wwPDB X-ray Structure Validation Summary Report (i)

Mar 18, 2026 – 11:34 AM UTC

PDB ID	:	7CJI / pdb_00007cji
Title	:	Photosystem II structure in the S1 state
Authors	:	Li, H.; Shen, J.-R.; Suga, M.
Deposited on	:	2020-07-11
Resolution	:	2.35 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:

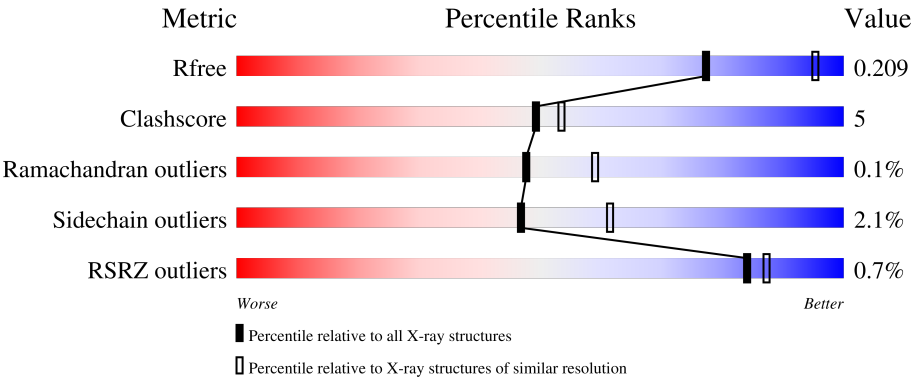
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.35 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.



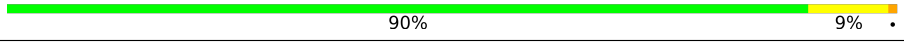
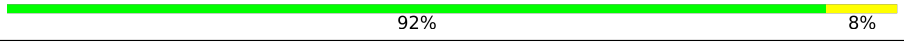
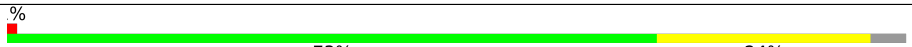
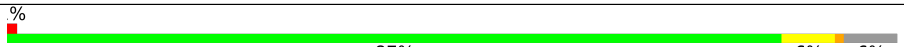
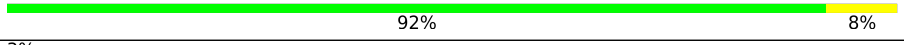
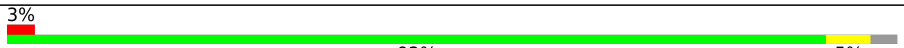
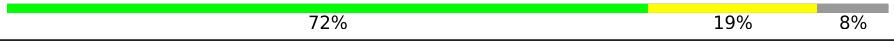
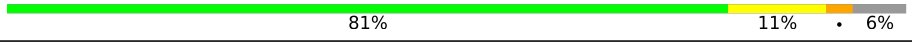
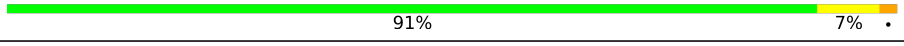
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	88% 9% .
1	a	344	% 88% 9% .
2	B	505	91% 8%
2	b	505	% 90% 9% .
3	C	455	88% 11% .

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	93% 7%
16	v	137	91% 8%
17	X	40	85% 10% 5%
17	x	40	85% 10% 5%
18	Y	30	7% 80% 17%
18	y	30	67% 23% 7%
19	Z	62	94% 5%
19	z	62	2% 87% 13%
20	R	34	15% 82% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
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23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53071 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	2	0
			2634	1725	433	461	15			
1	a	334	Total	C	N	O	S	0	3	0
			2642	1731	434	462	15			

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
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	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	4	0
			3513	2295	588	617	13			
3	c	455	Total	C	N	O	S	0	2	0
			3534	2311	591	619	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

- 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	1	0
			668	435	108	125			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

- 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	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	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
			277	185	43	48	1			

- 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	36	Total	C	N	O	0	1	0
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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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	3	0
			1886	1177	318	386	5			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	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	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total 281	C 188	N 45	O 48	0	0	0
17	x	38	Total 281	C 188	N 45	O 48	0	0	0

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total 273	C 186	N 47	O 40	0	0	0

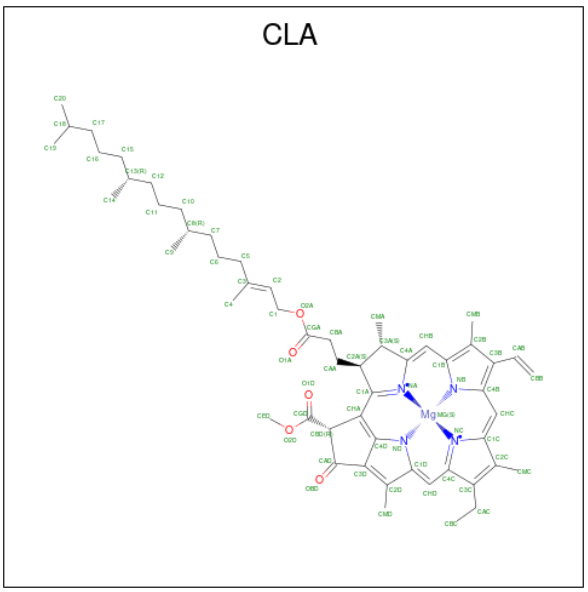
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- 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	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		
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		

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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	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	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		

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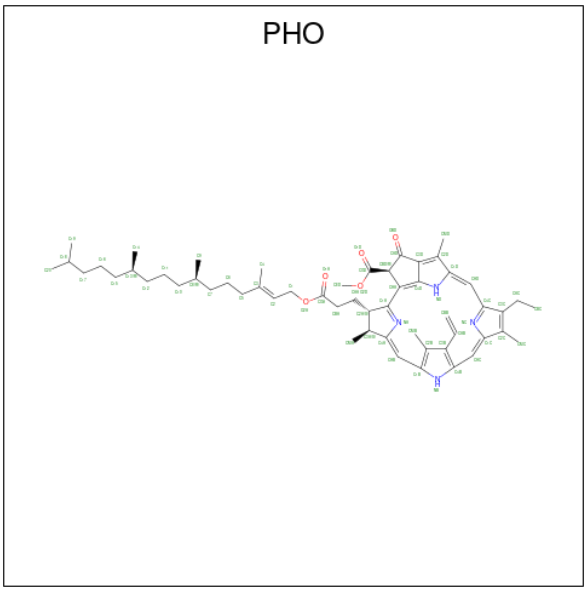
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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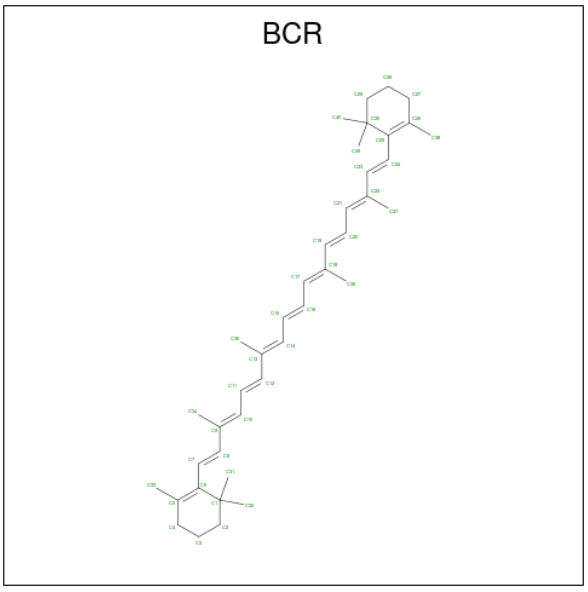
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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	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: $C_{55}H_{74}N_4O_5$).



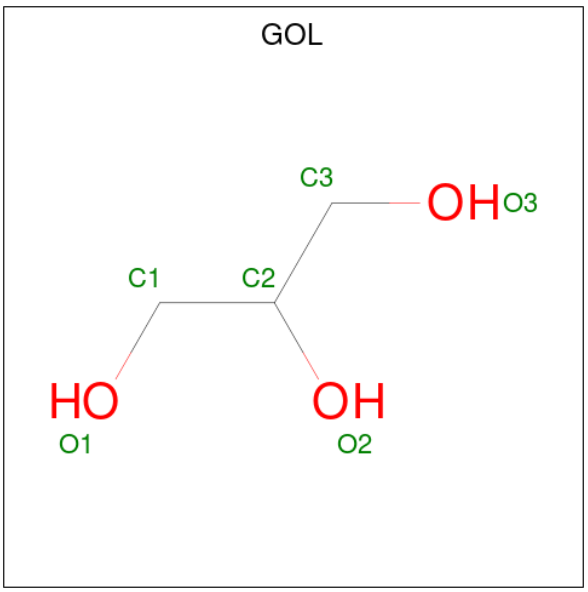
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- 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	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
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	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

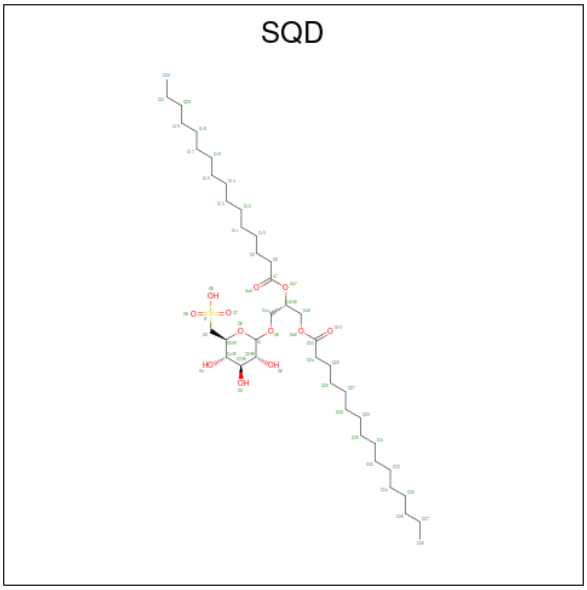
- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	0
			6	3	3		
26	O	1	Total	C	O	0	0
			6	3	3		
26	a	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	c	1	Total	C	O	0	0
			6	3	3		
26	c	1	Total	C	O	0	0
			6	3	3		
26	v	1	Total	C	O	0	0
			6	3	3		

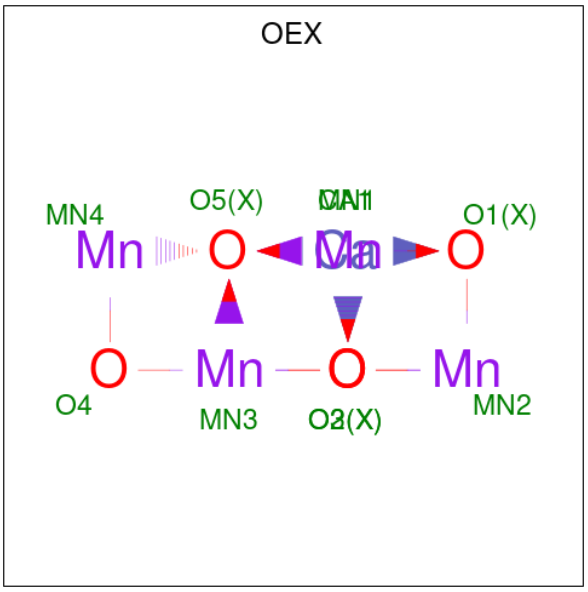
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



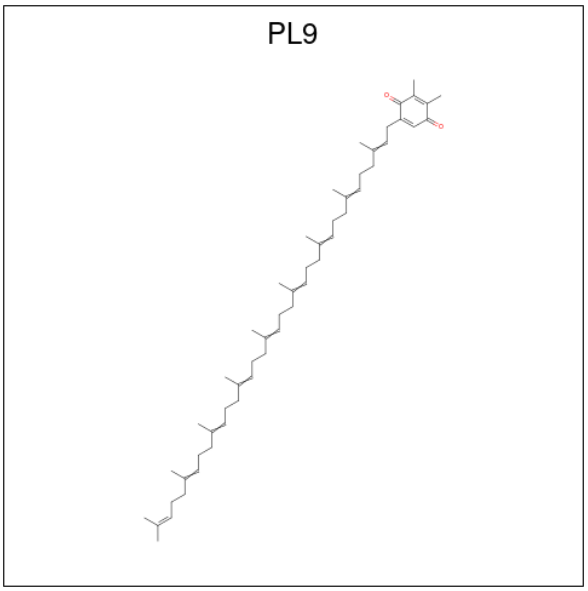
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	C	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0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

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 29 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
29	A	1	Total	C	O	0	0
			55	53	2		

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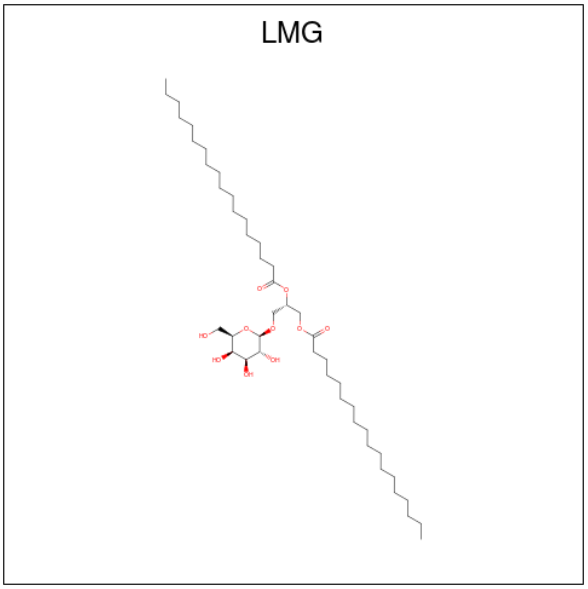
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total C O 55 53 2	0	0
29	a	1	Total C O 55 53 2	0	0
29	d	1	Total C O 55 53 2	0	0

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

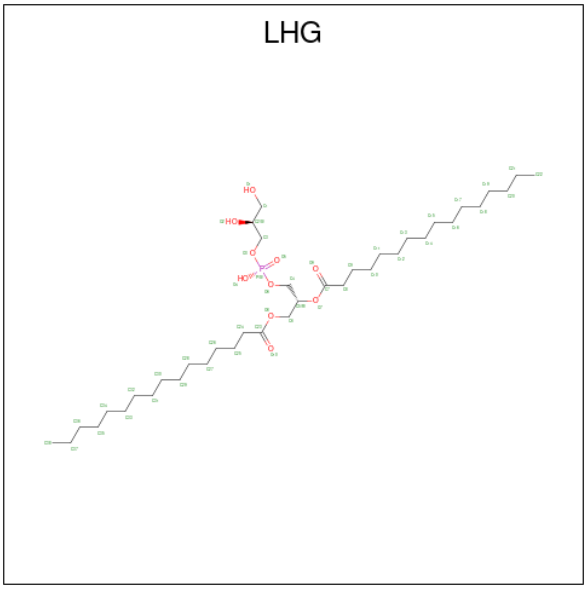
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	C	1	Total C O 34 29 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	M	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



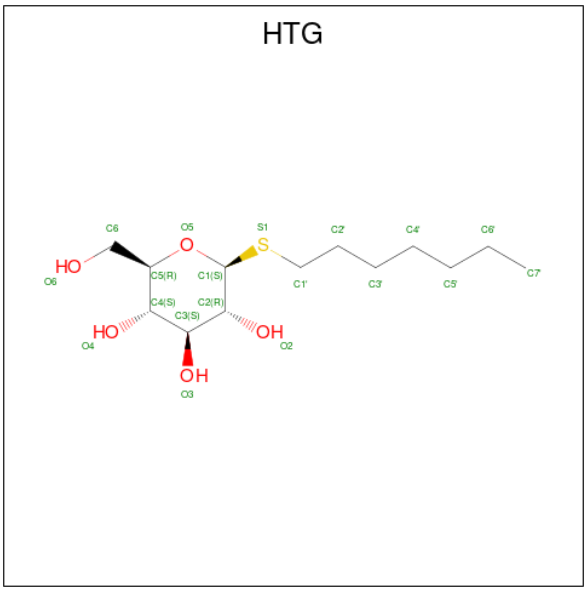
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
31	A	1	51	41	10	0	0
31	C	1	Total 51	C 41	O 10	0	0
31	C	1	Total 51	C 41	O 10	0	0
31	D	1	Total 51	C 41	O 10	0	0
31	M	1	Total 51	C 41	O 10	0	0
31	Z	1	Total 37	C 27	O 10	0	0
31	a	1	Total 51	C 41	O 10	0	0
31	c	1	Total 51	C 41	O 10	0	0
31	c	1	Total 51	C 41	O 10	0	0
31	d	1	Total 51	C 41	O 10	0	0
31	m	1	Total 51	C 41	O 10	0	0
31	z	1	Total 39	C 29	O 10	0	0

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



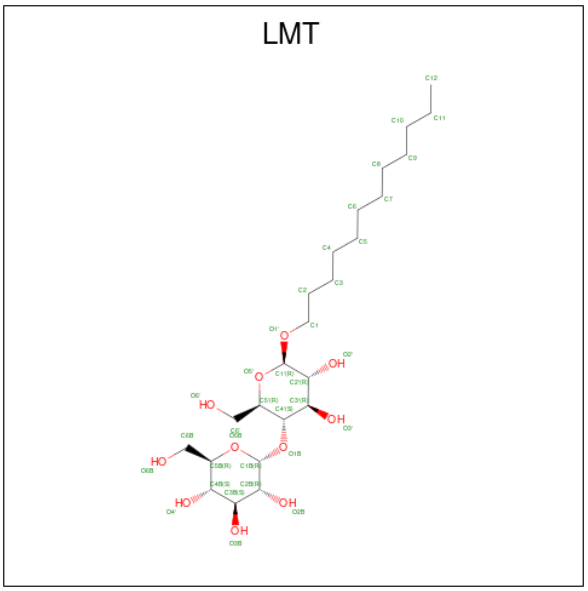
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			42	31	10	1		
32	b	1	Total	C	O	P	0	0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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



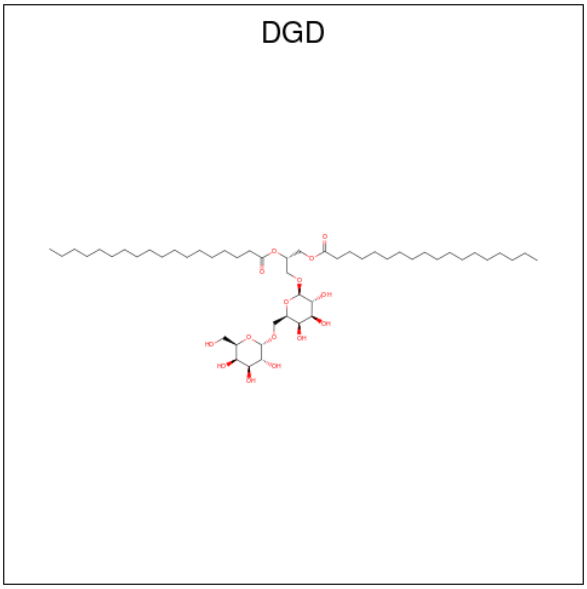
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	C	1	Total C O S 19 13 5 1	0	0
33	D	1	Total C O S 16 10 5 1	0	0
33	V	1	Total C O 11 6 5	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	c	1	Total C O S 19 13 5 1	0	0
33	h	1	Total C O S 16 10 5 1	0	0

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			25	19	6		
34	C	1	Total	C	O	0	0
			35	24	11		
34	D	1	Total	C	O	0	0
			35	24	11		
34	D	1	Total	C	O	0	0
			35	24	11		
34	E	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	b	1	Total	C	O	0	0
			25	19	6		
34	e	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

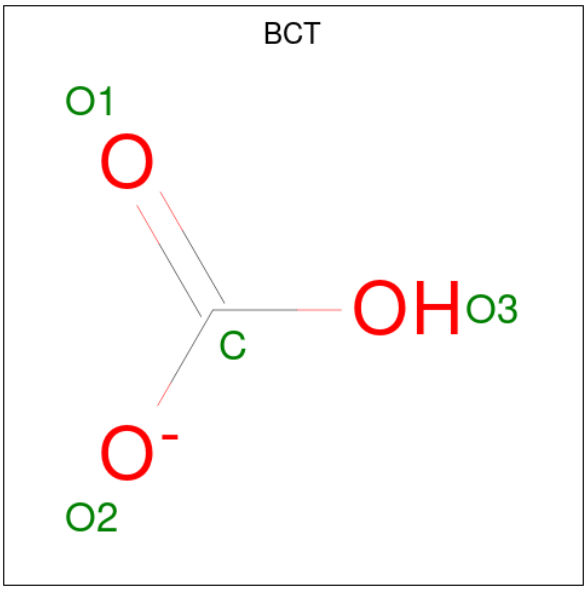
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0

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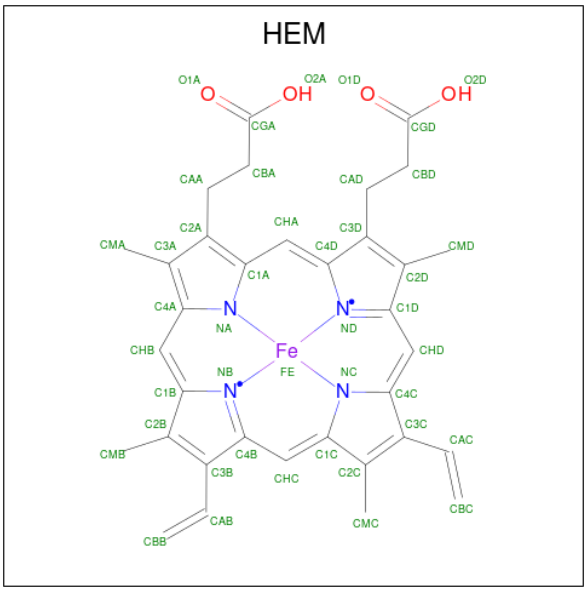
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	o	1	Total Ca 1 1	0	0
36	v	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 4 1 3	0	0
37	d	1	Total C O 4 1 3	0	0

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

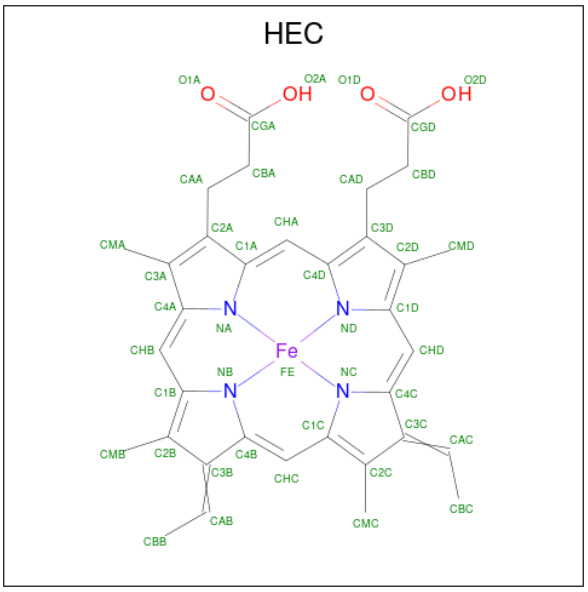


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	147	Total	O	0	0
			147	147		
41	B	207	Total	O	0	0
			207	207		
41	C	186	Total	O	0	0
			186	186		
41	D	132	Total	O	0	0
			132	132		
41	E	24	Total	O	0	0
			24	24		
41	F	8	Total	O	0	0
			8	8		
41	H	30	Total	O	0	0
			30	30		
41	I	3	Total	O	0	0
			3	3		
41	J	6	Total	O	0	0
			6	6		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 8 8	0	0
41	M	16	Total O 16 16	0	0
41	O	122	Total O 122 122	0	0
41	T	15	Total O 15 15	0	0
41	U	58	Total O 58 58	0	0
41	V	93	Total O 93 93	0	0
41	X	10	Total O 10 10	0	0
41	Y	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	144	Total O 144 144	0	0
41	b	222	Total O 222 222	0	0
41	c	166	Total O 166 166	0	0
41	d	127	Total O 127 127	0	0
41	e	13	Total O 13 13	0	0
41	f	5	Total O 5 5	0	0
41	h	24	Total O 24 24	0	0
41	i	2	Total O 2 2	0	0
41	j	3	Total O 3 3	0	0
41	k	5	Total O 5 5	0	0
41	l	7	Total O 7 7	0	0
41	m	11	Total O 11 11	0	0

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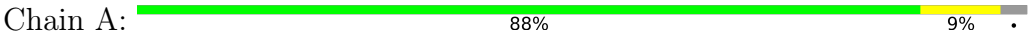
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	102	Total O 102 102	0	0
41	t	11	Total O 11 11	0	0
41	u	67	Total O 67 67	0	0
41	v	56	Total O 56 56	0	0
41	x	10	Total O 10 10	0	0
41	y	3	Total O 3 3	0	0

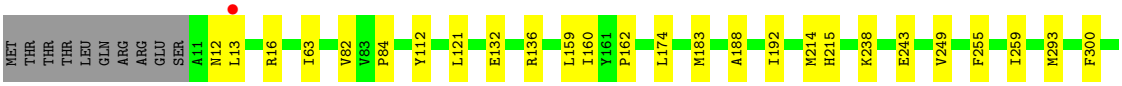
3 Residue-property plots (i)

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:

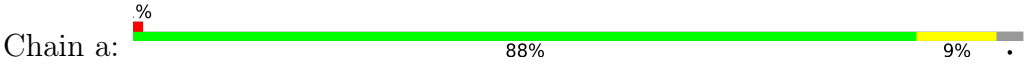


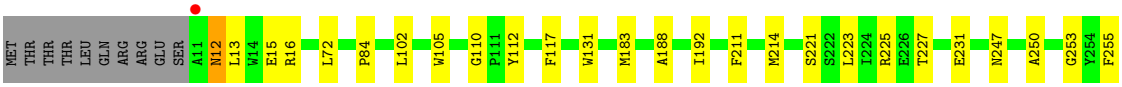




• Molecule 1: Photosystem II protein D1

Chain a:







• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



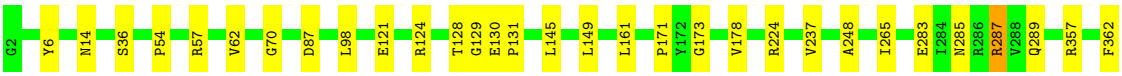


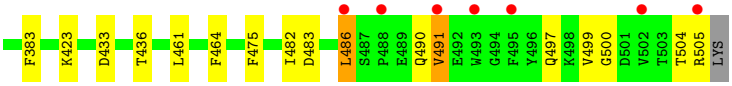


• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



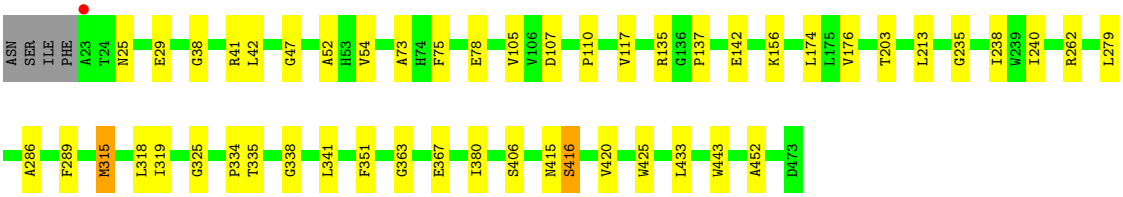




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

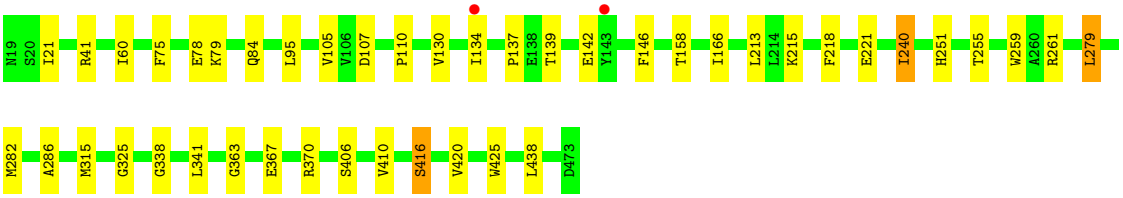




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:





• Molecule 4: Photosystem II D2 protein

Chain D:

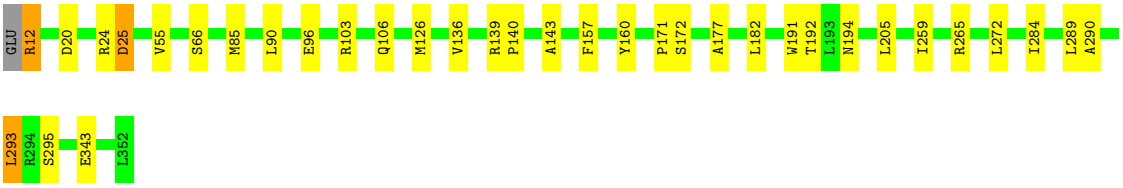




• Molecule 4: Photosystem II D2 protein

Chain d:

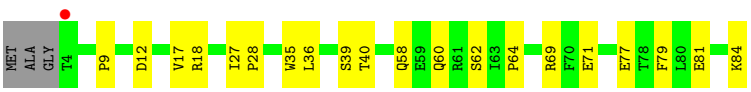




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

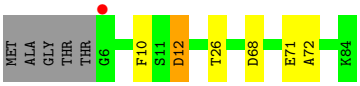




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

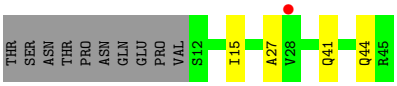




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

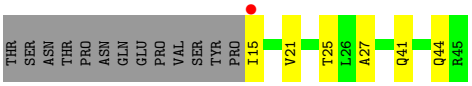




• Molecule 6: Cytochrome b559 subunit beta

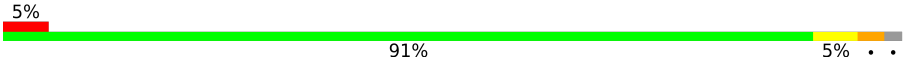
Chain f:

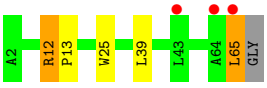




• Molecule 7: Photosystem II reaction center protein H

Chain H:

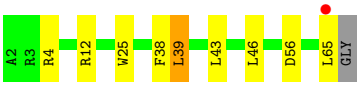




• Molecule 7: Photosystem II reaction center protein H

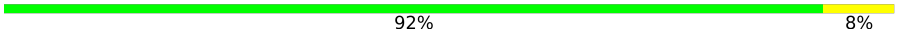
Chain h:





• Molecule 8: Photosystem II reaction center protein I

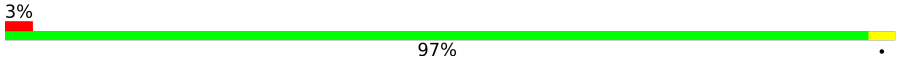
Chain I:





• Molecule 8: Photosystem II reaction center protein I

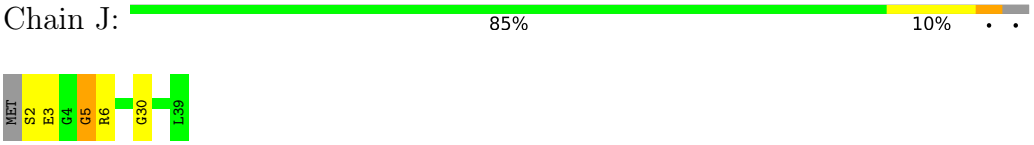
Chain i:





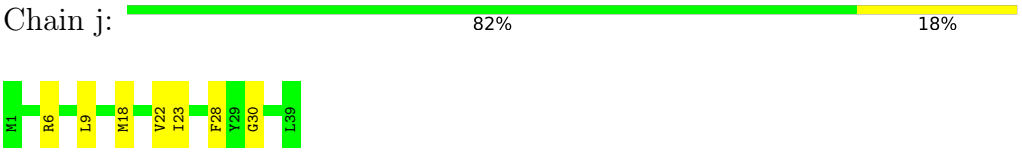
• Molecule 9: Photosystem II reaction center protein J

Chain J:



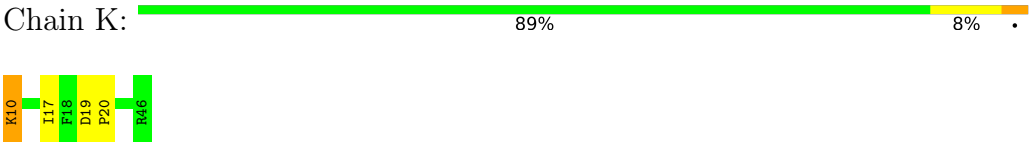
• Molecule 9: Photosystem II reaction center protein J

Chain j:



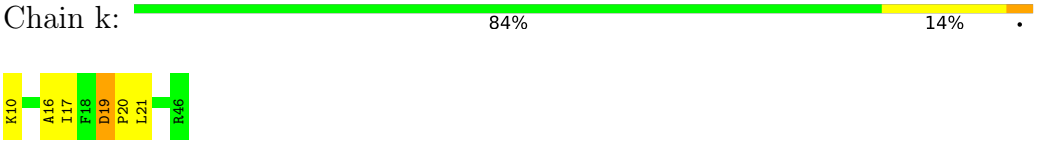
• Molecule 10: Photosystem II reaction center protein K

Chain K:



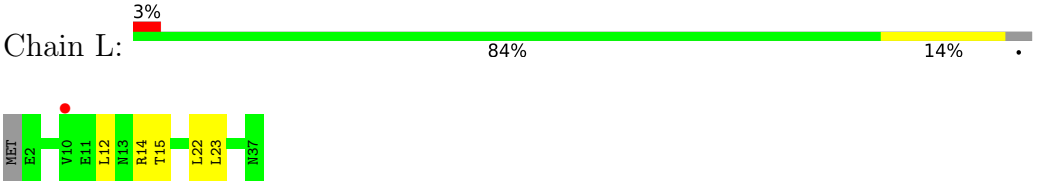
• Molecule 10: Photosystem II reaction center protein K

Chain k:



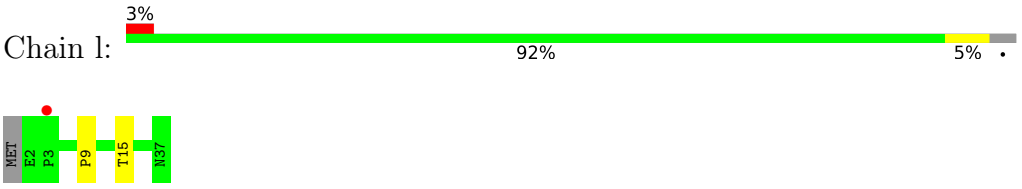
• Molecule 11: Photosystem II reaction center protein L

Chain L:



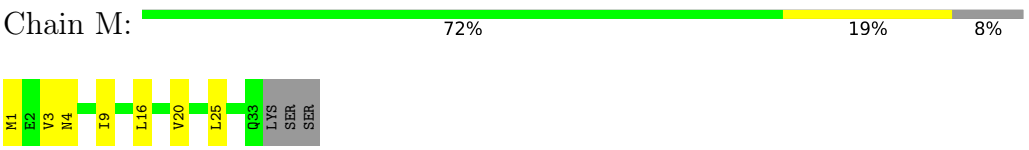
• Molecule 11: Photosystem II reaction center protein L

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:

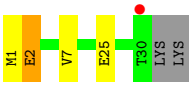




• Molecule 14: Photosystem II reaction center protein T

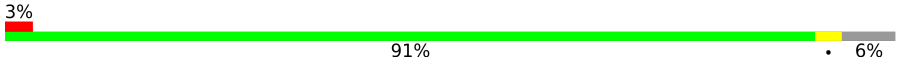
Chain T:





• Molecule 14: Photosystem II reaction center protein T

Chain t:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

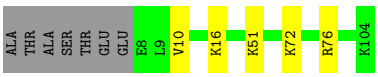




• Molecule 15: Photosystem II 12 kDa extrinsic protein

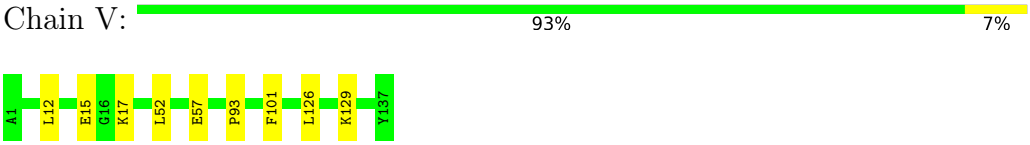
Chain u:





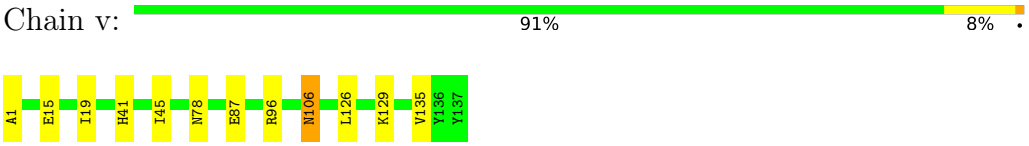
• Molecule 16: Cytochrome c-550

Chain V:



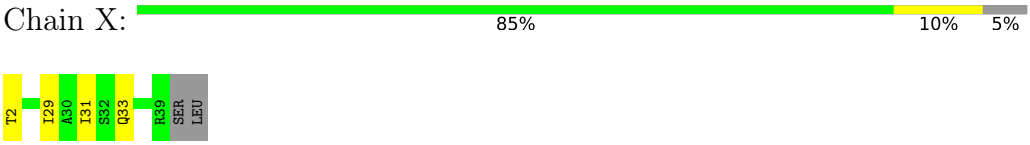
• Molecule 16: Cytochrome c-550

Chain v:



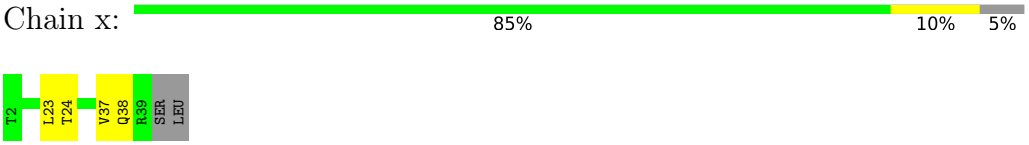
• Molecule 17: Photosystem II reaction center protein X

Chain X:



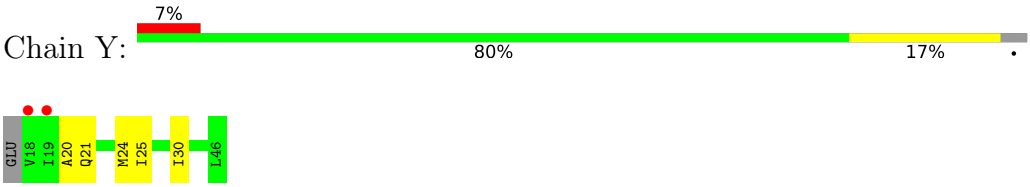
• Molecule 17: Photosystem II reaction center protein X

Chain x:



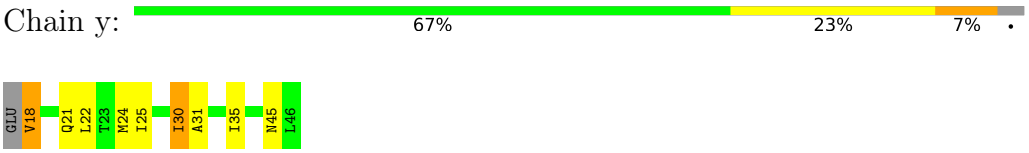
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



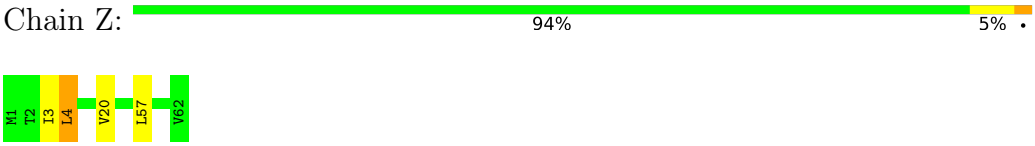
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 19: Photosystem II reaction center protein Z

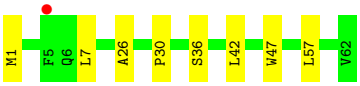
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

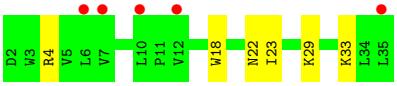




• Molecule 20: Photosystem II protein Y

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	126.02Å 231.70Å 288.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 2.35 39.93 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.93-2.35) 84.6 (39.93-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.160 , 0.208 0.162 , 0.209	Depositor DCC
R_{free} test set	17532 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 76.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53071	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 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/2719	0.53	0/3708
1	a	0.32	0/2727	0.49	0/3719
2	B	0.33	0/4190	0.48	0/5708
2	b	0.31	0/4138	0.47	0/5640
3	C	0.29	0/3626	0.47	0/4936
3	c	0.26	0/3648	0.44	0/4966
4	D	0.34	0/2821	0.52	0/3844
4	d	0.32	0/2812	0.50	0/3832
5	E	0.26	0/687	0.45	0/936
5	e	0.24	0/667	0.41	0/908
6	F	0.26	0/284	0.43	0/387
6	f	0.22	0/257	0.46	0/349
7	H	0.27	0/530	0.48	0/723
7	h	0.26	0/519	0.52	0/708
8	I	0.25	0/311	0.37	0/419
8	i	0.26	0/311	0.41	0/419
9	J	0.25	0/278	0.45	0/376
9	j	0.23	0/283	0.40	0/383
10	K	0.26	0/303	0.47	0/416
10	k	0.25	0/303	0.46	0/416
11	L	0.40	0/311	0.47	0/423
11	l	0.33	0/311	0.53	0/423
12	M	0.34	0/261	0.52	0/357
12	m	0.32	0/262	0.52	0/357
13	O	0.31	0/1917	0.49	0/2599
13	o	0.28	0/1910	0.46	0/2589
14	T	0.36	0/257	0.44	0/349
14	t	0.34	0/257	0.42	0/349
15	U	0.32	0/776	0.52	0/1052
15	u	0.29	0/785	0.51	0/1064
16	V	0.29	0/1085	0.45	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.27	0/1085	0.43	0/1473
17	X	0.22	0/284	0.37	0/384
17	x	0.20	0/284	0.34	0/384
18	Y	0.19	0/216	0.38	0/289
18	y	0.19	0/216	0.40	0/289
19	Z	0.19	0/490	0.35	0/669
19	z	0.18	0/490	0.31	0/669
20	R	0.19	0/279	0.34	0/383
All	All	0.30	0/42890	0.47	0/58368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2634	0	2531	20	0
1	a	2642	0	2541	25	0
2	B	4050	0	3894	33	0
2	b	3998	0	3852	40	0
3	C	3513	0	3424	35	0
3	c	3534	0	3445	34	0
4	D	2726	0	2627	20	0
4	d	2717	0	2621	26	0
5	E	668	0	652	14	0
5	e	648	0	634	4	0
6	F	275	0	282	4	0
6	f	250	0	261	5	0
7	H	517	0	542	5	0
7	h	506	0	529	10	0
8	I	314	0	328	3	0
8	i	314	0	328	0	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	4	0
10	K	293	0	305	2	0
10	k	293	0	305	4	0
11	L	304	0	314	4	0
11	l	304	0	314	2	0
12	M	268	0	285	4	0
12	m	269	0	288	4	0
13	O	1886	0	1856	15	0
13	o	1879	0	1850	12	0
14	T	258	0	261	3	0
14	t	258	0	261	0	0
15	U	765	0	767	6	0
15	u	774	0	773	3	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	8	0
17	X	281	0	312	2	0
17	x	281	0	312	5	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	1	0
19	z	479	0	516	3	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	12	0
23	B	1040	0	1152	37	0
23	C	845	0	936	31	0
23	D	130	0	144	3	0
23	a	195	0	216	8	0
23	b	1040	0	1152	38	0
23	c	845	0	936	46	0
23	d	195	0	216	8	0
24	A	64	0	74	1	0
24	D	64	0	74	1	0
24	a	128	0	148	5	0
25	A	40	0	56	1	0
25	B	120	0	168	11	0
25	C	80	0	112	3	0
25	D	40	0	56	0	0
25	H	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	K	40	0	56	2	0
25	T	40	0	56	8	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	8	0
25	c	80	0	112	4	0
25	d	40	0	56	1	0
25	h	40	0	56	3	0
25	k	80	0	112	3	0
25	t	40	0	56	3	0
26	A	6	0	8	0	0
26	B	18	0	24	1	0
26	C	6	0	8	0	0
26	O	6	0	8	0	0
26	a	6	0	8	0	0
26	b	12	0	16	1	0
26	c	12	0	16	2	0
26	v	6	0	8	1	0
27	A	54	0	78	0	0
27	B	54	0	78	0	0
27	C	54	0	78	3	0
27	D	43	0	53	2	0
27	L	54	0	78	4	0
27	a	108	0	155	3	0
27	f	43	0	53	2	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	3	0
29	D	55	0	80	1	0
29	a	55	0	80	6	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	C	34	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	51	0	72	2	0
31	C	102	0	144	4	0
31	D	51	0	72	0	0
31	M	51	0	72	3	0
31	Z	37	0	44	0	0
31	a	51	0	72	3	0
31	c	102	0	144	1	0
31	d	51	0	71	5	0
31	m	51	0	72	0	0
31	z	39	0	48	3	0
32	A	49	0	74	3	0
32	D	98	0	148	5	0
32	E	42	0	57	2	0
32	L	49	0	74	2	0
32	a	42	0	57	2	0
32	b	49	0	74	1	0
32	d	147	0	222	14	0
33	B	57	0	78	4	0
33	C	19	0	26	0	0
33	D	16	0	17	2	0
33	V	11	0	10	0	0
33	b	57	0	78	4	0
33	c	19	0	26	1	0
33	h	16	0	17	2	0
34	B	25	0	35	0	0
34	C	35	0	46	1	0
34	D	70	0	92	3	0
34	E	35	0	46	1	0
34	M	70	0	92	1	0
34	a	70	0	92	5	0
34	b	50	0	70	2	0
34	e	35	0	46	0	0
34	m	35	0	46	0	0
34	t	26	0	35	0	0
35	C	186	0	246	9	0
35	H	62	0	82	2	0
35	c	186	0	246	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	o	1	0	0	0	0
36	v	1	0	0	0	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	E	43	0	30	2	0
38	f	43	0	30	2	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	147	0	0	0	0
41	B	207	0	0	2	0
41	C	186	0	0	1	0
41	D	132	0	0	1	0
41	E	24	0	0	1	0
41	F	8	0	0	1	0
41	H	30	0	0	1	0
41	I	3	0	0	0	0
41	J	6	0	0	0	0
41	K	6	0	0	0	0
41	L	8	0	0	0	0
41	M	16	0	0	0	0
41	O	122	0	0	1	0
41	R	1	0	0	0	0
41	T	15	0	0	0	0
41	U	58	0	0	1	0
41	V	93	0	0	0	0
41	X	10	0	0	0	0
41	Y	1	0	0	0	0
41	a	144	0	0	1	0
41	b	222	0	0	0	0
41	c	166	0	0	5	0
41	d	127	0	0	0	0
41	e	13	0	0	0	0
41	f	5	0	0	1	0
41	h	24	0	0	0	0
41	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	3	0	0	0	0
41	k	5	0	0	1	0
41	l	7	0	0	0	0
41	m	11	0	0	0	0
41	o	102	0	0	0	0
41	t	11	0	0	0	0
41	u	67	0	0	2	0
41	v	56	0	0	0	0
41	x	10	0	0	0	0
41	y	3	0	0	1	0
All	All	53071	0	51934	551	0

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 5.

