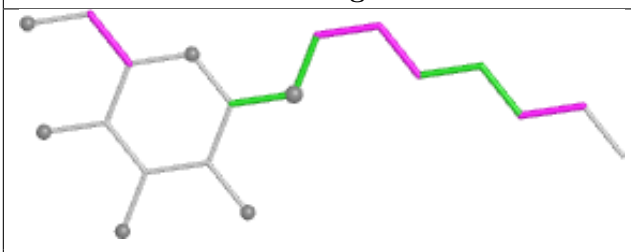
Ligand HTG B 622



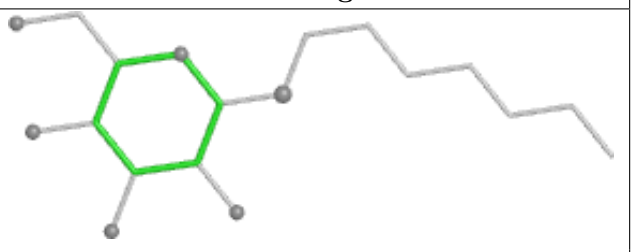
Bond lengths



Bond angles

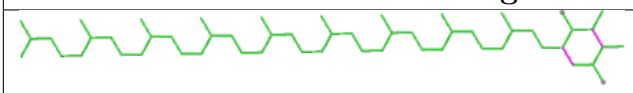


Torsions

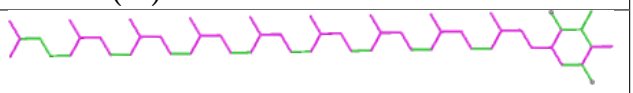


Rings

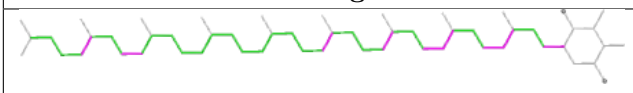
Ligand PL9 a 415 (A)



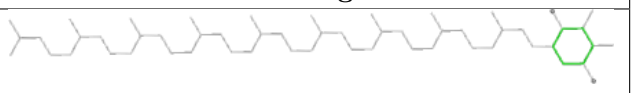
Bond lengths



Bond angles

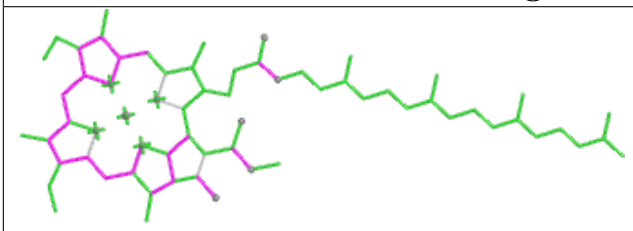


Torsions

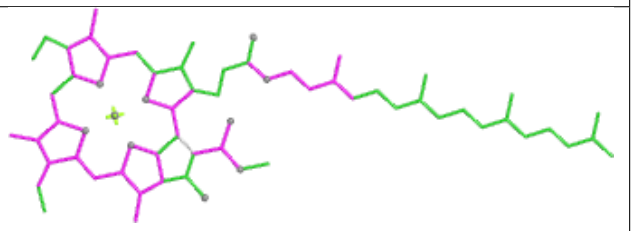


Rings

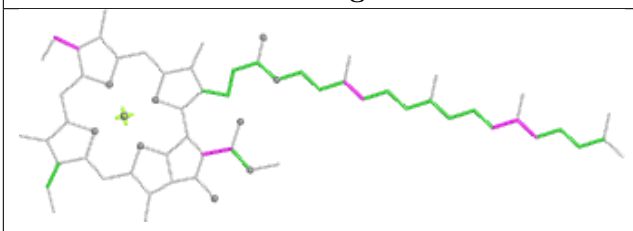
Ligand CLA C 506



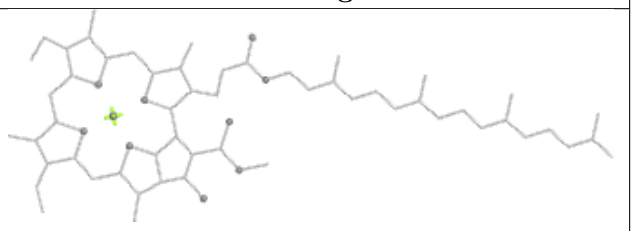
Bond lengths



Bond angles

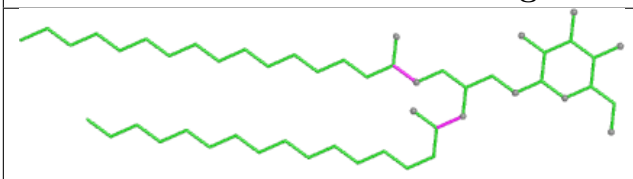


Torsions

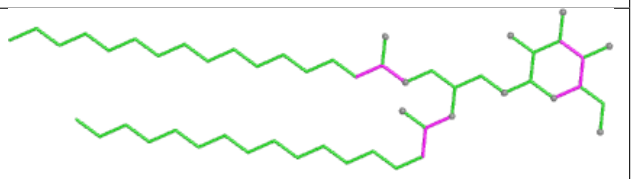


Rings

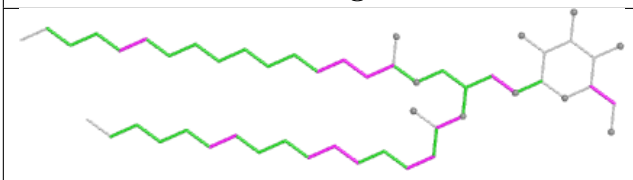
Ligand LMG C 520



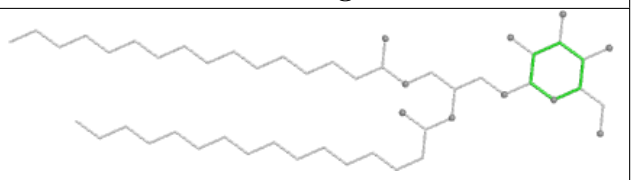
Bond lengths



Bond angles

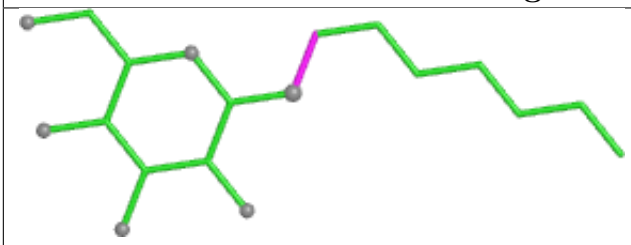


Torsions

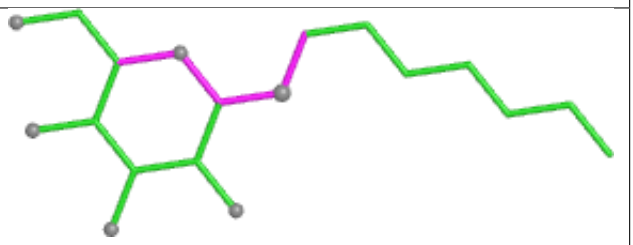


Rings

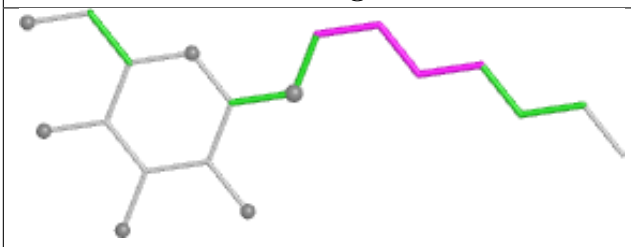
Ligand HTG b 602



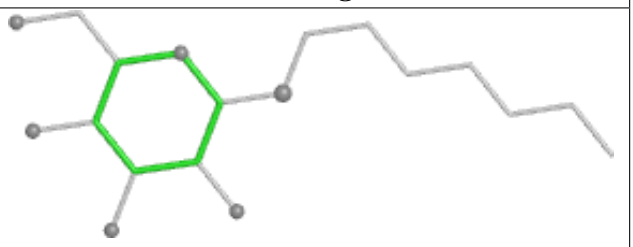
Bond lengths



Bond angles

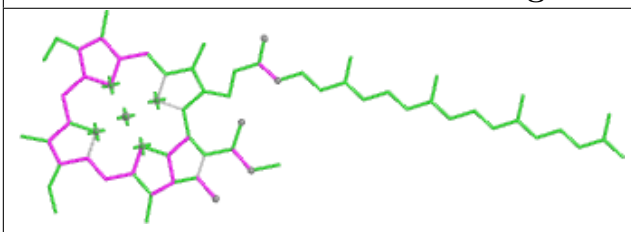


Torsions

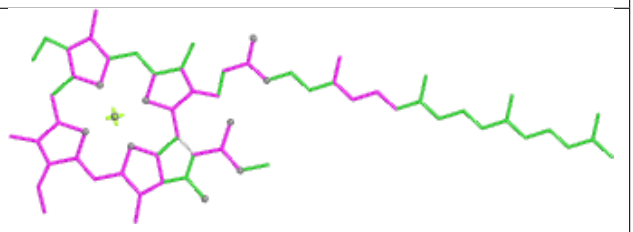


Rings

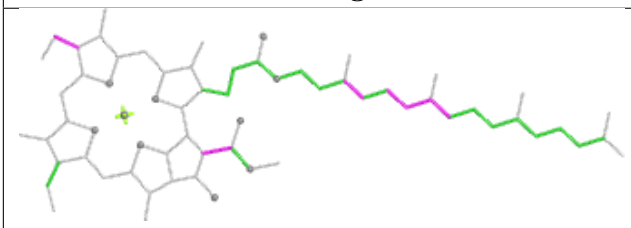
Ligand CLA b 612



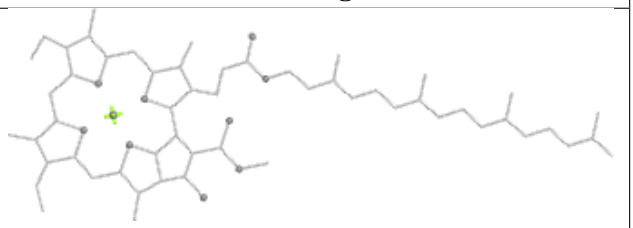
Bond lengths



Bond angles

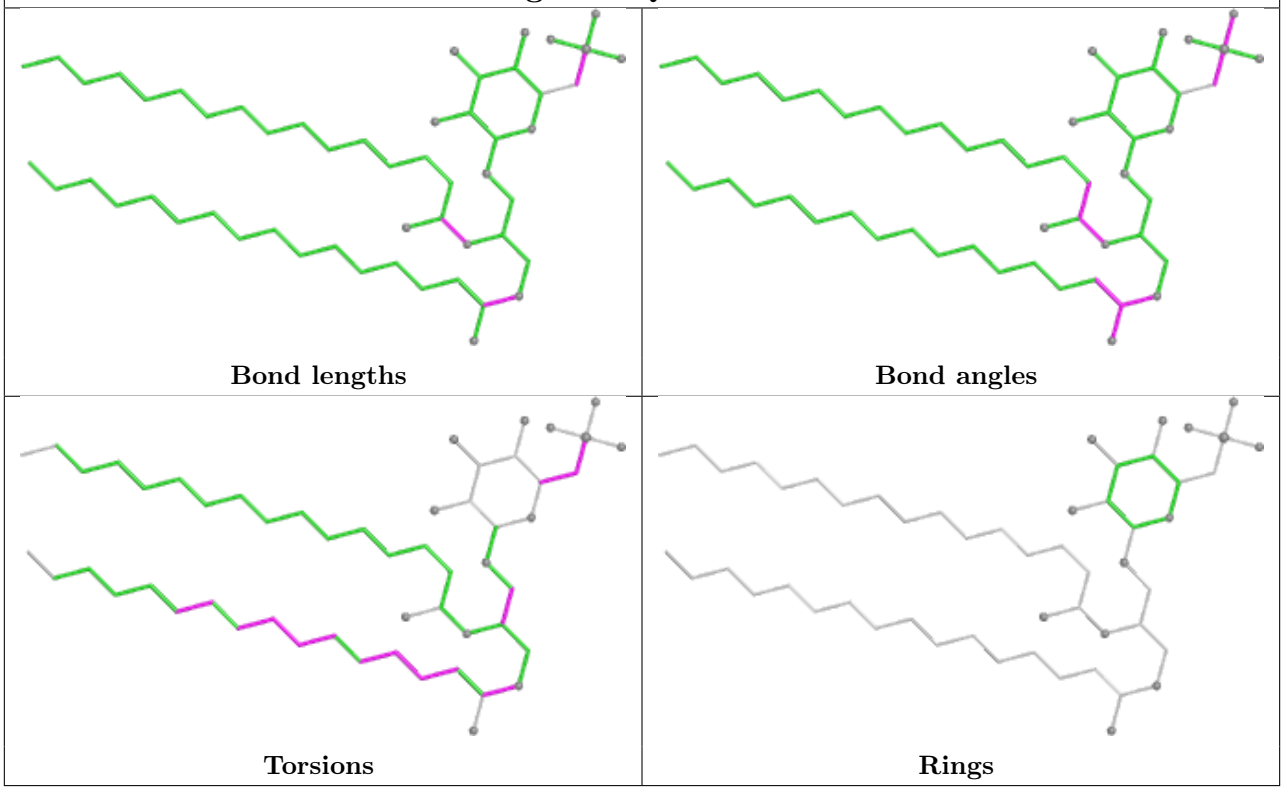


Torsions

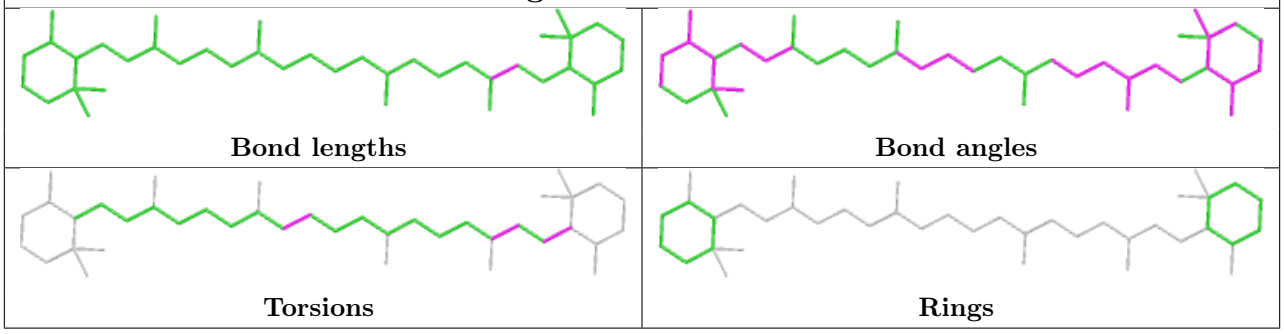


Rings

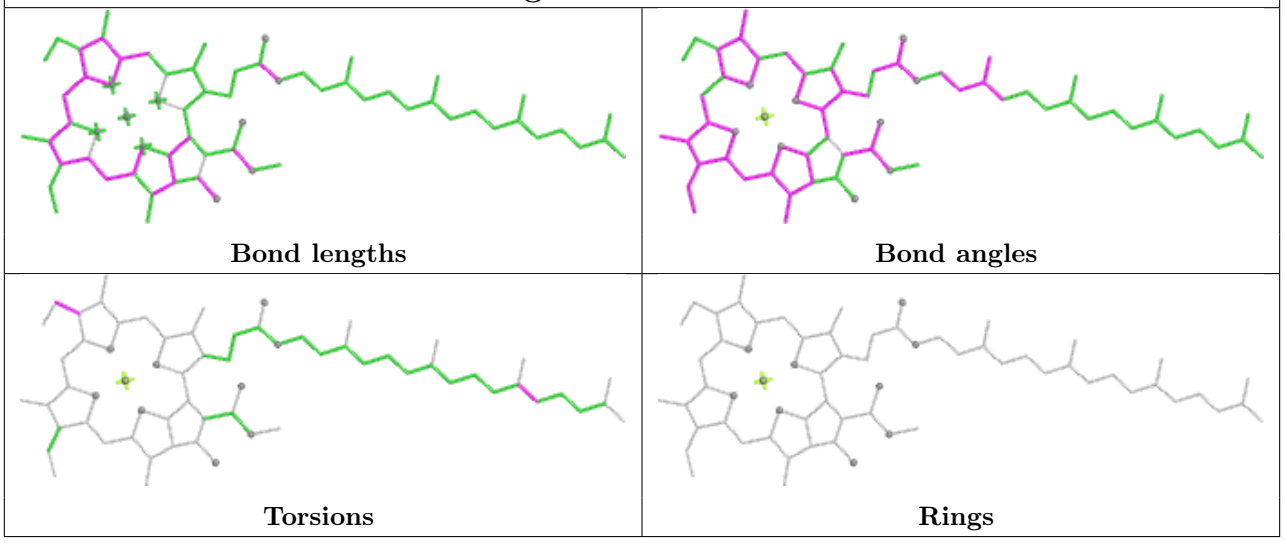
Ligand SQD B 636



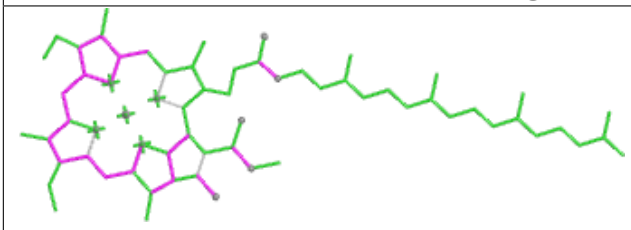
Ligand BCR d 406



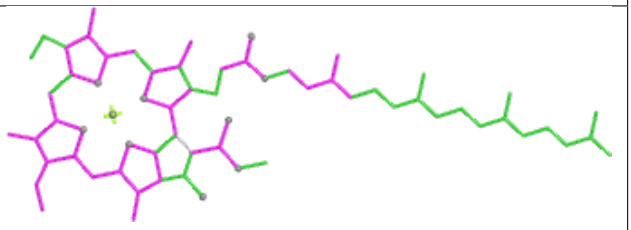
Ligand CLA D 405



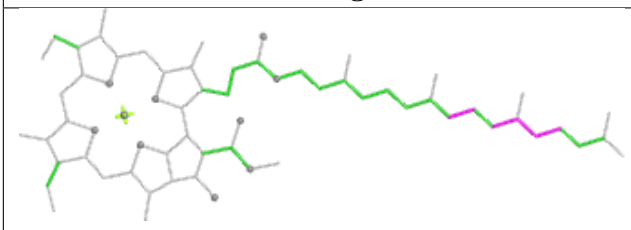
Ligand CLA B 612



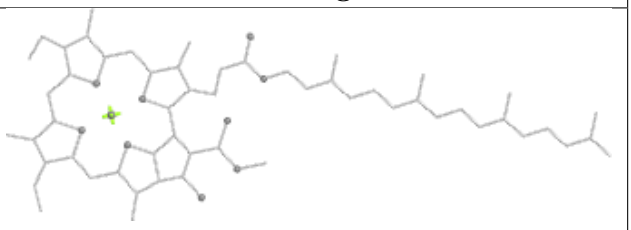
Bond lengths



Bond angles

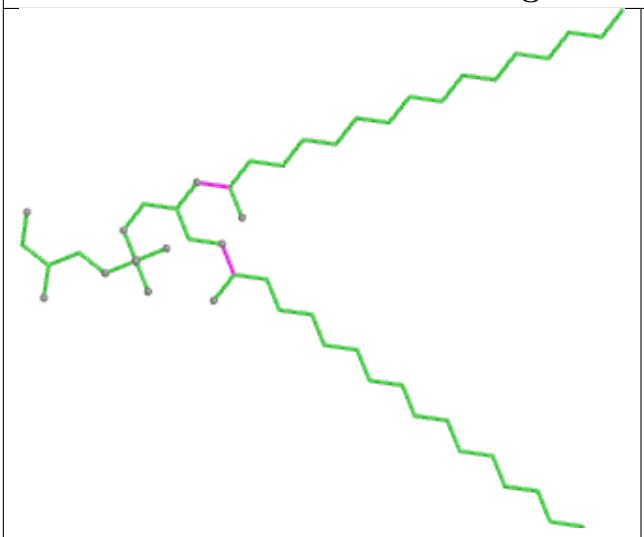


Torsions

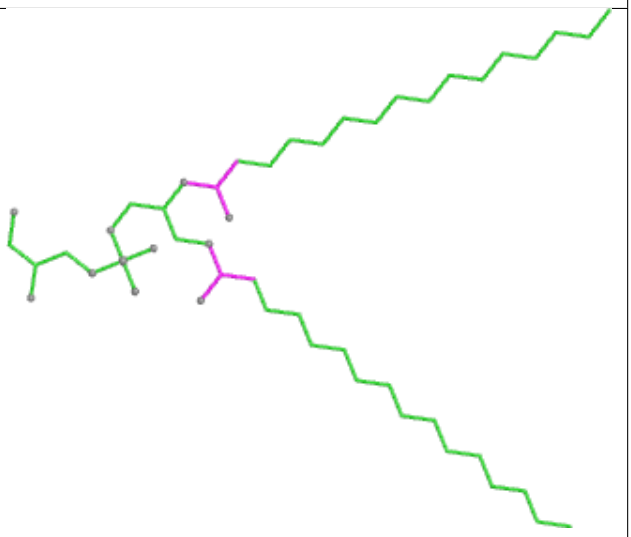


Rings

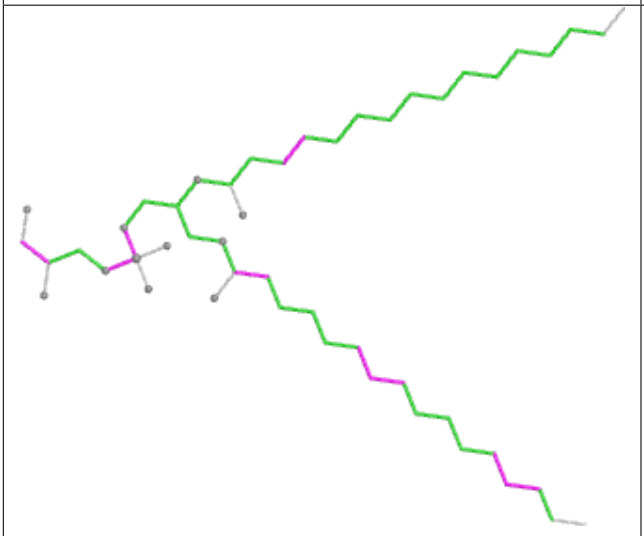
Ligand LHG D 410



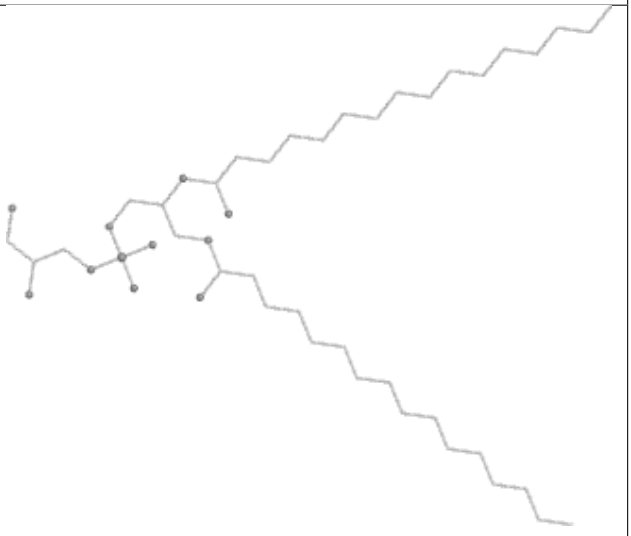
Bond lengths



Bond angles

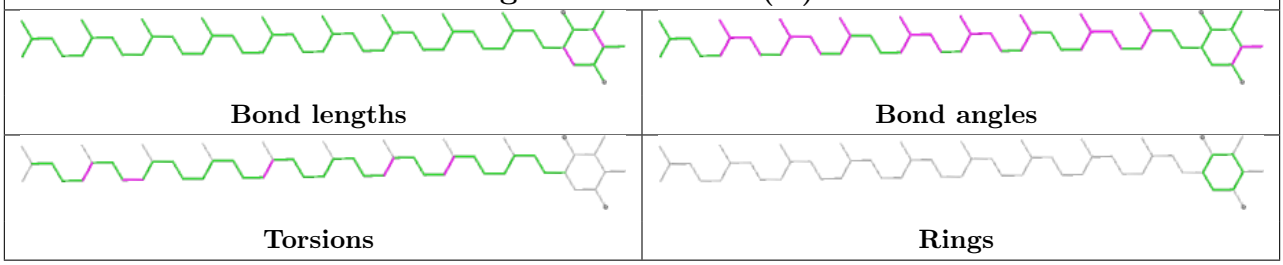


Torsions



Rings

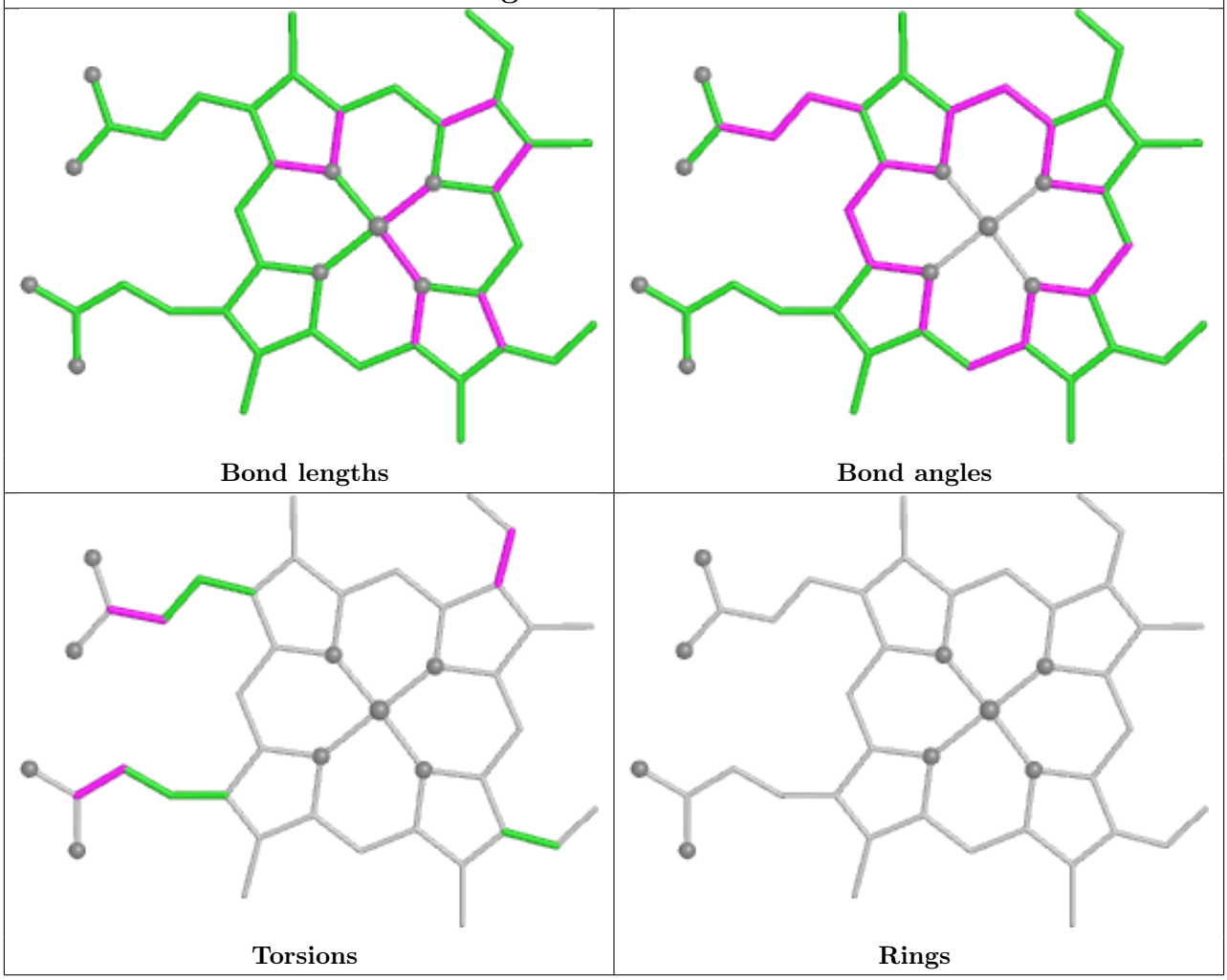
Ligand PL9 d 407 (A)



Bond lengths | Bond angles

Torsions | Rings

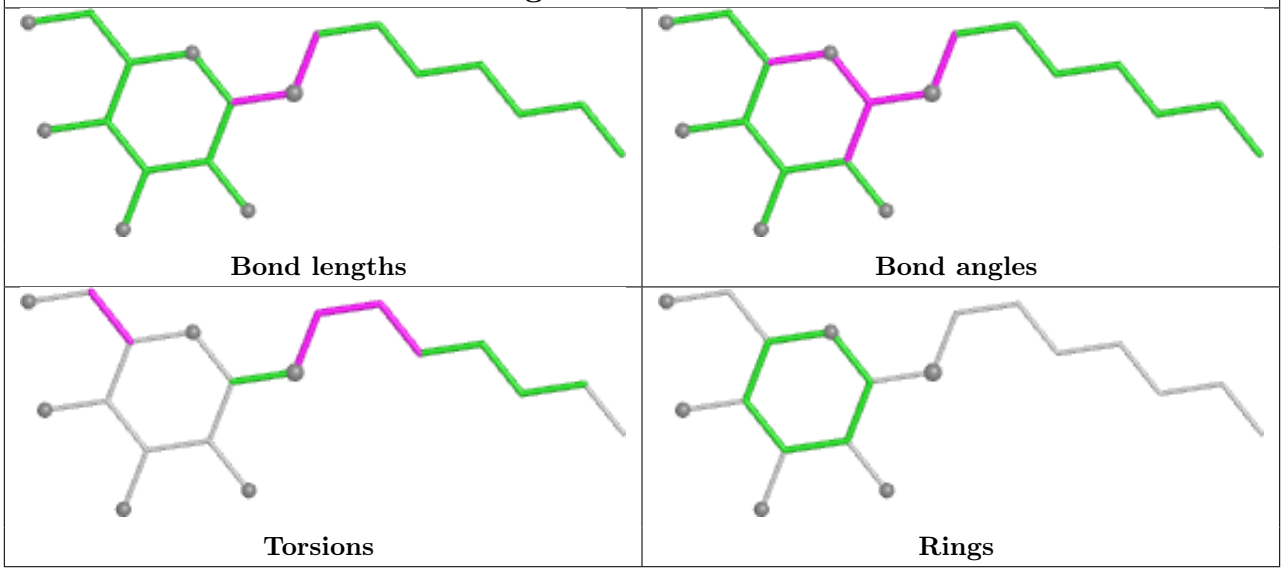
Ligand HEM e 101



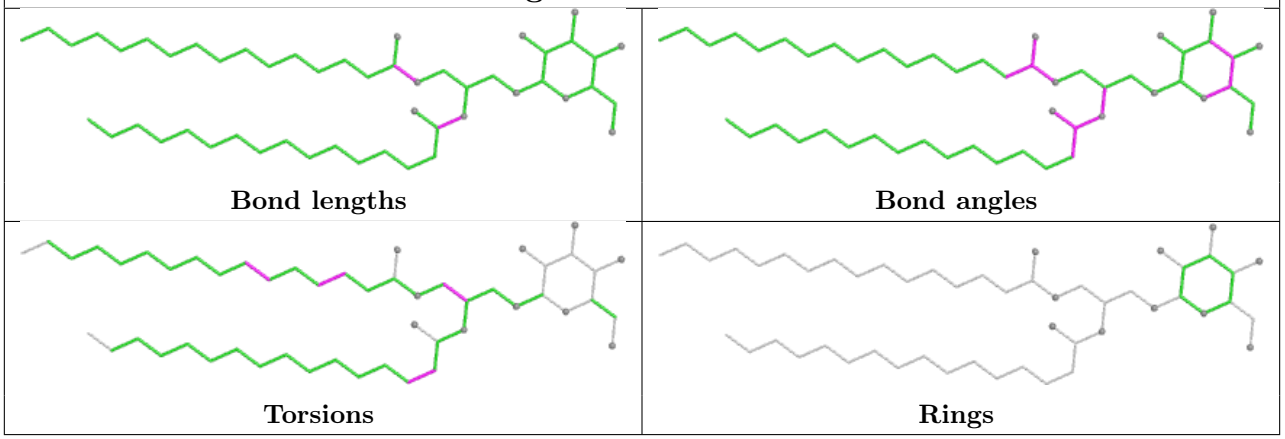
Bond lengths | Bond angles

Torsions | Rings

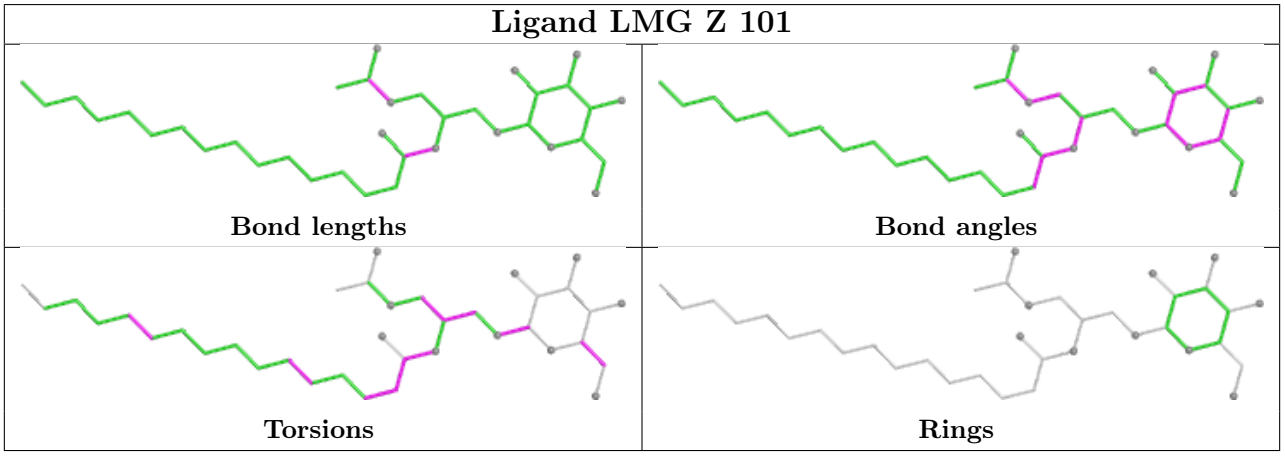
Ligand HTG b 632



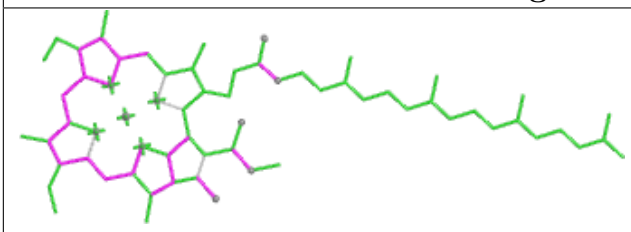
Ligand LMG c 522



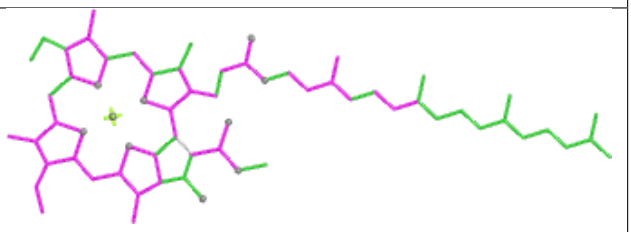
Ligand LMG Z 101



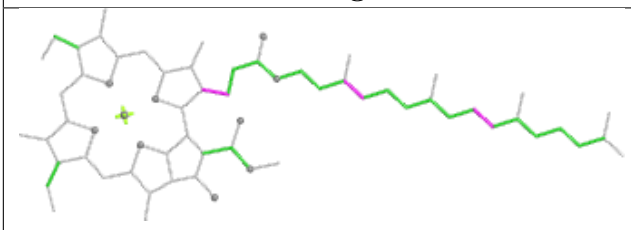
Ligand CLA c 517



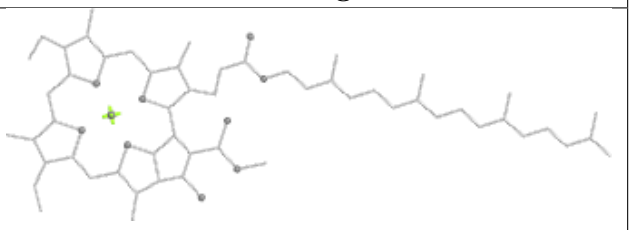
Bond lengths



Bond angles

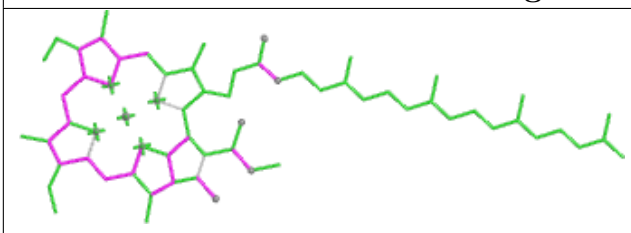


Torsions

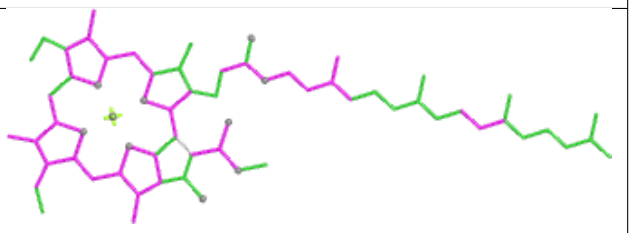


Rings

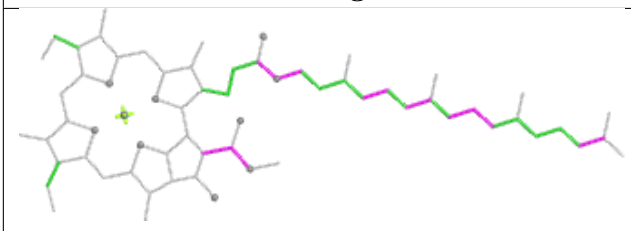
Ligand CLA C 510



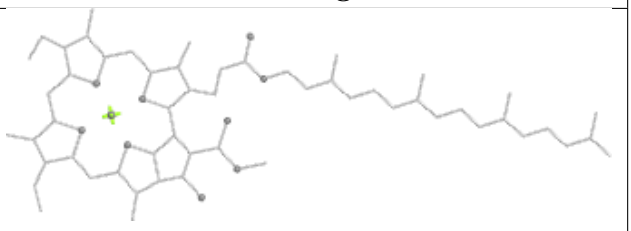
Bond lengths



Bond angles

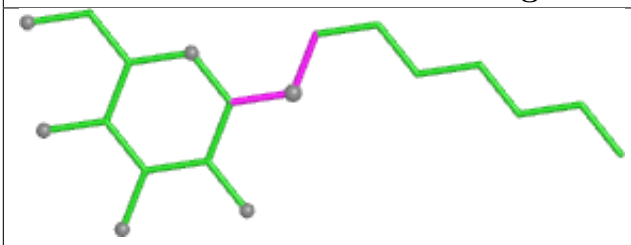


Torsions

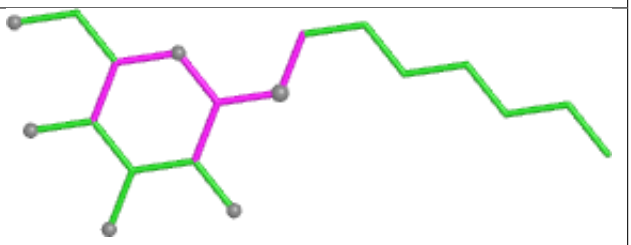


Rings

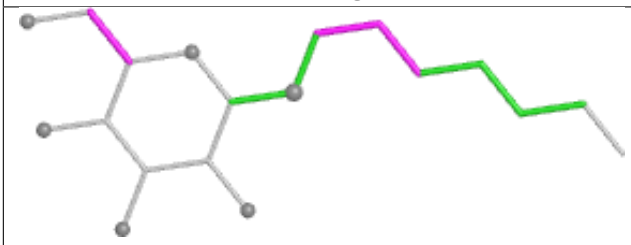
Ligand HTG C 523



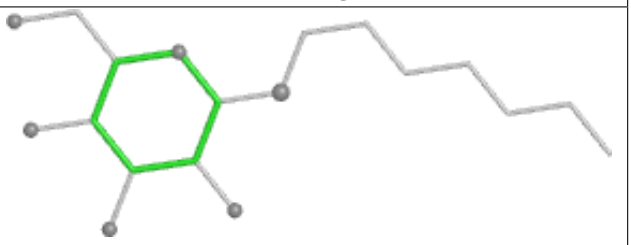
Bond lengths



Bond angles

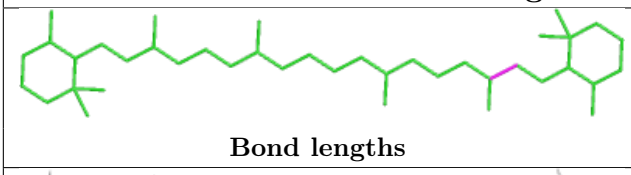


Torsions

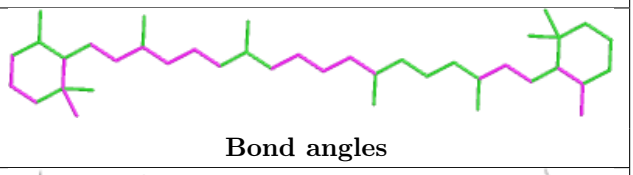


Rings

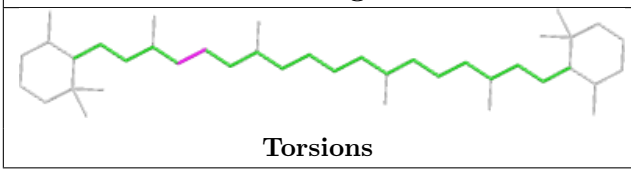
Ligand BCR h 101



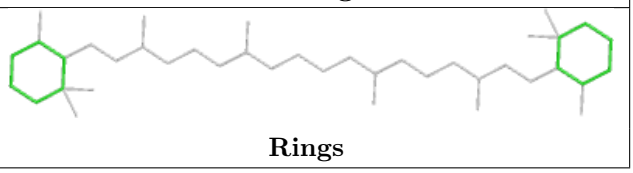
Bond lengths



Bond angles

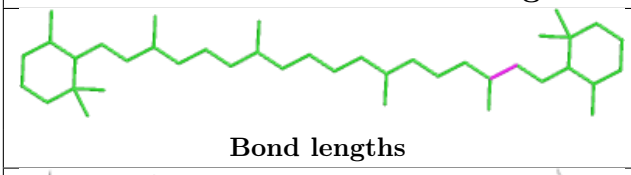


Torsions

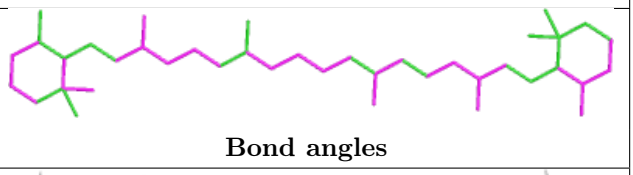


Rings

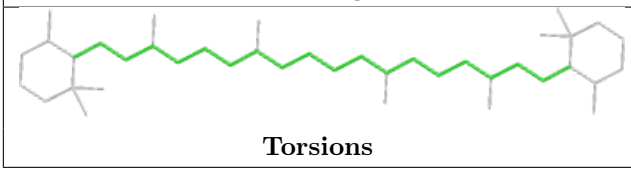
Ligand BCR B 620



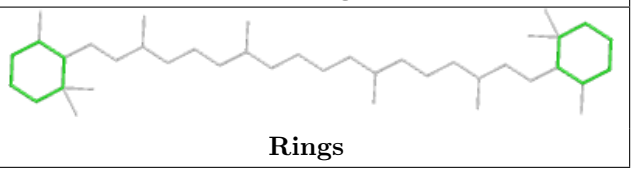
Bond lengths



Bond angles

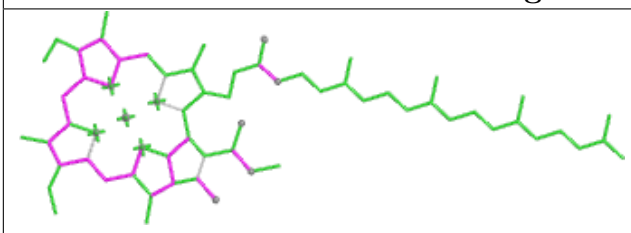


Torsions

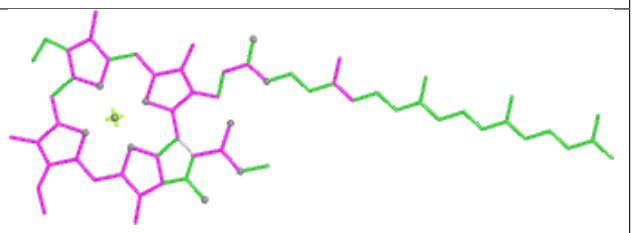


Rings

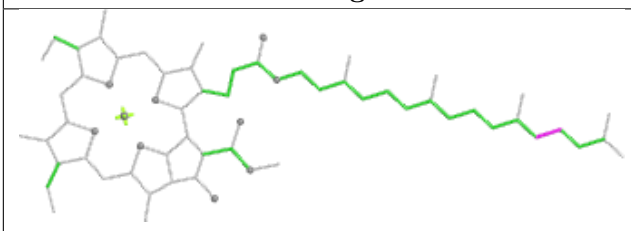
Ligand CLA B 609



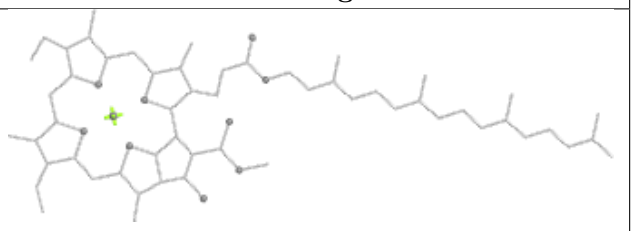
Bond lengths



Bond angles

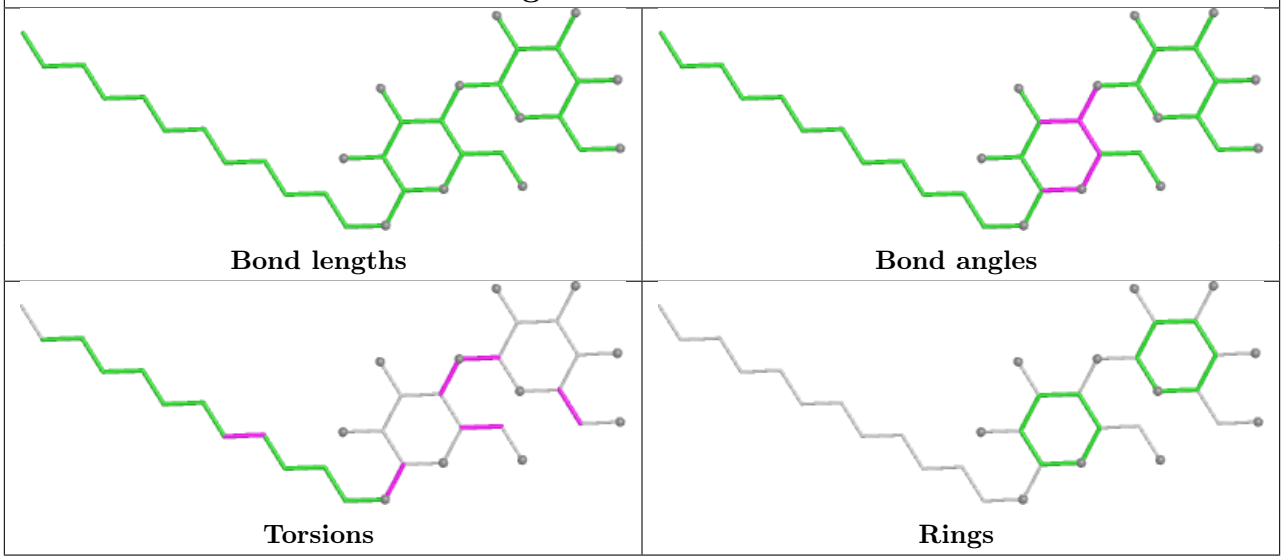


Torsions

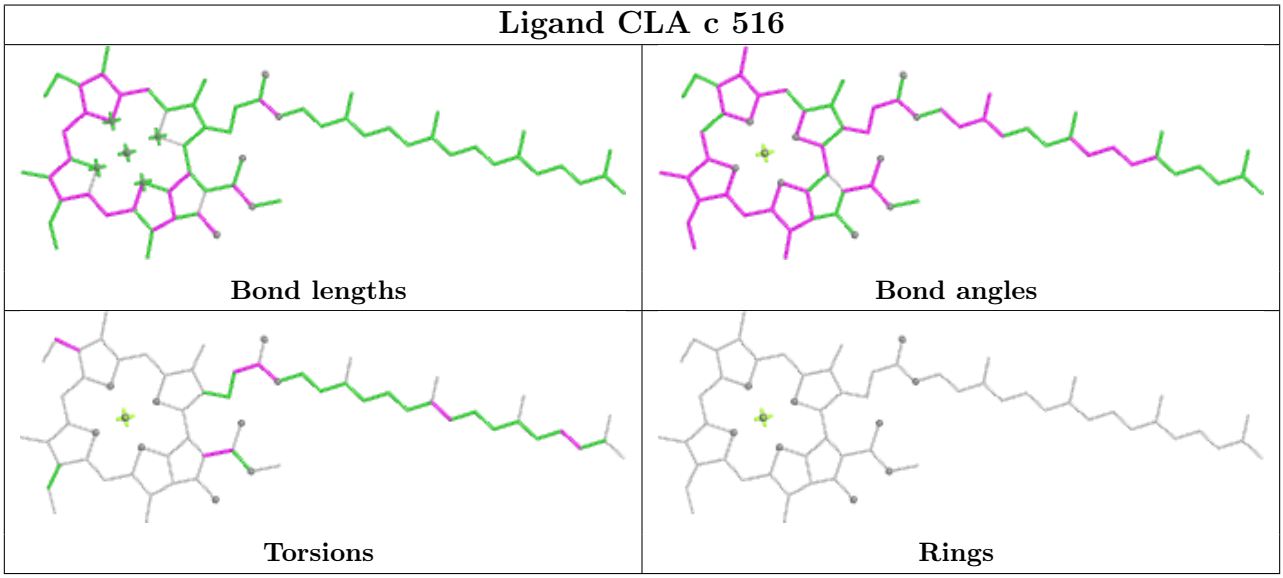


Rings

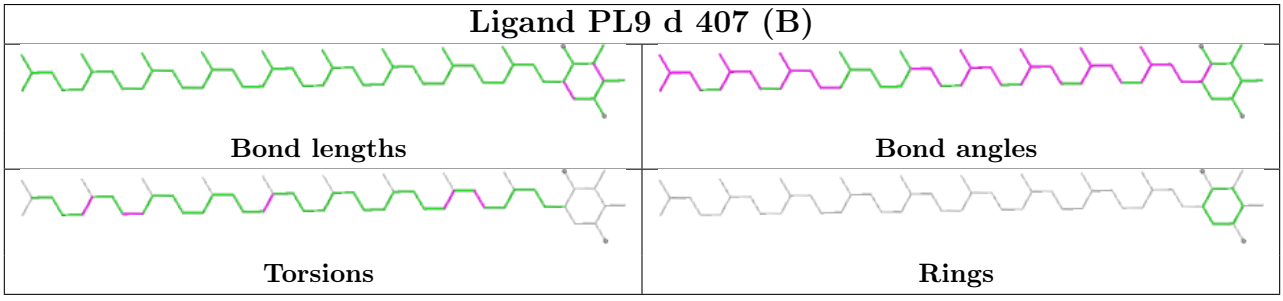
Ligand LMT C 521



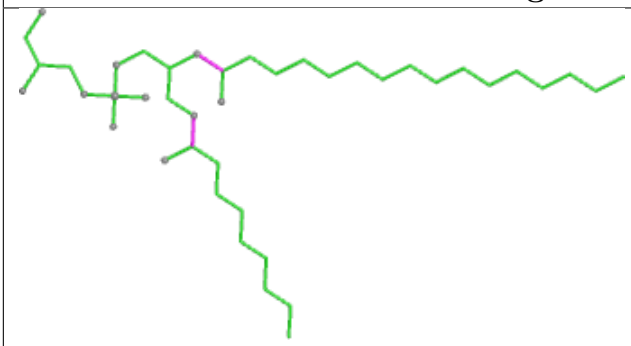
Ligand CLA c 516



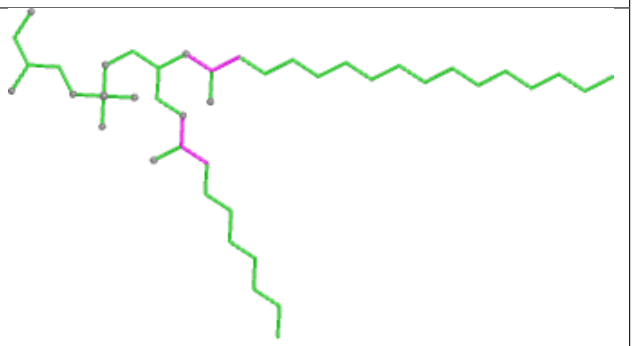
Ligand PL9 d 407 (B)