The worst 5 of 551 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)
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.42	1.02
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.59	0.83
1:A:214:MET:HG2	29:A:413:PL9:H102	1.59	0.83
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.62	0.81
23:B:601:CLA:H12	23:B:601:CLA:H71	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	36	43
1	a	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	36	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	30	34
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	43	52
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	329 (97%)	10 (3%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	31 (86%)	4 (11%)	1 (3%)	4	2
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	244/244 (100%)	237 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100 100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100 100
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100 100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 6
20	R	32/34 (94%)	32 (100%)	0	0	100 100
All	All	5246/5384 (97%)	5124 (98%)	115 (2%)	7 (0%)	48 59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
1	a	259	ILE
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	271/279 (97%)	268 (99%)	3 (1%)	65 79
1	a	272/279 (98%)	270 (99%)	2 (1%)	76 86
2	B	412/403 (102%)	409 (99%)	3 (1%)	76 86
2	b	406/403 (101%)	398 (98%)	8 (2%)	48 63
3	C	356/356 (100%)	350 (98%)	6 (2%)	53 68
3	c	358/356 (101%)	351 (98%)	7 (2%)	48 63
4	D	277/277 (100%)	273 (99%)	4 (1%)	59 73
4	d	276/277 (100%)	271 (98%)	5 (2%)	51 66
5	E	73/73 (100%)	71 (97%)	2 (3%)	39 52
5	e	70/73 (96%)	68 (97%)	2 (3%)	37 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	25/38 (66%)	25 (100%)	0	100 100
7	H	55/54 (102%)	51 (93%)	4 (7%)	13 14
7	h	54/54 (100%)	51 (94%)	3 (6%)	19 23
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	26/27 (96%)	24 (92%)	2 (8%)	12 13
10	K	30/30 (100%)	27 (90%)	3 (10%)	7 7
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 7
11	L	35/35 (100%)	34 (97%)	1 (3%)	37 49
11	l	35/35 (100%)	35 (100%)	0	100 100
12	M	30/32 (94%)	28 (93%)	2 (7%)	15 17
12	m	30/32 (94%)	28 (93%)	2 (7%)	15 17
13	O	209/207 (101%)	205 (98%)	4 (2%)	50 65
13	o	208/207 (100%)	203 (98%)	5 (2%)	43 57
14	T	26/28 (93%)	25 (96%)	1 (4%)	29 39
14	t	26/28 (93%)	26 (100%)	0	100 100
15	U	83/89 (93%)	79 (95%)	4 (5%)	23 29
15	u	84/89 (94%)	82 (98%)	2 (2%)	43 57
16	V	117/117 (100%)	116 (99%)	1 (1%)	70 82
16	v	117/117 (100%)	114 (97%)	3 (3%)	40 54
17	X	31/33 (94%)	30 (97%)	1 (3%)	34 46
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24 32
18	y	22/23 (96%)	19 (86%)	3 (14%)	3 3
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 22
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 39
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4352/4403 (99%)	4260 (98%)	92 (2%)	47 61

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	279	LEU
9	j	23	ILE
3	c	416	SER
5	e	12	ASP
12	m	5	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	186	GLN
13	o	80	GLN
15	u	81	HIS
13	o	132	ASN
15	U	78	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	0.70	0	8,9,11	1.33	1 (12%)
14	FME	t	1	14	8,9,10	0.68	0	8,9,11	1.80	2 (25%)
12	FME	M	1	12	8,9,10	0.64	0	8,9,11	1.55	3 (37%)
8	FME	i	1	8	8,9,10	0.61	0	8,9,11	1.02	1 (12%)
12	FME	m	1	12	8,9,10	0.62	0	8,9,11	1.29	1 (12%)
8	FME	I	1	8	8,9,10	0.73	0	8,9,11	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-3.48	117.47	122.82
12	M	1	FME	CA-N-CN	-2.93	118.32	122.82
14	T	1	FME	O-C-CA	-2.78	117.63	124.77
14	t	1	FME	O-C-CA	-2.43	118.52	124.77
12	M	1	FME	O-C-CA	-2.29	118.87	124.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	O-C-CA-CB
14	t	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.11	1 (6%)
27	SQD	A	411	-	52,54,54	1.00	2 (3%)	62,65,65	1.31	7 (11%)
31	LMG	c	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.05	4 (6%)
32	LHG	D	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	B	611	-	69,73,73	1.98	19 (27%)	82,113,113	2.72	31 (37%)
27	SQD	D	415	-	41,43,54	1.10	2 (4%)	51,54,65	1.80	10 (19%)
23	CLA	B	602	-	69,73,73	2.06	19 (27%)	82,113,113	2.77	31 (37%)
23	CLA	c	510	-	69,73,73	2.06	20 (28%)	82,113,113	2.70	30 (36%)
34	LMT	D	403	-	36,36,36	0.53	1 (2%)	47,47,47	0.83	2 (4%)
31	LMG	M	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.23	7 (11%)
23	CLA	b	605	-	69,73,73	1.95	21 (30%)	82,113,113	2.85	31 (37%)
23	CLA	B	612	-	69,73,73	1.91	19 (27%)	82,113,113	2.80	29 (35%)
26	GOL	v	202	-	5,5,5	1.03	0	5,5,5	0.99	0
27	SQD	a	411	-	52,54,54	0.97	2 (3%)	62,65,65	1.28	7 (11%)
25	BCR	K	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	11 (19%)
31	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.11	3 (6%)
23	CLA	B	614	-	69,73,73	1.93	20 (28%)	82,113,113	2.87	32 (39%)
25	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.70	11 (19%)
23	CLA	c	506	-	69,73,73	2.03	19 (27%)	82,113,113	2.60	29 (35%)
31	LMG	D	414	39	51,51,55	0.86	3 (5%)	59,59,63	0.99	3 (5%)
31	LMG	A	415	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	5 (8%)
23	CLA	b	606	-	69,73,73	1.96	20 (28%)	82,113,113	2.80	33 (40%)
38	HEM	E	103	5,6	50,50,50	1.56	8 (16%)	67,82,82	1.63	16 (23%)
23	CLA	B	606	-	69,73,73	1.98	20 (28%)	82,113,113	2.71	30 (36%)
23	CLA	c	507	-	69,73,73	2.03	20 (28%)	82,113,113	2.64	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	c	517	-	63,63,67	0.91	2 (3%)	77,77,81	1.03	3 (3%)
23	CLA	b	603	-	69,73,73	2.03	20 (28%)	82,113,113	2.76	32 (39%)
33	HTG	B	621	-	19,19,19	0.91	1 (5%)	23,24,24	1.49	4 (17%)
25	BCR	c	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.49	11 (19%)
23	CLA	c	504	-	69,73,73	2.03	19 (27%)	82,113,113	2.72	29 (35%)
33	HTG	C	522	-	19,19,19	0.84	1 (5%)	23,24,24	1.21	1 (4%)
29	PL9	D	408	-	55,55,55	0.68	2 (3%)	68,69,69	1.71	19 (27%)
23	CLA	c	508	41	69,73,73	2.06	18 (26%)	82,113,113	2.77	31 (37%)
23	CLA	D	406	-	69,73,73	2.03	17 (24%)	82,113,113	2.68	32 (39%)
23	CLA	A	408	-	69,73,73	2.02	20 (28%)	82,113,113	2.70	32 (39%)
23	CLA	d	402	41	69,73,73	2.04	18 (26%)	82,113,113	2.65	33 (40%)
25	BCR	D	407	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	15 (26%)
23	CLA	b	616	-	69,73,73	1.98	19 (27%)	82,113,113	2.81	33 (40%)
38	HEM	f	101	5,6	50,50,50	1.55	8 (16%)	67,82,82	1.63	12 (17%)
33	HTG	c	522	-	19,19,19	0.91	2 (10%)	23,24,24	1.22	1 (4%)
23	CLA	b	604	-	69,73,73	1.95	19 (27%)	82,113,113	2.64	34 (41%)
33	HTG	b	621	-	19,19,19	0.94	1 (5%)	23,24,24	1.32	2 (8%)
23	CLA	C	508	41	69,73,73	2.00	19 (27%)	82,113,113	2.61	32 (39%)
24	PHO	D	402	-	58,69,69	2.75	15 (25%)	55,99,99	2.98	17 (30%)
27	SQD	L	102	-	52,54,54	0.97	2 (3%)	62,65,65	1.60	10 (16%)
34	LMT	C	525	-	36,36,36	0.53	1 (2%)	47,47,47	1.16	3 (6%)
25	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.45	9 (16%)
34	LMT	b	626	-	25,25,36	0.57	1 (4%)	30,30,47	1.27	3 (10%)
33	HTG	b	624	-	19,19,19	0.96	2 (10%)	23,24,24	1.26	2 (8%)
23	CLA	b	611	-	69,73,73	1.94	20 (28%)	82,113,113	2.74	30 (36%)
33	HTG	h	101	-	16,16,19	1.05	2 (12%)	20,21,24	2.01	6 (30%)
23	CLA	c	514	-	69,73,73	2.06	20 (28%)	82,113,113	2.65	33 (40%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.11	8 (10%)
24	PHO	a	416	-	58,69,69	2.78	14 (24%)	55,99,99	2.97	15 (27%)
23	CLA	c	502	-	69,73,73	1.99	19 (27%)	82,113,113	2.62	32 (39%)
23	CLA	a	407	-	69,73,73	2.01	18 (26%)	82,113,113	2.68	32 (39%)
29	PL9	A	413	-	55,55,55	0.67	2 (3%)	68,69,69	2.01	22 (32%)
32	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.11	5 (9%)
25	BCR	T	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.69	13 (23%)
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	82,113,113	2.64	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	a	408	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	10 (17%)
35	DGD	C	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.02	4 (5%)
31	LMG	c	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.20	6 (10%)
23	CLA	a	405	41	69,73,73	1.93	19 (27%)	82,113,113	2.72	32 (39%)
23	CLA	c	512	3	69,73,73	2.01	18 (26%)	82,113,113	2.69	32 (39%)
34	LMT	B	628	-	25,25,36	0.46	0	30,30,47	1.01	1 (3%)
32	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.98	2 (4%)
33	HTG	B	624	-	19,19,19	0.97	2 (10%)	23,24,24	1.39	4 (17%)
23	CLA	A	405	41	69,73,73	2.02	19 (27%)	82,113,113	2.73	35 (42%)
29	PL9	d	406	-	55,55,55	0.72	2 (3%)	68,69,69	1.62	16 (23%)
35	DGD	h	103	-	63,63,67	0.92	3 (4%)	77,77,81	1.02	4 (5%)
25	BCR	b	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	10 (17%)
34	LMT	t	101	-	26,26,36	0.51	1 (3%)	31,31,47	1.05	2 (6%)
23	CLA	b	602	-	69,73,73	2.06	20 (28%)	82,113,113	2.75	33 (40%)
23	CLA	b	614	-	69,73,73	1.98	18 (26%)	82,113,113	2.74	31 (37%)
23	CLA	C	509	-	69,73,73	2.01	19 (27%)	82,113,113	2.71	26 (31%)
25	BCR	t	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	15 (26%)
26	GOL	B	626	-	5,5,5	0.88	0	5,5,5	1.21	0
28	OEX	A	412	41,3,1	0,15,15	-	-	-		
23	CLA	C	504	-	69,73,73	2.03	19 (27%)	82,113,113	2.71	29 (35%)
34	LMT	a	412	-	36,36,36	0.63	1 (2%)	47,47,47	1.26	5 (10%)
34	LMT	b	620	-	25,25,36	0.52	0	30,30,47	0.62	0
23	CLA	B	616	-	69,73,73	1.96	19 (27%)	82,113,113	2.73	31 (37%)
27	SQD	f	102	-	41,43,54	1.09	2 (4%)	51,54,65	1.26	6 (11%)
35	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.16	6 (7%)
23	CLA	B	604	-	69,73,73	1.96	20 (28%)	82,113,113	2.67	33 (40%)
33	HTG	b	622	-	19,19,19	0.92	1 (5%)	23,24,24	1.51	3 (13%)
32	LHG	A	416	-	48,48,48	0.90	2 (4%)	51,54,54	1.22	5 (9%)
25	BCR	b	617	-	41,41,41	1.14	1 (2%)	56,56,56	1.45	7 (12%)
23	CLA	B	607	41	69,73,73	1.95	19 (27%)	82,113,113	2.63	30 (36%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.86	15 (26%)
34	LMT	e	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.87	2 (4%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.62	11 (19%)
34	LMT	E	102	-	36,36,36	0.56	1 (2%)	47,47,47	1.11	4 (8%)
26	GOL	c	526	-	5,5,5	0.83	0	5,5,5	1.13	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	GOL	b	623	-	5,5,5	1.02	0	5,5,5	1.17	0
23	CLA	b	613	-	69,73,73	2.02	18 (26%)	82,113,113	2.64	30 (36%)
26	GOL	O	302	-	5,5,5	0.88	0	5,5,5	1.10	0
31	LMG	d	412	39	51,51,55	0.92	3 (5%)	59,59,63	0.90	3 (5%)
31	LMG	C	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.00	4 (6%)
23	CLA	b	607	41	69,73,73	1.98	18 (26%)	82,113,113	2.72	30 (36%)
25	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	11 (19%)
27	SQD	B	620	-	52,54,54	0.97	2 (3%)	62,65,65	1.53	10 (16%)
28	OEX	a	413	41,3,1	0,15,15	-	-	-		
23	CLA	A	406	41	69,73,73	2.00	20 (28%)	82,113,113	2.68	29 (35%)
23	CLA	c	503	-	69,73,73	1.95	19 (27%)	82,113,113	2.65	29 (35%)
31	LMG	a	417	-	51,51,55	0.93	2 (3%)	59,59,63	1.18	7 (11%)
23	CLA	B	608	-	69,73,73	1.97	20 (28%)	82,113,113	2.68	30 (36%)
25	BCR	h	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.33	7 (12%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	b	610	41	69,73,73	2.02	21 (30%)	82,113,113	2.76	31 (37%)
29	PL9	a	414	-	55,55,55	0.66	2 (3%)	68,69,69	2.04	20 (29%)
23	CLA	C	512	3	69,73,73	2.04	22 (31%)	82,113,113	2.64	31 (37%)
23	CLA	B	610	41	69,73,73	2.04	19 (27%)	82,113,113	2.69	30 (36%)
25	BCR	B	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.54	12 (21%)
23	CLA	D	405	-	69,73,73	1.96	19 (27%)	82,113,113	2.79	31 (37%)
23	CLA	C	511	-	69,73,73	2.02	19 (27%)	82,113,113	2.71	30 (36%)
37	BCT	d	401	21	3,3,3	0.43	0	2,3,3	1.94	1 (50%)
23	CLA	C	507	-	69,73,73	2.04	21 (30%)	82,113,113	2.70	34 (41%)
32	LHG	D	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.05	4 (7%)
32	LHG	L	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.15	4 (7%)
26	GOL	A	410	-	5,5,5	1.16	0	5,5,5	0.80	0
26	GOL	B	623	-	5,5,5	1.00	0	5,5,5	1.18	1 (20%)
23	CLA	b	612	-	69,73,73	2.00	20 (28%)	82,113,113	2.77	29 (35%)
32	LHG	d	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	3 (5%)
23	CLA	b	608	-	69,73,73	2.02	20 (28%)	82,113,113	2.66	30 (36%)
25	BCR	A	409	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	8 (14%)
26	GOL	b	627	-	5,5,5	0.99	0	5,5,5	1.11	1 (20%)
23	CLA	b	615	-	69,73,73	2.01	18 (26%)	82,113,113	2.67	30 (36%)
25	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.53	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMT	M	102	-	36,36,36	0.47	0	47,47,47	0.94	3 (6%)
23	CLA	B	603	-	69,73,73	2.02	19 (27%)	82,113,113	2.79	29 (35%)
34	LMT	m	103	-	36,36,36	0.44	0	47,47,47	1.03	3 (6%)
26	GOL	B	627	-	5,5,5	1.08	0	5,5,5	0.94	0
23	CLA	C	503	-	69,73,73	2.00	20 (28%)	82,113,113	2.58	31 (37%)
32	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.06	2 (4%)
23	CLA	C	505	41	69,73,73	2.00	21 (30%)	82,113,113	2.64	32 (39%)
23	CLA	B	615	-	69,73,73	1.95	18 (26%)	82,113,113	2.75	29 (35%)
33	HTG	B	622	-	19,19,19	0.77	1 (5%)	23,24,24	1.30	1 (4%)
23	CLA	a	404	-	69,73,73	1.98	18 (26%)	82,113,113	2.74	34 (41%)
23	CLA	B	613	-	69,73,73	1.96	20 (28%)	82,113,113	2.71	27 (32%)
32	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
23	CLA	c	511	-	69,73,73	1.96	20 (28%)	82,113,113	2.66	31 (37%)
23	CLA	B	601	41	69,73,73	2.07	20 (28%)	82,113,113	2.65	30 (36%)
24	PHO	A	407	-	58,69,69	2.66	13 (22%)	55,99,99	3.01	18 (32%)
26	GOL	c	501	-	5,5,5	1.07	0	5,5,5	0.94	0
33	HTG	D	413	-	16,16,19	1.02	2 (12%)	20,21,24	1.16	1 (5%)
26	GOL	C	523	-	5,5,5	1.21	0	5,5,5	1.01	0
40	HEC	v	203	16	46,50,50	1.91	5 (10%)	58,82,82	1.84	6 (10%)
31	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	3 (5%)
23	CLA	d	404	-	69,73,73	2.09	19 (27%)	82,113,113	2.78	32 (39%)
23	CLA	c	509	-	69,73,73	2.07	19 (27%)	82,113,113	2.68	31 (37%)
23	CLA	C	513	-	69,73,73	2.06	20 (28%)	82,113,113	2.65	34 (41%)
23	CLA	c	505	41	69,73,73	2.03	20 (28%)	82,113,113	2.71	34 (41%)
40	HEC	V	201	16	46,50,50	1.91	6 (13%)	58,82,82	1.84	11 (18%)
25	BCR	B	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.29	10 (17%)
23	CLA	c	513	-	69,73,73	2.04	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	C	510	-	69,73,73	2.08	20 (28%)	82,113,113	2.67	27 (32%)
23	CLA	B	609	-	69,73,73	1.98	18 (26%)	82,113,113	2.68	26 (31%)
25	BCR	d	405	-	41,41,41	1.17	2 (4%)	56,56,56	1.84	12 (21%)
35	DGD	c	519	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	6 (7%)
27	SQD	a	409	-	52,54,54	0.92	2 (3%)	62,65,65	1.63	11 (17%)
23	CLA	C	506	-	69,73,73	1.98	20 (28%)	82,113,113	2.59	29 (35%)
25	BCR	b	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.55	12 (21%)
25	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	BCT	D	401	21	3,3,3	0.44	0	2,3,3	1.16	0
23	CLA	b	609	-	69,73,73	2.02	22 (31%)	82,113,113	2.62	33 (40%)
26	GOL	a	410	-	5,5,5	0.85	0	5,5,5	1.08	0
34	LMT	M	104	-	36,36,36	0.50	0	47,47,47	1.18	3 (6%)
31	LMG	C	521	-	51,51,55	1.02	3 (5%)	59,59,63	1.36	7 (11%)
35	DGD	C	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.18	7 (9%)
32	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	4 (7%)
31	LMG	Z	101	-	37,37,55	1.03	3 (8%)	45,45,63	1.52	7 (15%)
23	CLA	C	514	-	69,73,73	2.00	19 (27%)	82,113,113	2.69	31 (37%)
35	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	4 (5%)
34	LMT	a	418	-	36,36,36	0.50	1 (2%)	47,47,47	0.95	2 (4%)
34	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.11	4 (8%)
23	CLA	B	605	-	69,73,73	2.03	19 (27%)	82,113,113	2.71	30 (36%)
27	SQD	C	501	-	52,54,54	0.90	2 (3%)	62,65,65	1.95	10 (16%)
23	CLA	A	404	-	69,73,73	1.97	19 (27%)	82,113,113	2.69	33 (40%)
24	PHO	a	406	-	58,69,69	2.68	13 (22%)	55,99,99	3.02	14 (25%)
23	CLA	C	502	-	69,73,73	1.98	20 (28%)	82,113,113	2.78	31 (37%)
23	CLA	d	403	-	69,73,73	1.90	19 (27%)	82,113,113	2.64	33 (40%)

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
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
31	LMG	c	520	-	-	9/46/66/70	0/1/1/1
32	LHG	D	410	-	-	14/53/53/53	-
23	CLA	B	611	-	1/1/15/20	4/39/115/115	-
27	SQD	D	415	-	-	15/38/58/69	0/1/1/1
23	CLA	B	602	-	1/1/15/20	9/39/115/115	-
23	CLA	c	510	-	1/1/15/20	11/39/115/115	-
34	LMT	D	403	-	-	8/21/61/61	0/2/2/2
31	LMG	M	101	-	-	10/46/66/70	0/1/1/1
23	CLA	b	605	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	-	1/1/15/20	3/39/115/115	-
26	GOL	v	202	-	-	2/4/4/4	-
27	SQD	a	411	-	-	16/49/69/69	0/1/1/1
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
31	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	10/39/115/115	-
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
23	CLA	c	506	-	1/1/15/20	4/39/115/115	-
31	LMG	D	414	39	-	9/46/66/70	0/1/1/1
31	LMG	A	415	-	-	24/46/66/70	0/1/1/1
23	CLA	b	606	-	1/1/15/20	7/39/115/115	-
38	HEM	E	103	5,6	-	4/14/54/54	-
23	CLA	B	606	-	1/1/15/20	11/39/115/115	-
23	CLA	c	507	-	1/1/15/20	11/39/115/115	-
35	DGD	c	517	-	-	18/51/91/95	0/2/2/2
23	CLA	b	603	-	1/1/15/20	6/39/115/115	-
33	HTG	B	621	-	-	2/10/30/30	0/1/1/1
25	BCR	c	516	-	-	2/29/63/63	0/2/2/2
23	CLA	c	504	-	1/1/15/20	0/39/115/115	-
33	HTG	C	522	-	-	1/10/30/30	0/1/1/1
29	PL9	D	408	-	-	9/53/73/73	0/1/1/1
23	CLA	c	508	41	1/1/15/20	11/39/115/115	-
23	CLA	D	406	-	1/1/15/20	8/39/115/115	-
23	CLA	A	408	-	1/1/15/20	10/39/115/115	-
23	CLA	d	402	41	1/1/15/20	8/39/115/115	-
25	BCR	D	407	-	-	6/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
38	HEM	f	101	5,6	-	5/14/54/54	-
33	HTG	c	522	-	-	3/10/30/30	0/1/1/1
23	CLA	b	604	-	1/1/15/20	8/39/115/115	-
33	HTG	b	621	-	-	4/10/30/30	0/1/1/1
23	CLA	C	508	41	1/1/15/20	6/39/115/115	-
24	PHO	D	402	-	-	0/37/103/103	0/5/6/6
27	SQD	L	102	-	-	19/49/69/69	0/1/1/1
34	LMT	C	525	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
34	LMT	b	626	-	-	9/17/37/61	0/1/1/2
33	HTG	b	624	-	-	2/10/30/30	0/1/1/1
23	CLA	b	611	-	1/1/15/20	5/39/115/115	-
33	HTG	h	101	-	-	1/7/27/30	0/1/1/1
23	CLA	c	514	-	1/1/15/20	13/39/115/115	-
35	DGD	H	102	-	-	18/51/91/95	0/2/2/2
24	PHO	a	416	-	-	6/37/103/103	0/5/6/6
23	CLA	c	502	-	1/1/15/20	5/39/115/115	-
23	CLA	a	407	-	1/1/15/20	11/39/115/115	-
29	PL9	A	413	-	-	16/53/73/73	0/1/1/1
32	LHG	d	407	-	-	16/53/53/53	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
23	CLA	b	601	41	1/1/15/20	14/39/115/115	-
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
35	DGD	C	519	-	-	9/51/91/95	0/2/2/2
31	LMG	c	521	-	-	9/46/66/70	0/1/1/1
23	CLA	a	405	41	-	8/39/115/115	-
23	CLA	c	512	3	1/1/15/20	4/39/115/115	-
34	LMT	B	628	-	-	2/17/37/61	0/1/1/2
32	LHG	a	419	-	-	14/46/46/53	-
33	HTG	B	624	-	-	4/10/30/30	0/1/1/1
23	CLA	A	405	41	1/1/15/20	2/39/115/115	-
29	PL9	d	406	-	-	7/53/73/73	0/1/1/1
35	DGD	h	103	-	-	12/51/91/95	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
23	CLA	b	614	-	1/1/15/20	10/39/115/115	-
23	CLA	C	509	-	1/1/15/20	5/39/115/115	-
25	BCR	t	102	-	-	6/29/63/63	0/2/2/2
26	GOL	B	626	-	-	3/4/4/4	-
23	CLA	C	504	-	-	4/39/115/115	-
34	LMT	a	412	-	-	7/21/61/61	0/2/2/2
34	LMT	b	620	-	-	7/17/37/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	616	-	1/1/15/20	7/39/115/115	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	6/39/115/115	-
33	HTG	b	622	-	-	3/10/30/30	0/1/1/1
32	LHG	A	416	-	-	15/53/53/53	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	607	41	1/1/15/20	4/39/115/115	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
34	LMT	e	101	-	-	10/21/61/61	0/2/2/2
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
34	LMT	E	102	-	-	6/21/61/61	0/2/2/2
26	GOL	c	526	-	-	0/4/4/4	-
26	GOL	b	623	-	-	2/4/4/4	-
23	CLA	b	613	-	1/1/15/20	7/39/115/115	-
26	GOL	O	302	-	-	4/4/4/4	-
31	LMG	d	412	39	-	7/46/66/70	0/1/1/1
31	LMG	C	520	-	-	13/46/66/70	0/1/1/1
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
27	SQD	B	620	-	-	15/49/69/69	0/1/1/1
31	LMG	a	417	-	-	13/46/66/70	0/1/1/1
23	CLA	c	503	-	1/1/15/20	5/39/115/115	-
23	CLA	A	406	41	-	5/39/115/115	-
23	CLA	B	608	-	-	2/39/115/115	-
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	b	610	41	1/1/15/20	8/39/115/115	-
29	PL9	a	414	-	-	18/53/73/73	0/1/1/1
23	CLA	C	512	3	1/1/15/20	3/39/115/115	-
23	CLA	B	610	41	1/1/15/20	5/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	D	405	-	1/1/15/20	5/39/115/115	-
23	CLA	C	511	-	1/1/15/20	10/39/115/115	-
23	CLA	C	507	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	D	409	-	-	15/53/53/53	-
32	LHG	L	101	-	-	12/53/53/53	-
26	GOL	A	410	-	-	4/4/4/4	-
26	GOL	B	623	-	-	2/4/4/4	-
23	CLA	b	612	-	1/1/15/20	3/39/115/115	-
32	LHG	d	409	-	-	9/53/53/53	-
23	CLA	b	608	-	-	3/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
26	GOL	b	627	-	-	0/4/4/4	-
23	CLA	b	615	-	1/1/15/20	11/39/115/115	-
25	BCR	c	515	-	-	2/29/63/63	0/2/2/2
34	LMT	M	102	-	-	6/21/61/61	0/2/2/2
23	CLA	B	603	-	1/1/15/20	8/39/115/115	-
34	LMT	m	103	-	-	5/21/61/61	0/2/2/2
26	GOL	B	627	-	-	0/4/4/4	-
23	CLA	C	503	-	-	10/39/115/115	-
32	LHG	E	101	-	-	15/46/46/53	-
23	CLA	C	505	41	1/1/15/20	7/39/115/115	-
23	CLA	B	615	-	1/1/15/20	7/39/115/115	-
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
23	CLA	a	404	-	1/1/15/20	6/39/115/115	-
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
32	LHG	b	628	-	-	17/53/53/53	-
23	CLA	c	511	-	1/1/15/20	7/39/115/115	-
23	CLA	B	601	41	1/1/15/20	10/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
26	GOL	c	501	-	-	0/4/4/4	-
33	HTG	D	413	-	-	2/7/27/30	0/1/1/1
26	GOL	C	523	-	-	0/4/4/4	-
40	HEC	v	203	16	-	6/14/54/54	-
31	LMG	m	101	-	-	12/46/66/70	0/1/1/1
23	CLA	d	404	-	1/1/15/20	6/39/115/115	-
23	CLA	c	509	-	1/1/15/20	7/39/115/115	-
23	CLA	C	513	-	1/1/15/20	12/39/115/115	-
23	CLA	c	505	41	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	201	16	-	6/14/54/54	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/15/20	10/39/115/115	-
23	CLA	C	510	-	1/1/15/20	4/39/115/115	-
23	CLA	B	609	-	1/1/15/20	4/39/115/115	-
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
27	SQD	a	409	-	-	13/49/69/69	0/1/1/1
23	CLA	C	506	-	1/1/15/20	9/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
23	CLA	b	609	-	1/1/15/20	10/39/115/115	-
26	GOL	a	410	-	-	4/4/4/4	-
34	LMT	M	104	-	-	8/21/61/61	0/2/2/2
31	LMG	C	521	-	-	14/46/66/70	0/1/1/1
35	DGD	C	517	-	-	16/51/91/95	0/2/2/2
32	LHG	d	408	-	-	18/53/53/53	-
31	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
23	CLA	C	514	-	1/1/15/20	13/39/115/115	-
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
34	LMT	D	404	-	-	9/21/61/61	0/2/2/2
23	CLA	B	605	-	1/1/15/20	6/39/115/115	-
27	SQD	C	501	-	-	12/49/69/69	0/1/1/1
23	CLA	A	404	-	1/1/15/20	2/39/115/115	-
24	PHO	a	406	-	-	2/37/103/103	0/5/6/6
23	CLA	C	502	-	1/1/15/20	4/39/115/115	-
23	CLA	d	403	-	1/1/15/20	6/39/115/115	-

The worst 5 of 1579 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416	PHO	C1B-C2B	9.40	1.49	1.39
24	A	407	PHO	C1D-C2D	9.07	1.49	1.39
24	a	406	PHO	C1B-C2B	8.99	1.49	1.39
24	a	416	PHO	C1D-C2D	8.90	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	PHO	C1D-C2D	8.68	1.49	1.39

The worst 5 of 2859 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	PHO	C2D-C1D-ND	11.91	118.04	109.43
24	D	402	PHO	C2D-C1D-ND	11.72	117.90	109.43
24	a	416	PHO	C2D-C1D-ND	11.42	117.68	109.43
23	a	405	CLA	C1D-ND-C4D	-10.77	98.76	106.31
24	A	407	PHO	C2D-C1D-ND	10.76	117.21	109.43

5 of 64 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

5 of 1277 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C14-C13-C15-C16

There are no ring outliers.

146 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	520	LMG	1	0
32	D	410	LHG	4	0
27	D	415	SQD	2	0
23	B	602	CLA	6	0
23	c	510	CLA	3	0
34	D	403	LMT	2	0
31	M	101	LMG	3	0
23	b	605	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	612	CLA	2	0
26	v	202	GOL	1	0
25	K	101	BCR	2	0
31	z	101	LMG	3	0
25	k	102	BCR	2	0
23	c	506	CLA	7	0
31	A	415	LMG	2	0
23	b	606	CLA	2	0
38	E	103	HEM	2	0
23	B	606	CLA	1	0
23	c	507	CLA	4	0
35	c	517	DGD	2	0
23	b	603	CLA	5	0
33	B	621	HTG	1	0
25	c	516	BCR	3	0
23	c	504	CLA	4	0
29	D	408	PL9	1	0
23	c	508	CLA	4	0
23	A	408	CLA	5	0
23	d	402	CLA	4	0
23	b	616	CLA	3	0
38	f	101	HEM	2	0
33	c	522	HTG	1	0
23	b	604	CLA	5	0
33	b	621	HTG	3	0
23	C	508	CLA	2	0
24	D	402	PHO	1	0
27	L	102	SQD	4	0
34	C	525	LMT	1	0
25	H	101	BCR	3	0
34	b	626	LMT	1	0
33	b	624	HTG	1	0
23	b	611	CLA	1	0
33	h	101	HTG	2	0
23	c	514	CLA	3	0
35	H	102	DGD	2	0
24	a	416	PHO	3	0
23	c	502	CLA	3	0
23	a	407	CLA	3	0
29	A	413	PL9	3	0
32	d	407	LHG	4	0
25	T	101	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	601	CLA	1	0
25	a	408	BCR	1	0
35	C	519	DGD	1	0
23	a	405	CLA	2	0
23	c	512	CLA	3	0
32	a	419	LHG	2	0
33	B	624	HTG	1	0
23	A	405	CLA	5	0
29	d	406	PL9	1	0
25	b	618	BCR	4	0
23	b	602	CLA	2	0
23	b	614	CLA	1	0
23	C	509	CLA	3	0
25	t	102	BCR	3	0
26	B	626	GOL	1	0
23	C	504	CLA	4	0
34	a	412	LMT	2	0
34	b	620	LMT	1	0
23	B	616	CLA	6	0
27	f	102	SQD	2	0
35	C	518	DGD	3	0
23	B	604	CLA	3	0
32	A	416	LHG	3	0
25	b	617	BCR	1	0
23	B	607	CLA	2	0
25	Y	101	BCR	2	0
25	k	101	BCR	1	0
34	E	102	LMT	1	0
23	b	613	CLA	5	0
31	d	412	LMG	5	0
31	C	520	LMG	3	0
25	C	516	BCR	1	0
23	A	406	CLA	1	0
23	c	503	CLA	4	0
31	a	417	LMG	3	0
25	h	102	BCR	3	0
25	C	515	BCR	2	0
23	b	610	CLA	4	0
29	a	414	PL9	6	0
23	C	512	CLA	3	0
23	B	610	CLA	2	0
25	B	618	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	405	CLA	3	0
23	C	511	CLA	4	0
23	C	507	CLA	5	0
32	D	409	LHG	1	0
32	L	101	LHG	2	0
32	d	409	LHG	8	0
23	b	608	CLA	3	0
25	A	409	BCR	1	0
26	b	627	GOL	1	0
23	b	615	CLA	4	0
25	c	515	BCR	1	0
34	M	102	LMT	1	0
23	B	603	CLA	4	0
23	C	503	CLA	4	0
32	E	101	LHG	2	0
23	C	505	CLA	2	0
23	B	615	CLA	2	0
33	B	622	HTG	2	0
23	a	404	CLA	3	0
23	B	613	CLA	4	0
32	b	628	LHG	1	0
23	c	511	CLA	2	0
23	B	601	CLA	2	0
24	A	407	PHO	1	0
26	c	501	GOL	2	0
33	D	413	HTG	2	0
23	d	404	CLA	2	0
23	c	509	CLA	3	0
23	C	513	CLA	2	0
23	c	505	CLA	5	0
40	V	201	HEC	1	0
25	B	619	BCR	5	0
23	c	513	CLA	8	0
23	C	510	CLA	1	0
23	B	609	CLA	1	0
25	d	405	BCR	1	0
35	c	519	DGD	2	0
27	a	409	SQD	3	0
23	C	506	CLA	1	0
25	b	619	BCR	3	0
25	B	617	BCR	2	0
31	C	521	LMG	1	0

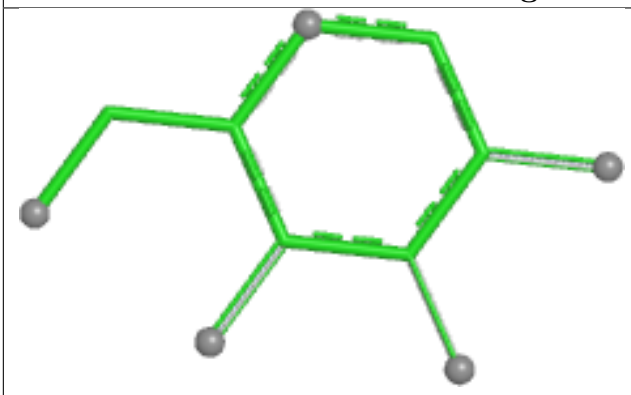
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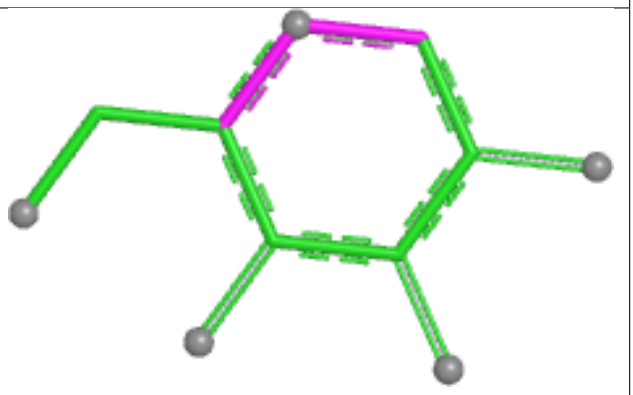
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	517	DGD	5	0
32	d	408	LHG	2	0
23	C	514	CLA	1	0
35	c	518	DGD	1	0
34	a	418	LMT	3	0
34	D	404	LMT	1	0
23	B	605	CLA	6	0
27	C	501	SQD	3	0
23	A	404	CLA	2	0
24	a	406	PHO	2	0
23	C	502	CLA	3	0
23	d	403	CLA	2	0

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.

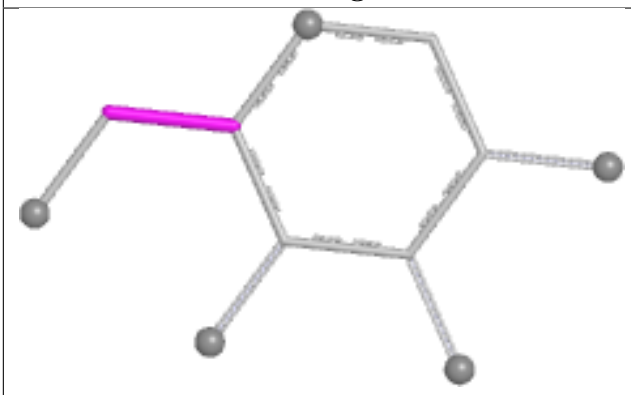
Ligand HTG V 202



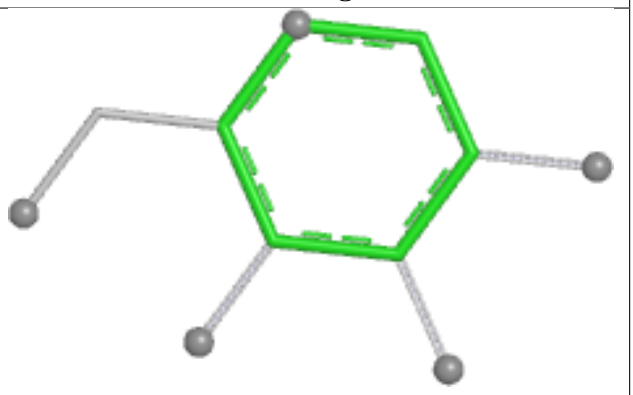
Bond lengths



Bond angles

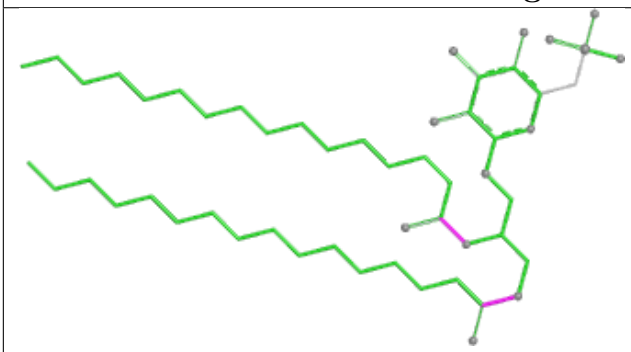


Torsions

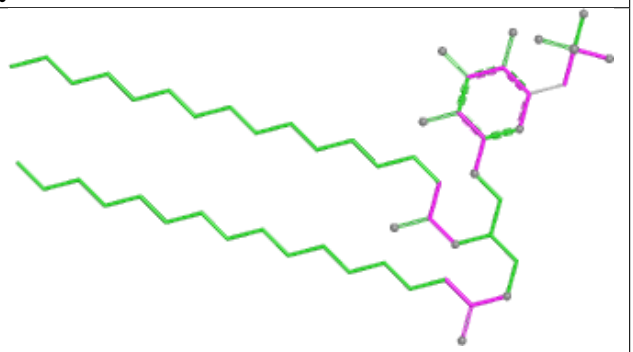


Rings

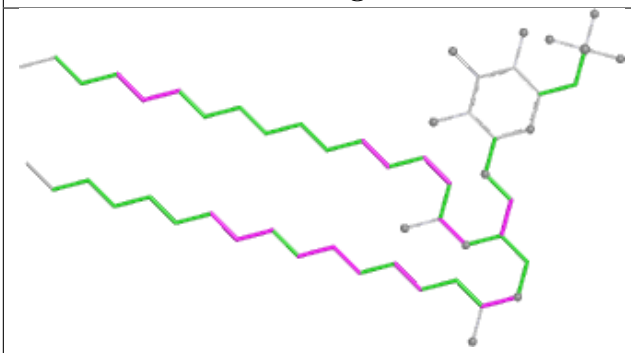
Ligand SQD A 411



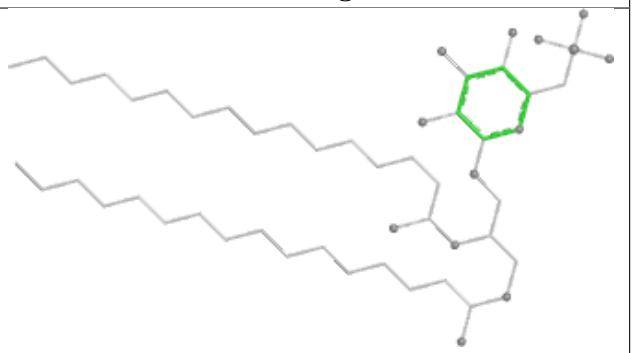
Bond lengths



Bond angles

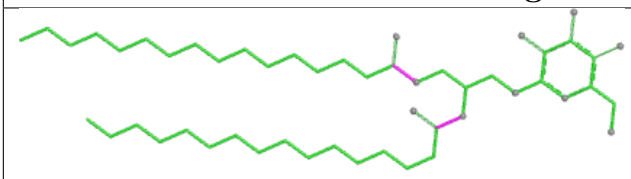


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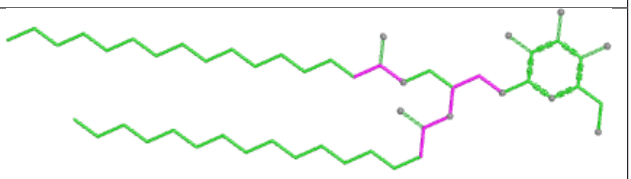


Rings

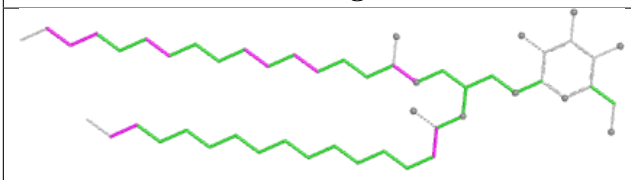
Ligand LMG c 520



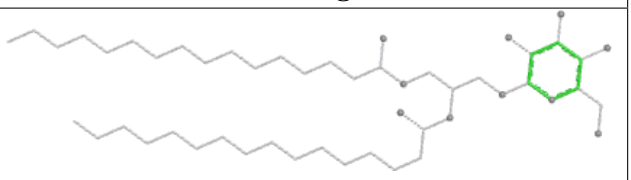
Bond lengths



Bond angles

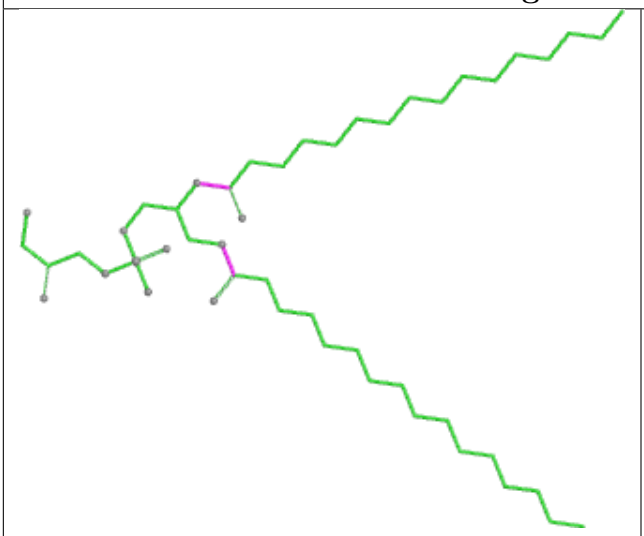


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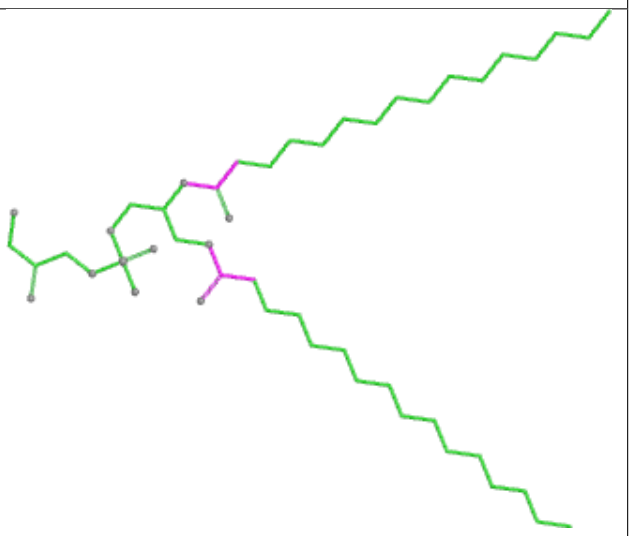


Rings

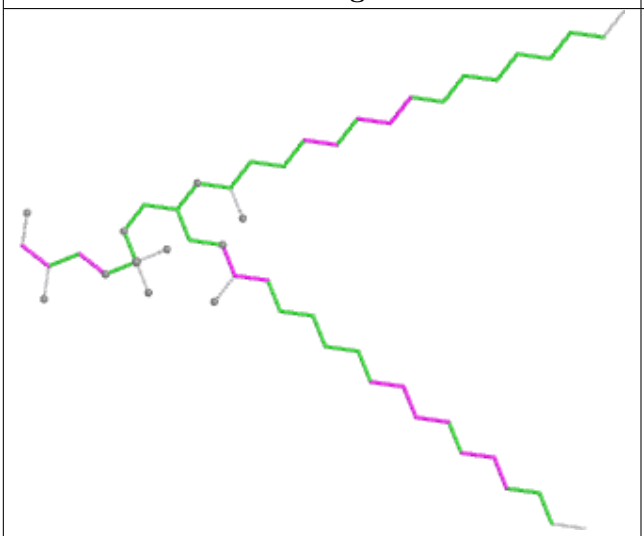
Ligand LHG D 410



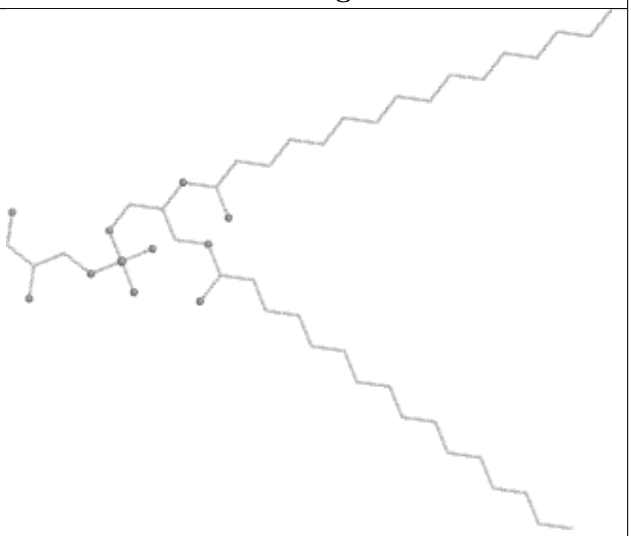
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Bond angles

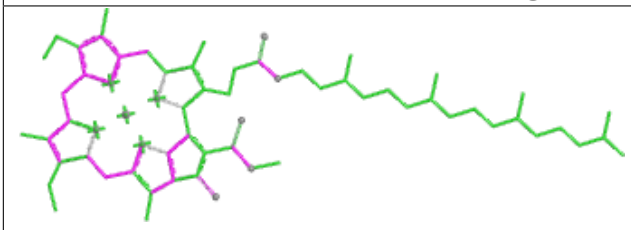


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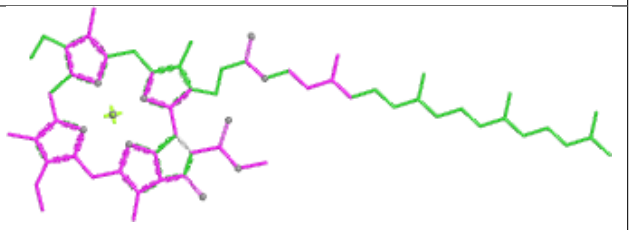


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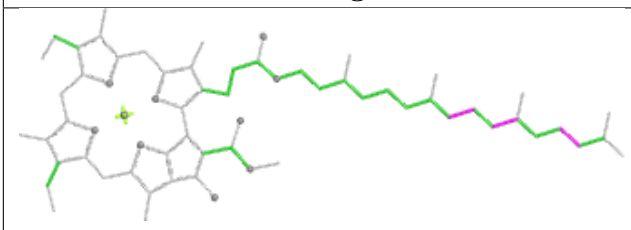
Ligand CLA B 611



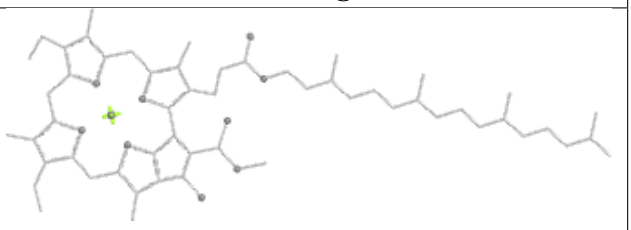
Bond lengths



Bond angles

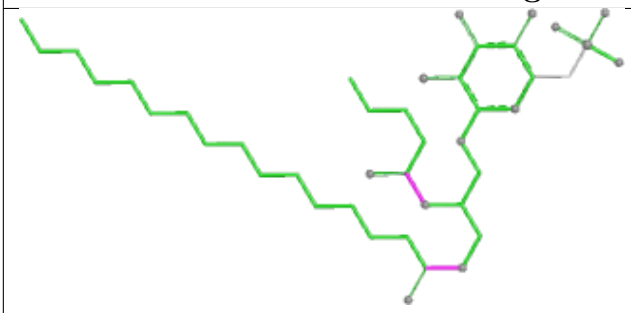


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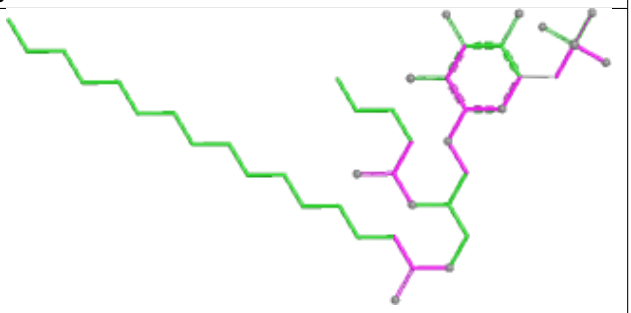


Rings

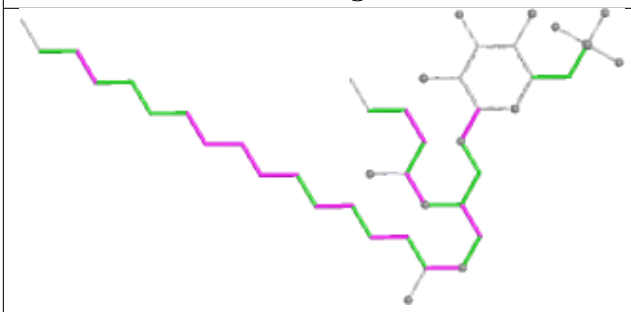
Ligand SQD D 415



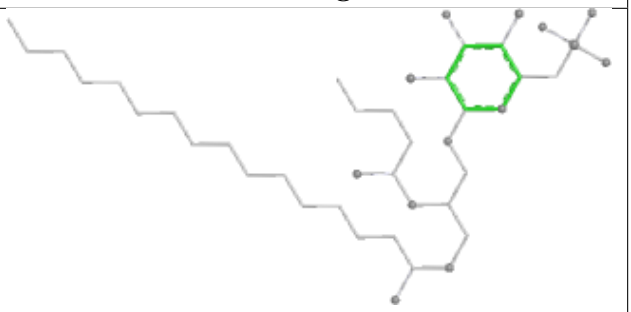
Bond lengths



Bond angles

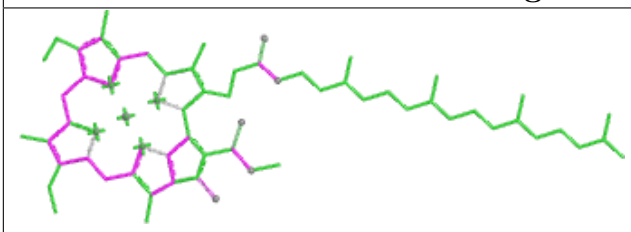


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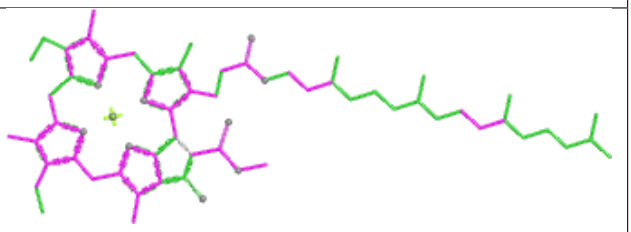


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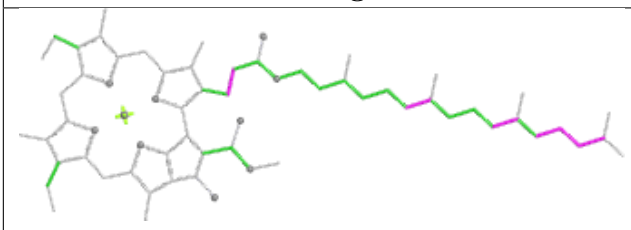
Ligand CLA B 602



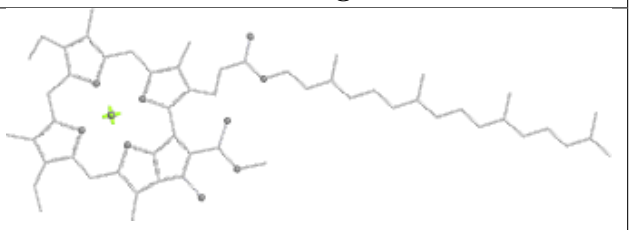
Bond lengths



Bond angles

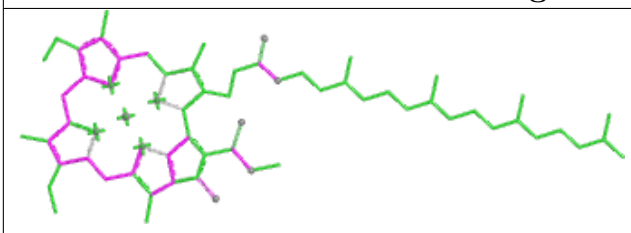


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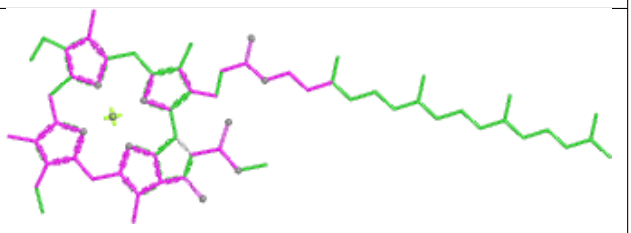


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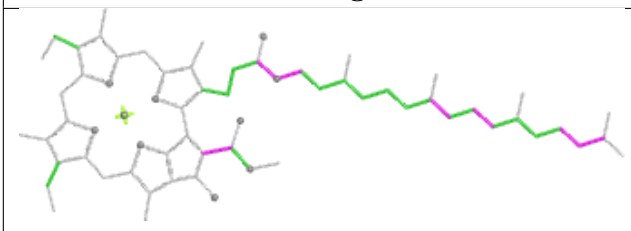
Ligand CLA c 510



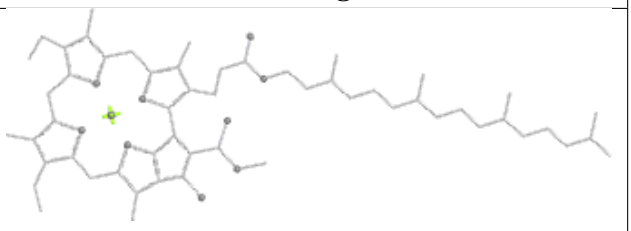
Bond lengths



Bond angles

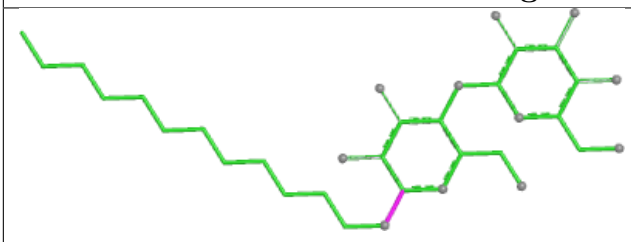


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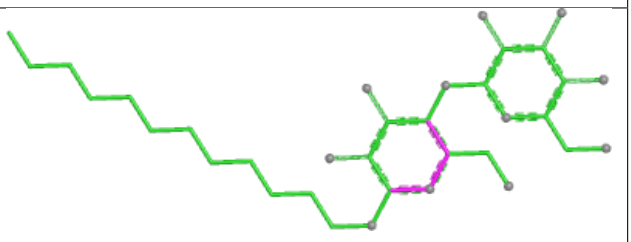


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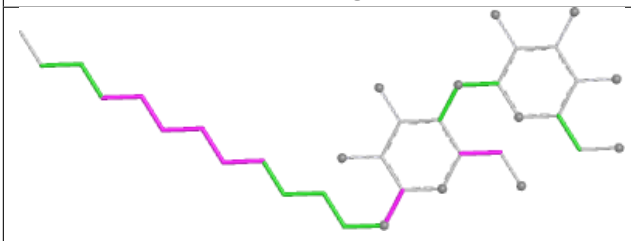
Ligand LMT D 403



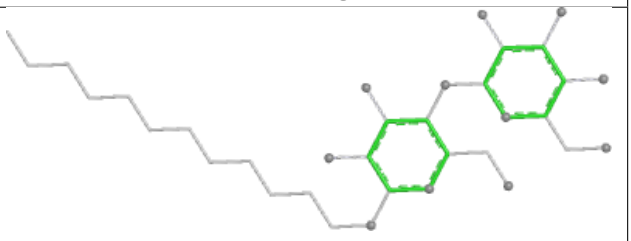
Bond lengths



Bond angles

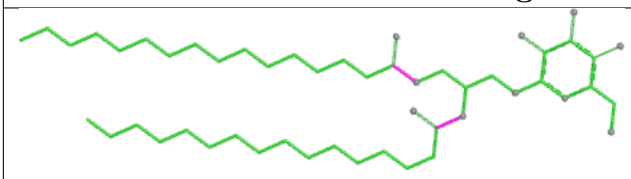


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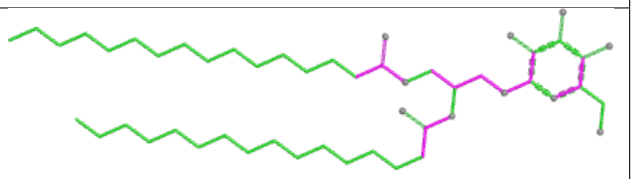


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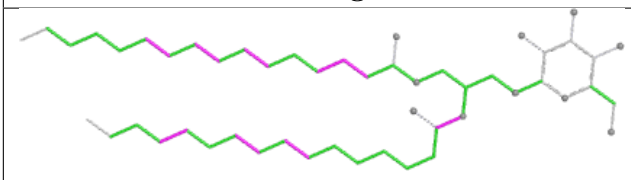
Ligand LMG M 101



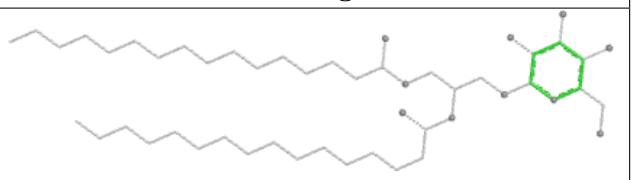
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Bond angles

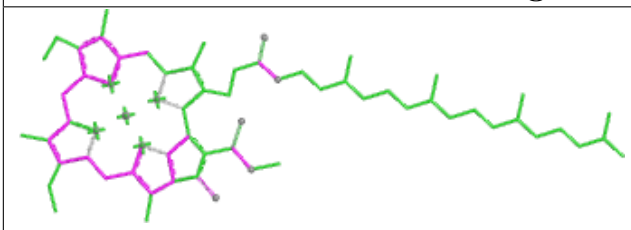


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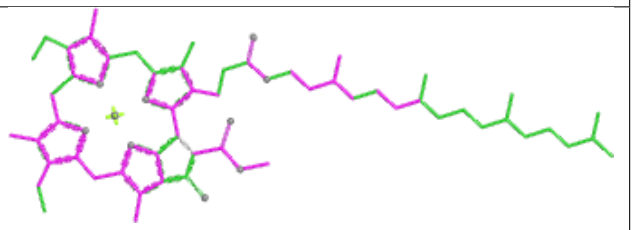


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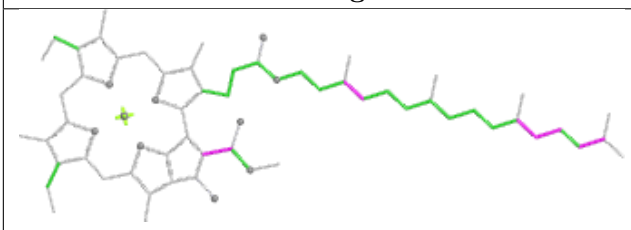
Ligand CLA b 605



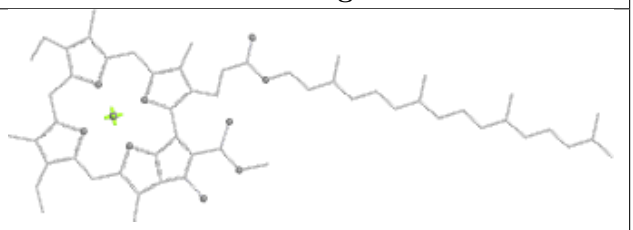
Bond lengths



Bond angles

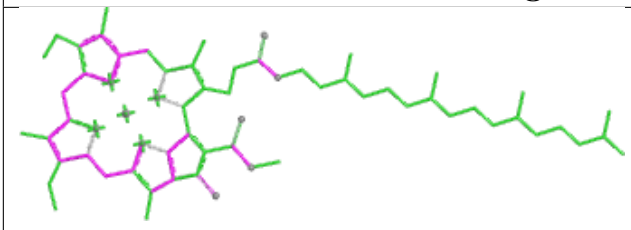


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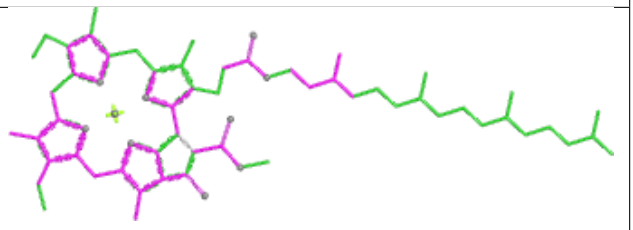


Rings

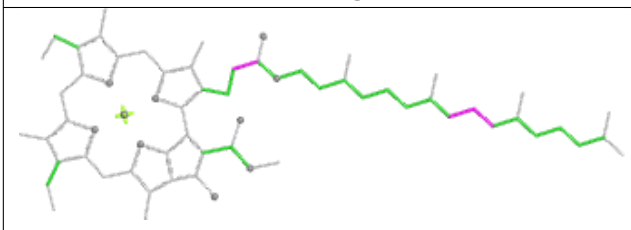
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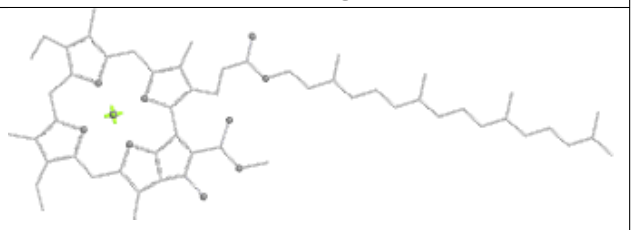
Bond lengths



Bond angles

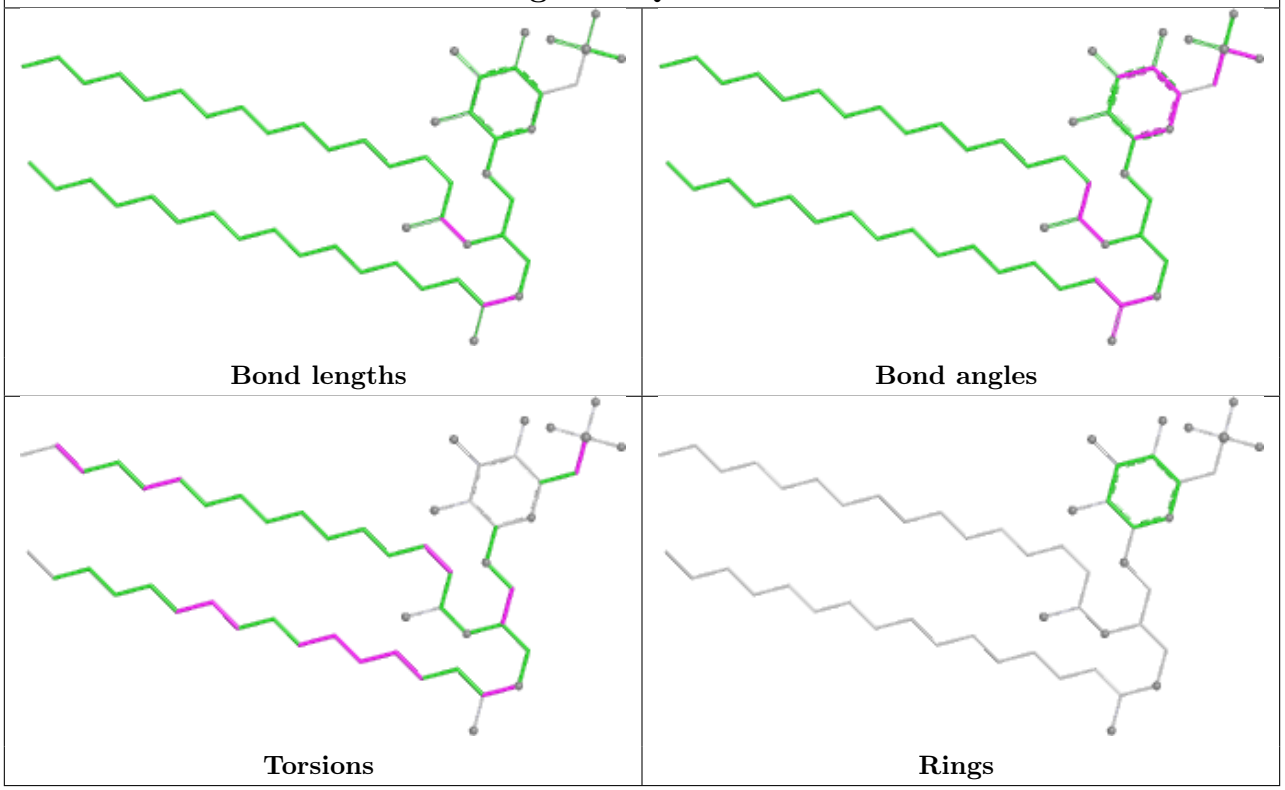


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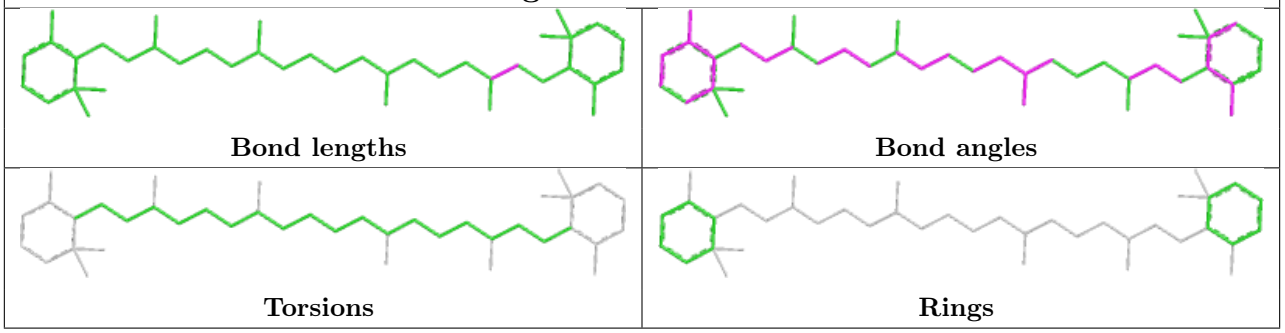


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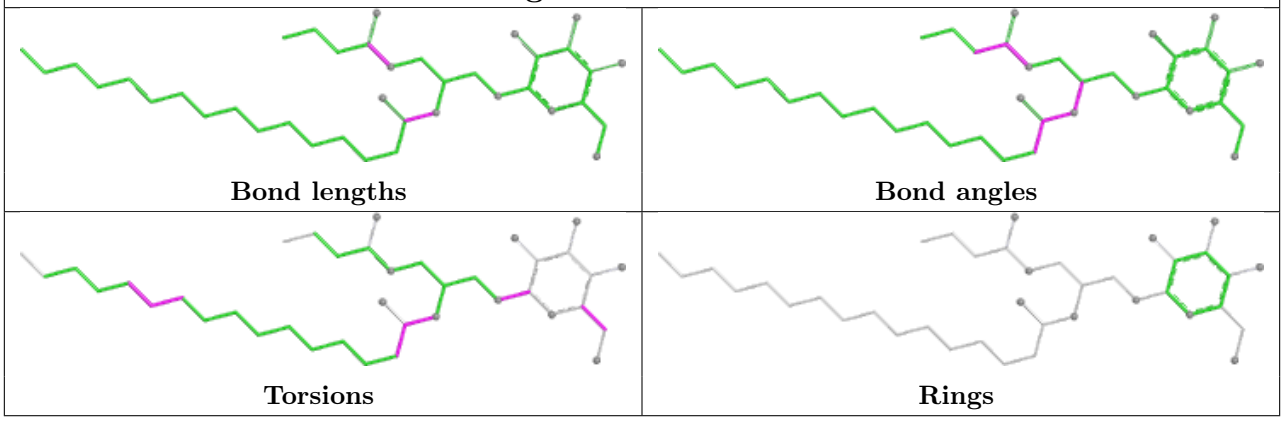
Ligand SQD a 411



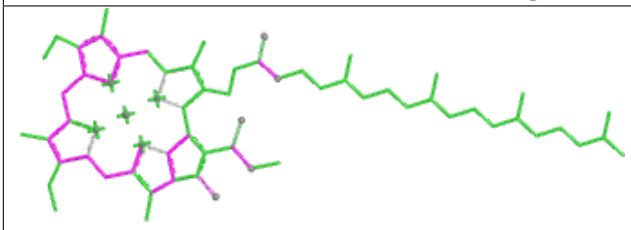
Ligand BCR K 101



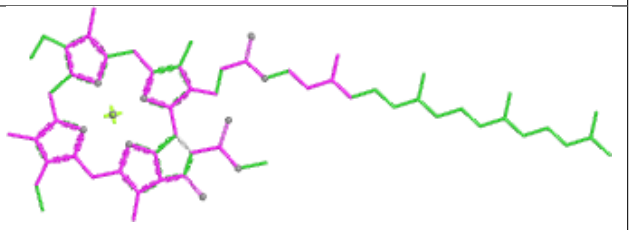
Ligand LMG z 101



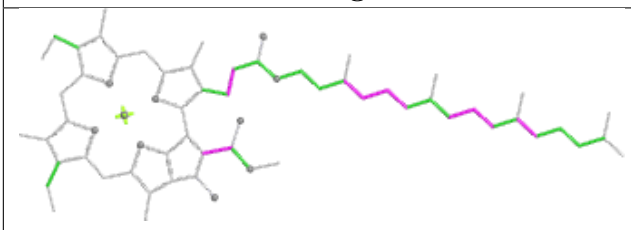
Ligand CLA B 614



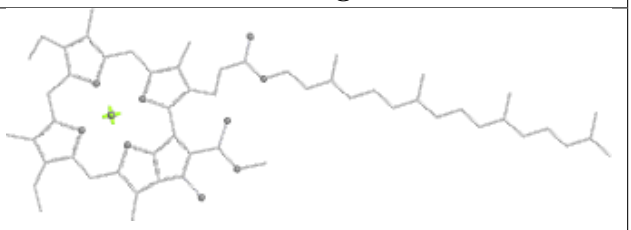
Bond lengths



Bond angles



Torsions

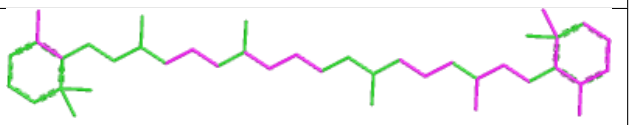


Rings

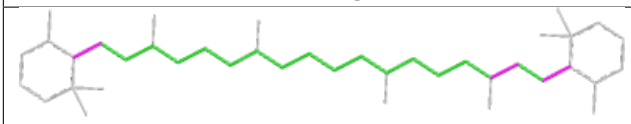
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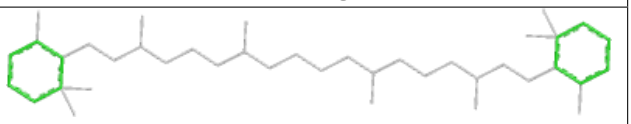
Bond lengths



Bond angles

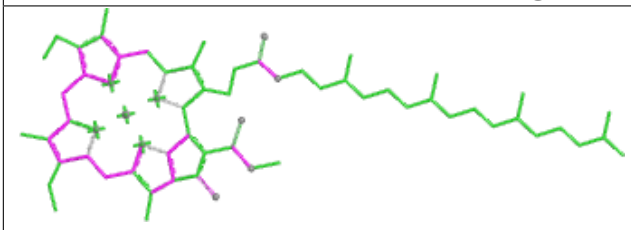


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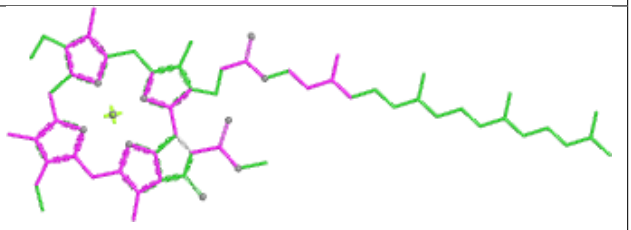


Rings

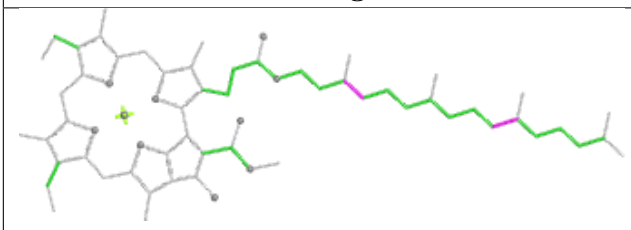
Ligand CLA c 506



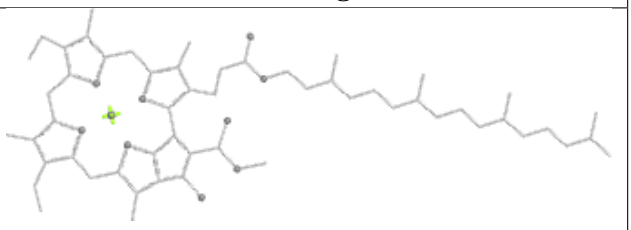
Bond lengths



Bond angles

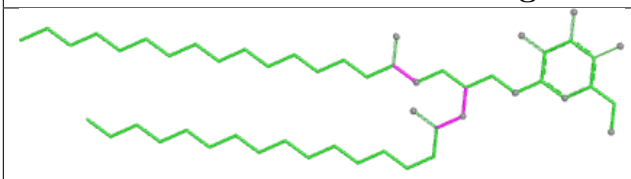


Torsions

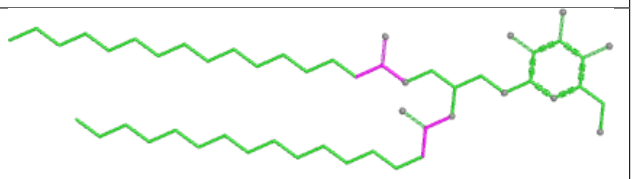


Rings

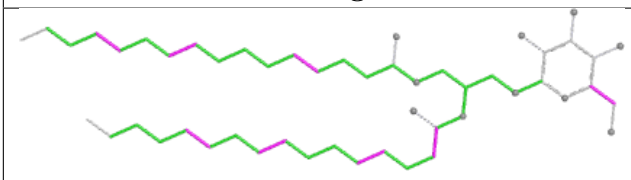
Ligand LMG D 414



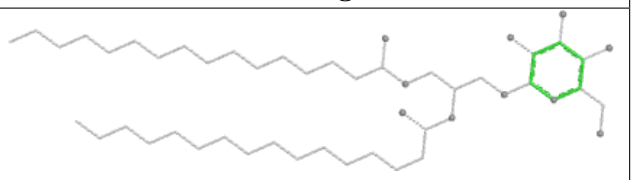
Bond lengths



Bond angles

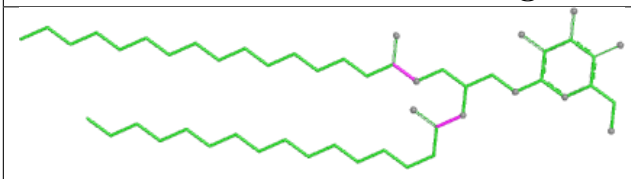


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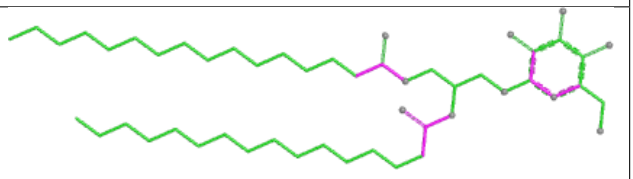


Rings

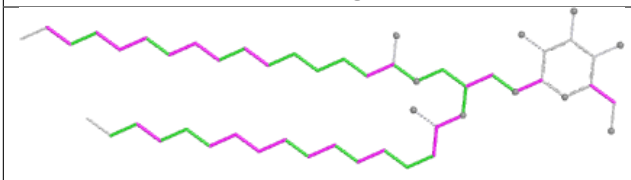
Ligand LMG A 415



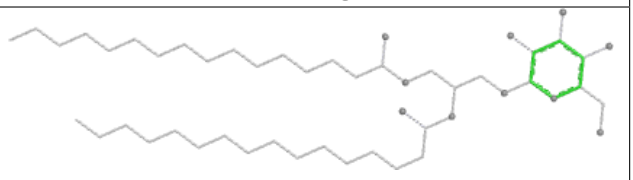
Bond lengths



Bond angles

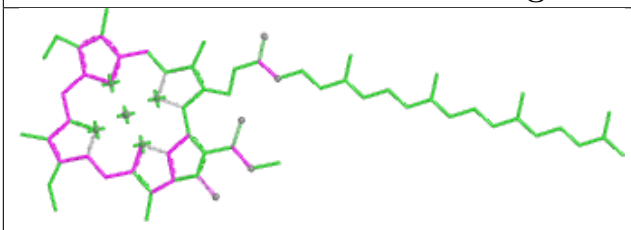


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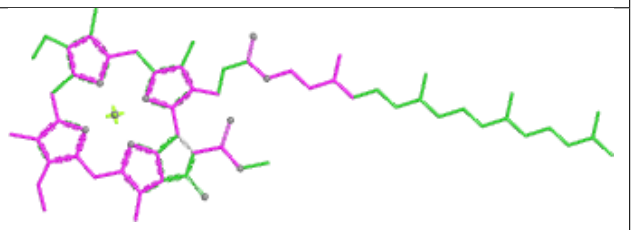


Rings

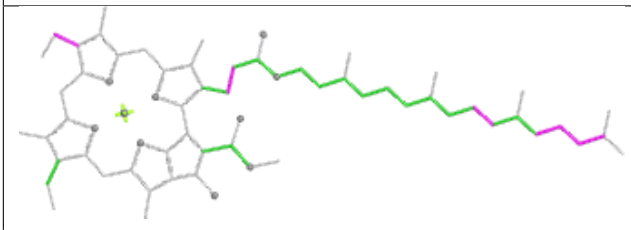
Ligand CLA b 606



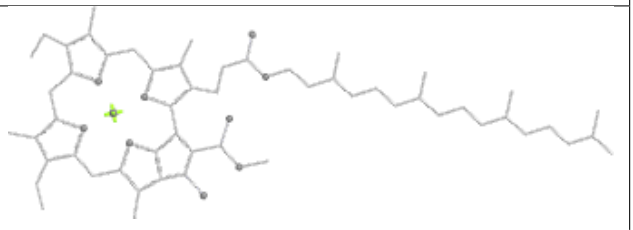
Bond lengths



Bond angles

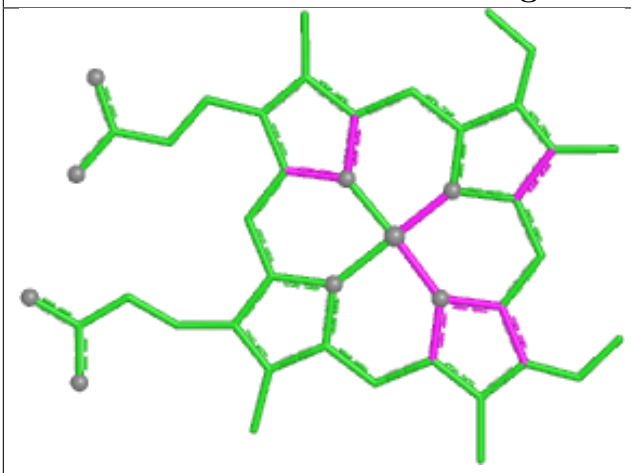


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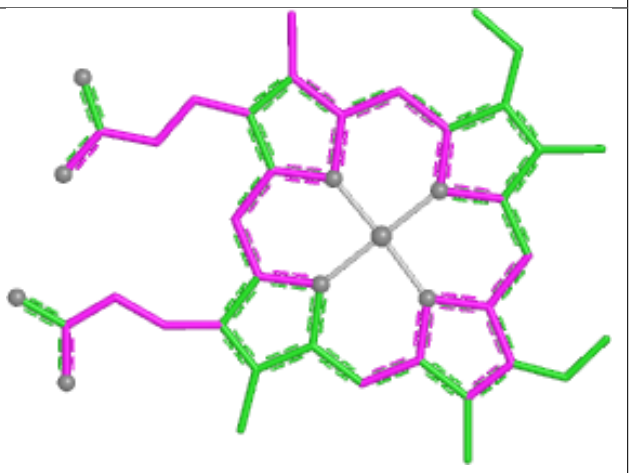


Rings

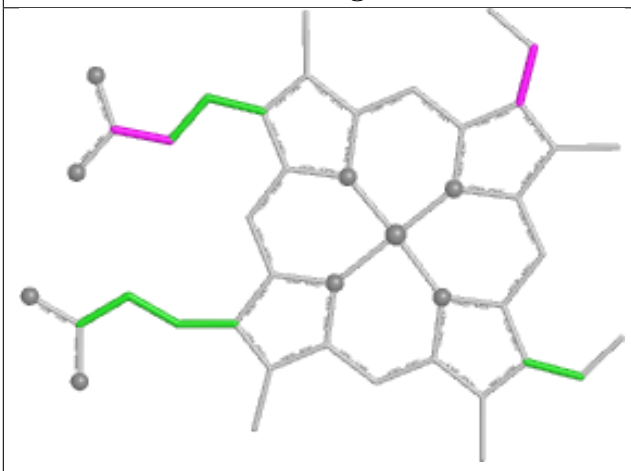
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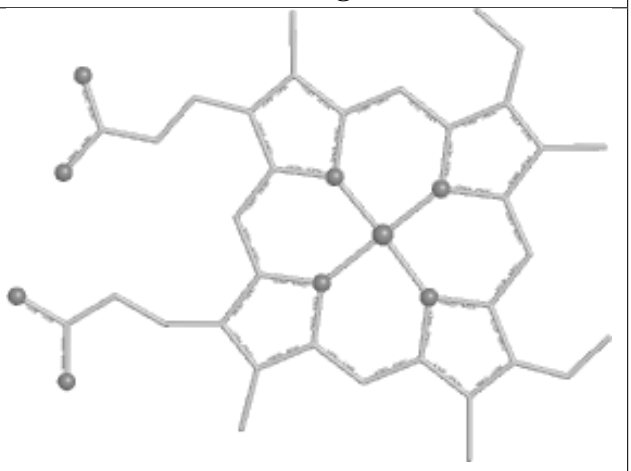
Bond lengths



Bond angles

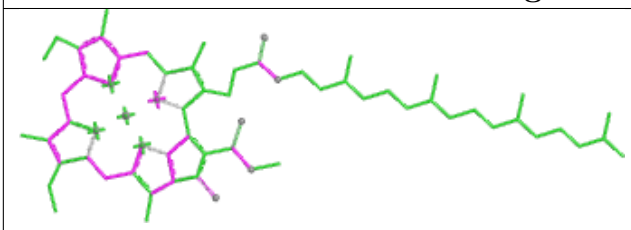


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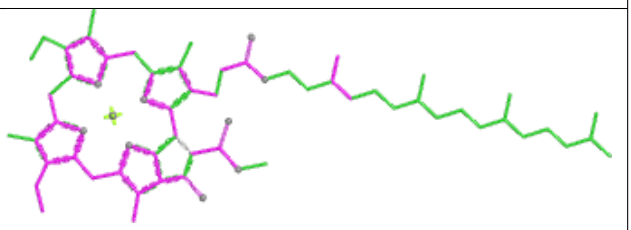


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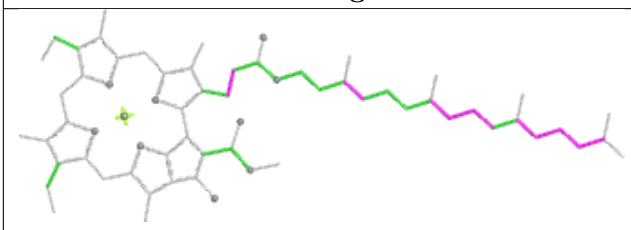
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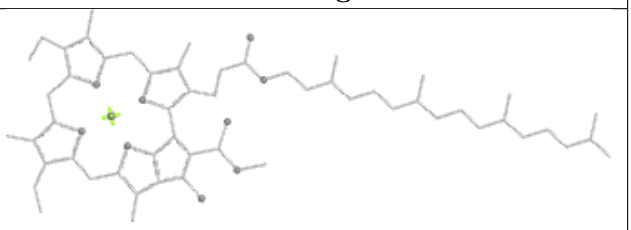
Bond lengths



Bond angles

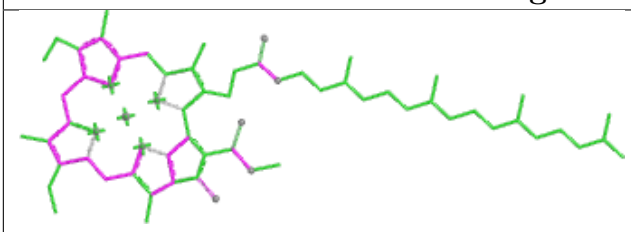


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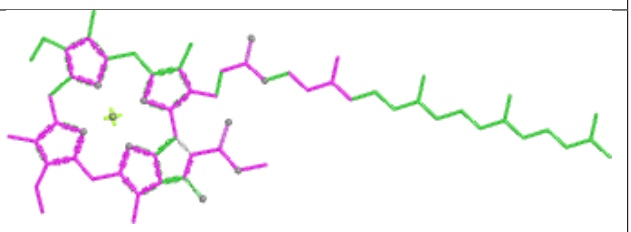


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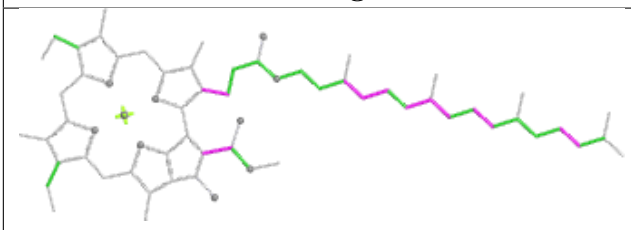
Ligand CLA c 507



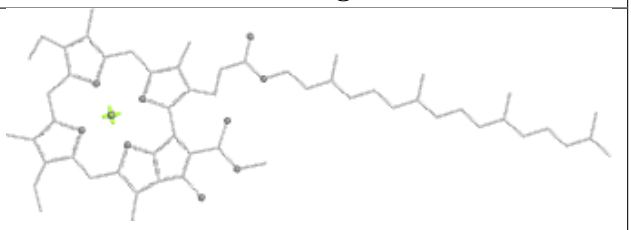
Bond lengths



Bond angles

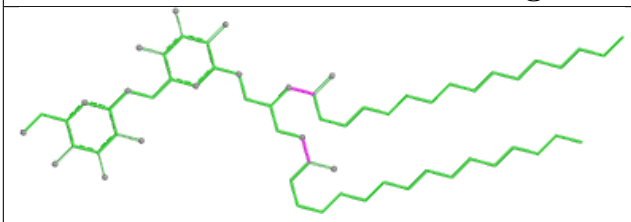


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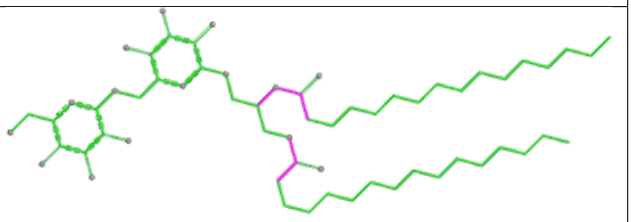


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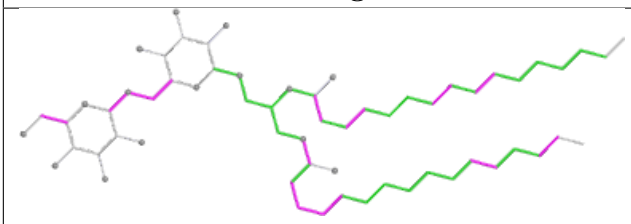
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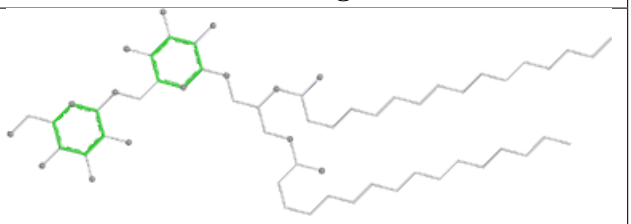
Bond lengths



Bond angles

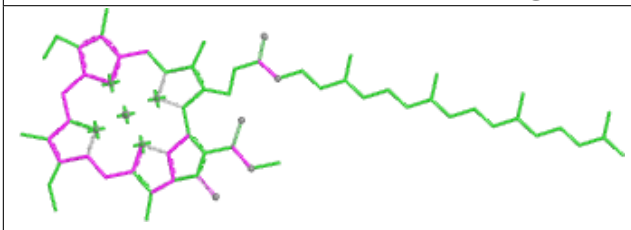


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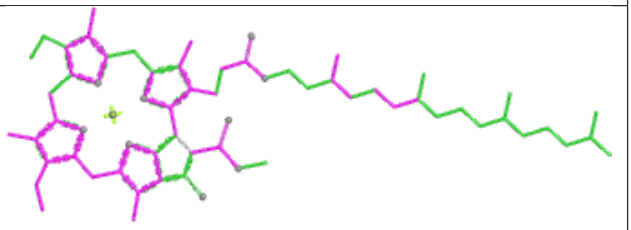


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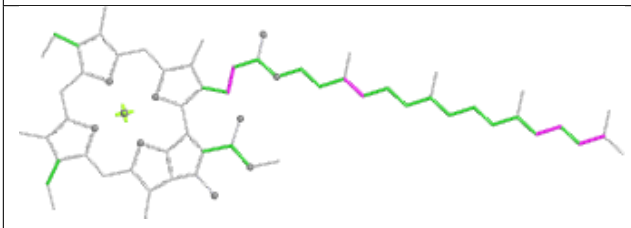
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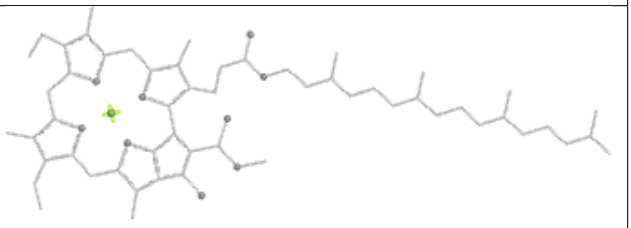
Bond lengths



Bond angles

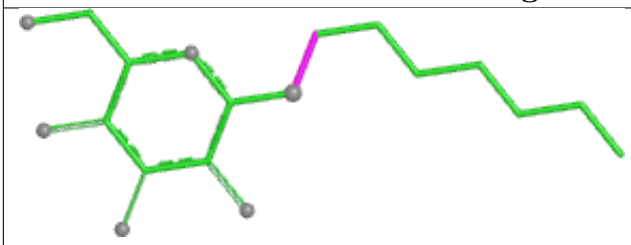


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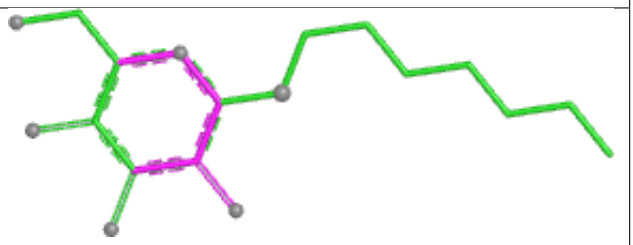


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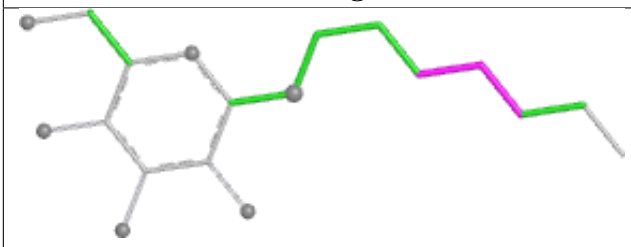
Ligand HTG B 621



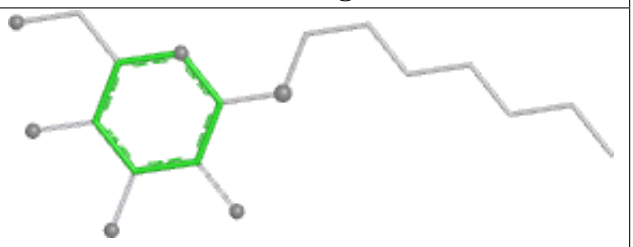
Bond lengths



Bond angles



Torsions

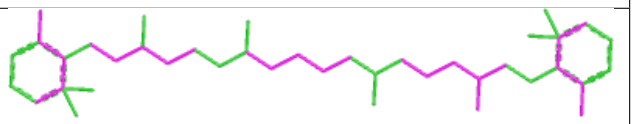


Rings

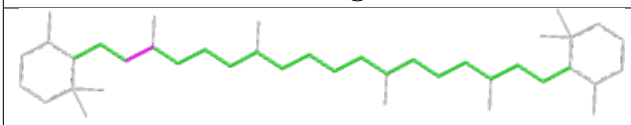
Ligand BCR c 516



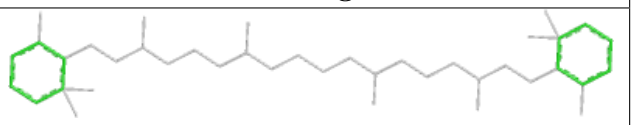
Bond lengths



Bond angles

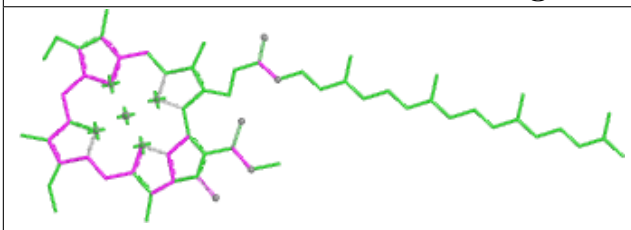


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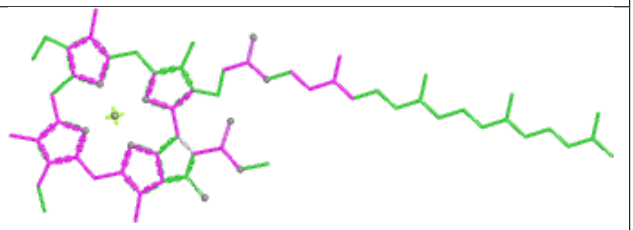


Rings

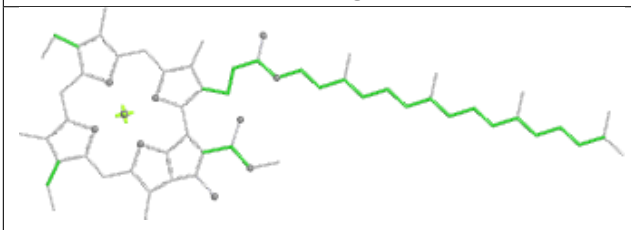
Ligand CLA c 504



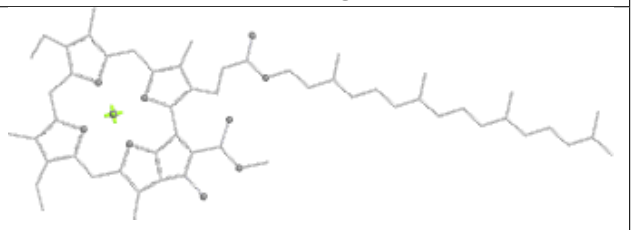
Bond lengths



Bond angles

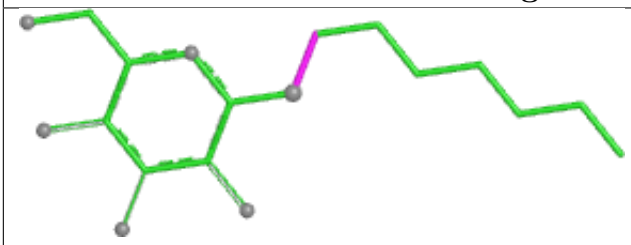


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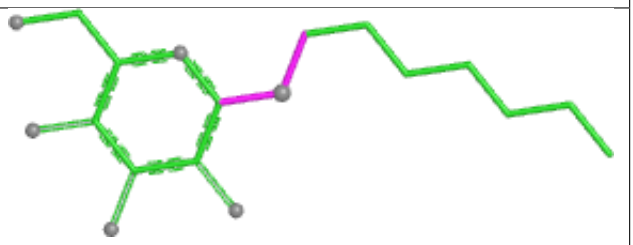


Rings

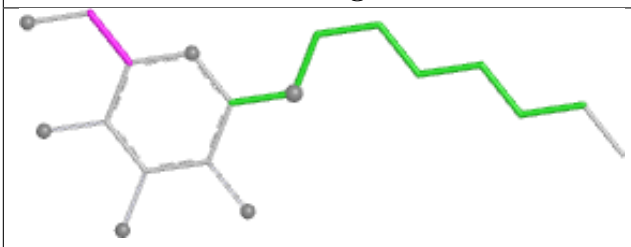
Ligand HTG C 522



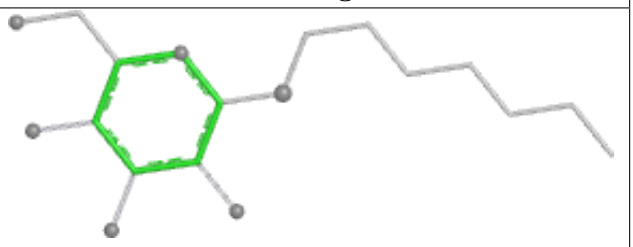
Bond lengths



Bond angles



Torsions



Rings

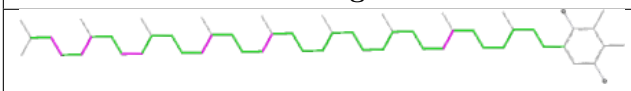
Ligand PL9 D 408



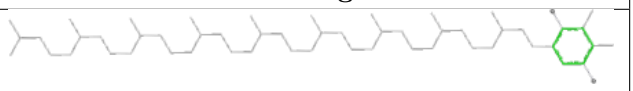
Bond lengths



Bond angles

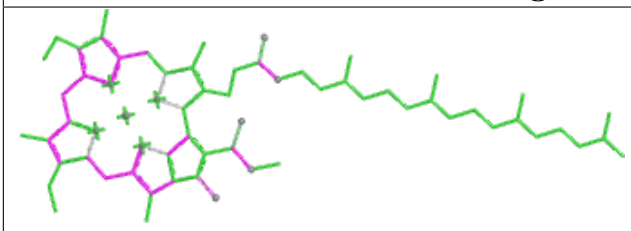


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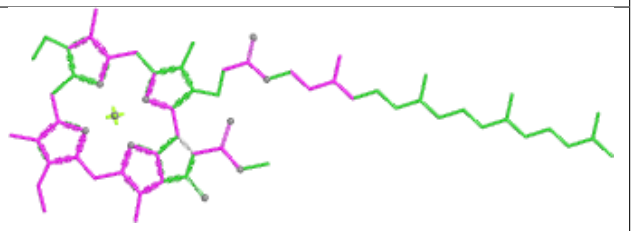


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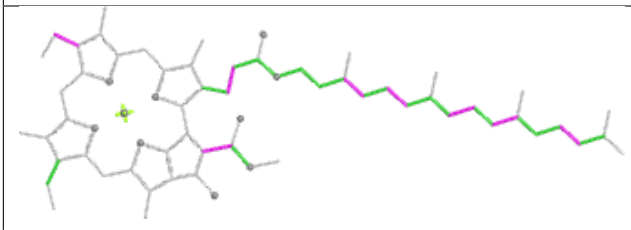
Ligand CLA c 508



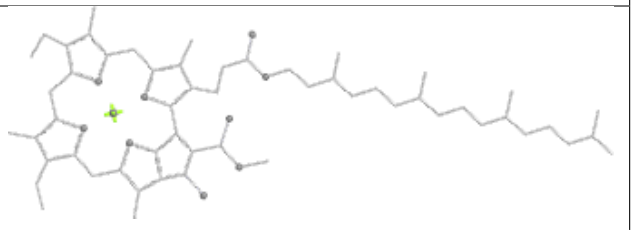
Bond lengths



Bond angles

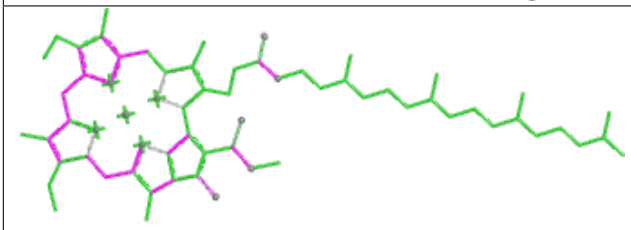


Torsions

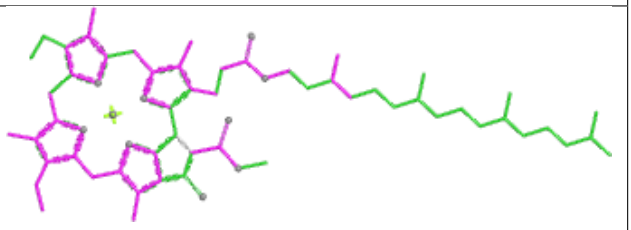


Rings

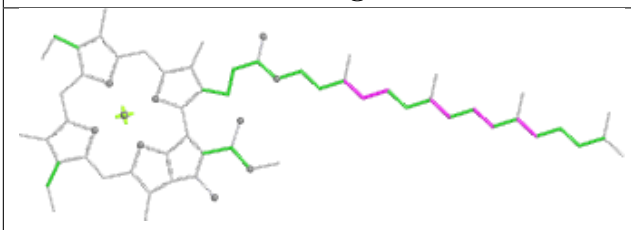
Ligand CLA D 406



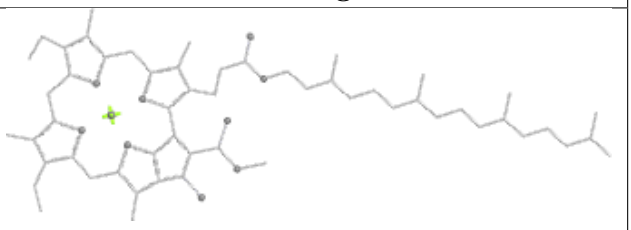
Bond lengths



Bond angles

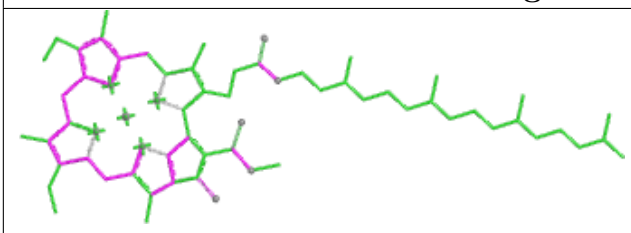


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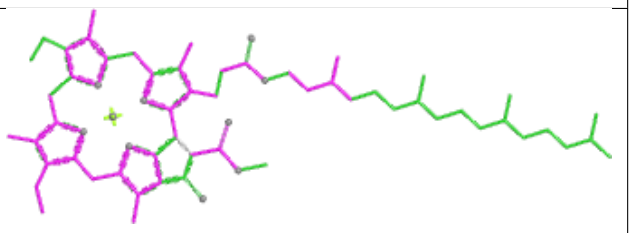