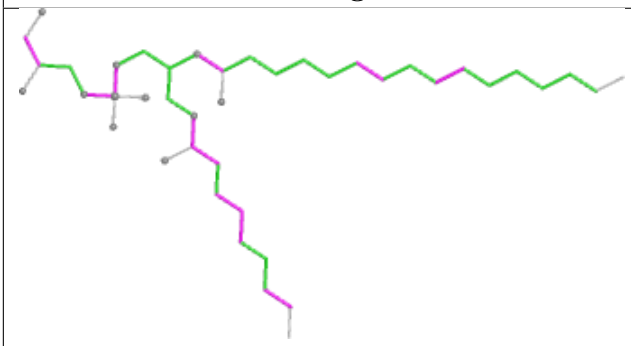
Ligand LHG a 419



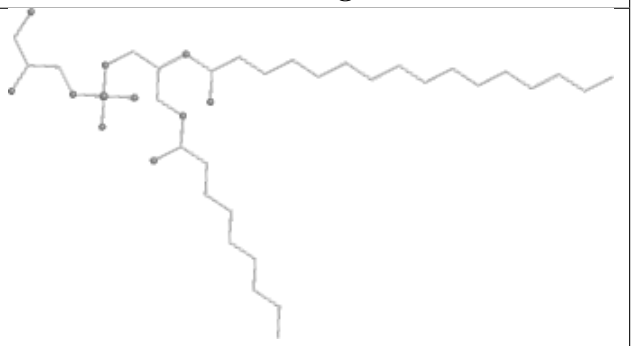
Bond lengths



Bond angles

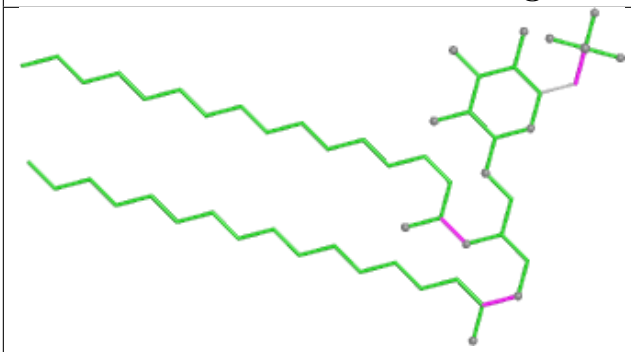


Torsions

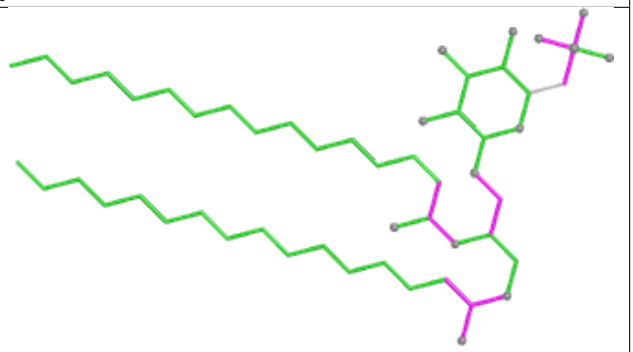


Rings

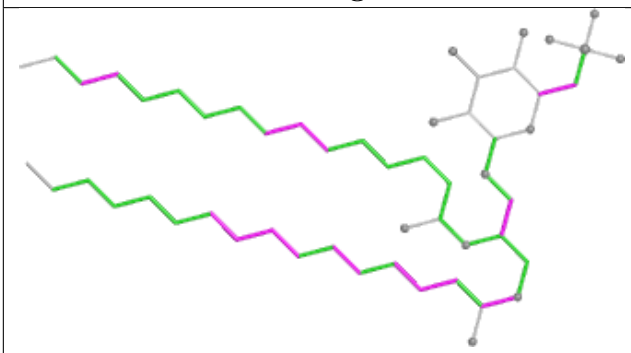
Ligand SQD A 413



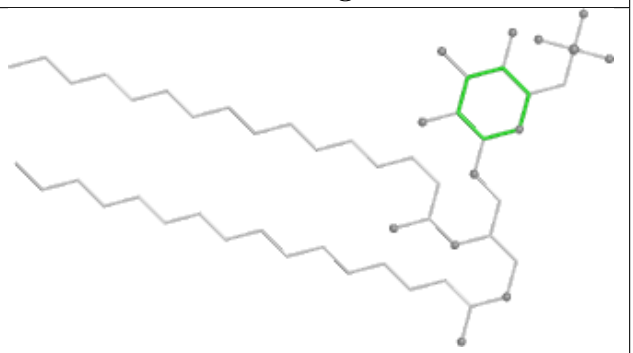
Bond lengths



Bond angles

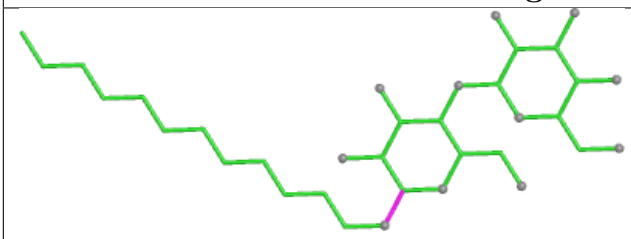


Torsions

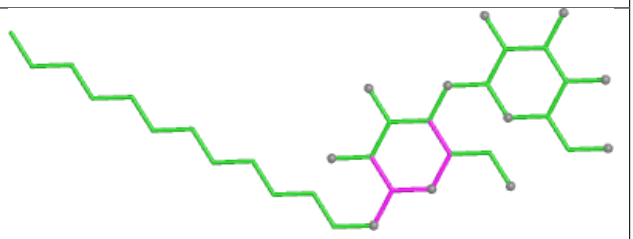


Rings

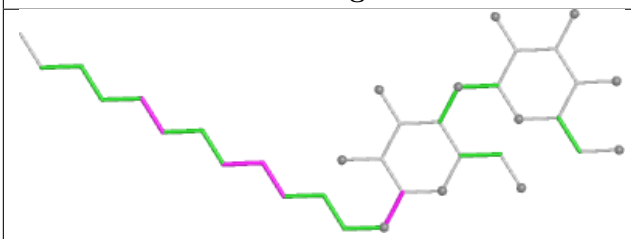
Ligand LMT a 404



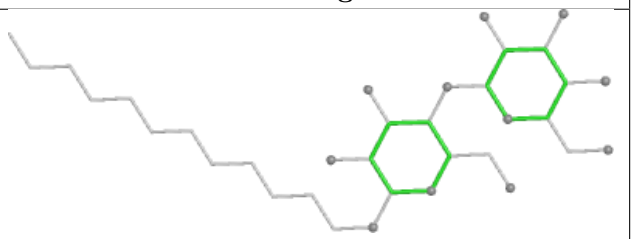
Bond lengths



Bond angles

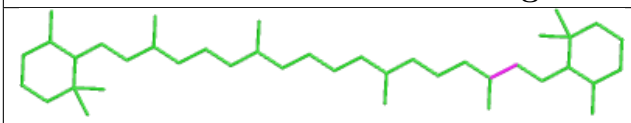


Torsions

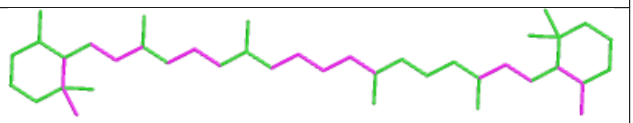


Rings

Ligand BCR H 101



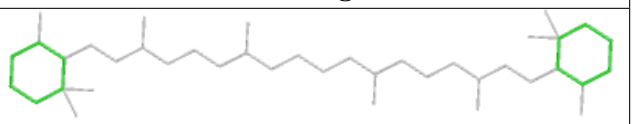
Bond lengths



Bond angles

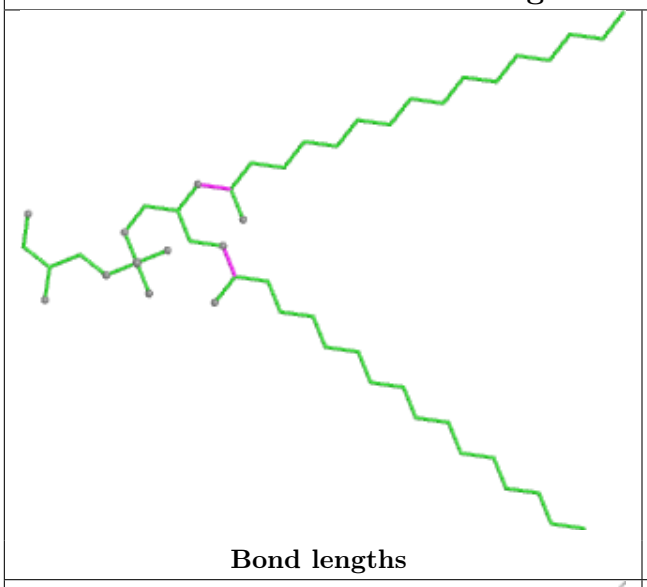


Torsions

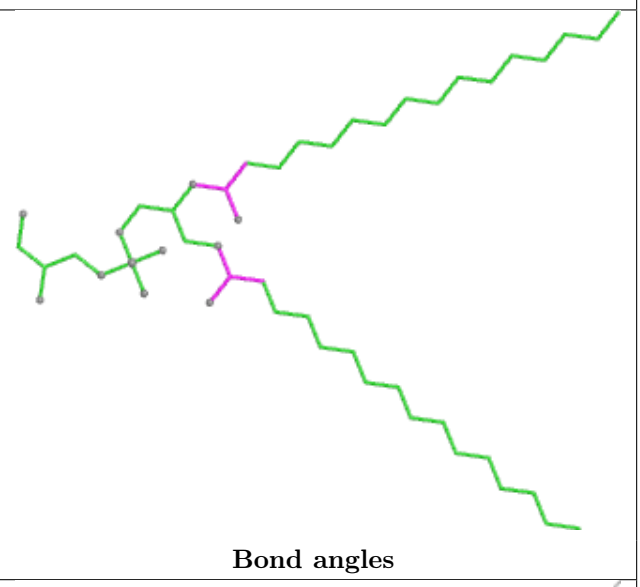


Rings

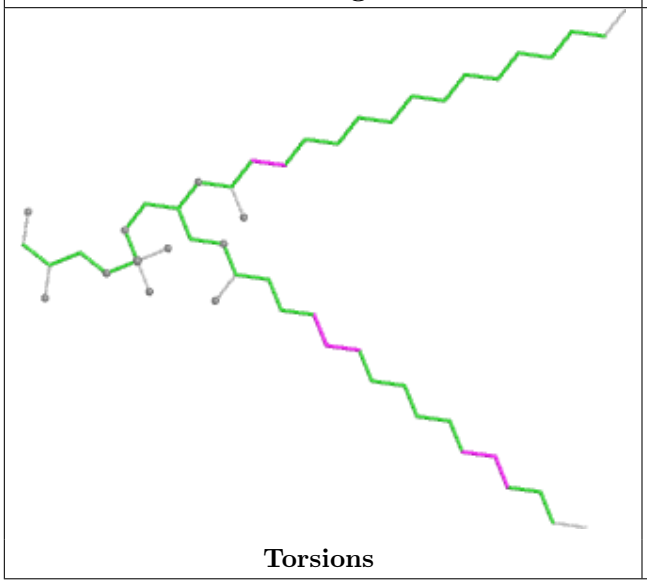
Ligand LHG d 409



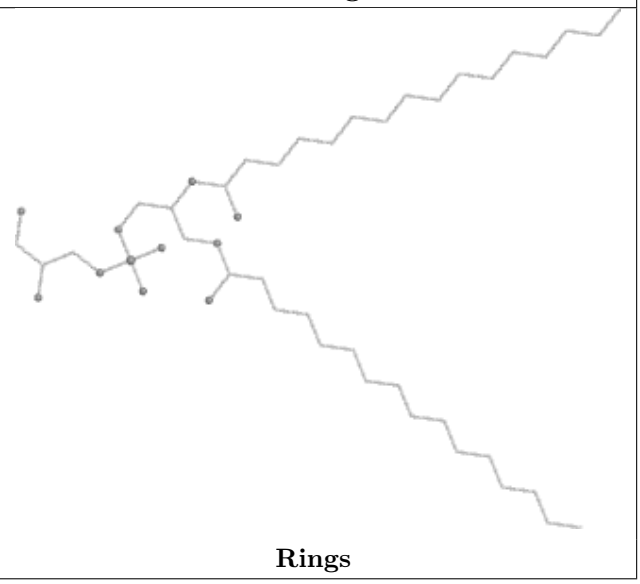
Bond lengths



Bond angles

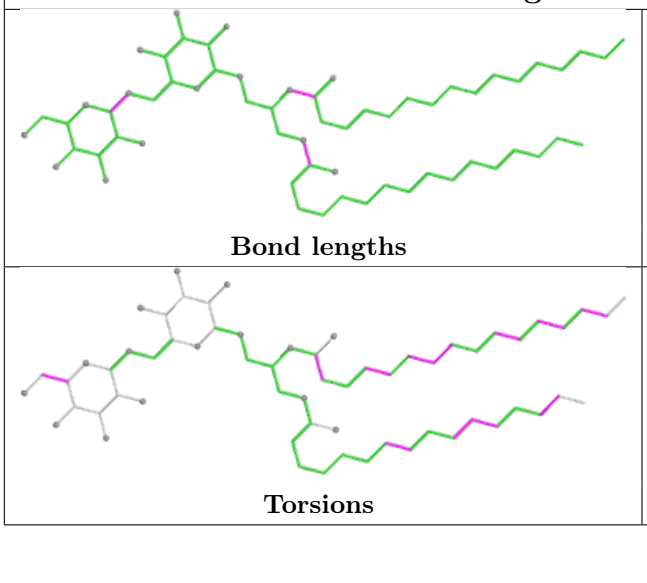


Torsions

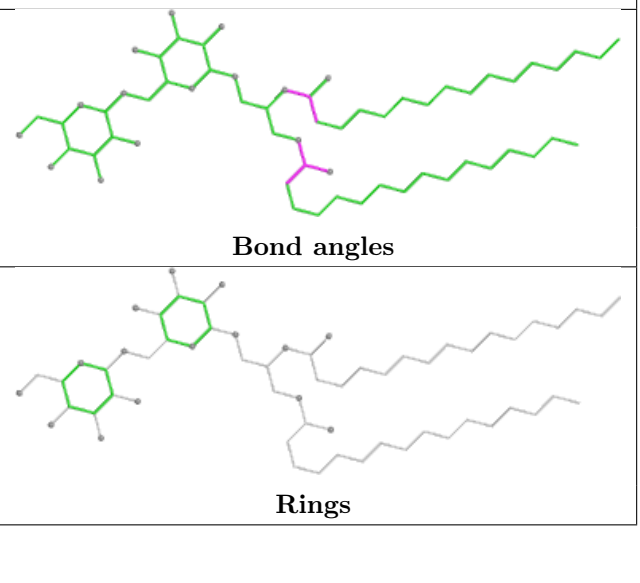


Rings

Ligand DGD h 102



Bond lengths

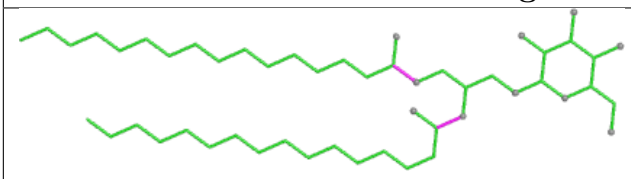


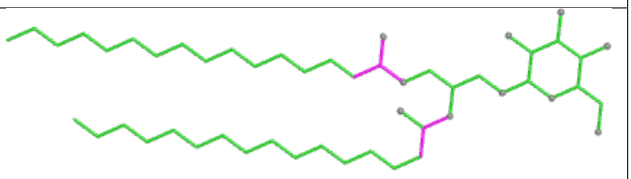
Bond angles

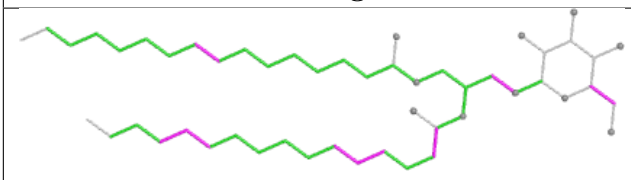
Torsions

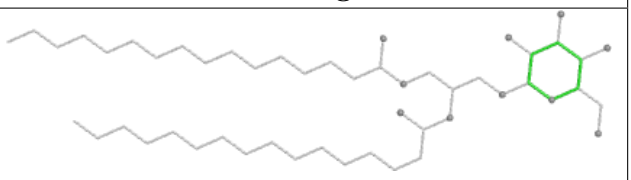
Rings

Ligand LMG D 416

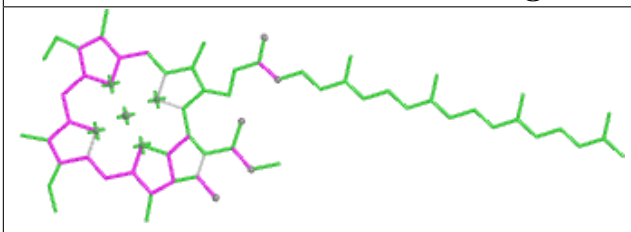

Bond lengths

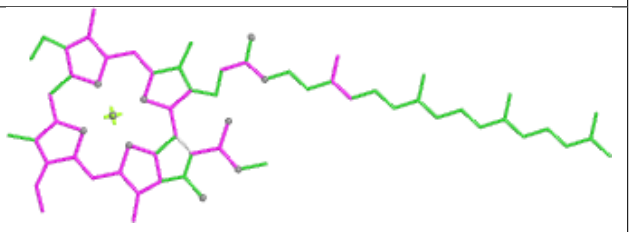

Bond angles

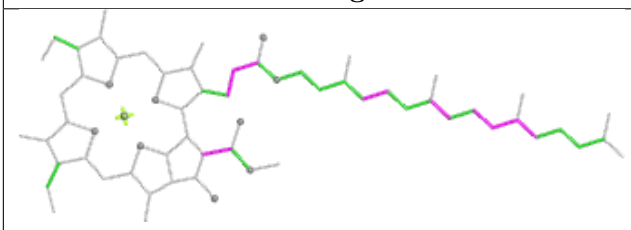

Torsions

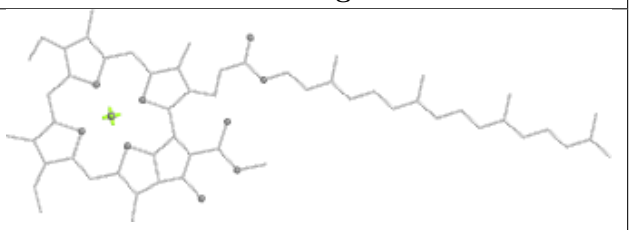

Rings

Ligand CLA B 602

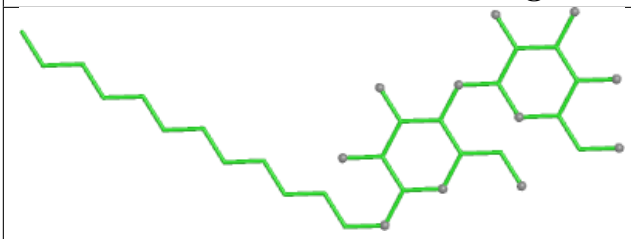

Bond lengths

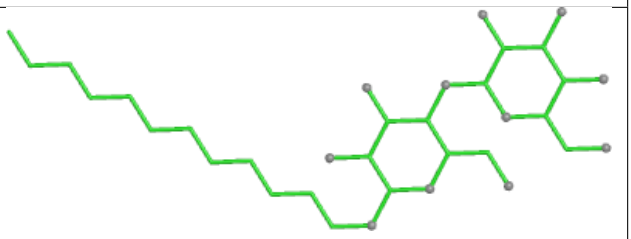

Bond angles

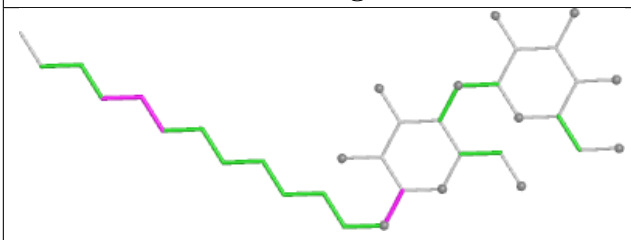

Torsions

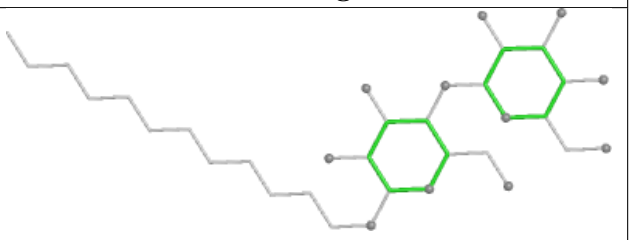

Rings

Ligand LMT a 418

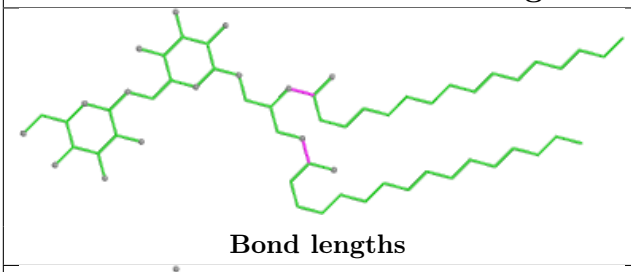

Bond lengths


Bond angles

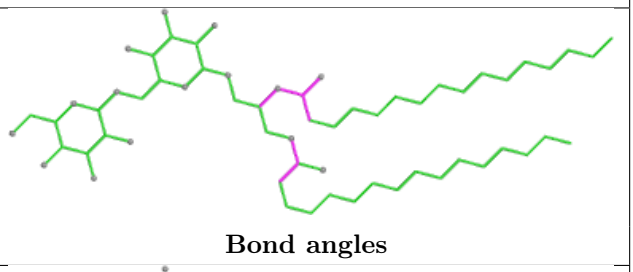

Torsions


Rings

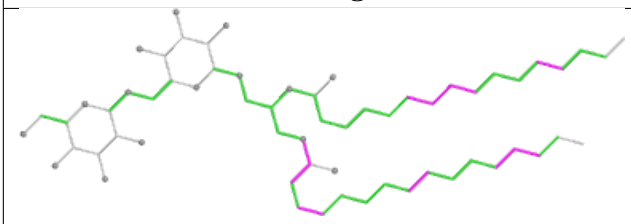
Ligand DGD c 521



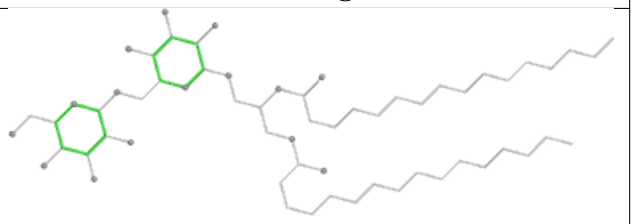
Bond lengths



Bond angles

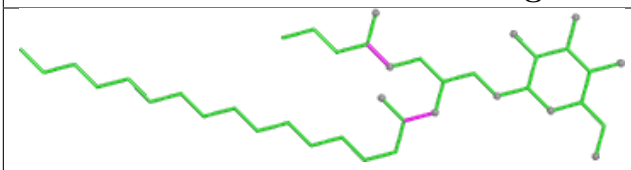


Torsions

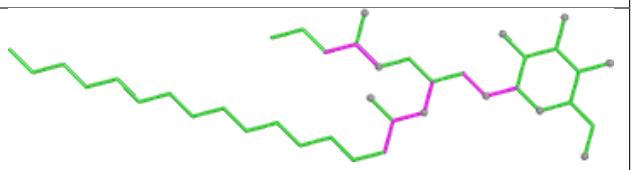


Rings

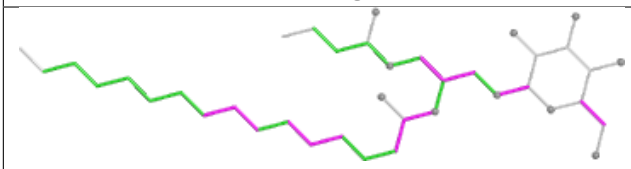
Ligand LMG z 101



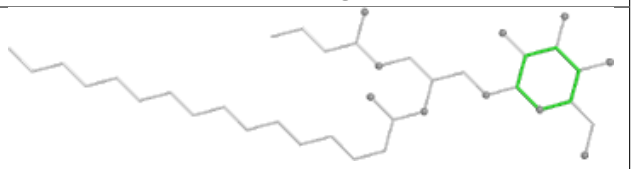
Bond lengths



Bond angles

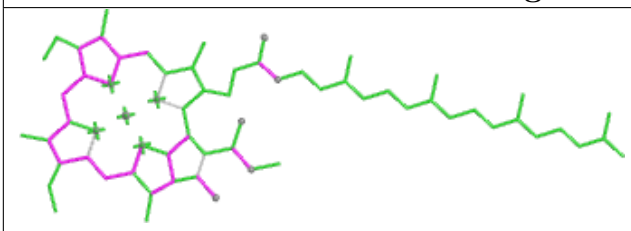


Torsions

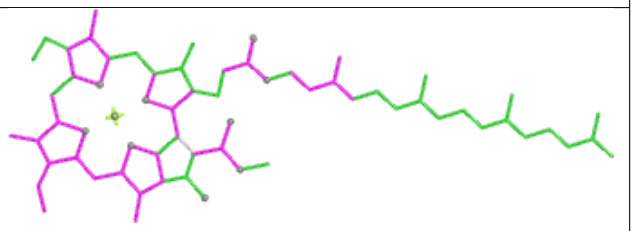


Rings

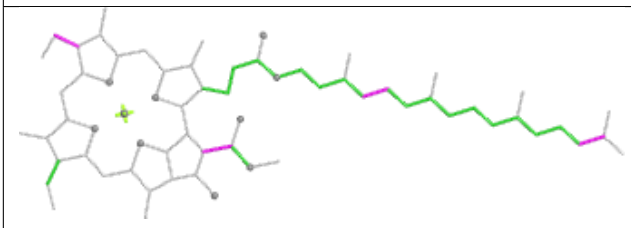
Ligand CLA C 503



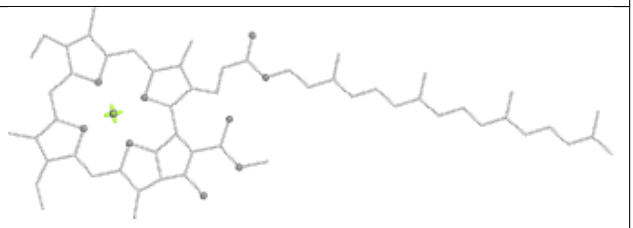
Bond lengths



Bond angles

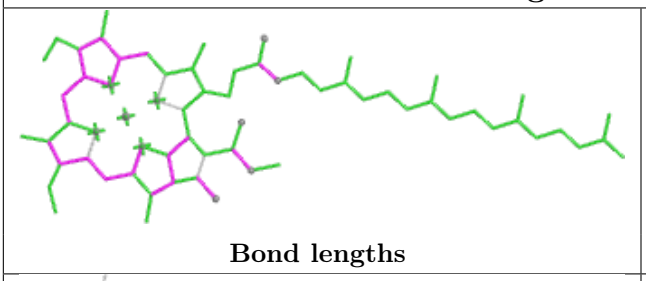


Torsions

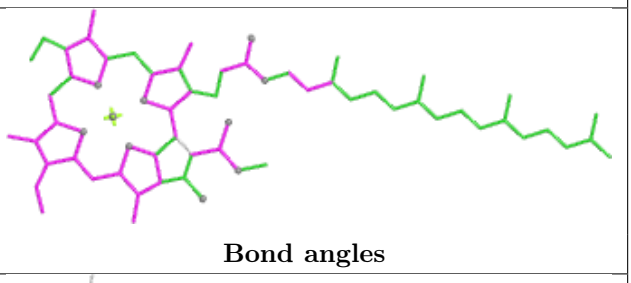


Rings

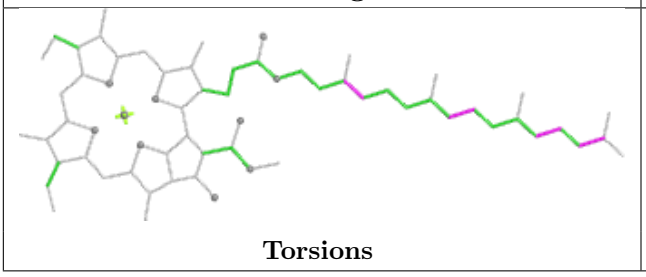
Ligand CLA b 620



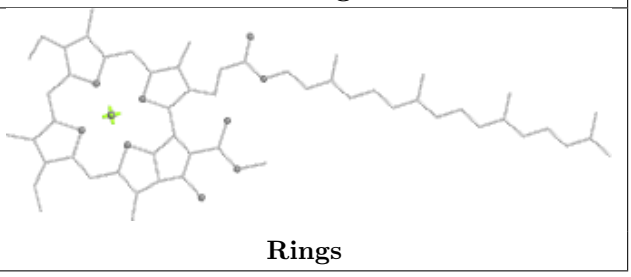
Bond lengths



Bond angles

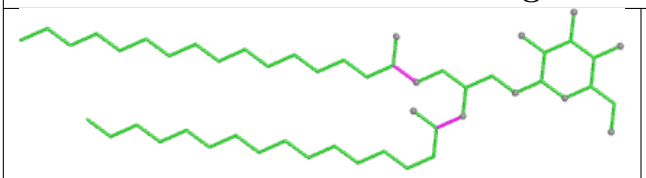


Torsions

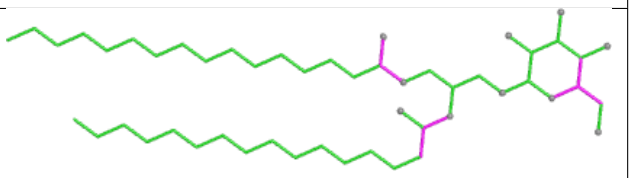


Rings

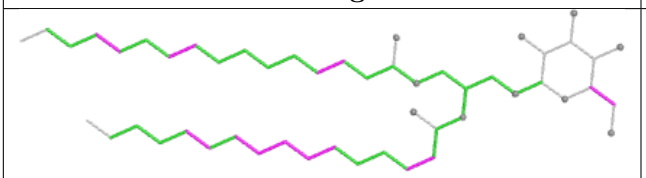
Ligand LMG d 416



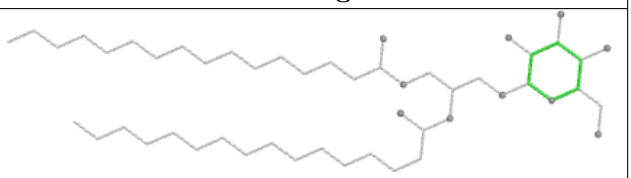
Bond lengths



Bond angles



Torsions

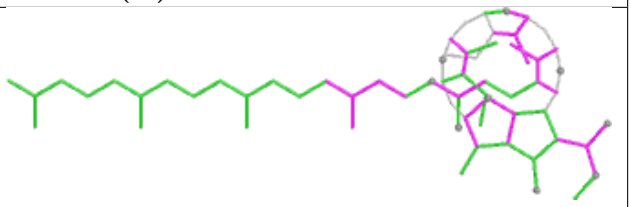


Rings

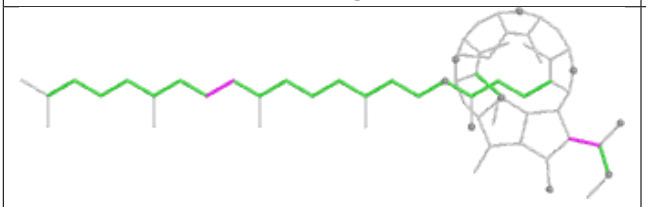
Ligand PHO d 402 (B)