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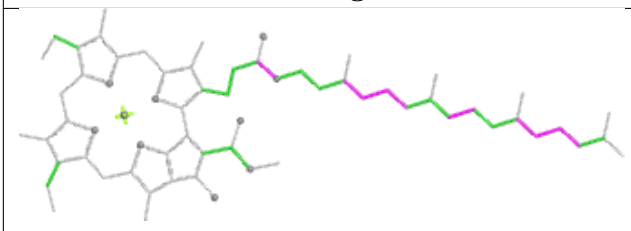
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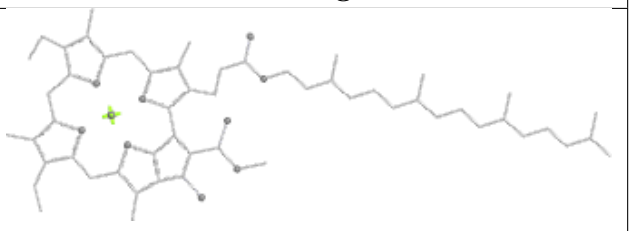
Bond lengths



Bond angles

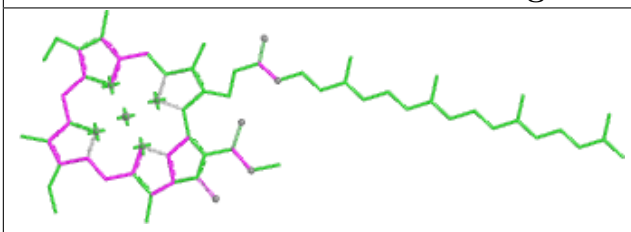


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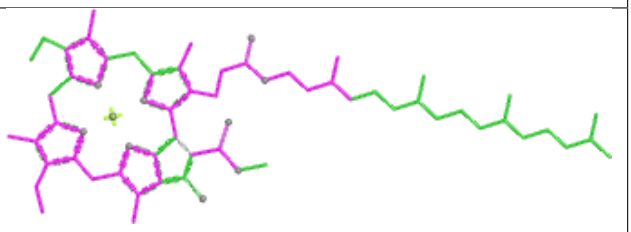


Rings

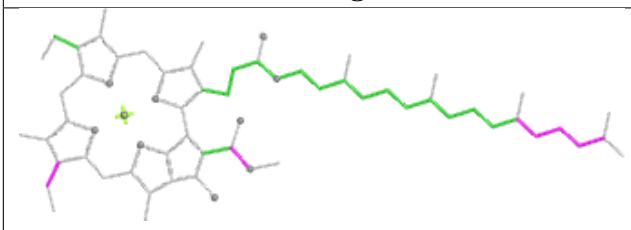
Ligand CLA d 402



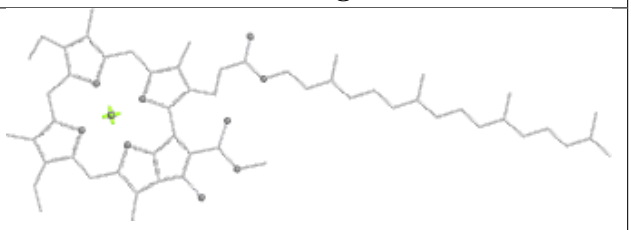
Bond lengths



Bond angles

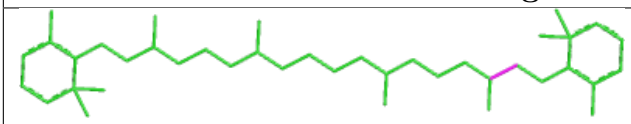


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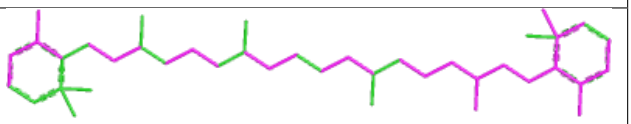


Rings

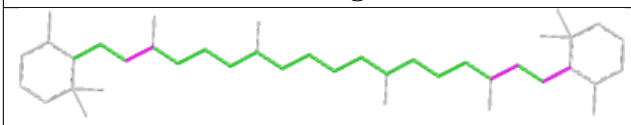
Ligand BCR D 407



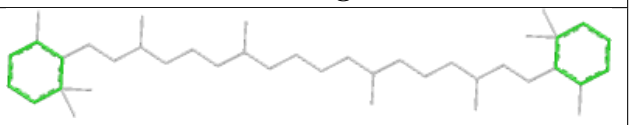
Bond lengths



Bond angles

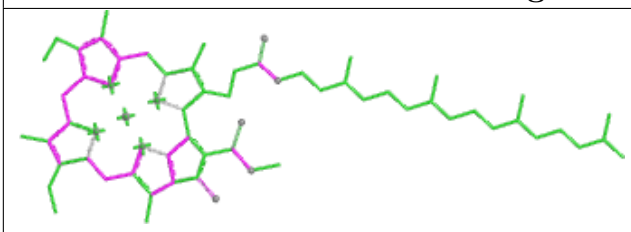


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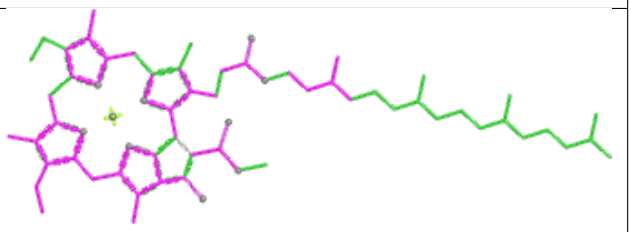


Rings

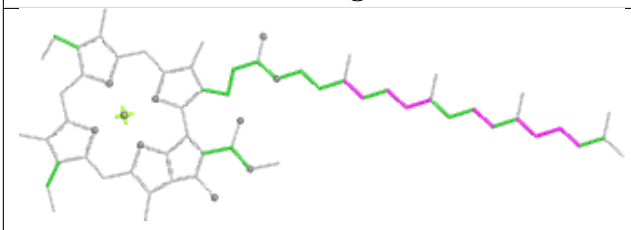
Ligand CLA b 616



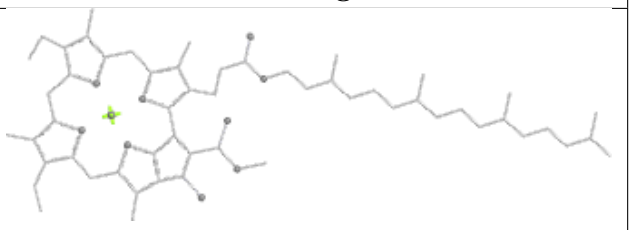
Bond lengths



Bond angles

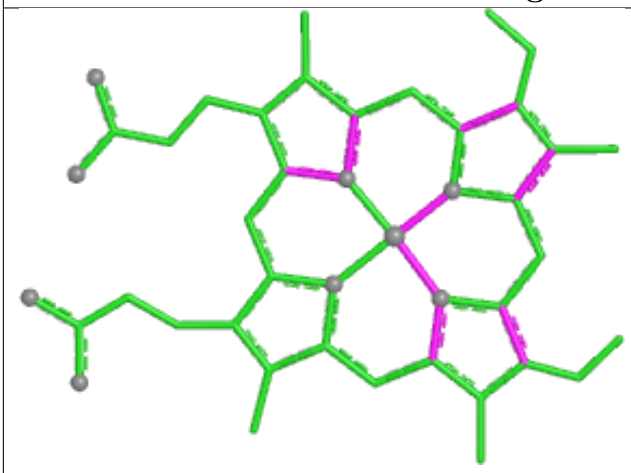


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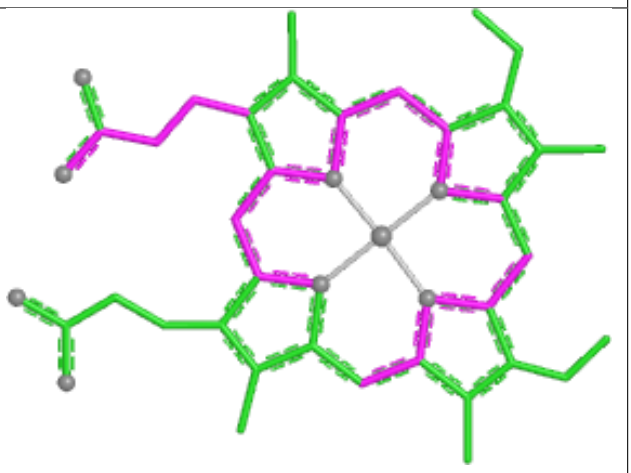


Rings

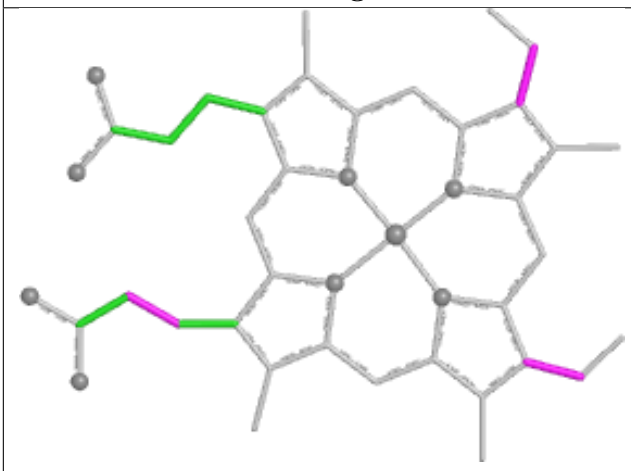
Ligand HEM f 101



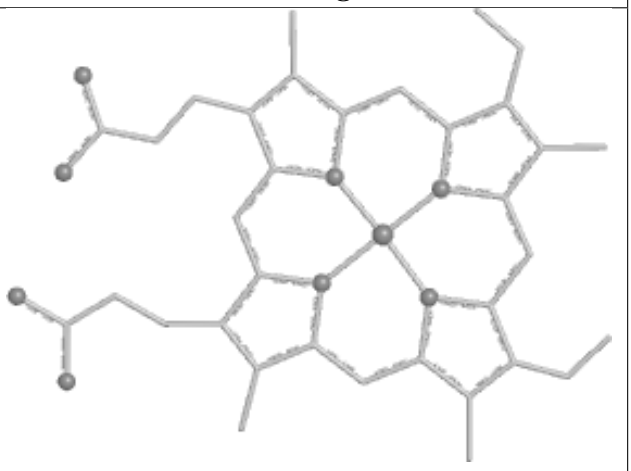
Bond lengths



Bond angles

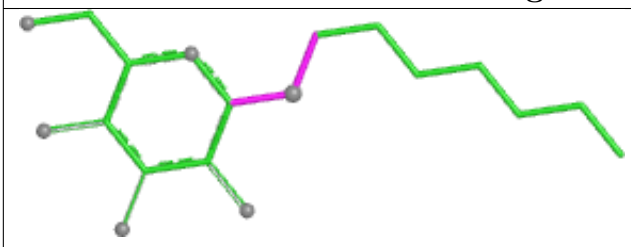


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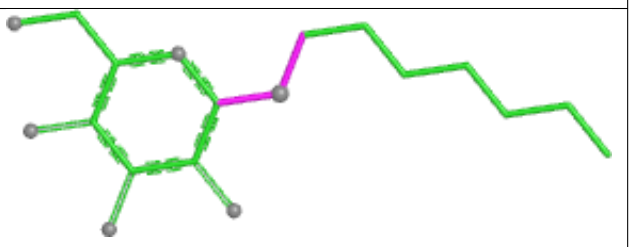


Rings

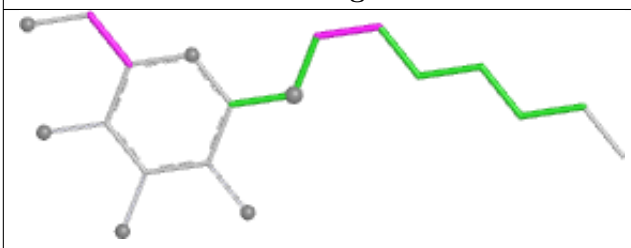
Ligand HTG c 522



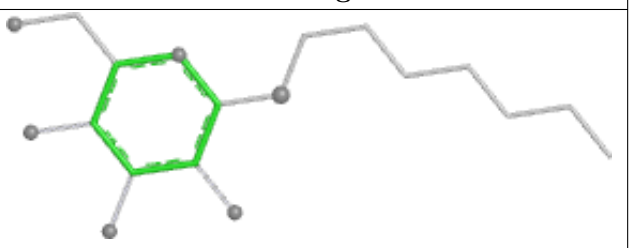
Bond lengths



Bond angles

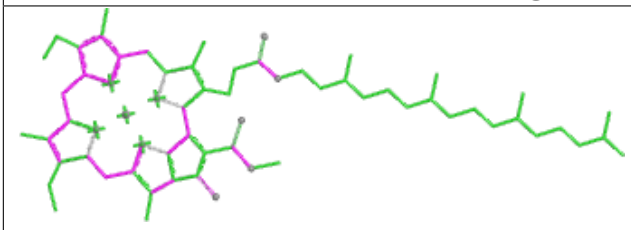


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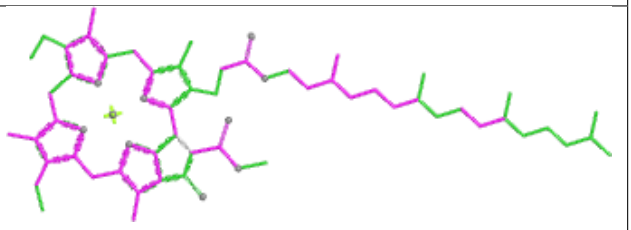


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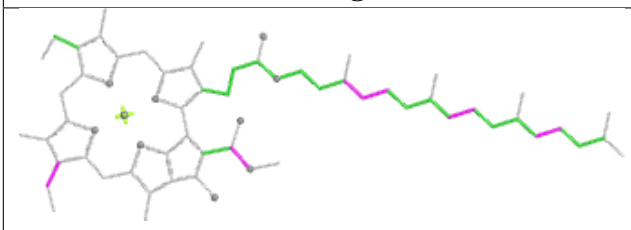
Ligand CLA b 604



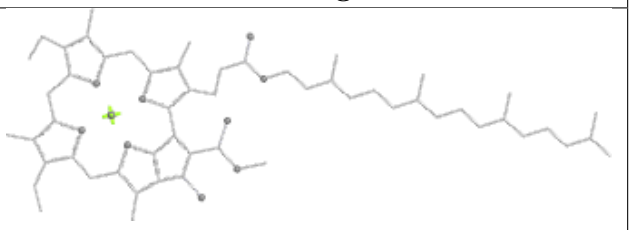
Bond lengths



Bond angles

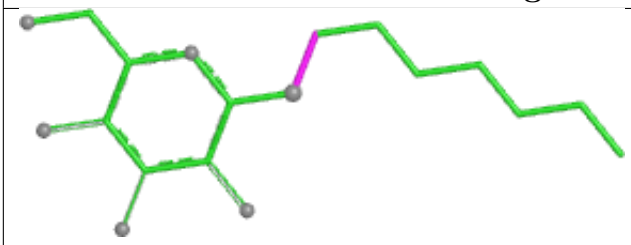


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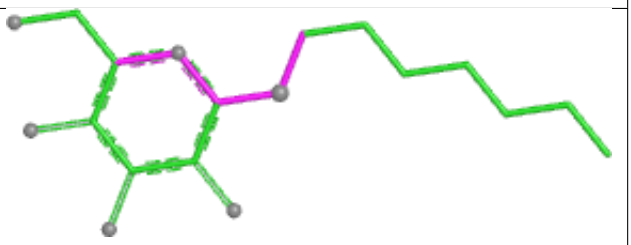


Rings

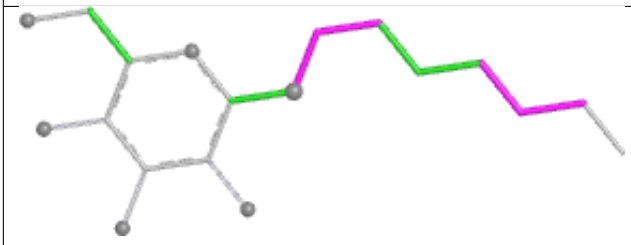
Ligand HTG b 621



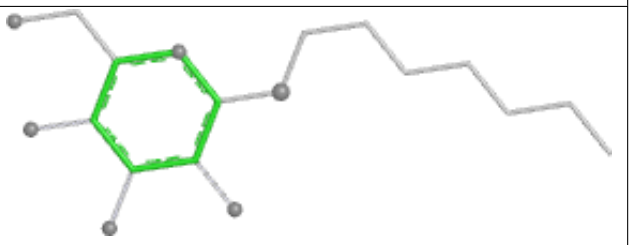
Bond lengths



Bond angles

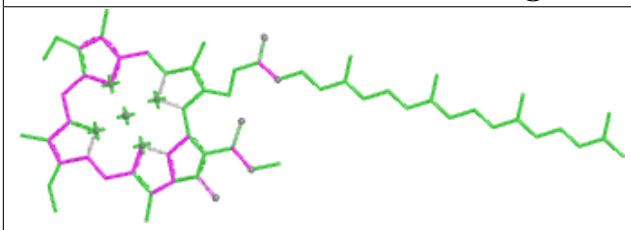


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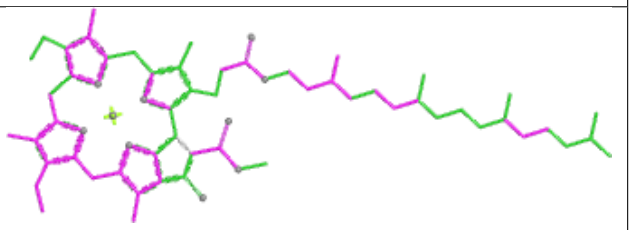


Rings

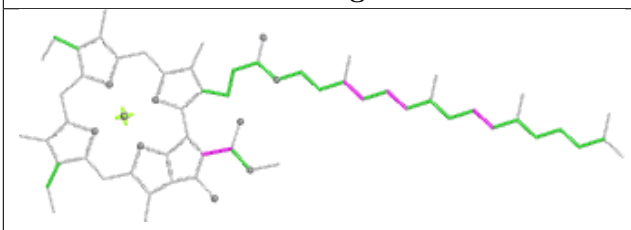
Ligand CLA C 508



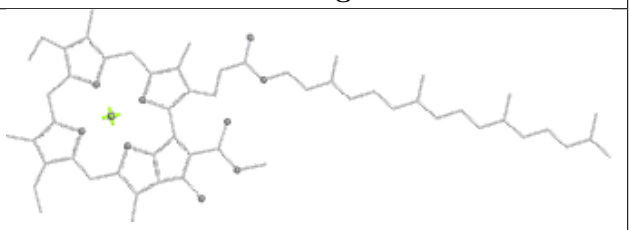
Bond lengths



Bond angles

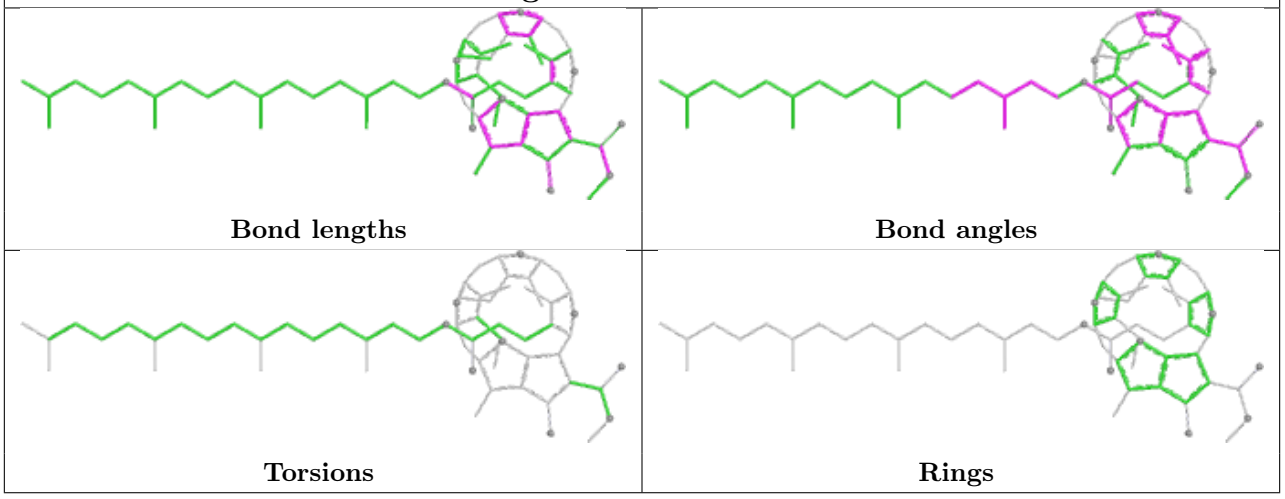


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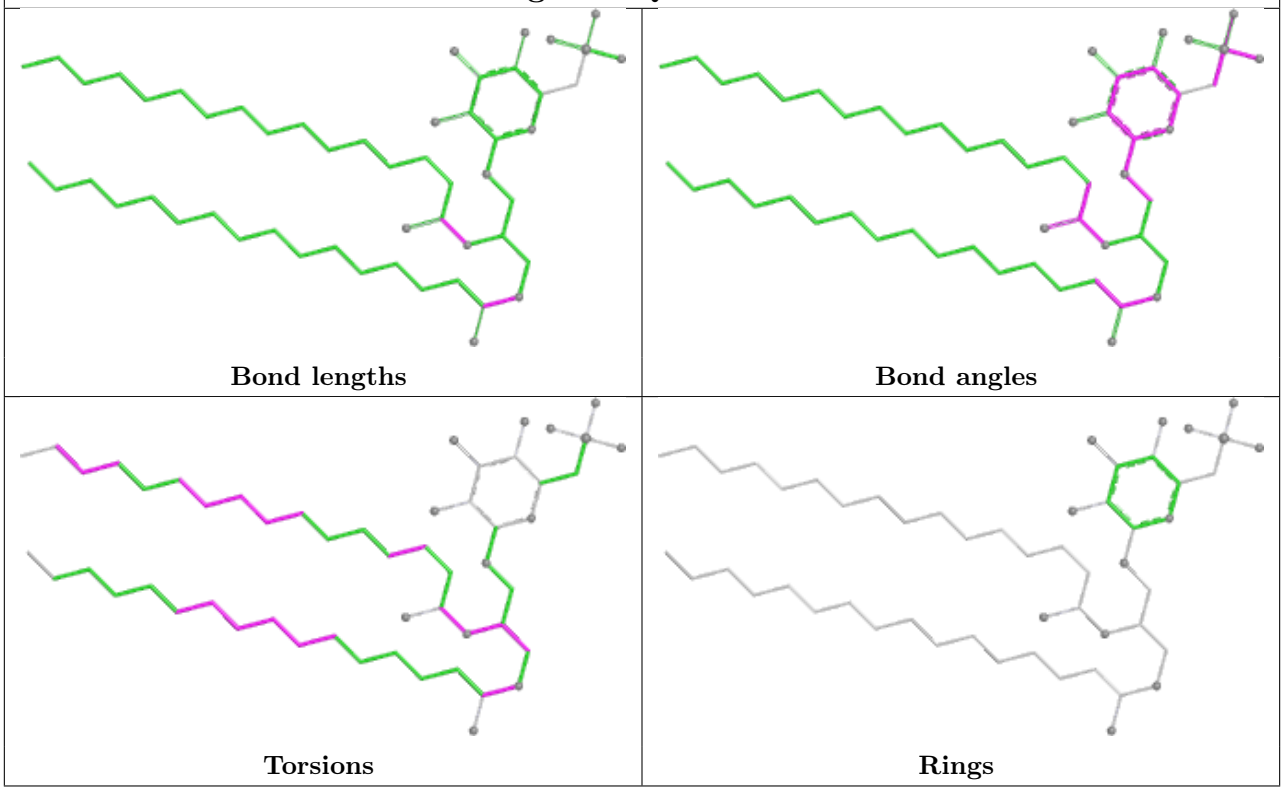


Rings

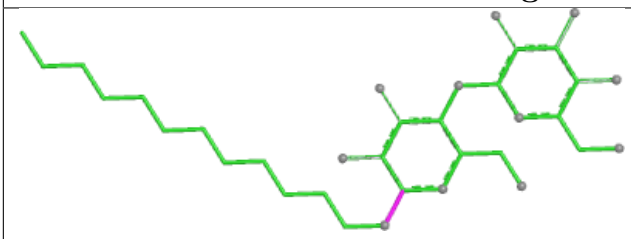
Ligand PHO D 402



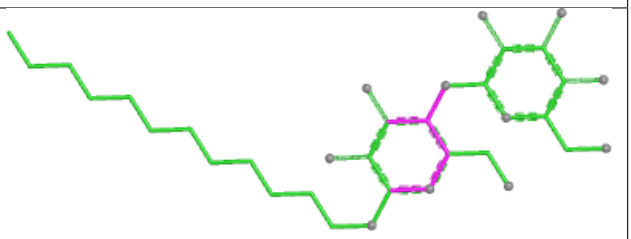
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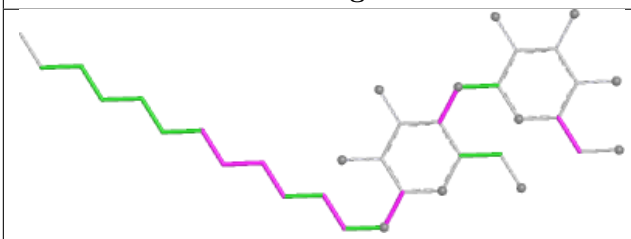
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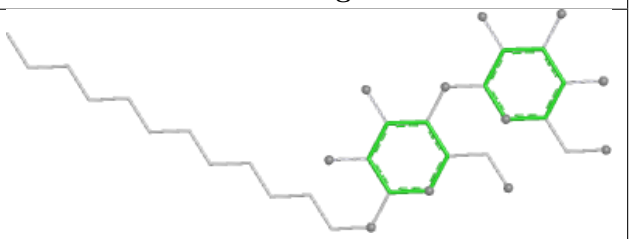
Bond lengths



Bond angles

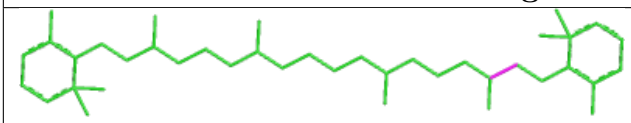


Torsions

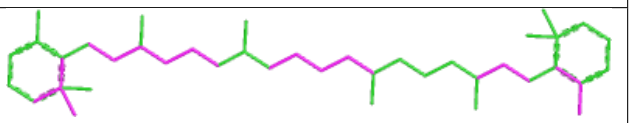


Rings

Ligand BCR H 101



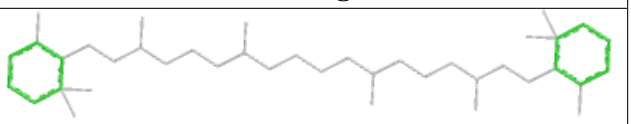
Bond lengths



Bond angles

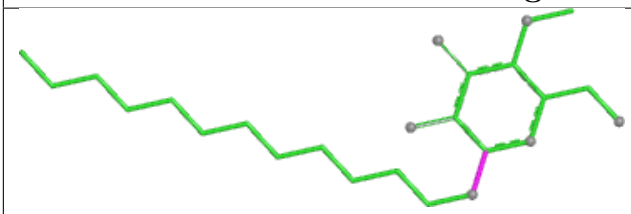


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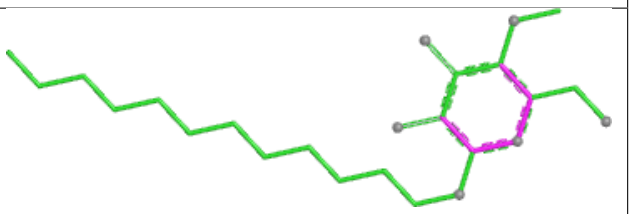


Rings

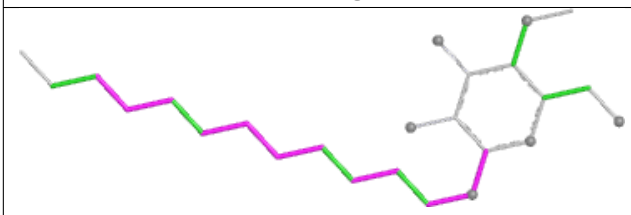
Ligand LMT b 626



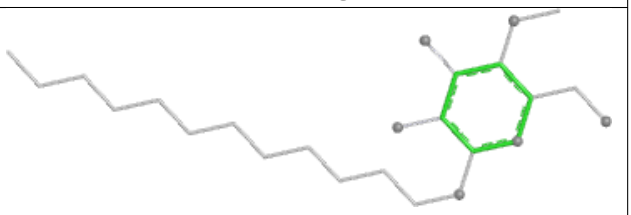
Bond lengths



Bond angles

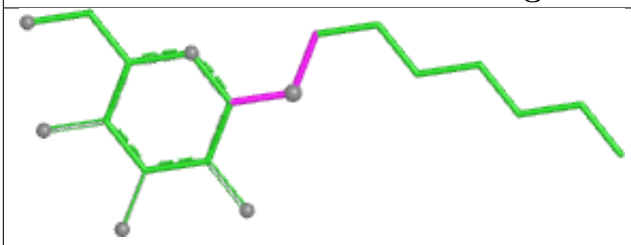


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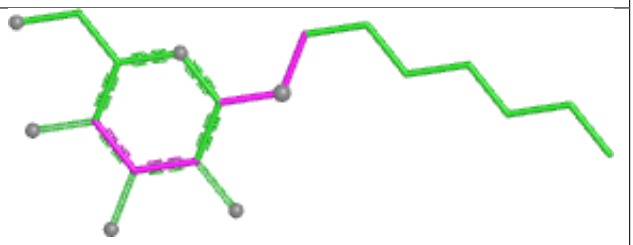


Rings

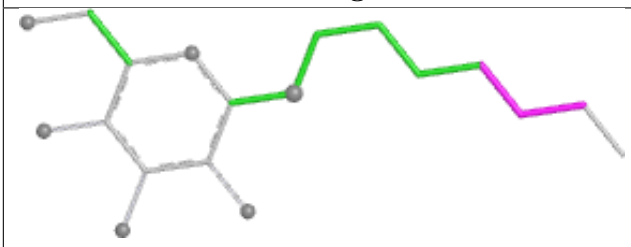
Ligand HTG b 624



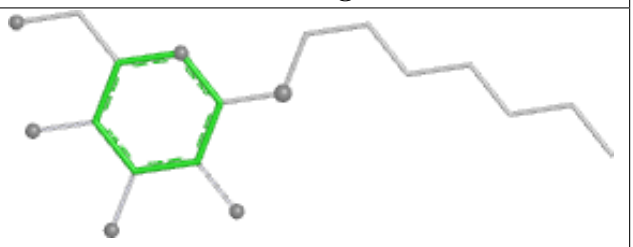
Bond lengths



Bond angles

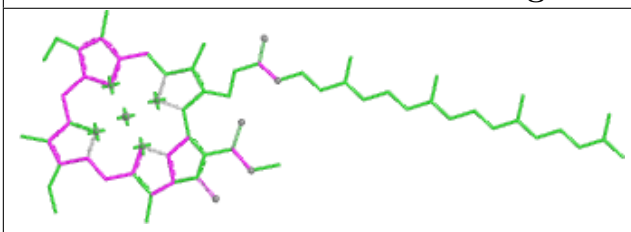


Torsions

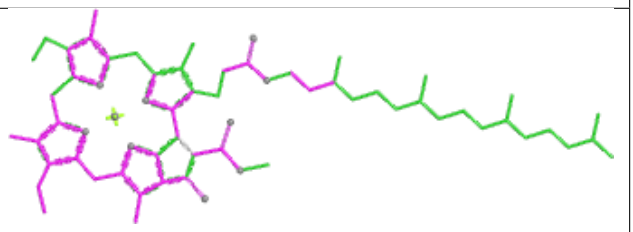


Rings

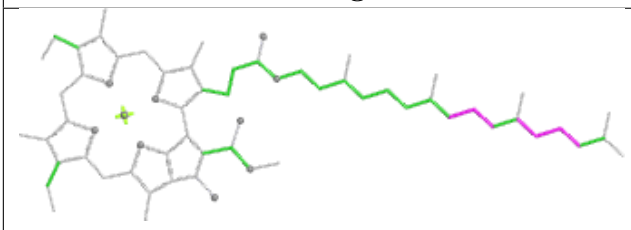
Ligand CLA b 611



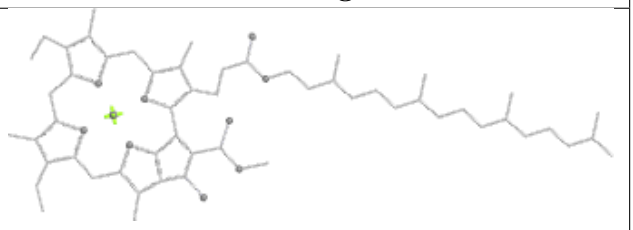
Bond lengths



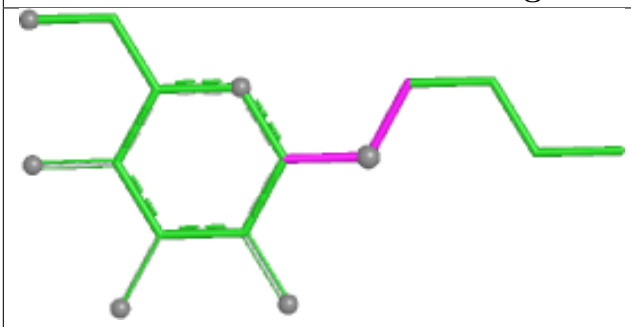
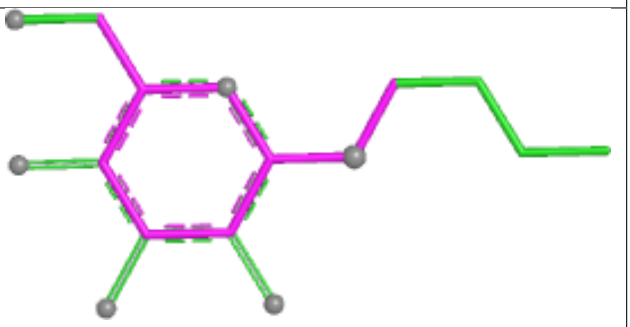
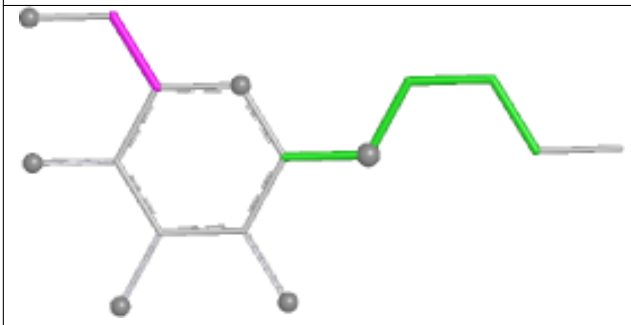
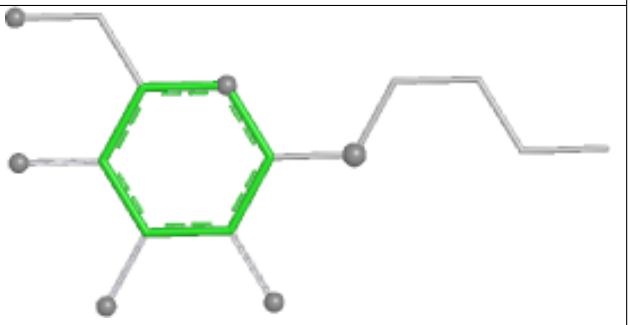
Bond angles

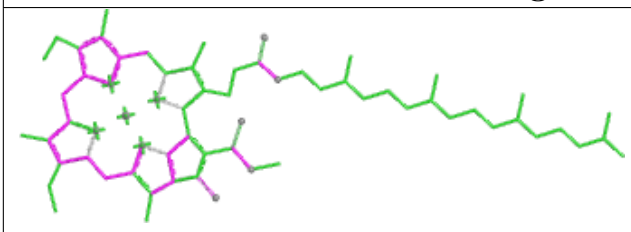
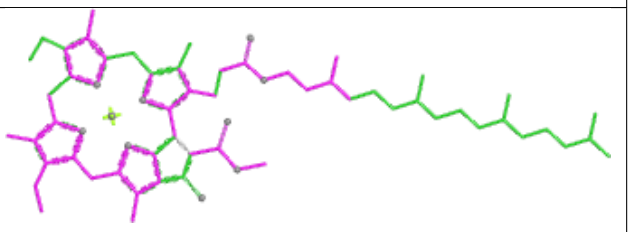
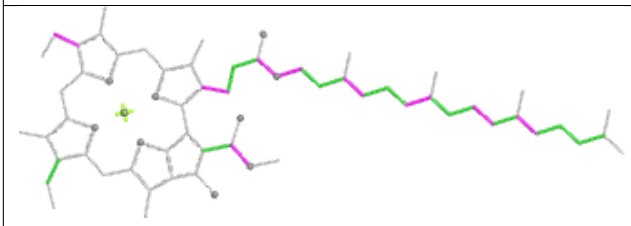
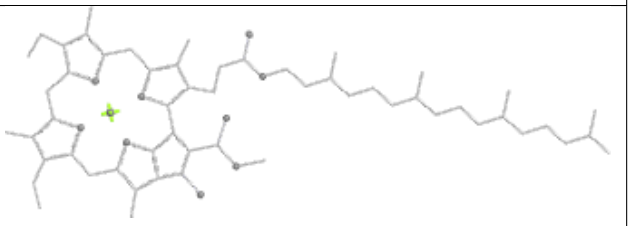


Torsions

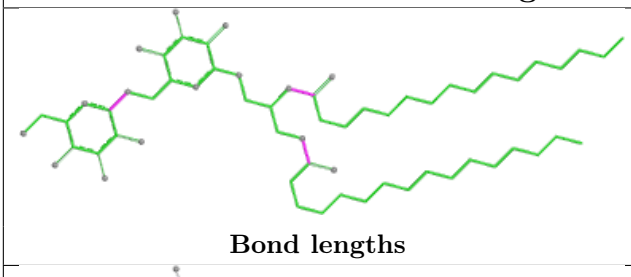


Rings

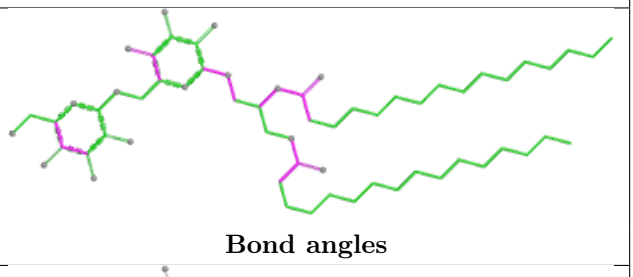
Ligand HTG h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

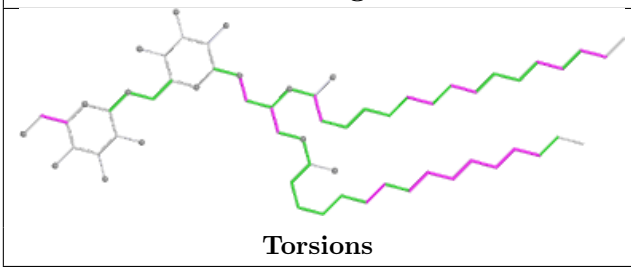
Ligand DGD H 102



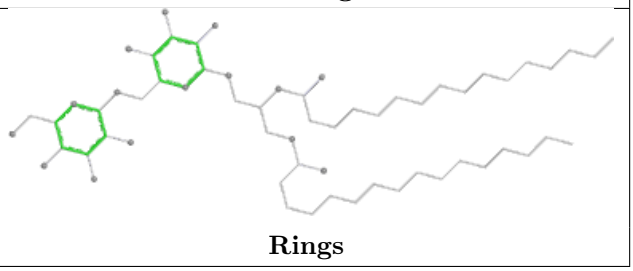
Bond lengths



Bond angles

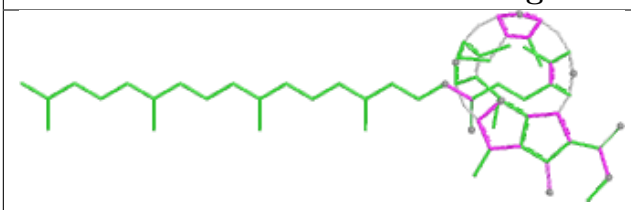


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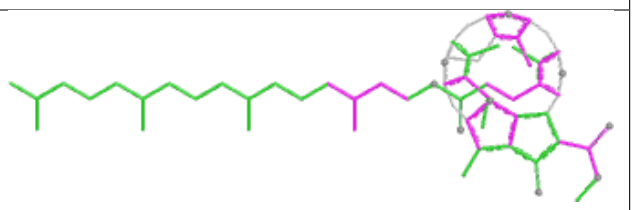


Rings

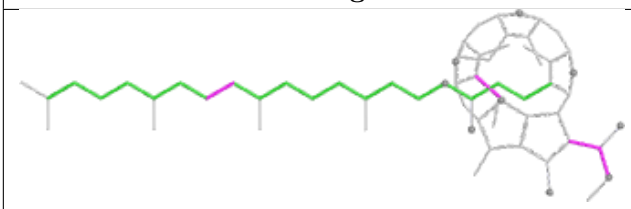
Ligand PHO a 416



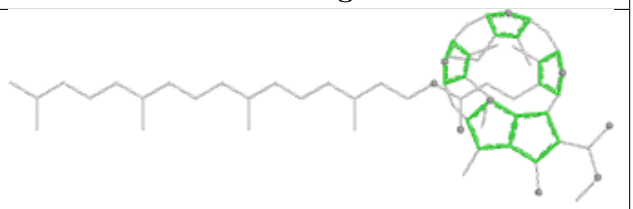
Bond lengths



Bond angles

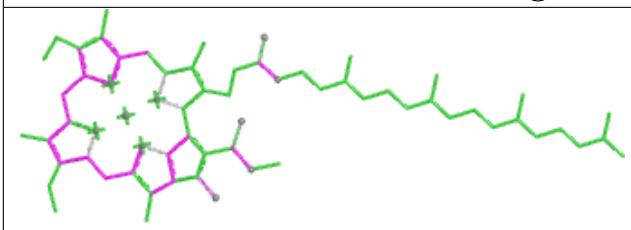


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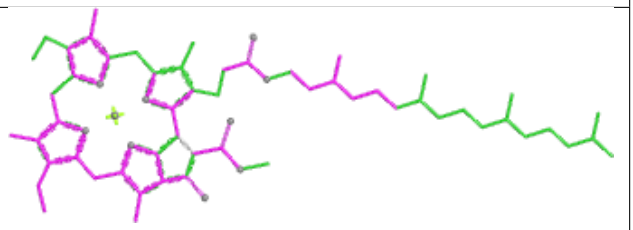


Rings

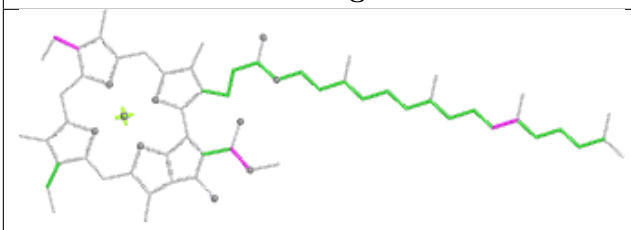
Ligand CLA c 502



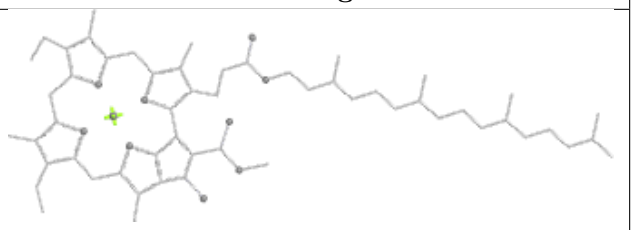
Bond lengths



Bond angles

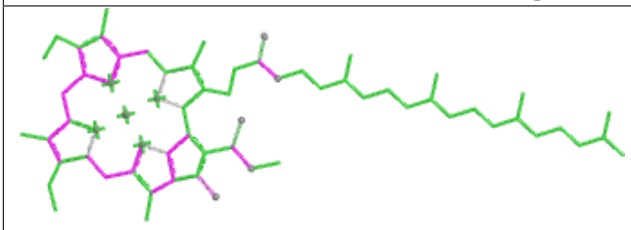


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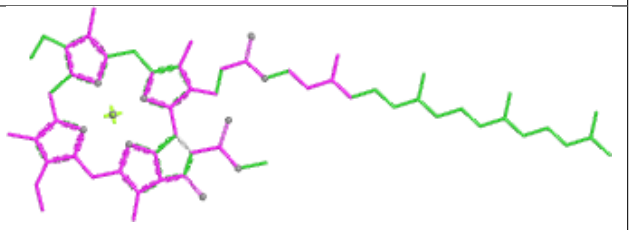


Rings

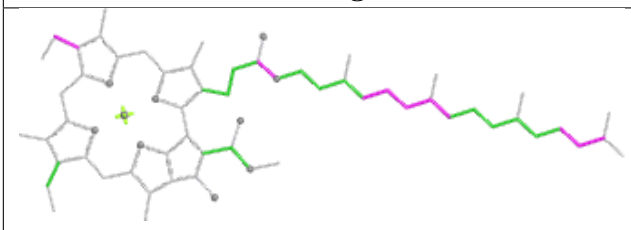
Ligand CLA a 407



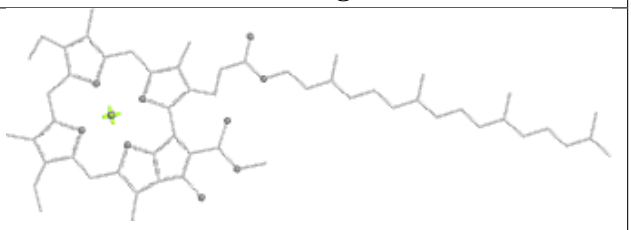
Bond lengths



Bond angles



Torsions

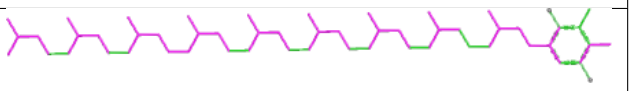


Rings

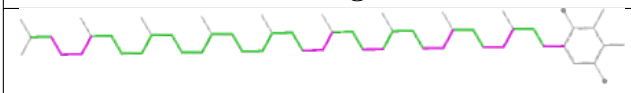
Ligand PL9 A 413



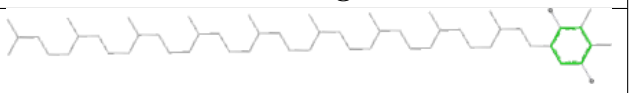
Bond lengths



Bond angles

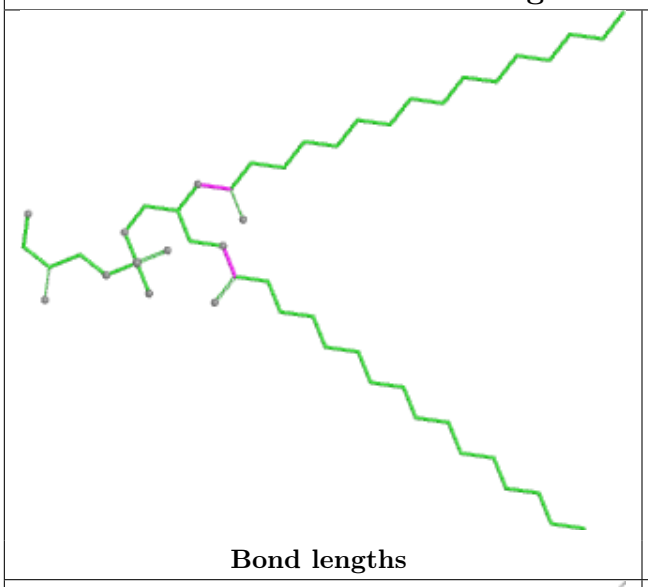


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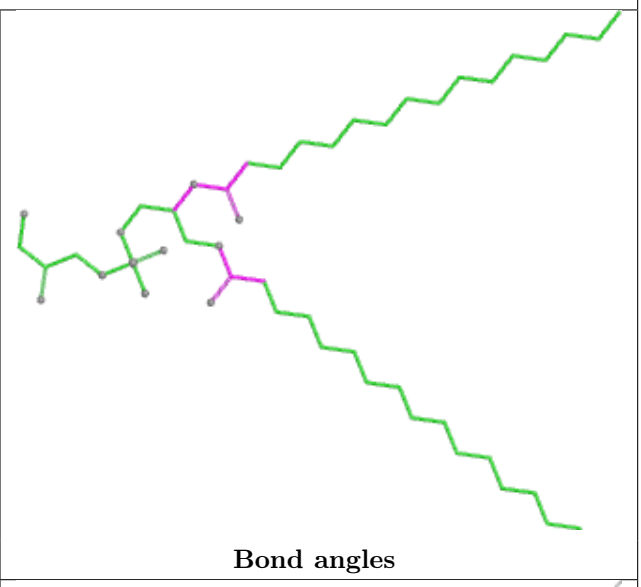


Rings

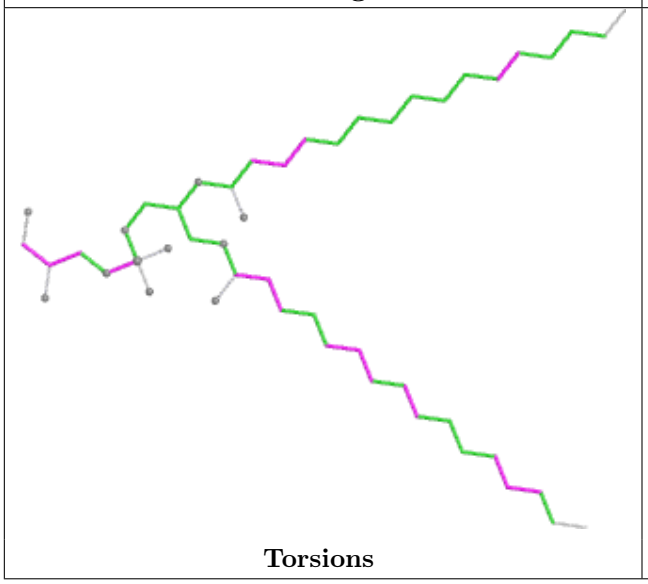
Ligand LHG d 407



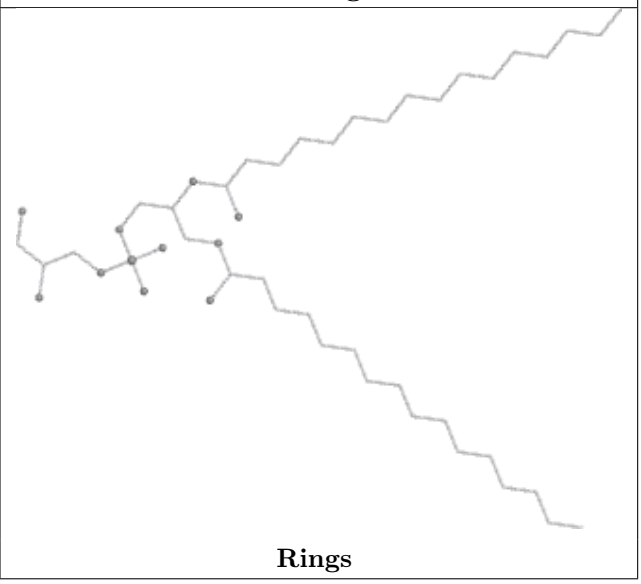
Bond lengths



Bond angles



Torsions

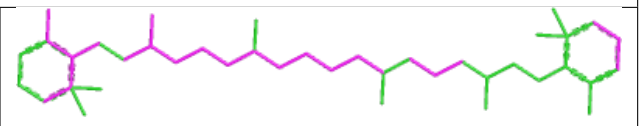


Rings

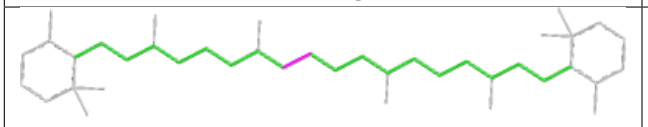
Ligand BCR T 101



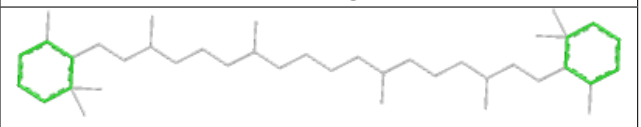
Bond lengths



Bond angles

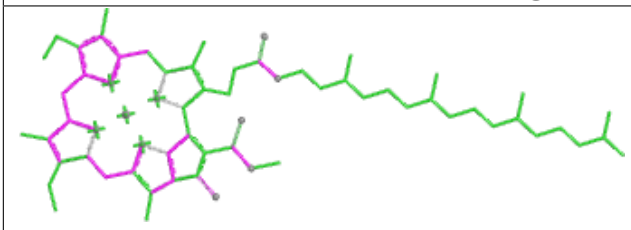


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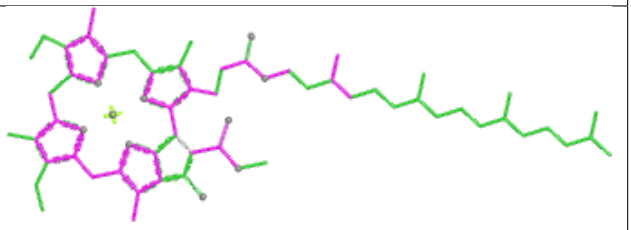


Rings

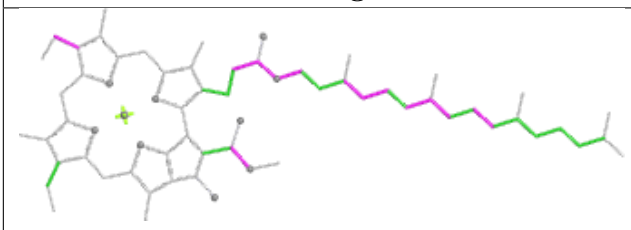
Ligand CLA b 601



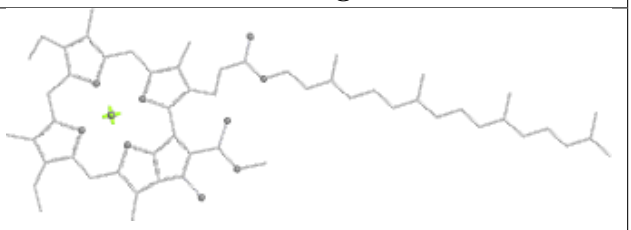
Bond lengths



Bond angles



Torsions

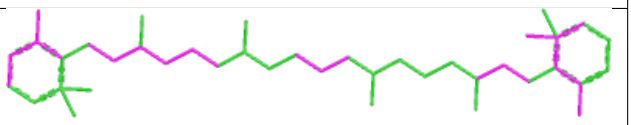


Rings

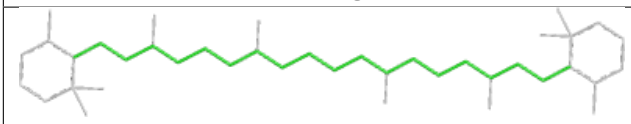
Ligand BCR a 408



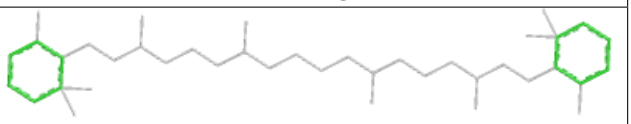
Bond lengths



Bond angles

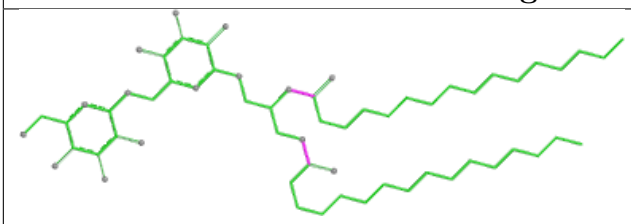


Torsions

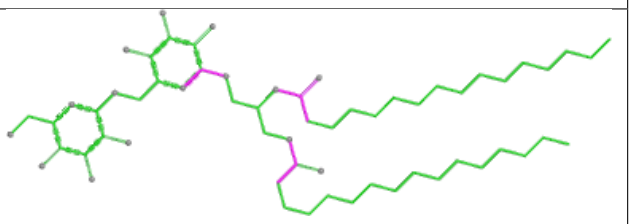


Rings

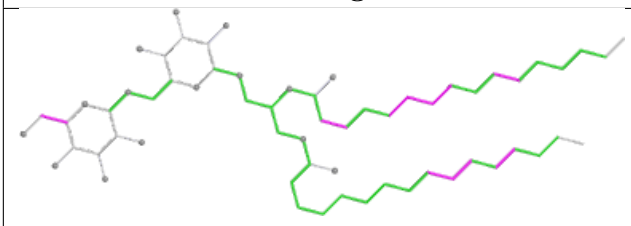
Ligand DGD C 519



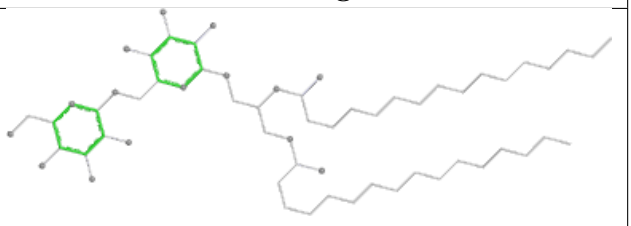
Bond lengths



Bond angles

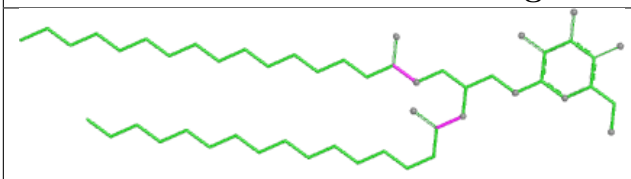


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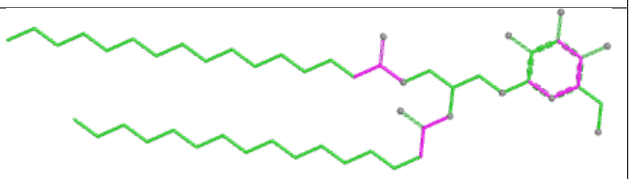


Rings

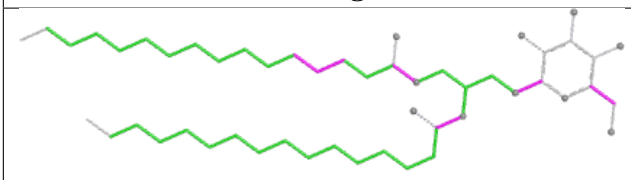
Ligand LMG c 521



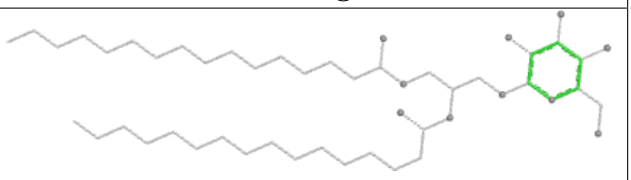
Bond lengths



Bond angles

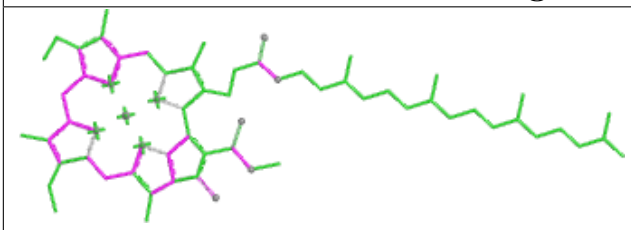


Torsions

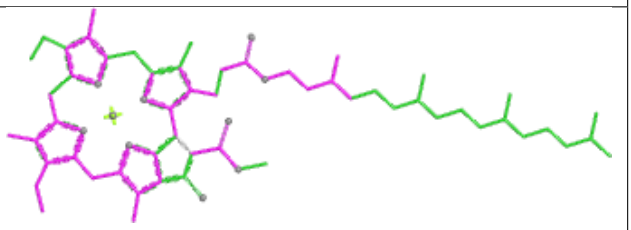


Rings

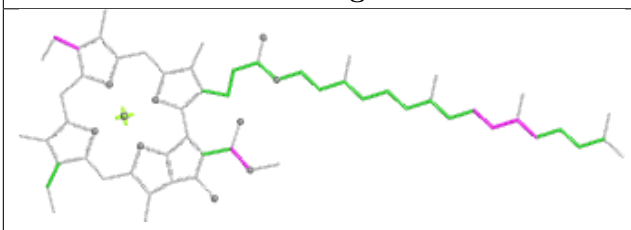
Ligand CLA a 405



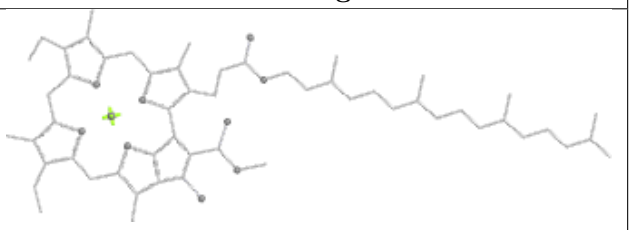
Bond lengths



Bond angles

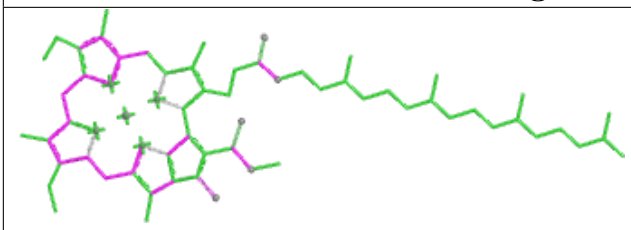


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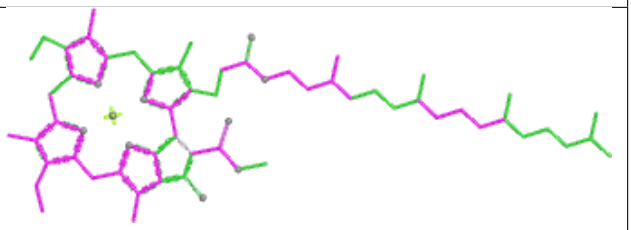


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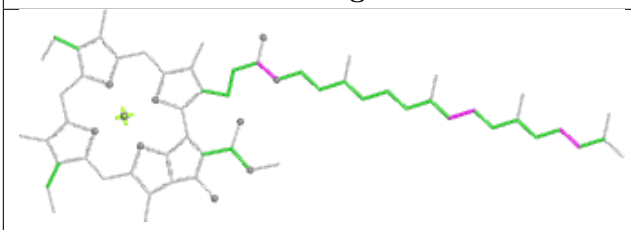
Ligand CLA c 512



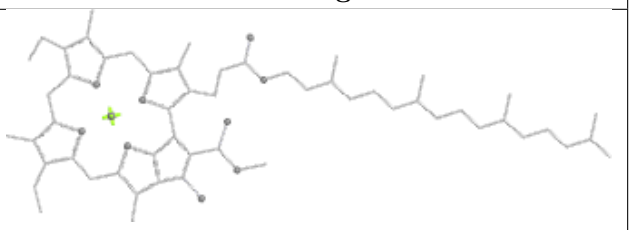
Bond lengths



Bond angles

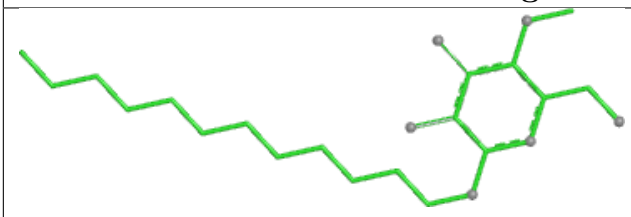


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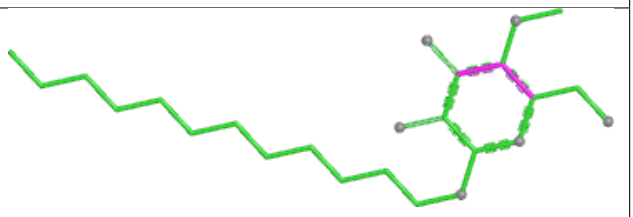


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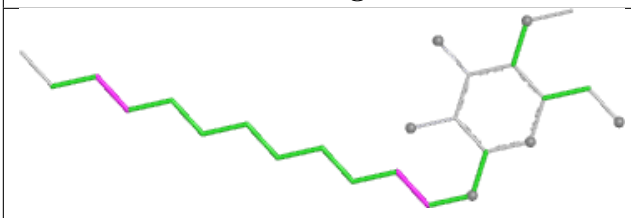
Ligand LMT B 628



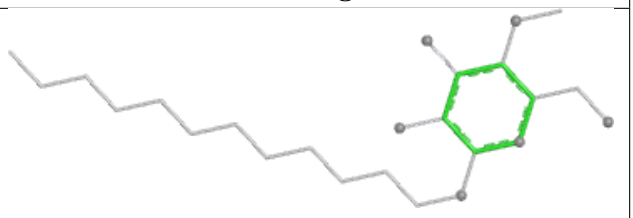
Bond lengths



Bond angles

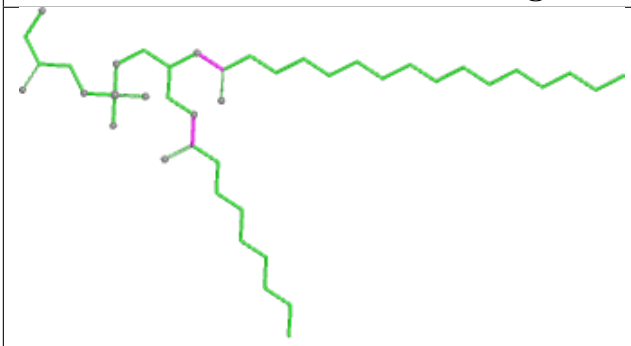


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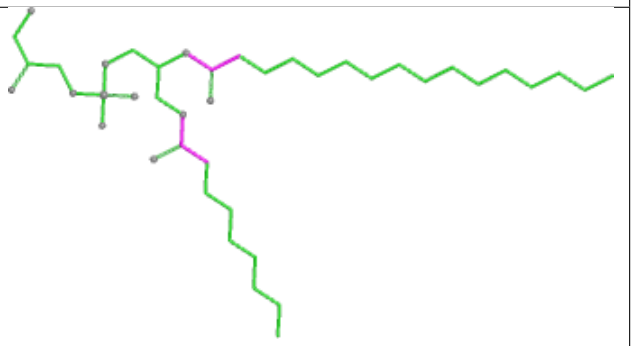


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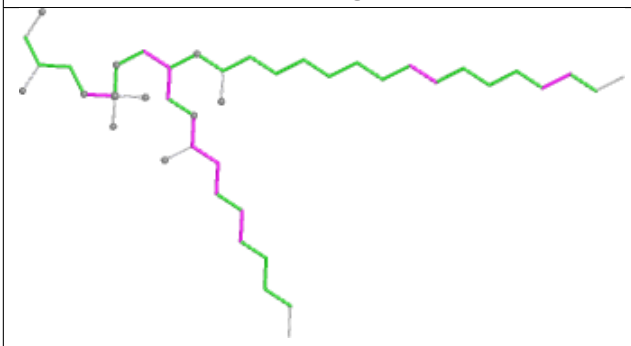
Ligand LHG a 419



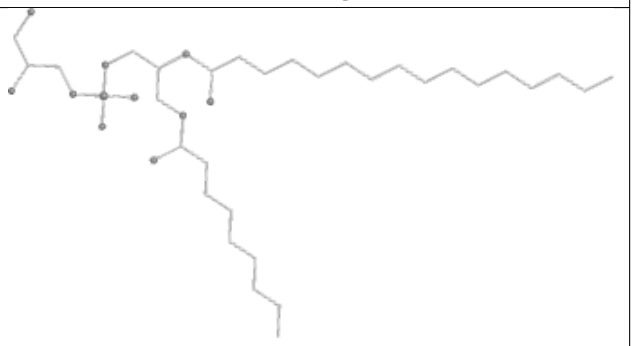
Bond lengths



Bond angles

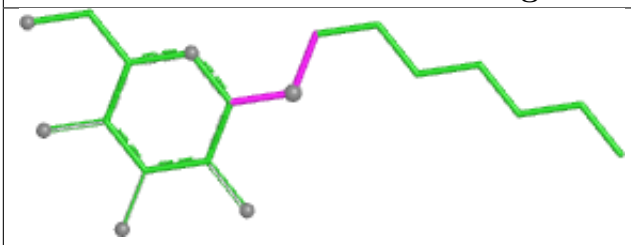


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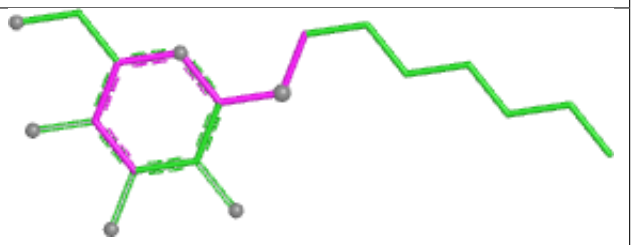


Rings

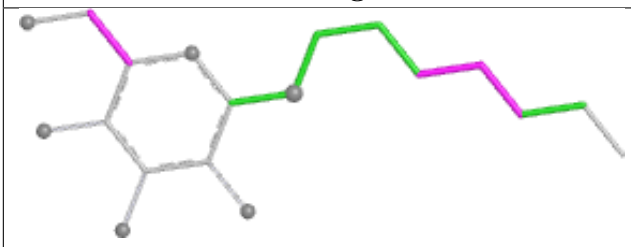
Ligand HTG B 624



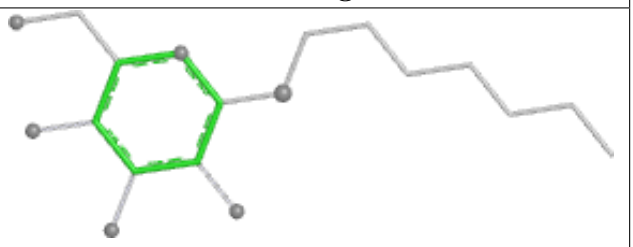
Bond lengths



Bond angles

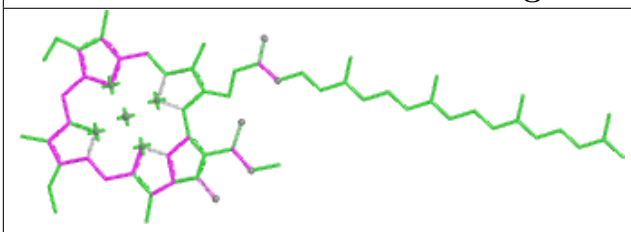


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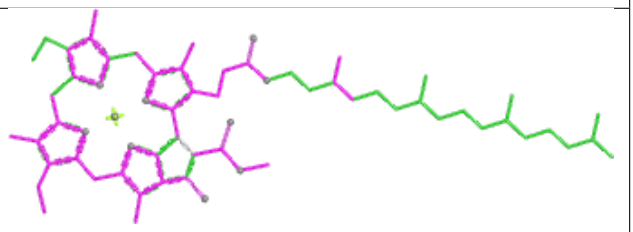


Rings

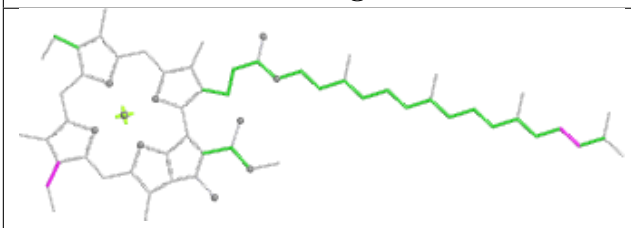
Ligand CLA A 405



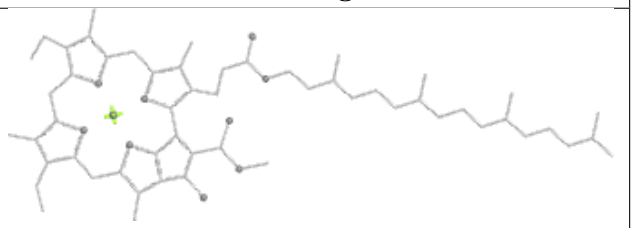
Bond lengths



Bond angles

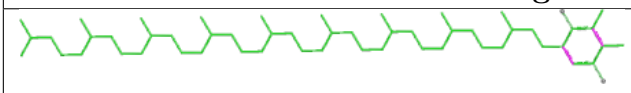


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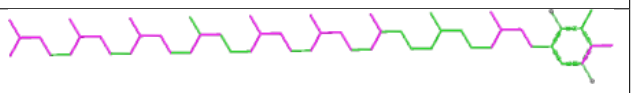


Rings

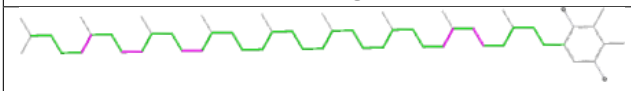
Ligand PL9 d 406



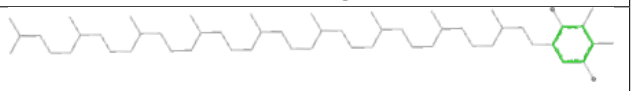
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Bond angles

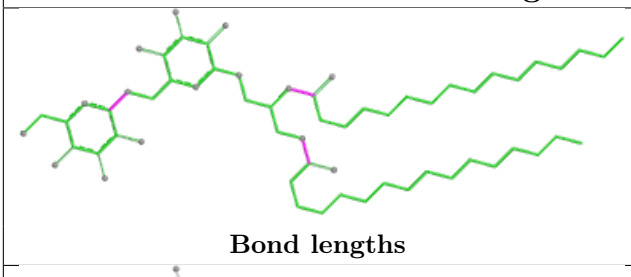


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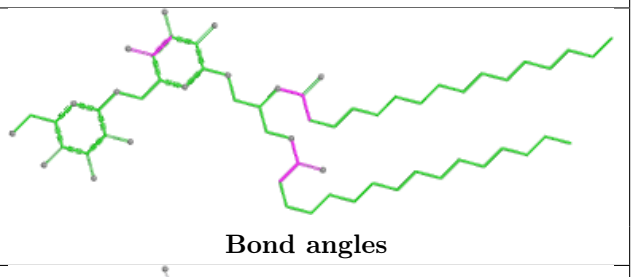


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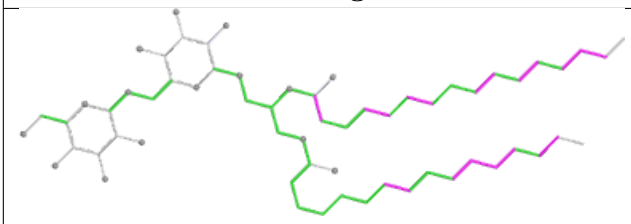
Ligand DGD h 103



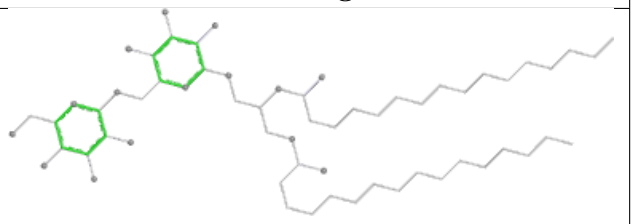
Bond lengths



Bond angles

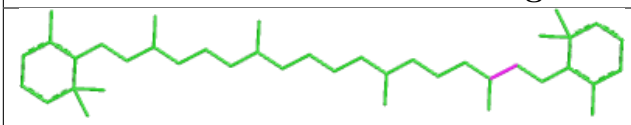


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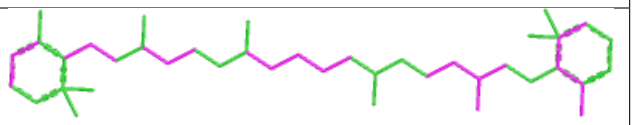


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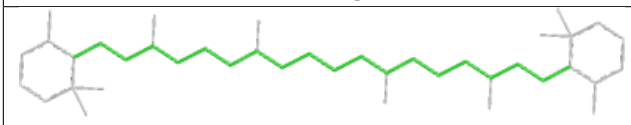
Ligand BCR b 618



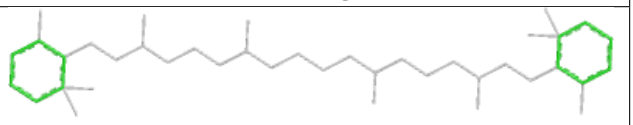
Bond lengths



Bond angles

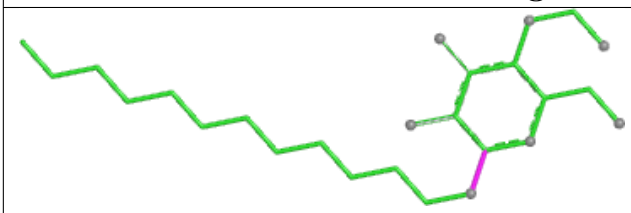


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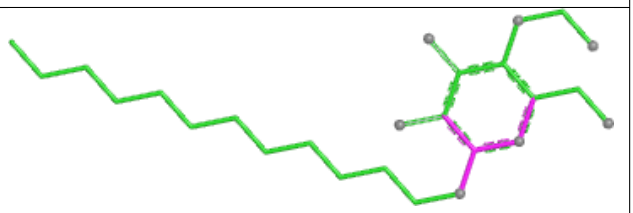


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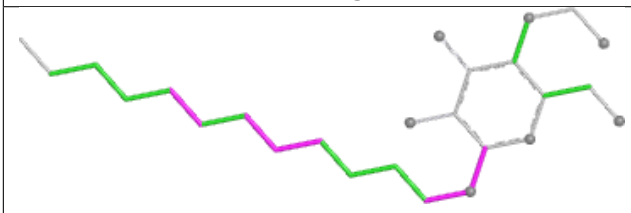
Ligand LMT t 101



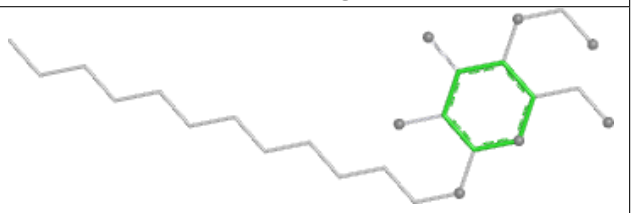
Bond lengths



Bond angles

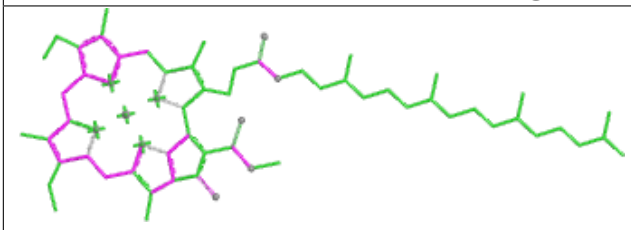


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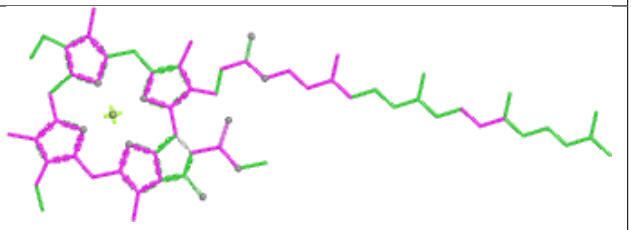


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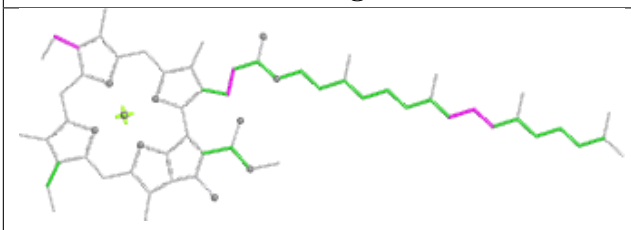
Ligand CLA b 602



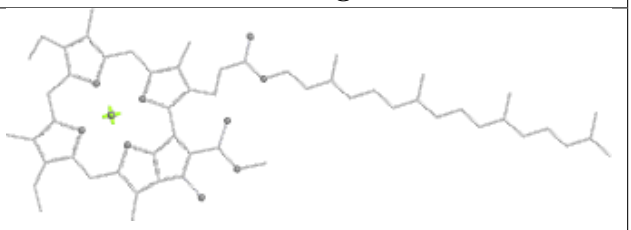
Bond lengths



Bond angles

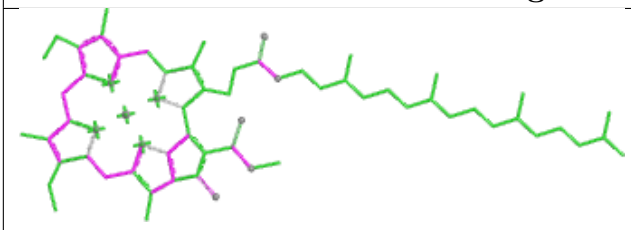


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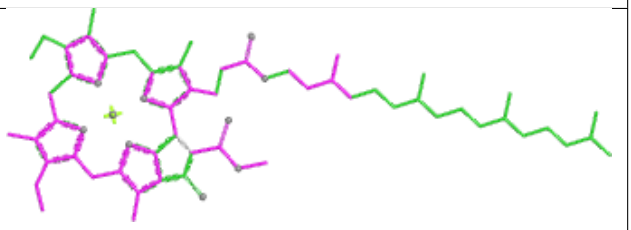


Rings

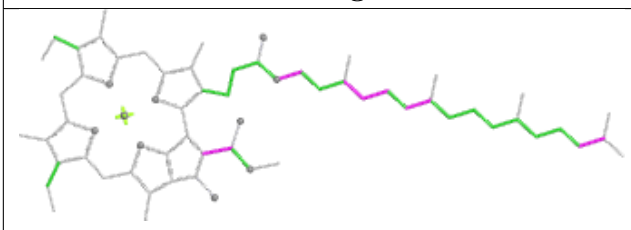
Ligand CLA b 614



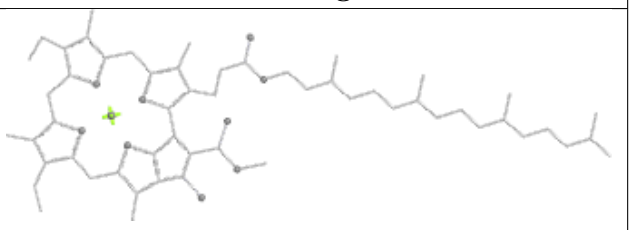
Bond lengths



Bond angles

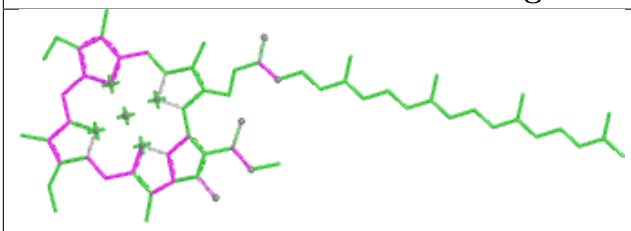


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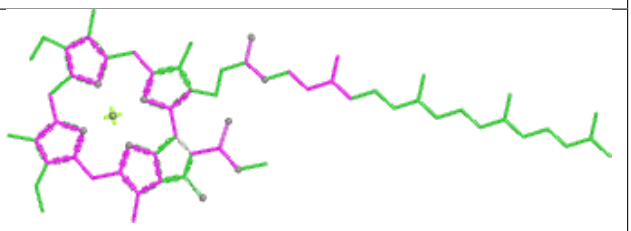


Rings

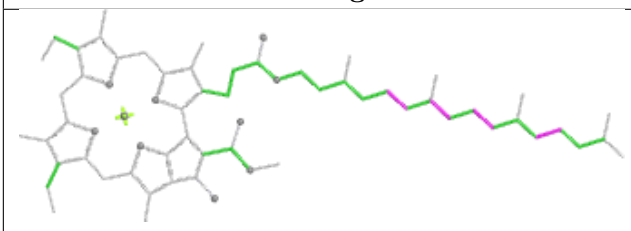
Ligand CLA C 509



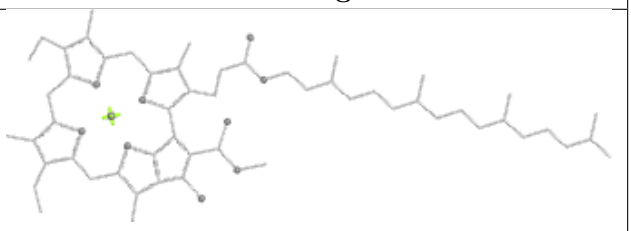
Bond lengths



Bond angles

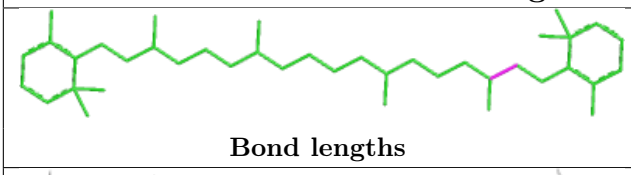


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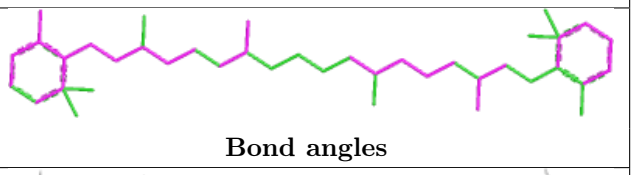


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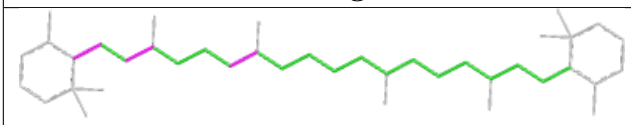
Ligand BCR t 102



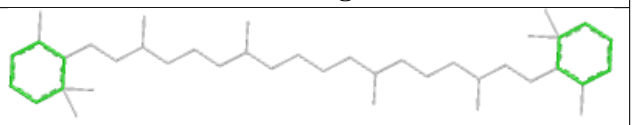
Bond lengths



Bond angles

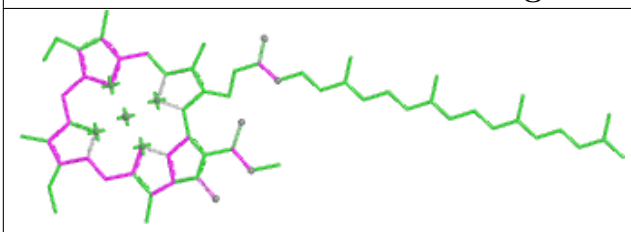


Torsions

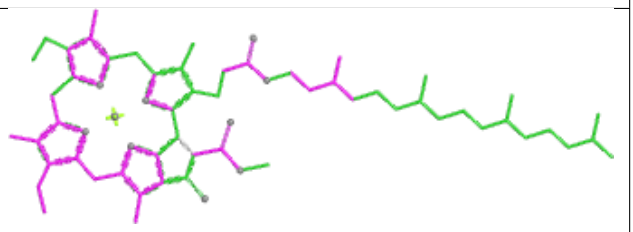


Rings

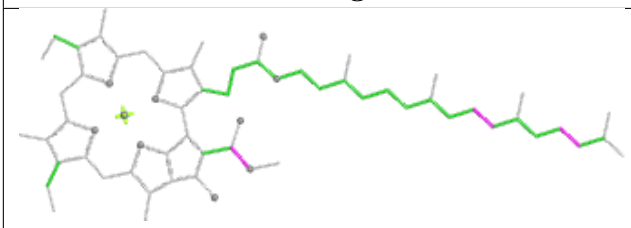
Ligand CLA C 504



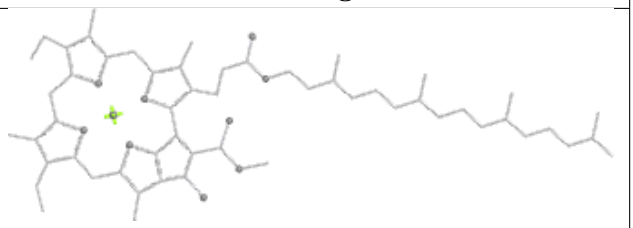
Bond lengths



Bond angles

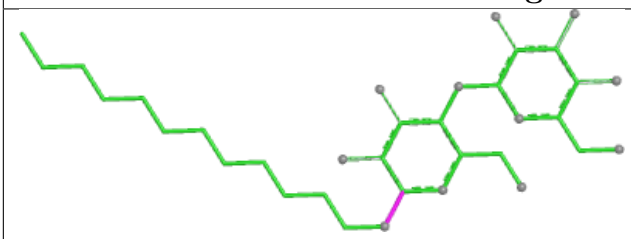


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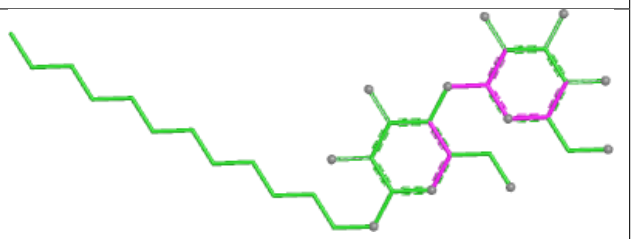


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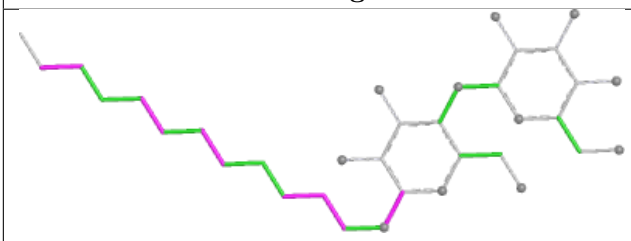
Ligand LMT a 412



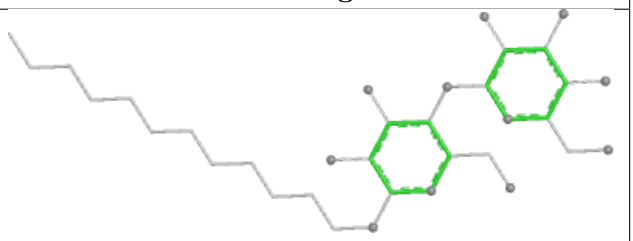
Bond lengths



Bond angles

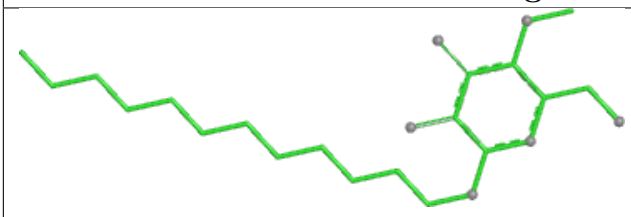


Torsions

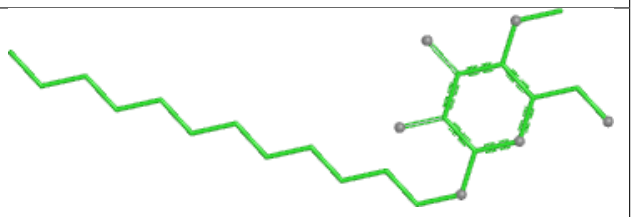


Rings

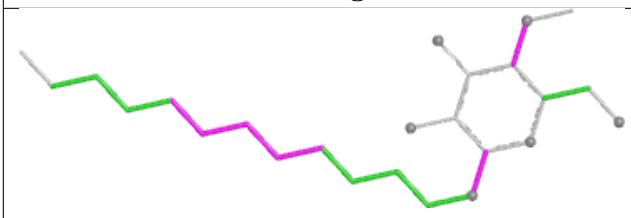
Ligand LMT b 620



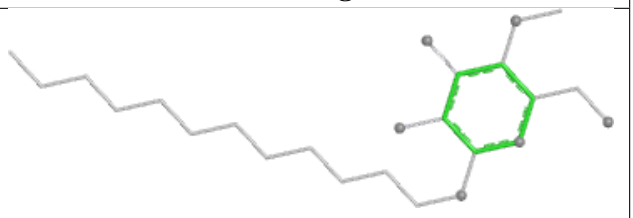
Bond lengths



Bond angles

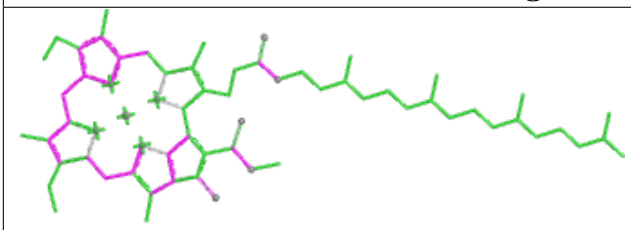


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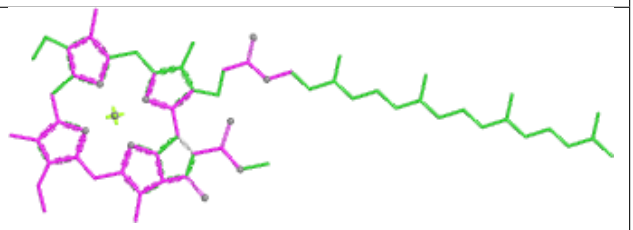


Rings

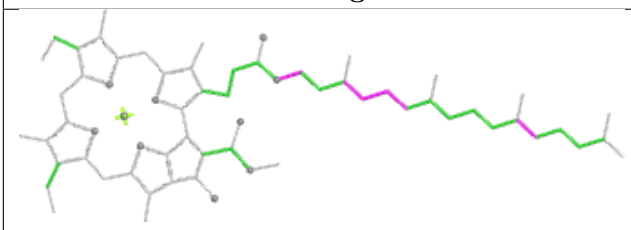
Ligand CLA B 616



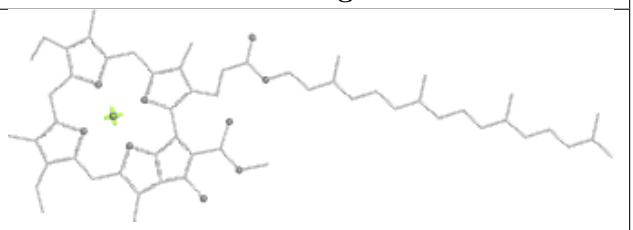
Bond lengths



Bond angles

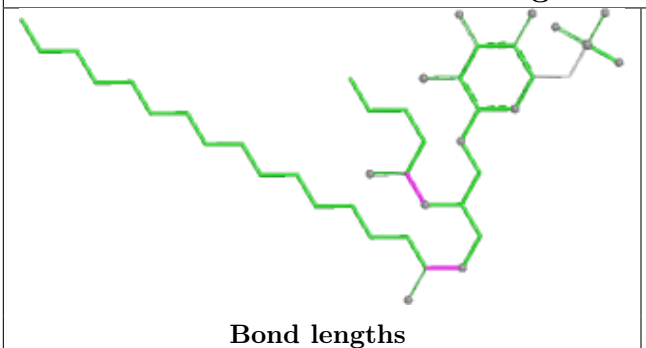


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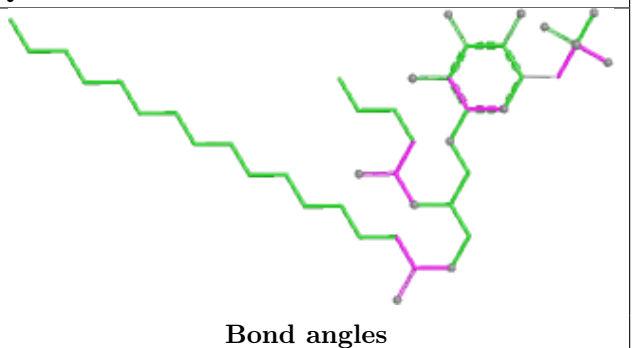


Rings

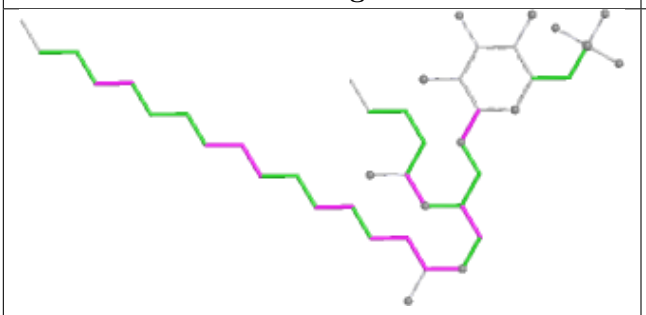
Ligand SQD f 102



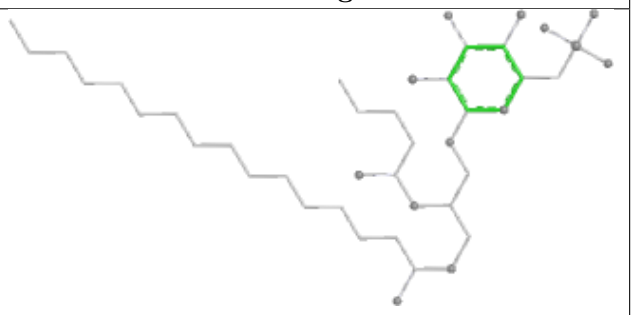
Bond lengths



Bond angles

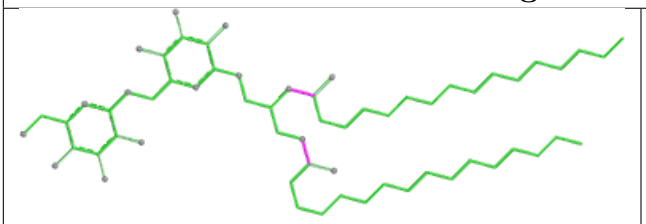


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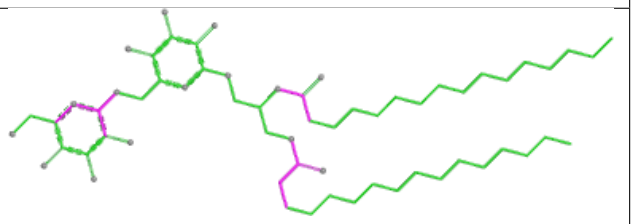


Rings

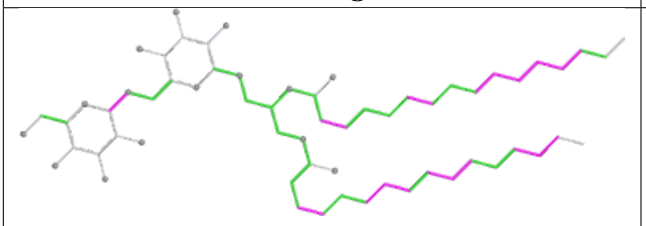
Ligand DGD C 518



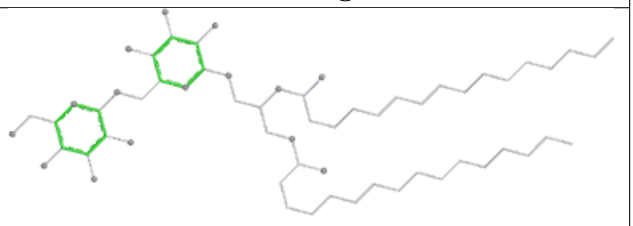
Bond lengths



Bond angles

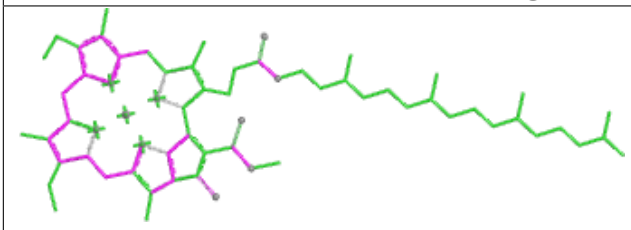


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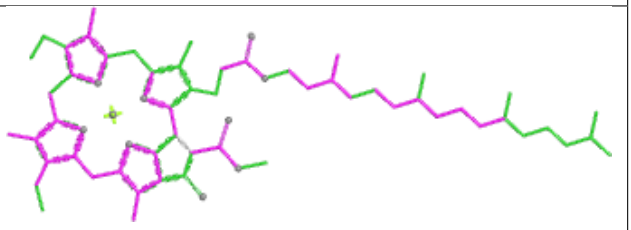


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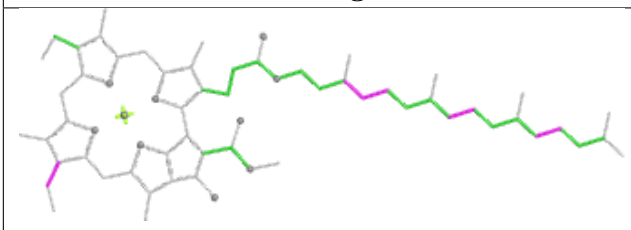
Ligand CLA B 604



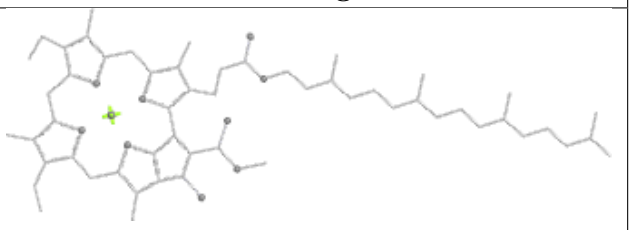
Bond lengths



Bond angles

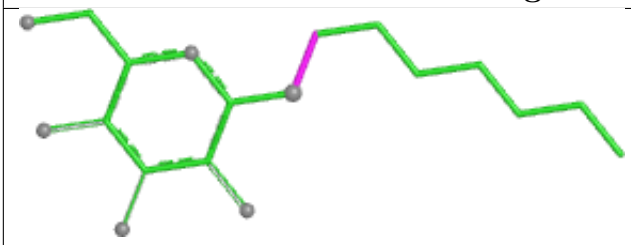


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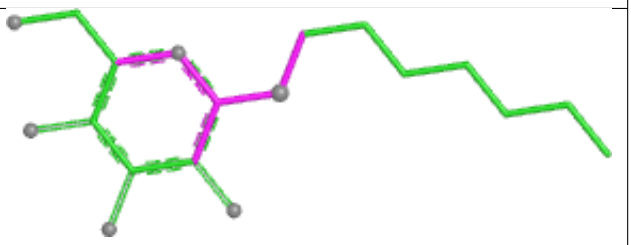