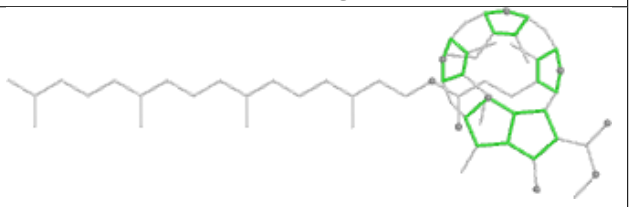
Bond lengths



Bond angles

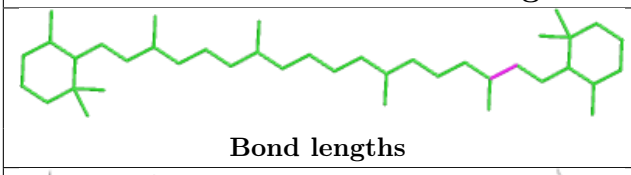


Torsions

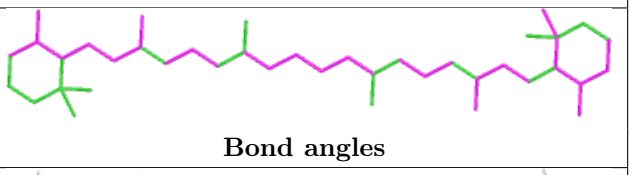


Rings

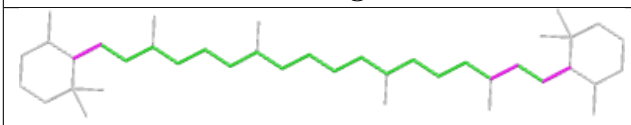
Ligand BCR Y 101



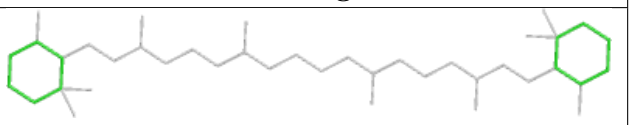
Bond lengths



Bond angles

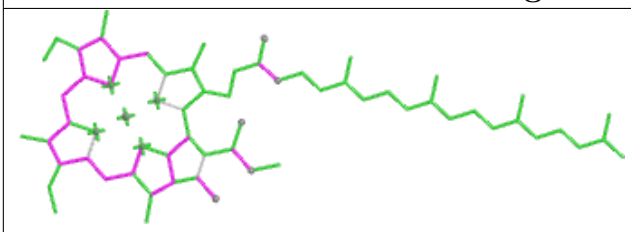


Torsions

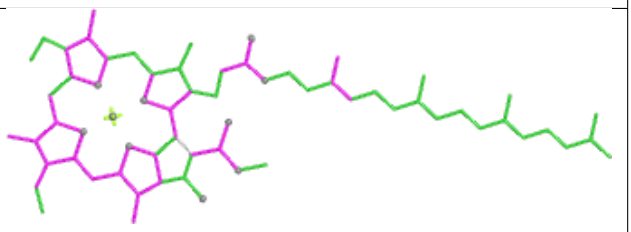


Rings

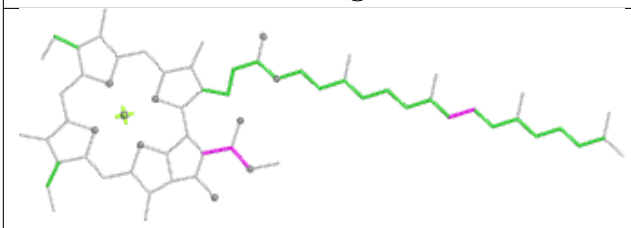
Ligand CLA C 504



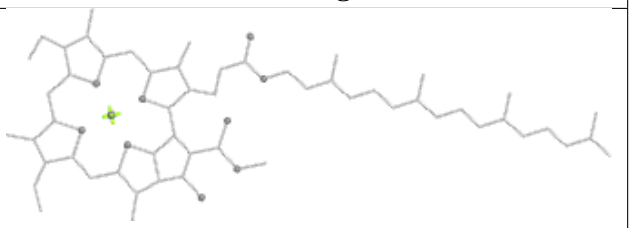
Bond lengths



Bond angles

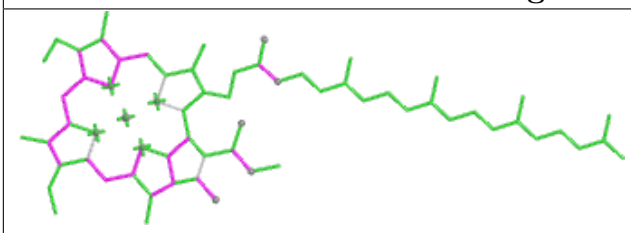


Torsions

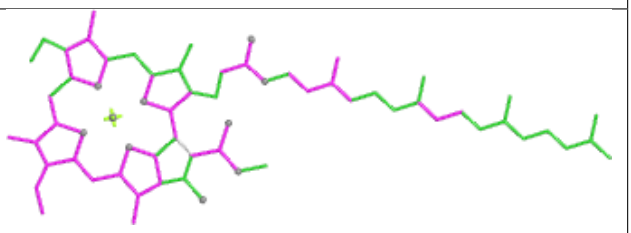


Rings

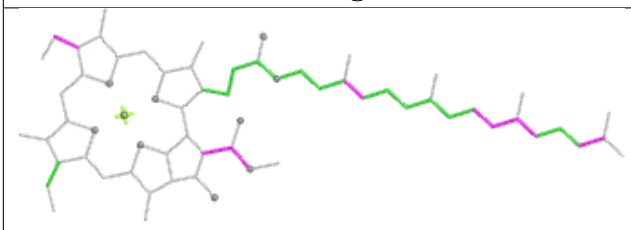
Ligand CLA b 625



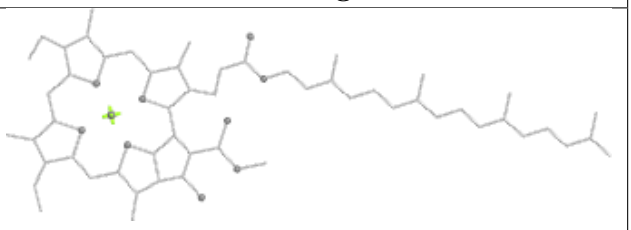
Bond lengths



Bond angles

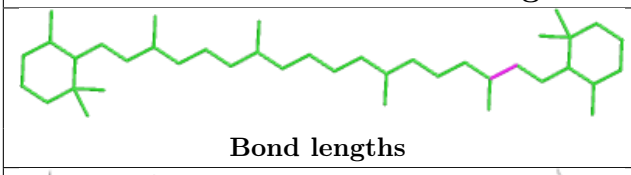


Torsions

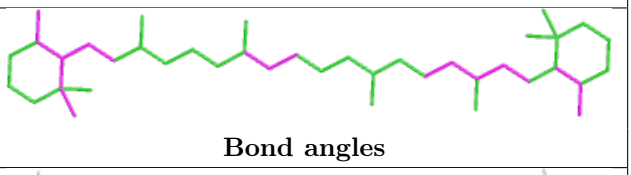


Rings

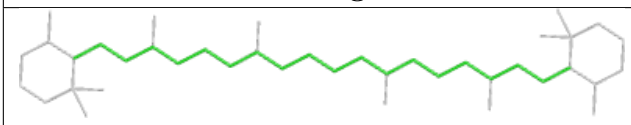
Ligand BCR A 409



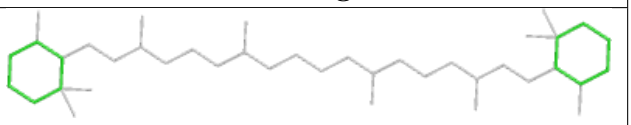
Bond lengths



Bond angles

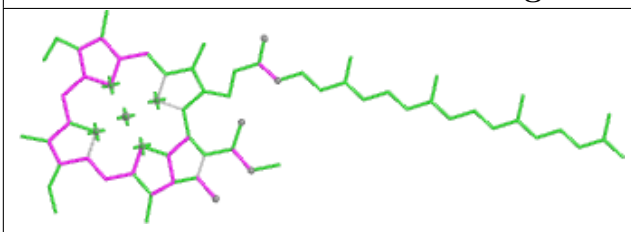


Torsions

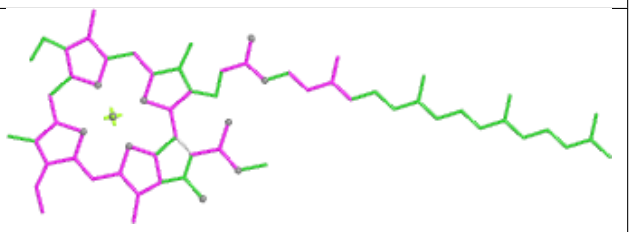


Rings

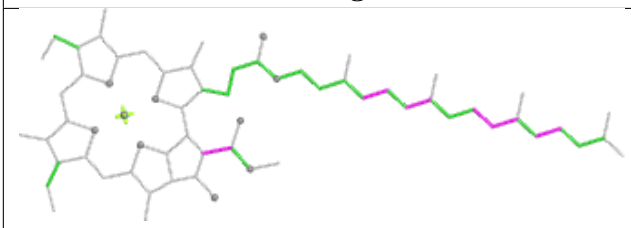
Ligand CLA C 509



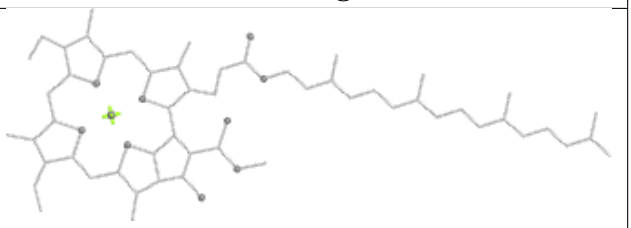
Bond lengths



Bond angles

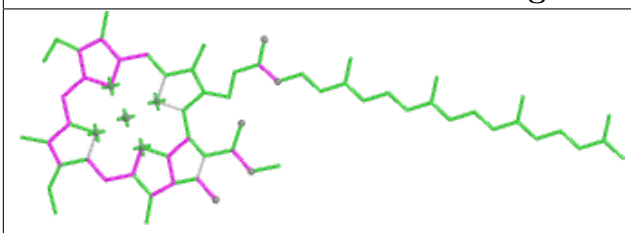


Torsions

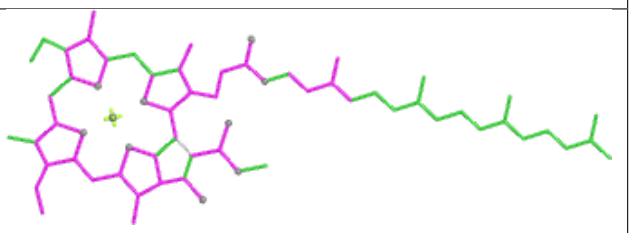


Rings

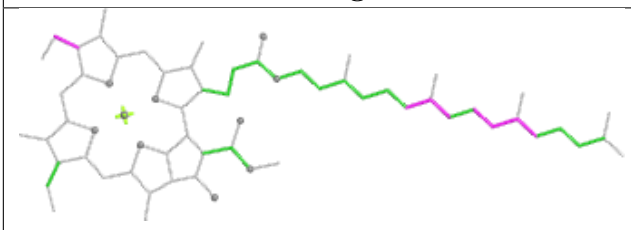
Ligand CLA a 409



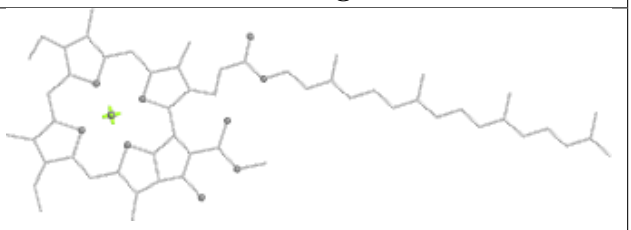
Bond lengths



Bond angles

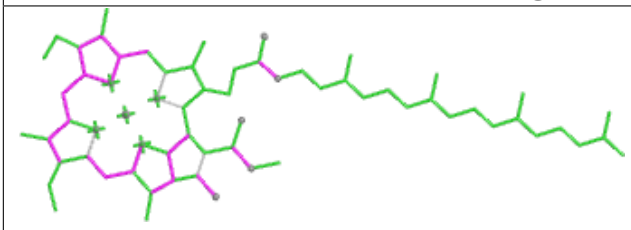


Torsions

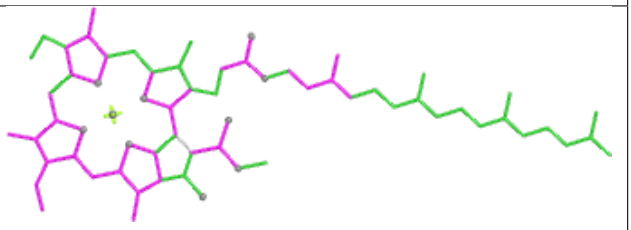


Rings

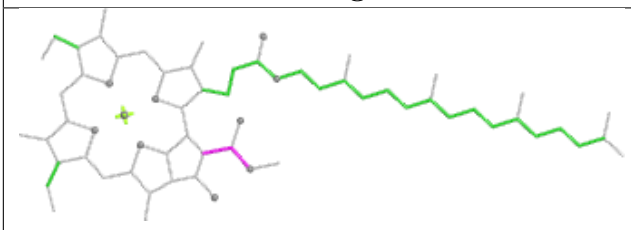
Ligand CLA c 507



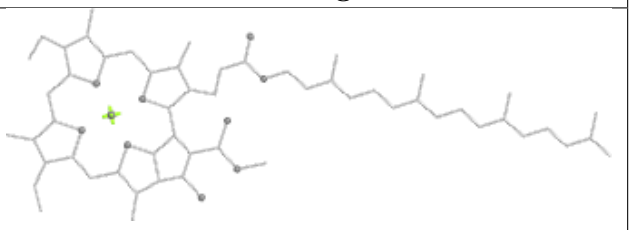
Bond lengths



Bond angles

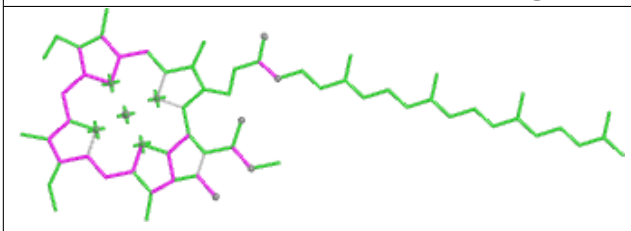


Torsions

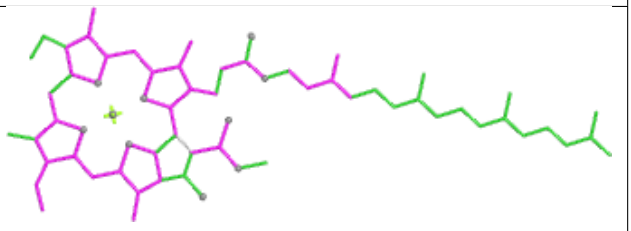


Rings

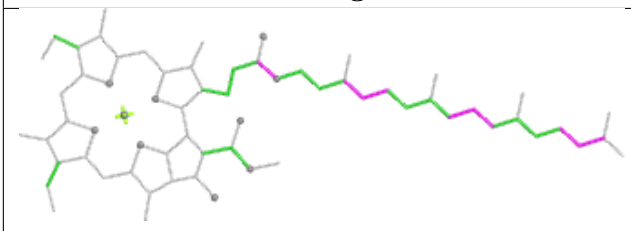
Ligand CLA a 411



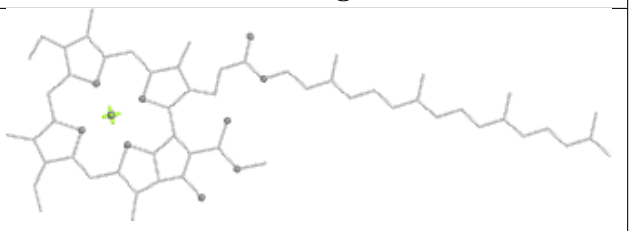
Bond lengths



Bond angles

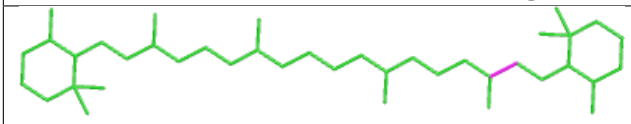


Torsions

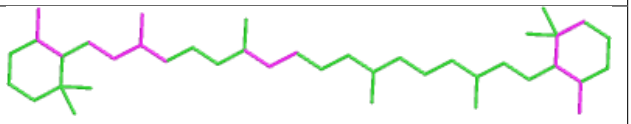


Rings

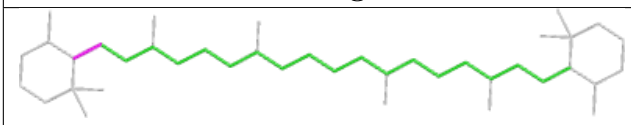
Ligand BCR B 618



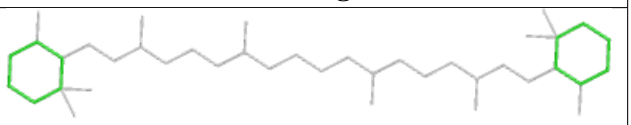
Bond lengths



Bond angles

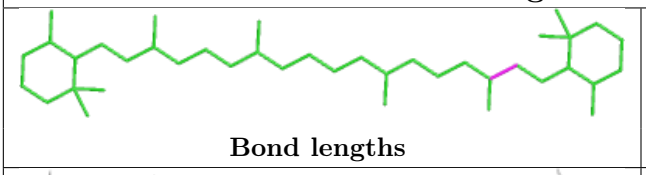


Torsions

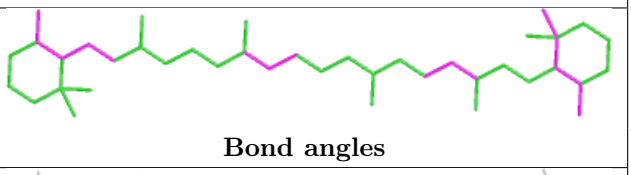


Rings

Ligand BCR a 412



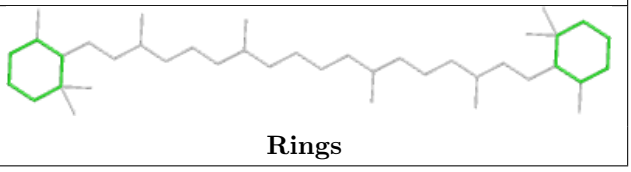
Bond lengths



Bond angles

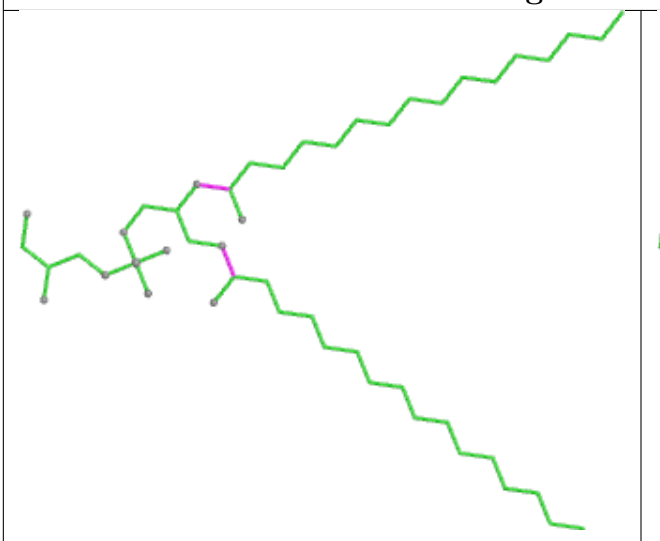


Torsions

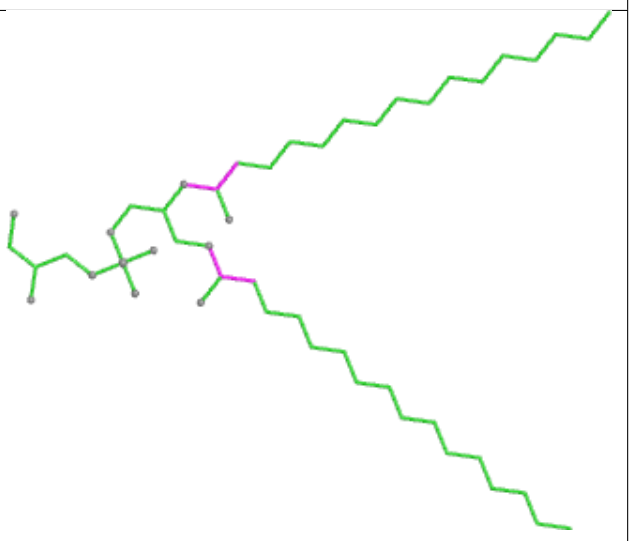


Rings

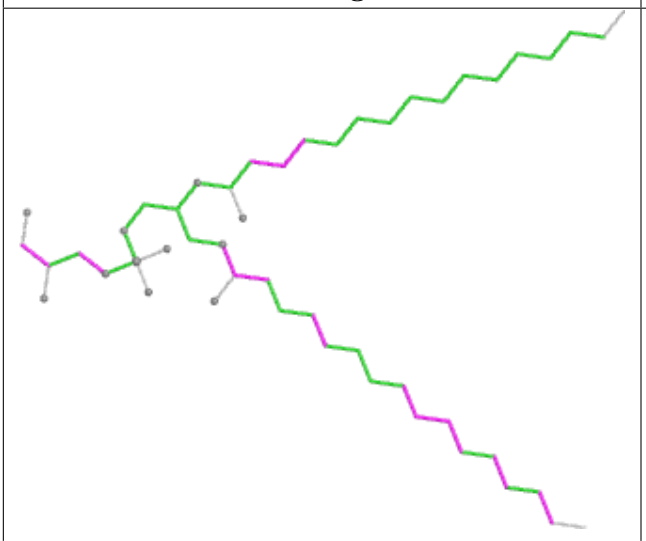
Ligand LHG d 411



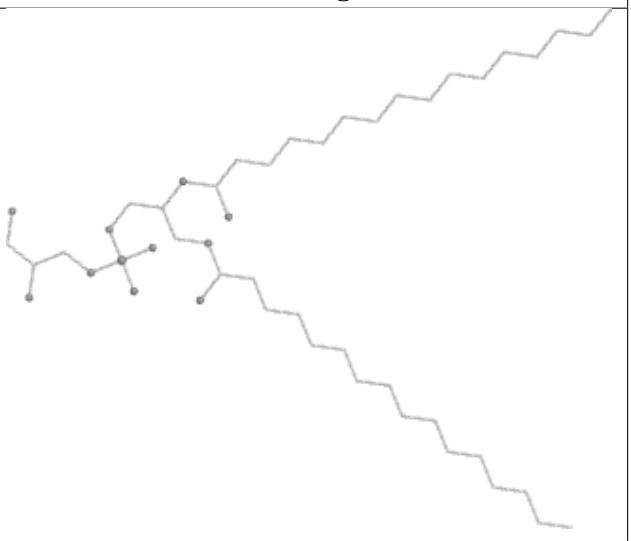
Bond lengths



Bond angles

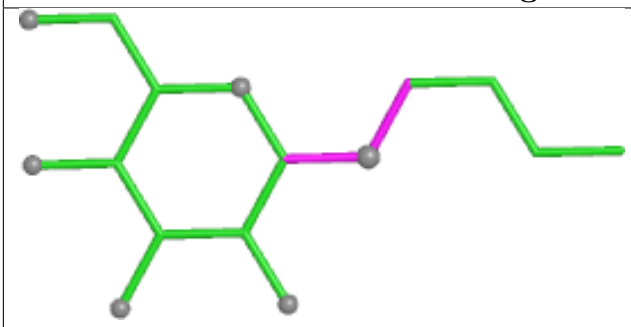


Torsions

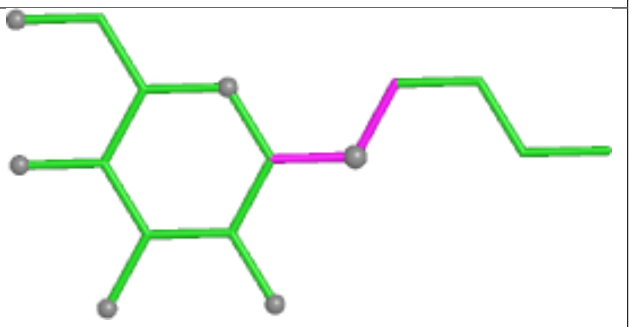


Rings

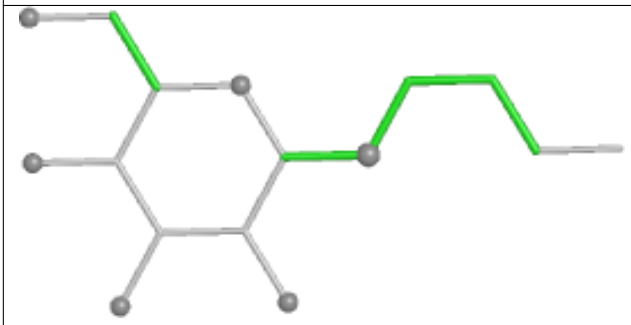
Ligand HTG D 415



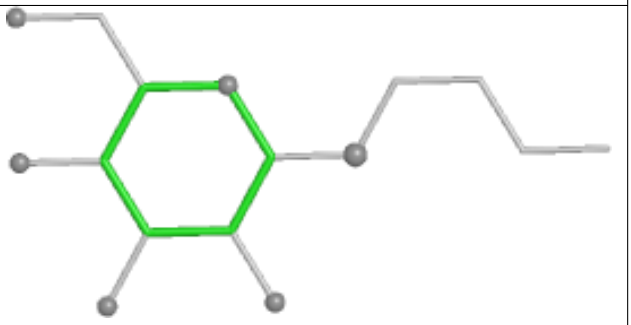
Bond lengths



Bond angles

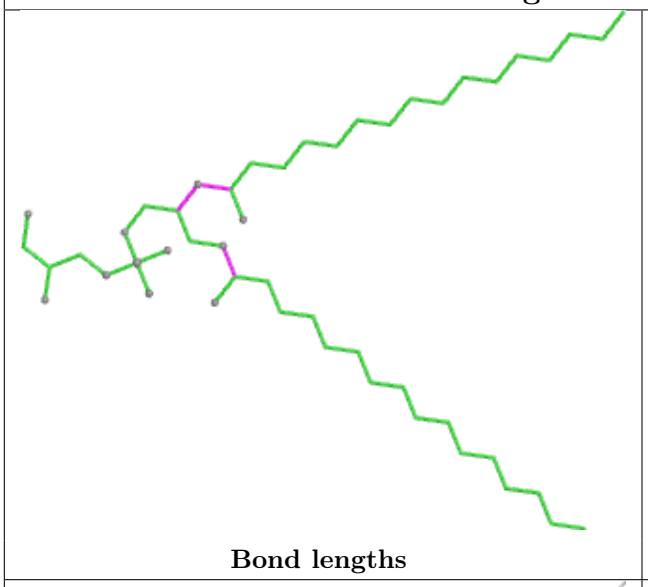


Torsions

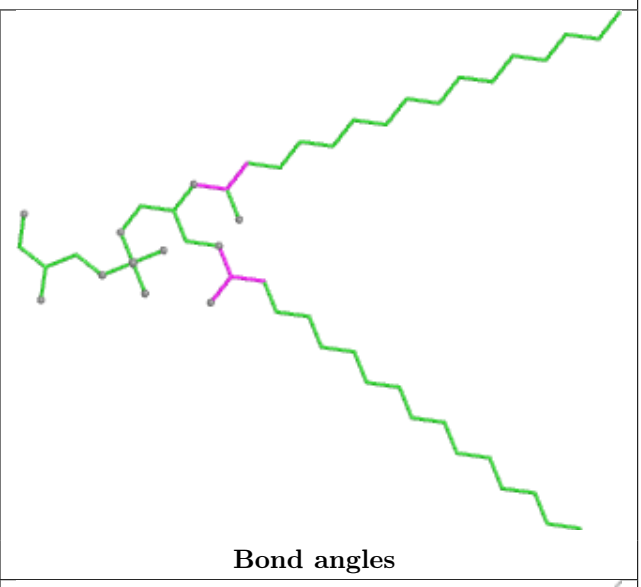


Rings

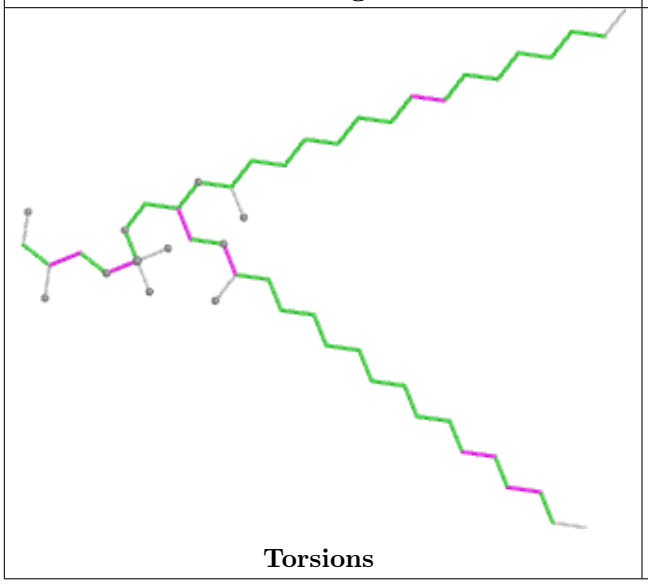
Ligand LHG D 411



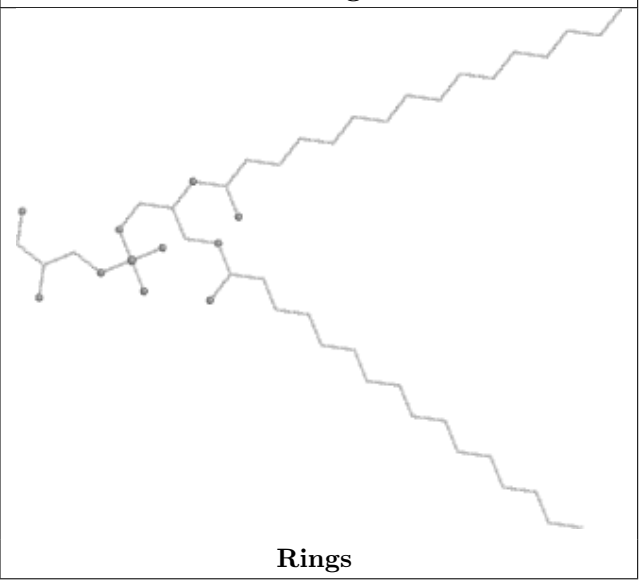
Bond lengths



Bond angles

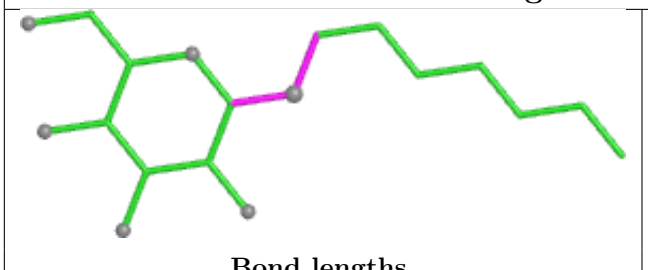


Torsions

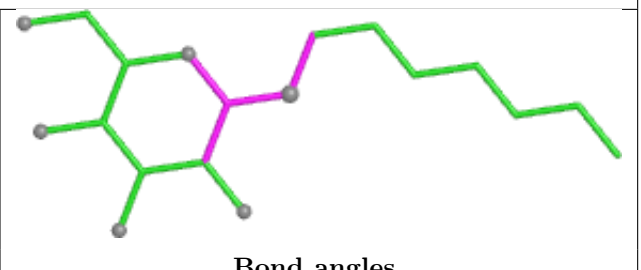


Rings

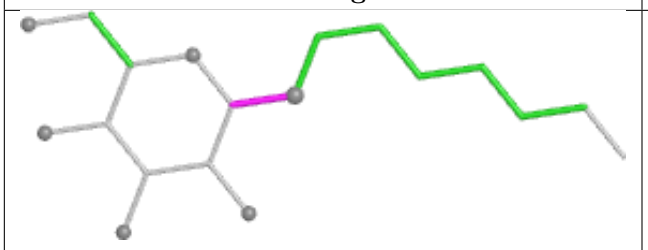
Ligand HTG b 608



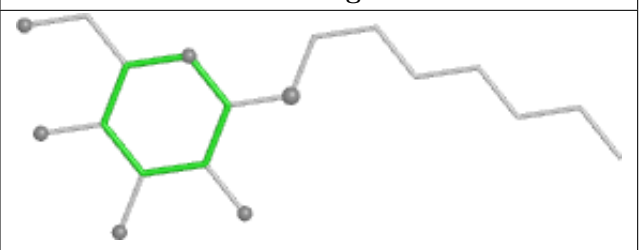
Bond lengths



Bond angles

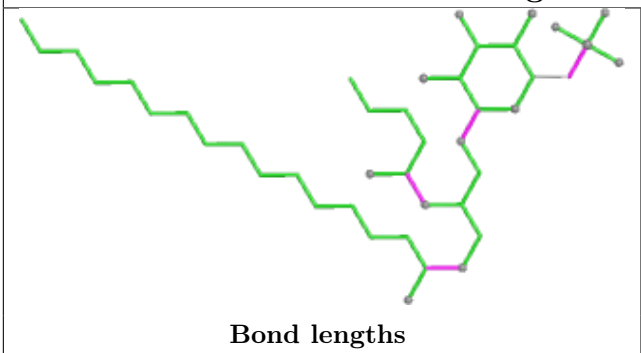


Torsions

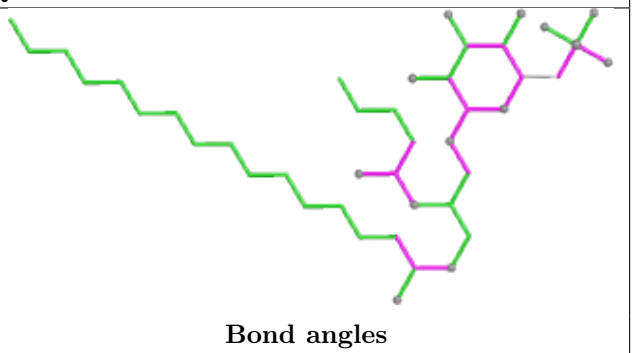


Rings

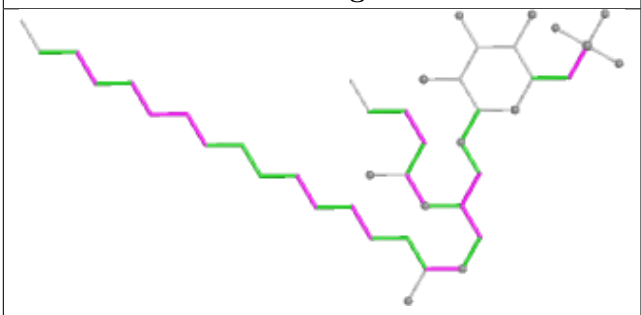
Ligand SQD F 104



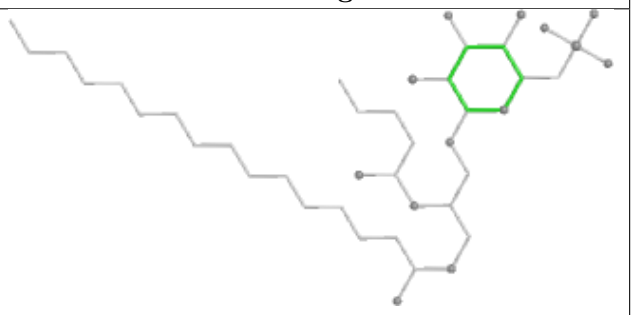
Bond lengths



Bond angles

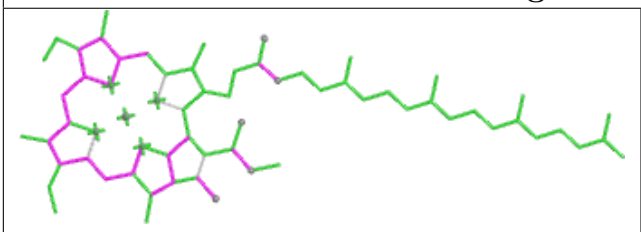


Torsions

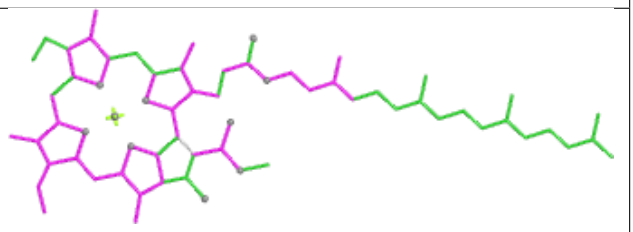


Rings

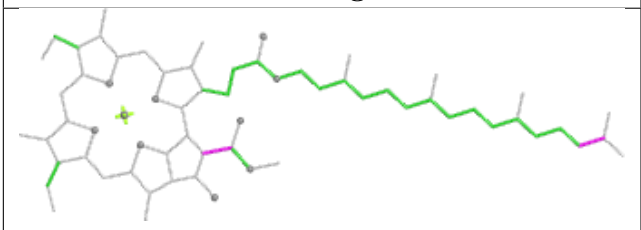
Ligand CLA b 611



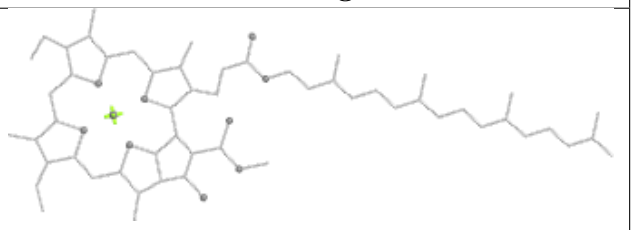
Bond lengths



Bond angles

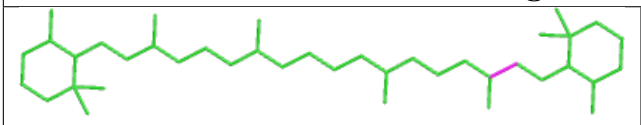


Torsions

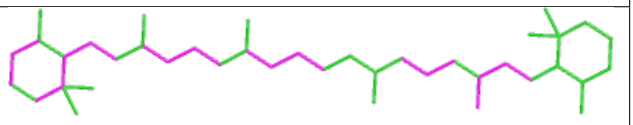


Rings

Ligand BCR b 628



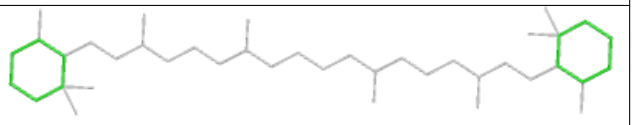
Bond lengths



Bond angles

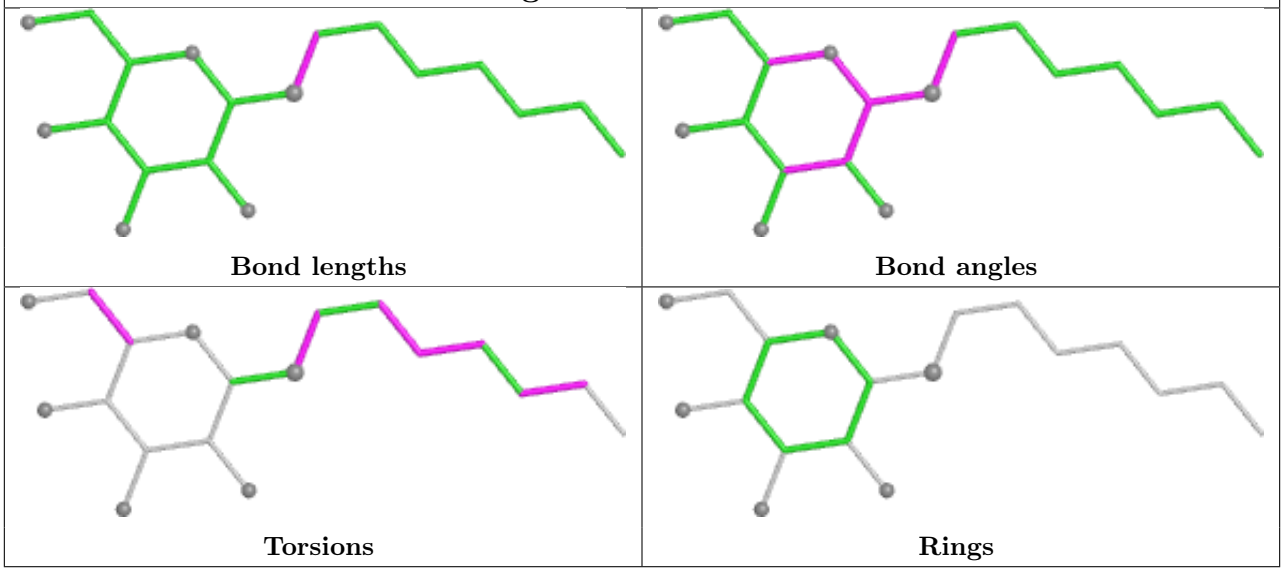


Torsions

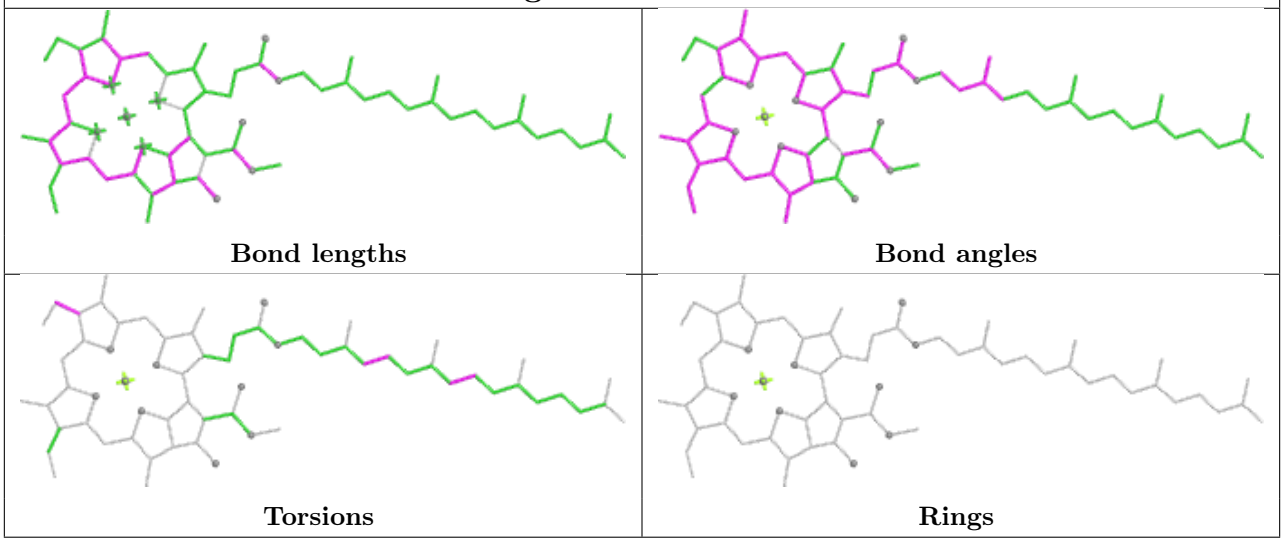


Rings

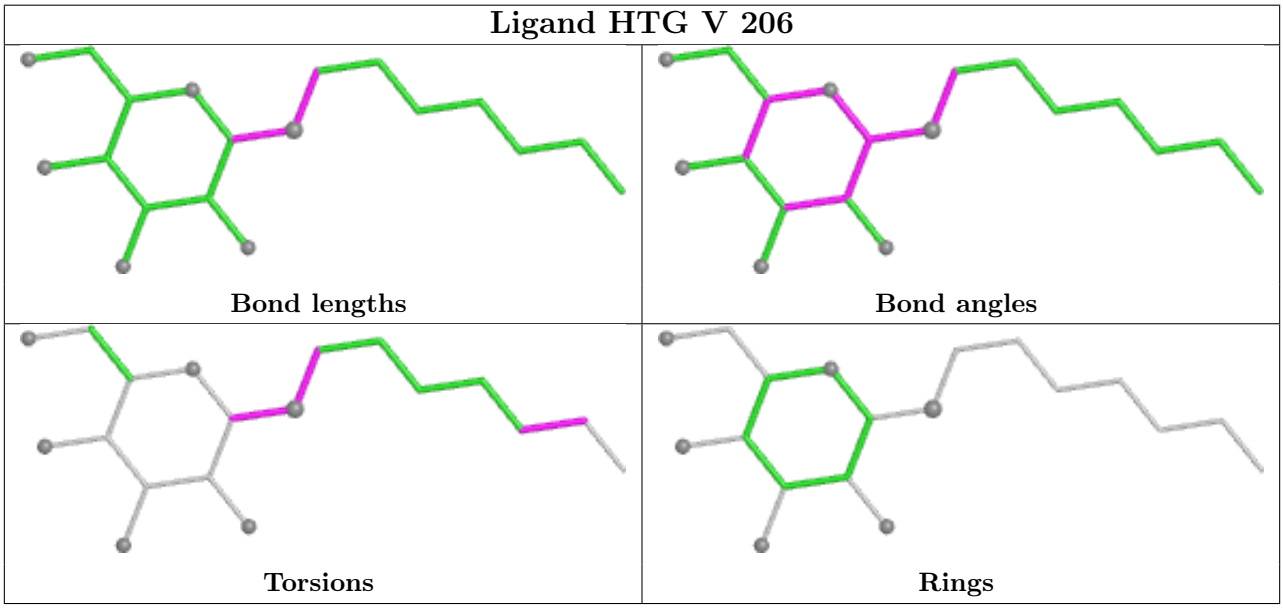
Ligand HTG B 623



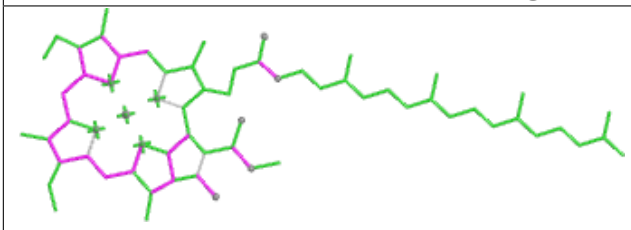
Ligand CLA D 406



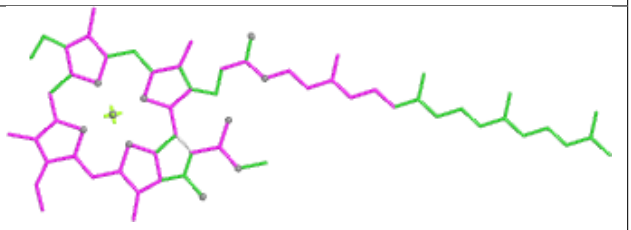
Ligand HTG V 206



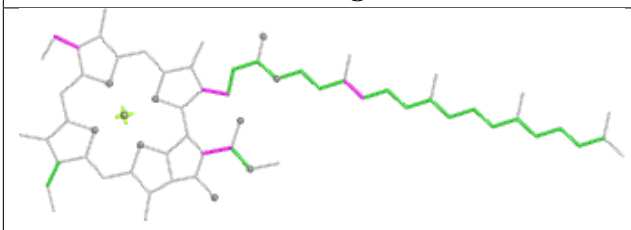
Ligand CLA B 610



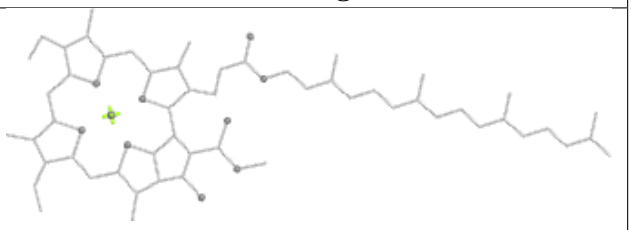
Bond lengths



Bond angles

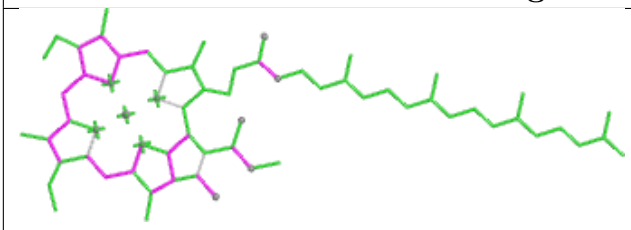


Torsions

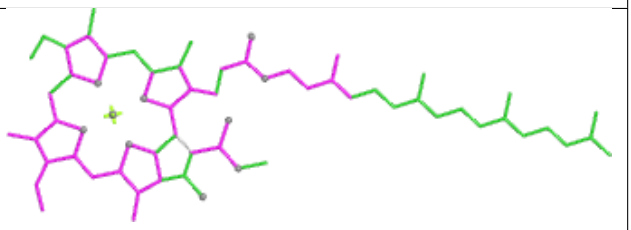


Rings

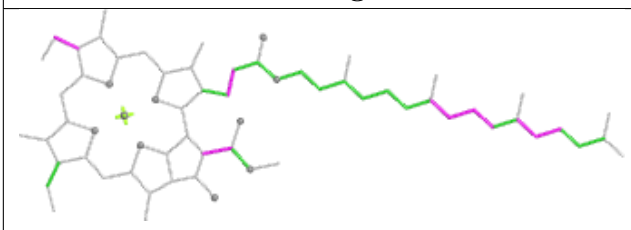
Ligand CLA b 615



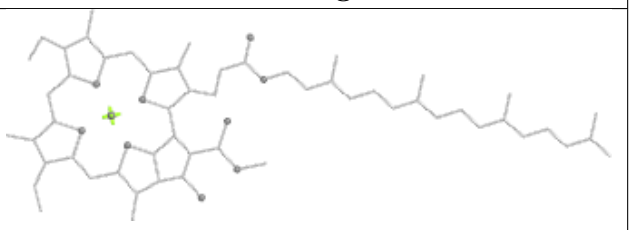
Bond lengths



Bond angles

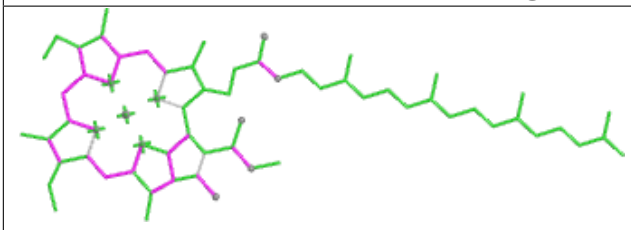


Torsions

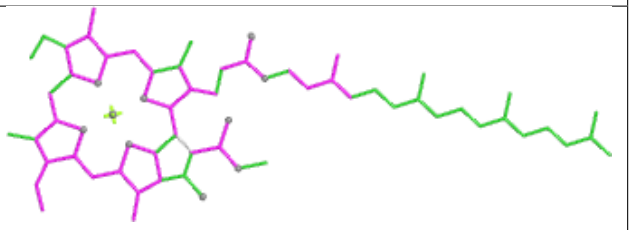


Rings

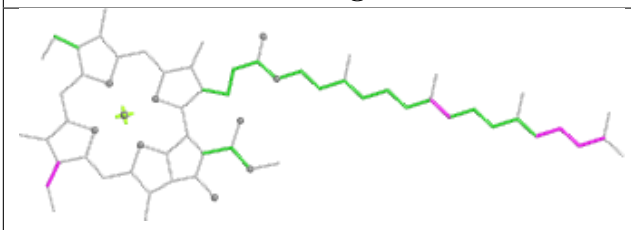
Ligand CLA A 406



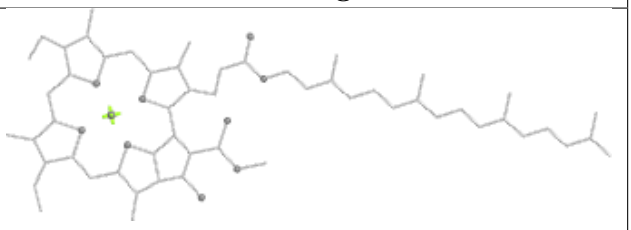
Bond lengths



Bond angles

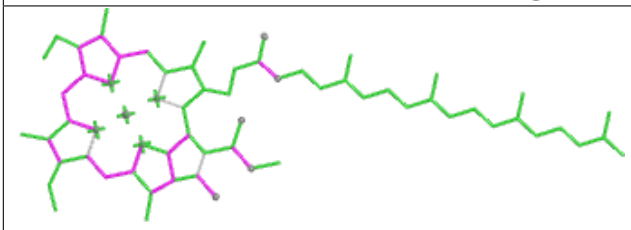


Torsions

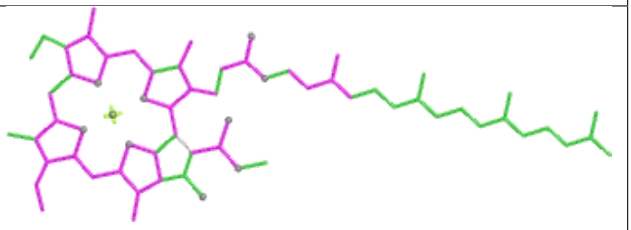


Rings

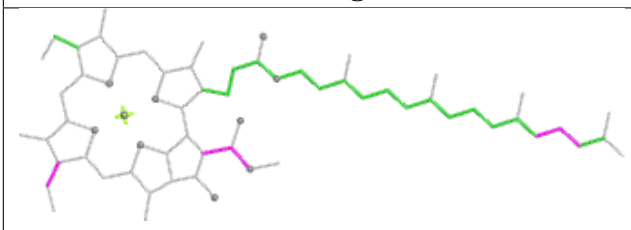
Ligand CLA d 403



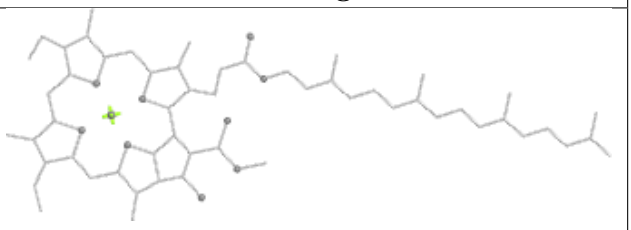
Bond lengths



Bond angles



Torsions

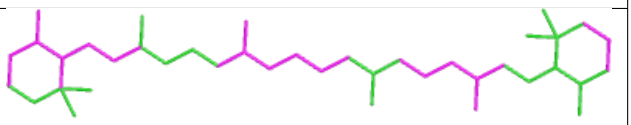


Rings

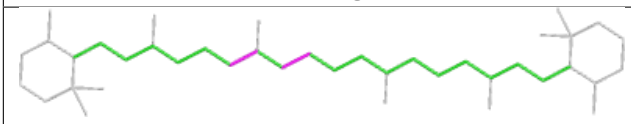
Ligand BCR t 101



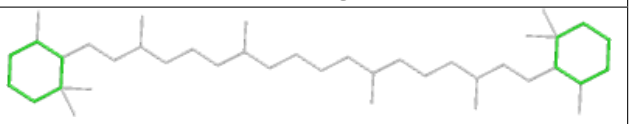
Bond lengths



Bond angles

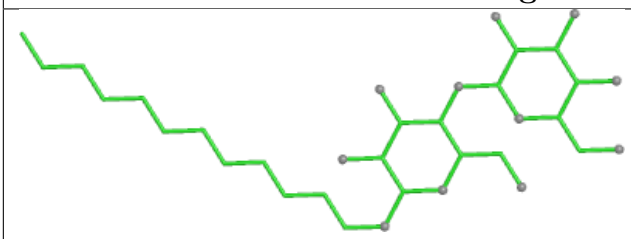


Torsions

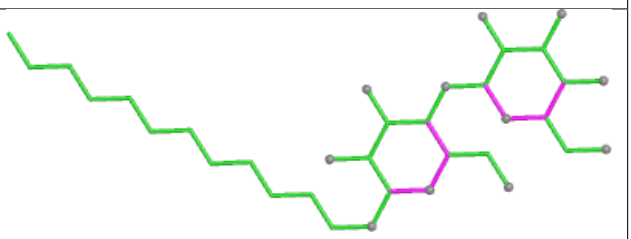


Rings

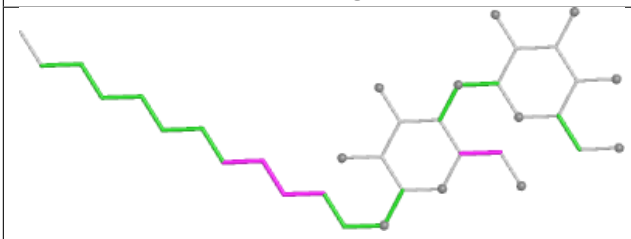
Ligand LMT m 102



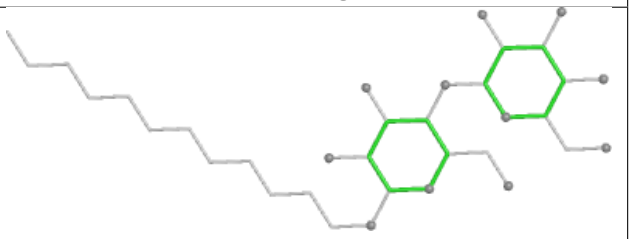
Bond lengths



Bond angles

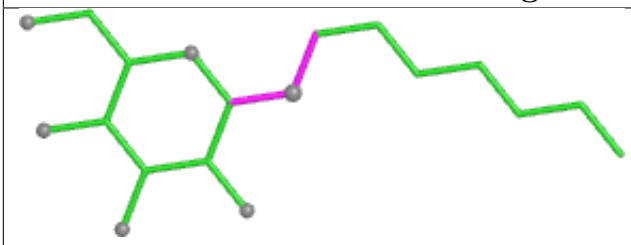


Torsions

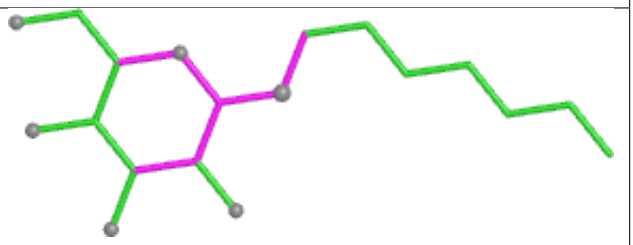


Rings

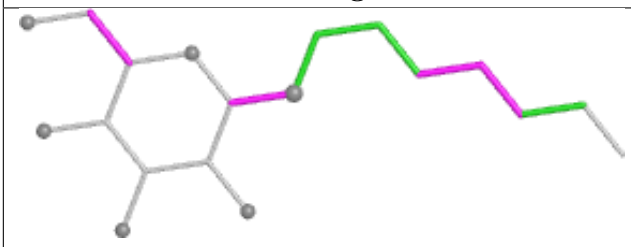
Ligand HTG B 624



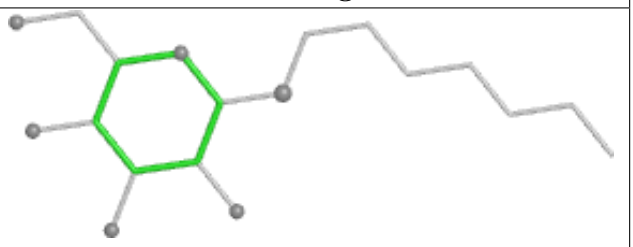
Bond lengths



Bond angles

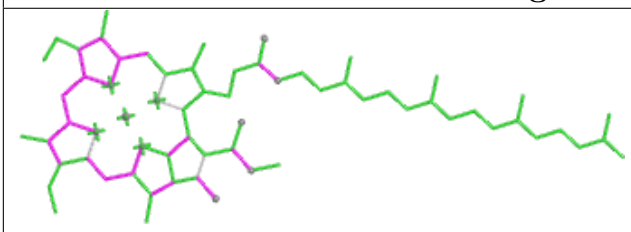


Torsions

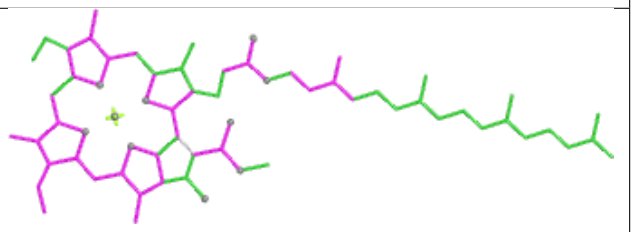


Rings

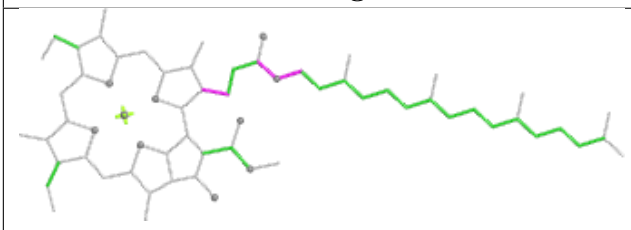
Ligand CLA c 515



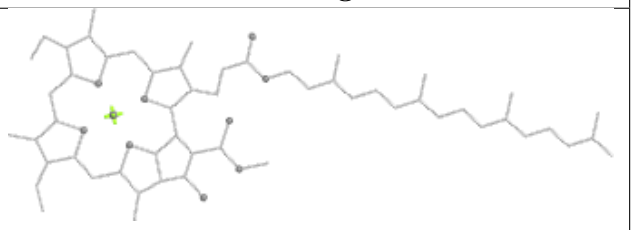
Bond lengths



Bond angles

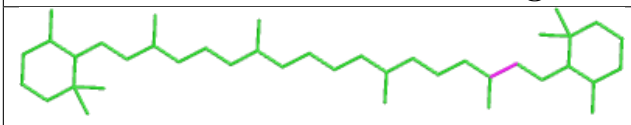


Torsions

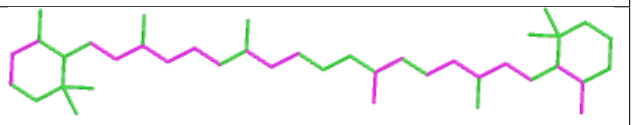


Rings

Ligand BCR k 102



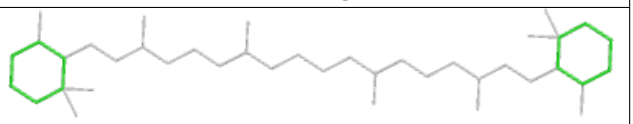
Bond lengths



Bond angles

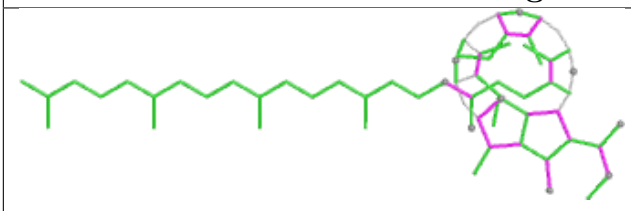


Torsions

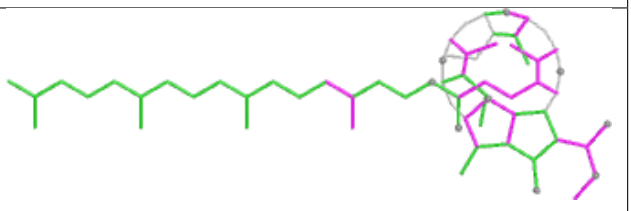


Rings

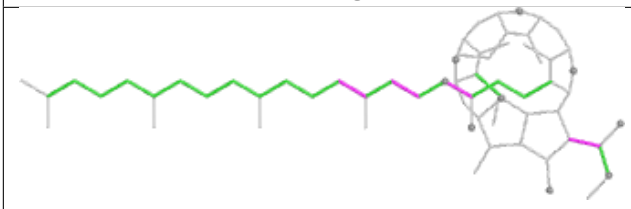
Ligand PHO a 410



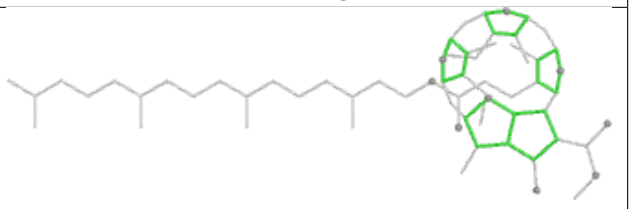
Bond lengths



Bond angles

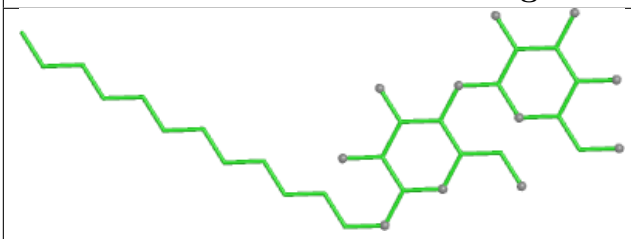


Torsions

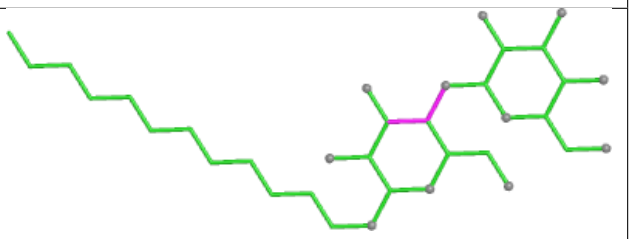


Rings

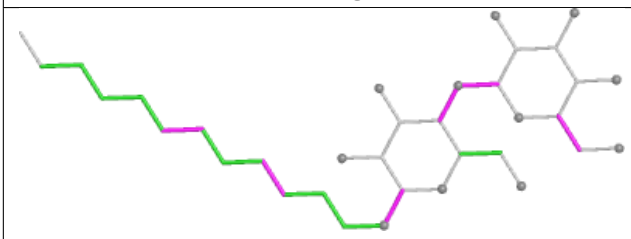
Ligand LMT D 404



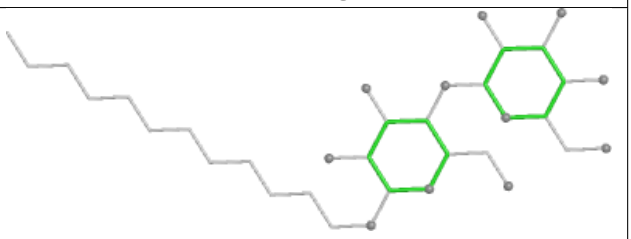
Bond lengths



Bond angles

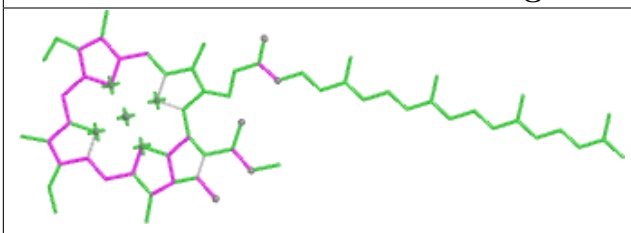


Torsions

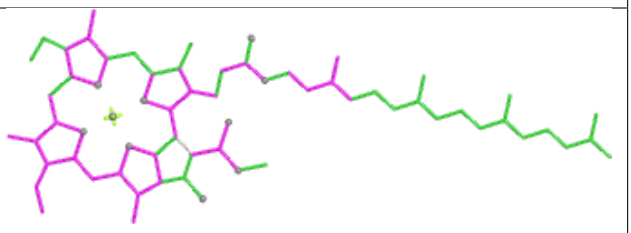


Rings

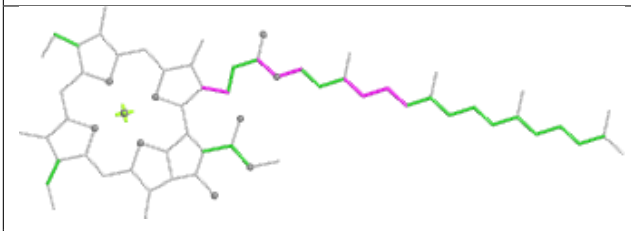
Ligand CLA C 514



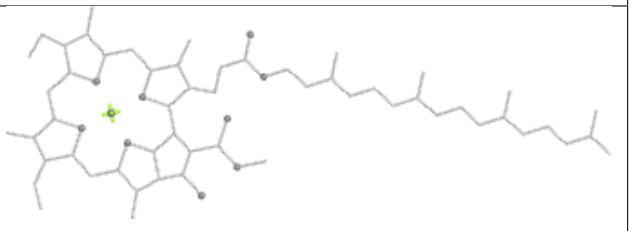
Bond lengths



Bond angles

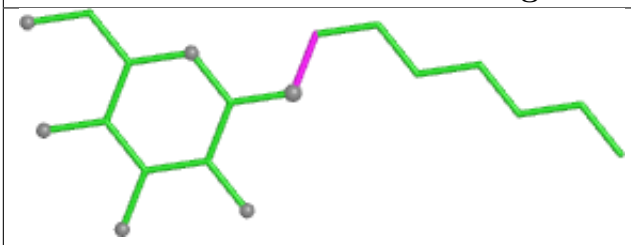


Torsions

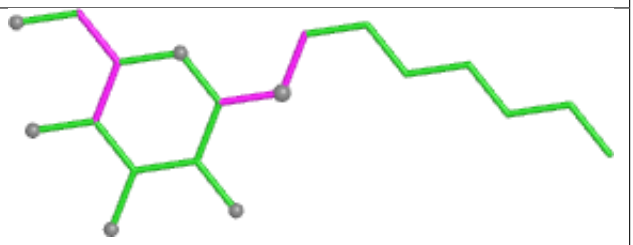


Rings

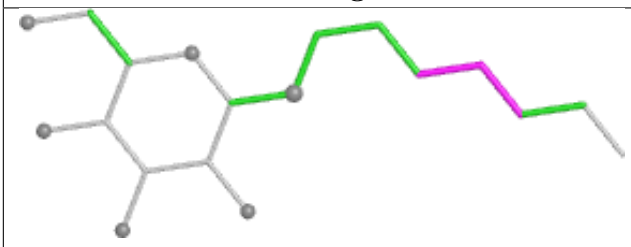
Ligand HTG B 631



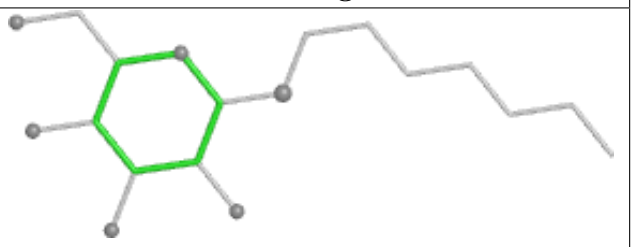
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.58	0 100 100	21, 46, 74, 127	54 (16%)
1	a	334/344 (97%)	-0.61	1 (0%) 90 88	21, 48, 80, 155	54 (16%)
2	B	504/505 (99%)	-0.54	2 (0%) 88 86	29, 53, 90, 153	10 (1%)
2	b	503/505 (99%)	-0.49	4 (0%) 82 80	31, 53, 97, 199	12 (2%)
3	C	451/455 (99%)	-0.48	0 100 100	24, 62, 89, 152	12 (2%)
3	c	455/455 (100%)	-0.49	0 100 100	24, 66, 87, 137	20 (4%)
4	D	341/342 (99%)	-0.66	0 100 100	23, 49, 76, 132	16 (4%)
4	d	341/342 (99%)	-0.65	0 100 100	24, 50, 71, 113	16 (4%)
5	E	81/84 (96%)	-0.01	0 100 100	39, 83, 115, 160	2 (2%)
5	e	81/84 (96%)	-0.17	2 (2%) 58 54	43, 80, 131, 187	2 (2%)
6	F	34/44 (77%)	-0.14	0 100 100	59, 72, 119, 124	0
6	f	32/44 (72%)	-0.32	1 (3%) 51 47	59, 69, 132, 147	0
7	H	65/65 (100%)	-0.33	2 (3%) 51 47	41, 64, 89, 158	1 (1%)
7	h	65/65 (100%)	-0.47	1 (1%) 72 68	53, 65, 84, 165	0
8	I	37/38 (97%)	-0.11	0 100 100	51, 65, 133, 192	0
8	i	37/38 (97%)	-0.24	1 (2%) 56 52	52, 63, 125, 165	0
9	J	38/39 (97%)	-0.00	1 (2%) 57 53	59, 78, 159, 185	0
9	j	39/39 (100%)	-0.13	1 (2%) 57 53	58, 71, 156, 185	0
10	K	37/37 (100%)	-0.27	0 100 100	64, 78, 100, 110	0
10	k	37/37 (100%)	-0.38	0 100 100	62, 77, 98, 117	0
11	L	37/37 (100%)	-0.67	0 100 100	25, 43, 99, 128	1 (2%)
11	l	37/37 (100%)	-0.60	0 100 100	26, 45, 105, 131	1 (2%)
12	M	33/36 (91%)	-0.63	0 100 100	28, 43, 74, 122	1 (3%)
12	m	33/36 (91%)	-0.59	0 100 100	35, 45, 82, 117	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.58	0 100 100	33, 58, 106, 157	8 (3%)
13	o	243/244 (99%)	-0.52	0 100 100	32, 62, 116, 177	5 (2%)
14	T	29/32 (90%)	-0.67	0 100 100	34, 45, 77, 142	1 (3%)
14	t	29/32 (90%)	-0.61	1 (3%) 48 44	33, 44, 72, 149	1 (3%)
15	U	97/104 (93%)	-0.68	0 100 100	44, 58, 91, 126	0
15	u	97/104 (93%)	-0.64	0 100 100	47, 61, 83, 126	0
16	V	137/137 (100%)	-0.64	0 100 100	25, 59, 84, 114	2 (1%)
16	v	137/137 (100%)	-0.54	0 100 100	26, 69, 102, 141	1 (0%)
17	Y	29/30 (96%)	0.84	5 (17%) 4 3	79, 96, 194, 213	0
17	y	29/30 (96%)	0.22	1 (3%) 48 44	79, 97, 147, 168	0
18	X	39/40 (97%)	-0.09	0 100 100	63, 75, 126, 149	0
18	x	38/40 (95%)	0.18	1 (2%) 57 53	64, 72, 135, 162	0
19	Z	62/62 (100%)	-0.02	0 100 100	81, 98, 134, 146	0
19	z	62/62 (100%)	0.16	1 (1%) 70 66	80, 98, 144, 190	0
20	R	18/34 (52%)	1.87	11 (61%) 0 0	104, 152, 180, 185	0
All	All	5275/5384 (97%)	-0.48	36 (0%) 84 81	21, 58, 108, 213	220 (4%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	3.8
18	x	37	VAL	3.6
20	R	15	ALA	3.6
7	H	65	LEU	3.4
5	e	4	THR	3.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.94	0.07	32,41,50,93	0
12	FME	m	1	10/11	0.95	0.09	35,51,99,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.95	0.07	38,51,69,90	0
8	FME	I	1	10/11	0.97	0.06	42,55,62,63	0
8	FME	i	1	10/11	0.97	0.06	40,61,72,73	0
12	FME	M	1	10/11	0.98	0.06	37,50,94,100	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
28	LMT	F	101	35/35	0.68	0.19	133,168,178,179	0
32	UNL	J	101	10/-	0.69	0.23	80,97,103,105	0
37	DGD	d	408	62/66	0.70	0.17	83,130,177,185	0
32	UNL	M	103	10/-	0.72	0.13	54,61,84,85	0
32	UNL	m	101	10/-	0.74	0.16	58,66,81,82	0
26	SQD	f	102	43/54	0.74	0.16	102,125,159,165	0
33	LHG	a	419	42/49	0.75	0.12	83,141,183,185	0
37	DGD	D	409	52/66	0.75	0.15	75,108,154,165	0
28	LMT	b	630	25/35	0.75	0.16	84,108,161,164	0
28	LMT	C	521	35/35	0.76	0.14	102,138,166,166	0
32	UNL	j	101	10/-	0.76	0.15	69,87,97,98	0
28	LMT	a	418	35/35	0.77	0.14	97,135,160,164	0
32	UNL	K	102	34/-	0.77	0.14	91,128,136,139	0
32	UNL	i	101	40/-	0.78	0.14	67,89,140,142	0
33	LHG	A	419	42/49	0.79	0.12	77,120,144,148	0
32	UNL	a	403	30/-	0.79	0.13	75,97,125,131	0
32	UNL	A	418	28/-	0.80	0.13	64,91,111,115	0
34	CA	b	609	1/1	0.80	0.09	147,147,147,147	0
36	LMG	C	520	51/55	0.80	0.12	67,119,131,134	0
28	LMT	D	404	35/35	0.80	0.12	78,132,156,159	0
28	LMT	e	102	35/35	0.80	0.13	92,137,158,159	0
28	LMT	A	414	35/35	0.81	0.12	56,91,113,122	0
26	SQD	F	104	43/54	0.81	0.13	90,122,138,144	0
35	HTG	V	206	19/19	0.81	0.12	77,106,125,227	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	HTG	D	415	16/19	0.82	0.12	74,138,159,163	0
27	GOL	O	301	6/6	0.82	0.10	83,92,94,97	0
32	UNL	I	101	40/-	0.82	0.15	51,88,154,155	0
28	LMT	M	104	35/35	0.82	0.13	54,102,153,155	0
28	LMT	a	404	35/35	0.82	0.13	57,98,122,147	0
27	GOL	V	201	6/6	0.83	0.15	83,92,94,96	0
36	LMG	Z	101	37/55	0.83	0.15	80,131,148,151	0
32	UNL	d	413	36/-	0.84	0.12	60,91,132,138	0
35	HTG	b	608	19/19	0.84	0.10	58,111,145,147	0
35	HTG	d	414	16/19	0.84	0.12	83,103,113,126	0
35	HTG	B	624	19/19	0.84	0.11	74,126,137,186	0
35	HTG	B	632	19/19	0.84	0.11	57,113,139,189	0
35	HTG	C	523	19/19	0.84	0.11	87,108,129,139	0
32	UNL	D	414	40/-	0.84	0.12	59,87,128,135	0
35	HTG	c	524	19/19	0.85	0.11	82,117,127,131	0
28	LMT	B	634	25/35	0.85	0.13	56,85,147,154	0
27	GOL	a	402	6/6	0.85	0.14	96,103,108,109	0
32	UNL	B	633	33/-	0.85	0.13	60,86,131,134	0
36	LMG	z	101	39/55	0.85	0.14	80,131,153,162	0
34	CA	f	103	1/1	0.85	0.06	135,135,135,135	0
32	UNL	c	525	32/-	0.85	0.12	80,99,140,150	0
28	LMT	T	104	25/35	0.86	0.14	47,81,132,142	0
28	LMT	m	102	35/35	0.86	0.11	50,108,132,133	0
32	UNL	b	633	33/-	0.86	0.14	56,92,143,145	0
31	PL9	A	417[A]	55/55	0.86	0.15	85,107,123,125	55
31	PL9	A	417[B]	55/55	0.86	0.15	85,107,122,125	55
26	SQD	b	601	54/54	0.86	0.10	49,79,130,144	0
35	HTG	c	523	19/19	0.86	0.10	92,106,118,124	0
35	HTG	C	522	19/19	0.87	0.10	86,100,123,126	0
26	SQD	A	413	54/54	0.87	0.11	56,80,130,138	0
36	LMG	C	519	51/55	0.87	0.11	61,104,123,126	0
26	SQD	B	621	54/54	0.87	0.11	48,81,143,150	0
35	HTG	B	623	19/19	0.87	0.12	62,78,91,92	0
36	LMG	c	522	51/55	0.87	0.11	64,114,125,127	0
31	PL9	a	415[A]	55/55	0.87	0.15	91,111,122,122	55
35	HTG	b	632	19/19	0.87	0.11	84,140,154,155	0
31	PL9	a	415[B]	55/55	0.87	0.15	92,111,122,123	55
23	CLA	C	514	65/65	0.88	0.10	64,87,119,126	0
26	SQD	B	636	54/54	0.88	0.09	45,81,130,132	0
27	GOL	t	102	6/6	0.88	0.16	71,91,105,109	0
27	GOL	v	203	6/6	0.88	0.13	93,105,109,120	0
35	HTG	b	631	19/19	0.88	0.13	71,83,97,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	A	412	6/6	0.88	0.12	76,82,86,90	0
27	GOL	C	524	6/6	0.88	0.15	81,88,106,110	0
21	CL	U	201	1/1	0.88	0.16	116,116,116,116	0
32	UNL	X	101	18/-	0.89	0.11	61,78,113,117	0
36	LMG	C	501	51/55	0.89	0.10	58,91,106,111	0
22	BCT	d	401[A]	4/4	0.89	0.10	74,74,76,78	4
27	GOL	v	202	6/6	0.89	0.12	86,100,101,109	0
27	GOL	T	101	6/6	0.89	0.17	69,87,92,93	0
36	LMG	a	414	51/55	0.89	0.10	60,86,102,110	0
28	LMT	M	105	35/35	0.89	0.11	58,95,126,127	0
36	LMG	k	101	51/55	0.89	0.10	67,96,122,125	0
22	BCT	d	401[B]	4/4	0.89	0.10	73,74,76,78	4
23	CLA	C	507	65/65	0.89	0.10	54,78,117,123	0
27	GOL	b	606	6/6	0.89	0.12	79,90,98,98	0
27	GOL	B	627	6/6	0.90	0.10	71,79,86,91	0
27	GOL	c	502	6/6	0.90	0.14	76,97,108,111	0
27	GOL	o	301	6/6	0.90	0.11	84,90,99,104	0
27	GOL	T	102	6/6	0.90	0.11	100,114,116,120	0
27	GOL	b	605	6/6	0.90	0.16	67,86,109,116	0
21	CL	v	205	1/1	0.91	0.08	124,124,124,124	0
23	CLA	B	602	65/65	0.91	0.10	52,74,118,137	0
23	CLA	b	610	65/65	0.91	0.10	52,80,123,129	0
32	UNL	d	412	17/-	0.91	0.10	59,72,96,98	0
28	LMT	M	102	35/35	0.91	0.10	44,94,118,130	0
26	SQD	A	410	54/54	0.91	0.10	54,94,105,109	0
27	GOL	B	635	6/6	0.91	0.09	57,59,66,69	0
33	LHG	D	412	49/49	0.92	0.10	53,70,117,124	0
27	GOL	B	629	6/6	0.92	0.13	51,65,75,83	0
34	CA	B	601	1/1	0.92	0.06	123,123,123,123	0
34	CA	F	105	1/1	0.92	0.07	112,112,112,112	0
32	UNL	d	415	18/-	0.92	0.10	67,74,111,117	0
23	CLA	c	517	65/65	0.92	0.09	85,97,108,112	0
25	BCR	K	101	40/40	0.92	0.09	62,87,98,98	0
25	BCR	y	101	40/40	0.92	0.09	56,72,84,92	0
37	DGD	C	517	62/66	0.92	0.08	52,73,103,110	0
35	HTG	B	631	19/19	0.92	0.09	52,94,118,125	0
23	CLA	C	505	65/65	0.92	0.09	47,65,96,110	0
25	BCR	K	103	40/40	0.93	0.09	59,74,89,92	0
25	BCR	Y	101	40/40	0.93	0.09	65,78,92,103	0
27	GOL	V	202	6/6	0.93	0.10	54,67,81,83	0
27	GOL	V	204	6/6	0.93	0.11	96,100,106,117	0
27	GOL	A	411	6/6	0.93	0.09	54,57,60,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	BCT	A	403[A]	4/4	0.93	0.11	76,81,81,92	4
23	CLA	b	615	65/65	0.93	0.08	41,54,92,97	0
36	LMG	D	416	51/55	0.93	0.09	52,75,120,131	0
36	LMG	M	101	51/55	0.93	0.08	40,60,77,89	0
23	CLA	c	510	65/65	0.93	0.08	56,74,97,104	0
27	GOL	f	101	6/6	0.93	0.09	95,101,102,103	0
23	CLA	C	513	65/65	0.93	0.08	61,83,93,101	0
36	LMG	d	416	51/55	0.93	0.09	55,68,107,118	0
25	BCR	D	407	40/40	0.93	0.08	51,65,105,115	0
35	HTG	b	602	19/19	0.93	0.09	49,64,75,79	0
35	HTG	b	607	19/19	0.93	0.08	49,81,95,101	0
22	BCT	A	403[B]	4/4	0.93	0.11	72,82,83,95	4
26	SQD	a	413	54/54	0.93	0.08	53,88,106,109	0
23	CLA	c	512	65/65	0.94	0.07	46,58,125,136	0
23	CLA	c	516	65/65	0.94	0.07	62,77,93,97	0
23	CLA	B	615	65/65	0.94	0.09	32,45,99,106	0
23	CLA	a	411	65/65	0.94	0.10	39,57,122,128	0
25	BCR	H	101	40/40	0.94	0.08	43,64,79,81	0
23	CLA	C	509	65/65	0.94	0.08	49,66,130,139	0
23	CLA	C	511	65/65	0.94	0.07	54,71,81,84	0
23	CLA	b	625	65/65	0.94	0.08	44,61,111,117	0
25	BCR	b	627	40/40	0.94	0.06	34,47,64,72	0
27	GOL	B	626	6/6	0.94	0.09	53,67,81,92	0
25	BCR	c	526	40/40	0.94	0.09	68,87,98,99	0
36	LMG	b	629	51/55	0.94	0.07	43,57,75,87	0
25	BCR	d	406	40/40	0.94	0.08	51,64,84,86	0
25	BCR	h	101	40/40	0.94	0.07	52,67,77,78	0
23	CLA	c	507	65/65	0.94	0.07	52,65,76,93	0
31	PL9	D	408[A]	55/55	0.94	0.07	31,43,50,58	55
37	DGD	C	516	62/66	0.94	0.08	42,55,89,91	0
31	PL9	D	408[B]	55/55	0.94	0.07	32,43,51,56	55
37	DGD	C	518	62/66	0.94	0.08	49,66,88,97	0
27	GOL	F	103	6/6	0.94	0.09	104,108,111,111	0
37	DGD	c	520	62/66	0.94	0.08	52,65,117,131	0
23	CLA	A	408	65/65	0.94	0.08	38,56,120,128	0
23	CLA	c	515	65/65	0.95	0.08	55,71,88,95	0
23	CLA	C	508	65/65	0.95	0.08	51,70,83,91	0
31	PL9	d	407[A]	55/55	0.95	0.07	33,44,54,60	55
31	PL9	d	407[B]	55/55	0.95	0.07	34,44,54,60	55
23	CLA	C	504	65/65	0.95	0.07	50,66,79,84	0
23	CLA	d	405	65/65	0.95	0.08	49,59,108,118	0
32	UNL	D	413	17/-	0.95	0.07	50,76,96,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PHO	d	402[A]	64/64	0.95	0.07	37,51,57,59	64
24	PHO	d	402[B]	64/64	0.95	0.07	39,50,56,59	64
25	BCR	A	409	40/40	0.95	0.07	36,47,55,56	0
25	BCR	B	620	40/40	0.95	0.06	41,52,62,66	0
27	GOL	v	204	6/6	0.95	0.10	63,69,78,81	0
25	BCR	C	515	40/40	0.95	0.07	50,64,76,78	0
23	CLA	B	607	65/65	0.95	0.08	35,53,96,98	0
23	CLA	b	618	65/65	0.95	0.07	46,55,65,68	0
27	GOL	B	628	6/6	0.95	0.10	61,71,81,83	0
23	CLA	b	620	65/65	0.95	0.06	33,47,57,64	0
23	CLA	b	623	65/65	0.95	0.07	33,46,93,110	0
23	CLA	C	512	65/65	0.95	0.08	57,76,93,108	0
27	GOL	C	525	6/6	0.95	0.11	56,58,70,72	0
27	GOL	D	403	6/6	0.95	0.12	52,56,67,70	0
23	CLA	C	506	65/65	0.95	0.07	48,58,74,83	0
23	CLA	c	508	65/65	0.95	0.07	51,65,81,89	0
33	LHG	D	410	49/49	0.95	0.07	40,53,65,67	0
23	CLA	B	617	65/65	0.95	0.10	43,58,134,136	0
23	CLA	c	511	65/65	0.95	0.08	52,68,77,82	0
33	LHG	d	411	49/49	0.95	0.09	49,64,116,122	0
25	BCR	k	102	40/40	0.95	0.08	59,75,87,90	0
25	BCR	t	101	40/40	0.95	0.06	33,52,66,68	0
27	GOL	V	203	6/6	0.95	0.10	64,71,80,84	0
23	CLA	D	406	65/65	0.95	0.08	45,61,114,119	0
37	DGD	c	519	62/66	0.95	0.08	41,60,100,103	0
35	HTG	B	622	19/19	0.95	0.09	48,68,85,91	0
37	DGD	c	521	62/66	0.95	0.07	48,62,94,109	0
23	CLA	c	513	65/65	0.95	0.08	54,68,82,91	0
37	DGD	h	102	62/66	0.95	0.07	38,58,80,85	0
27	GOL	B	630	6/6	0.96	0.14	50,85,91,96	0
25	BCR	B	619	40/40	0.96	0.06	36,48,61,67	0
23	CLA	b	617	65/65	0.96	0.06	41,56,64,70	0
23	CLA	B	614	65/65	0.96	0.06	31,43,66,84	0
23	CLA	b	619	65/65	0.96	0.07	42,54,63,70	0
23	CLA	B	603	65/65	0.96	0.06	41,52,63,70	0
23	CLA	b	621	65/65	0.96	0.06	36,47,56,65	0
23	CLA	b	622	65/65	0.96	0.06	34,47,60,67	0
25	BCR	T	103	40/40	0.96	0.05	30,50,64,66	0
23	CLA	C	510	65/65	0.96	0.08	54,73,88,95	0
25	BCR	a	412	40/40	0.96	0.06	37,47,54,57	0
25	BCR	b	626	40/40	0.96	0.05	38,47,56,58	0
23	CLA	b	624	65/65	0.96	0.07	43,53,73,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	a	401	6/6	0.96	0.08	52,63,72,75	0
25	BCR	b	628	40/40	0.96	0.07	40,59,69,70	0
25	BCR	c	518	40/40	0.96	0.07	52,64,77,80	0
23	CLA	B	616	65/65	0.96	0.06	40,54,71,78	0
23	CLA	c	505	65/65	0.96	0.07	52,66,75,79	0
23	CLA	c	506	65/65	0.96	0.07	48,62,79,87	0
23	CLA	A	406	65/65	0.96	0.06	34,45,102,111	0
23	CLA	C	502	65/65	0.96	0.06	50,63,78,92	0
23	CLA	c	509	65/65	0.96	0.06	43,55,72,76	0
23	CLA	C	503	65/65	0.96	0.07	45,65,72,76	0
23	CLA	B	608	65/65	0.96	0.06	28,43,57,64	0
23	CLA	a	409	65/65	0.96	0.07	37,48,109,116	0
23	CLA	B	610	65/65	0.96	0.06	45,54,62,68	0
23	CLA	c	514	65/65	0.96	0.06	51,63,72,82	0
23	CLA	B	611	65/65	0.96	0.07	40,57,67,70	0
23	CLA	b	611	65/65	0.96	0.07	42,54,61,68	0
23	CLA	b	612	65/65	0.96	0.07	41,54,64,70	0
23	CLA	b	613	65/65	0.96	0.06	33,45,71,77	0
24	PHO	D	402[A]	64/64	0.96	0.06	37,49,59,63	64
33	LHG	b	634	49/49	0.96	0.07	38,52,68,85	0
33	LHG	d	409	49/49	0.96	0.07	41,55,68,69	0
37	DGD	H	102	62/66	0.96	0.07	42,58,97,102	0
33	LHG	d	410	49/49	0.96	0.07	37,48,64,91	0
24	PHO	D	402[B]	64/64	0.96	0.06	36,48,58,63	64
23	CLA	b	614	65/65	0.96	0.07	35,46,60,65	0
23	CLA	B	613	65/65	0.96	0.07	34,45,54,58	0
23	CLA	b	616	65/65	0.96	0.06	29,42,51,58	0
39	HEM	F	102	43/43	0.96	0.09	60,81,105,113	0
39	HEM	e	101	43/43	0.96	0.10	72,91,130,138	0
27	GOL	b	604	6/6	0.97	0.07	63,68,80,82	0
23	CLA	B	609	65/65	0.97	0.06	41,51,67,70	0
23	CLA	A	404	65/65	0.97	0.06	33,40,53,66	0
23	CLA	A	405	65/65	0.97	0.05	30,40,48,53	0
23	CLA	B	612	65/65	0.97	0.05	32,44,55,60	0
23	CLA	D	405	65/65	0.97	0.06	31,42,64,67	0
23	CLA	d	403	65/65	0.97	0.05	36,44,51,62	0
27	GOL	v	201	6/6	0.97	0.08	72,80,88,97	0
23	CLA	d	404	65/65	0.97	0.06	35,43,58,69	0
23	CLA	B	604	65/65	0.97	0.06	46,55,63,66	0
24	PHO	A	407	64/64	0.97	0.06	30,41,50,55	0
23	CLA	a	408	65/65	0.97	0.06	35,42,50,62	0
23	CLA	B	605	65/65	0.97	0.06	32,44,76,81	0

Continued on next page...

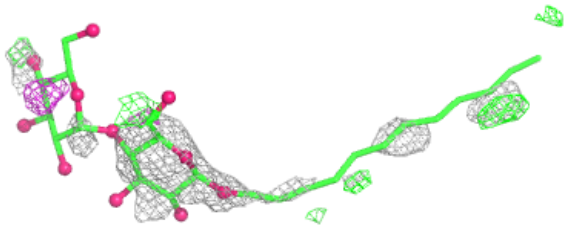
Continued from previous page...