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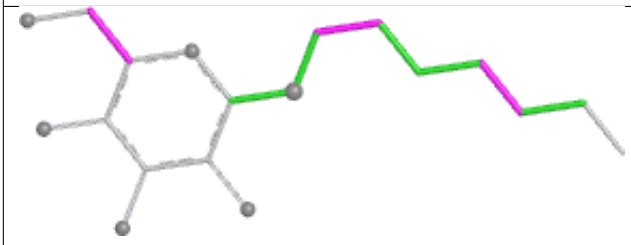
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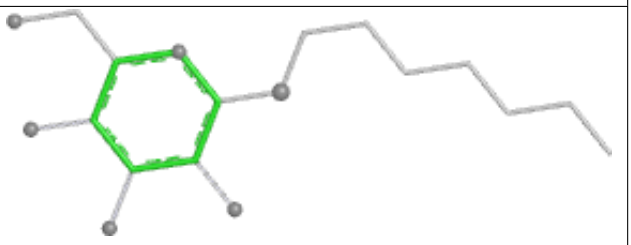
Bond lengths



Bond angles

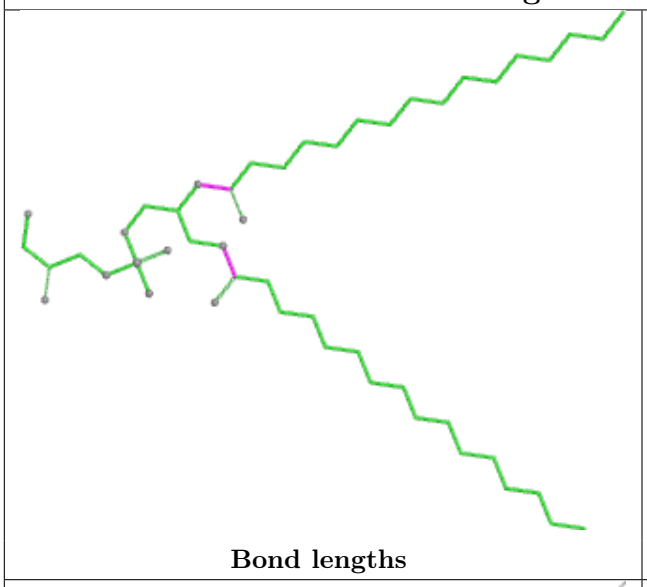


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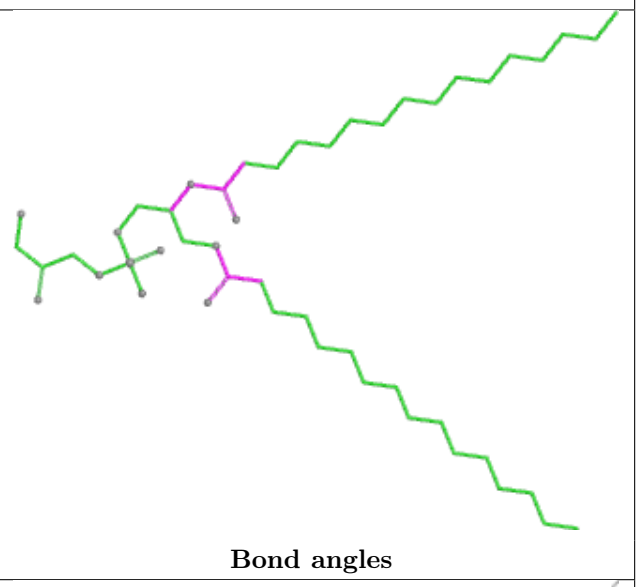


Rings

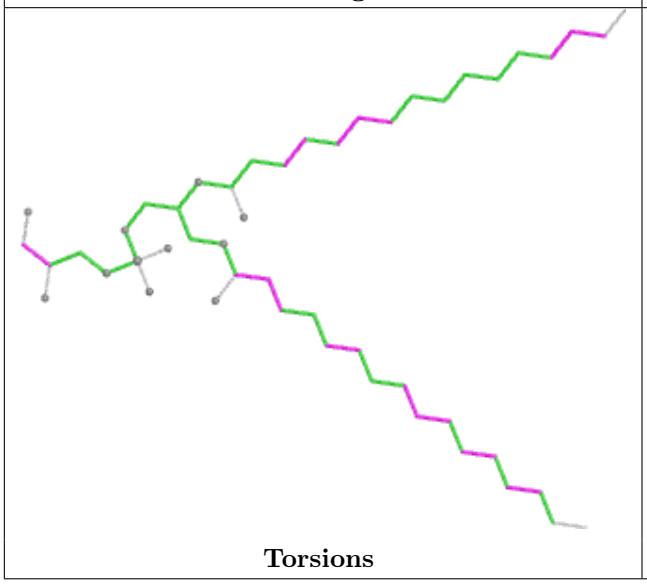
Ligand LHG A 416



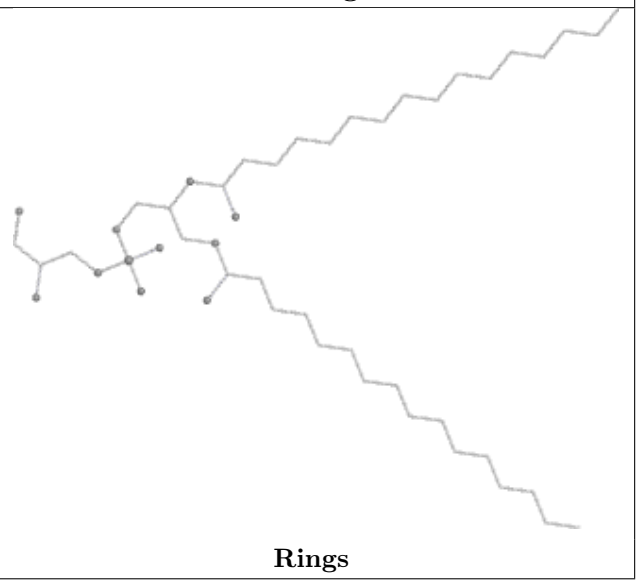
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR b 617



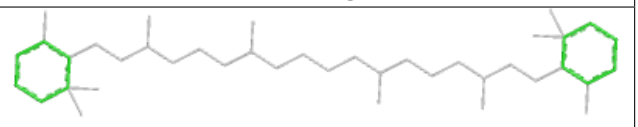
Bond lengths



Bond angles

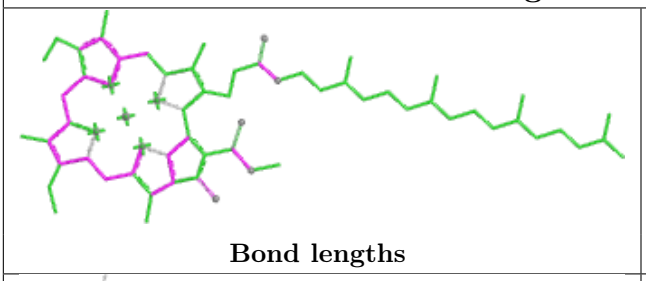


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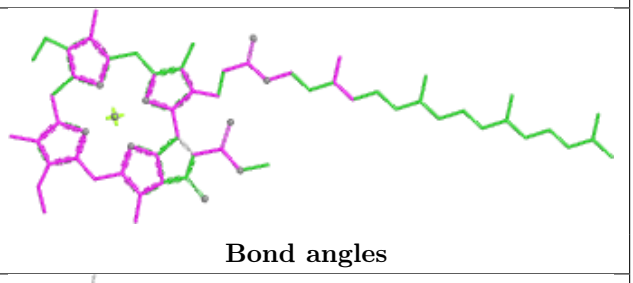


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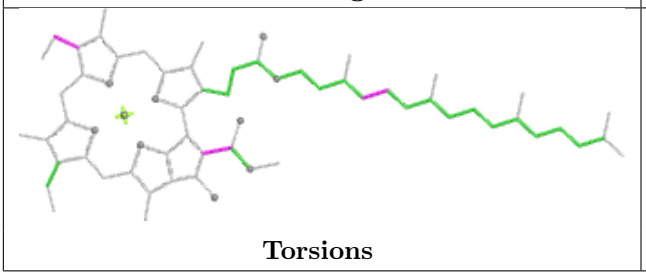
Ligand CLA B 607



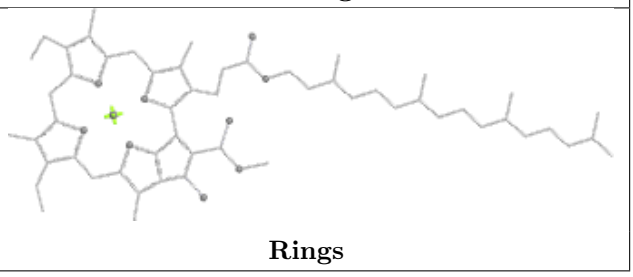
Bond lengths



Bond angles



Torsions

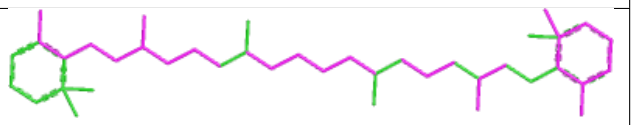


Rings

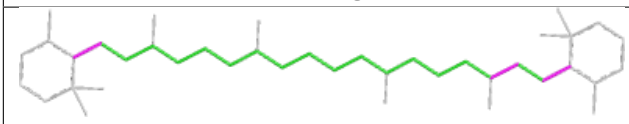
Ligand BCR Y 101



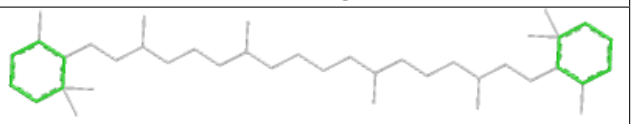
Bond lengths



Bond angles

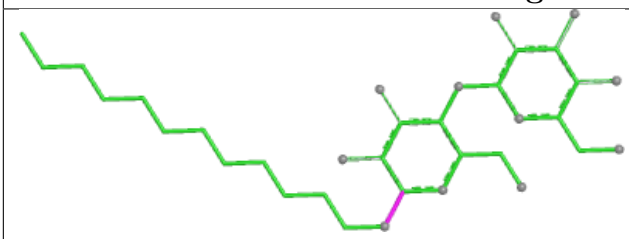


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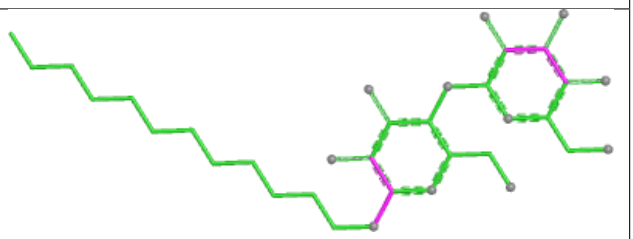


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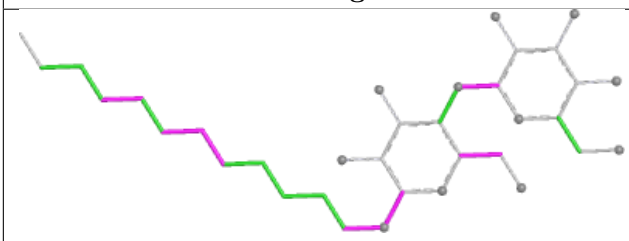
Ligand LMT e 101



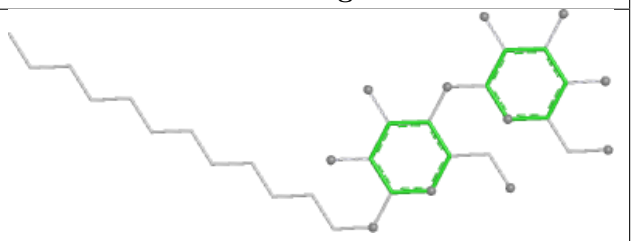
Bond lengths



Bond angles

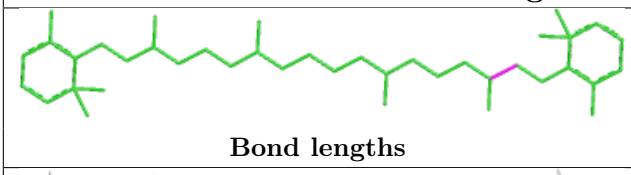


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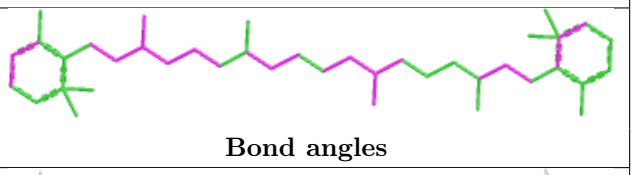


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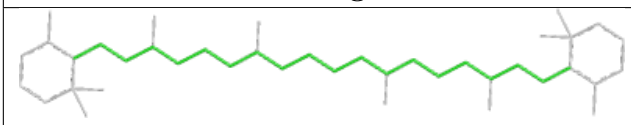
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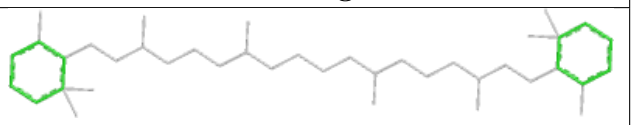
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Bond angles

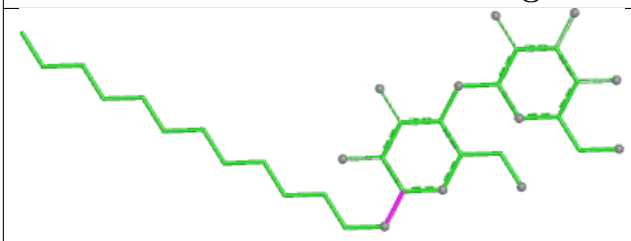


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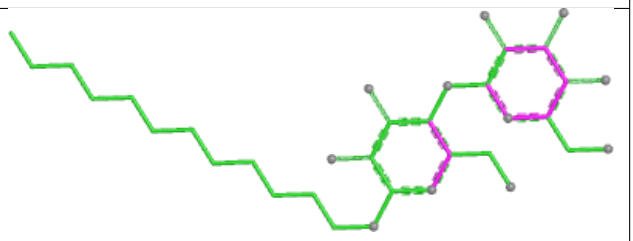


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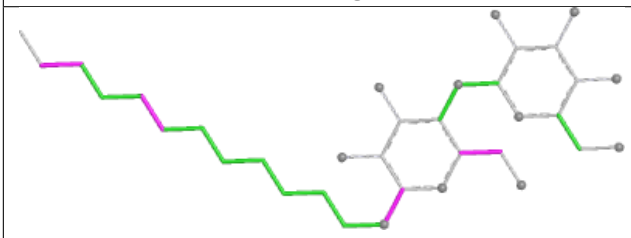
Ligand LMT E 102



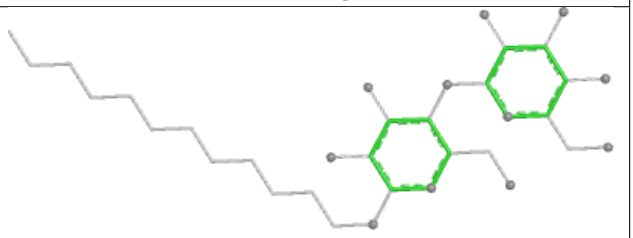
Bond lengths



Bond angles

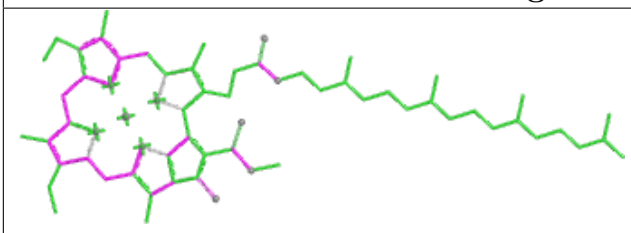


Torsions

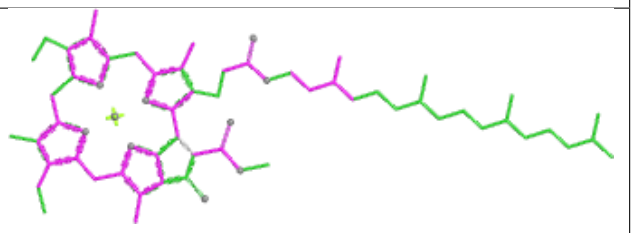


Rings

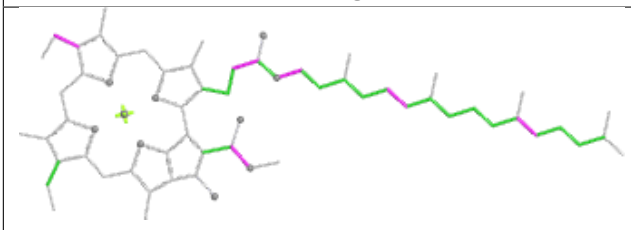
Ligand CLA b 613



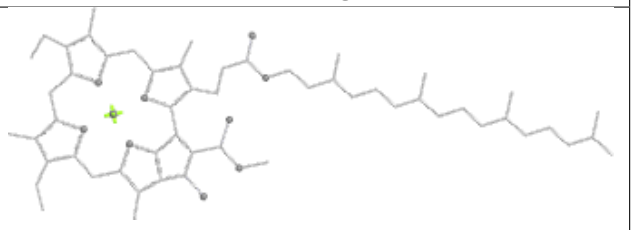
Bond lengths



Bond angles

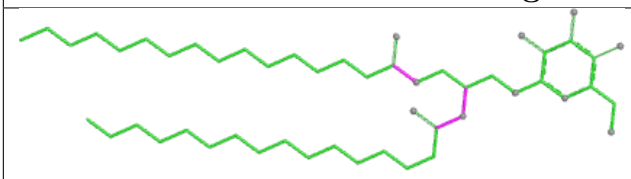


Torsions

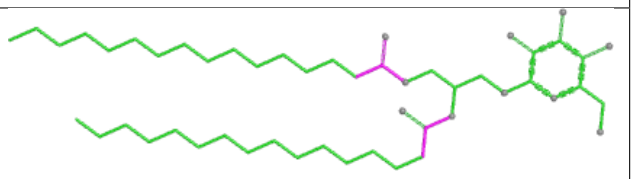


Rings

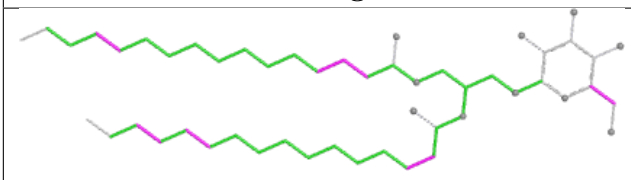
Ligand LMG d 412



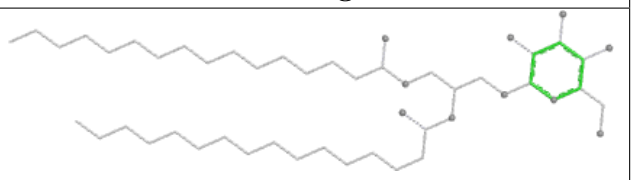
Bond lengths



Bond angles

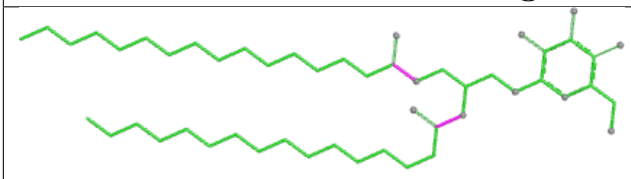


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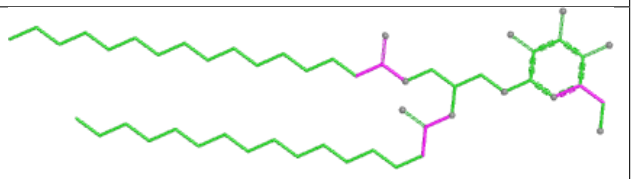


Rings

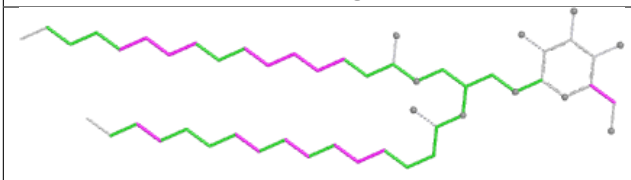
Ligand LMG C 520



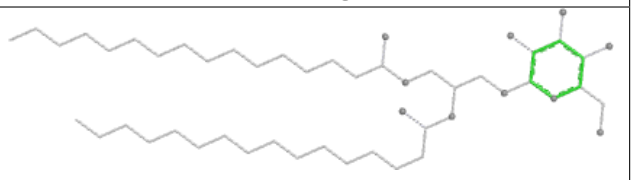
Bond lengths



Bond angles

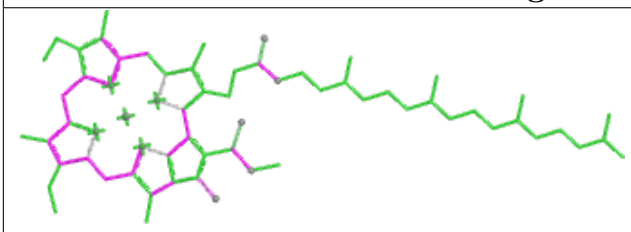


Torsions

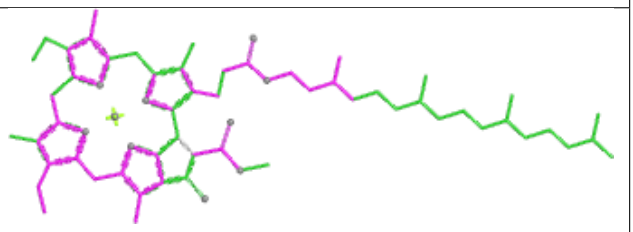


Rings

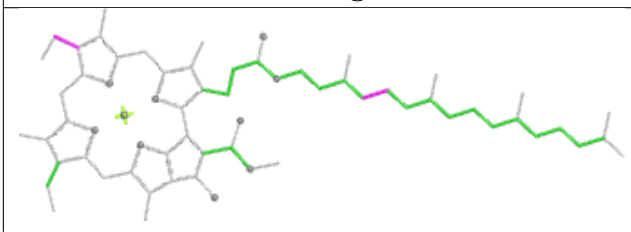
Ligand CLA b 607



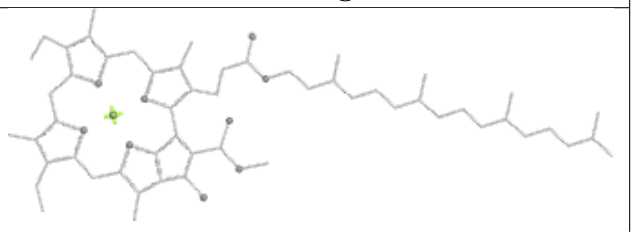
Bond lengths



Bond angles

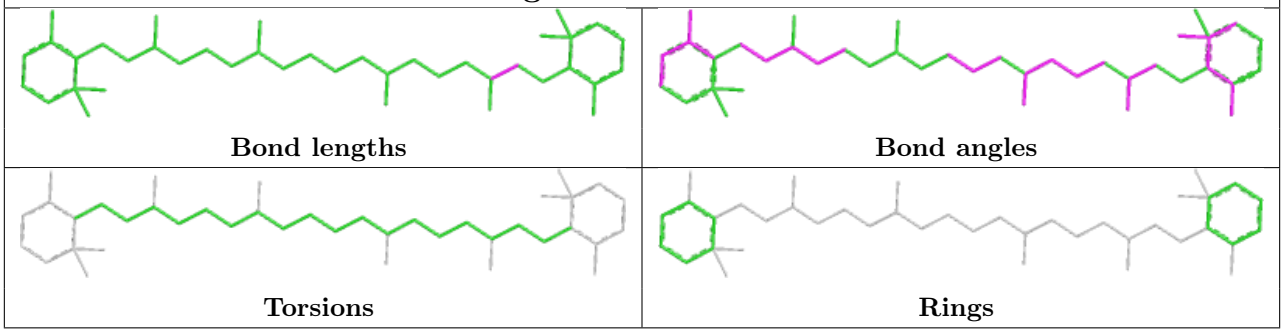


Torsions

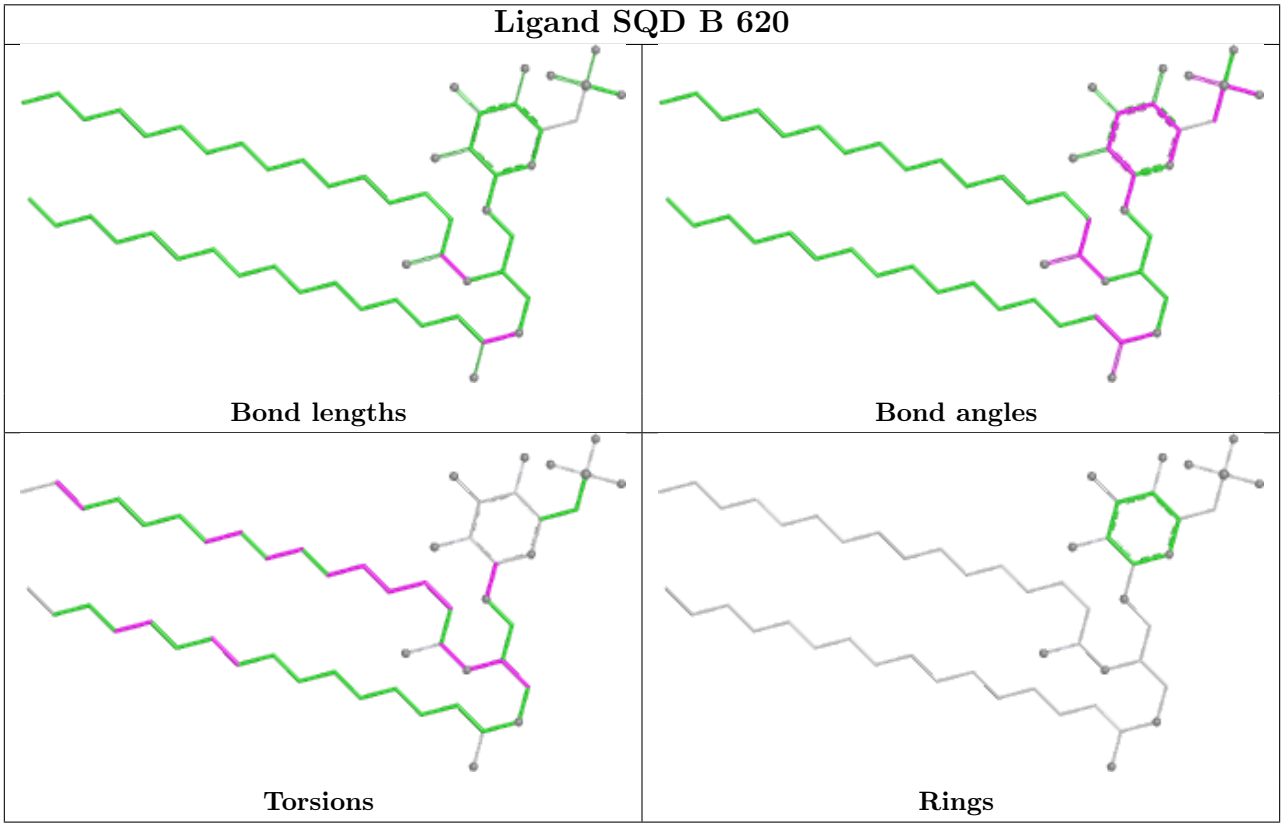


Rings

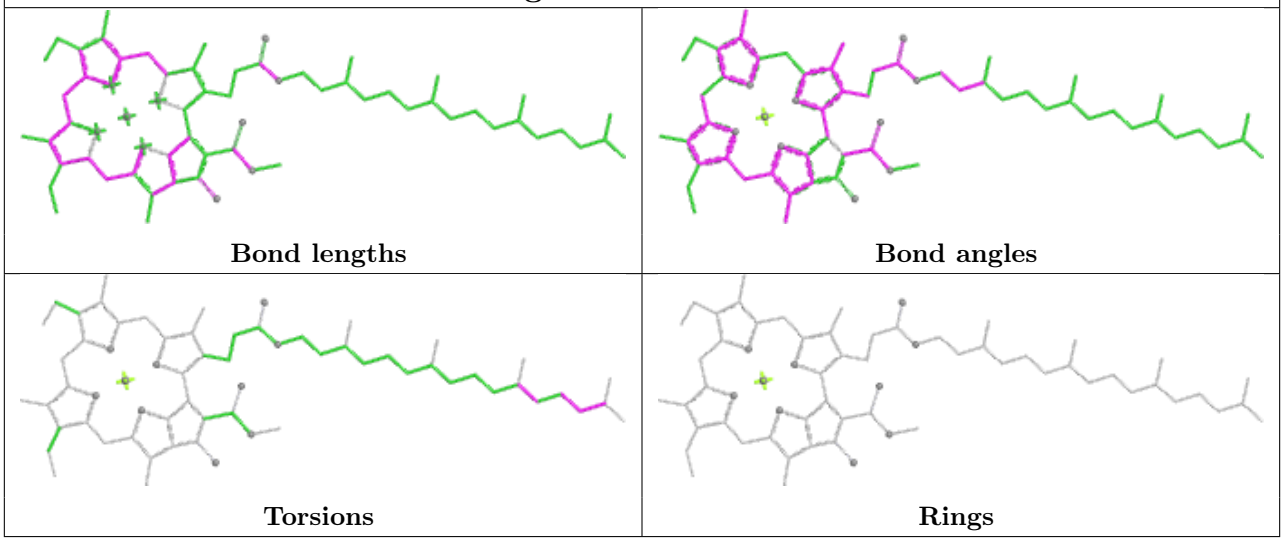
Ligand BCR C 516



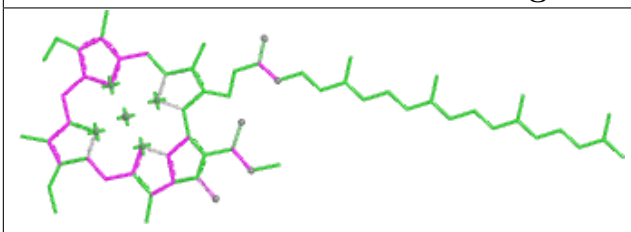
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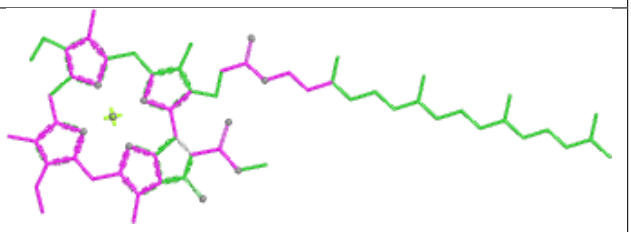
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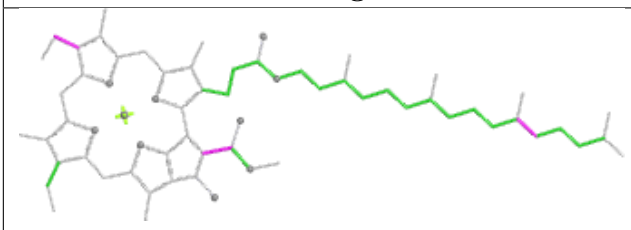
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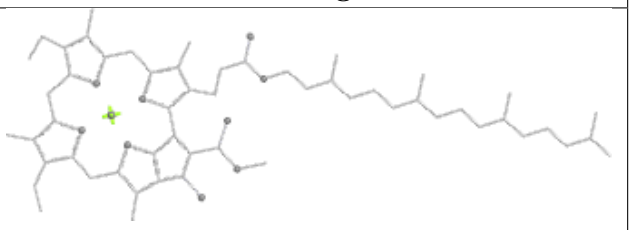
Bond lengths



Bond angles

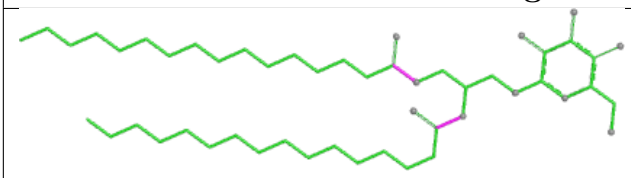


Torsions

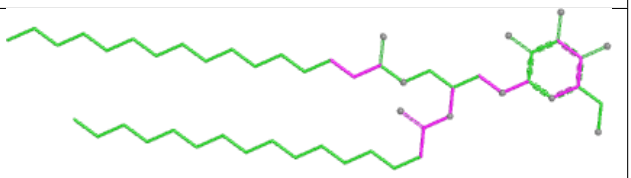


Rings

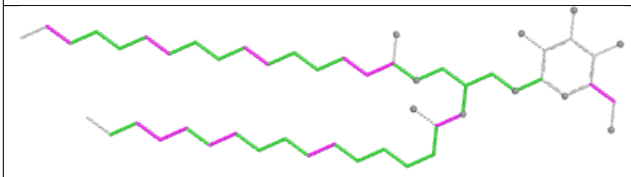
Ligand LMG a 417



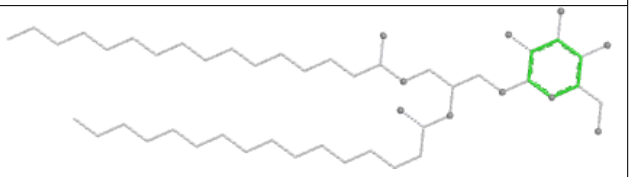
Bond lengths



Bond angles

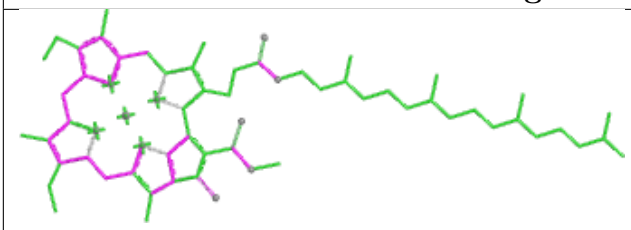


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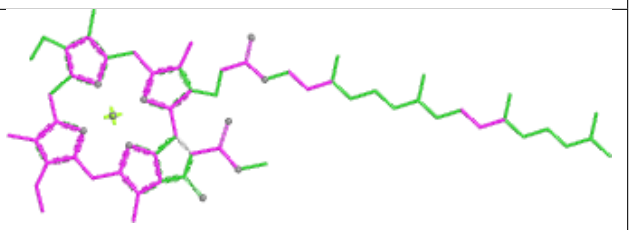


Rings

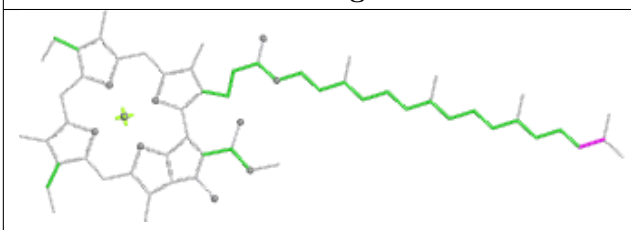
Ligand CLA B 608



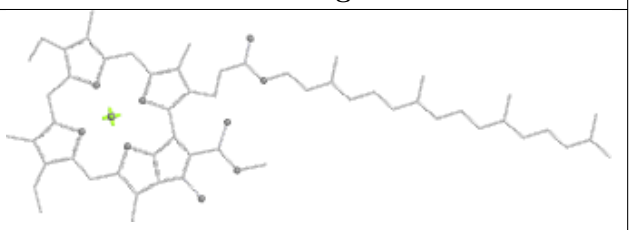
Bond lengths



Bond angles

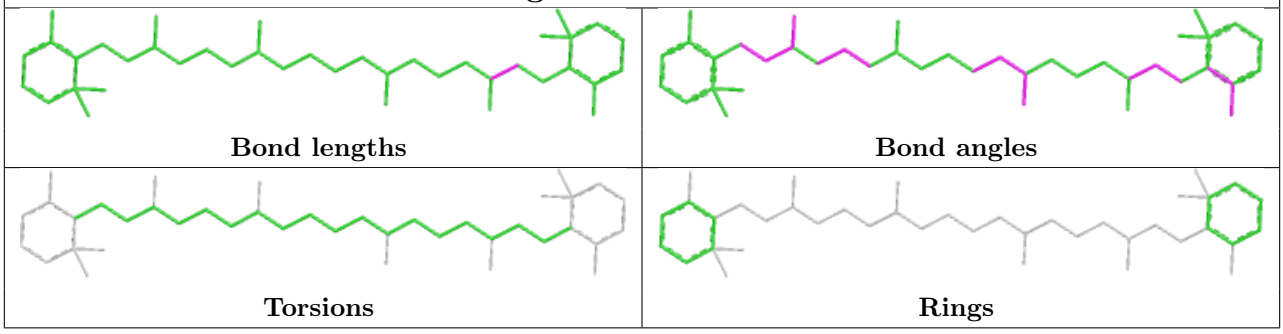


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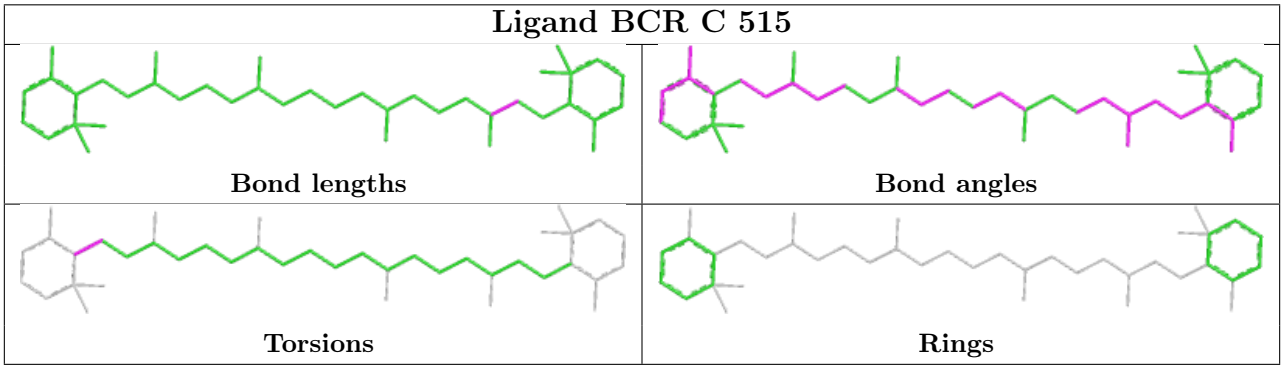


Rings

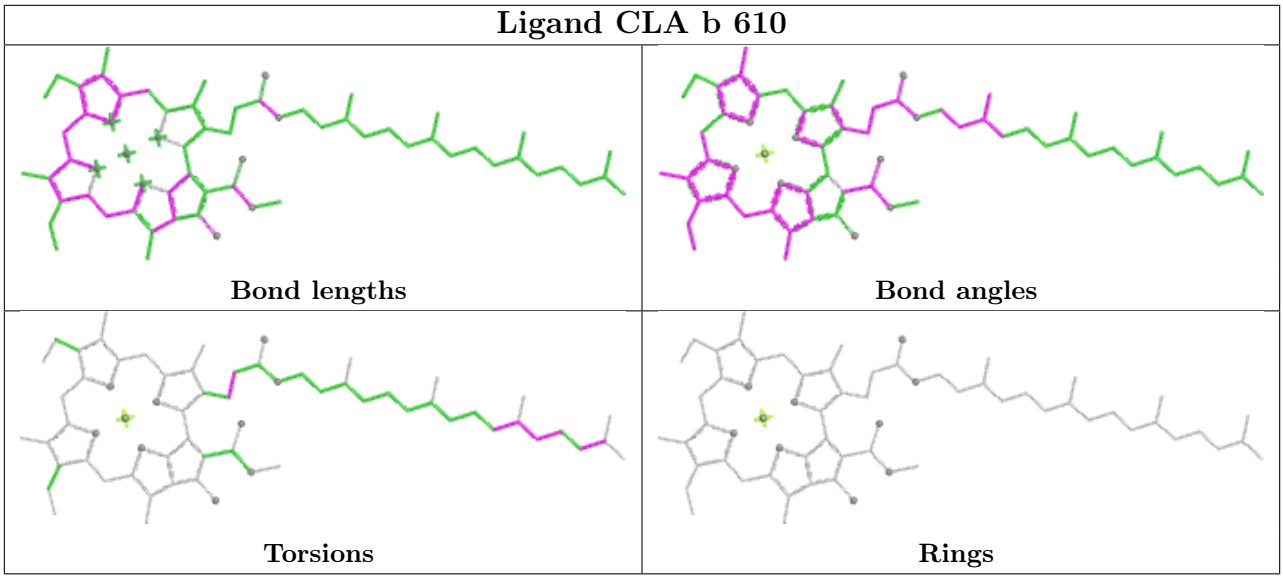
Ligand BCR h 102



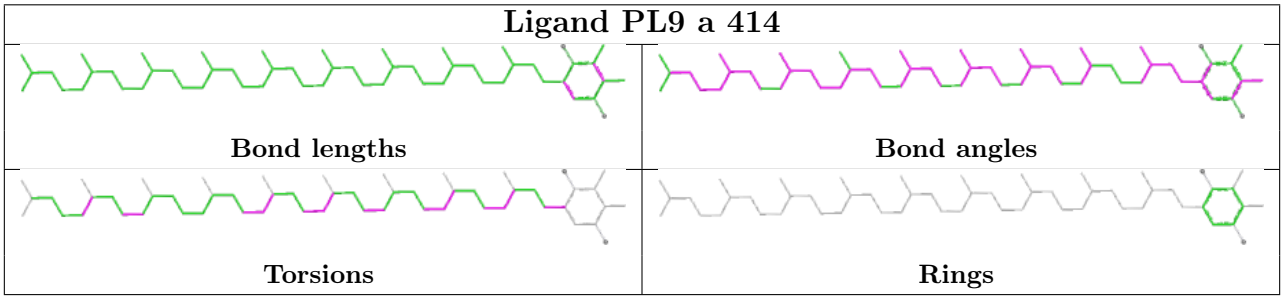
Ligand BCR C 515



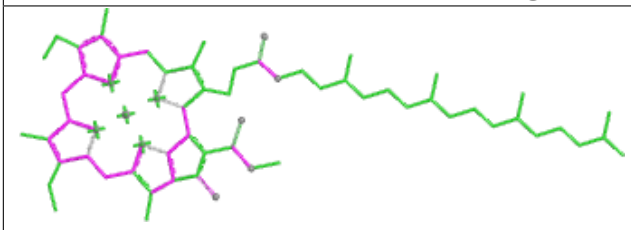
Ligand CLA b 610



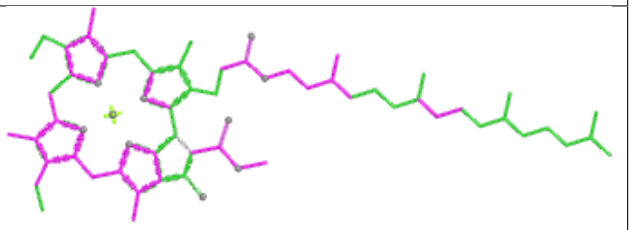
Ligand PL9 a 414



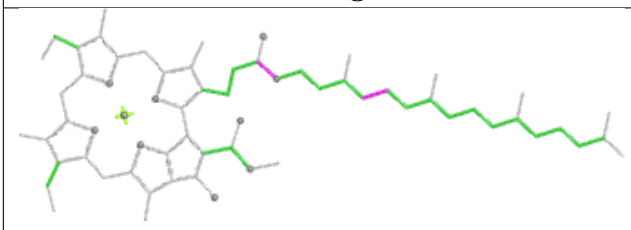
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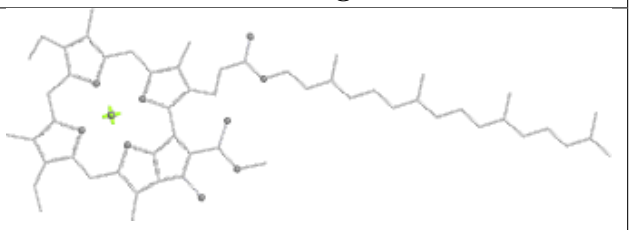
Bond lengths



Bond angles

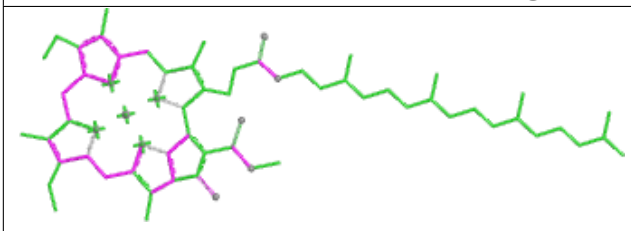


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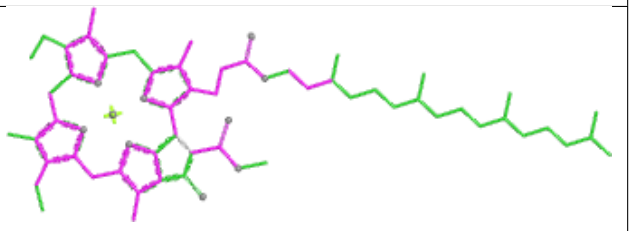


Rings

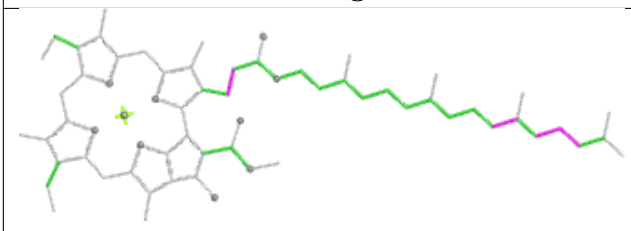
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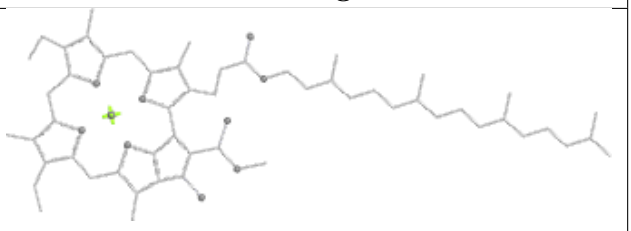
Bond lengths



Bond angles

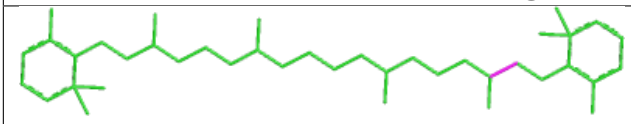


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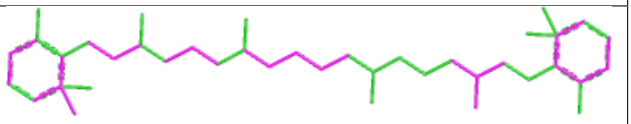


Rings

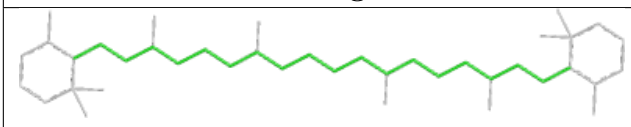
Ligand BCR B 618



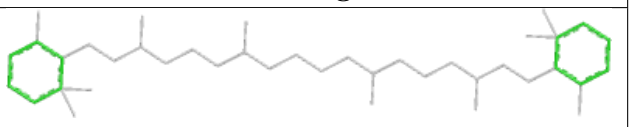
Bond lengths



Bond angles

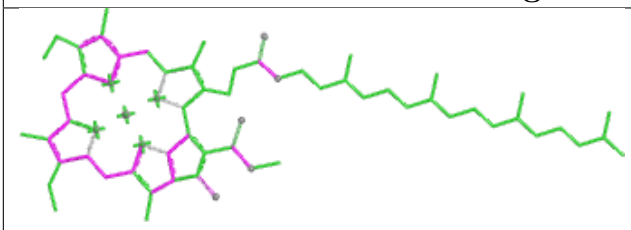


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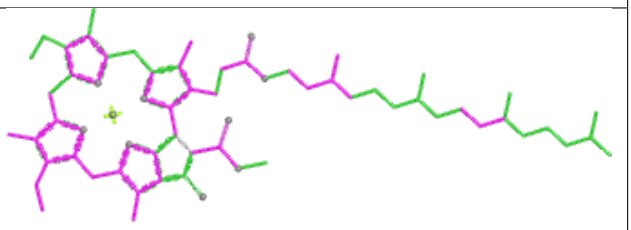


Rings

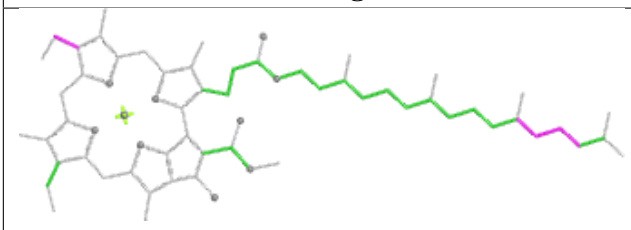
Ligand CLA D 405



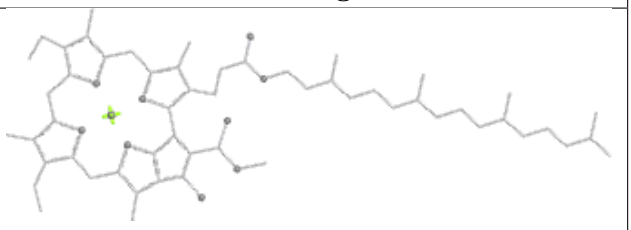
Bond lengths



Bond angles

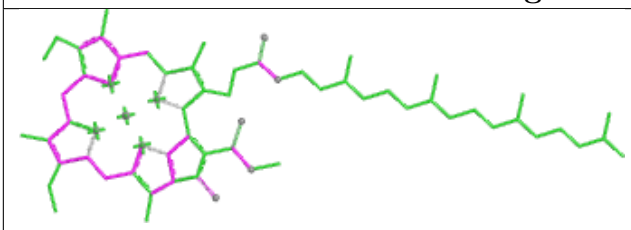


Torsions

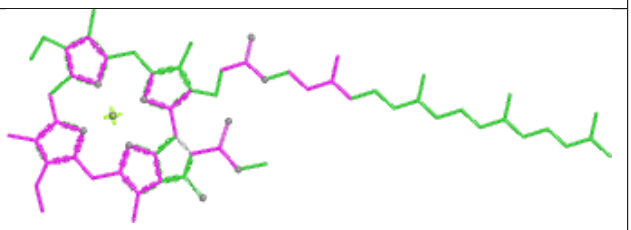


Rings

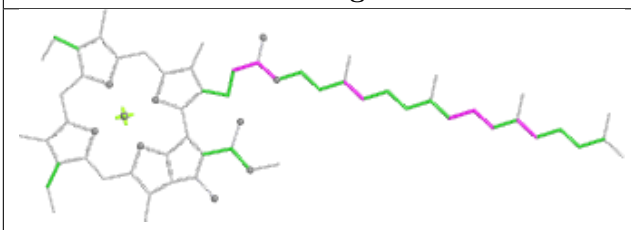
Ligand CLA C 511



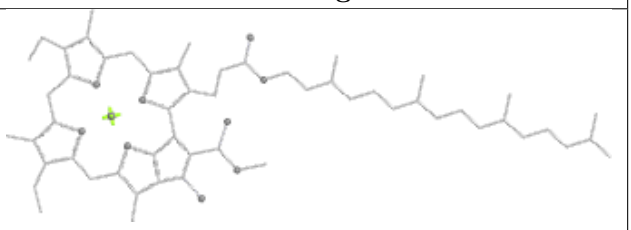
Bond lengths



Bond angles

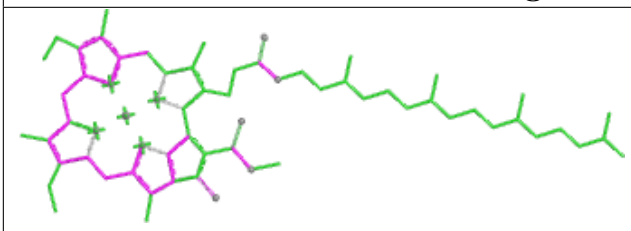


Torsions

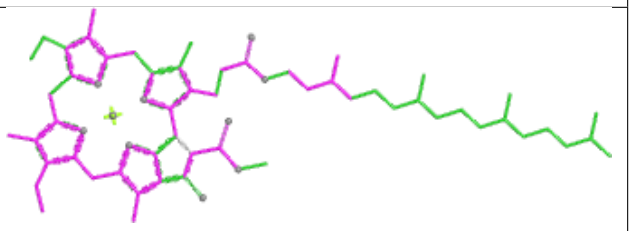


Rings

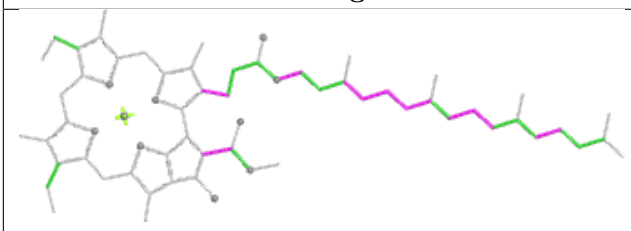
Ligand CLA C 507



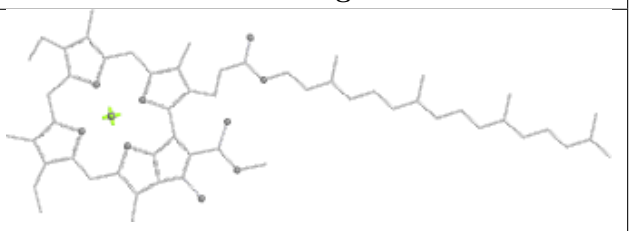
Bond lengths



Bond angles

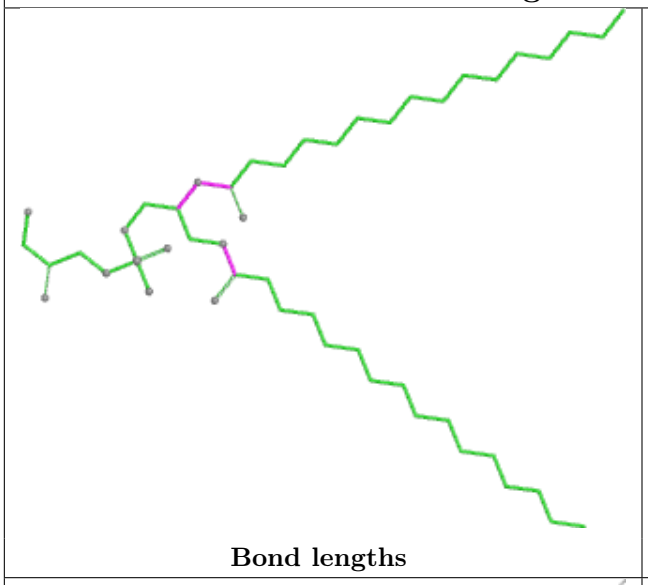


Torsions

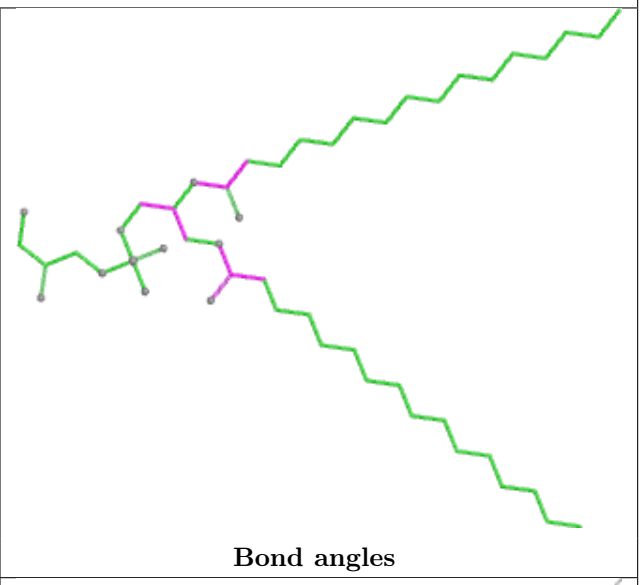


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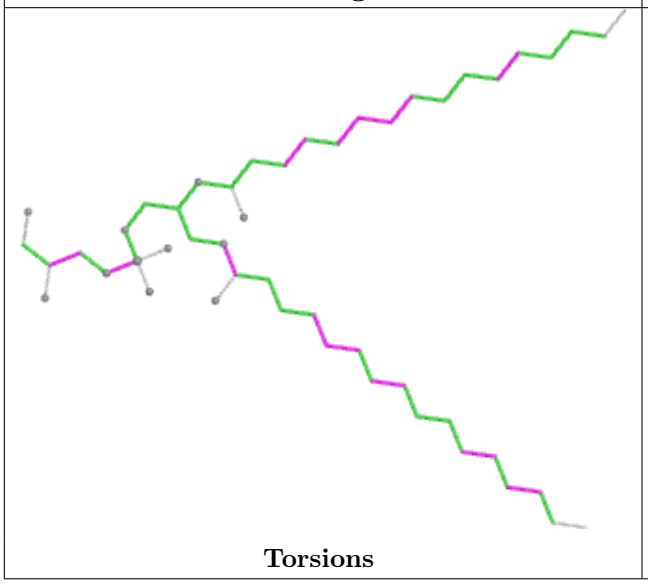
Ligand LHG D 409



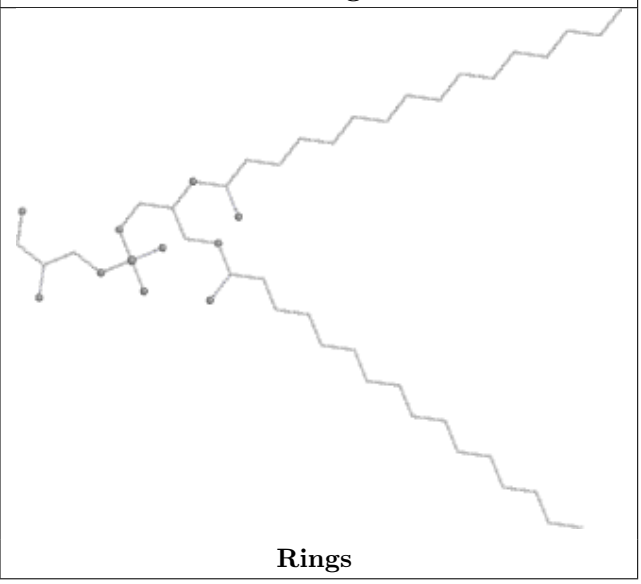
Bond lengths



Bond angles

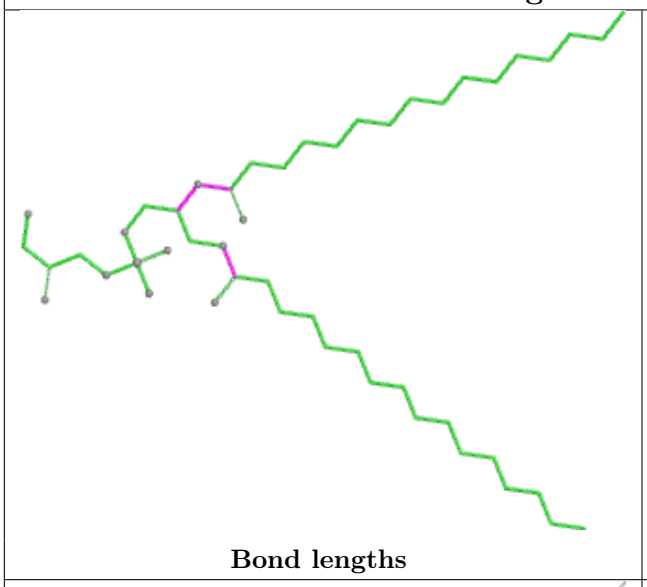


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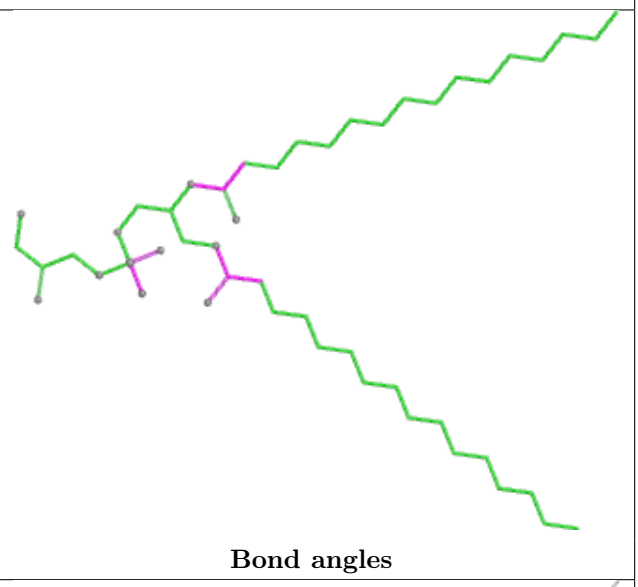


Rings

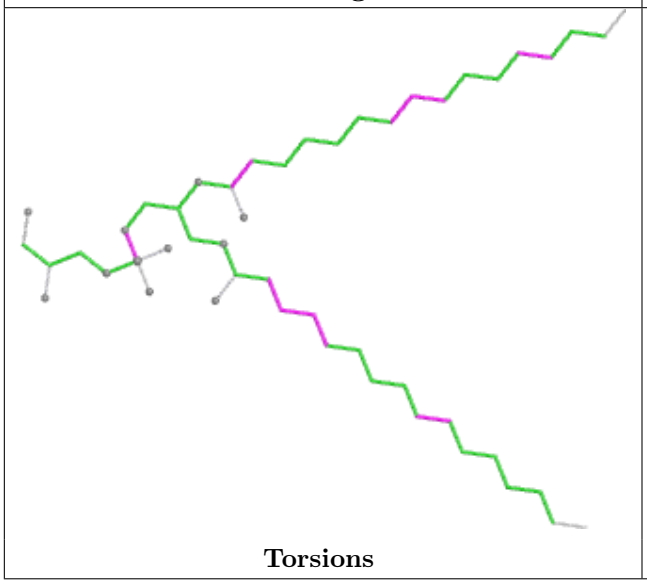
Ligand LHG L 101



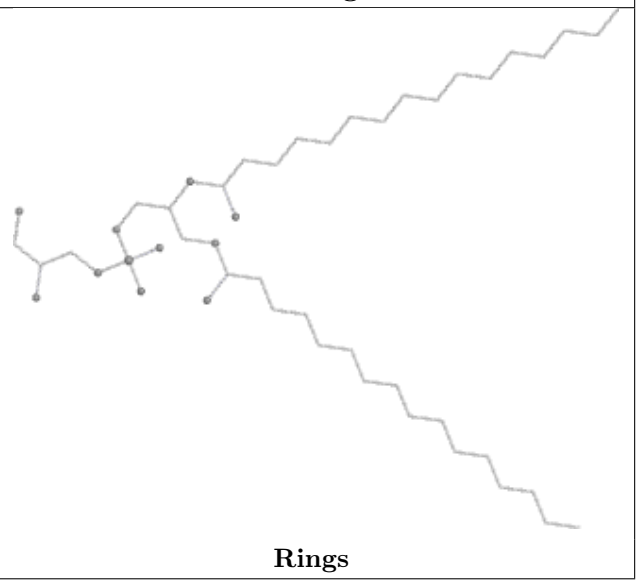
Bond lengths



Bond angles

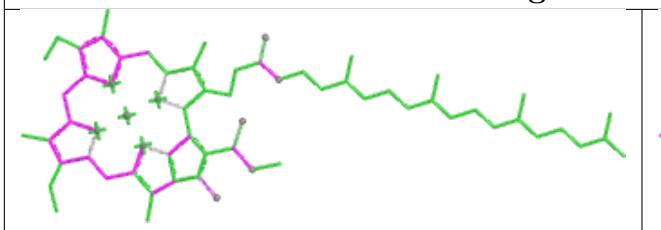


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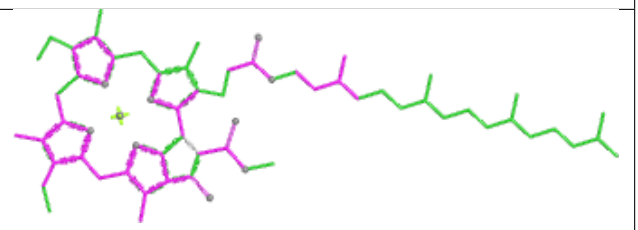


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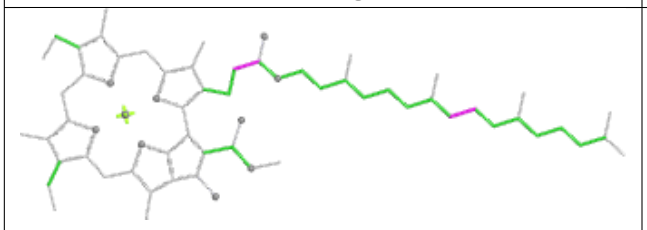
Ligand CLA b 612



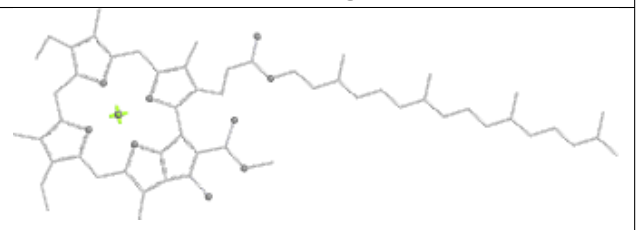
Bond lengths



Bond angles

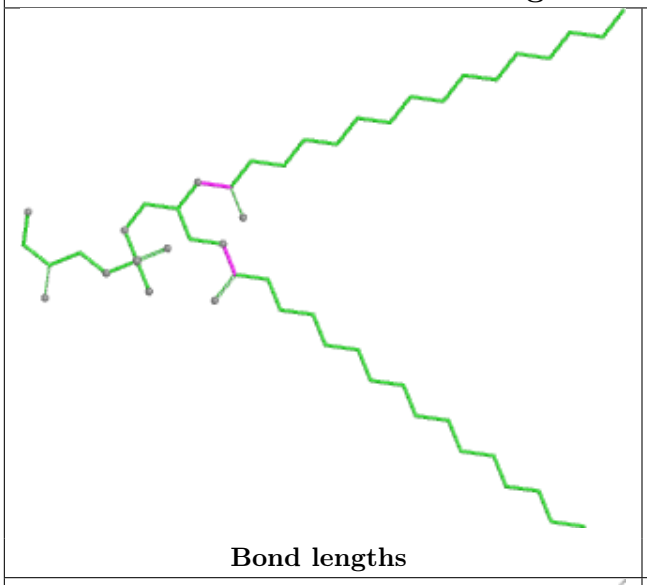


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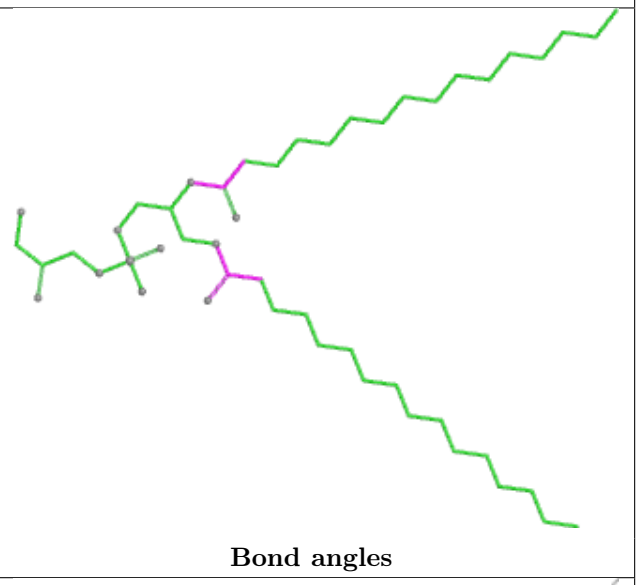


Rings

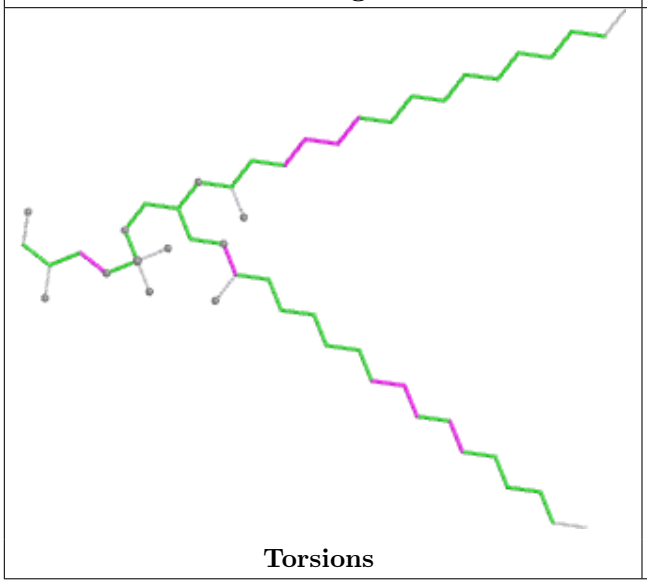
Ligand LHG d 409



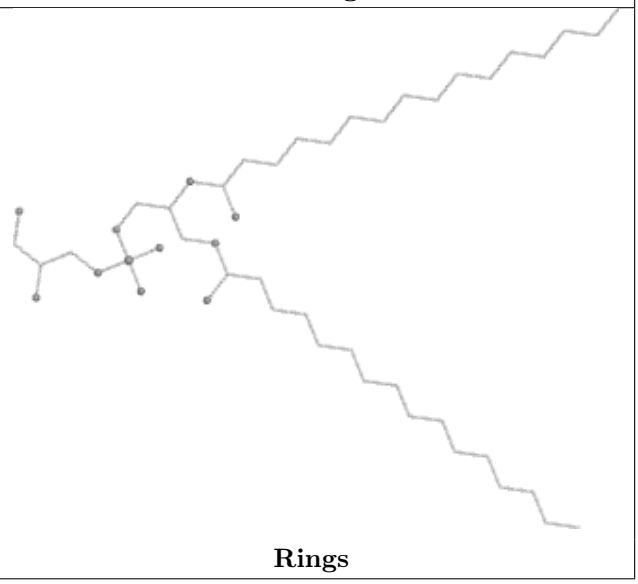
Bond lengths



Bond angles

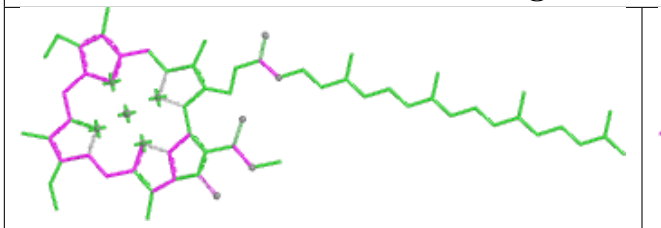


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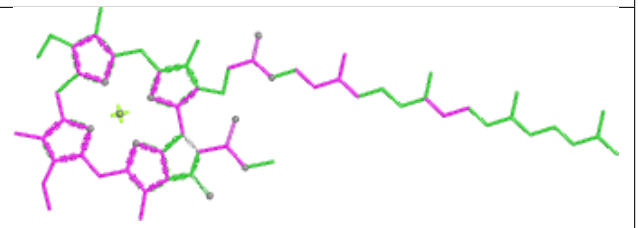


Rings

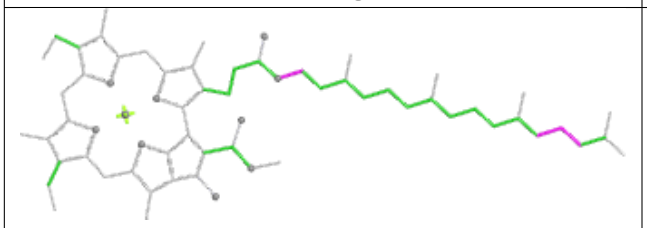
Ligand CLA b 608



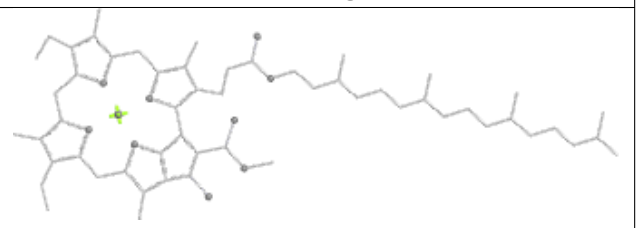
Bond lengths



Bond angles

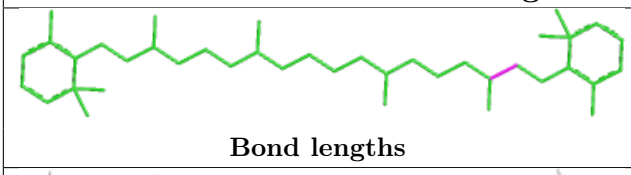


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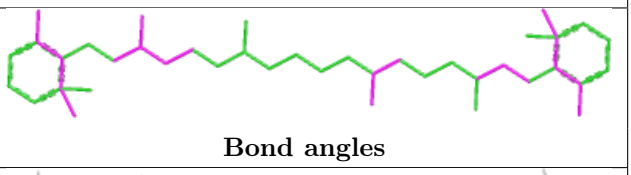


Rings

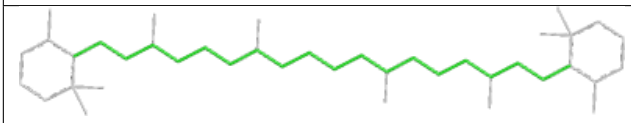
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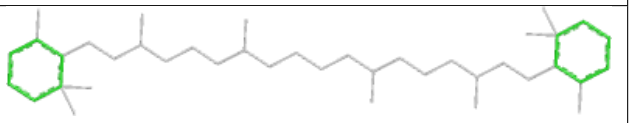
Bond lengths



Bond angles

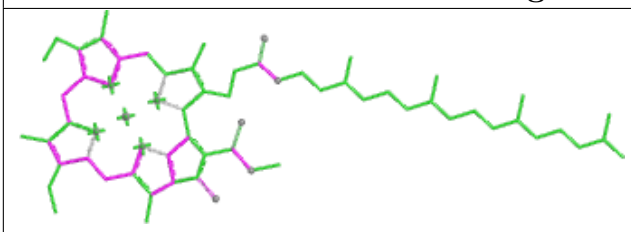


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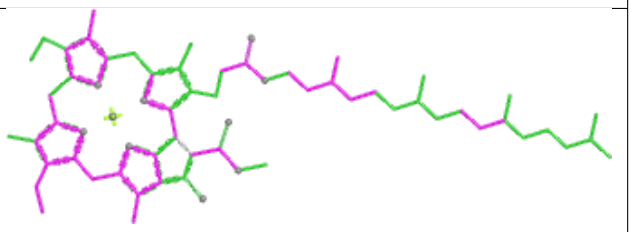


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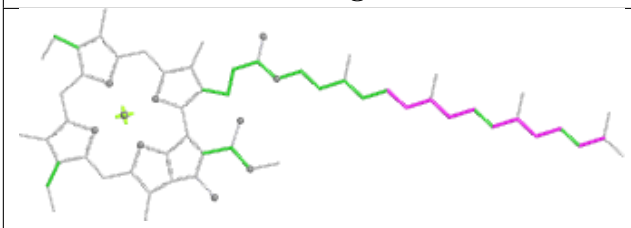
Ligand CLA b 615



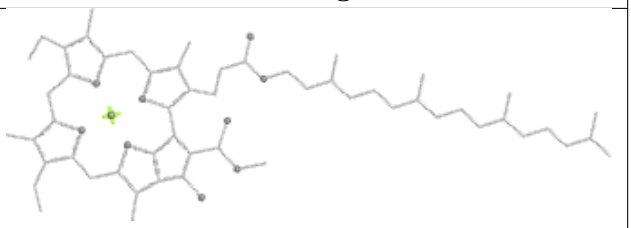
Bond lengths



Bond angles

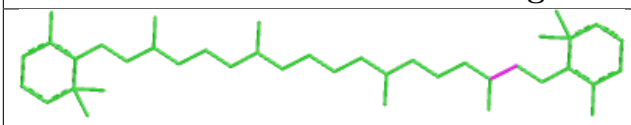


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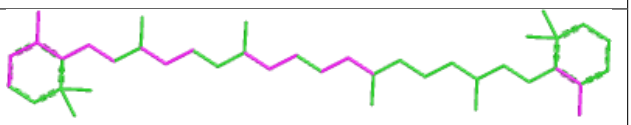


Rings

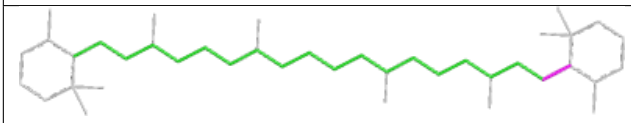
Ligand BCR c 515



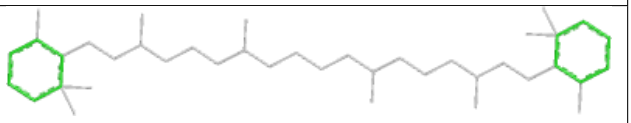
Bond lengths



Bond angles

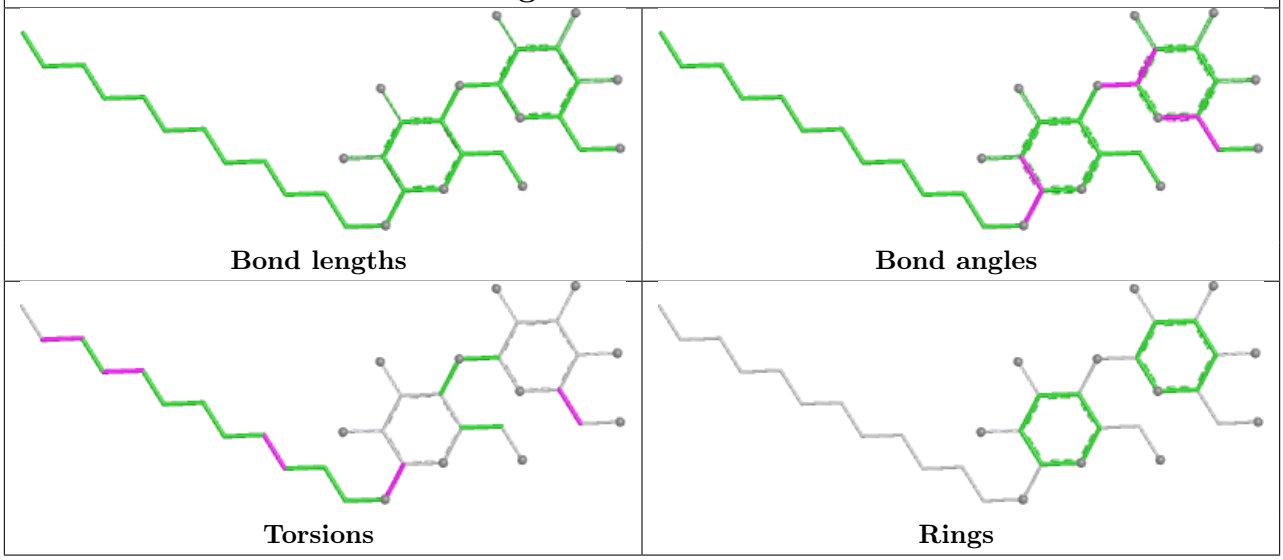


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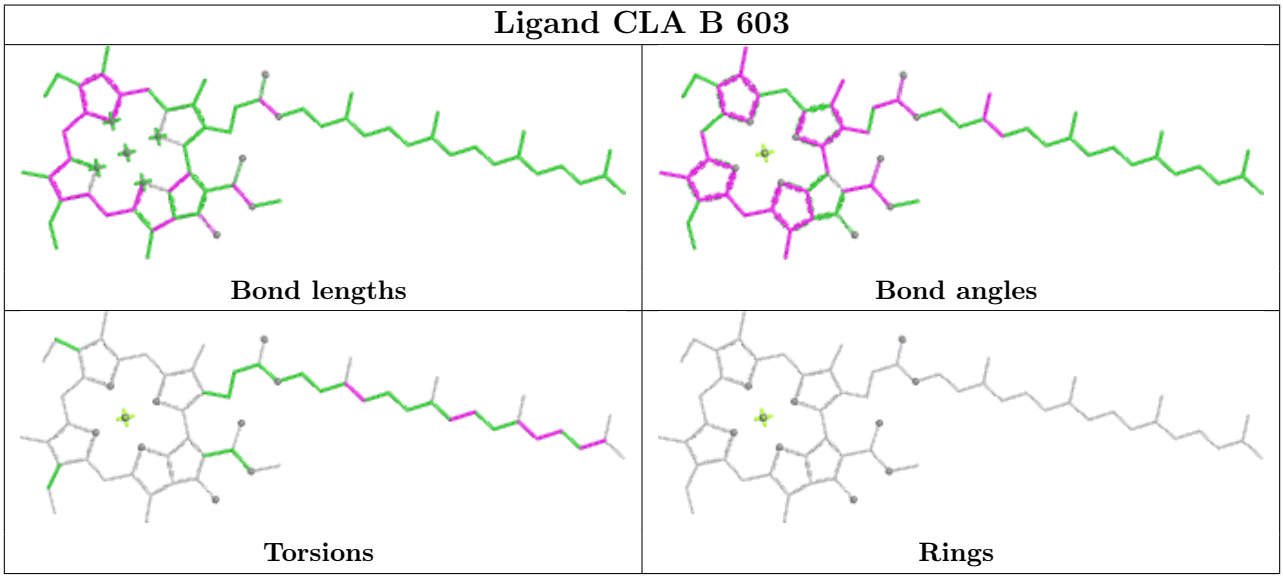


Rings

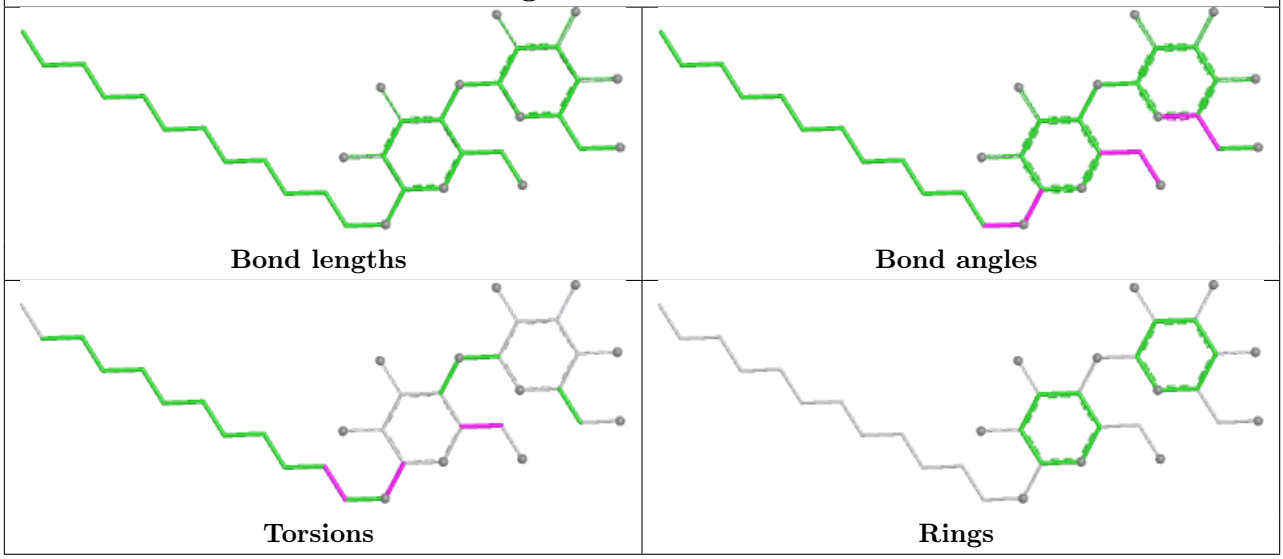
Ligand LMT M 102



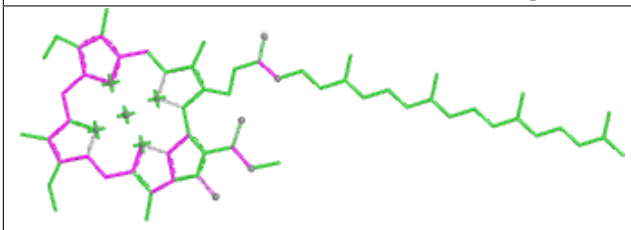
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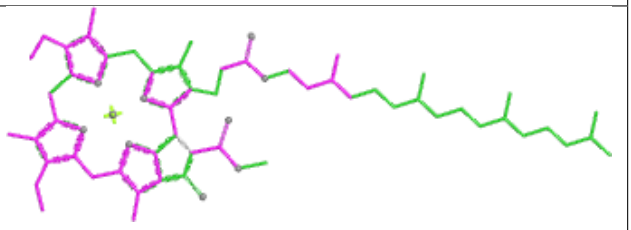
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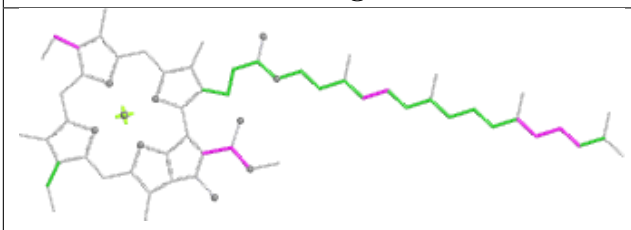
Ligand CLA C 503



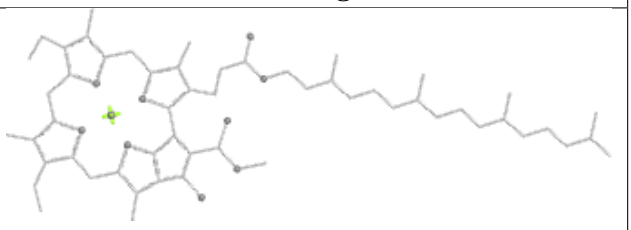
Bond lengths



Bond angles

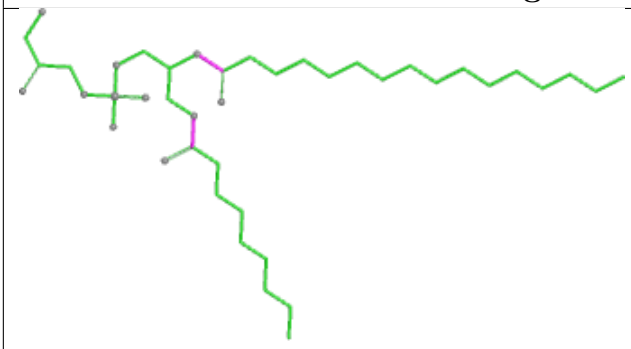


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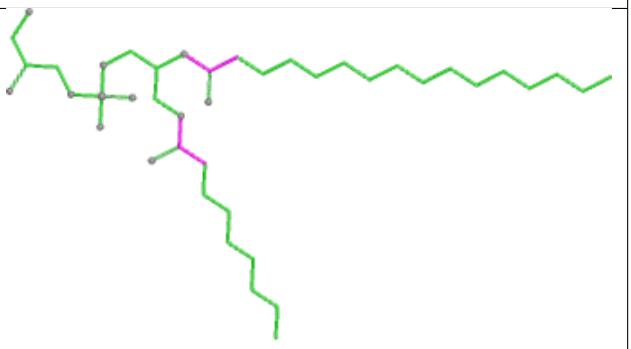


Rings

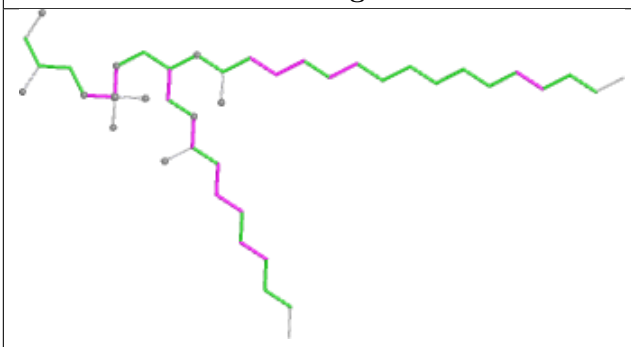
Ligand LHG E 101



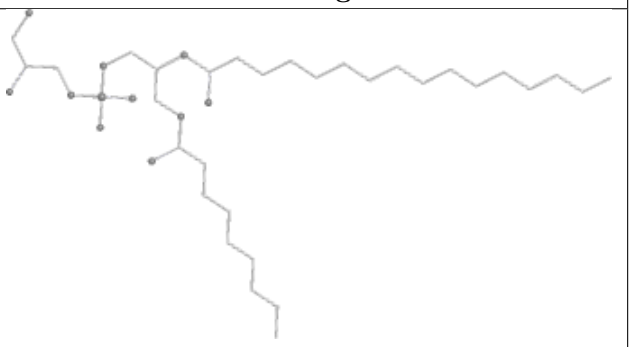
Bond lengths



Bond angles

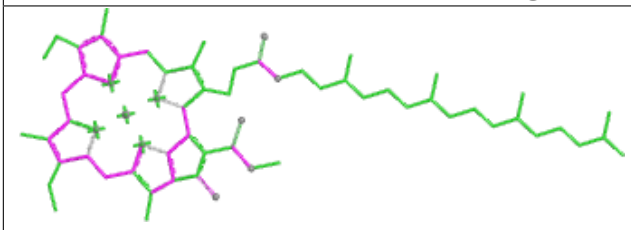


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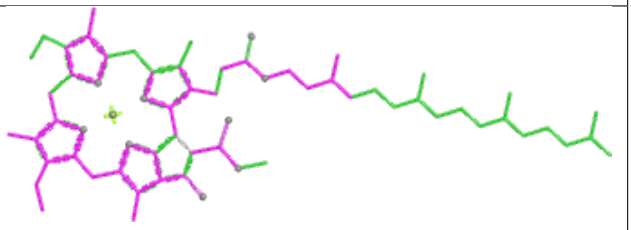


Rings

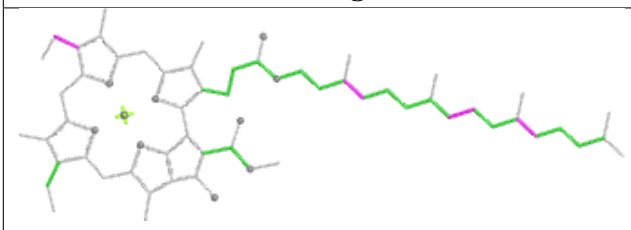
Ligand CLA C 505



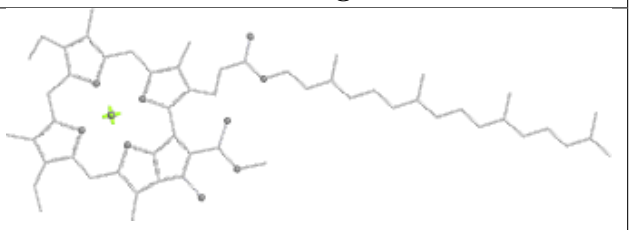
Bond lengths



Bond angles

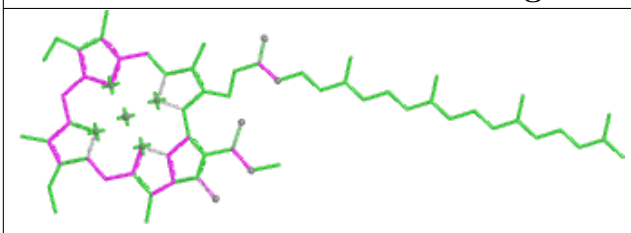


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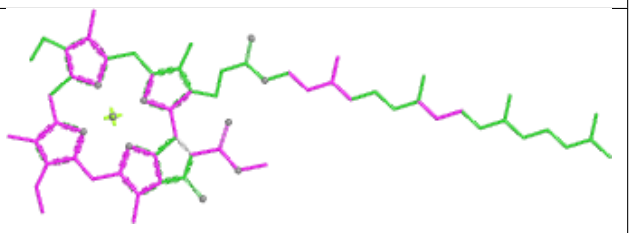


Rings

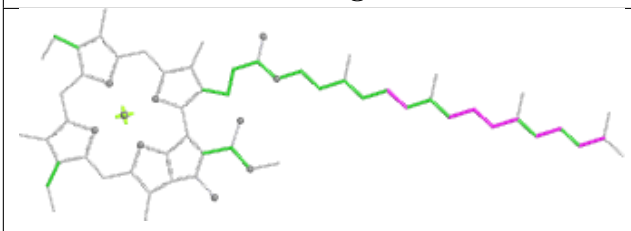
Ligand CLA B 615



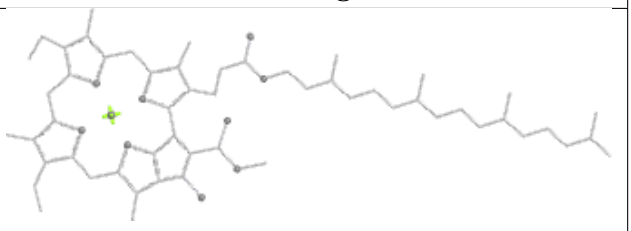
Bond lengths



Bond angles

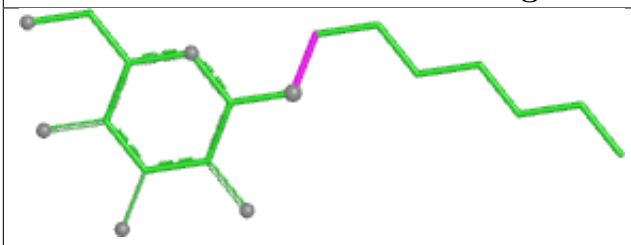


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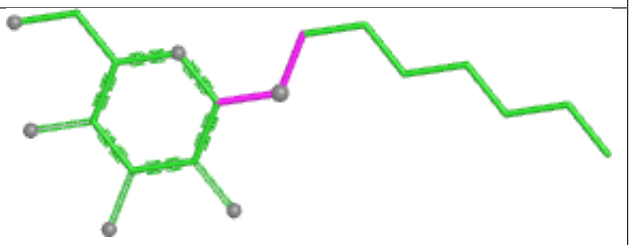


Rings

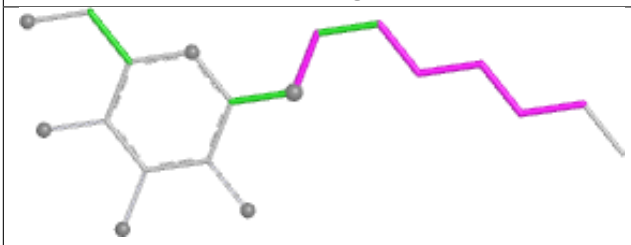
Ligand HTG B 622



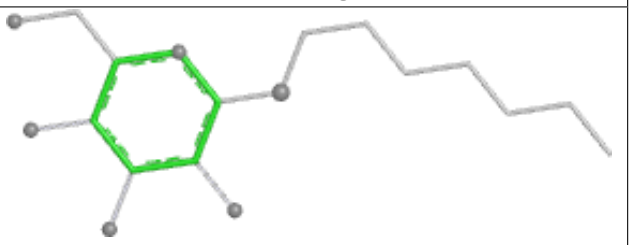
Bond lengths



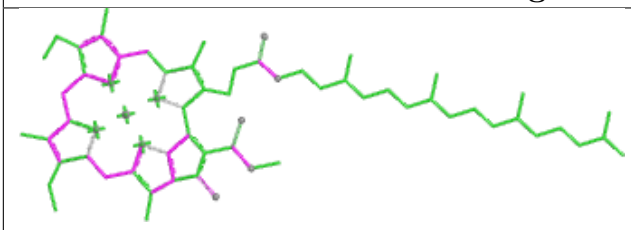
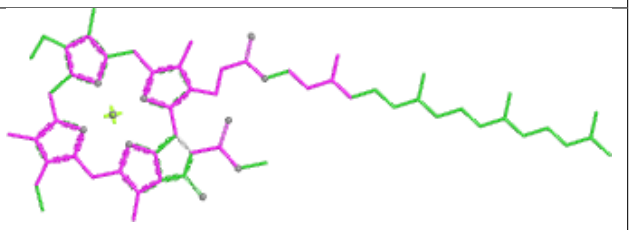
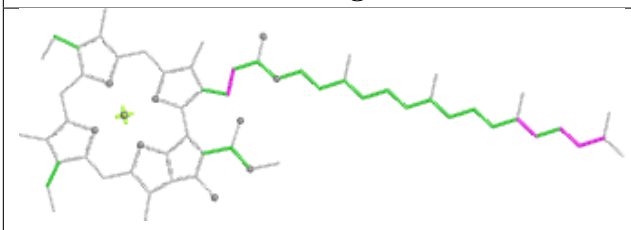
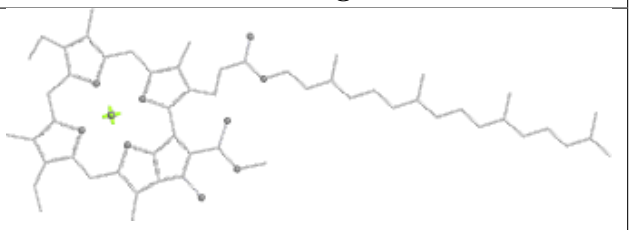
Bond angles

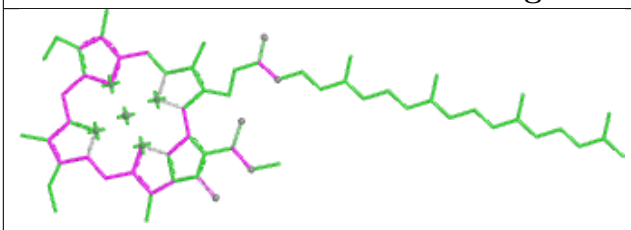
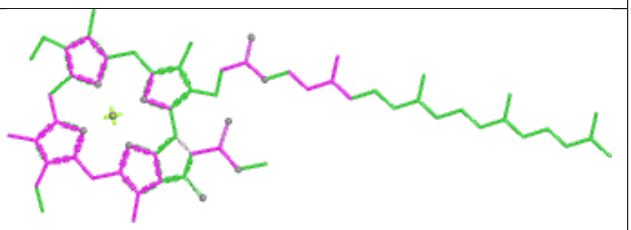
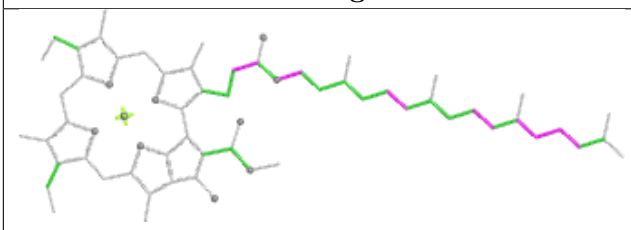
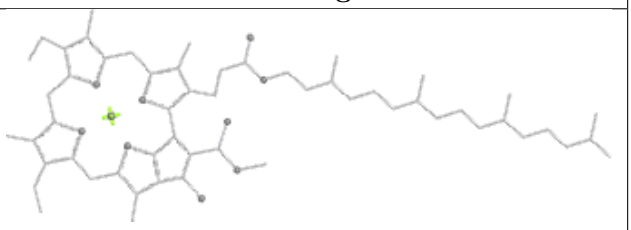


Torsions

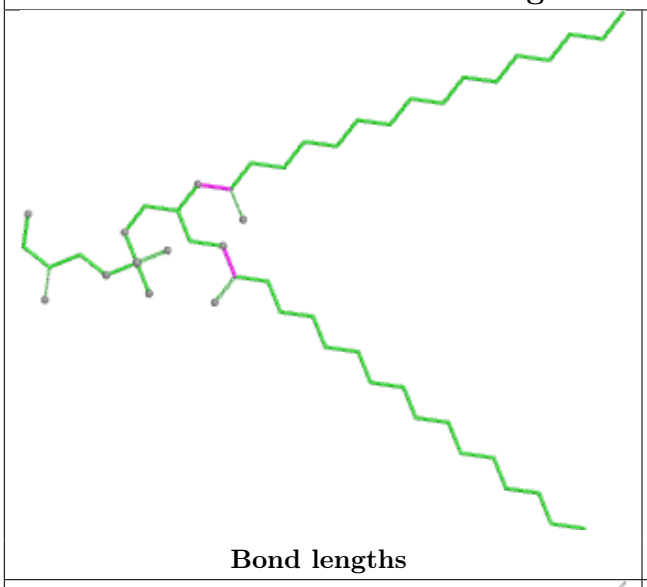


Rings

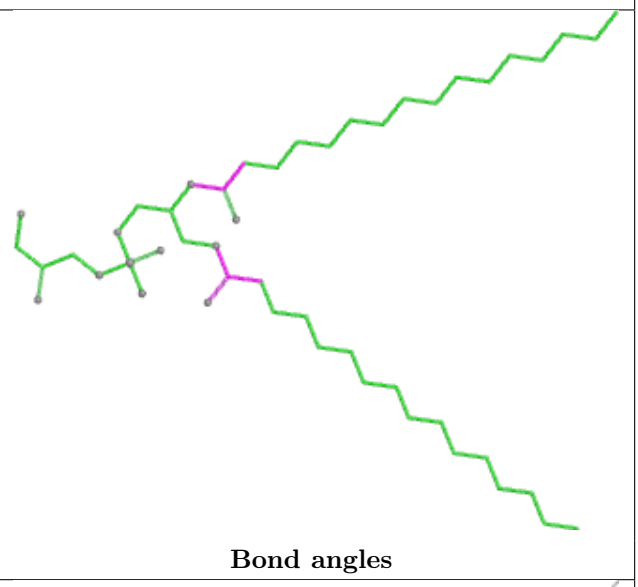
Ligand CLA a 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