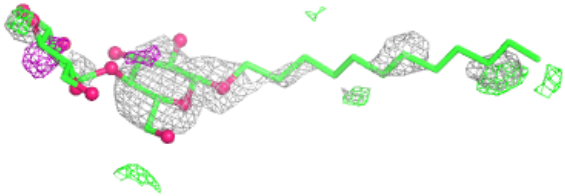
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LHG	D	411	49/49	0.97	0.07	32,49,73,81	0
24	PHO	a	410	64/64	0.97	0.05	36,44,50,53	0
33	LHG	L	101	49/49	0.97	0.06	41,50,59,62	0
23	CLA	B	606	65/65	0.97	0.05	35,44,57,61	0
21	CL	A	402[A]	1/1	0.97	0.08	44,44,44,44	1
27	GOL	B	625	6/6	0.97	0.06	53,63,67,79	0
21	CL	A	402[B]	1/1	0.97	0.08	46,46,46,46	1
25	BCR	B	618	40/40	0.97	0.05	34,45,56,58	0
27	GOL	b	603	6/6	0.97	0.08	58,75,83,86	0
21	CL	A	401[A]	1/1	0.98	0.03	42,42,42,42	1
34	CA	c	503	1/1	0.98	0.06	78,78,78,78	0
21	CL	a	406[A]	1/1	0.98	0.04	46,46,46,46	1
34	CA	o	302	1/1	0.98	0.03	96,96,96,96	0
21	CL	a	406[B]	1/1	0.98	0.04	47,47,47,47	1
21	CL	A	401[B]	1/1	0.98	0.03	39,39,39,39	1
34	CA	C	526	1/1	0.98	0.04	88,88,88,88	0
27	GOL	c	501	6/6	0.98	0.09	56,62,65,68	0
34	CA	O	302	1/1	0.98	0.03	96,96,96,96	0
40	MG	J	102	1/1	0.98	0.05	64,64,64,64	0
40	MG	j	102	1/1	0.98	0.08	71,71,71,71	0
41	HEC	V	205	43/43	0.98	0.06	46,53,60,62	0
41	HEC	v	206	43/43	0.98	0.06	55,68,73,77	0
30	OEY	a	417[B]	11/11	0.99	0.03	40,48,57,78	11
38	FE2	D	401[A]	1/1	0.99	0.05	70,70,70,70	1
38	FE2	D	401[B]	1/1	0.99	0.05	69,69,69,69	1
38	FE2	a	405[B]	1/1	0.99	0.04	62,62,62,62	0
34	CA	c	504	1/1	0.99	0.02	85,85,85,85	0
21	CL	a	407[A]	1/1	0.99	0.04	52,52,52,52	1
21	CL	a	407[B]	1/1	0.99	0.04	47,47,47,47	1
29	OEX	A	415[A]	10/10	0.99	0.03	47,56,62,72	10
29	OEX	a	416[A]	10/10	0.99	0.03	41,48,53,56	10
30	OEY	A	416[B]	11/11	0.99	0.03	43,53,64,72	11

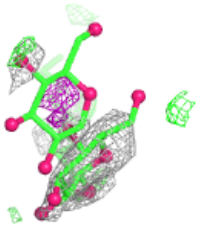
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

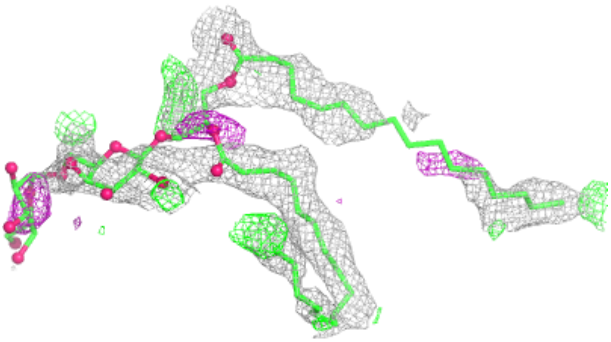


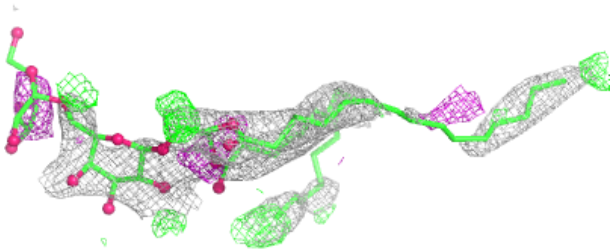


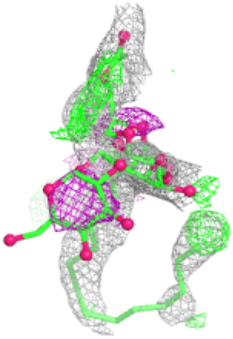


Electron density around DGD d 408:

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

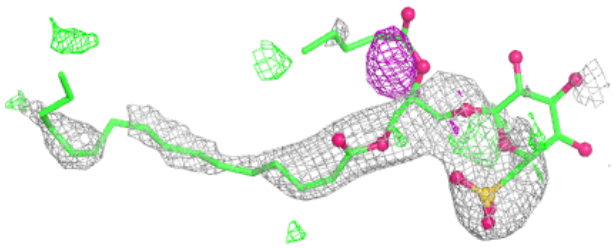


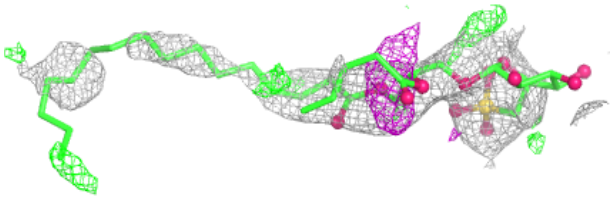


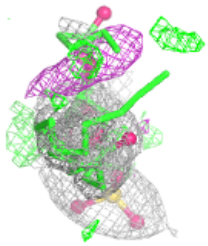


Electron density around SQD f 102:

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

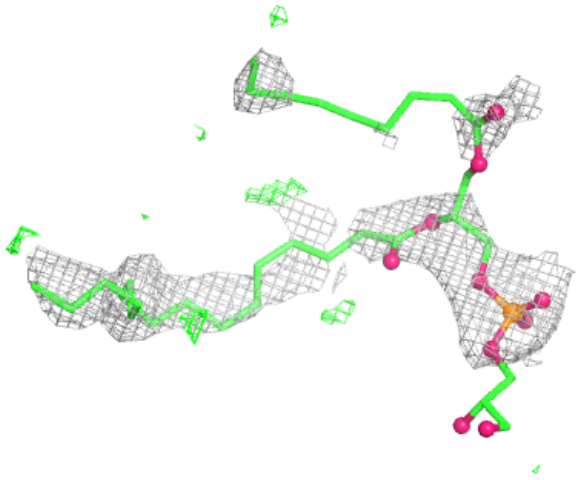


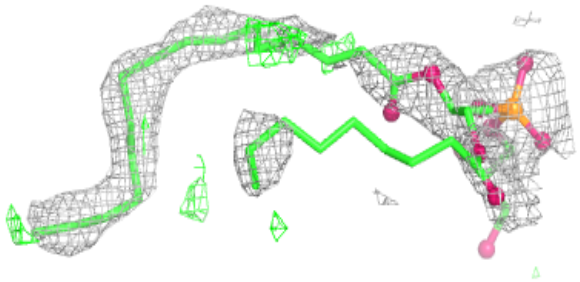


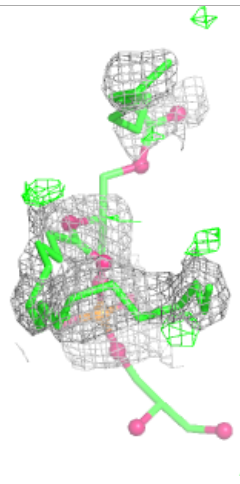


Electron density around LHG a 419:

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

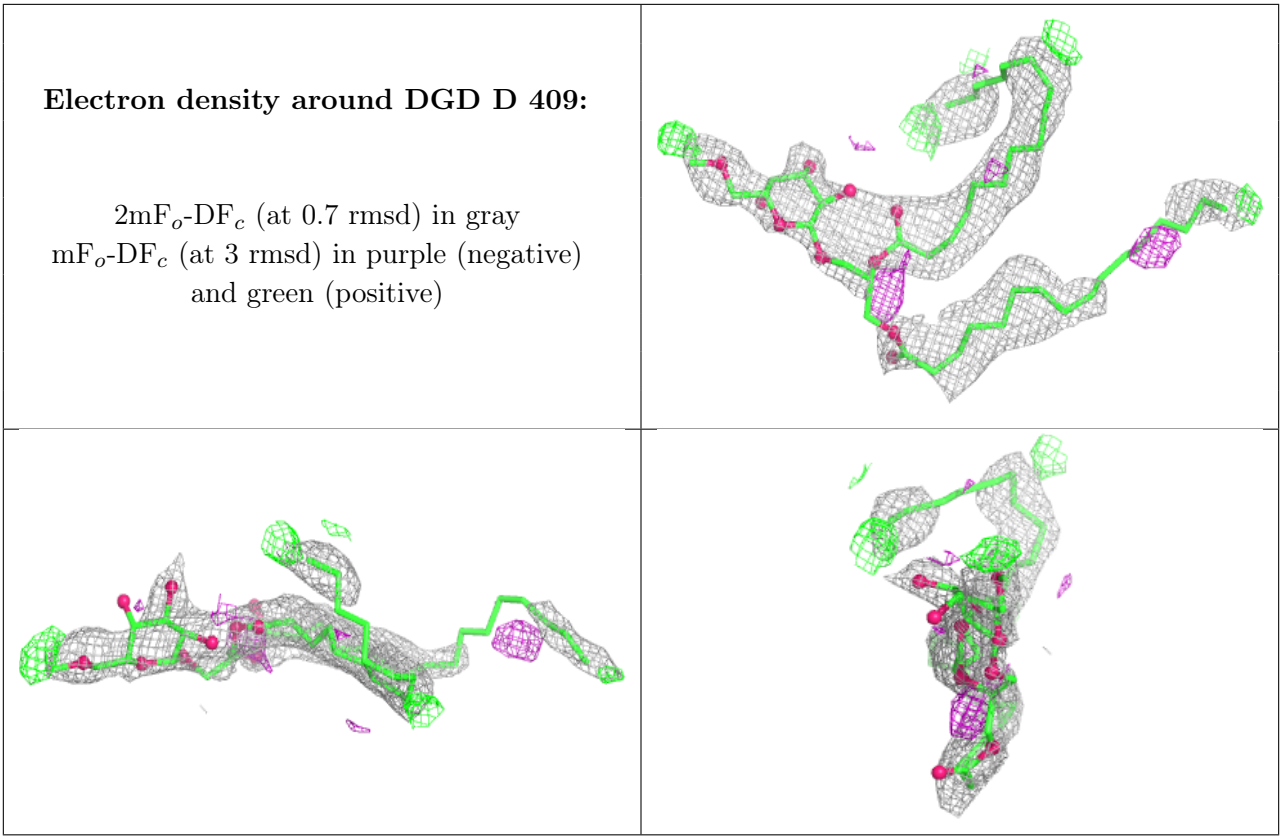






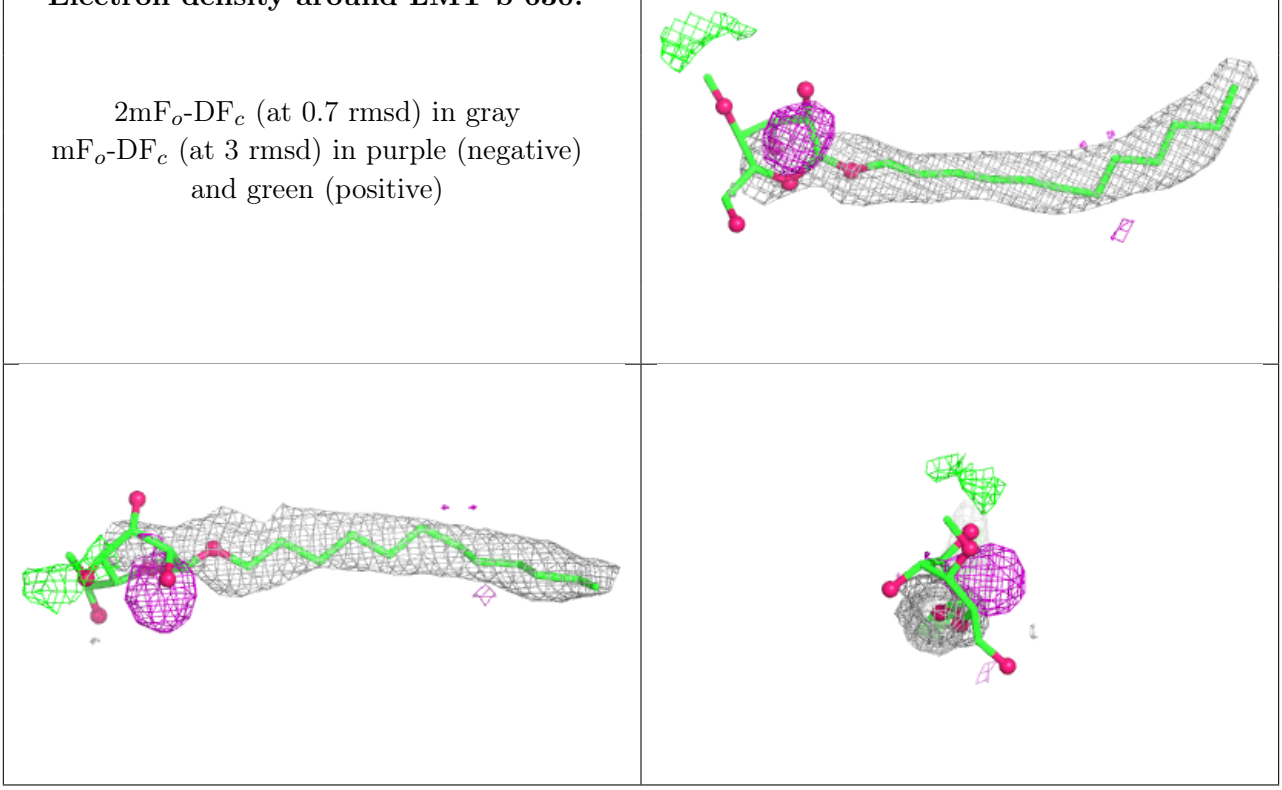
Electron density around DGD D 409:

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



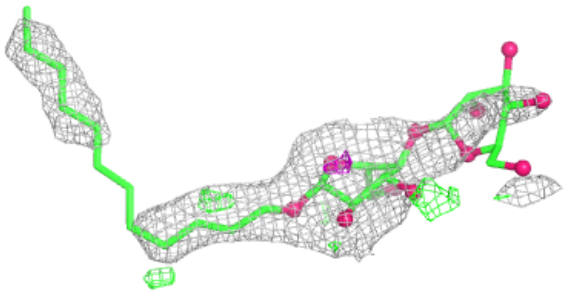
Electron density around LMT b 630:

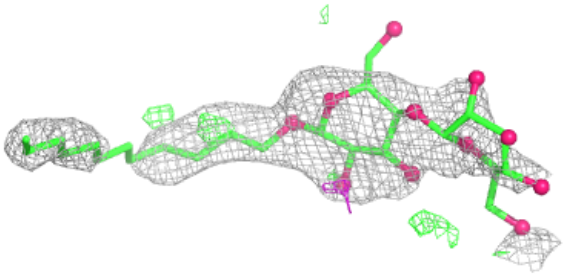
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

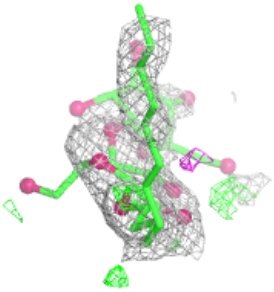


Electron density around LMT C 521:

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

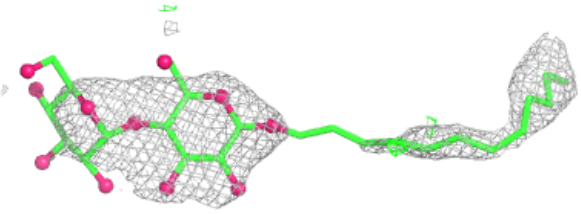


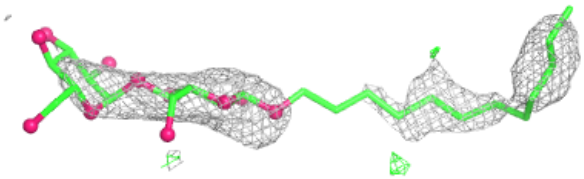


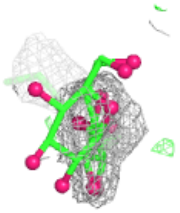


Electron density around LMT a 418:

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

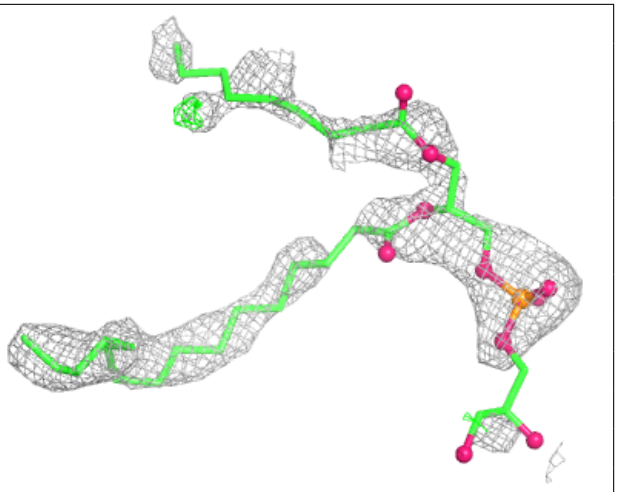


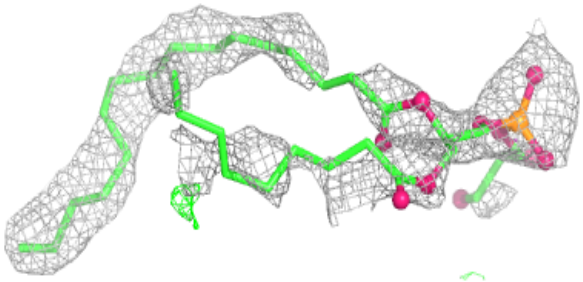


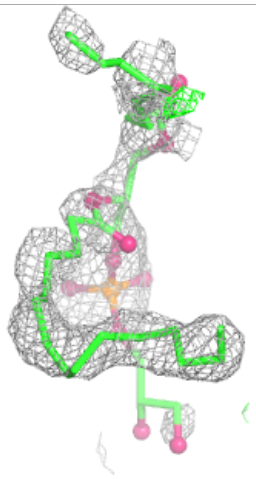


Electron density around LHG A 419:

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

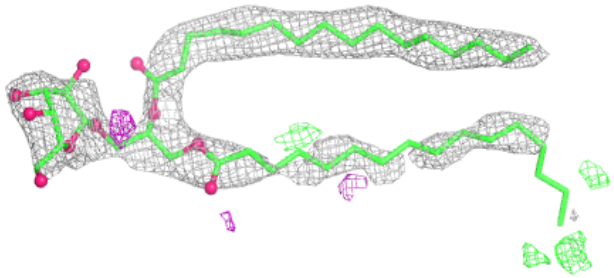


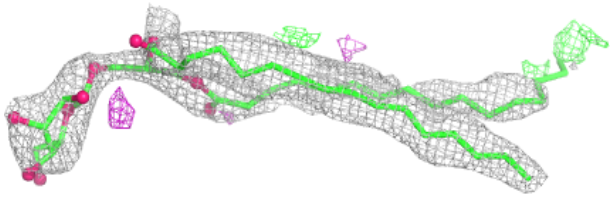


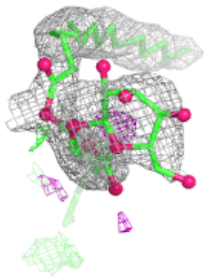


Electron density around LMG C 520:

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

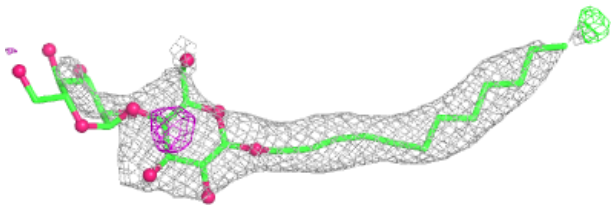


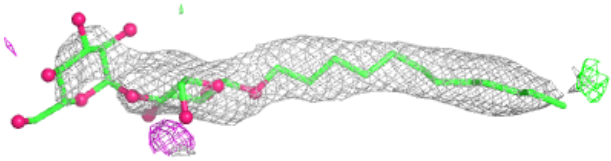


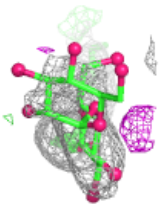


Electron density around LMT D 404:

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

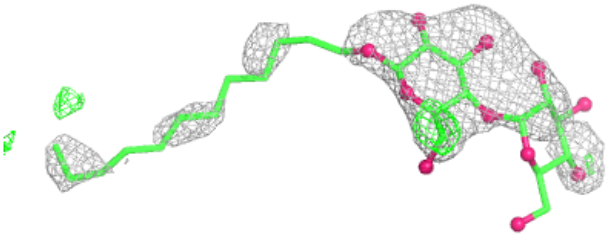


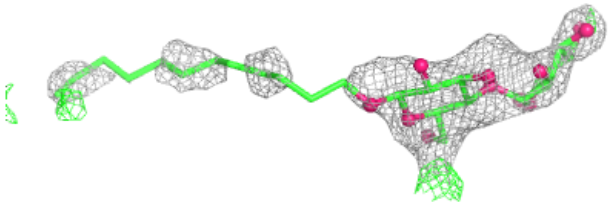


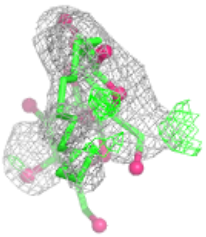


Electron density around LMT e 102:

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

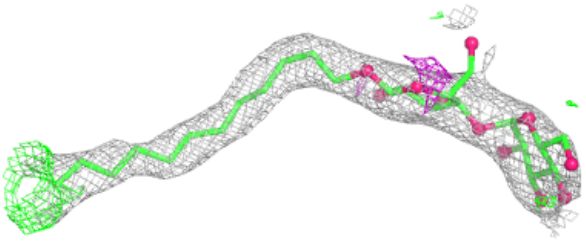


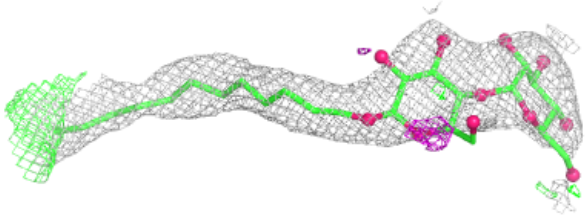


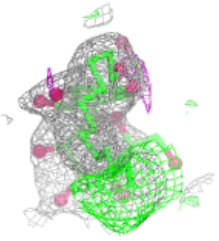


Electron density around LMT A 414:

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

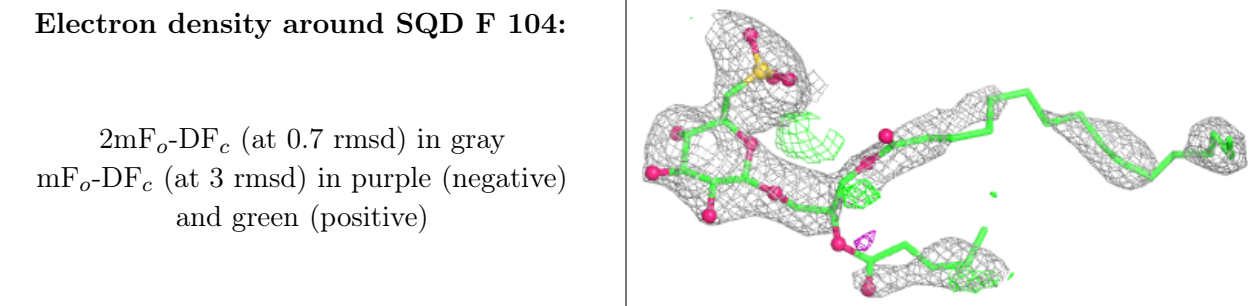


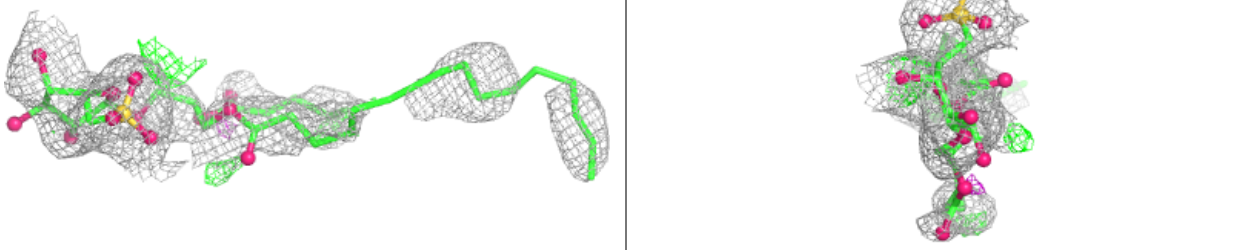




Electron density around SQD F 104:

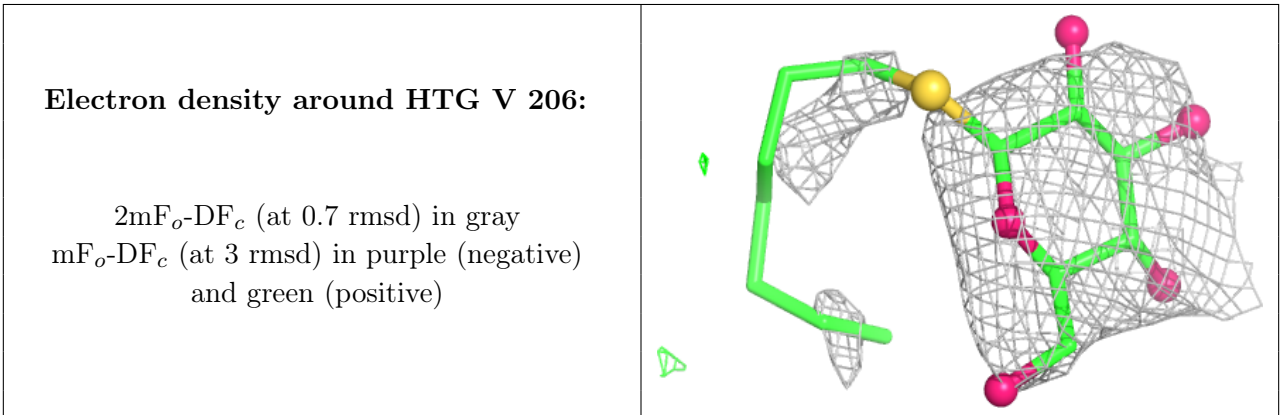
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

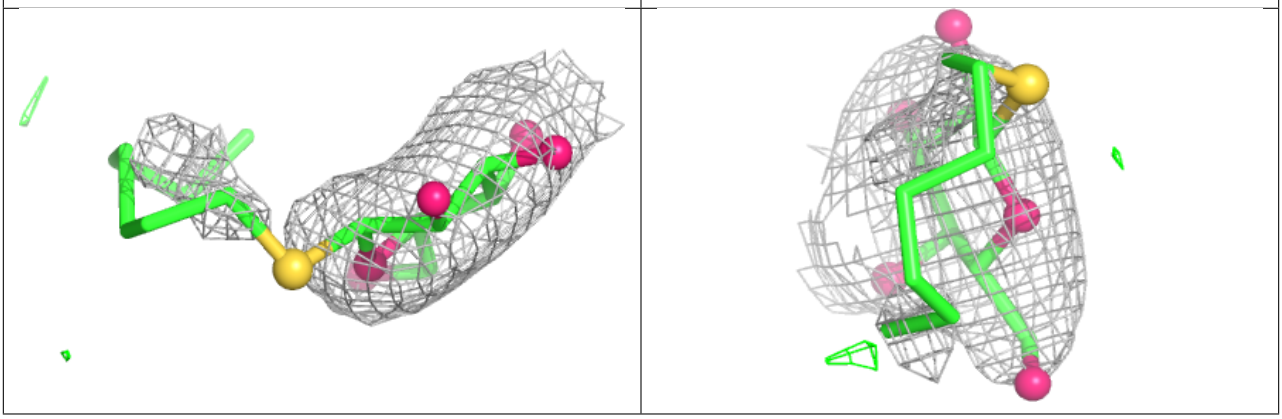




Electron density around HTG V 206:

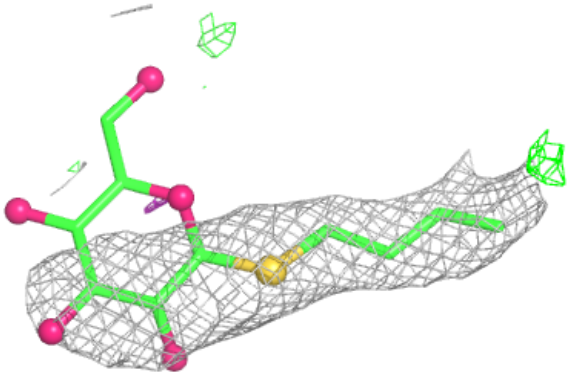
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

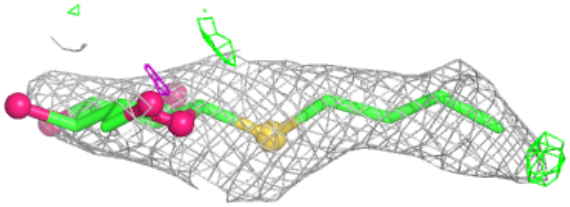


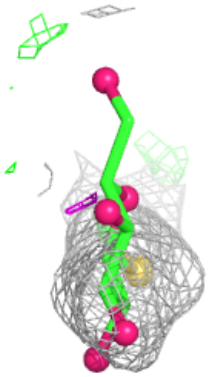


Electron density around HTG D 415:

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

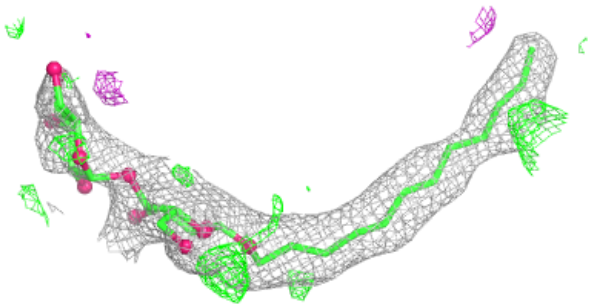


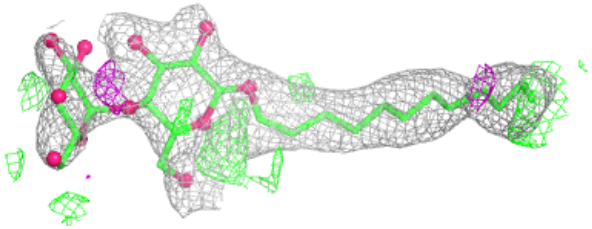


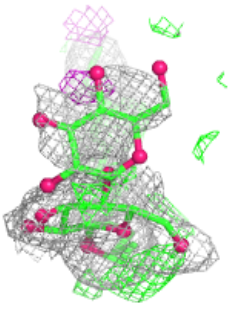


Electron density around LMT M 104:

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

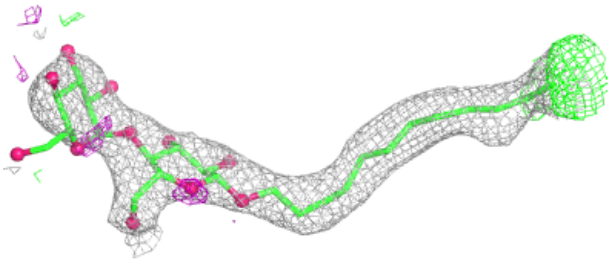


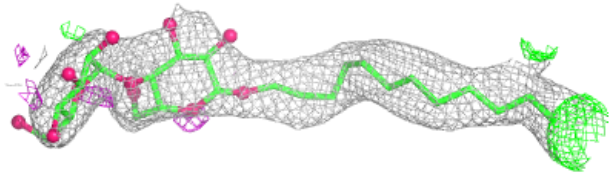


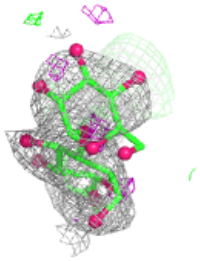


Electron density around LMT a 404:

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

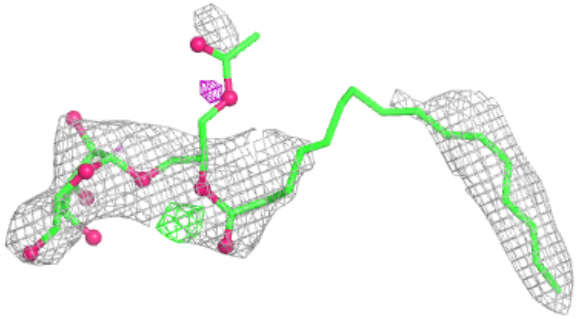


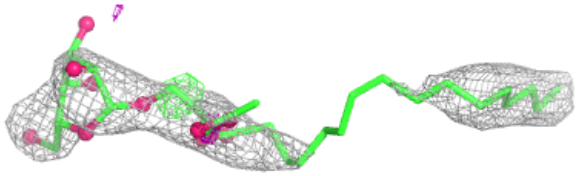


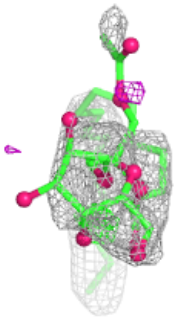


Electron density around LMG Z 101:

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

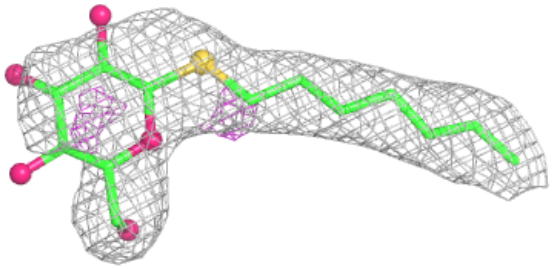


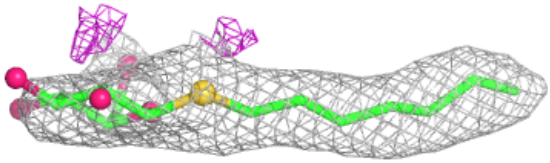


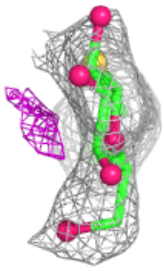


Electron density around HTG b 608:

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

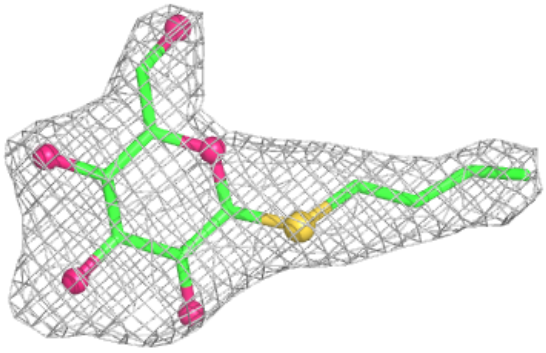


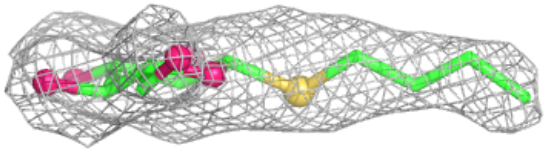


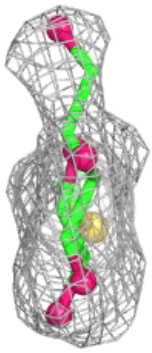


Electron density around HTG d 414:

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

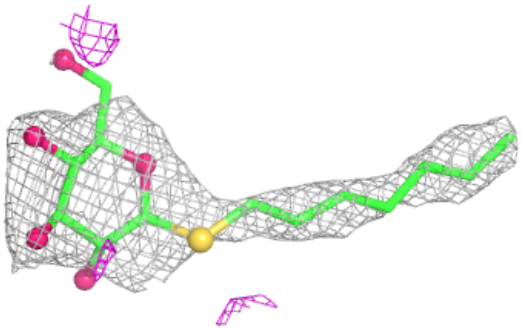


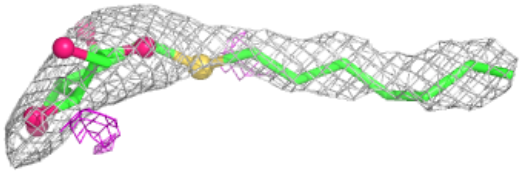


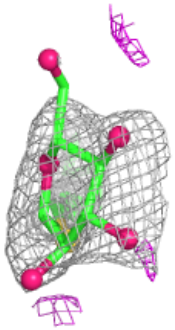


Electron density around HTG B 624:

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

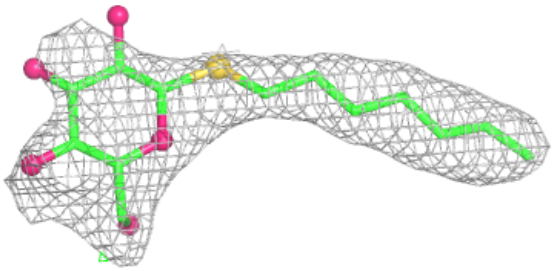


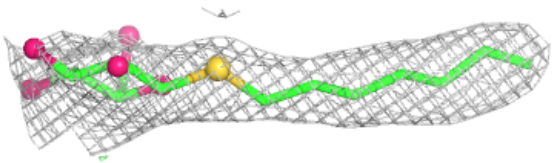


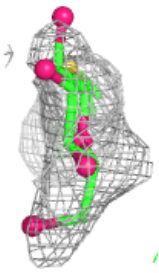


Electron density around HTG B 632:

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

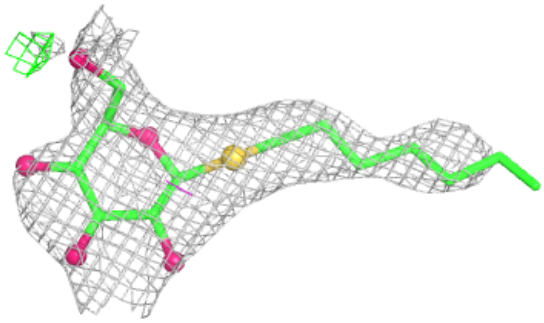


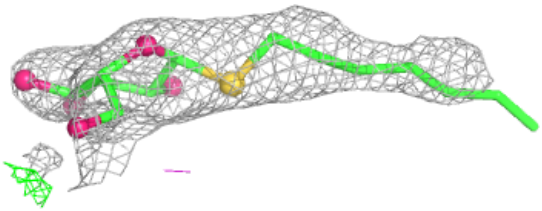


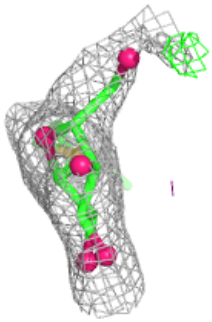


Electron density around HTG C 523:

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

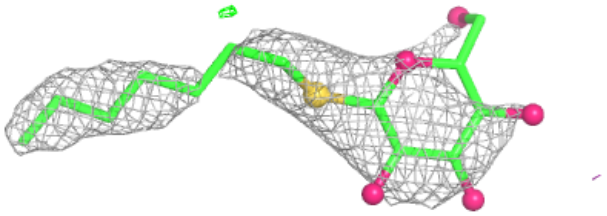


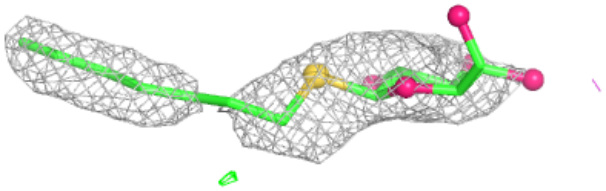


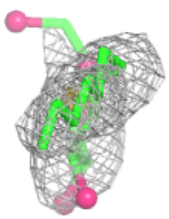


Electron density around HTG c 524:

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

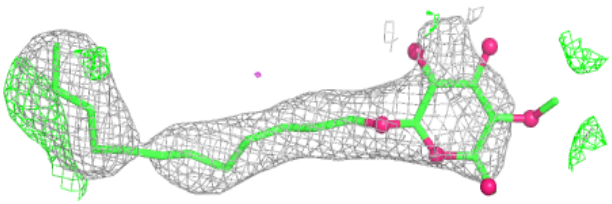


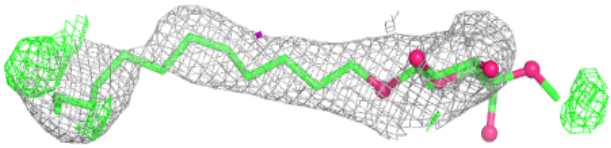


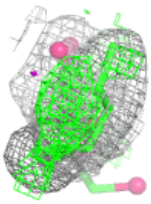


Electron density around LMT B 634:

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

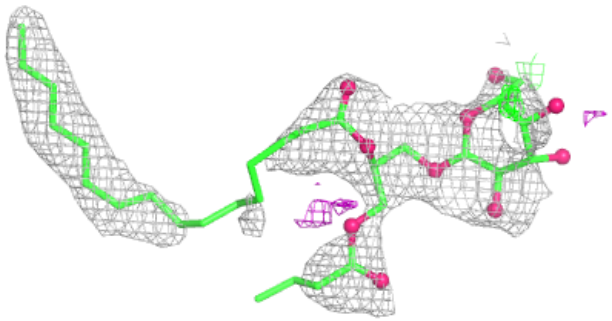


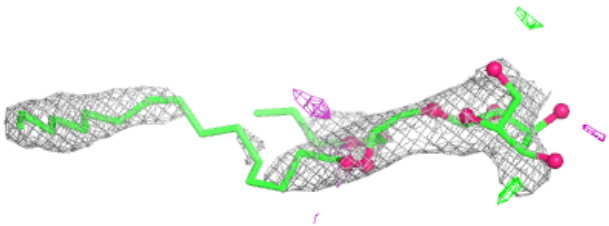


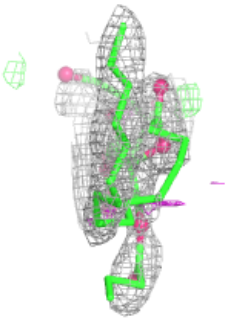


Electron density around LMG z 101:

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

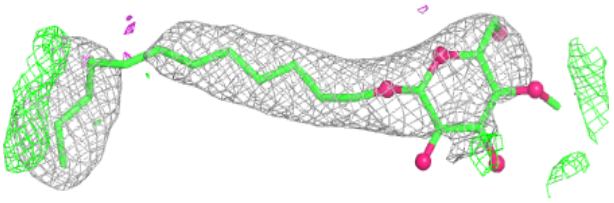


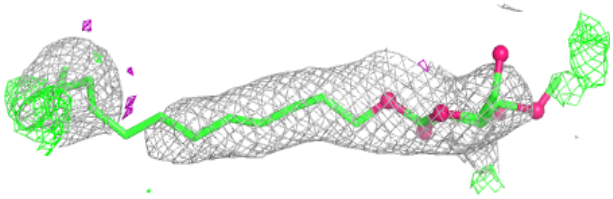


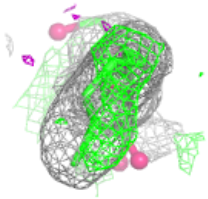


Electron density around LMT T 104:

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

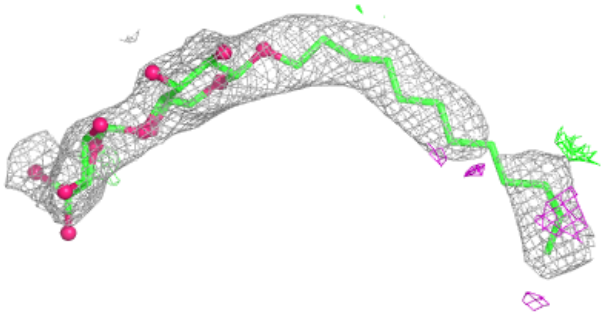


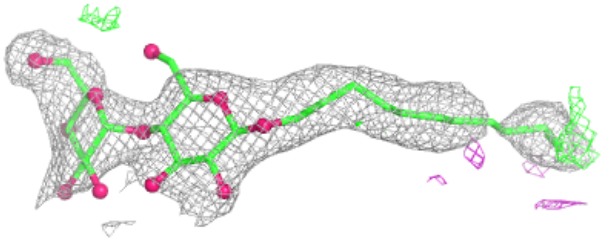


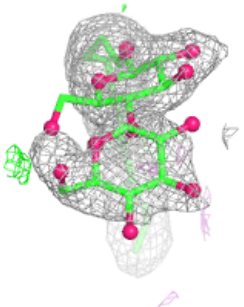


Electron density around LMT m 102:

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

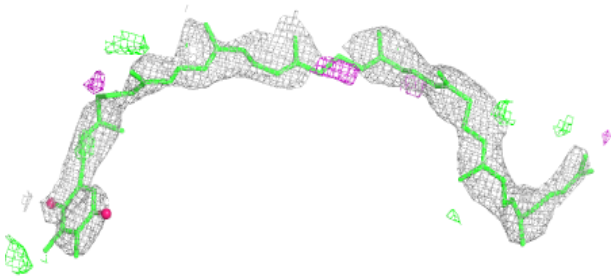


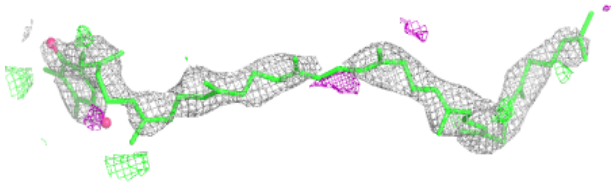


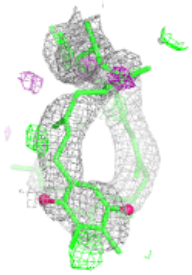


Electron density around PL9 A 417 (A):

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

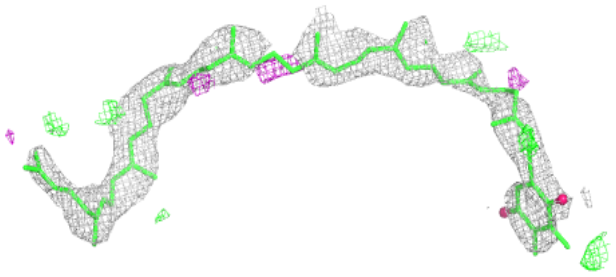


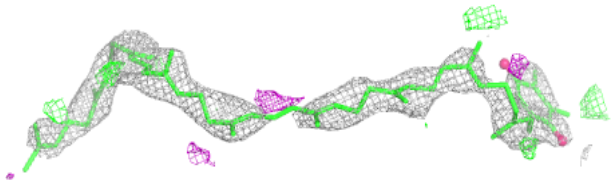


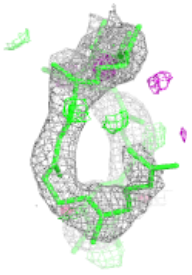


Electron density around PL9 A 417 (B):

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

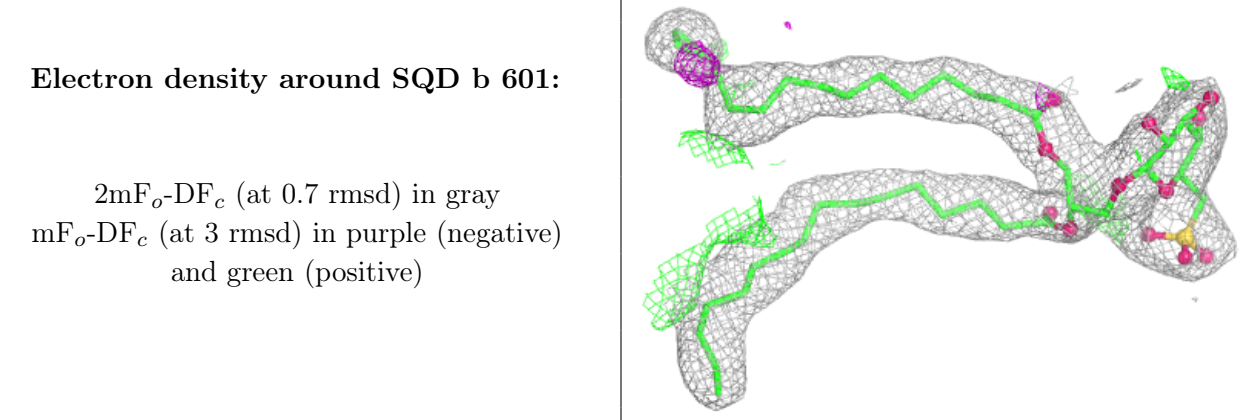


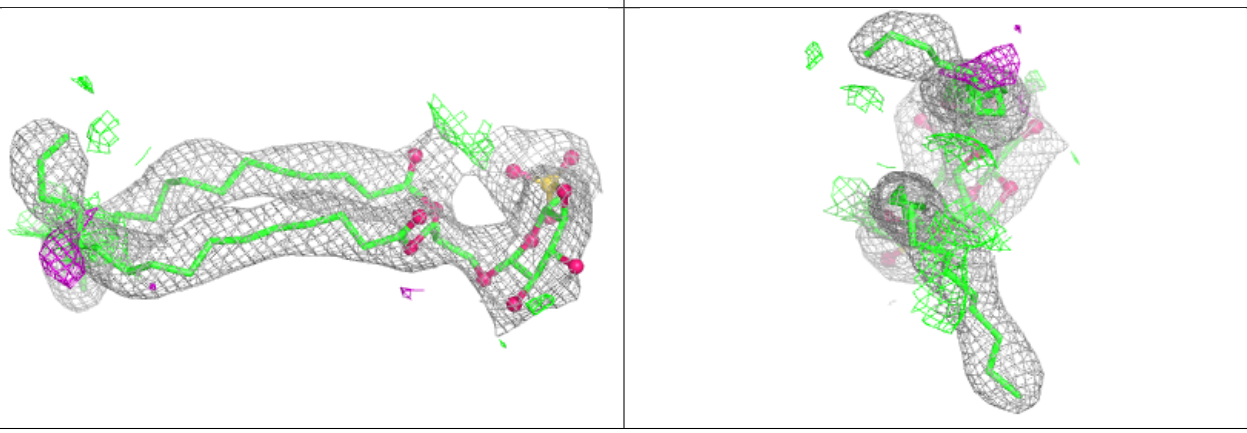




Electron density around SQD b 601:

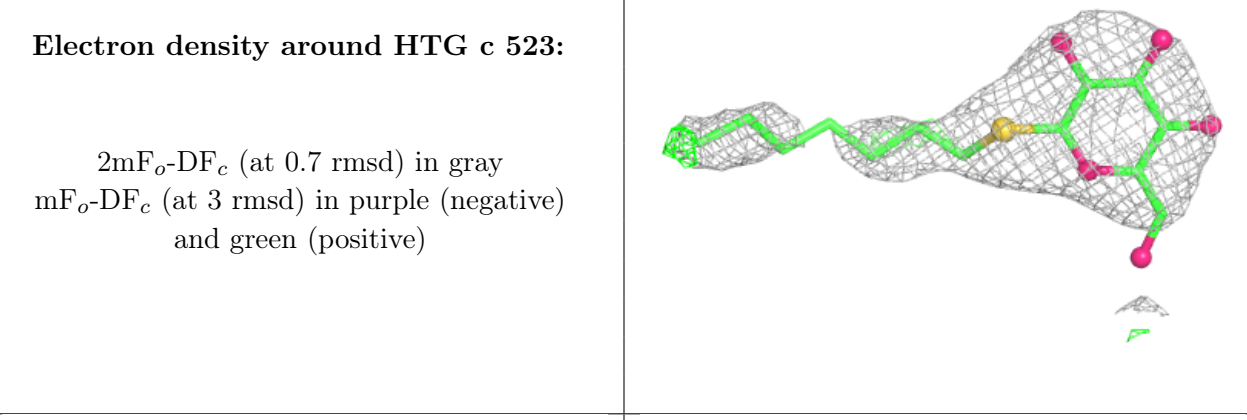
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

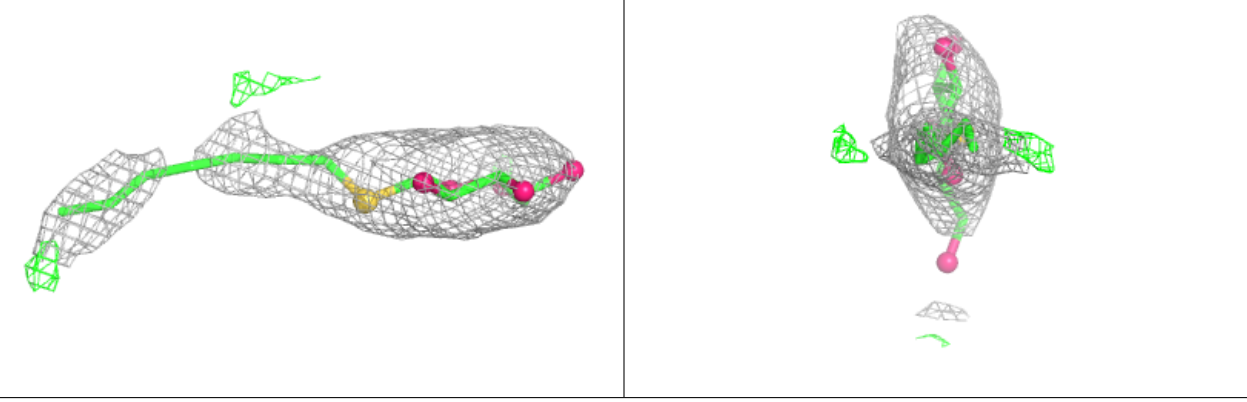




Electron density around HTG c 523:

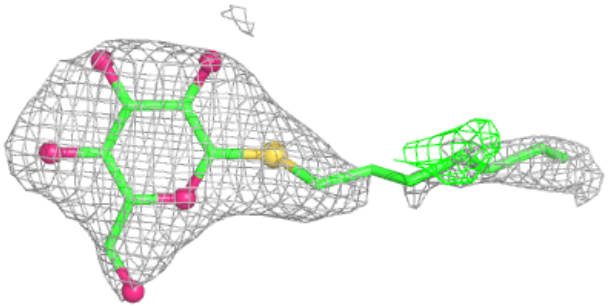
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

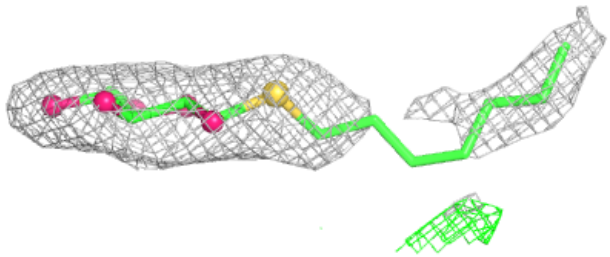


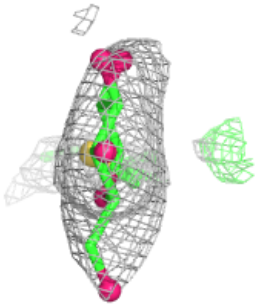


Electron density around HTG C 522:

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

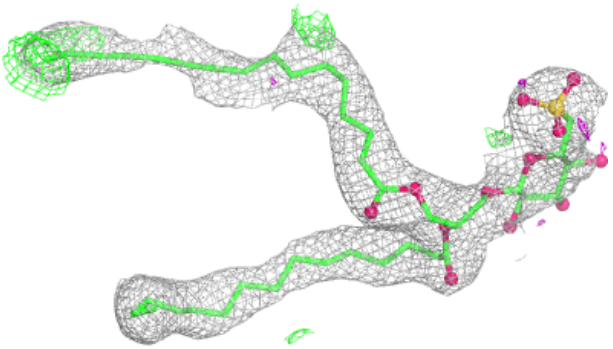


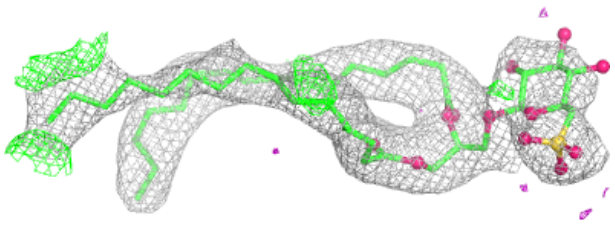


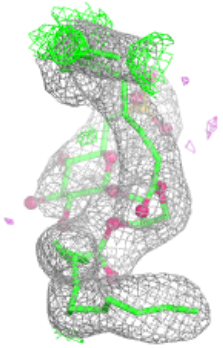


Electron density around SQD A 413:

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

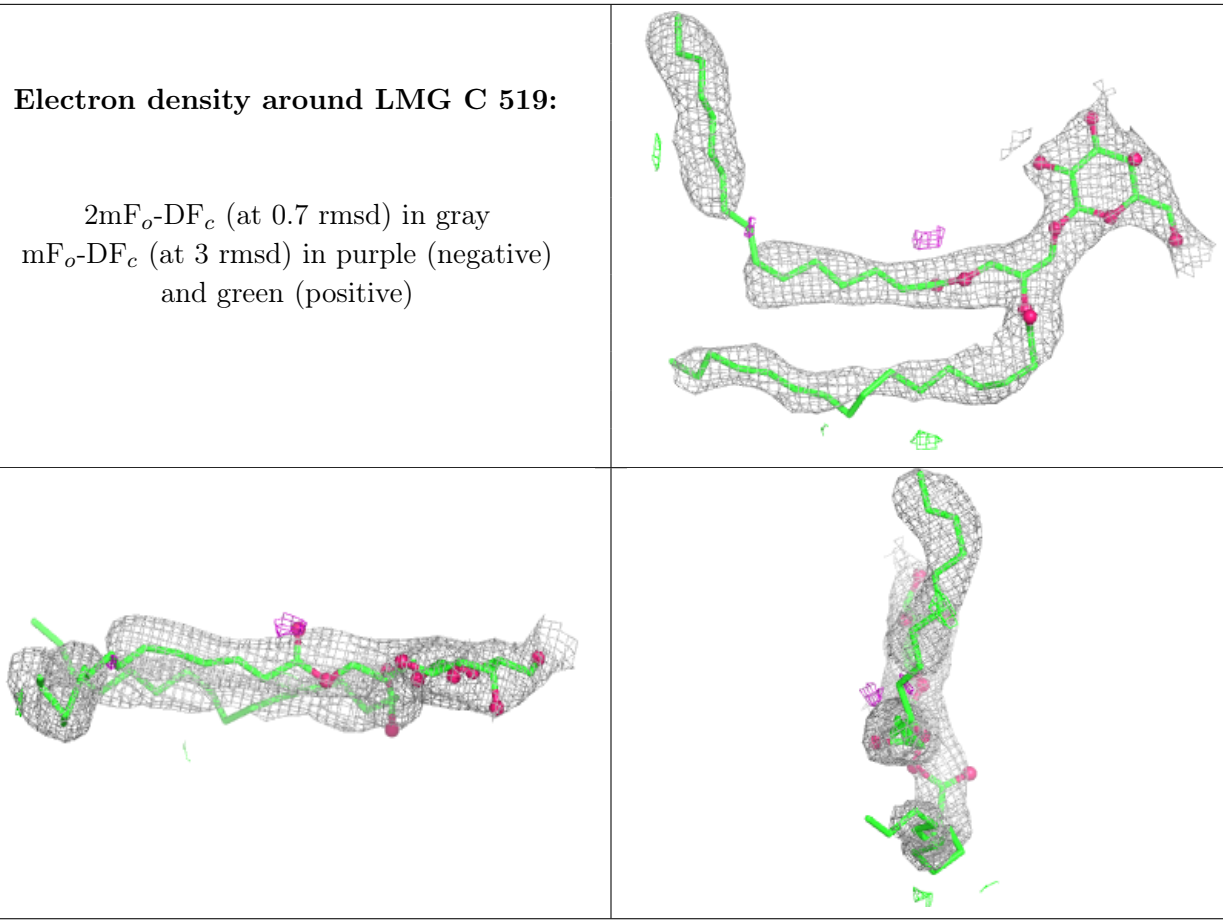






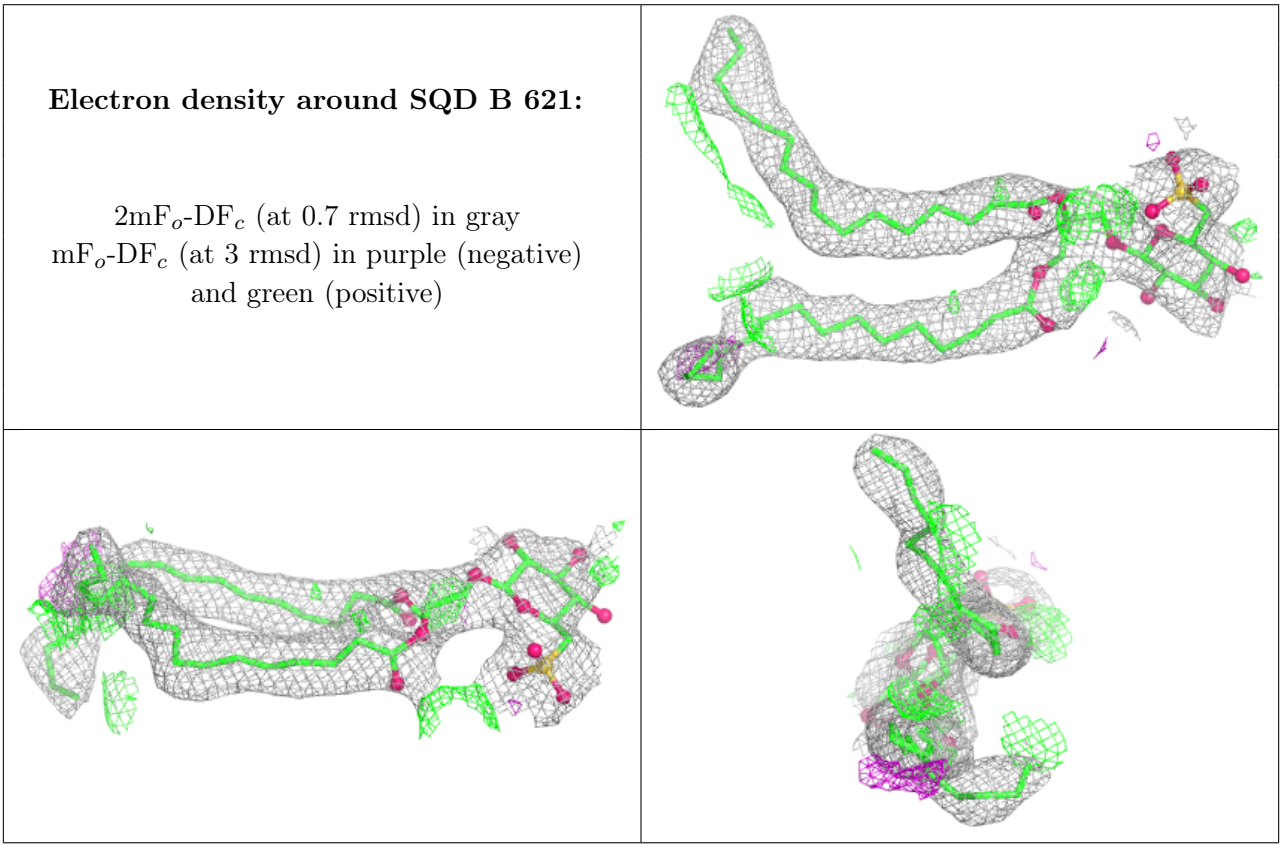
Electron density around LMG C 519:

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



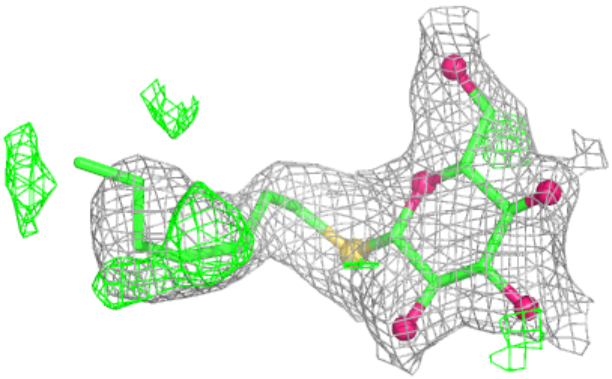
Electron density around SQD B 621:

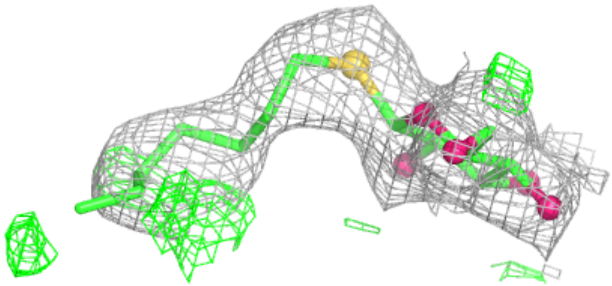
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

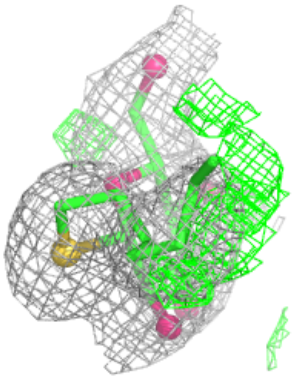


Electron density around HTG B 623:

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

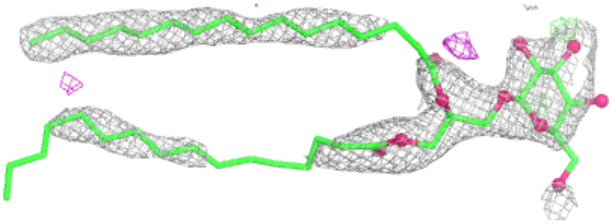


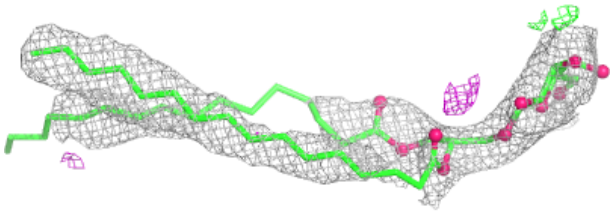


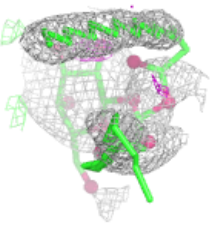


Electron density around LMG c 522:

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

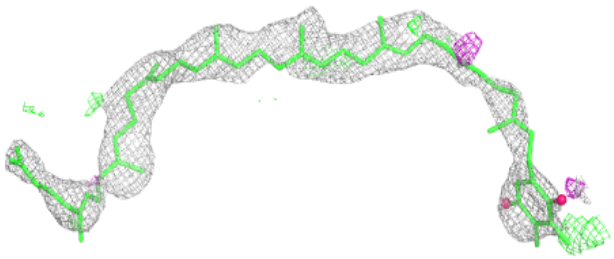


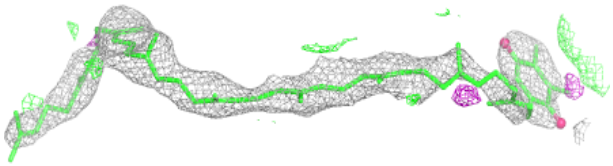


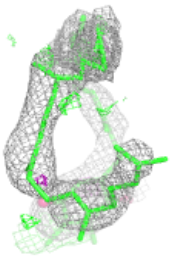


Electron density around PL9 a 415 (A):

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

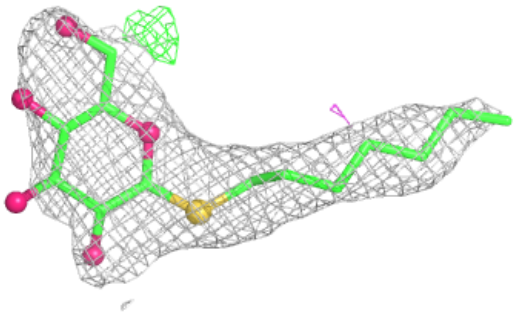


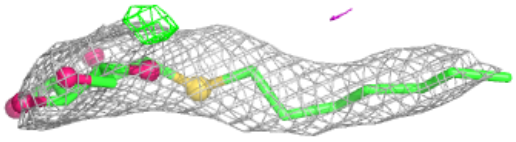


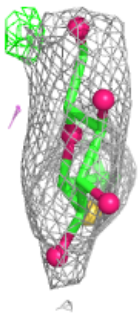


Electron density around HTG b 632:

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

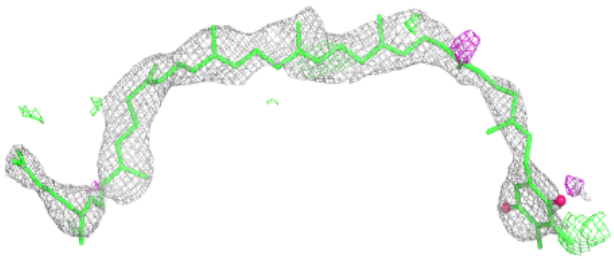


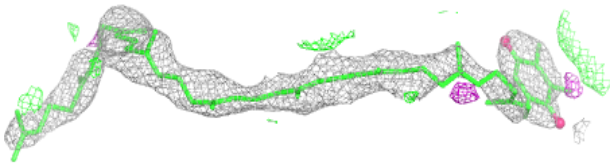


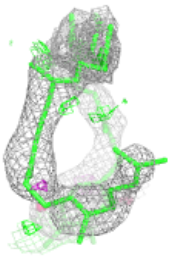


Electron density around PL9 a 415 (B):

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

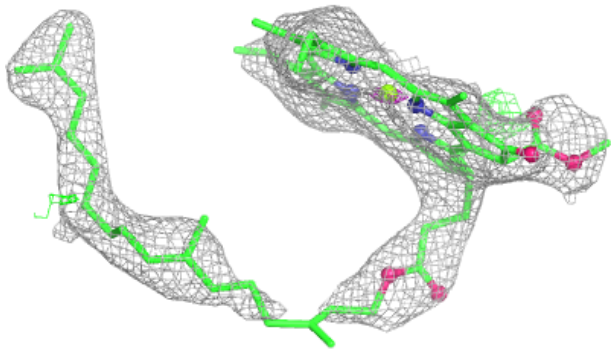


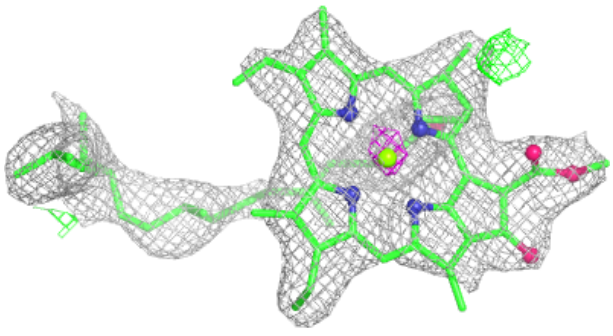


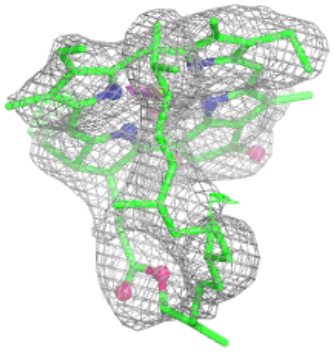


Electron density around CLA C 514:

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

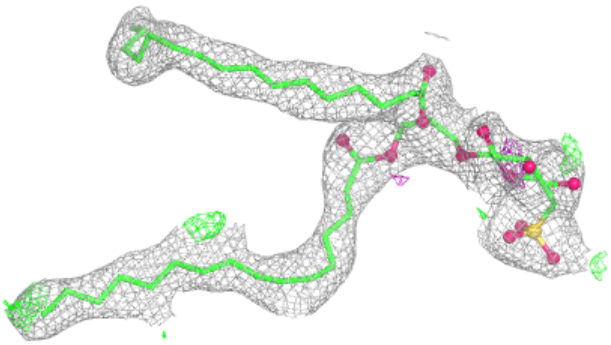


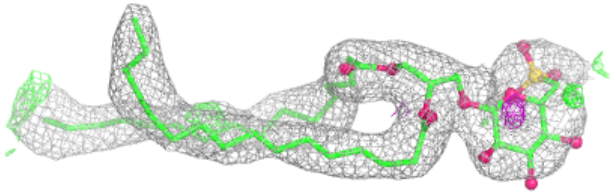


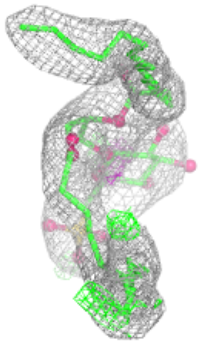


Electron density around SQD B 636:

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

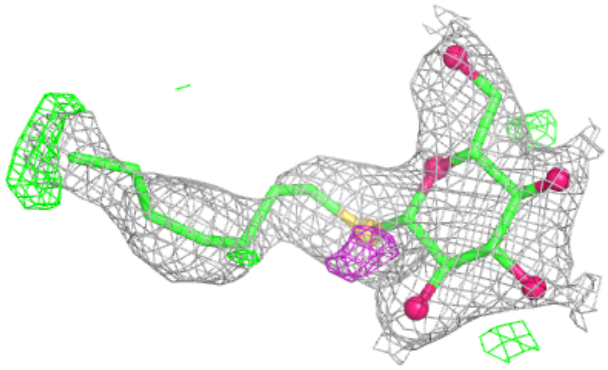


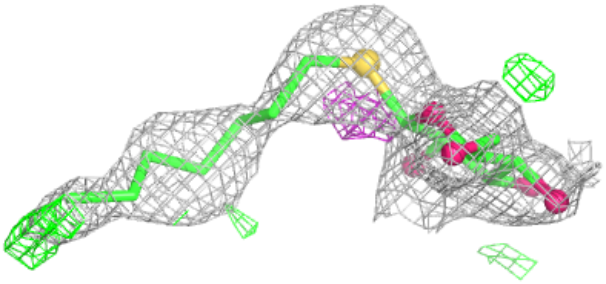


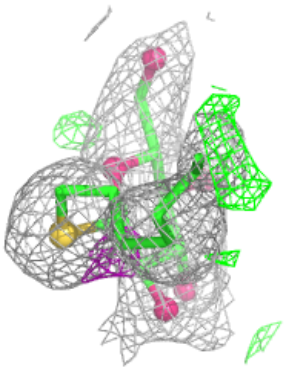


Electron density around HTG b 631:

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

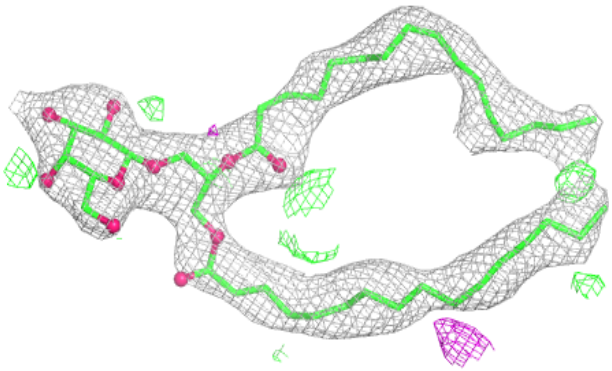


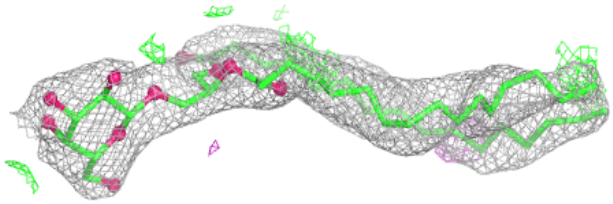


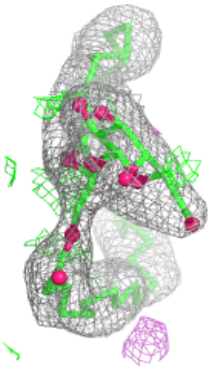


Electron density around LMG C 501:

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

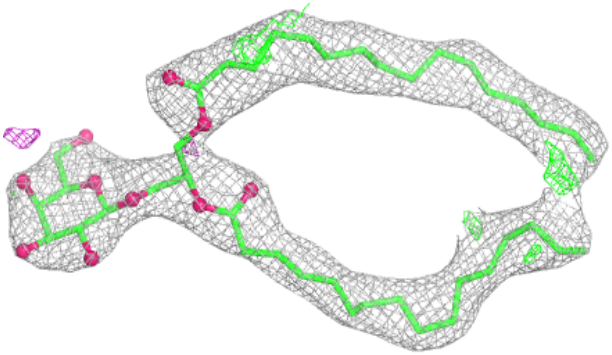


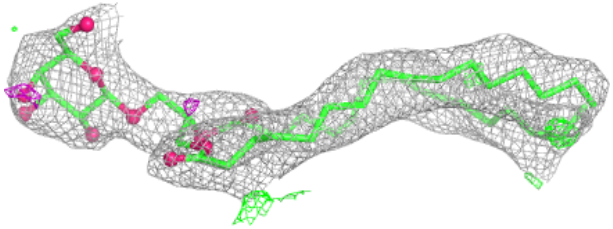


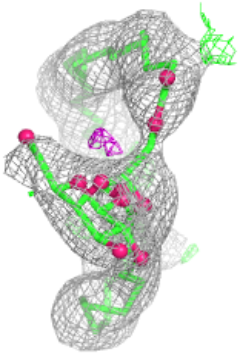


Electron density around LMG a 414:

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

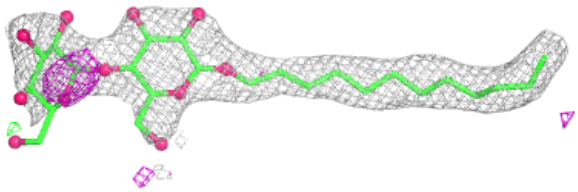


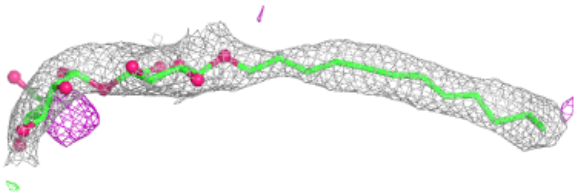


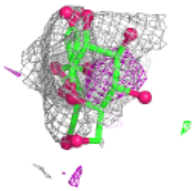


Electron density around LMT M 105:

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

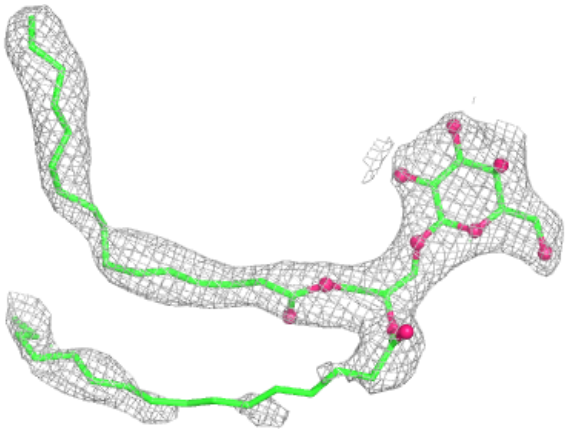


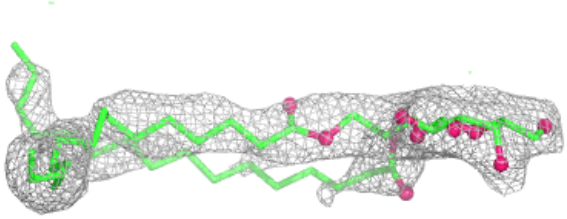


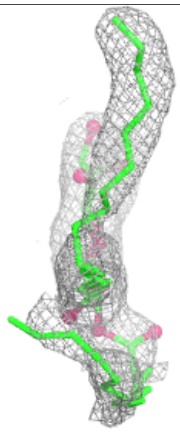


Electron density around LMG k 101:

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

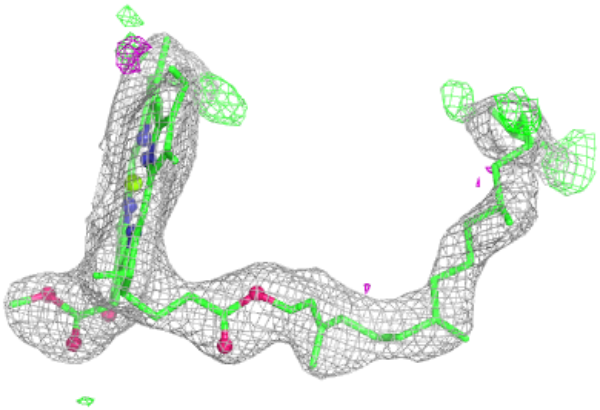


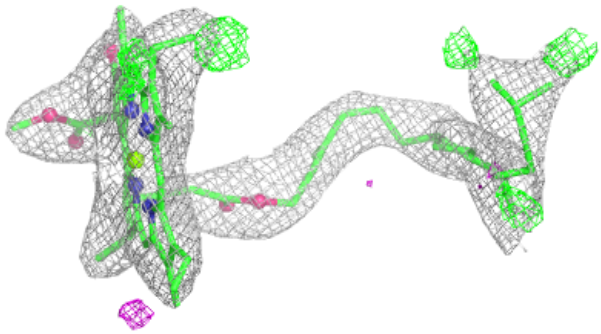


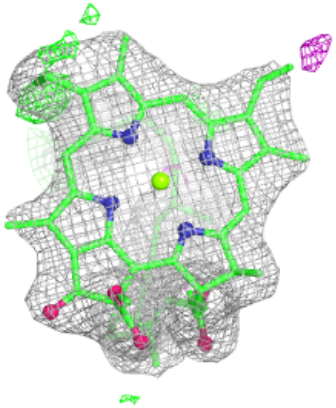


Electron density around CLA C 507:

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

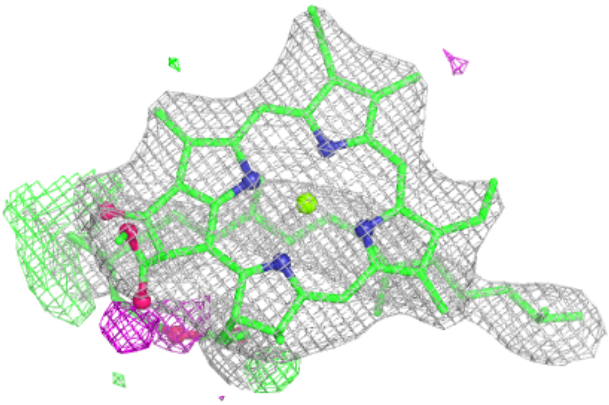


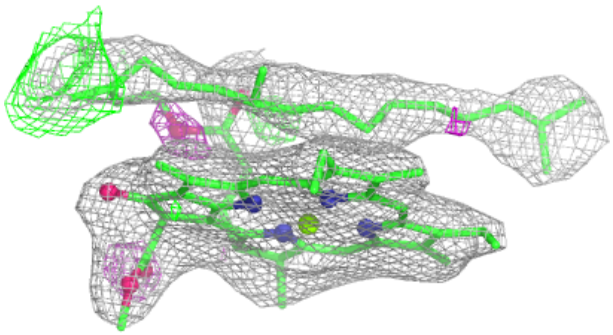


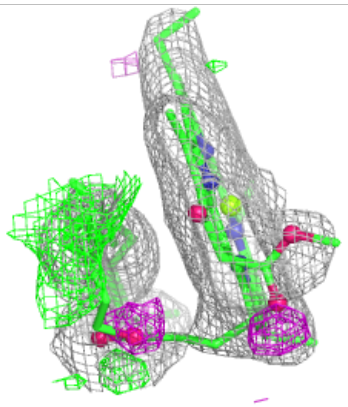


Electron density around CLA B 602:

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

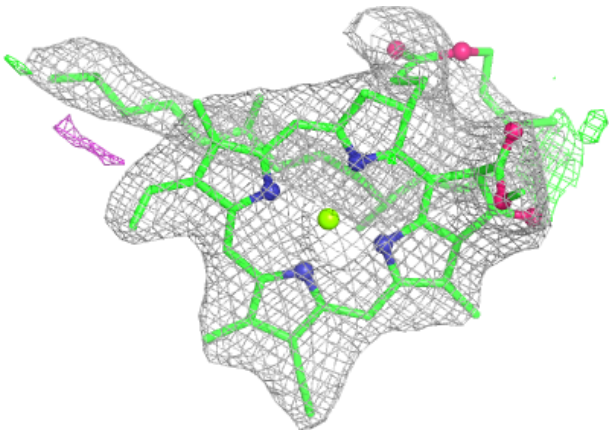


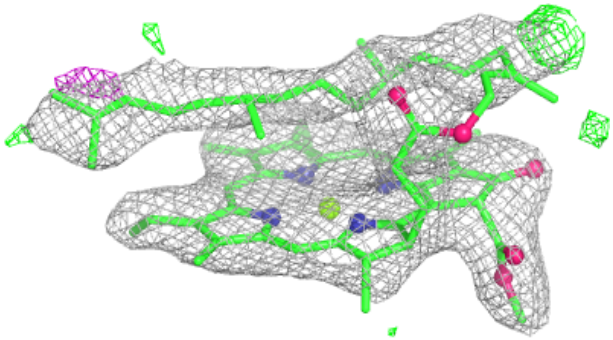


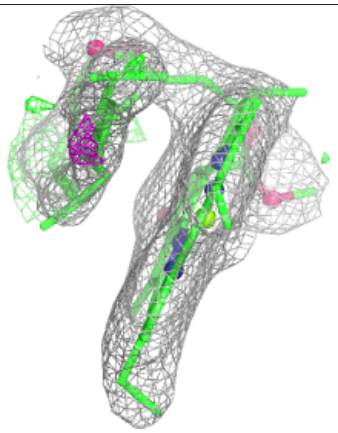


Electron density around CLA b 610:

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

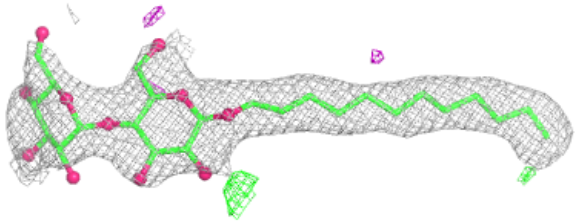


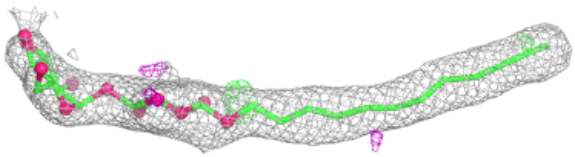


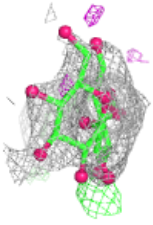


Electron density around LMT M 102:

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

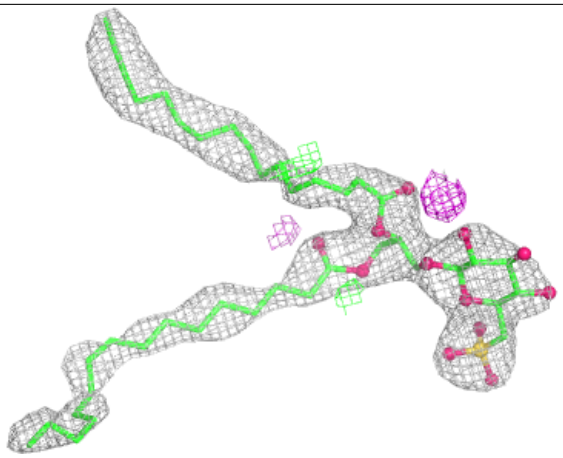


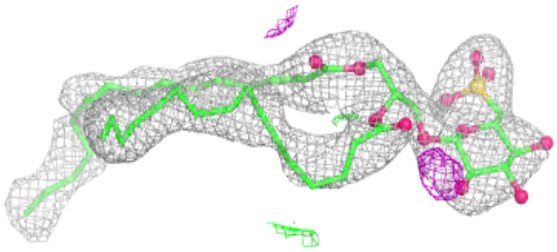


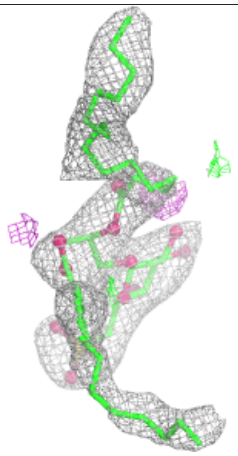


Electron density around SQD A 410:

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

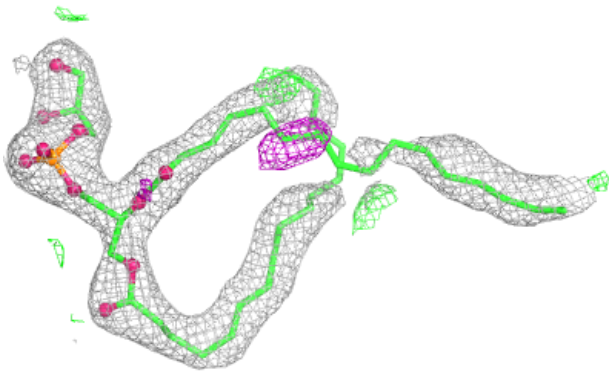


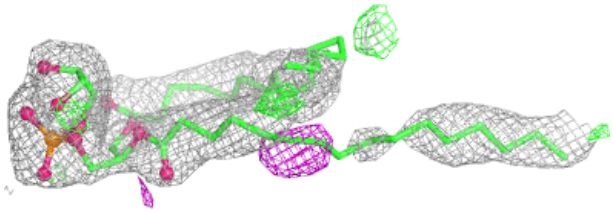


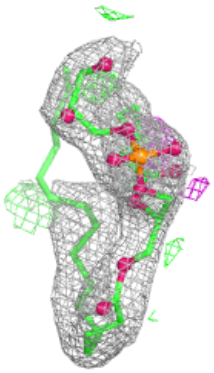


Electron density around LHG D 412:

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

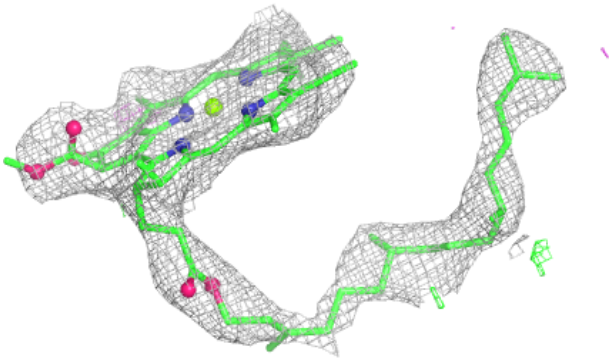


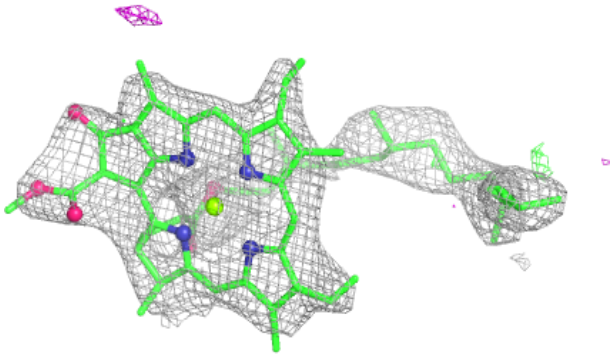


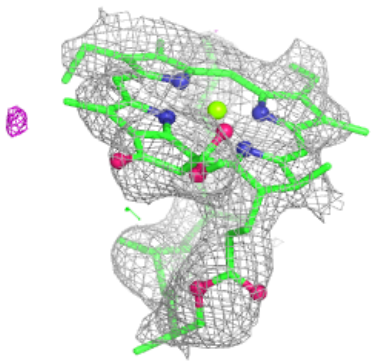


Electron density around CLA c 517:

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

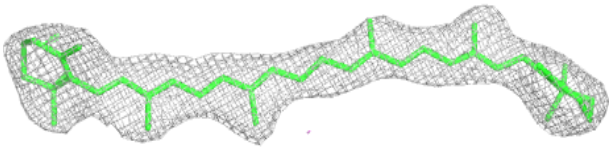


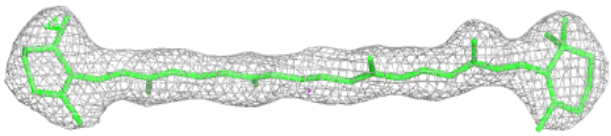


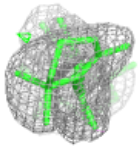


Electron density around BCR K 101:

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

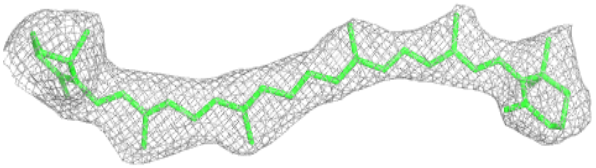


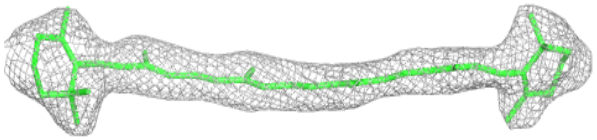


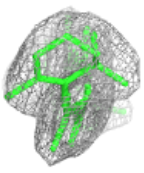


Electron density around BCR y 101:

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

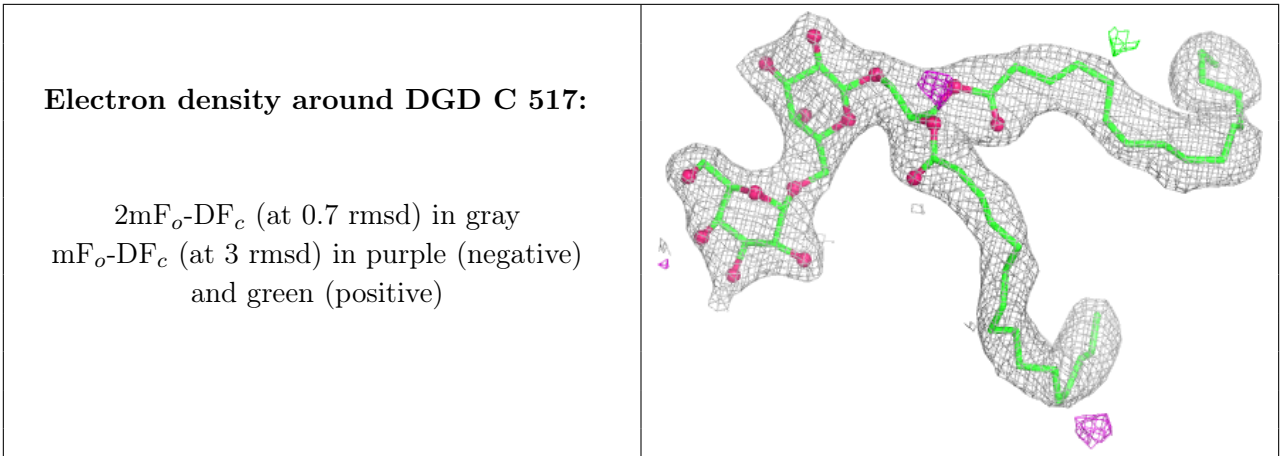






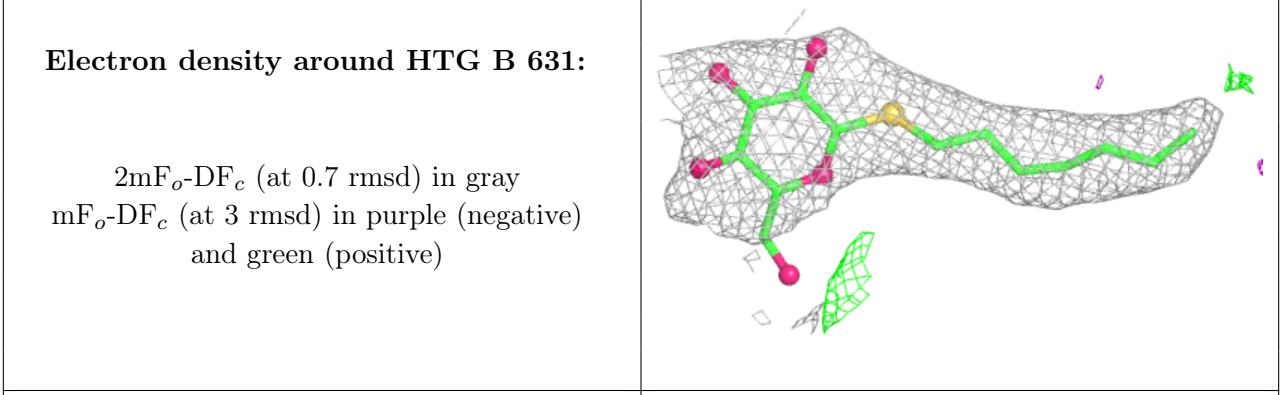
Electron density around DGD C 517:

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



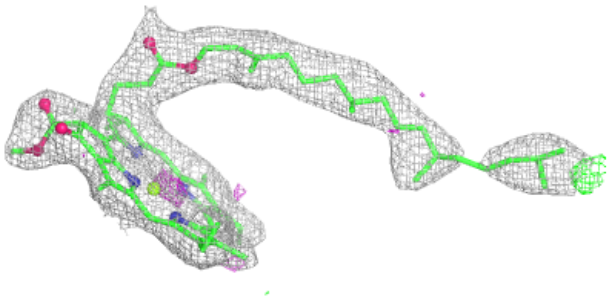
Electron density around HTG B 631:

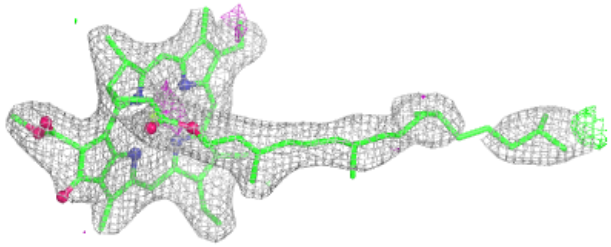
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

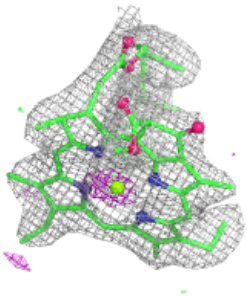


Electron density around CLA C 505:

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

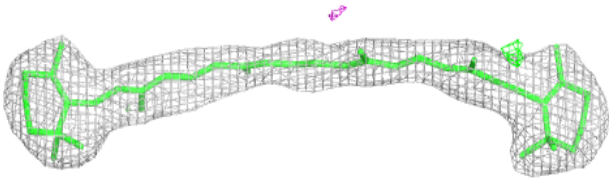


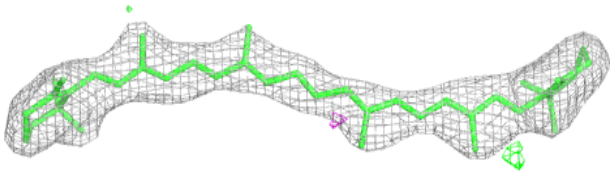


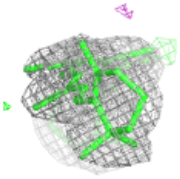


Electron density around BCR K 103:

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

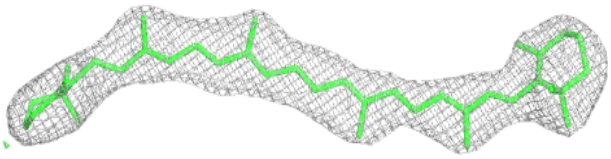


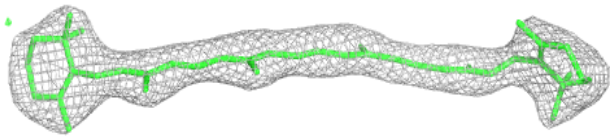


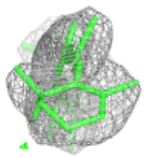


Electron density around BCR Y 101:

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

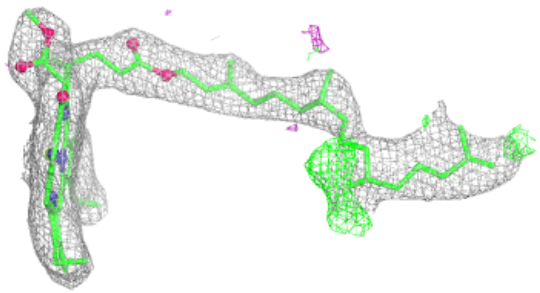


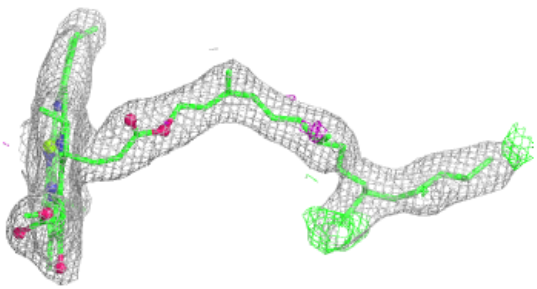


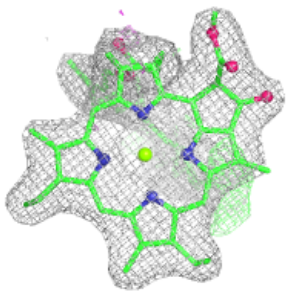


Electron density around CLA b 615:

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

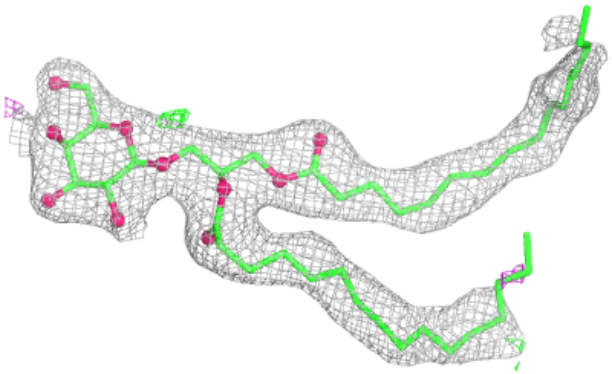


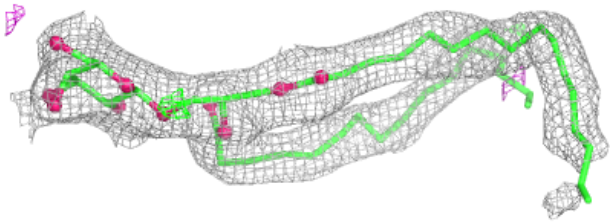




Electron density around LMG D 416:

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

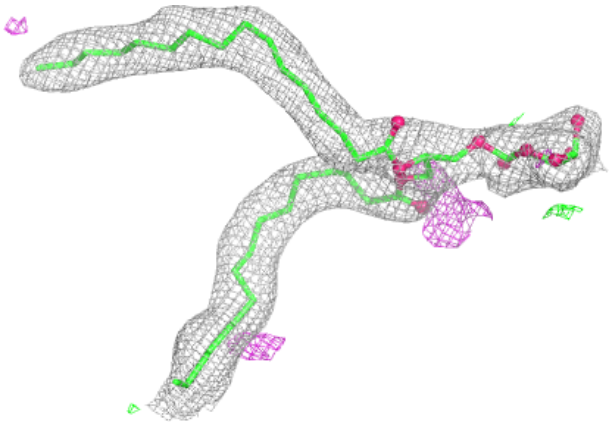


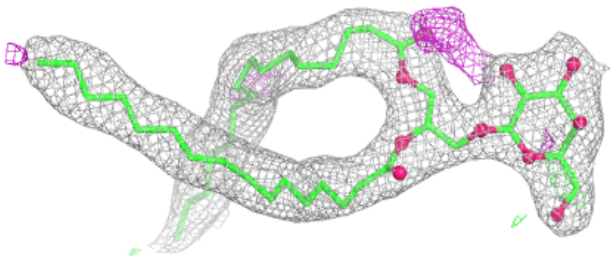


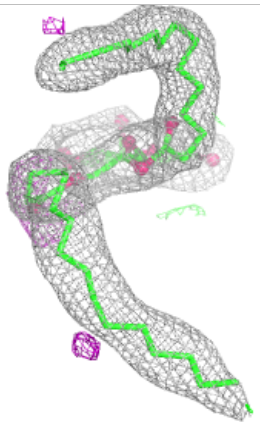


Electron density around LMG M 101:

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

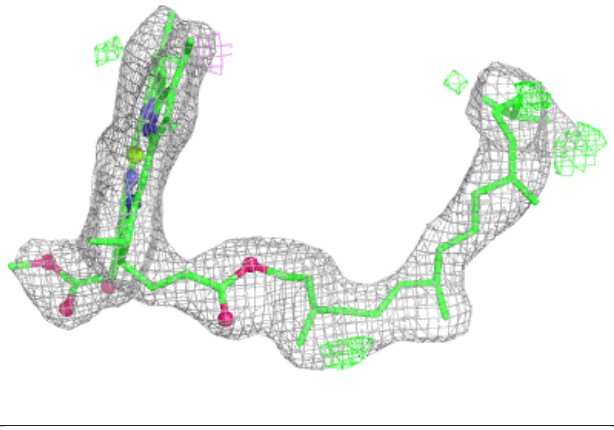


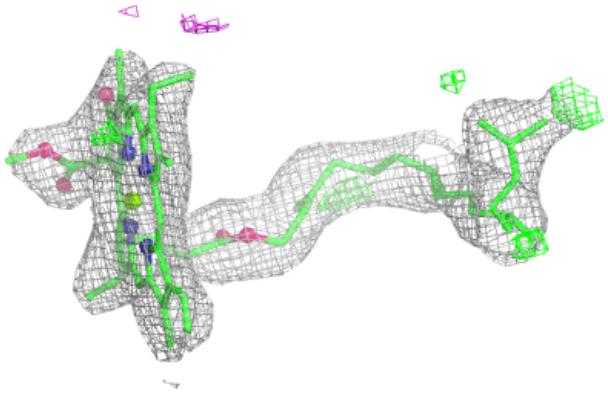


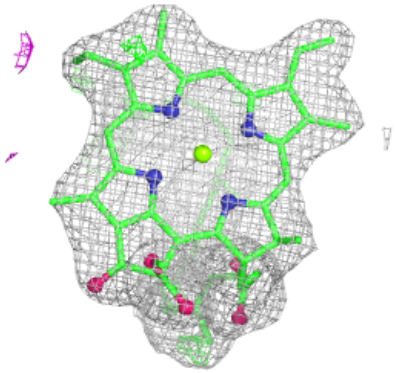


Electron density around CLA c 510:

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

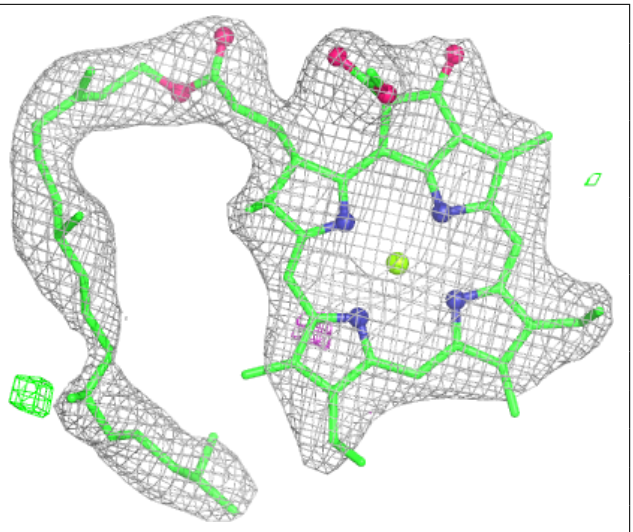


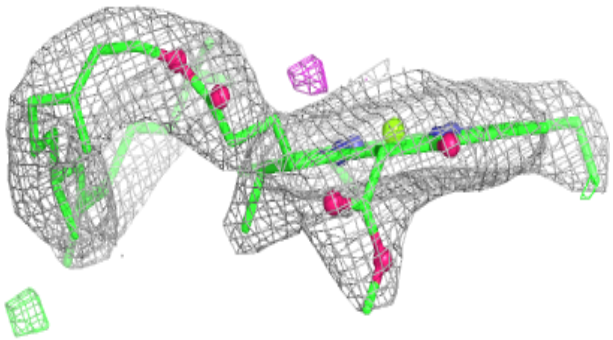


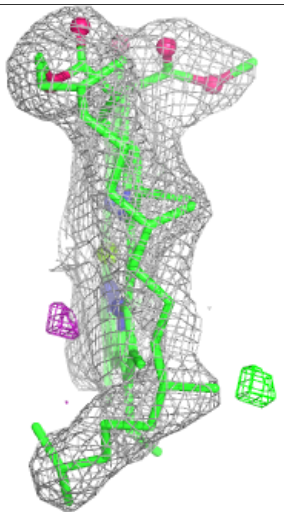


Electron density around CLA C 513:

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

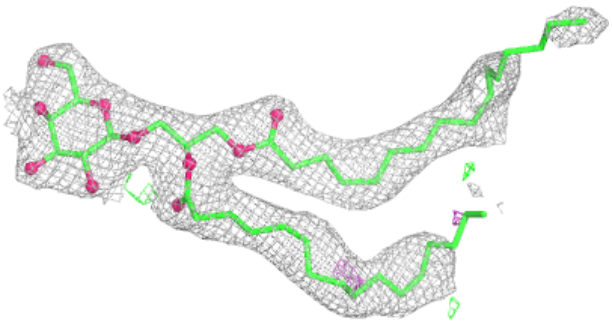


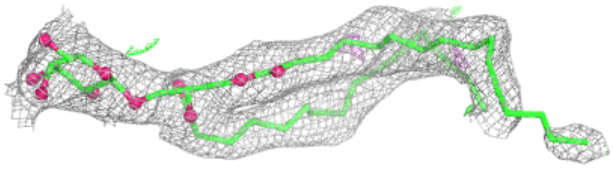


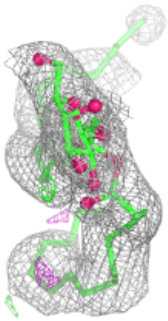


Electron density around LMG d 416:

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

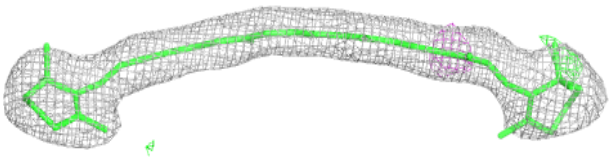


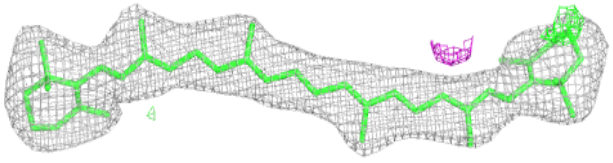


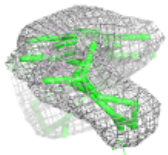


Electron density around BCR D 407:

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

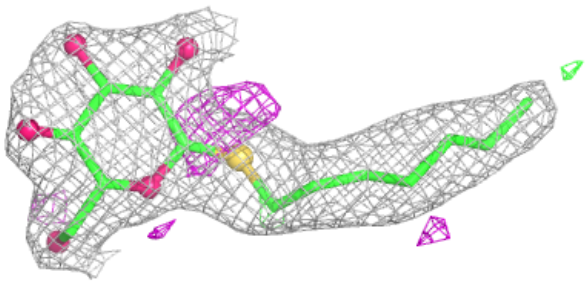


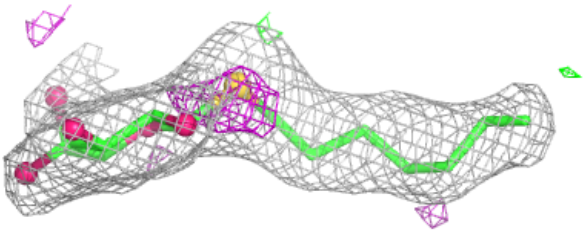


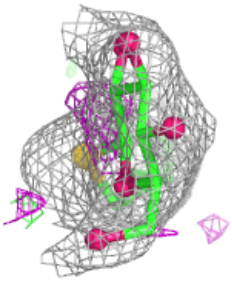


Electron density around HTG b 602:

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

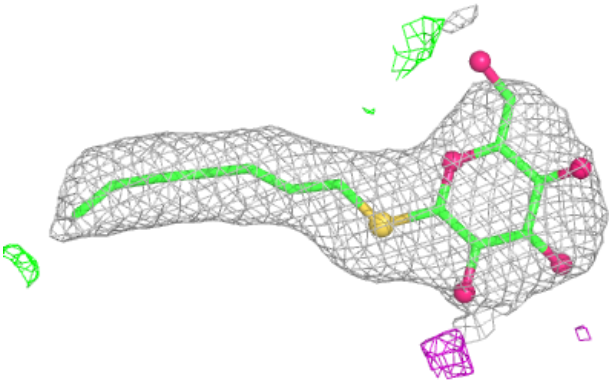


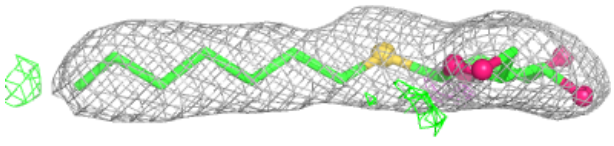


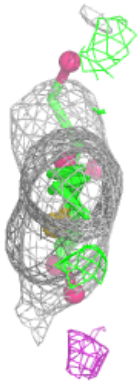


Electron density around HTG b 607:

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

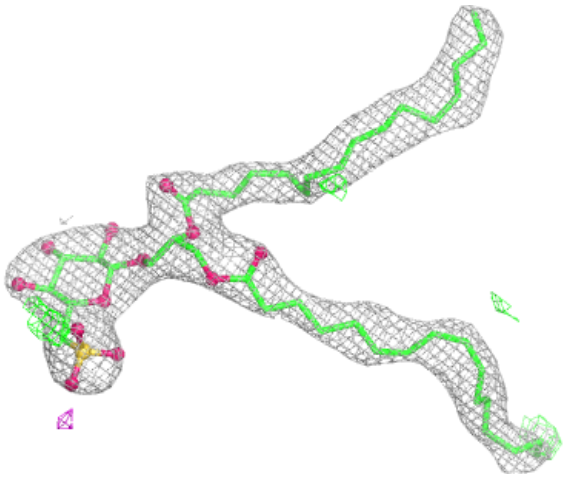


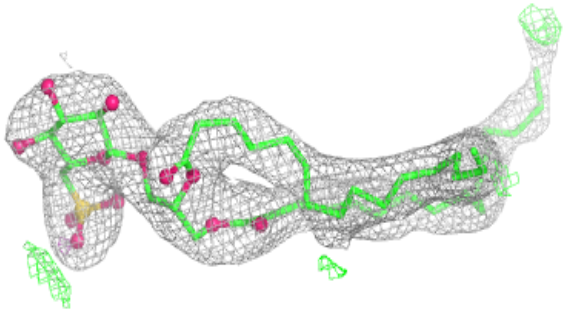




Electron density around SQD a 413:

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

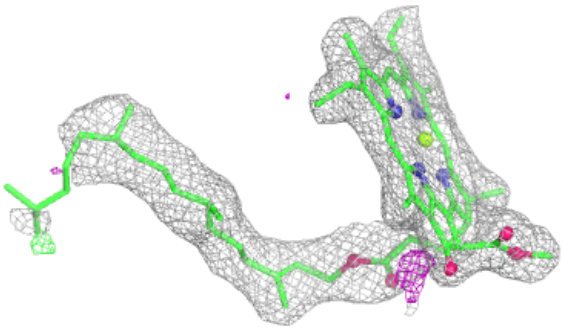


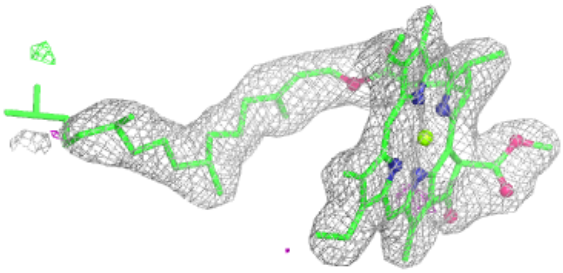


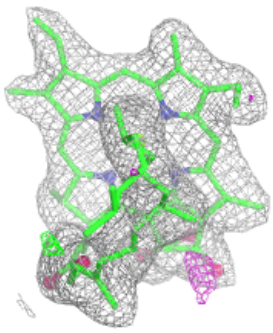


Electron density around CLA c 512:

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

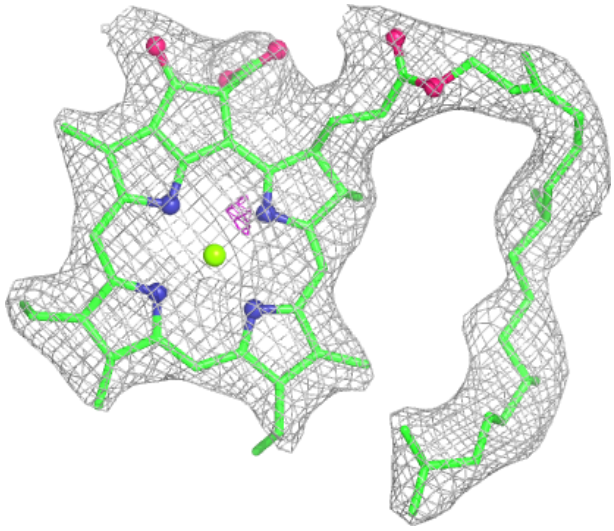


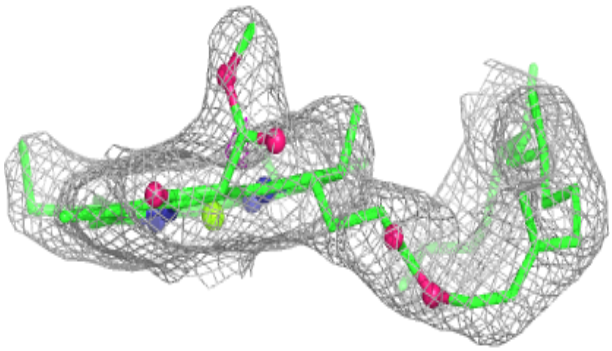


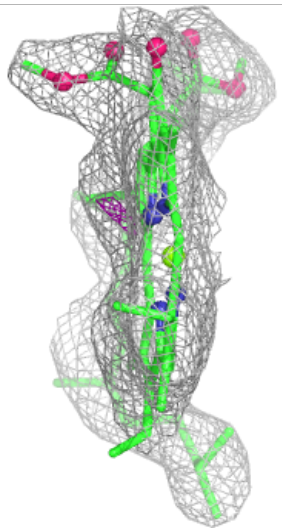


Electron density around CLA c 516:

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

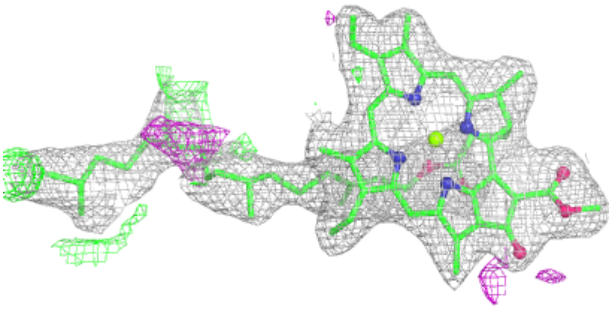


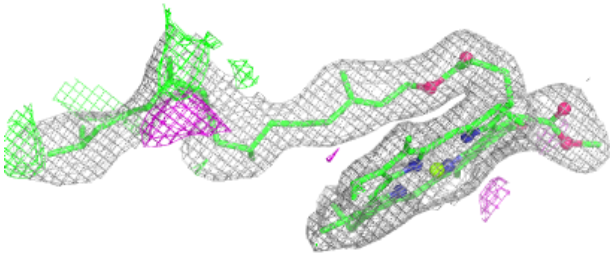


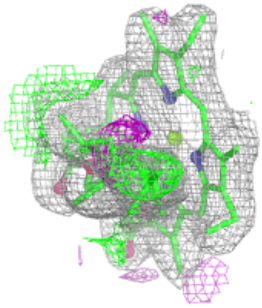


Electron density around CLA B 615:

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

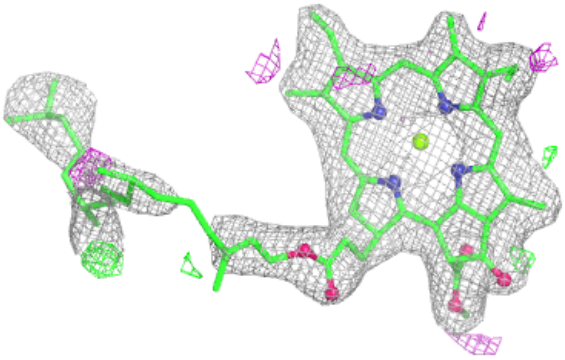


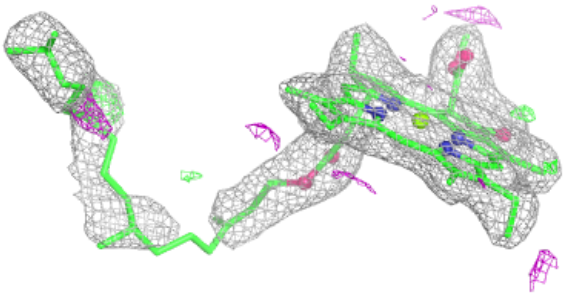


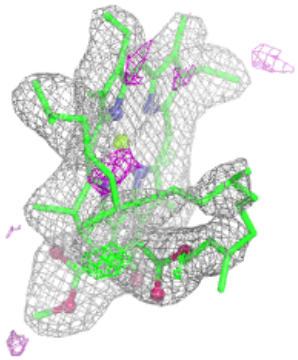


Electron density around CLA a 411:

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

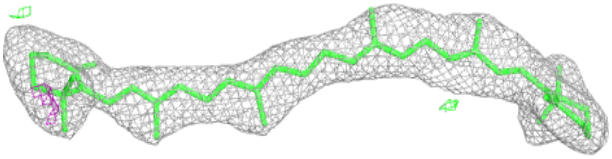


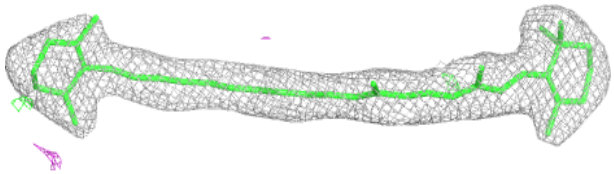


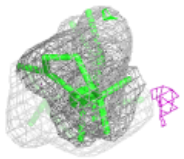


Electron density around BCR H 101:

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

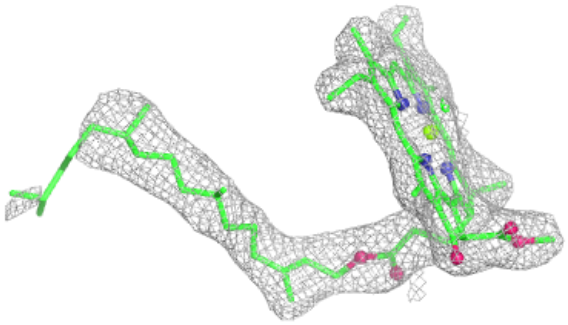


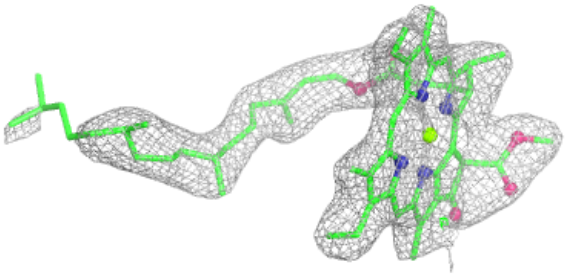


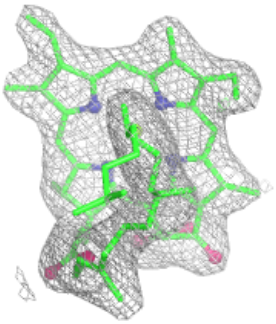


Electron density around CLA C 509:

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

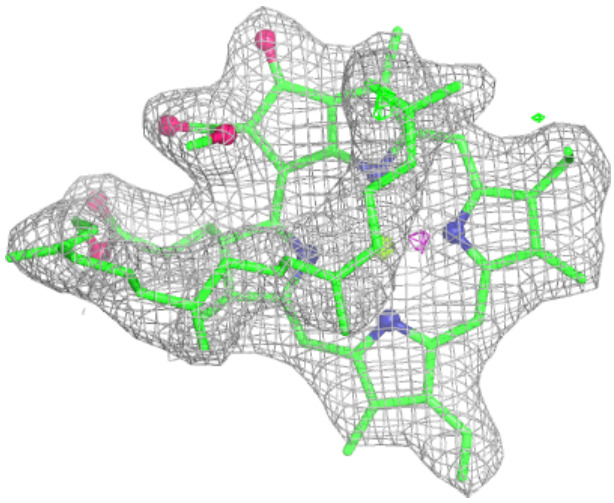


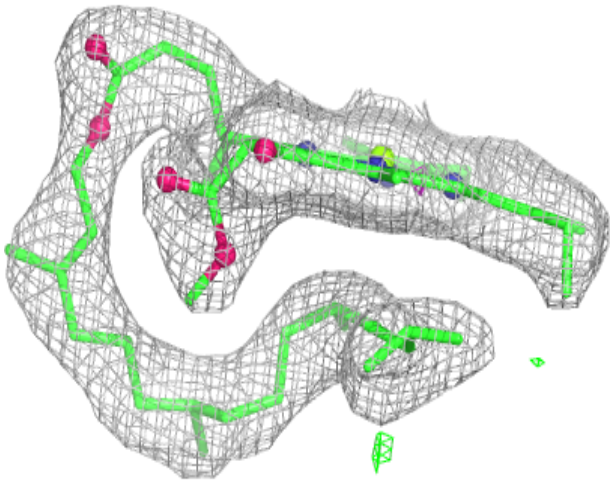


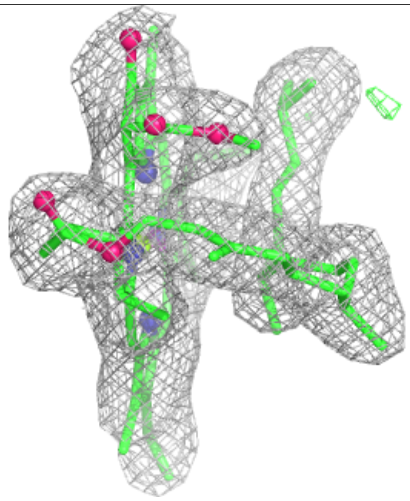


Electron density around CLA C 511:

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

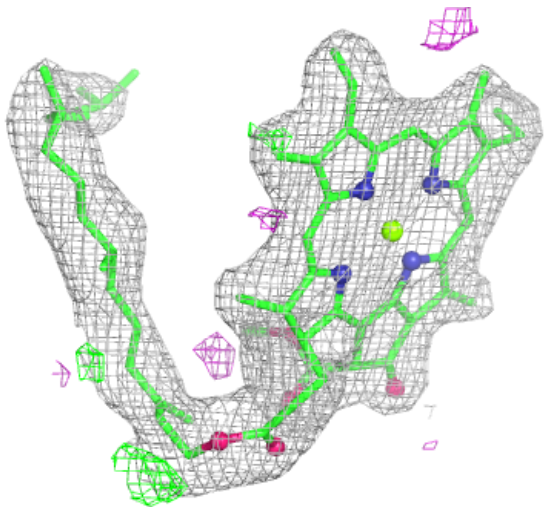


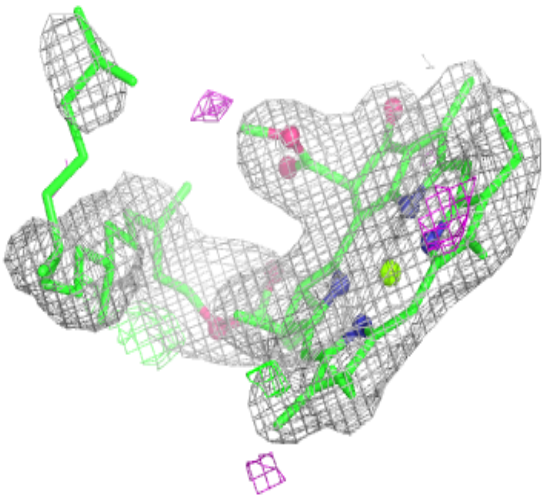


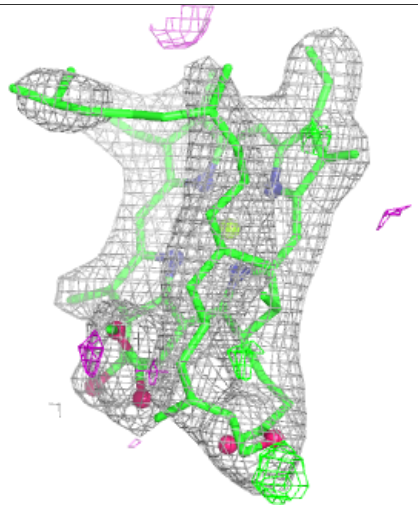


Electron density around CLA b 625:

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

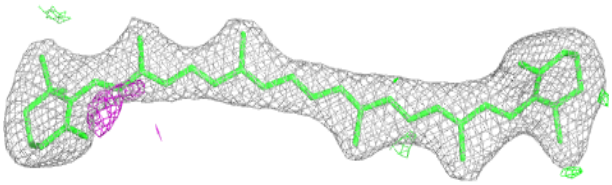


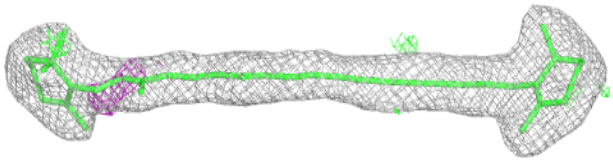


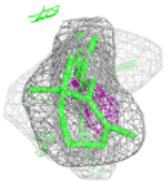


Electron density around BCR b 627:

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

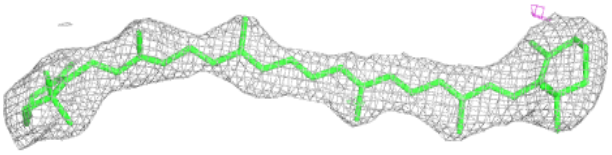


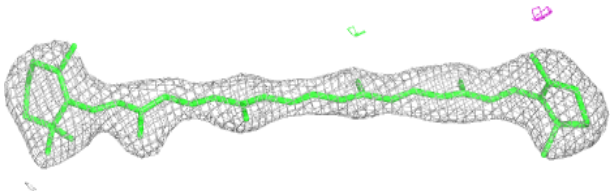


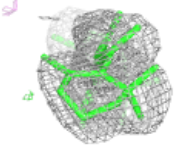


Electron density around BCR c 526:

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

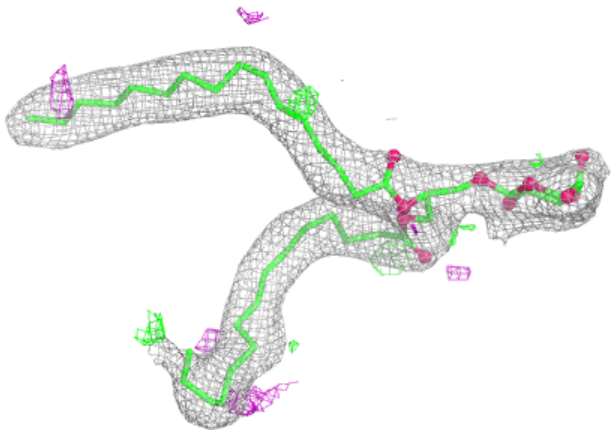


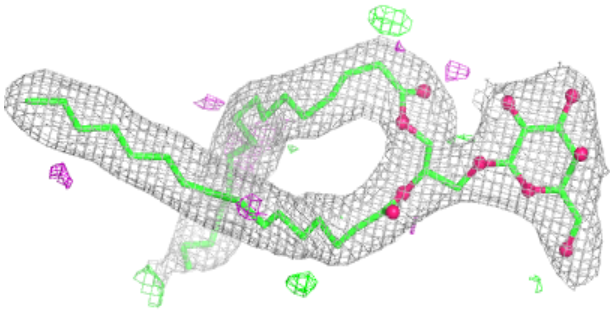


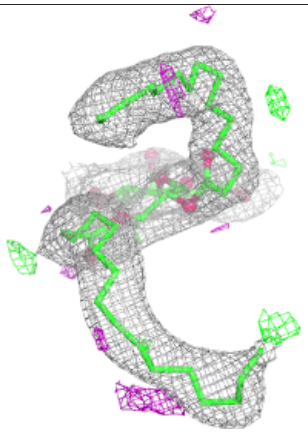


Electron density around LMG b 629:

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

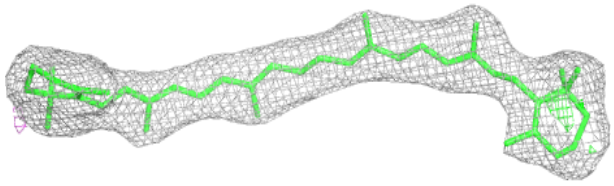


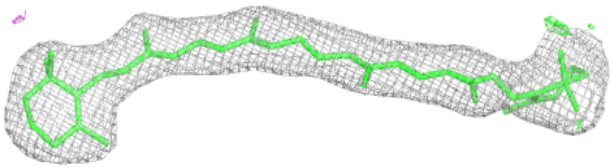


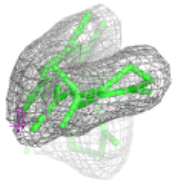


Electron density around BCR d 406:

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

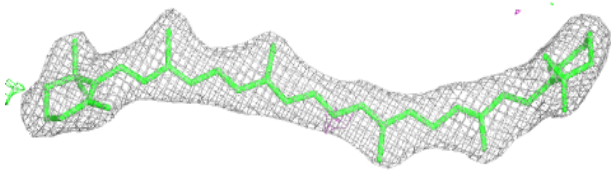


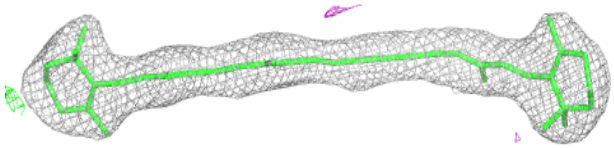


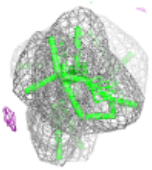


Electron density around BCR h 101:

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

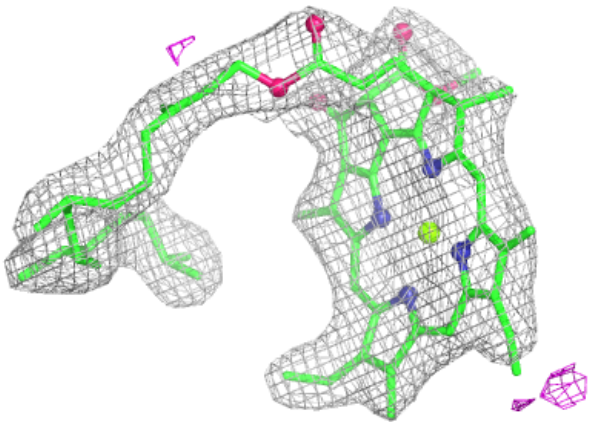


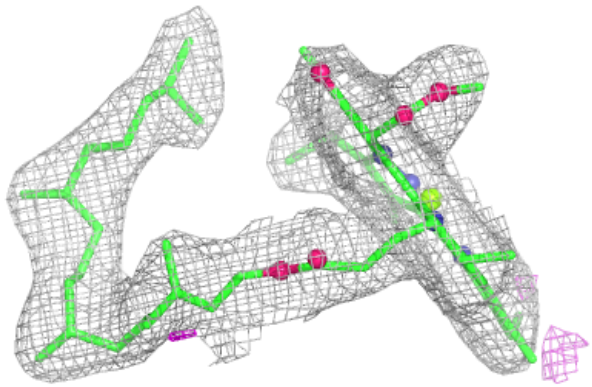


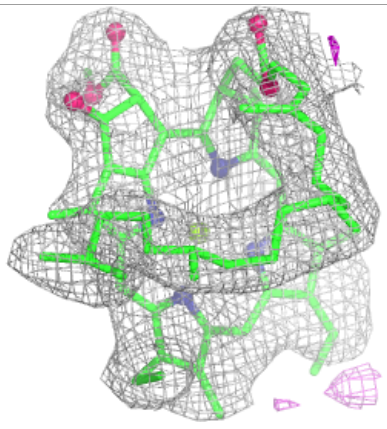


Electron density around CLA c 507:

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

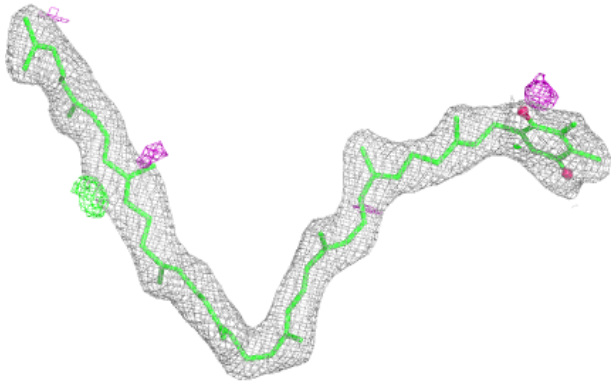


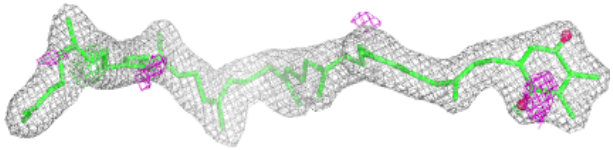


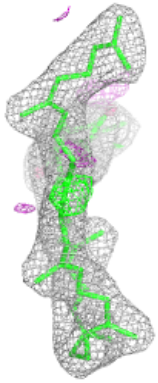


Electron density around PL9 D 408 (A):

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

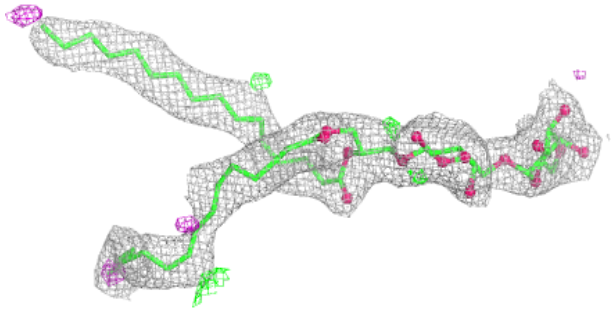


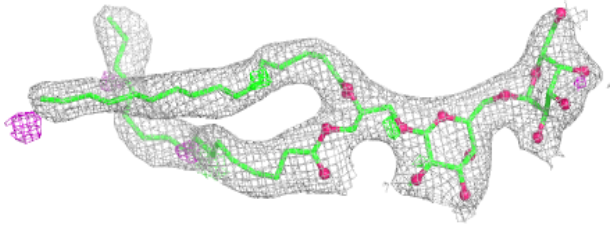


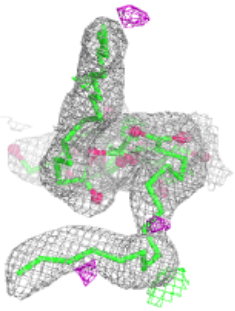


Electron density around DGD C 516:

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

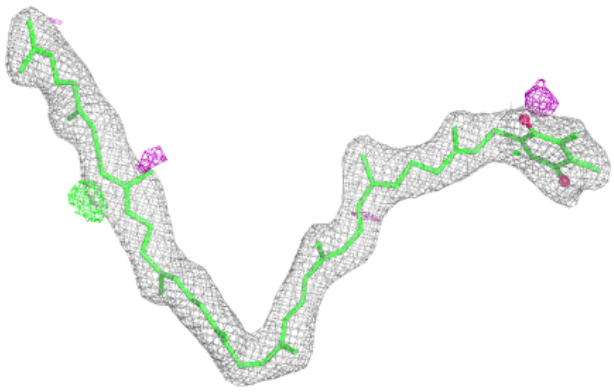


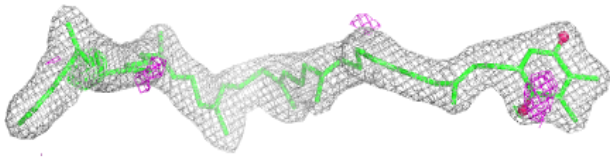


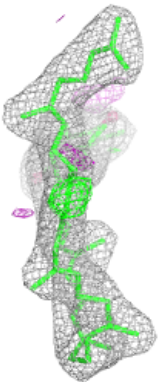


Electron density around PL9 D 408 (B):

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

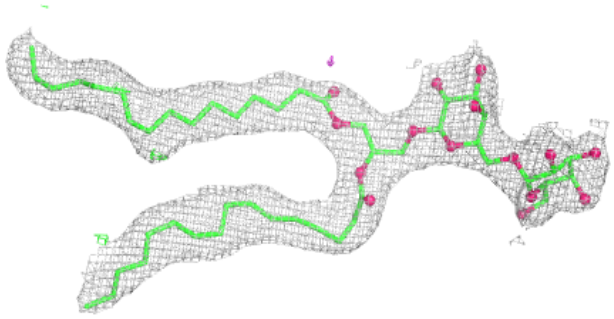


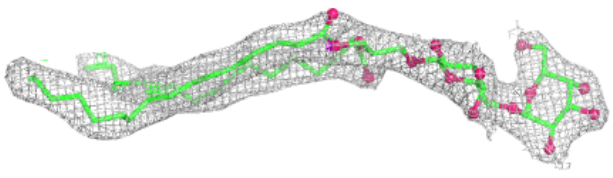


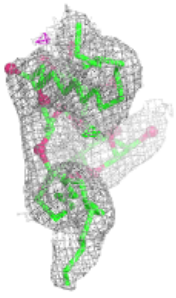


Electron density around DGD C 518:

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

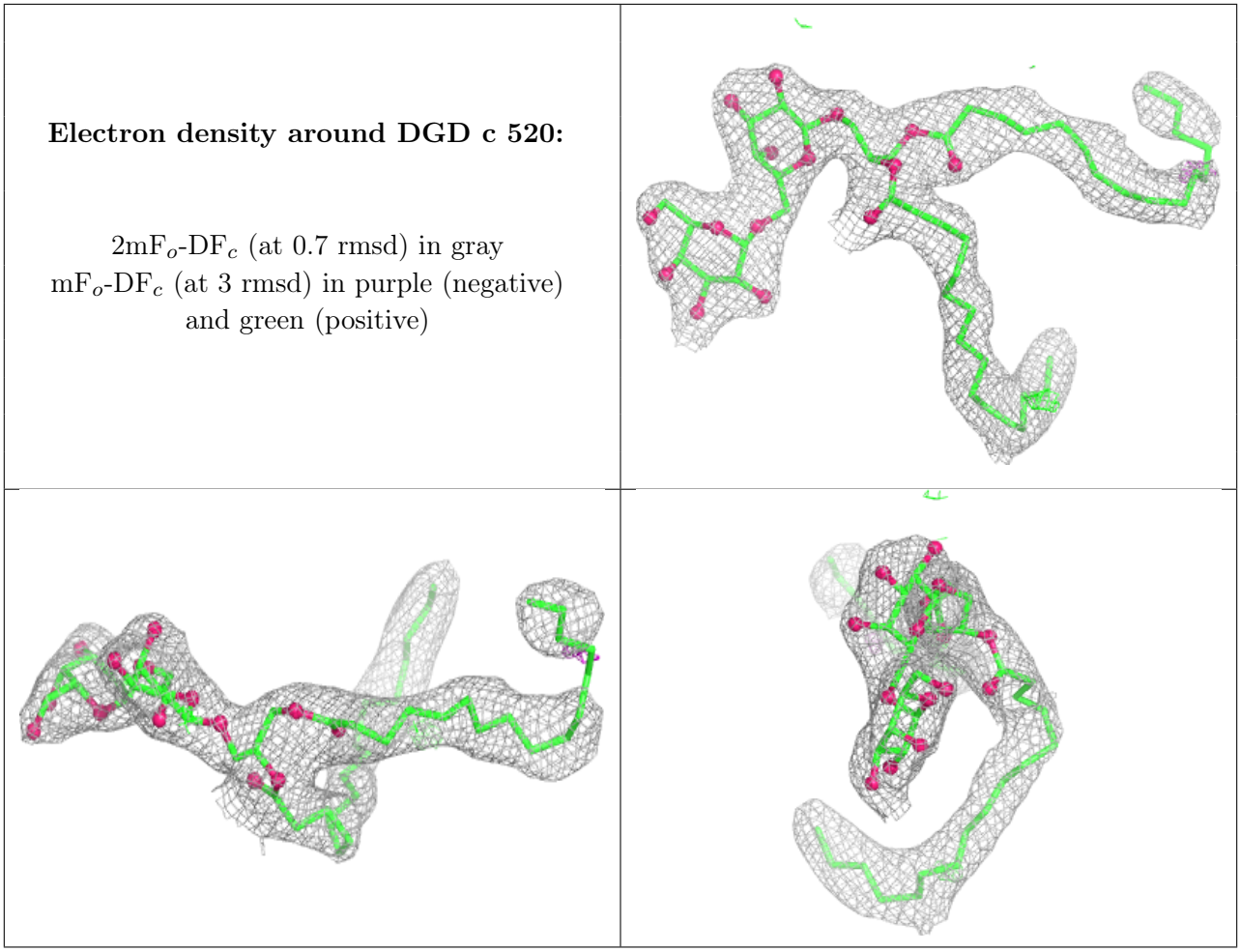






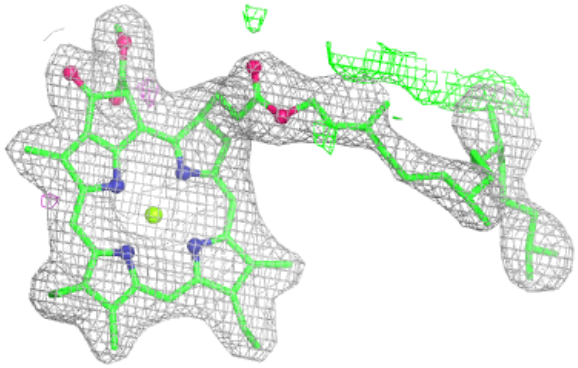
Electron density around DGD c 520:

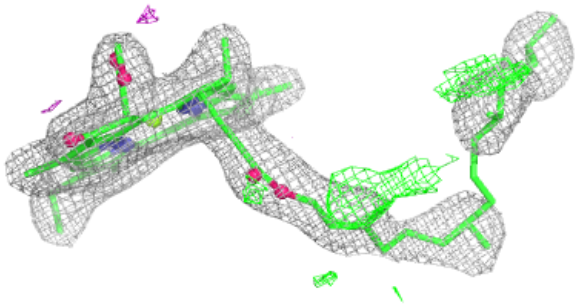
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

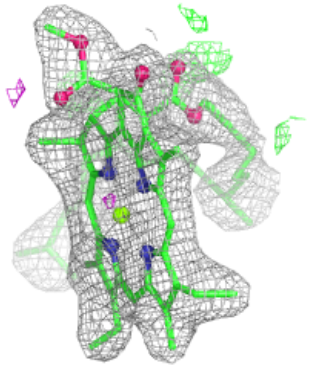


Electron density around CLA A 408:

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

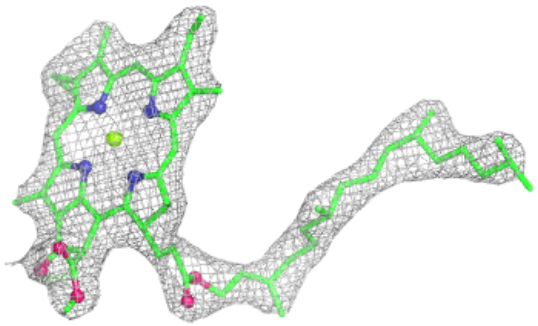


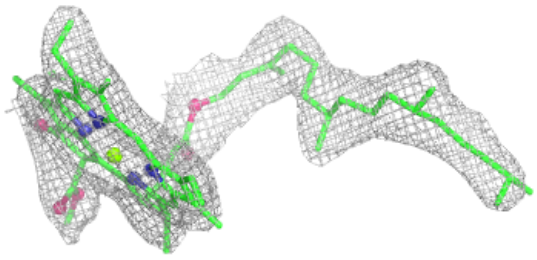


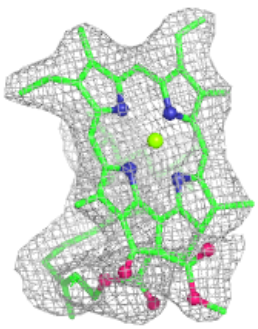


Electron density around CLA c 515:

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

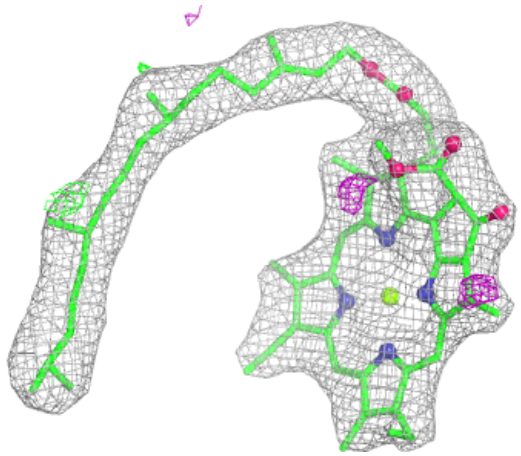


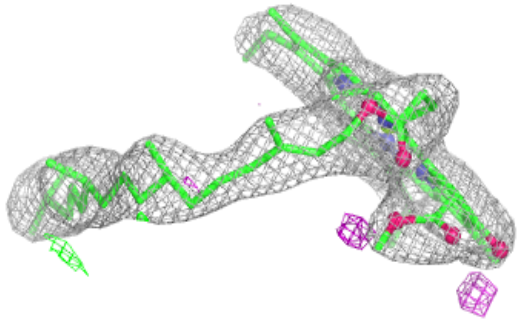


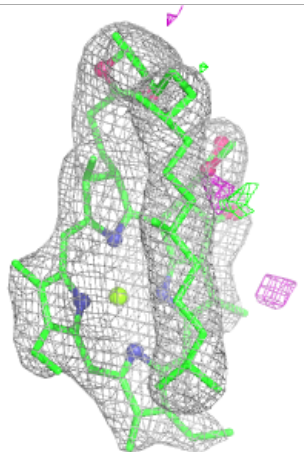


Electron density around CLA C 508:

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

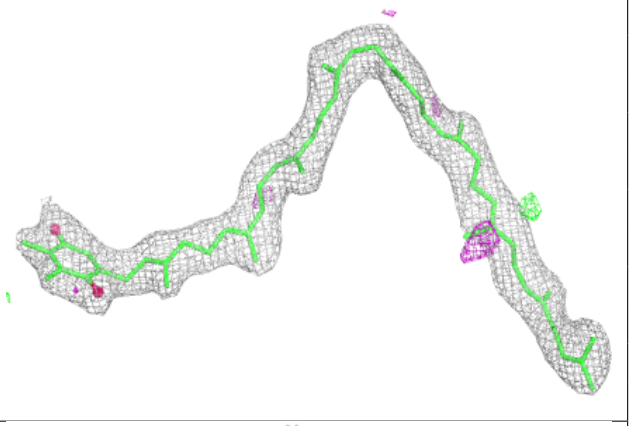


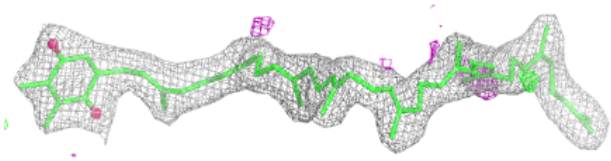




Electron density around PL9 d 407 (A):

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

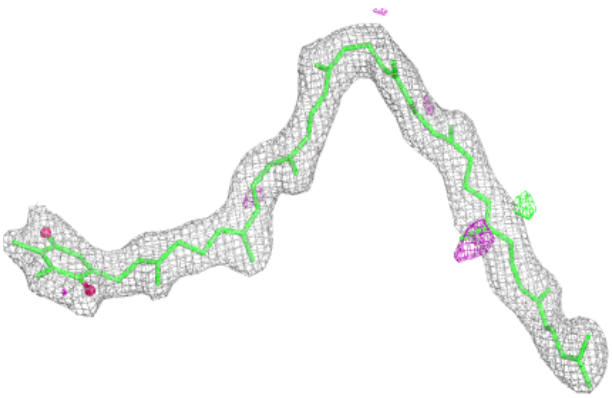


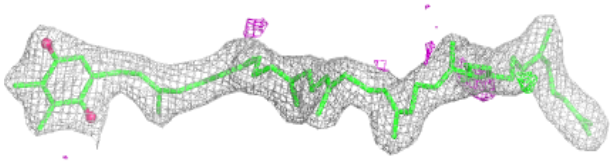




Electron density around PL9 d 407 (B):

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

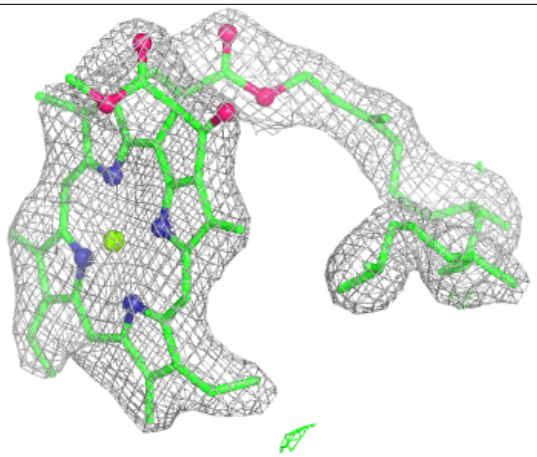


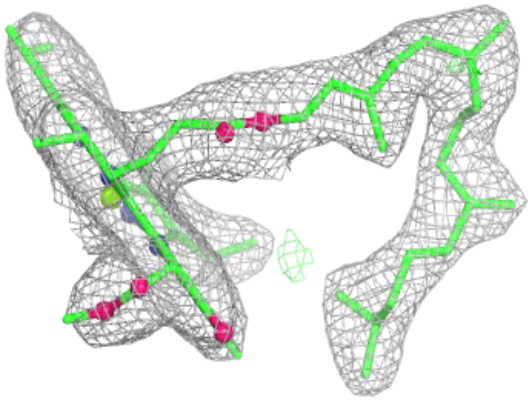


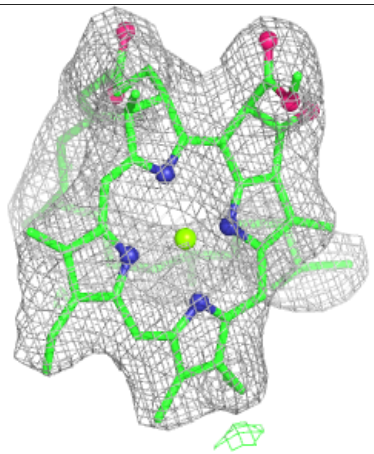


Electron density around CLA C 504:

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

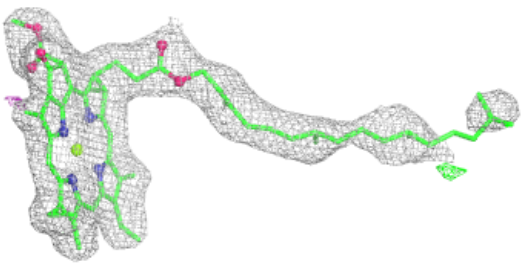


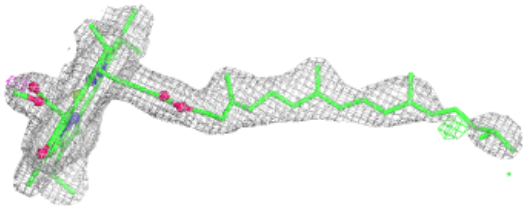


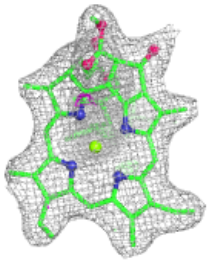


Electron density around CLA d 405:

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

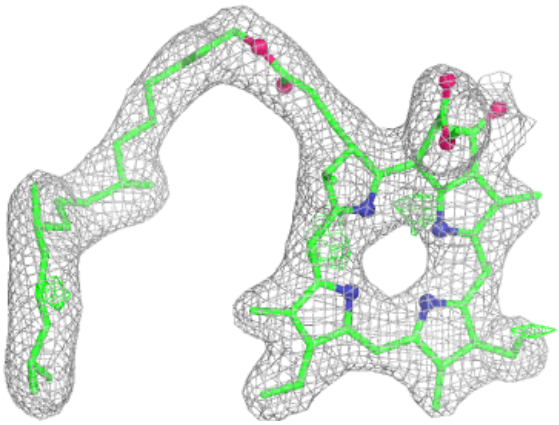


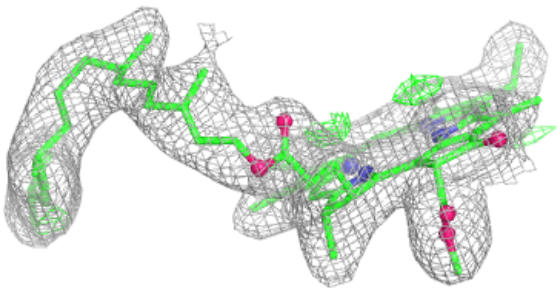


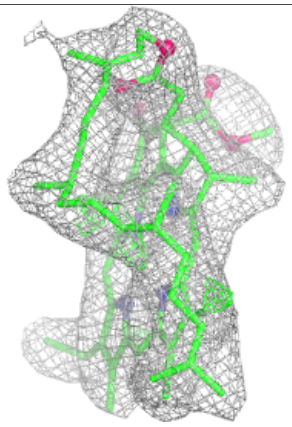


Electron density around PHO d 402 (A):

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

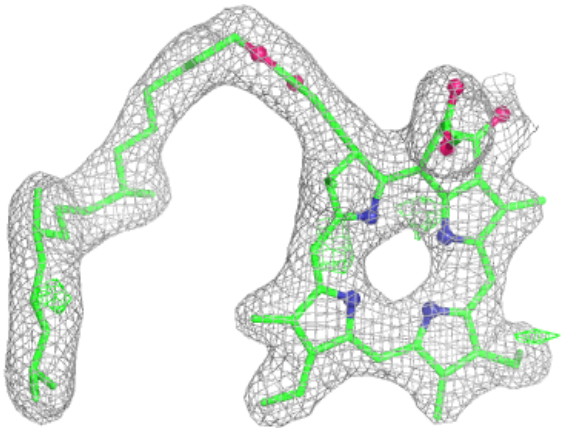


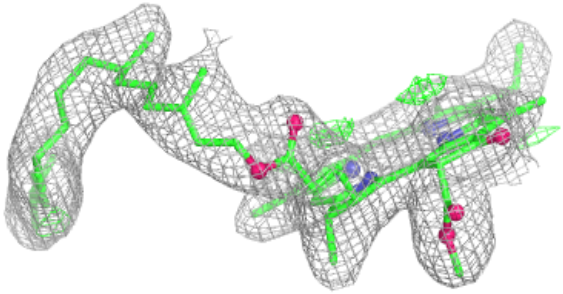


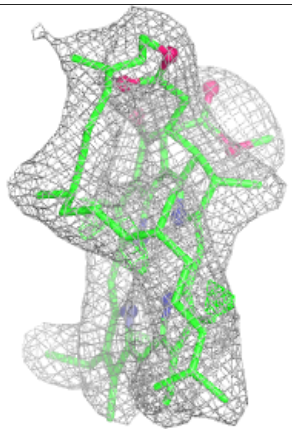


Electron density around PHO d 402 (B):

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

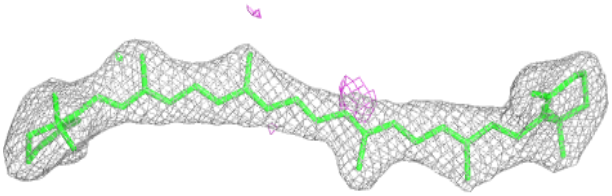


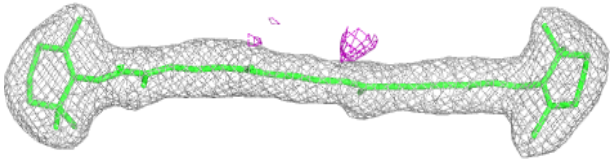


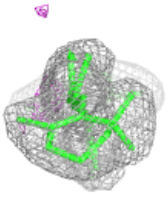


Electron density around BCR A 409:

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

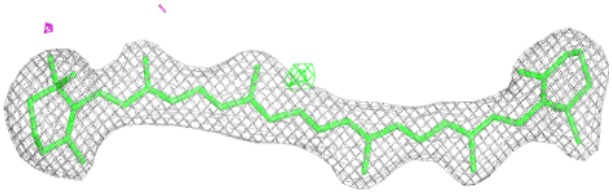


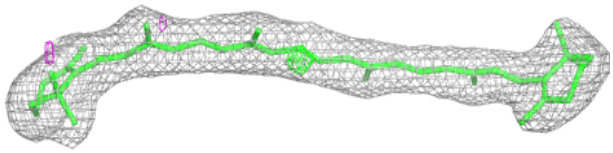


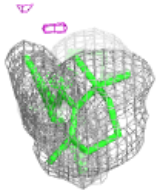


Electron density around BCR B 620:

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

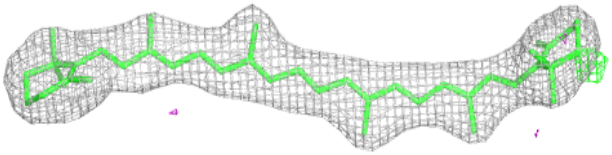


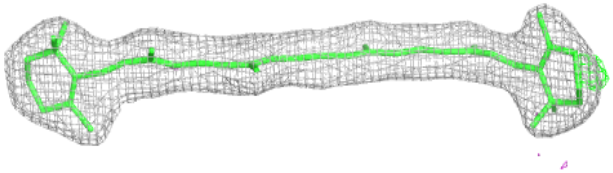


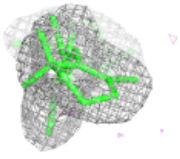


Electron density around BCR C 515:

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

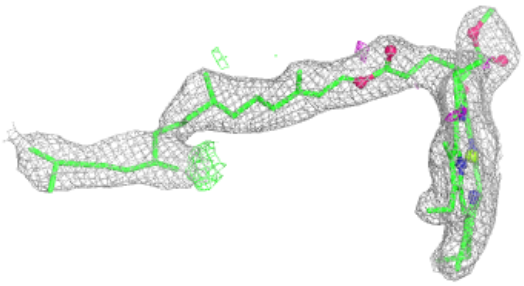


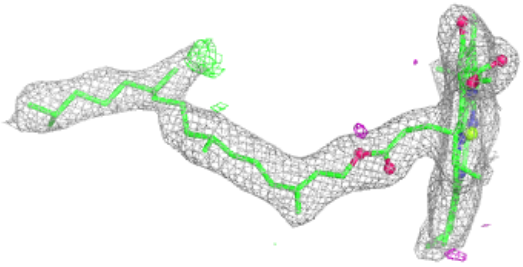


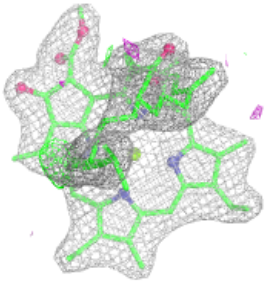


Electron density around CLA B 607:

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

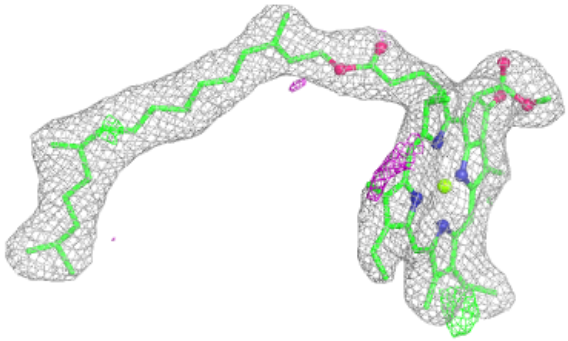


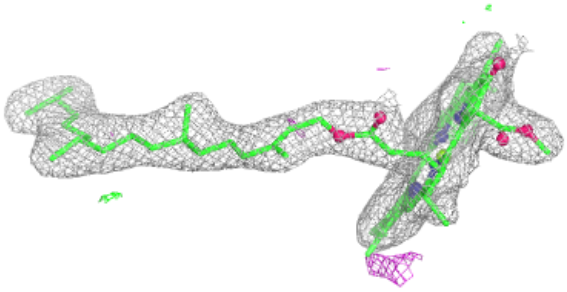


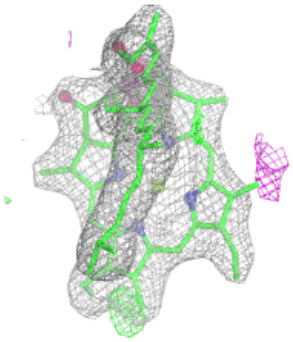


Electron density around CLA b 618:

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

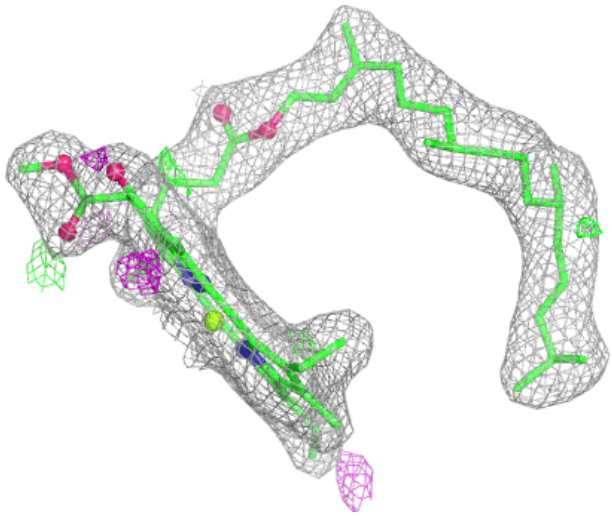


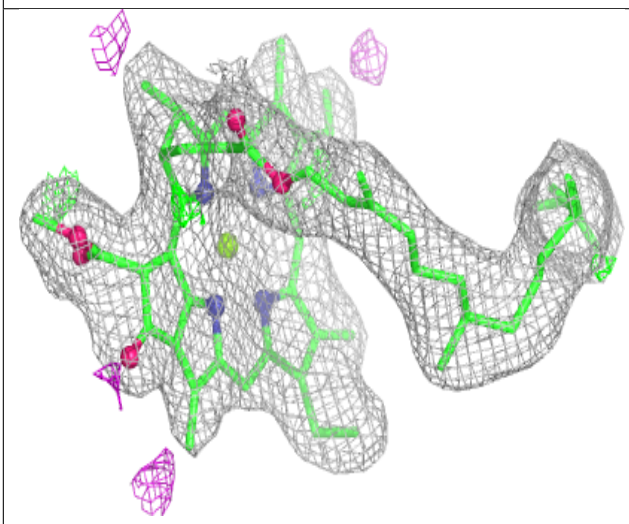


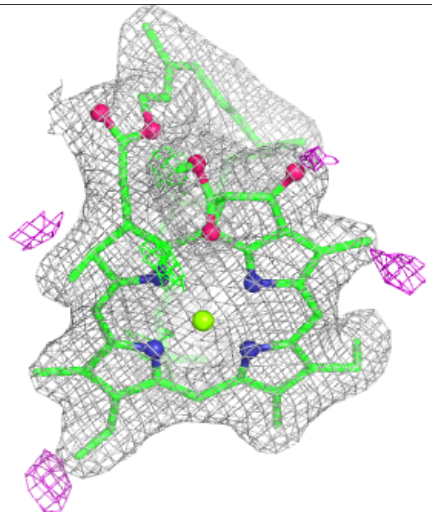


Electron density around CLA b 620:

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

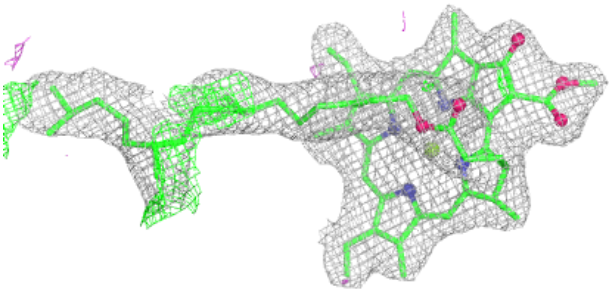


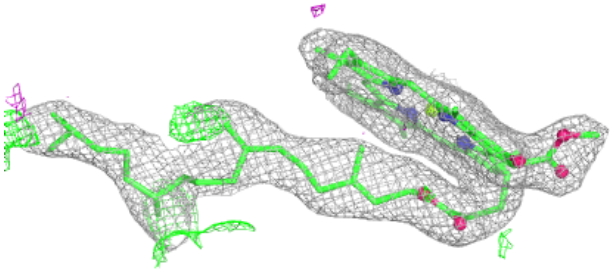


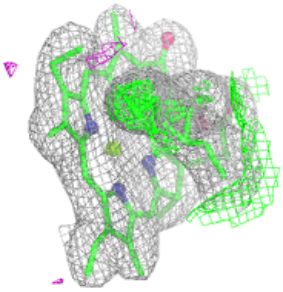


Electron density around CLA b 623:

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

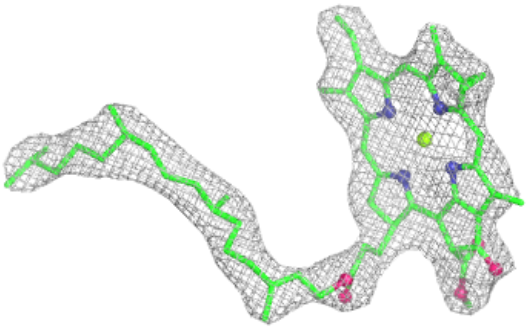


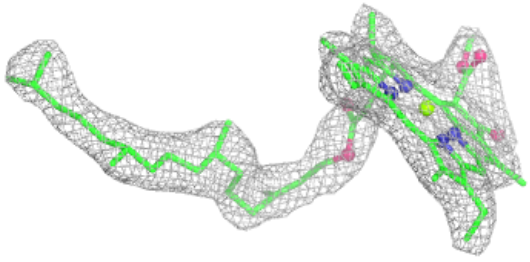


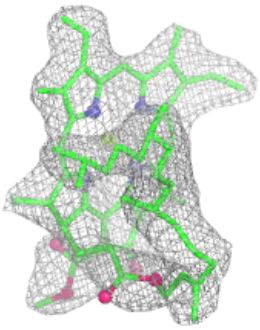


Electron density around CLA C 512:

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

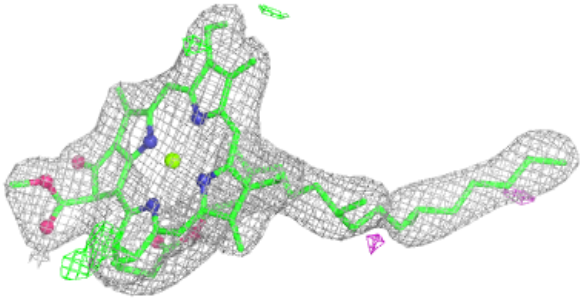


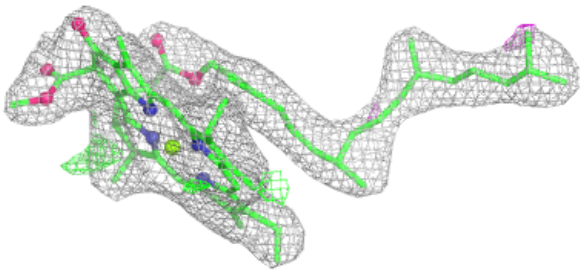


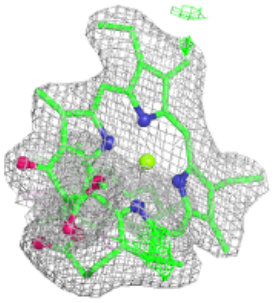


Electron density around CLA C 506:

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

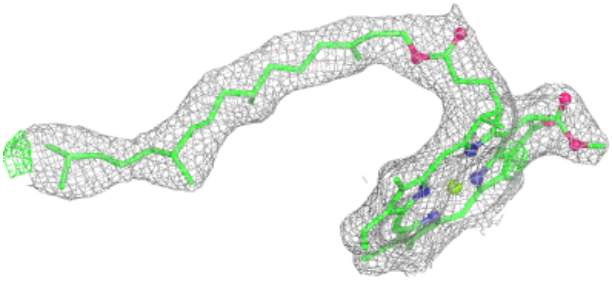


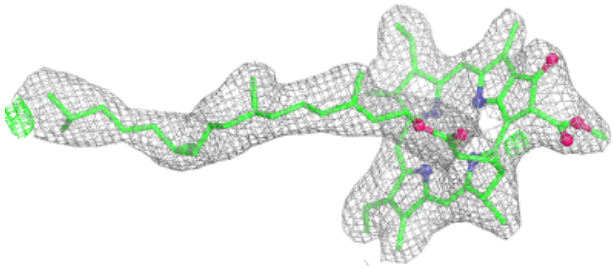


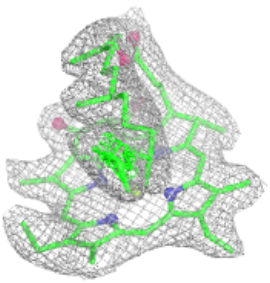


Electron density around CLA c 508:

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

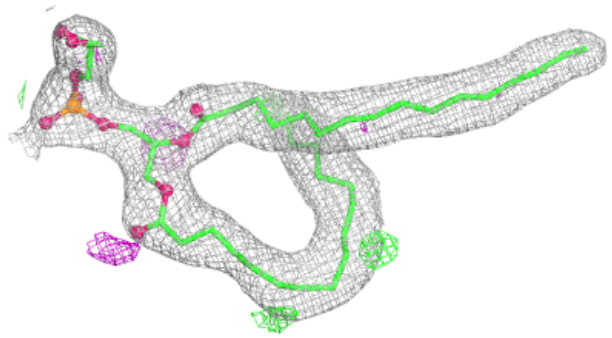


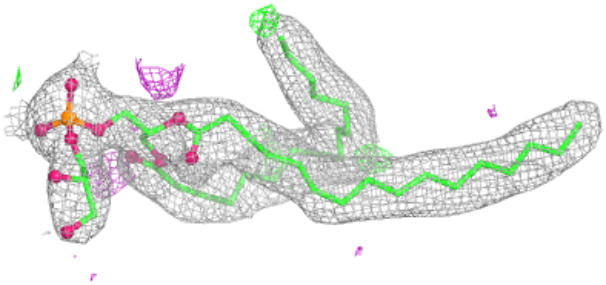




Electron density around LHG D 410:

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

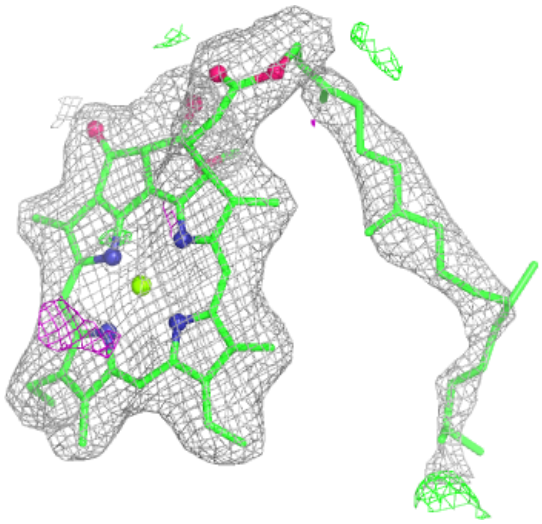


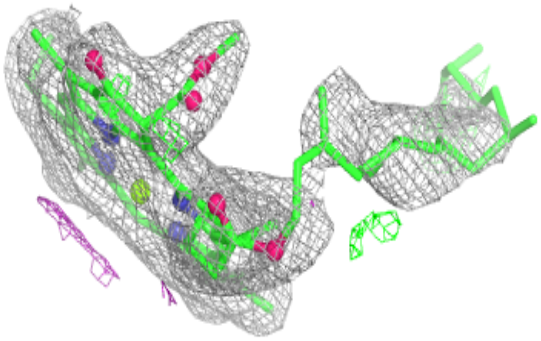


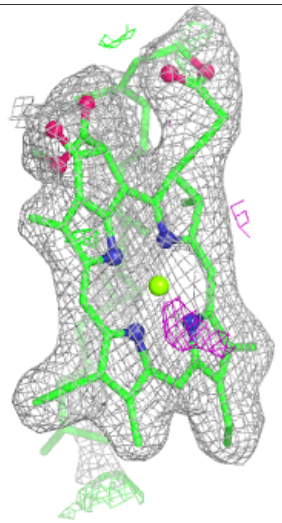


Electron density around CLA B 617:

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

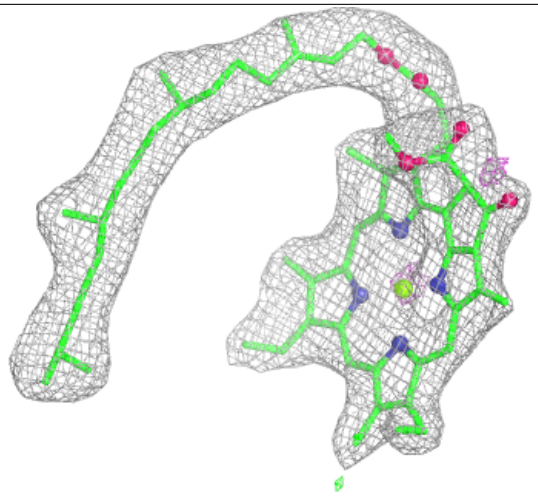


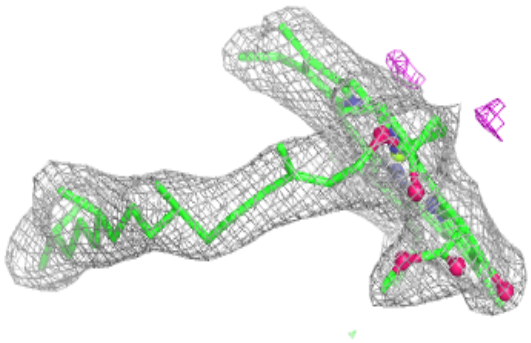


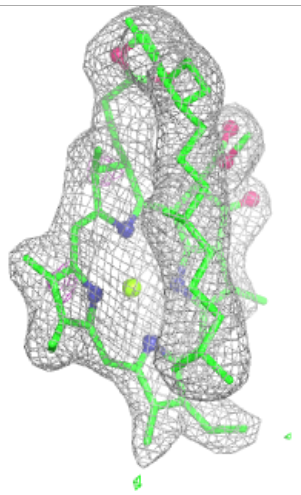


Electron density around CLA c 511:

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

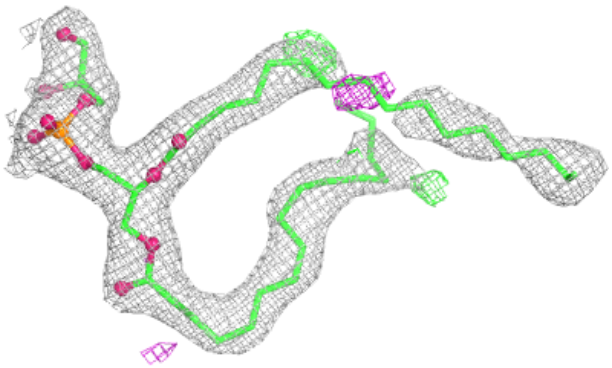


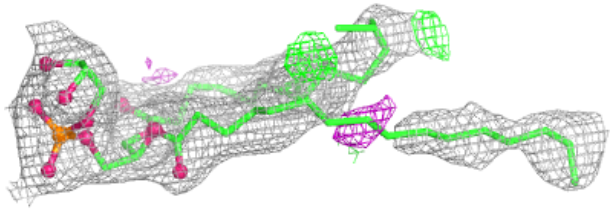


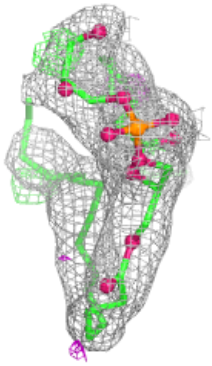


Electron density around LHG d 411:

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

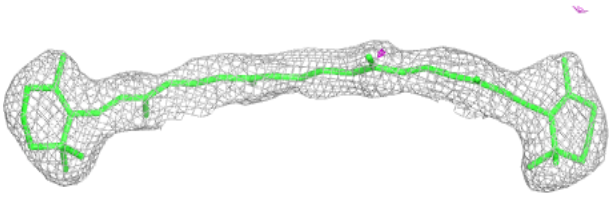


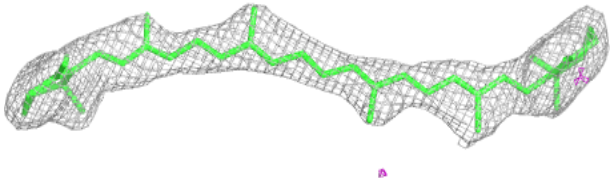


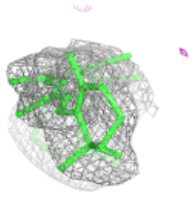


Electron density around BCR k 102:

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

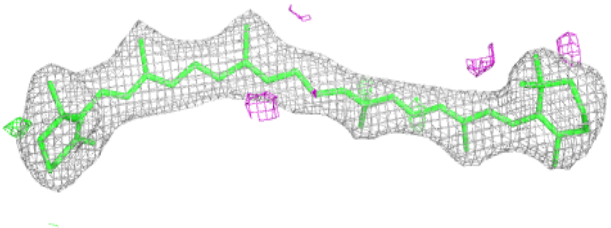


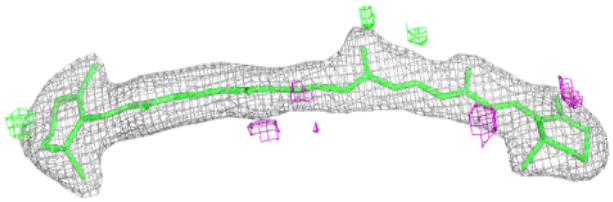


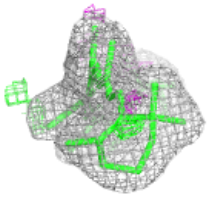


Electron density around BCR t 101:

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

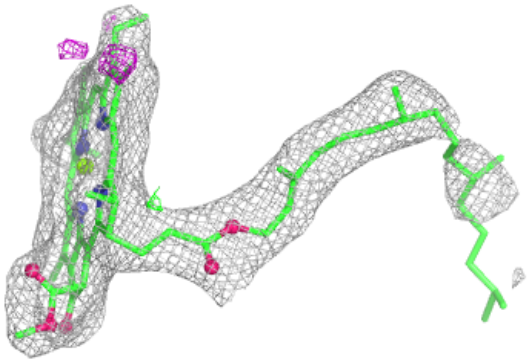


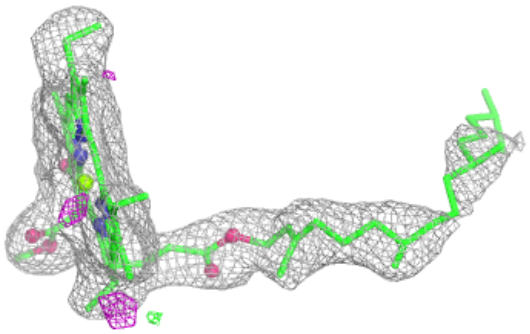


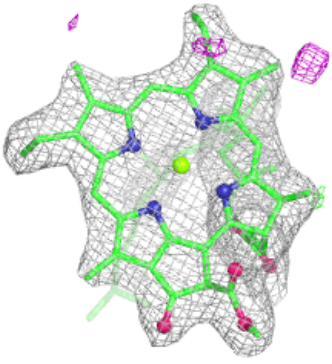


Electron density around CLA D 406:

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

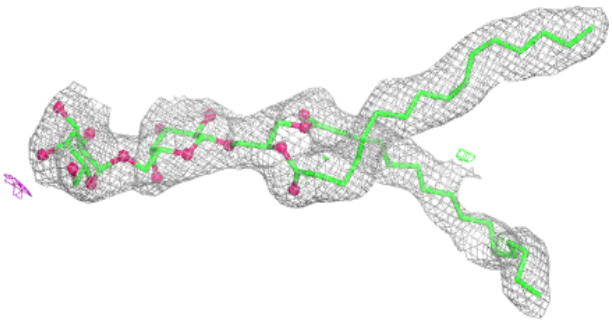


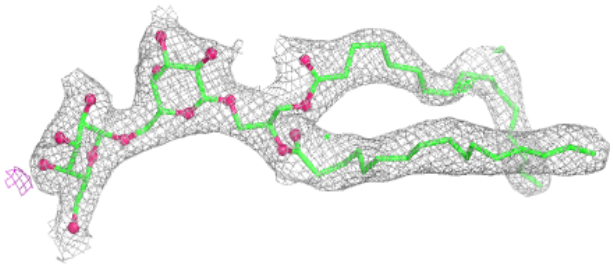


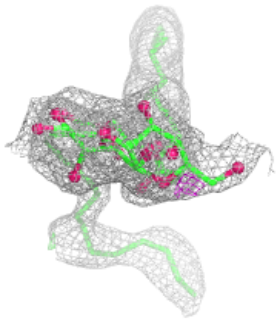


Electron density around DGD c 519:

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

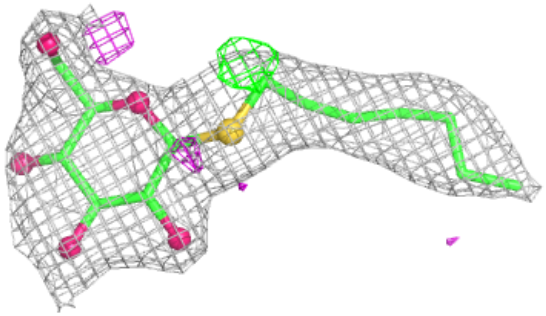


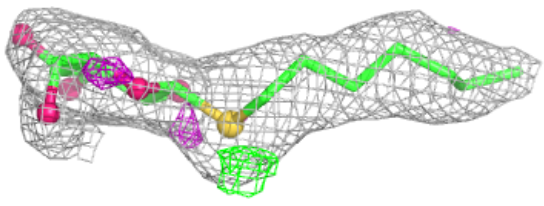


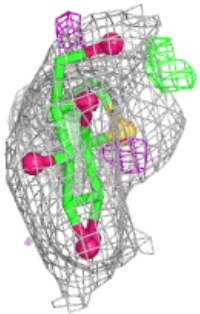


Electron density around HTG B 622:

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

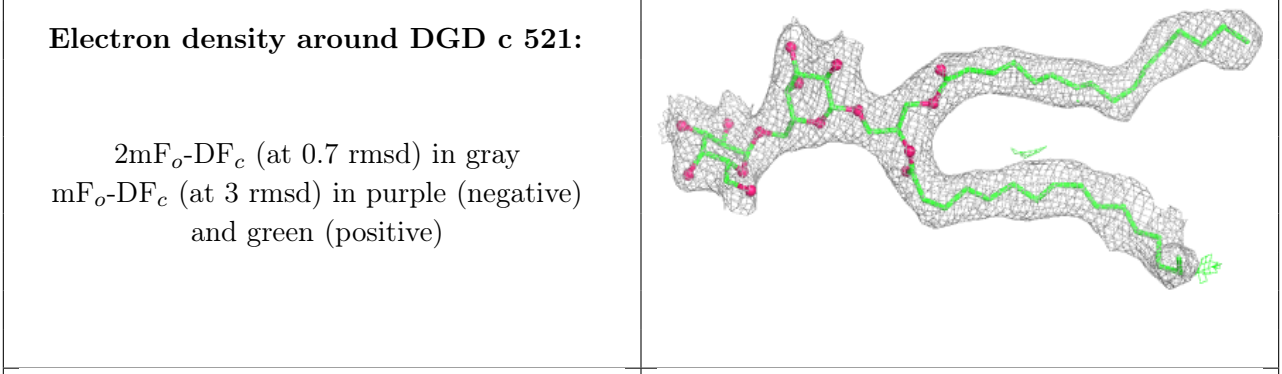






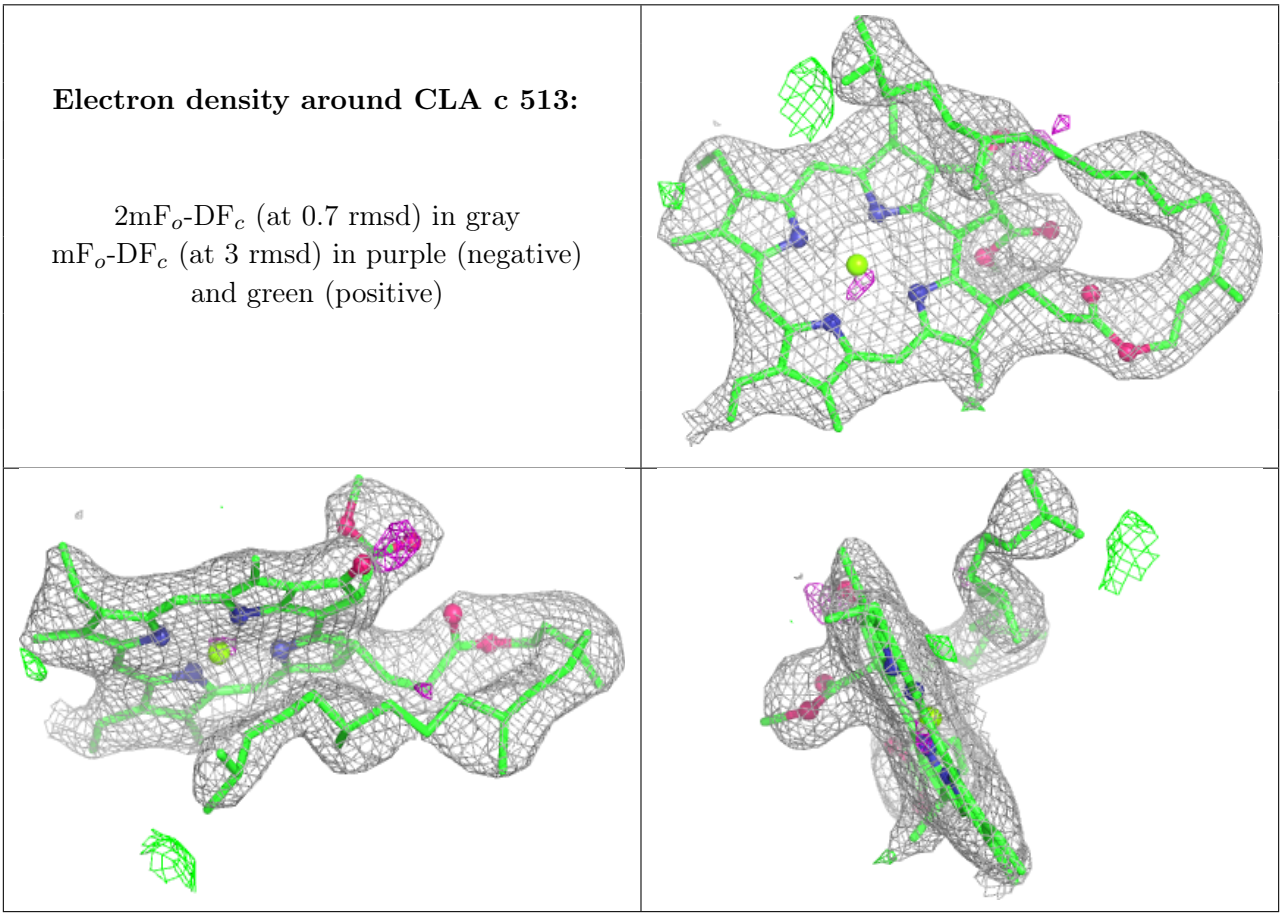
Electron density around DGD c 521:

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



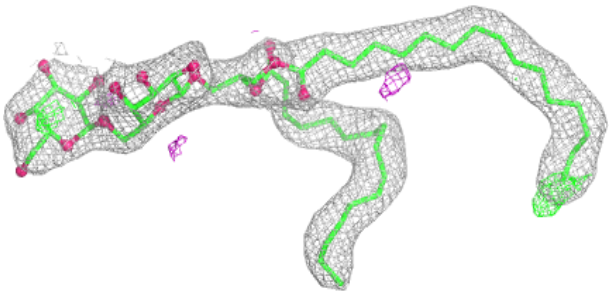
Electron density around CLA c 513:

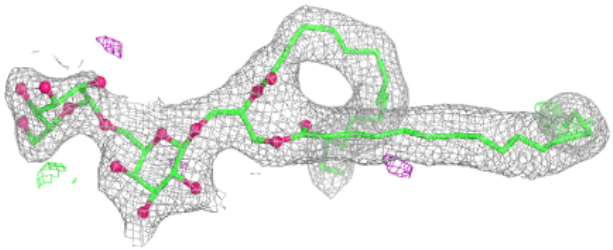
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

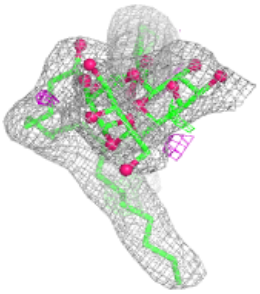


Electron density around DGD h 102:

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

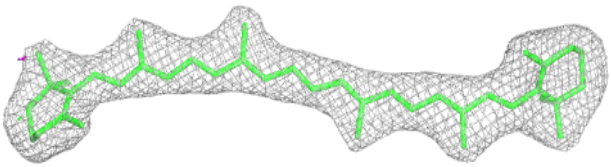


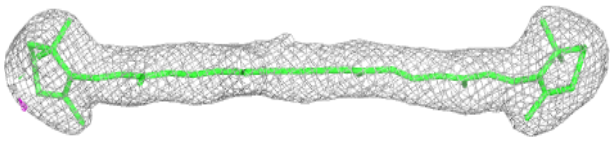


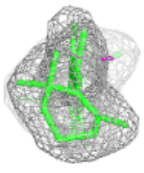


Electron density around BCR B 619:

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

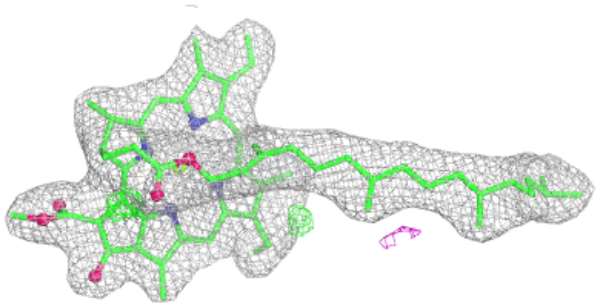


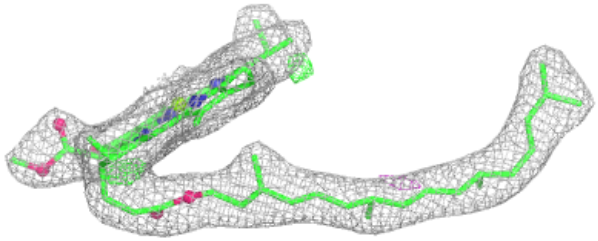


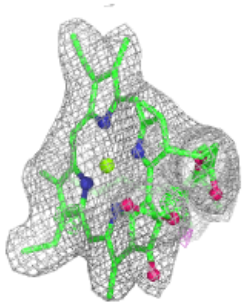


Electron density around CLA b 617:

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

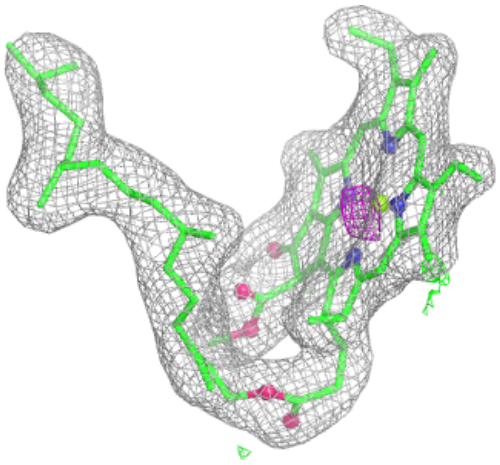


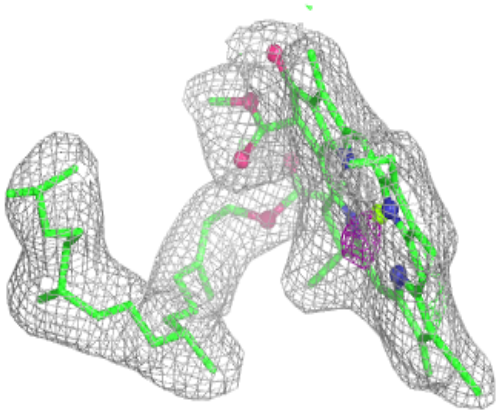


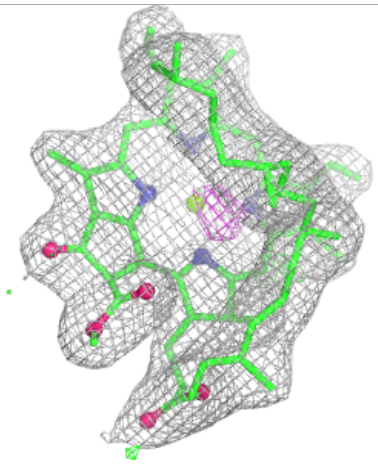


Electron density around CLA B 614:

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

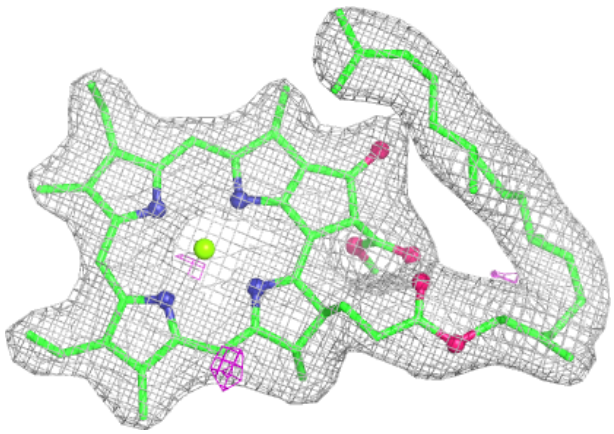


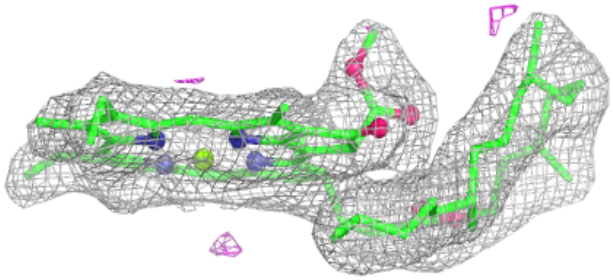


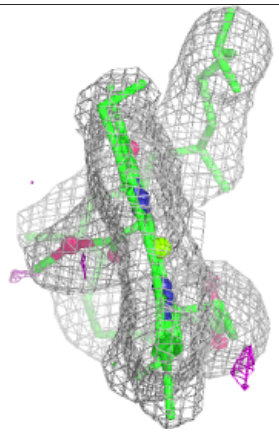


Electron density around CLA b 619:

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

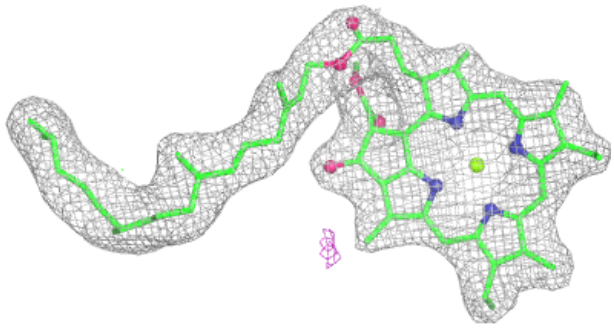


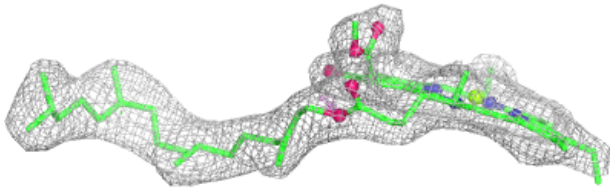


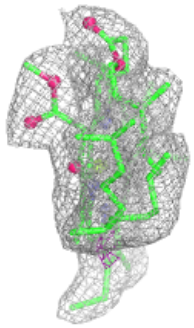


Electron density around CLA B 603:

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

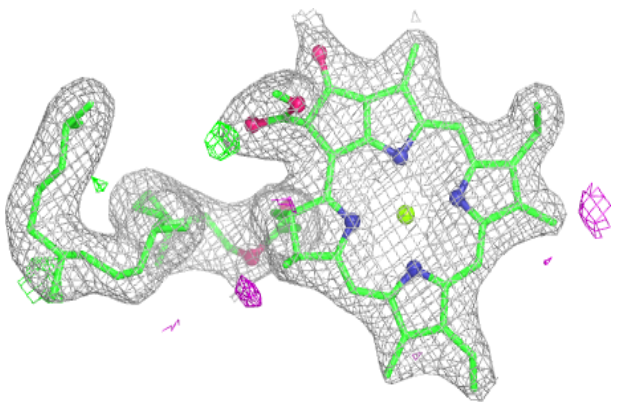


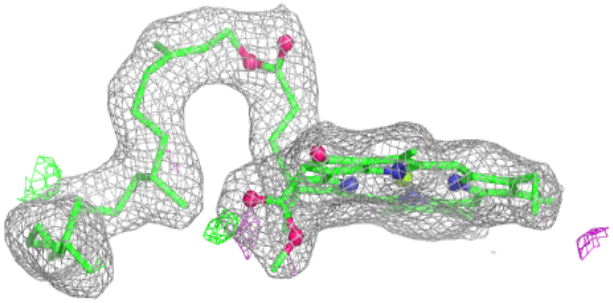


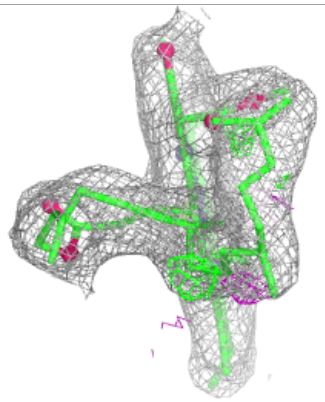


Electron density around CLA b 621:

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

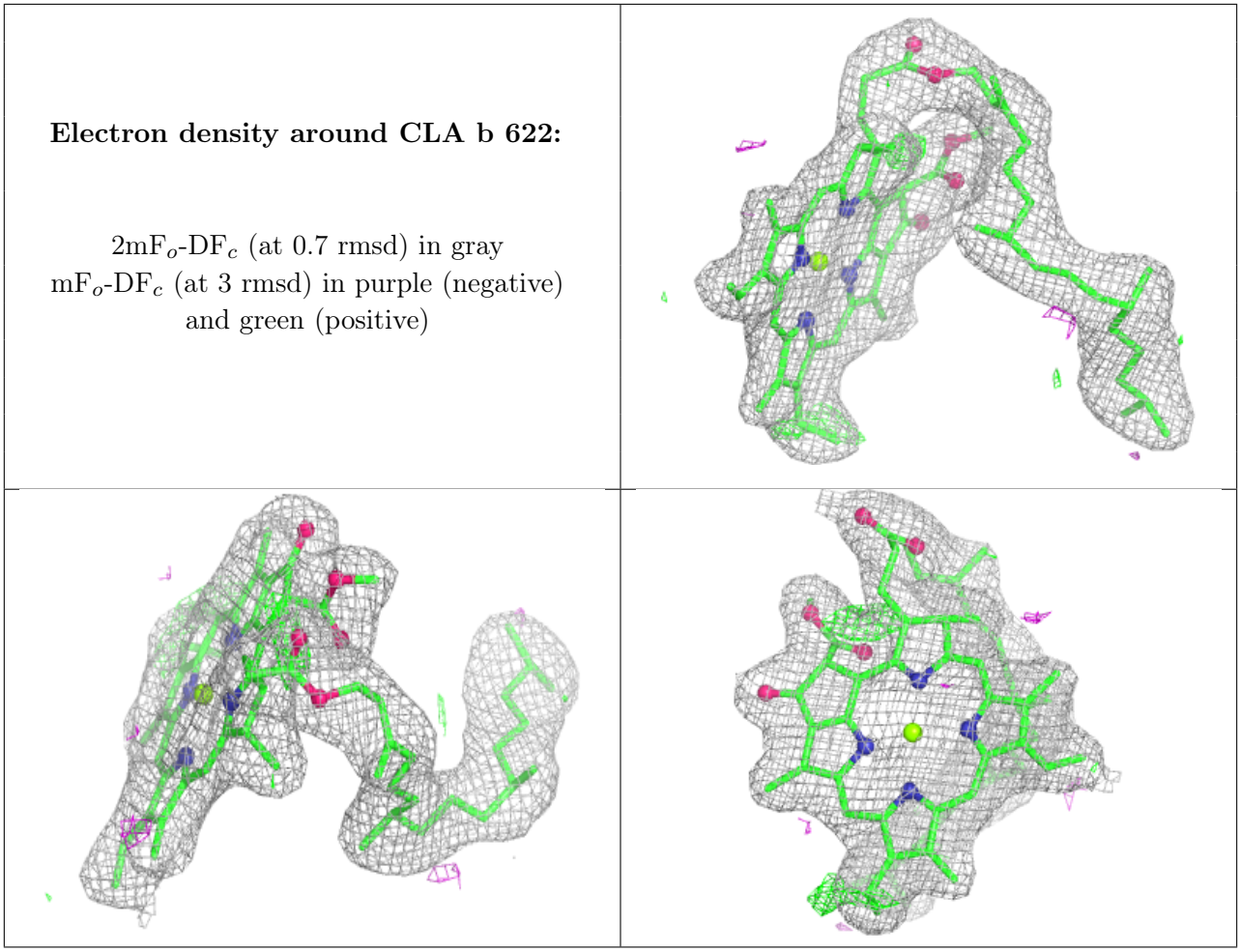






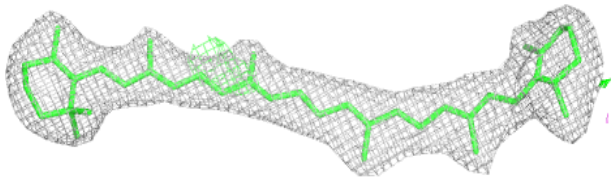
Electron density around CLA b 622:

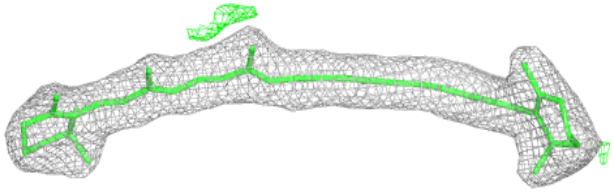
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

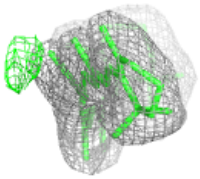


Electron density around BCR T 103:

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

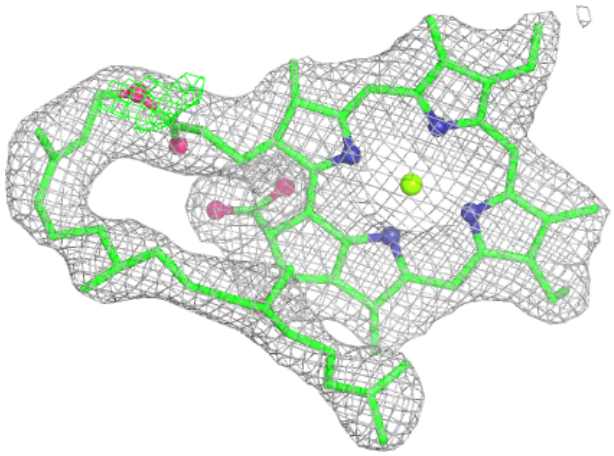


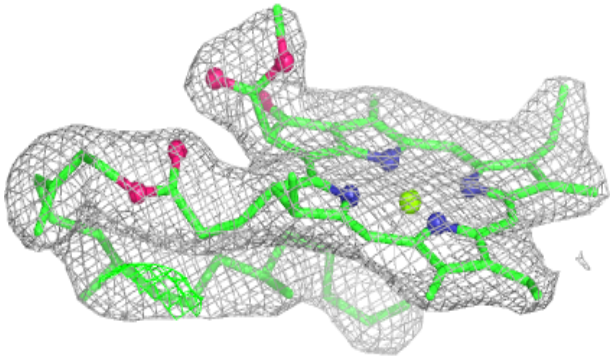




Electron density around CLA C 510:

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

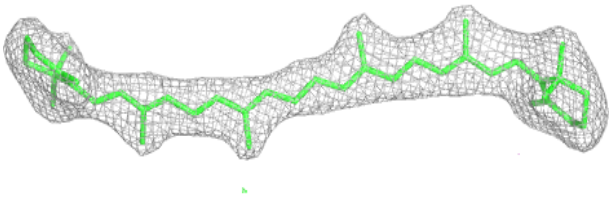


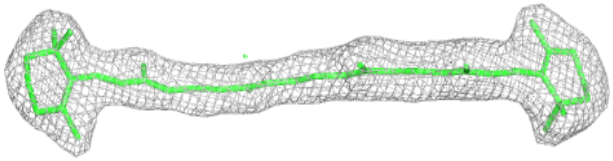


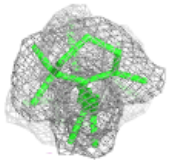


Electron density around BCR a 412:

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

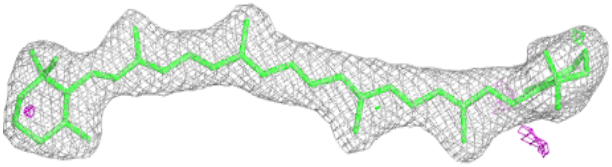


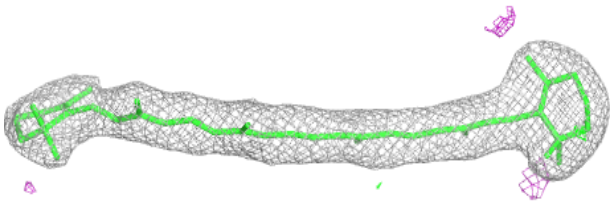


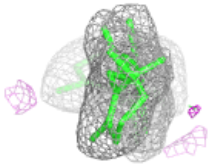


Electron density around BCR b 626:

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

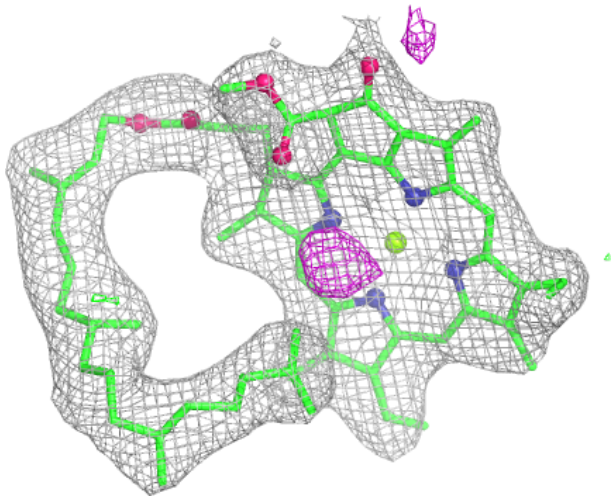


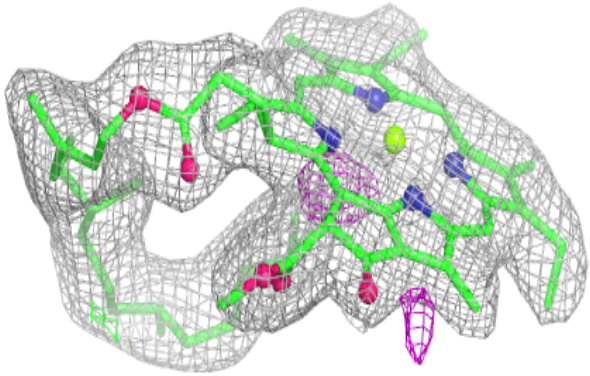


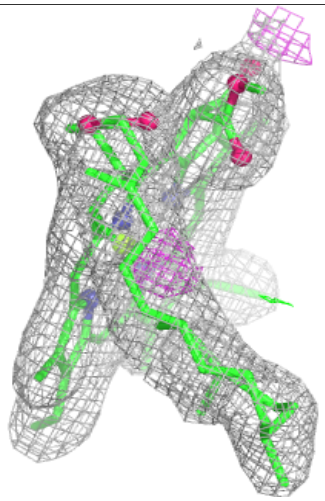


Electron density around CLA b 624:

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

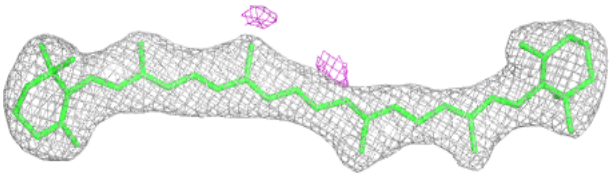


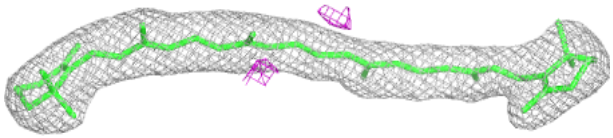


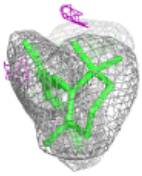


Electron density around BCR b 628:

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

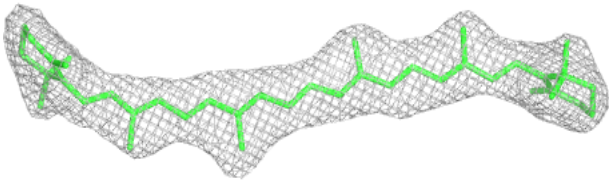


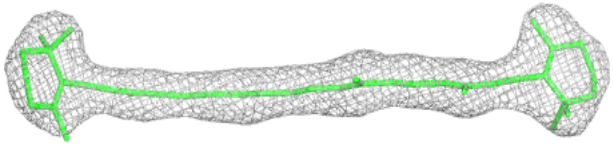


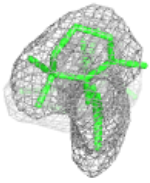


Electron density around BCR c 518:

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

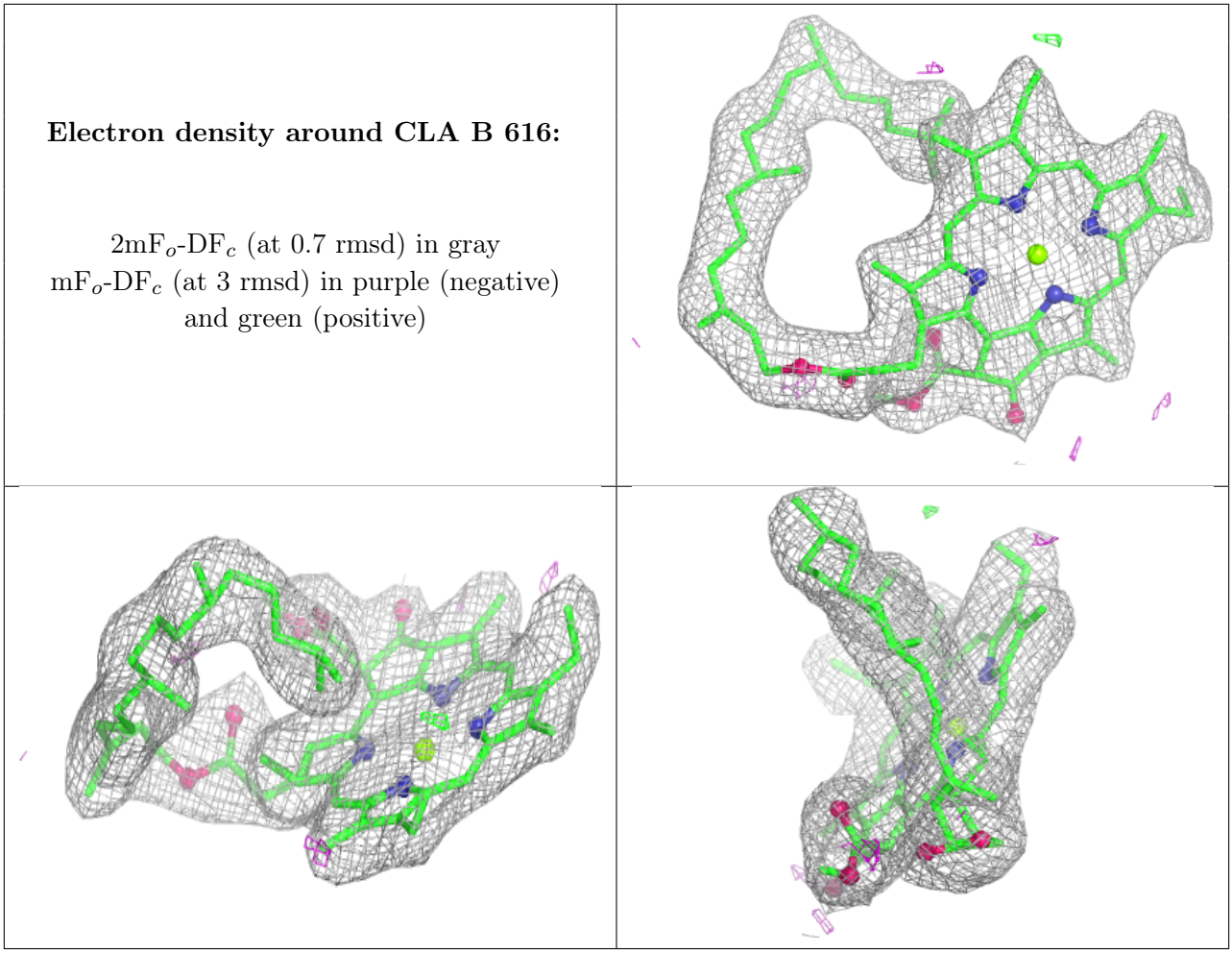






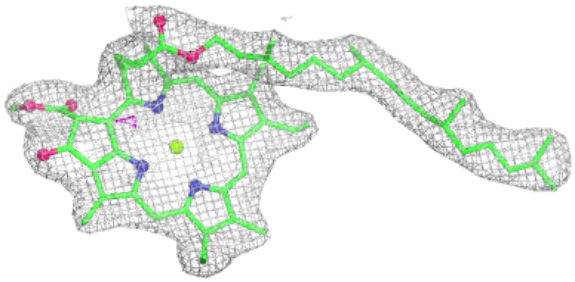
Electron density around CLA B 616:

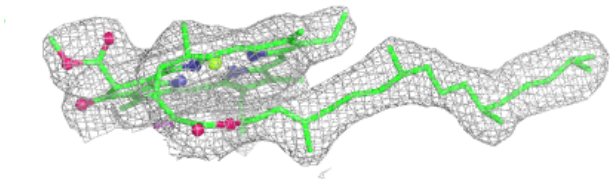
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

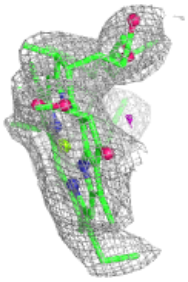


Electron density around CLA c 505:

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

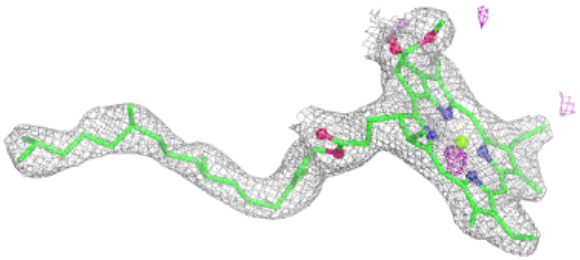


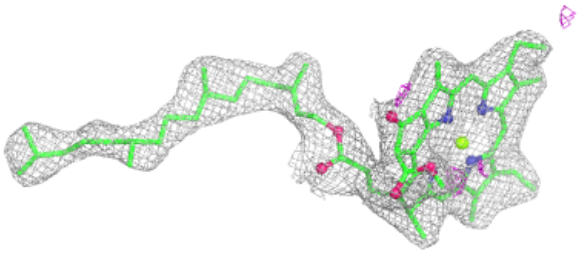


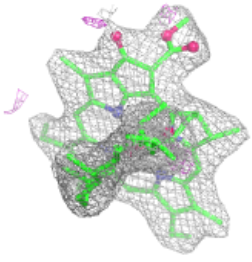


Electron density around CLA c 506:

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

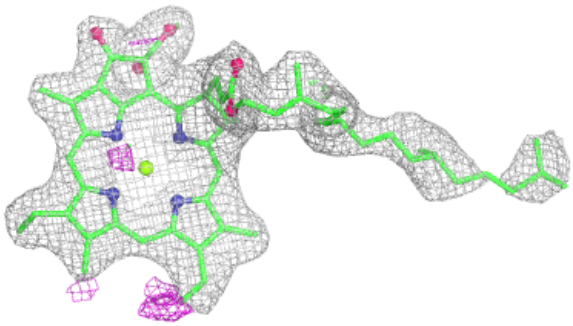


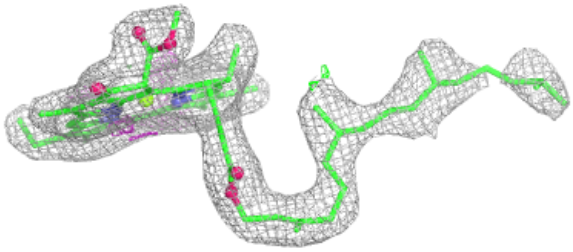


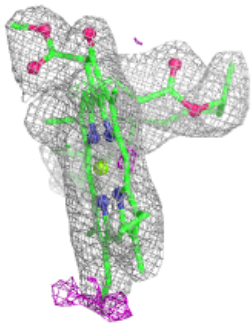


Electron density around CLA A 406:

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

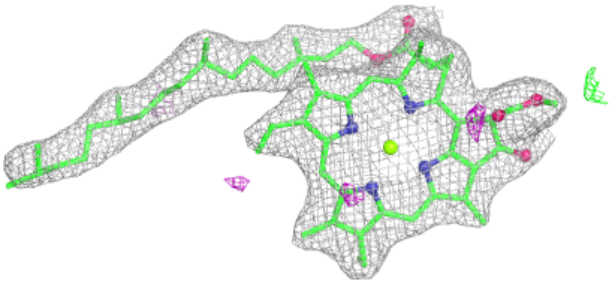


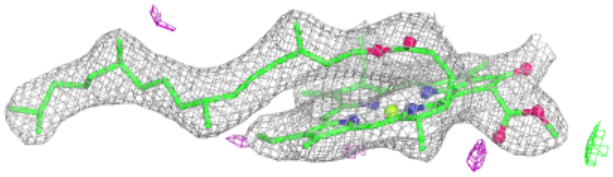


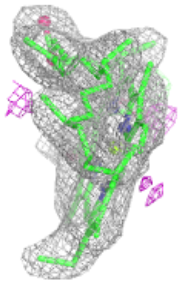


Electron density around CLA C 502:

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

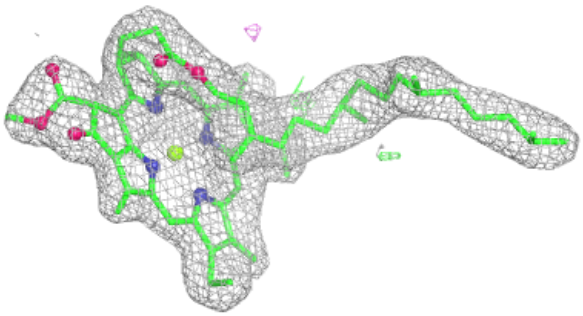


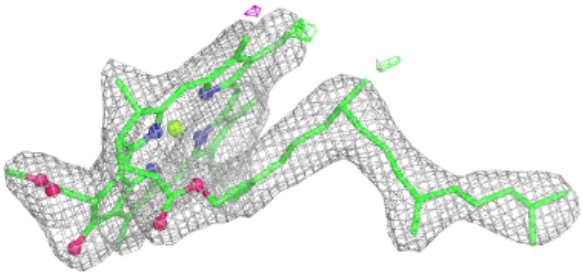


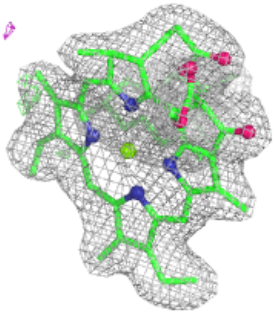


Electron density around CLA c 509:

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

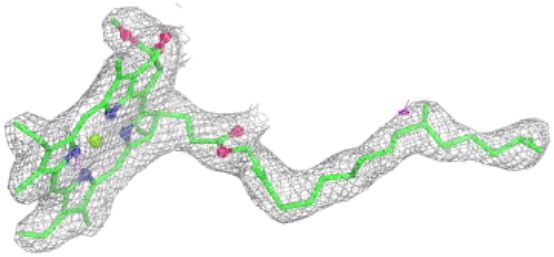


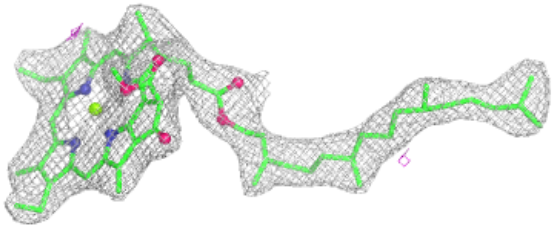


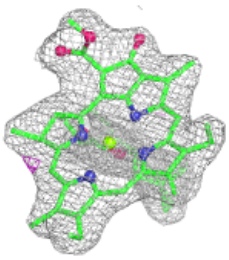


Electron density around CLA C 503:

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

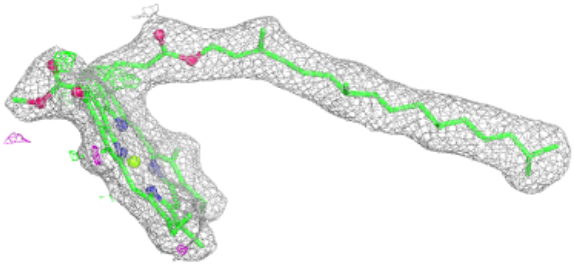


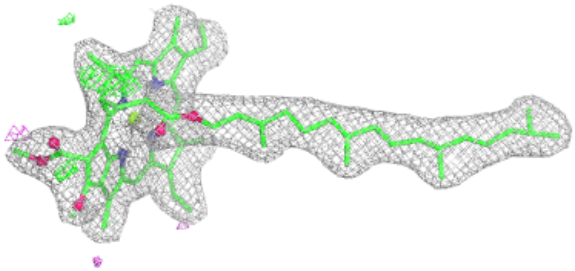


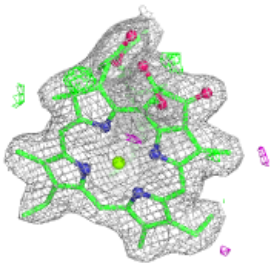


Electron density around CLA B 608:

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

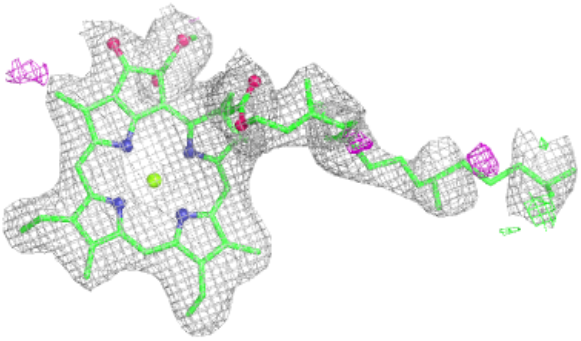


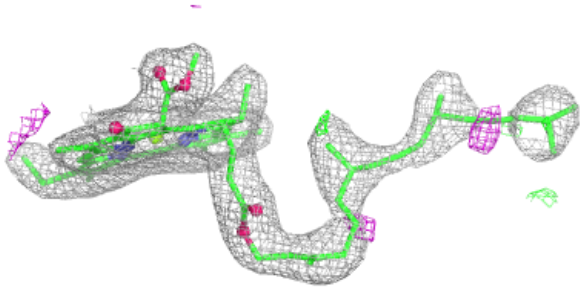


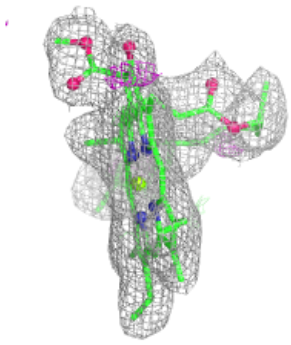


Electron density around CLA a 409:

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

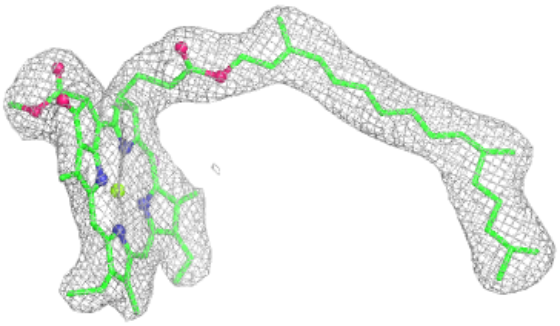


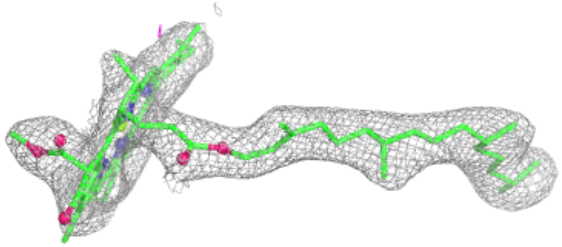


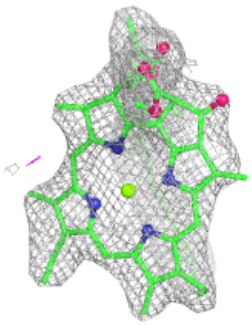


Electron density around CLA B 610:

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

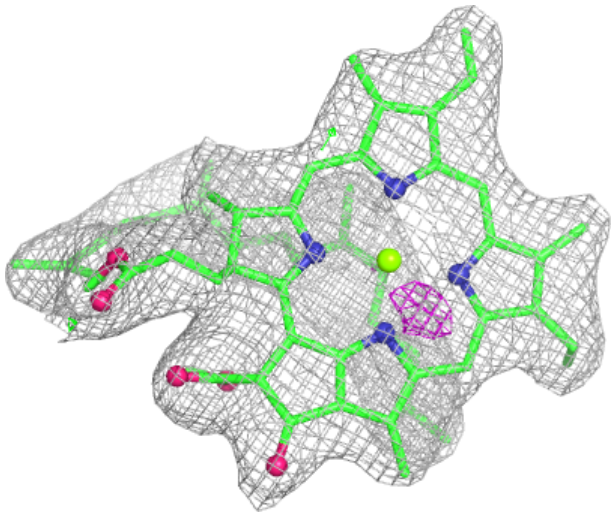


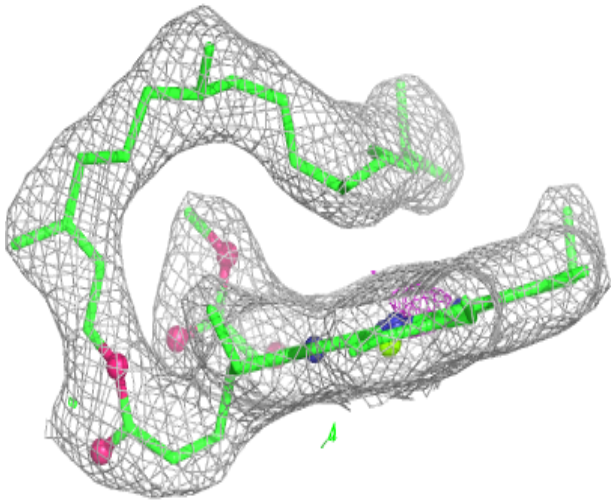


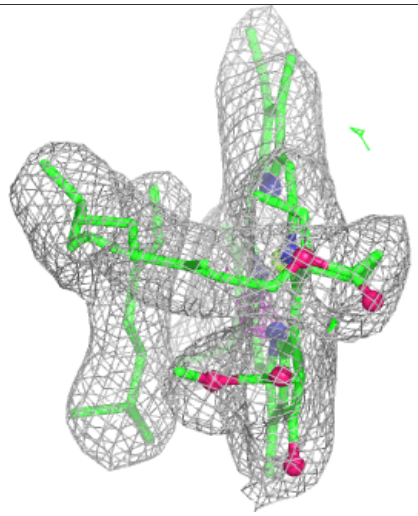


Electron density around CLA c 514:

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

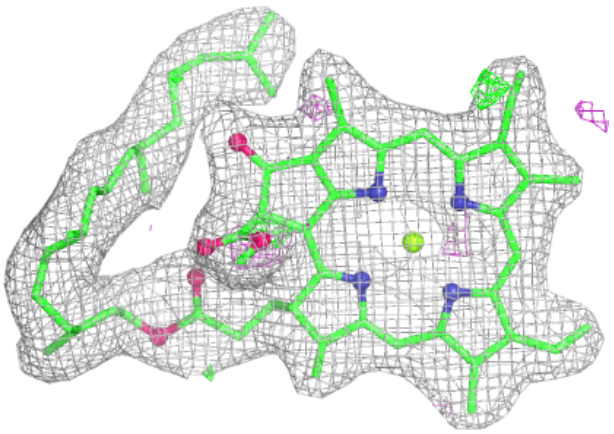


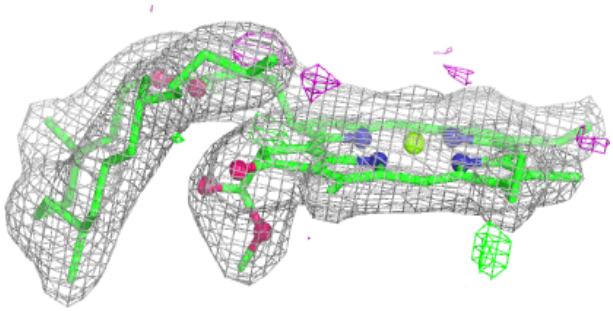


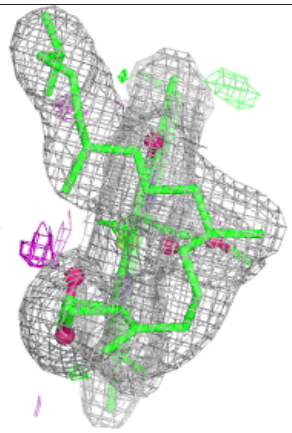


Electron density around CLA B 611:

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

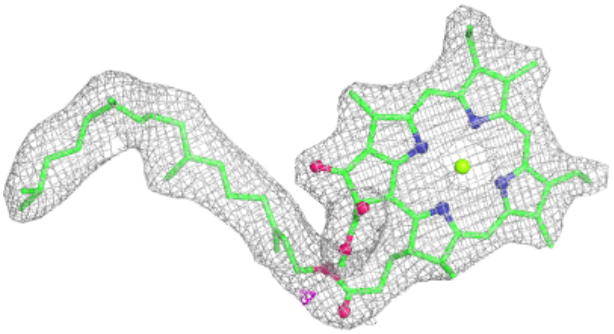


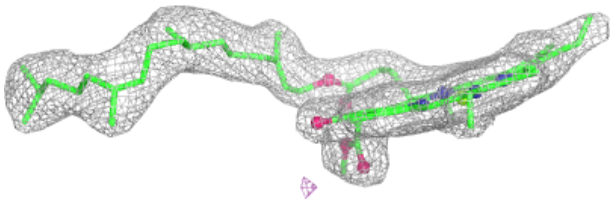


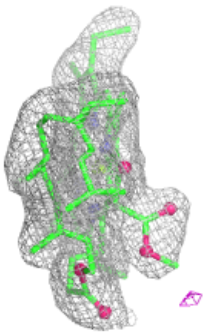


Electron density around CLA b 611:

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

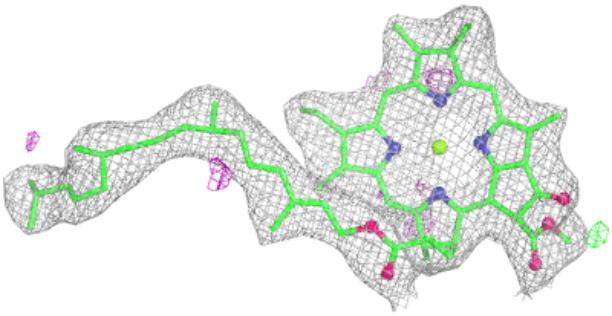


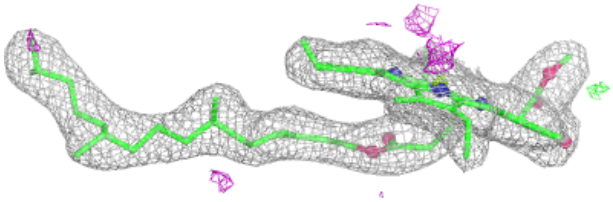


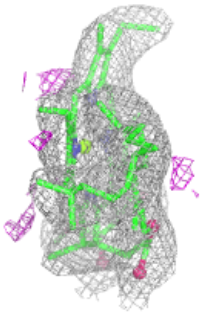


Electron density around CLA b 612:

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

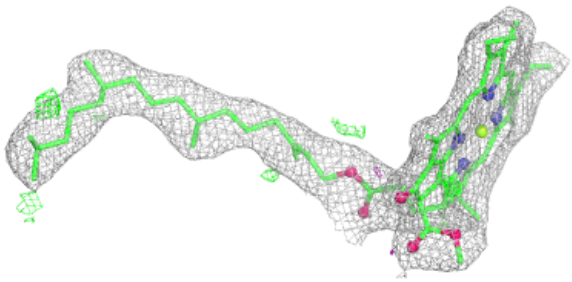


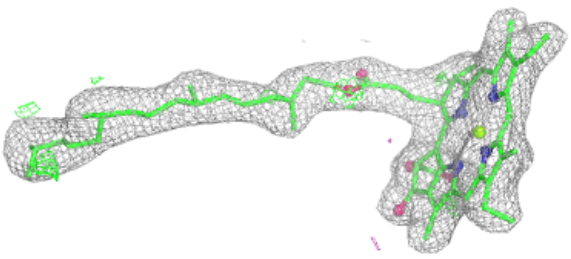




Electron density around CLA b 613:

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

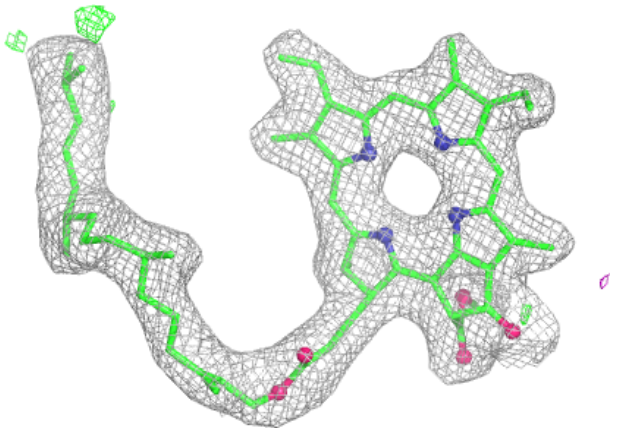


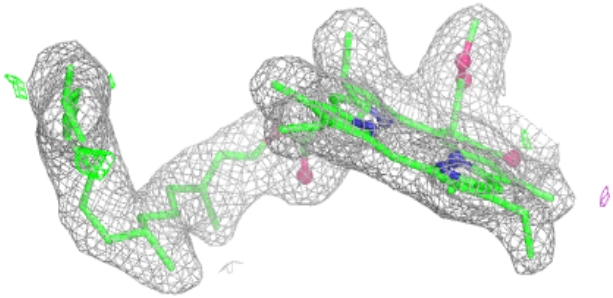




Electron density around PHO D 402 (A):

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

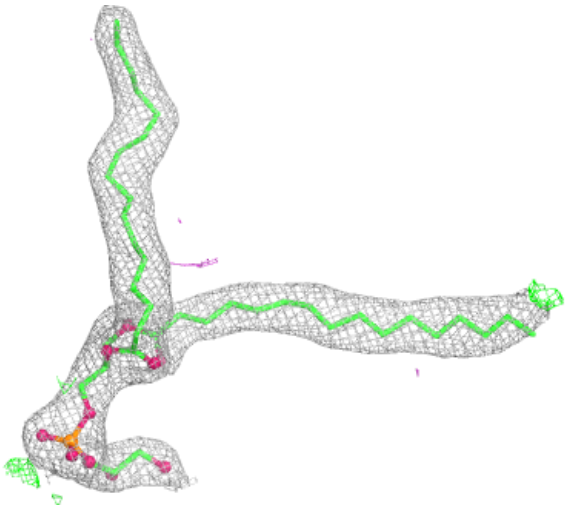


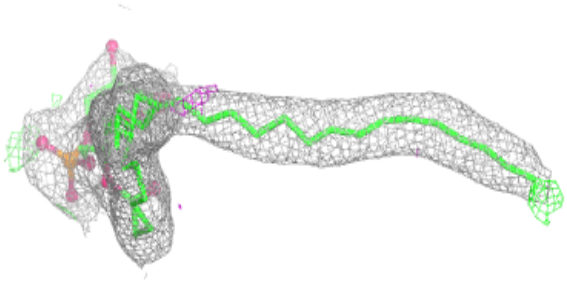


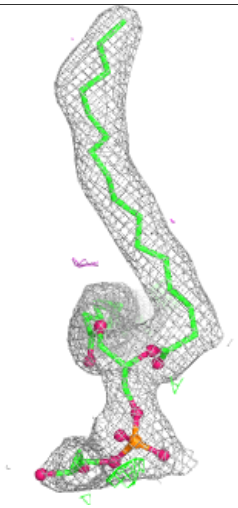


Electron density around LHG b 634:

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

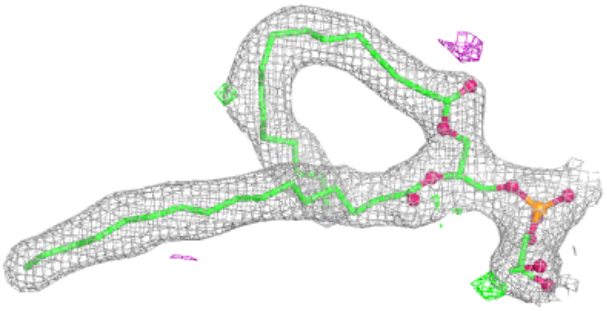


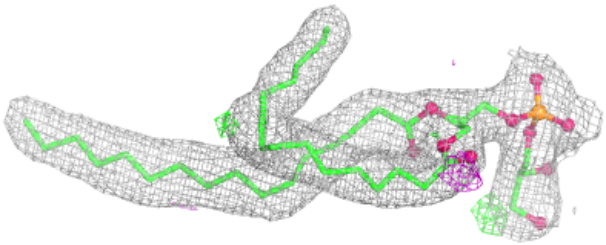


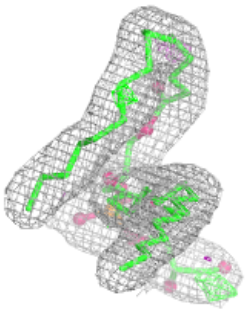


Electron density around LHG d 409:

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

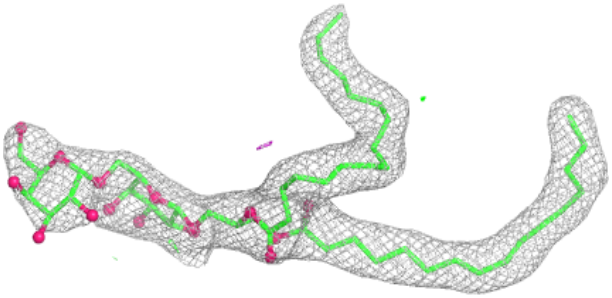


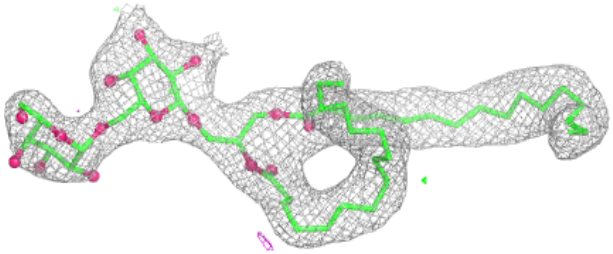


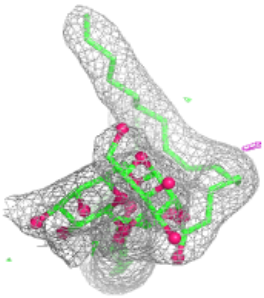


Electron density around DGD H 102:

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

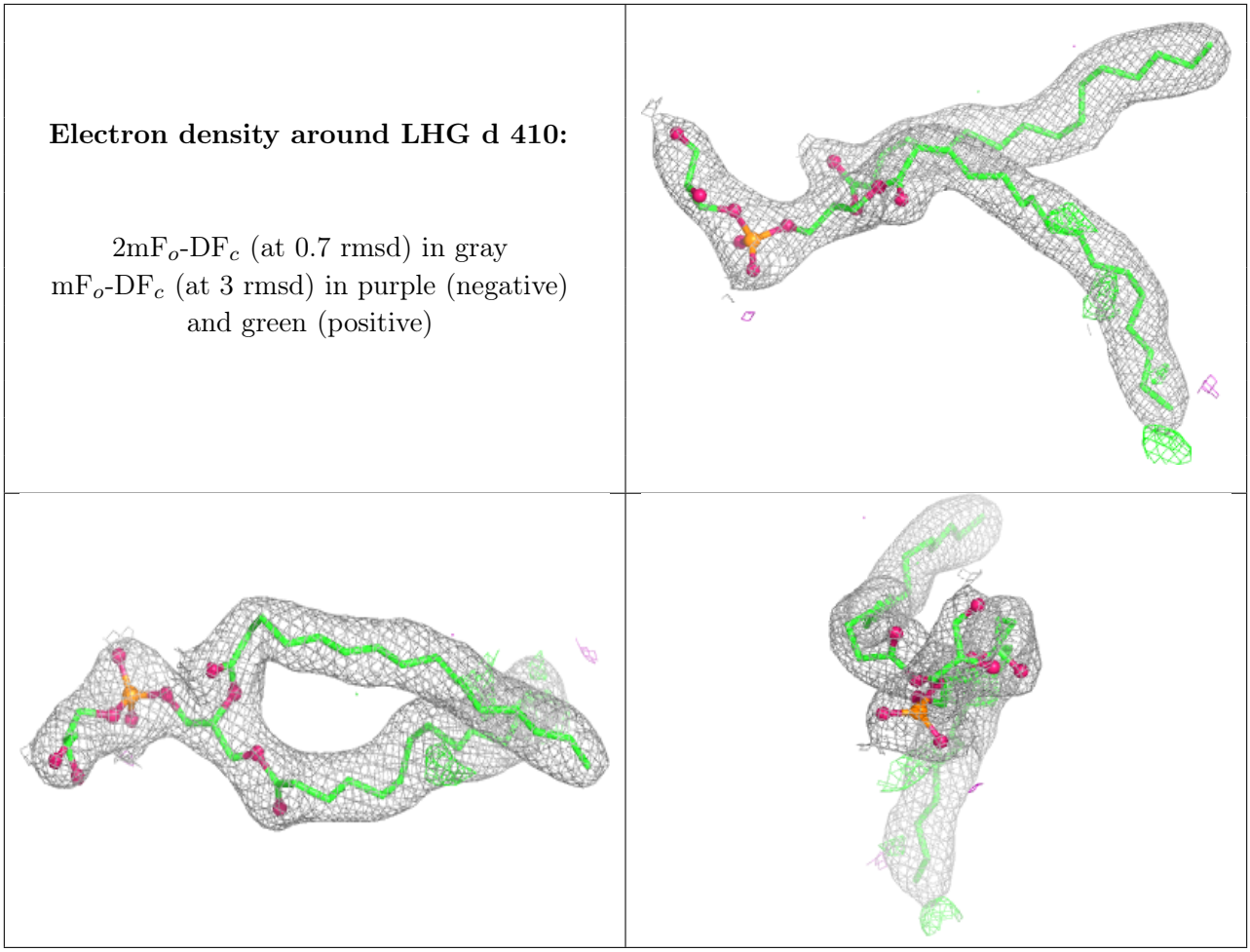






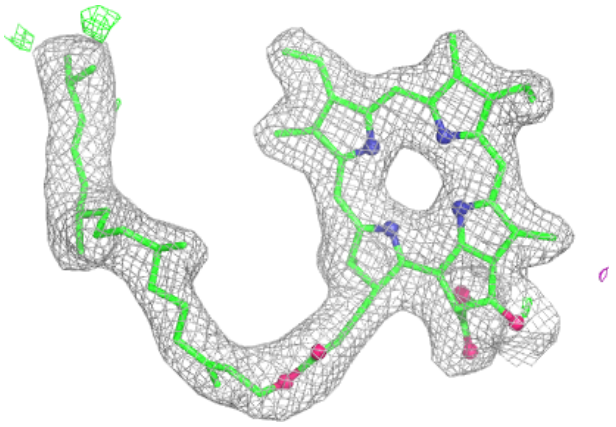
Electron density around LHG d 410:

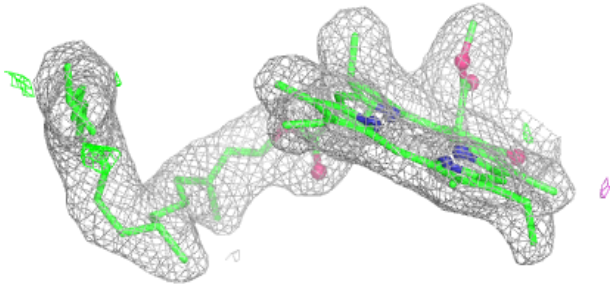
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO D 402 (B):

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

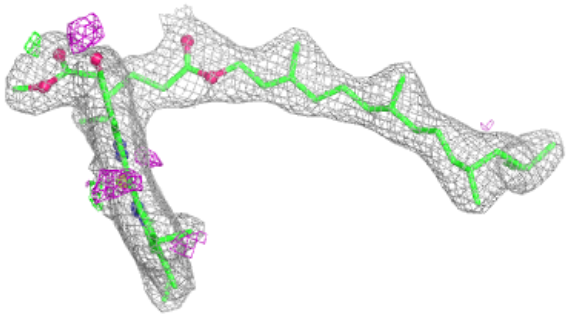


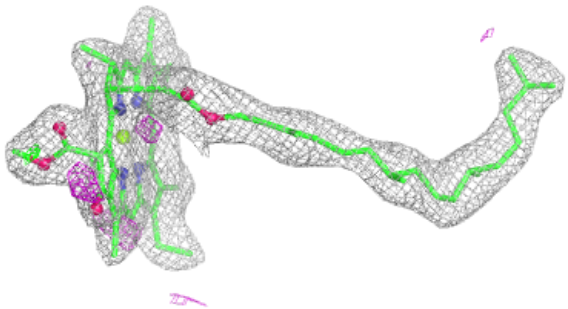


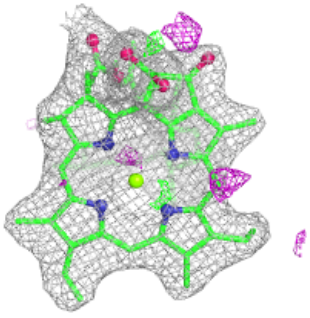


Electron density around CLA b 614:

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

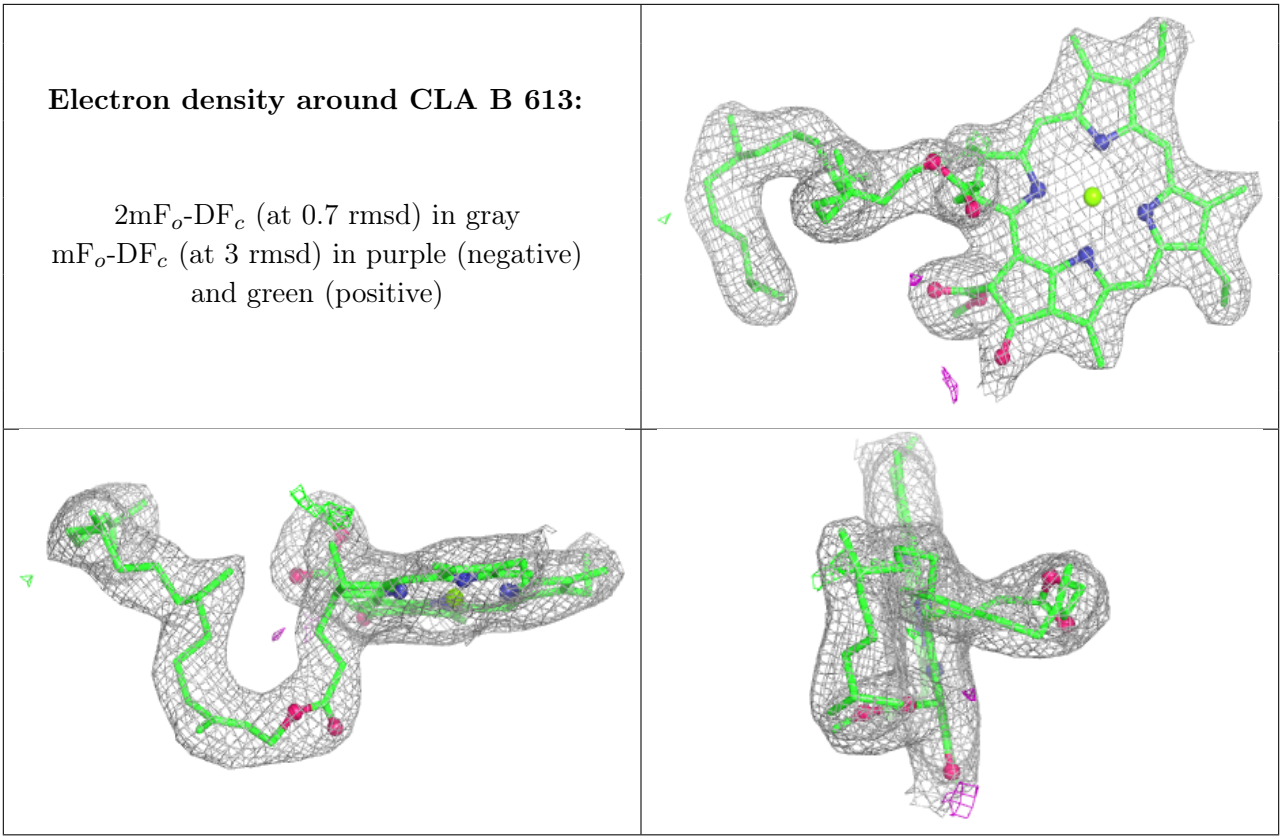






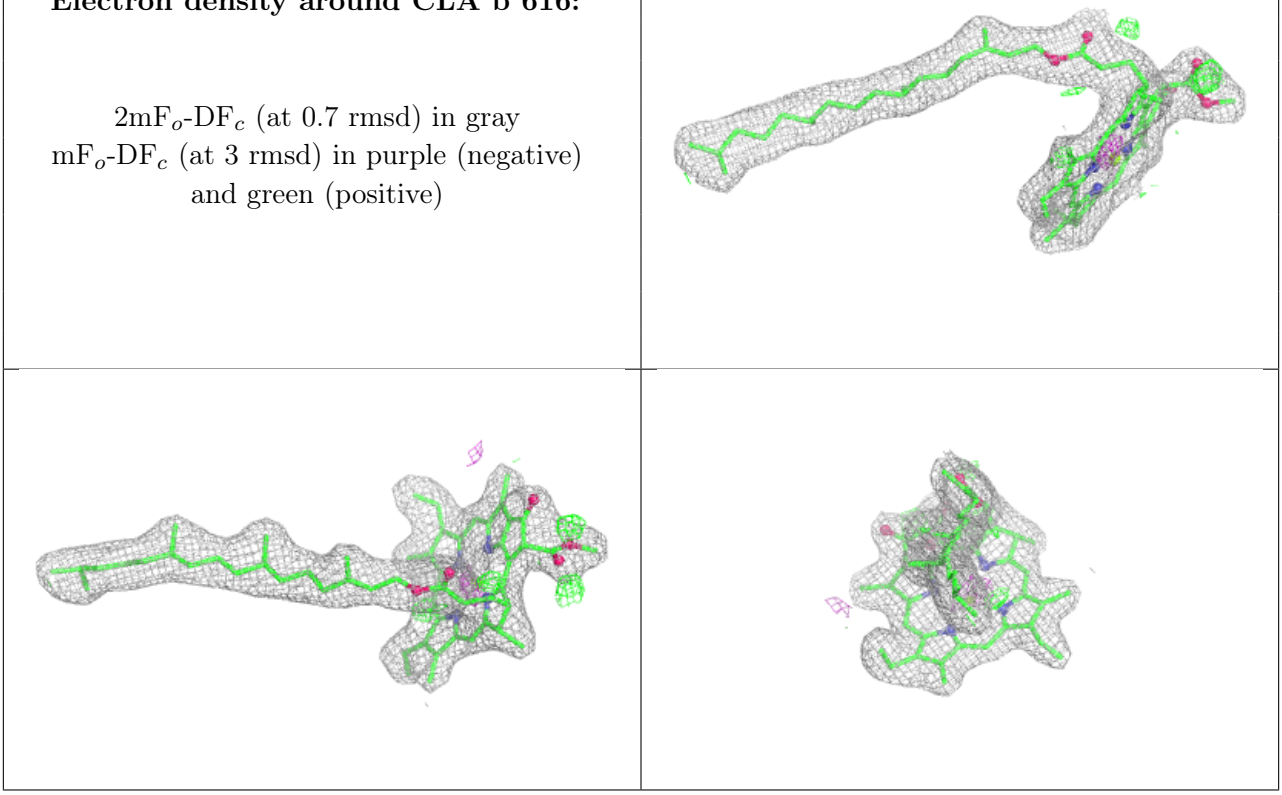
Electron density around CLA B 613:

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



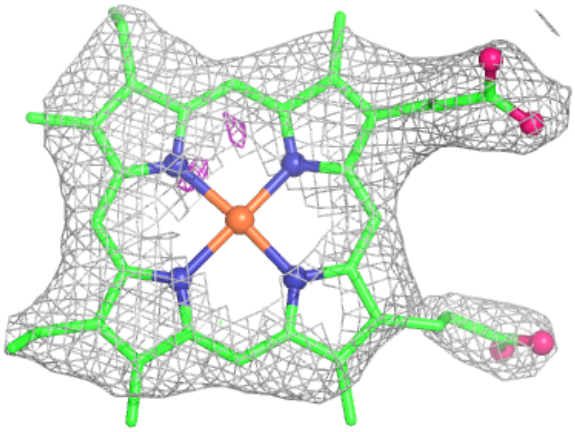
Electron density around CLA b 616:

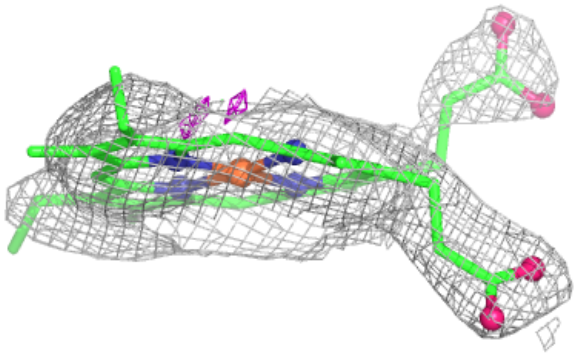
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

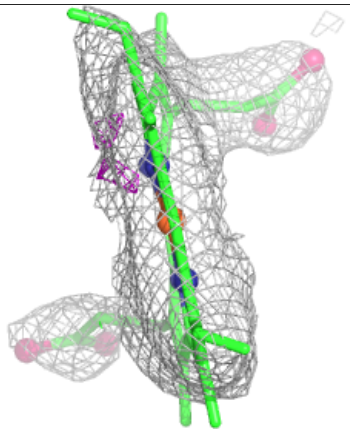


Electron density around HEM F 102:

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

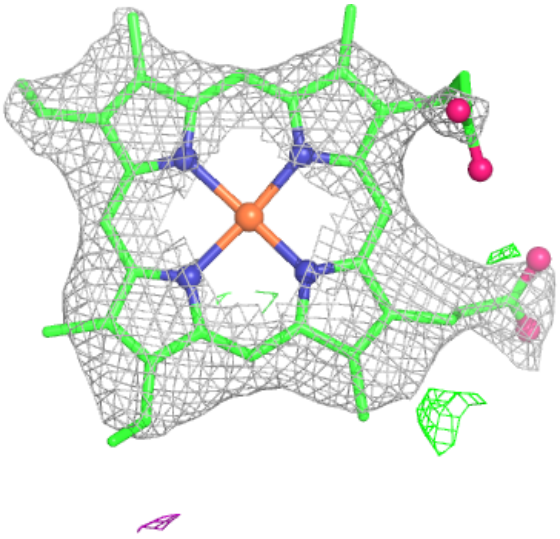


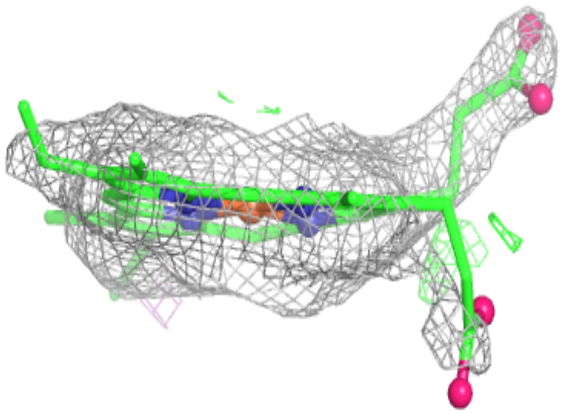


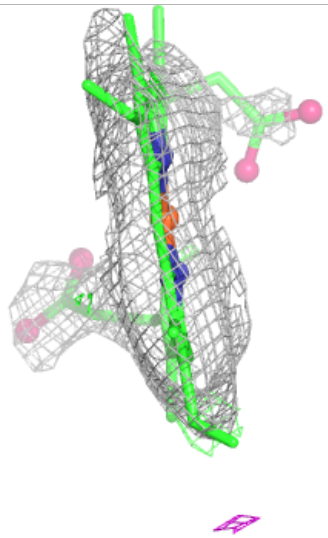


Electron density around HEM e 101:

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

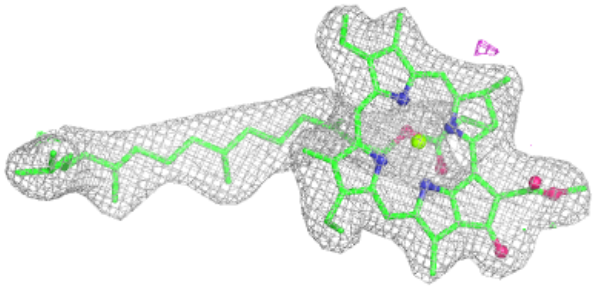


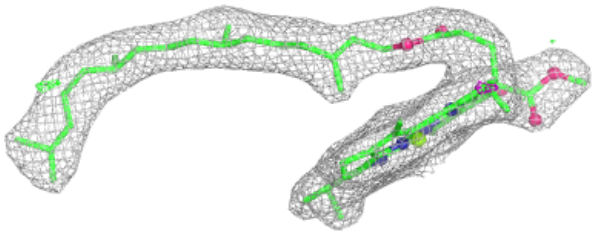




Electron density around CLA B 609:

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

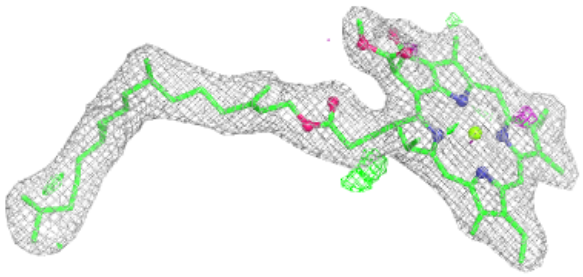


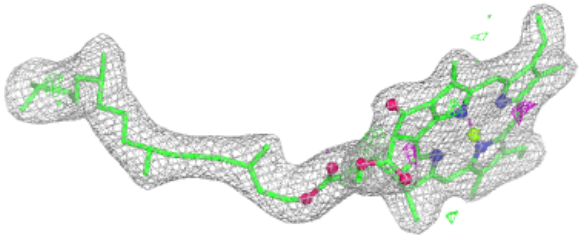


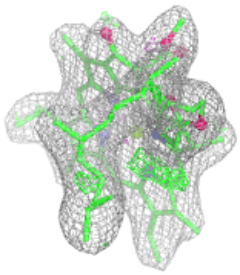


Electron density around CLA A 404:

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

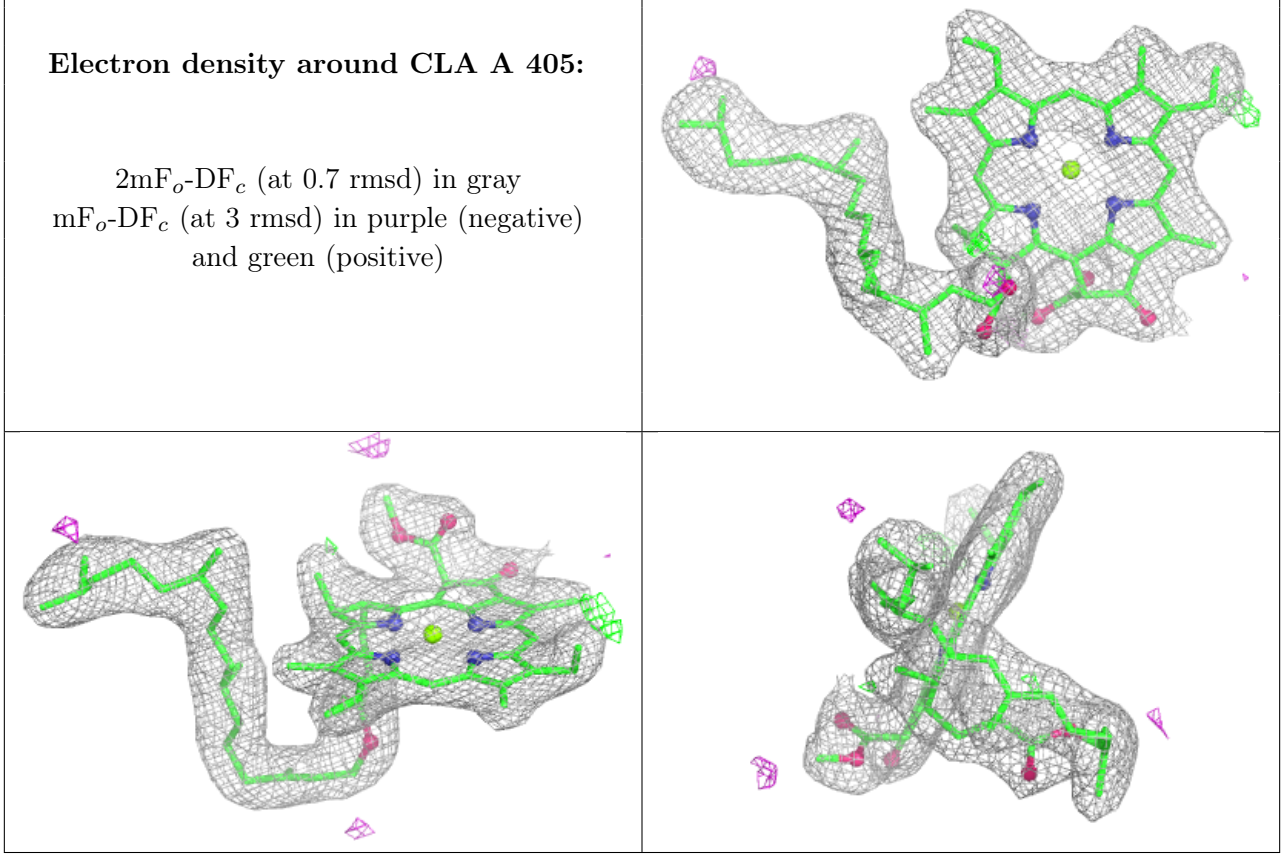






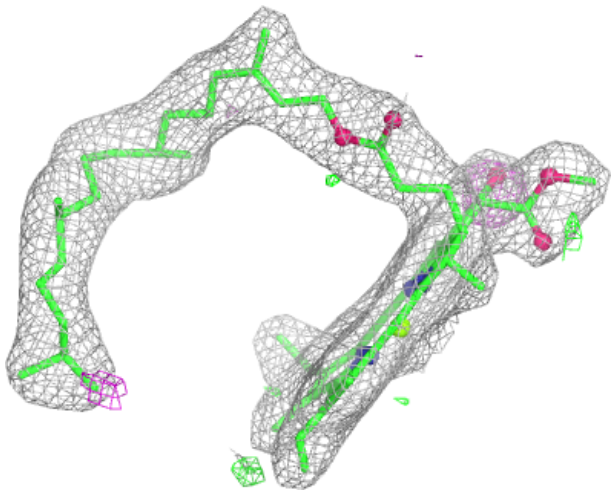
Electron density around CLA A 405:

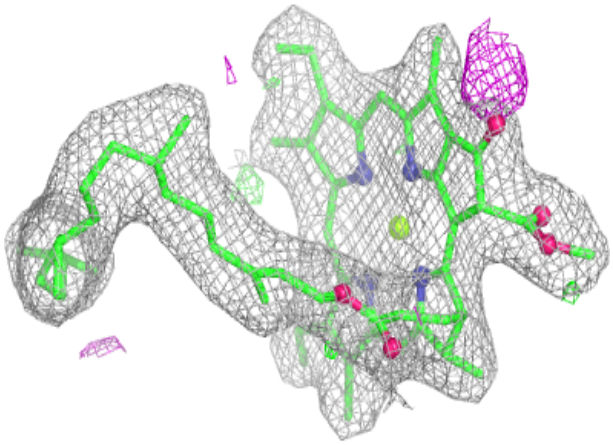
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

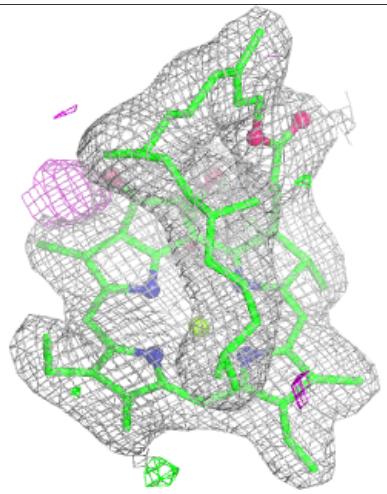


Electron density around CLA B 612:

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

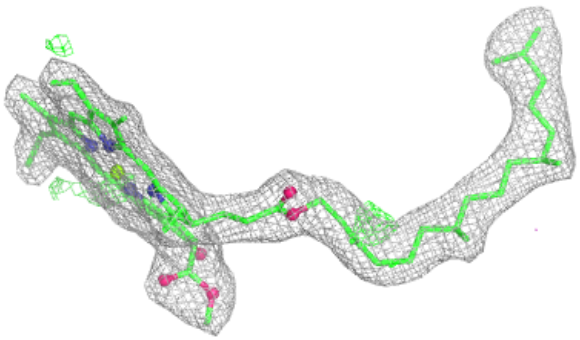


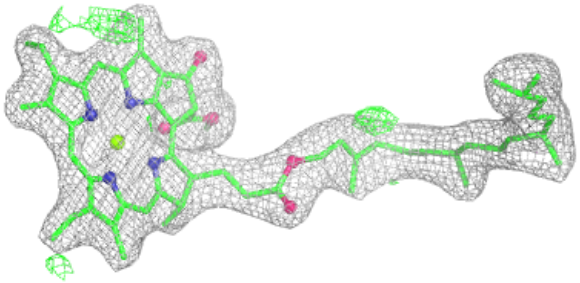


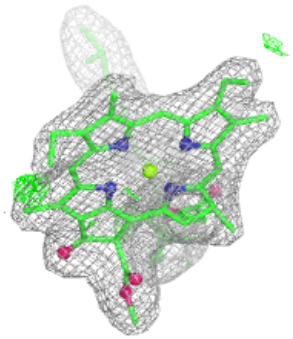


Electron density around CLA D 405:

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

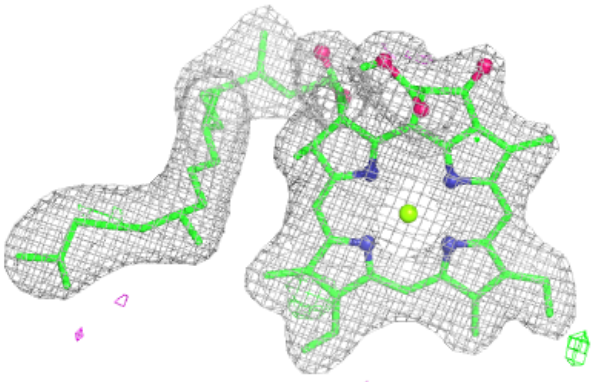


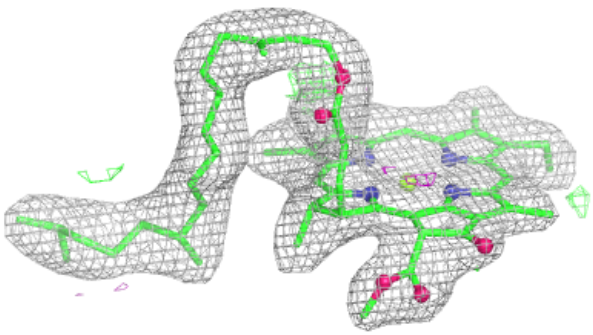


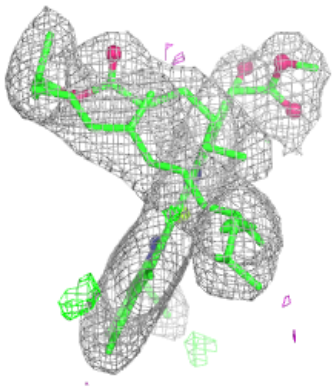


Electron density around CLA d 403:

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

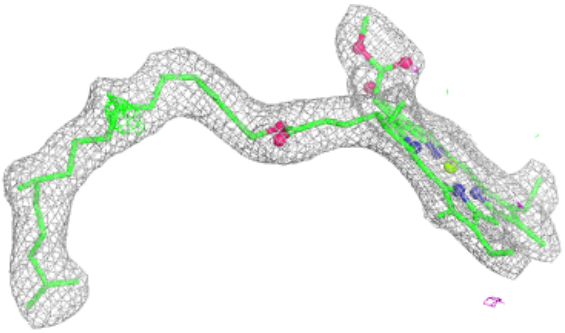


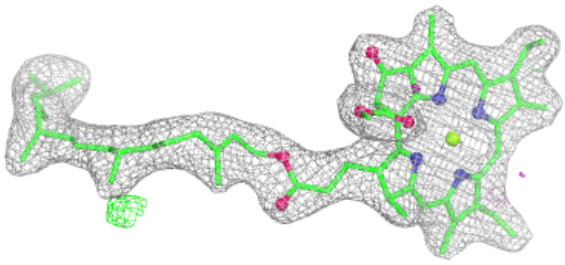


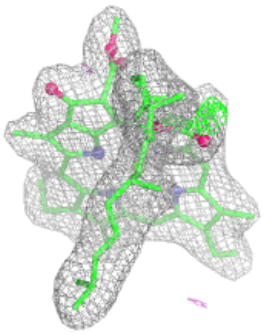


Electron density around CLA d 404:

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

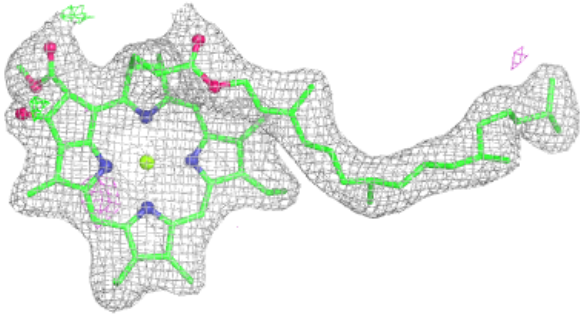


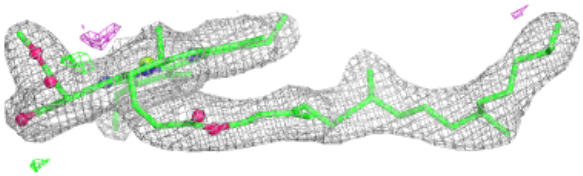


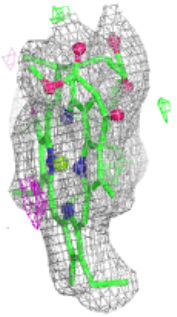


Electron density around CLA B 604:

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

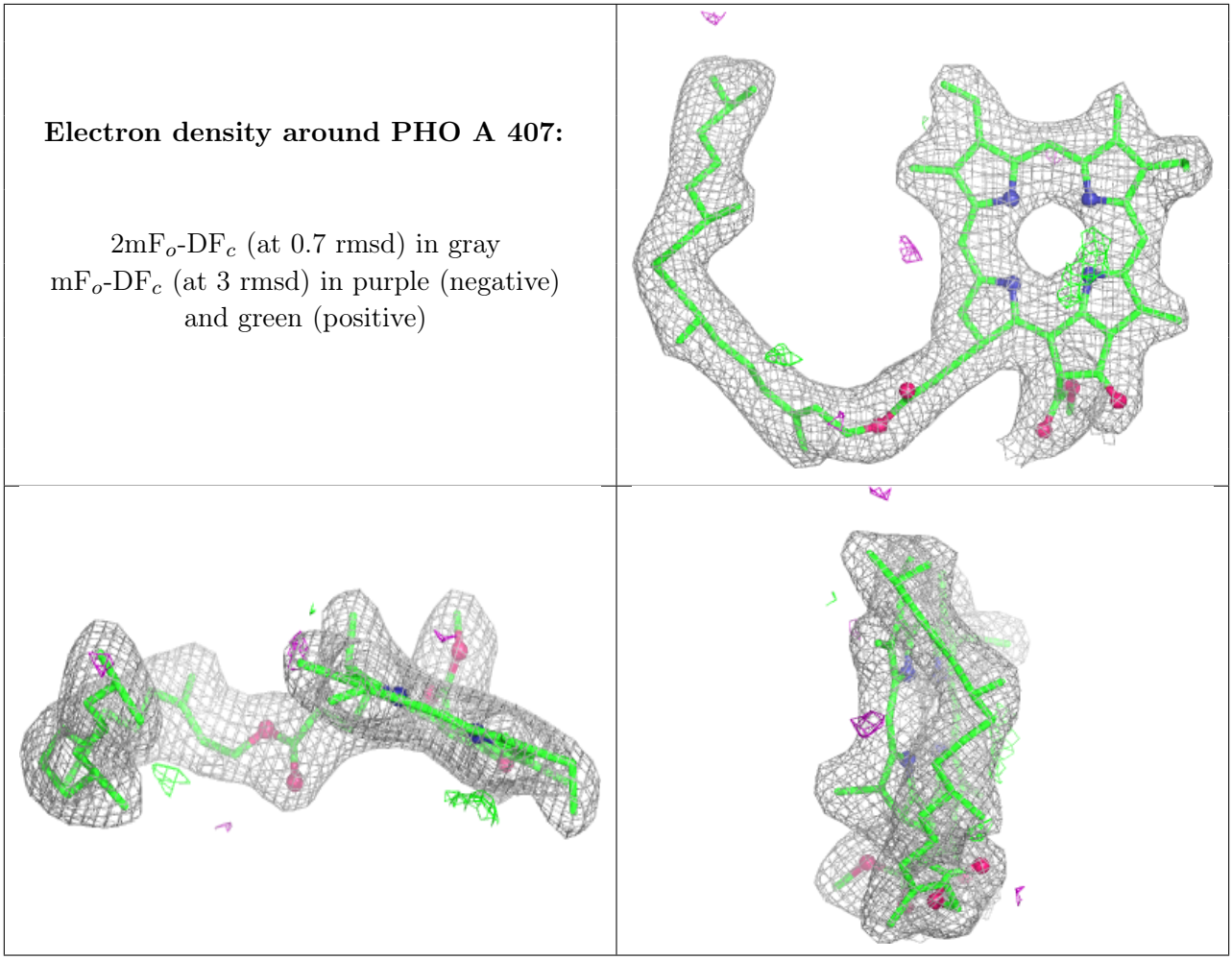






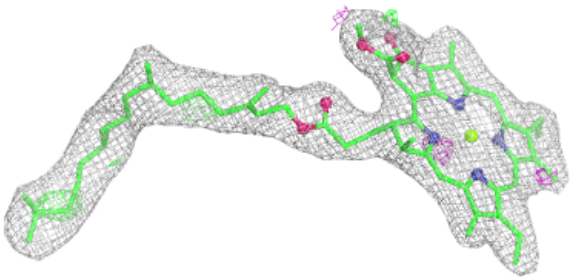
Electron density around PHO A 407:

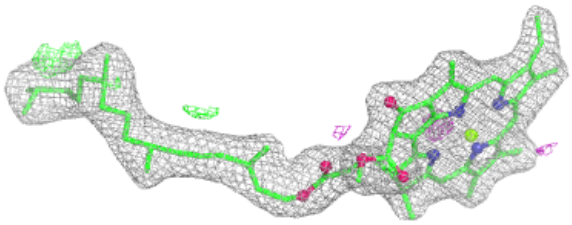
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

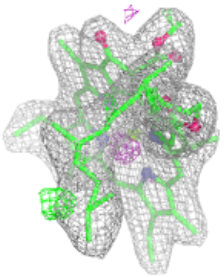


Electron density around CLA a 408:

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

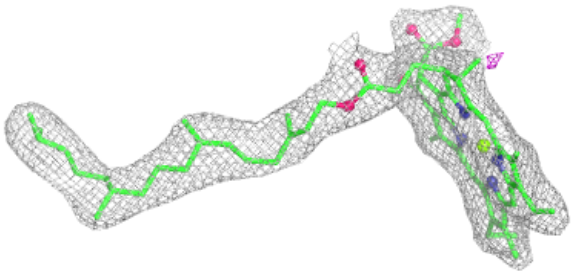


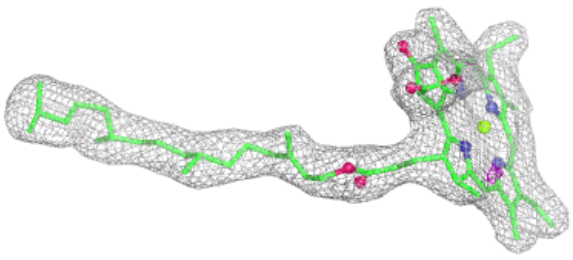


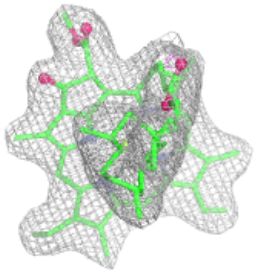


Electron density around CLA B 605:

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

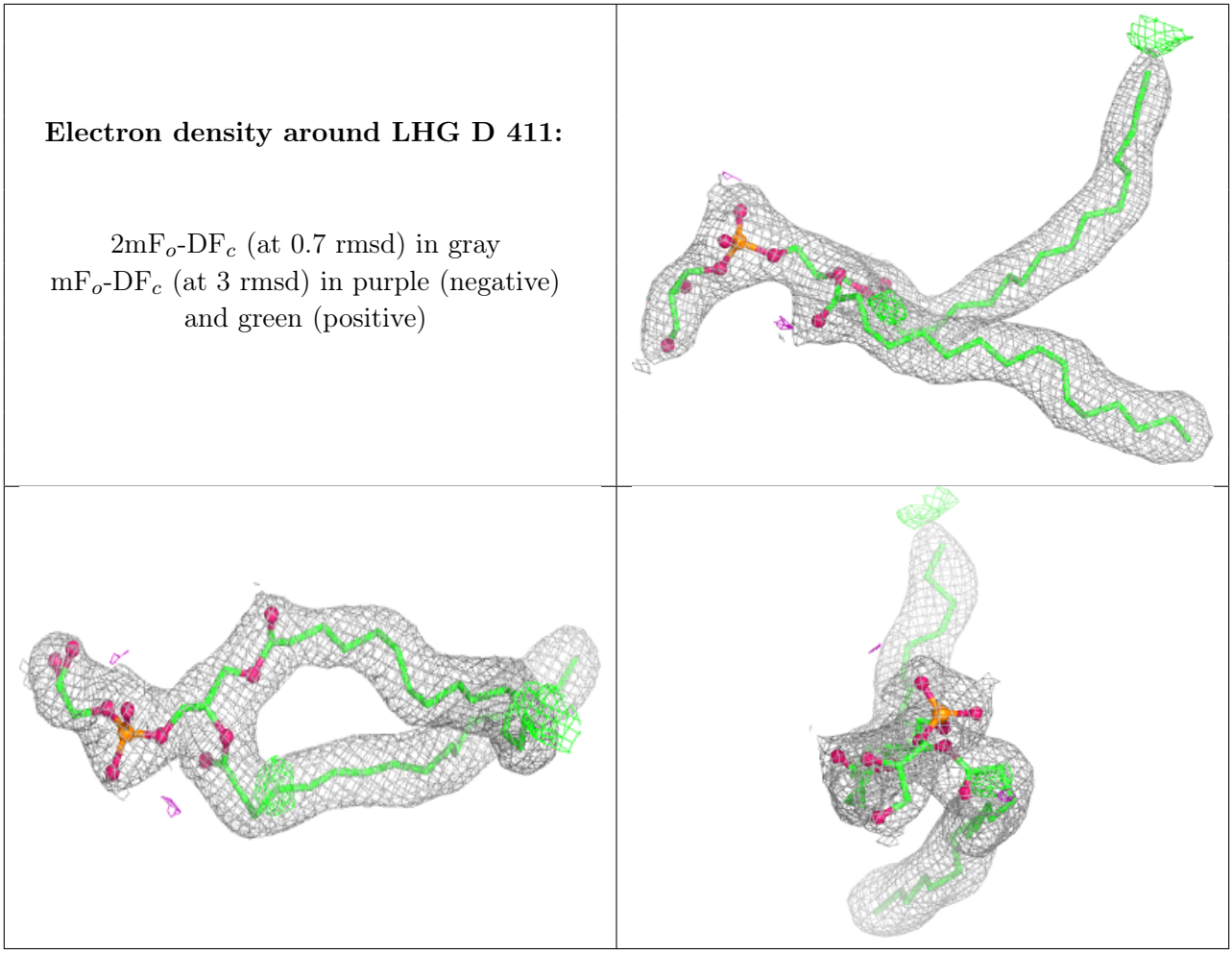






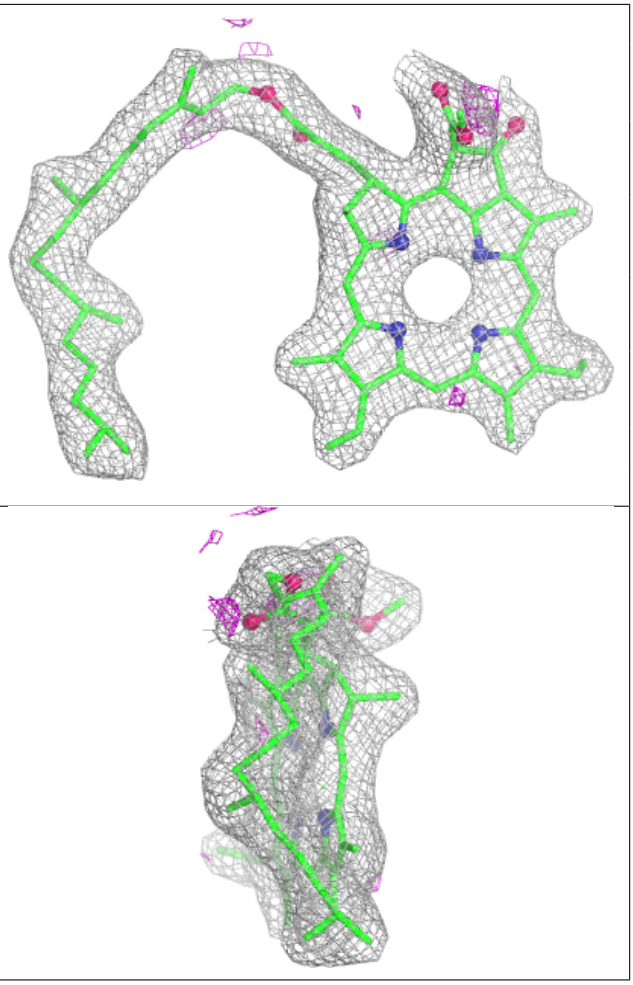
Electron density around LHG D 411:

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



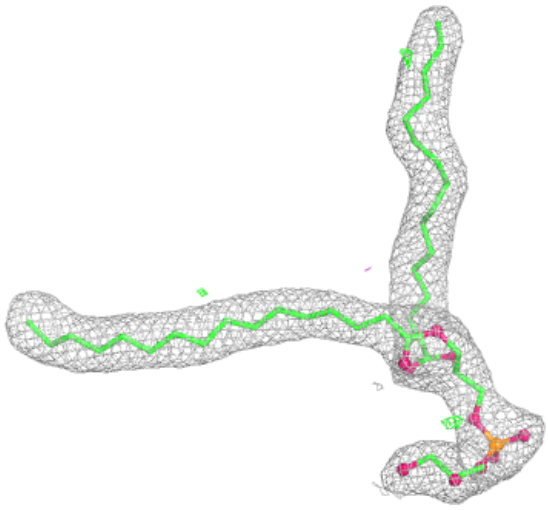
Electron density around PHO a 410:

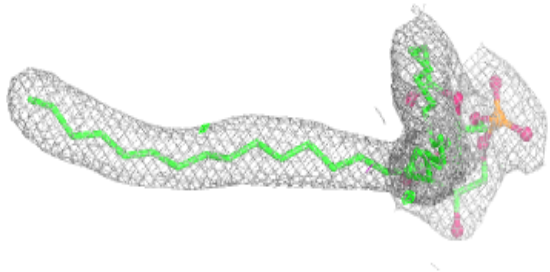
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

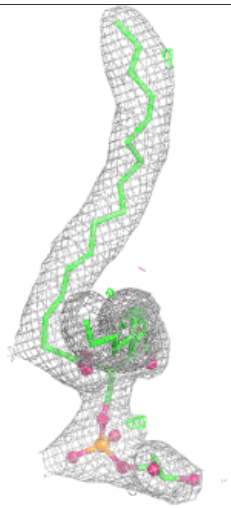


Electron density around LHG L 101:

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

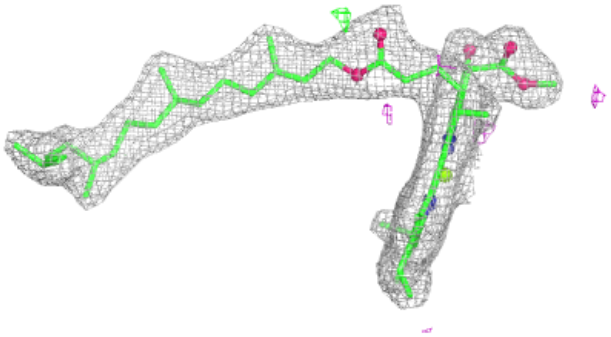


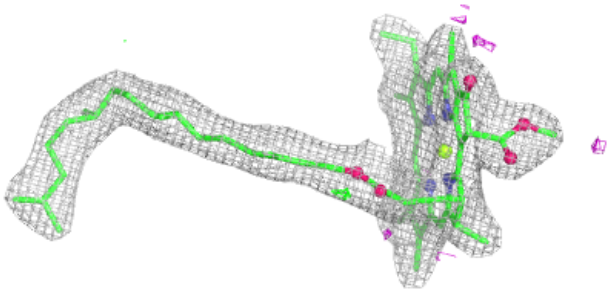


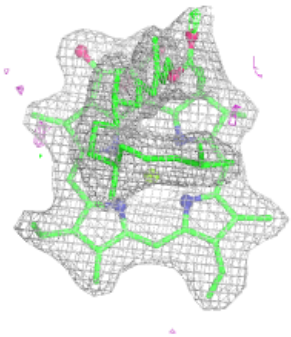


Electron density around CLA B 606:

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

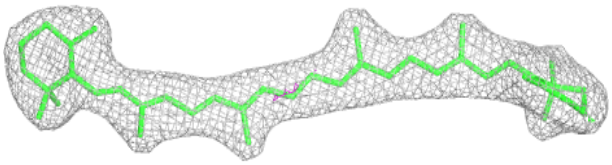


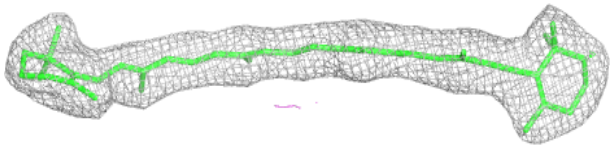


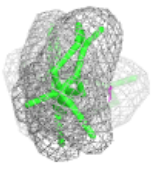


Electron density around BCR B 618:

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

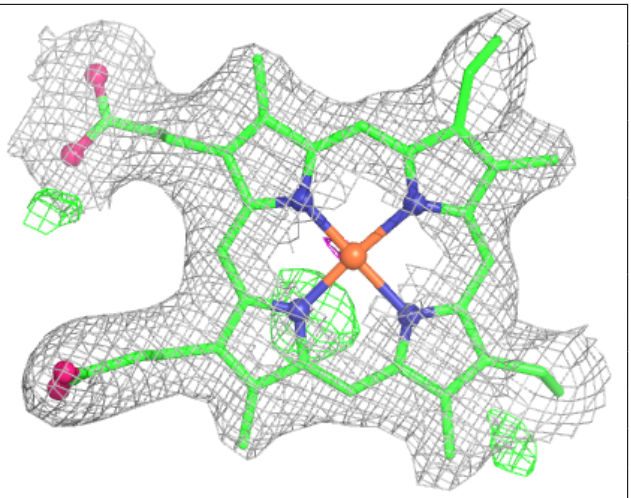


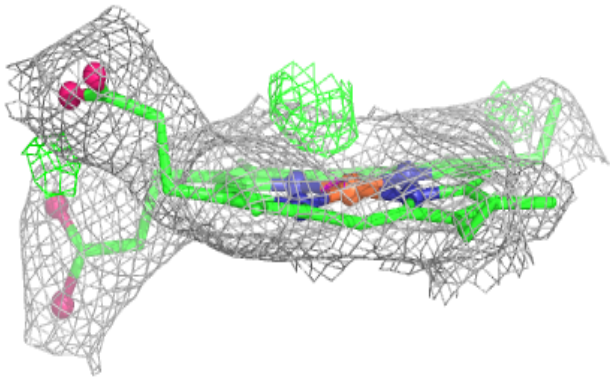




Electron density around HEC V 205:

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

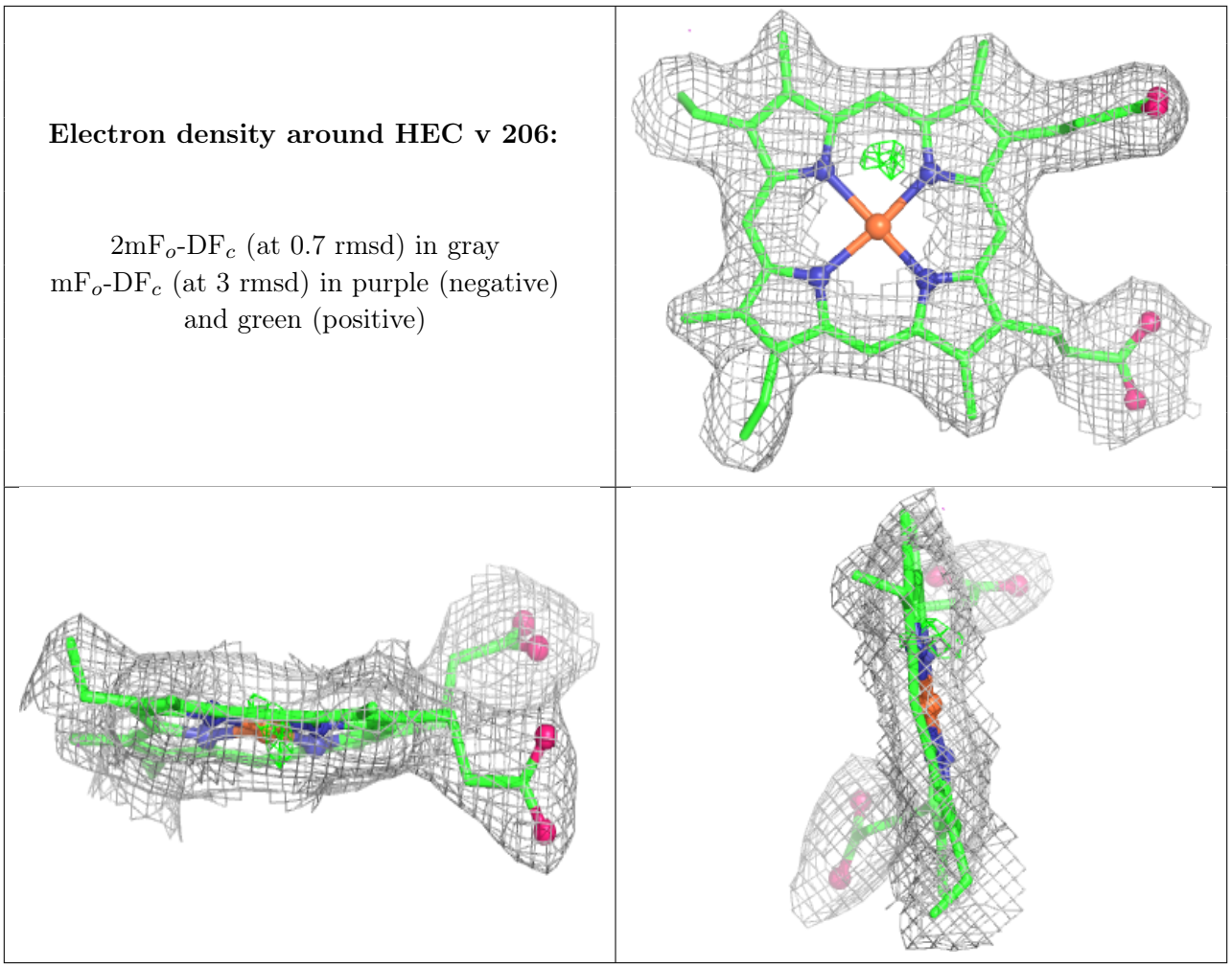






Electron density around HEC v 206:

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



6.5 Other polymers (i)

There are no such residues in this entry.