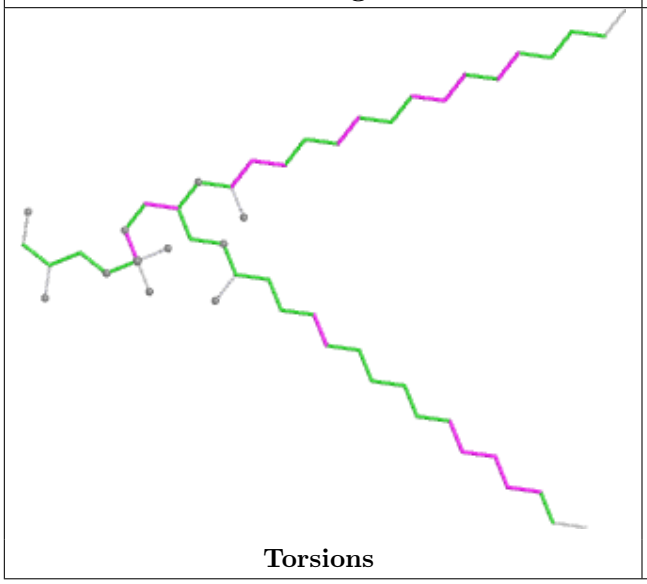
Ligand LHG b 628



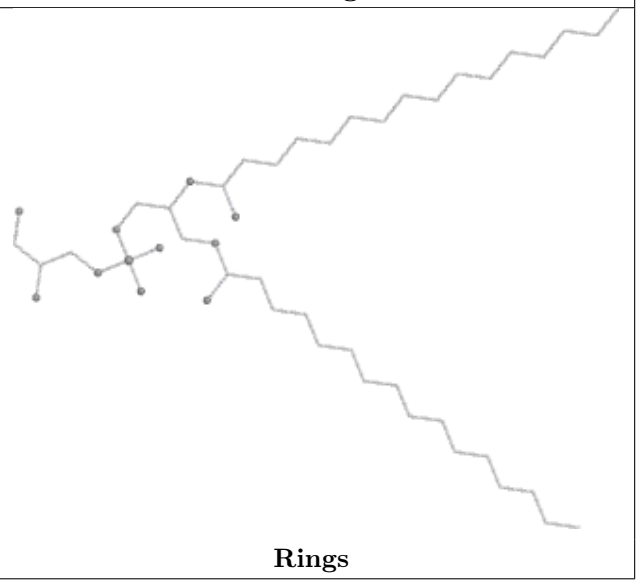
Bond lengths



Bond angles

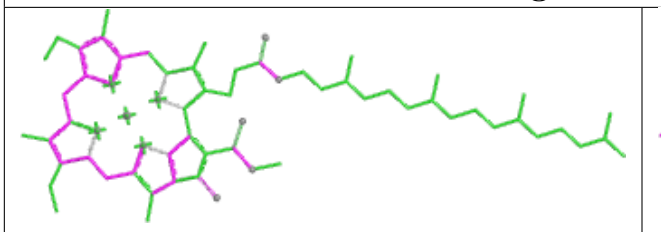


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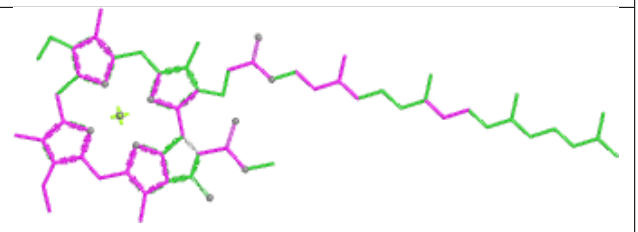


Rings

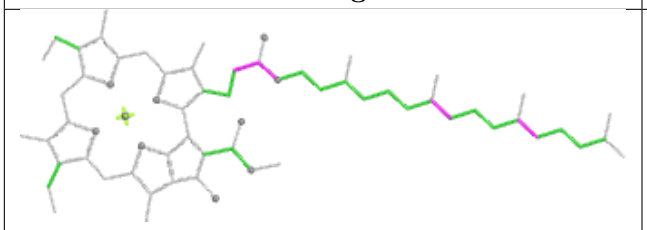
Ligand CLA c 511



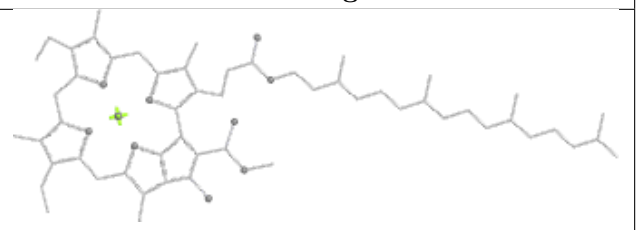
Bond lengths



Bond angles

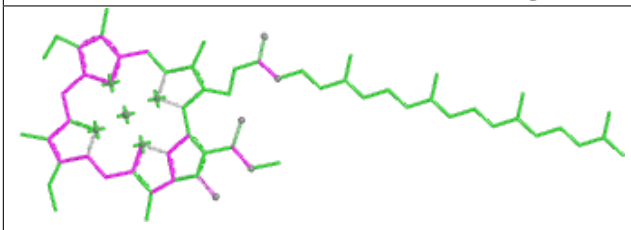


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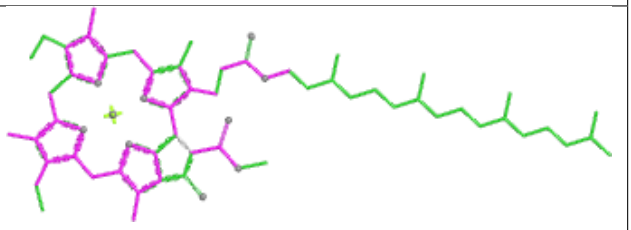


Rings

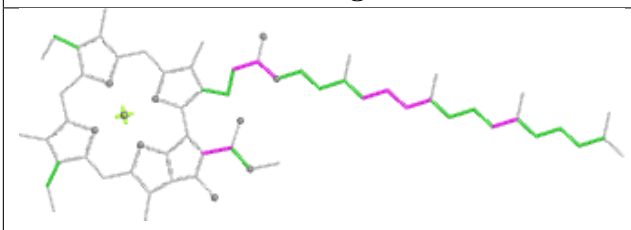
Ligand CLA B 601



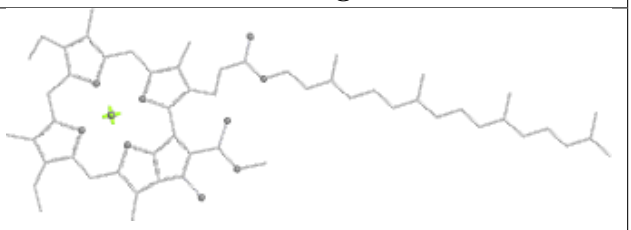
Bond lengths



Bond angles



Torsions

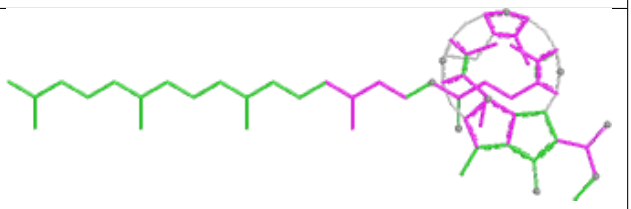


Rings

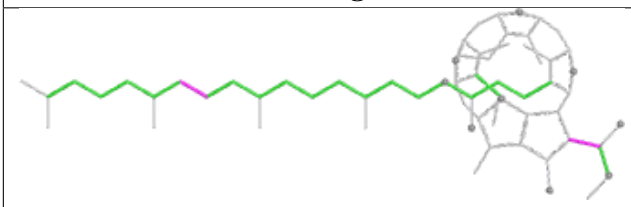
Ligand PHO A 407



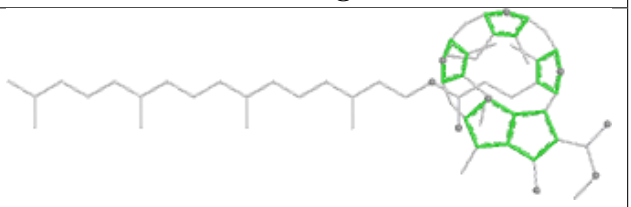
Bond lengths



Bond angles

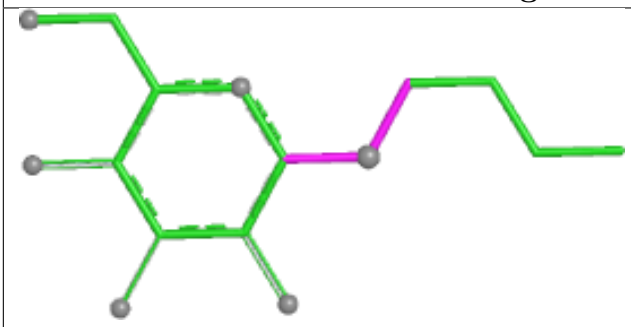


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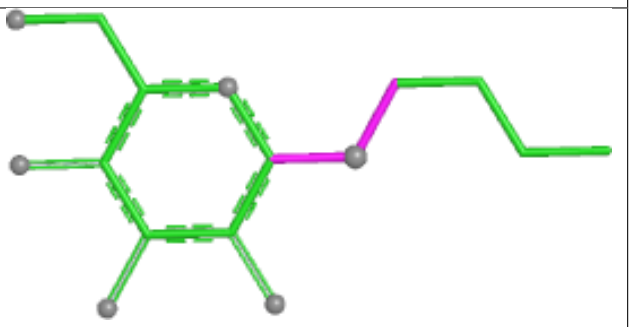


Rings

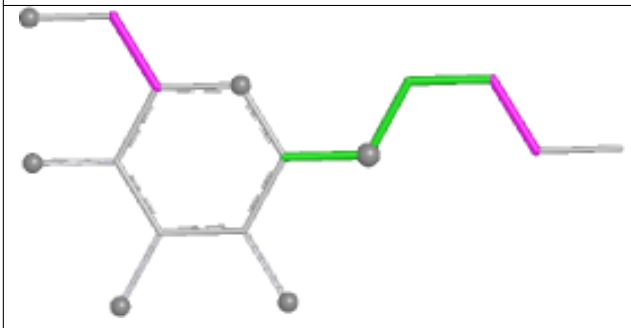
Ligand HTG D 413



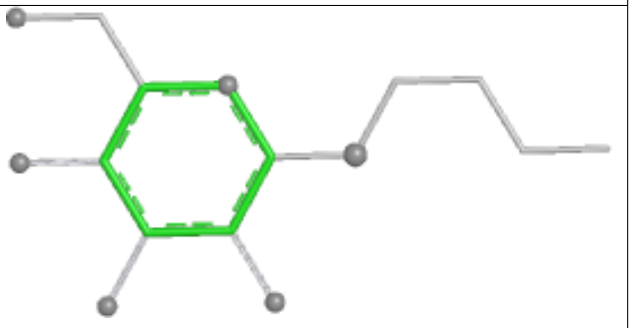
Bond lengths



Bond angles

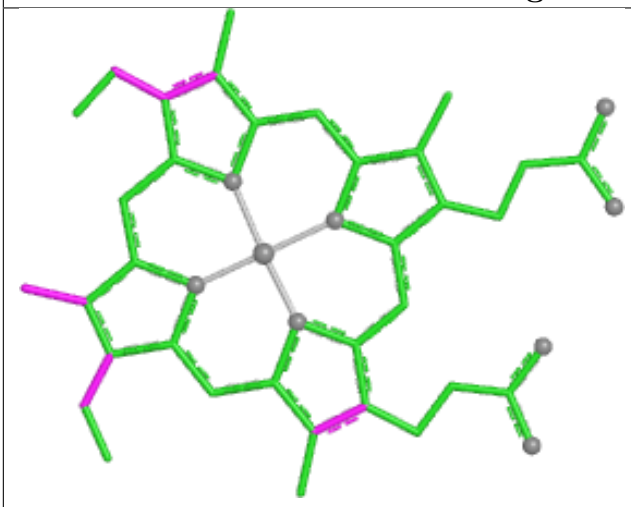


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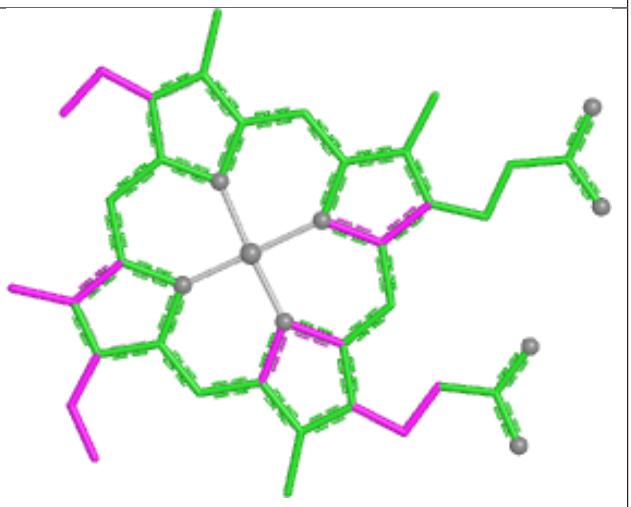


Rings

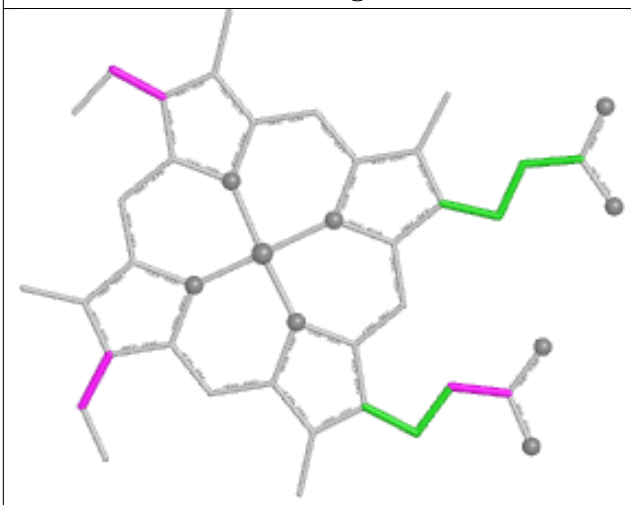
Ligand HEC v 203



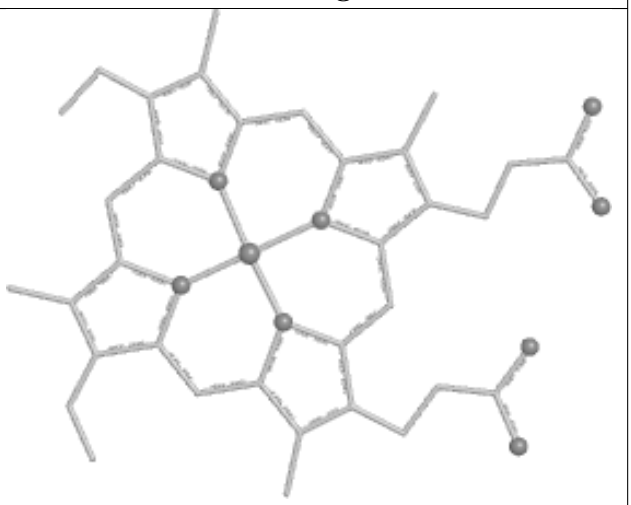
Bond lengths



Bond angles

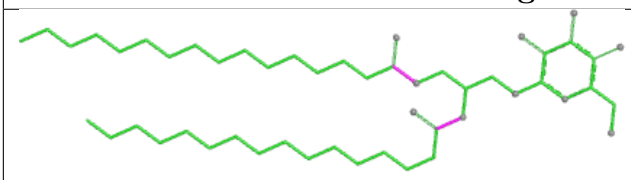


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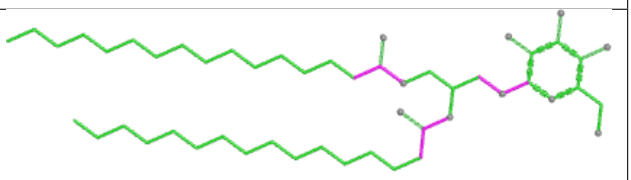


Rings

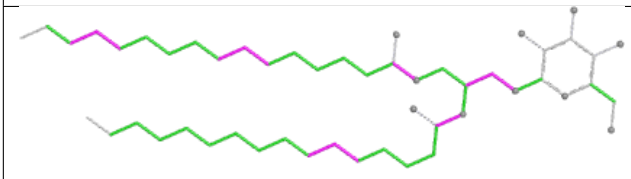
Ligand LMG m 101



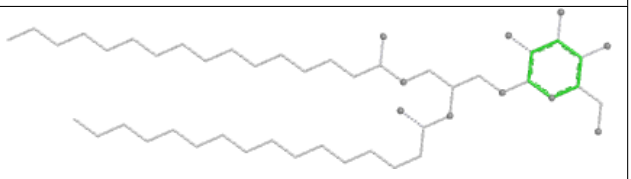
Bond lengths



Bond angles

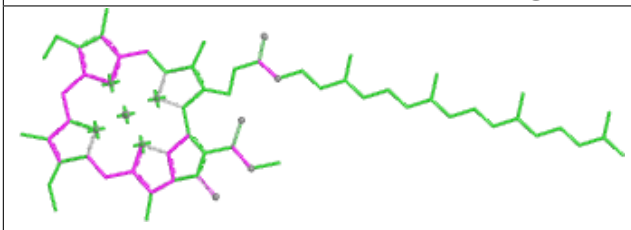


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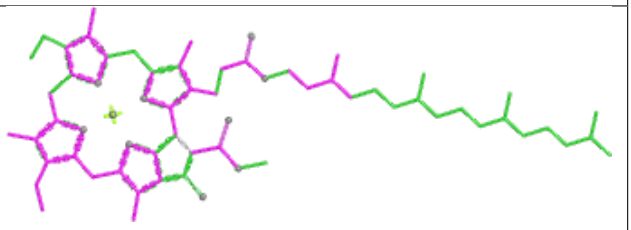


Rings

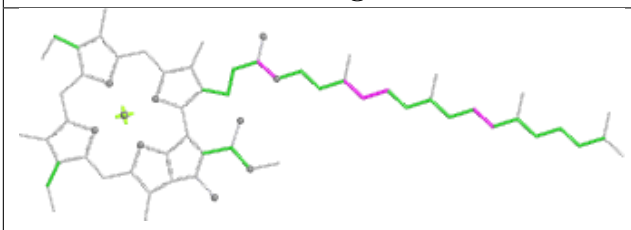
Ligand CLA d 404



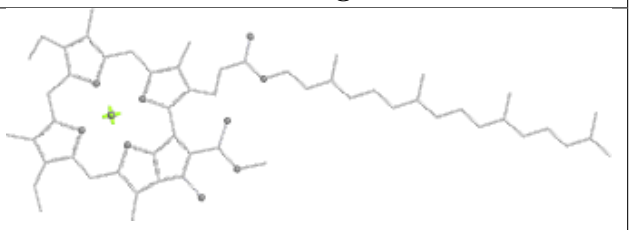
Bond lengths



Bond angles

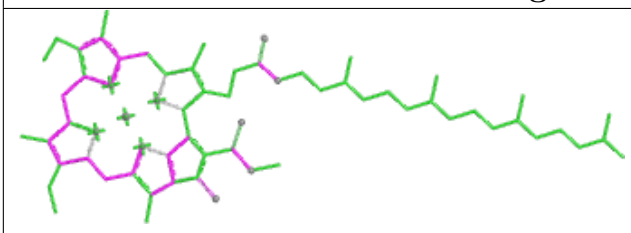


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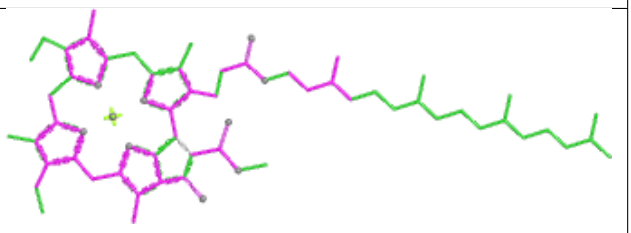


Rings

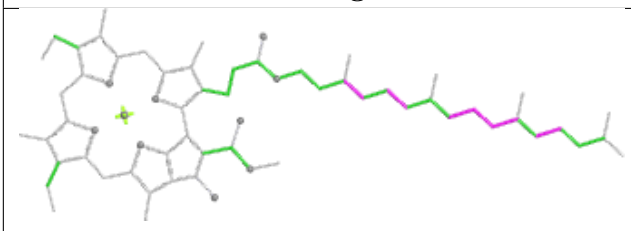
Ligand CLA c 509



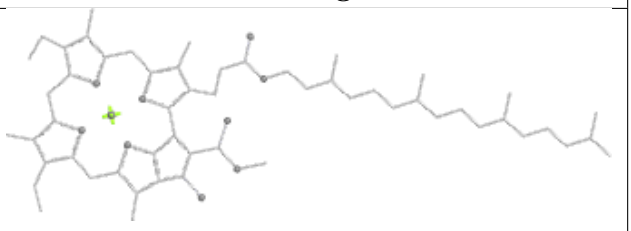
Bond lengths



Bond angles

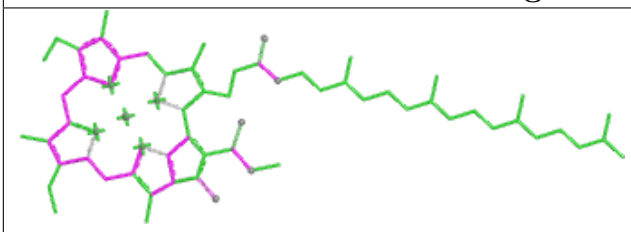


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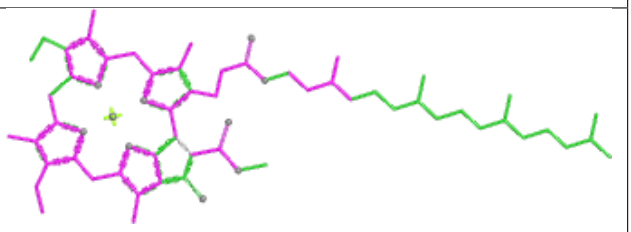


Rings

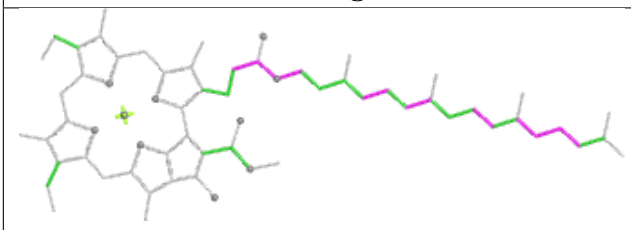
Ligand CLA C 513



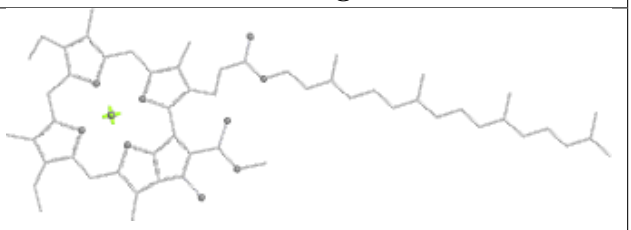
Bond lengths



Bond angles

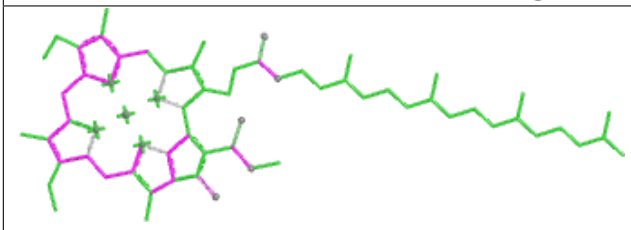


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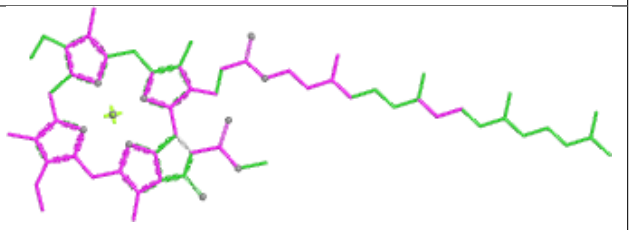


Rings

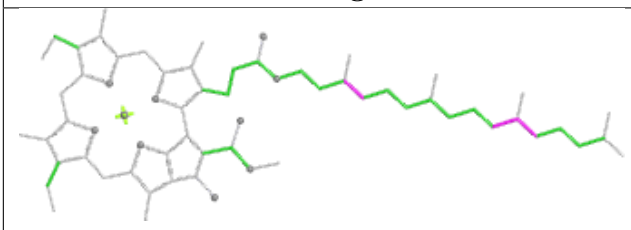
Ligand CLA c 505



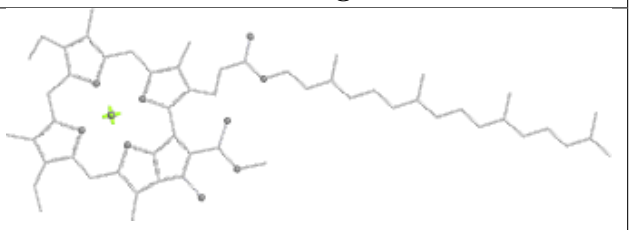
Bond lengths



Bond angles

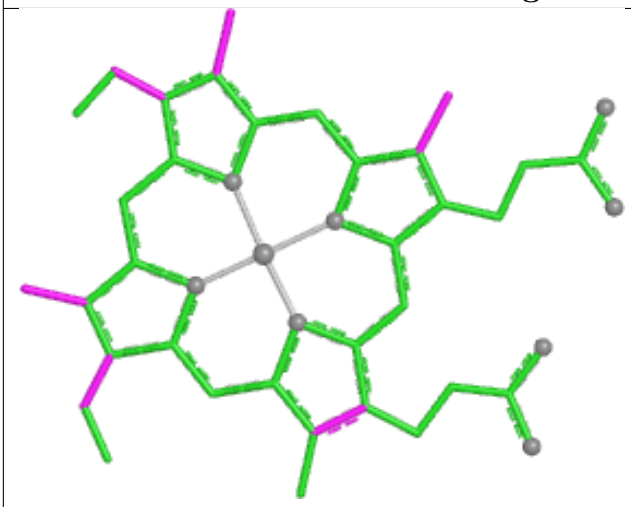


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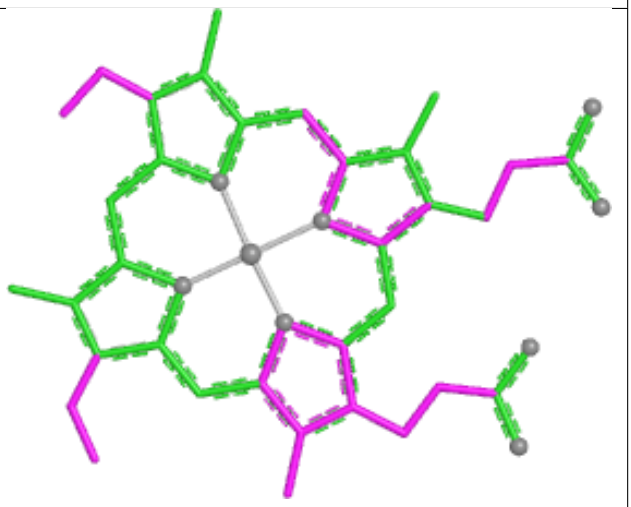


Rings

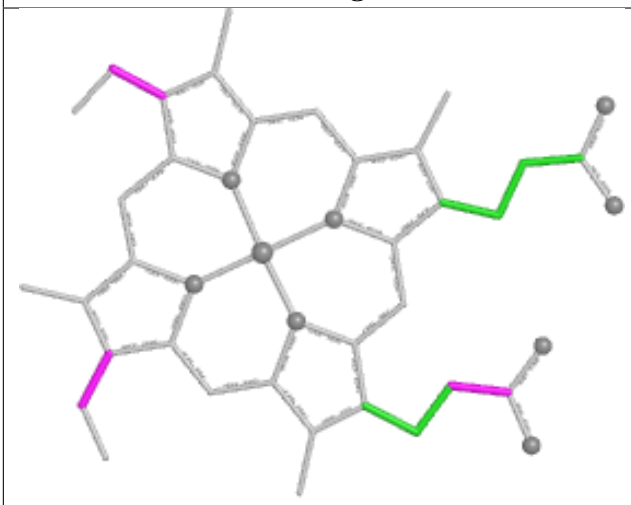
Ligand HEC V 201



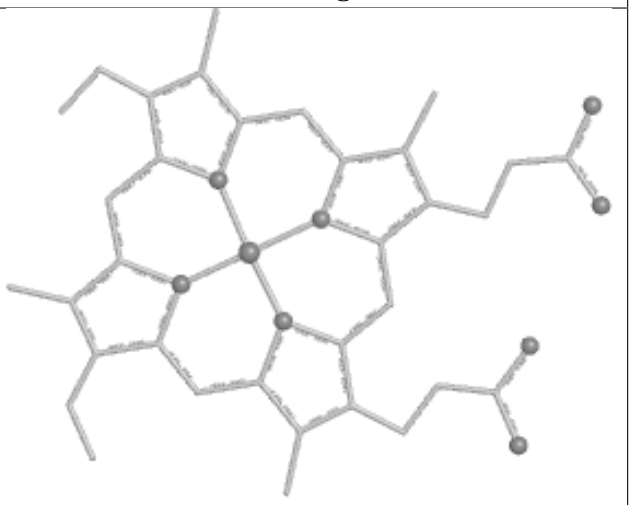
Bond lengths



Bond angles

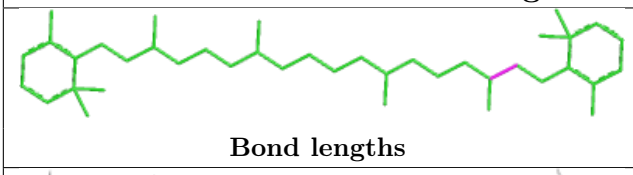


Torsions

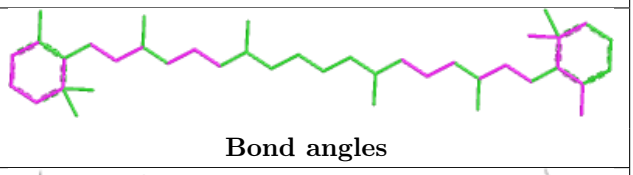


Rings

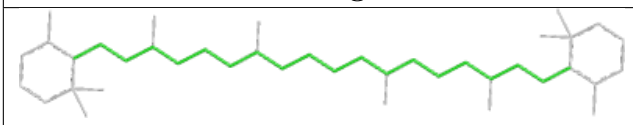
Ligand BCR B 619



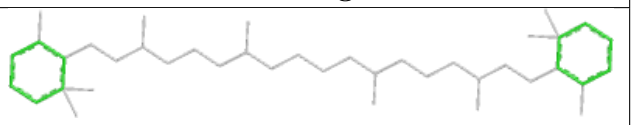
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Bond angles

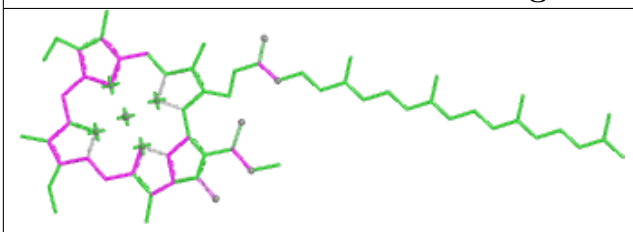


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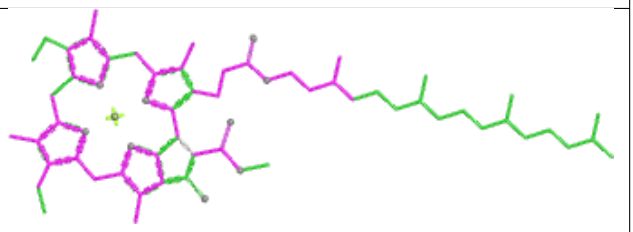


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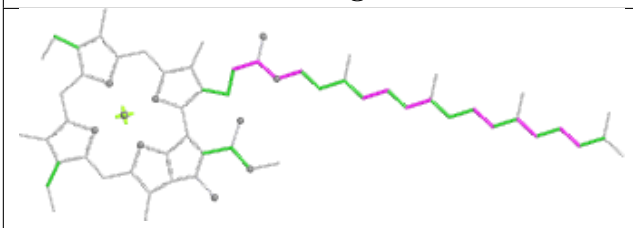
Ligand CLA c 513



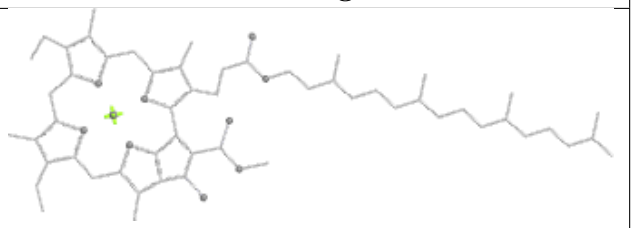
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Bond angles

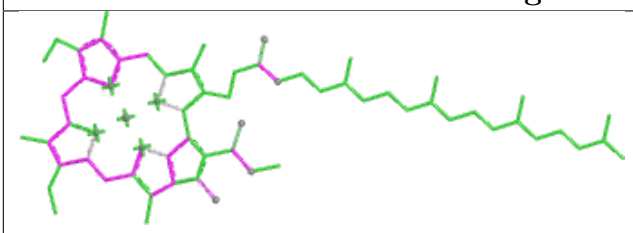


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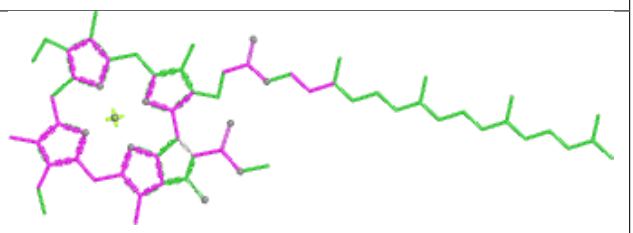


Rings

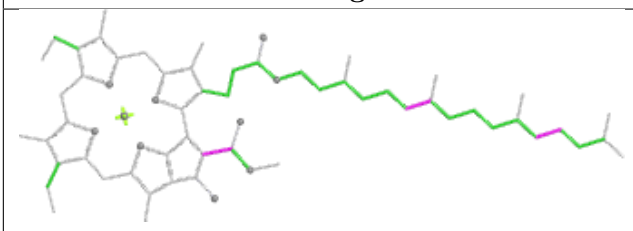
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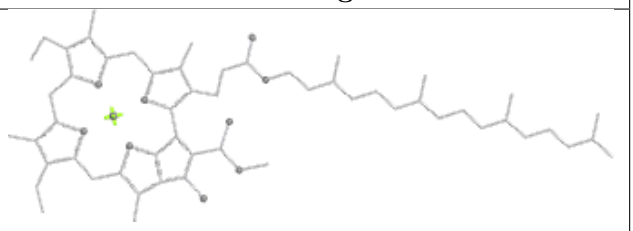
Bond lengths



Bond angles

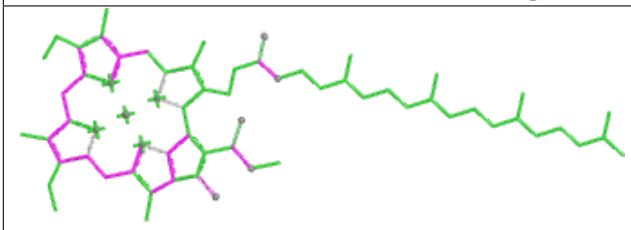


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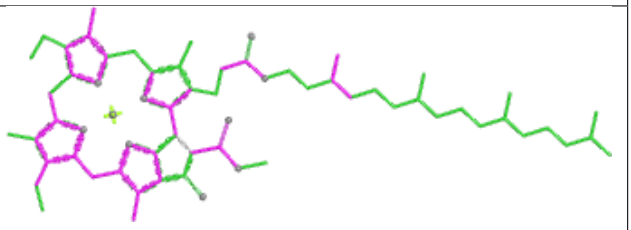


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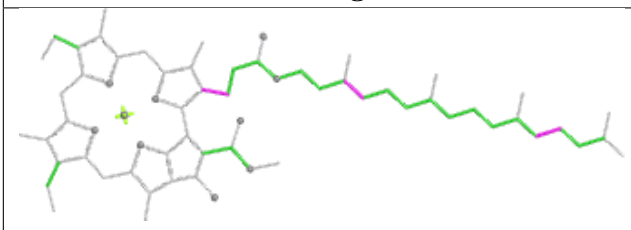
Ligand CLA B 609



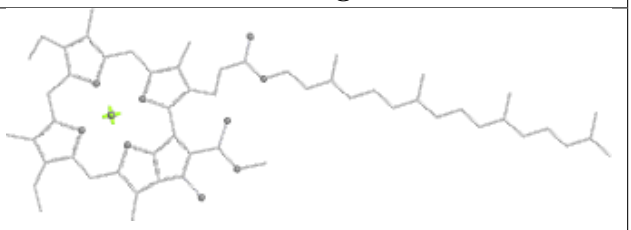
Bond lengths



Bond angles



Torsions

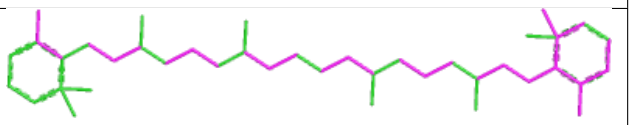


Rings

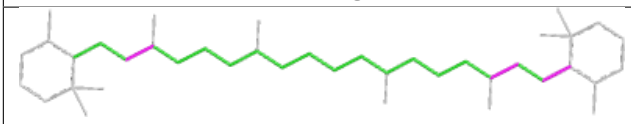
Ligand BCR d 405



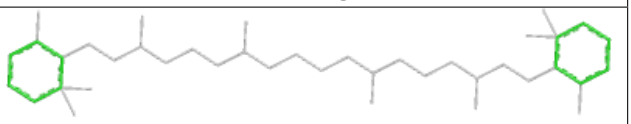
Bond lengths



Bond angles

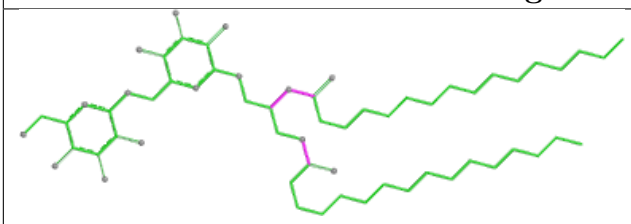


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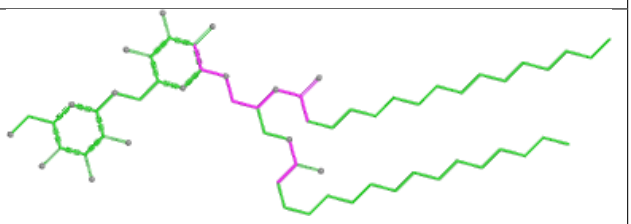


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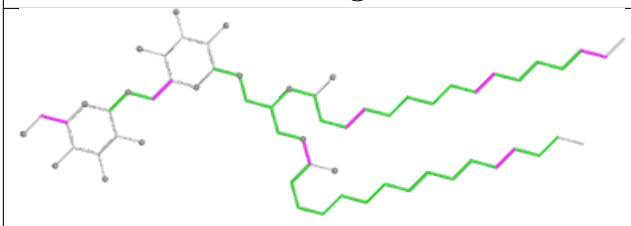
Ligand DGD c 519



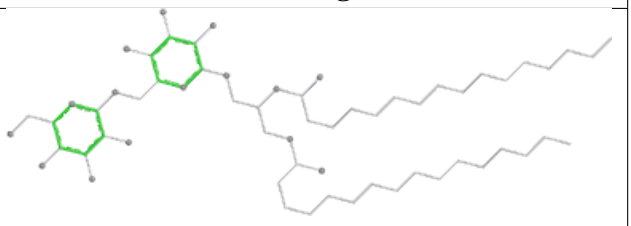
Bond lengths



Bond angles

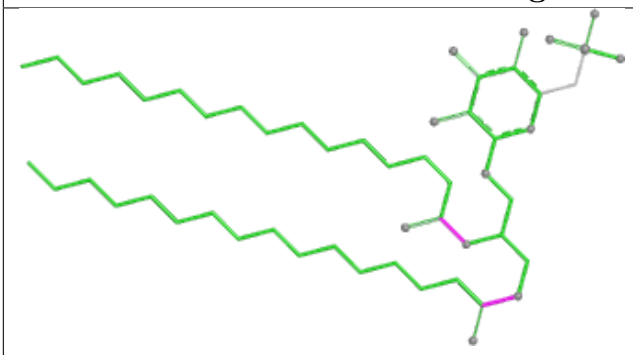


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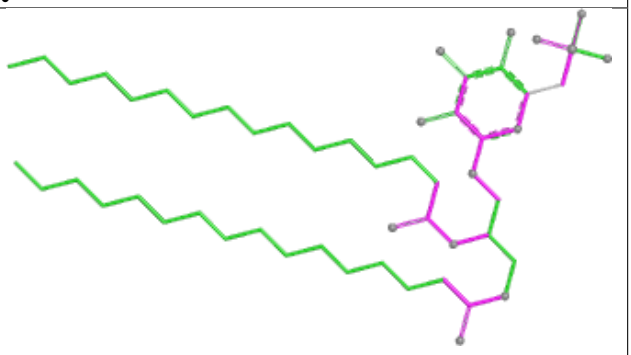


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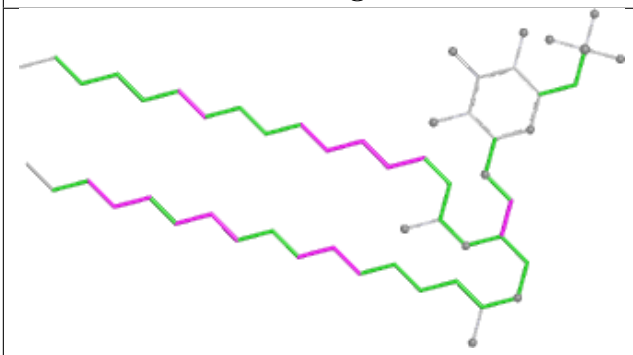
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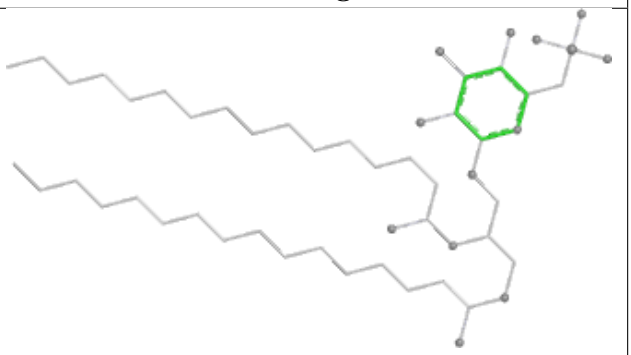
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Bond angles

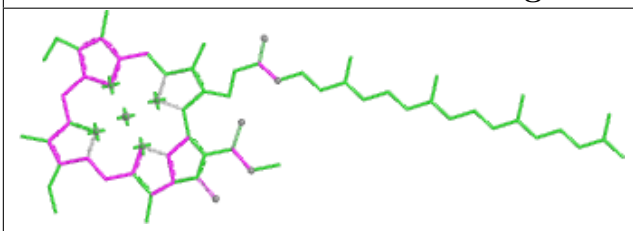


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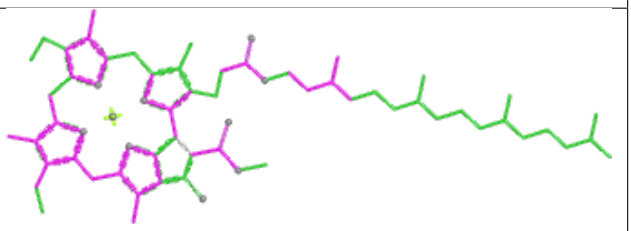


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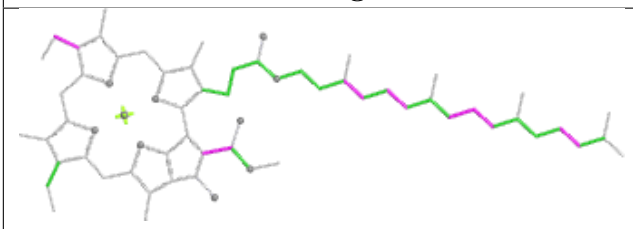
Ligand CLA C 506



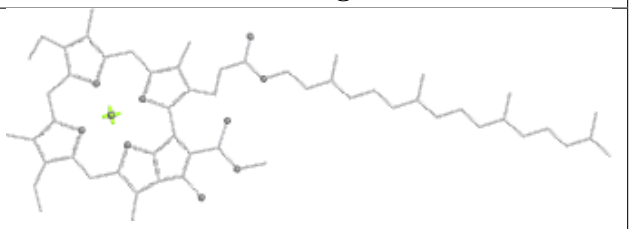
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Bond angles

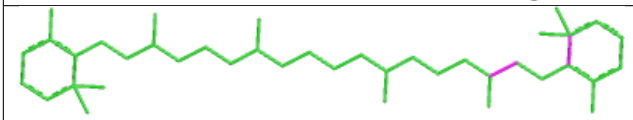


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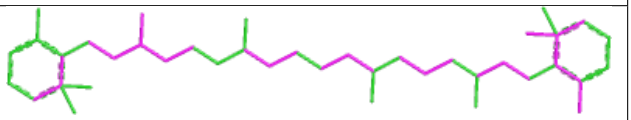


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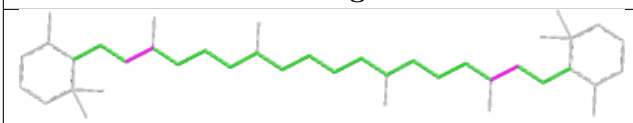
Ligand BCR b 619



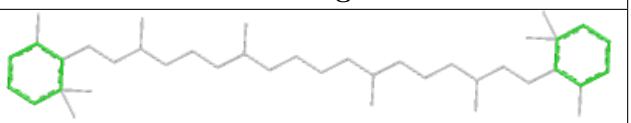
Bond lengths



Bond angles

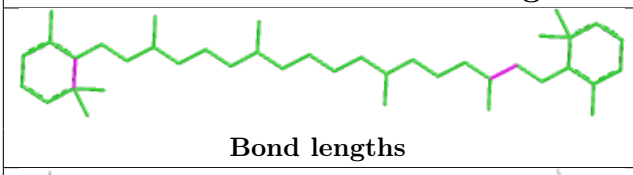


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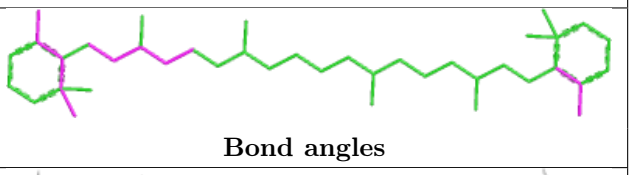


Rings

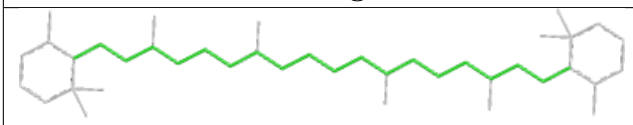
Ligand BCR B 617



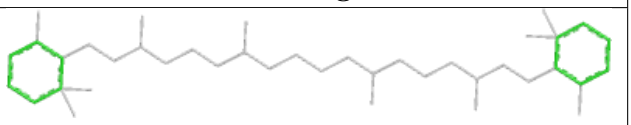
Bond lengths



Bond angles

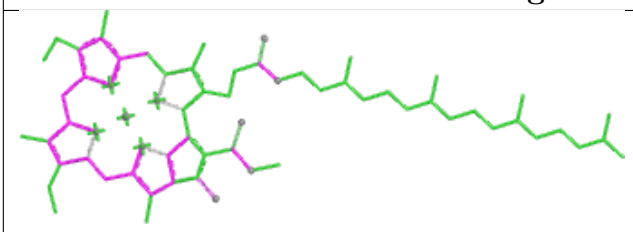


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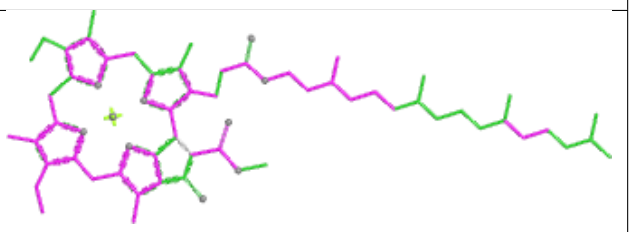


Rings

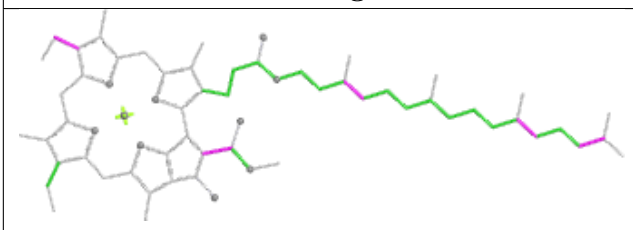
Ligand CLA b 609



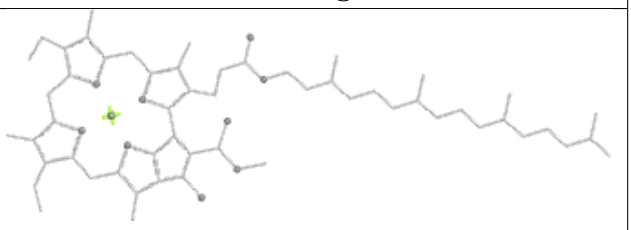
Bond lengths



Bond angles

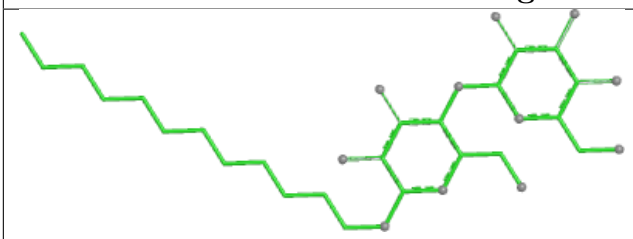


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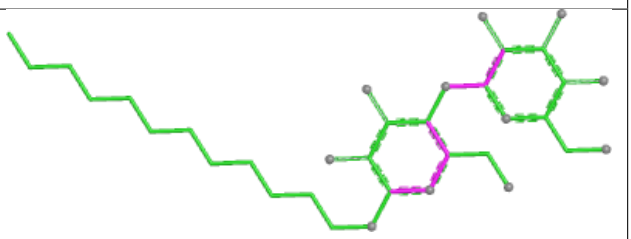


Rings

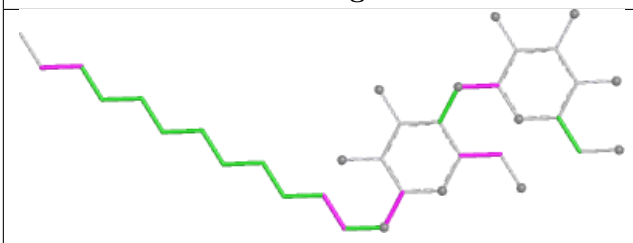
Ligand LMT M 104



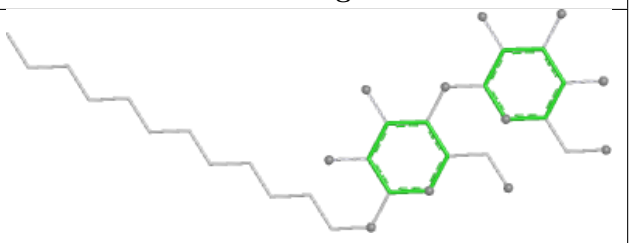
Bond lengths



Bond angles

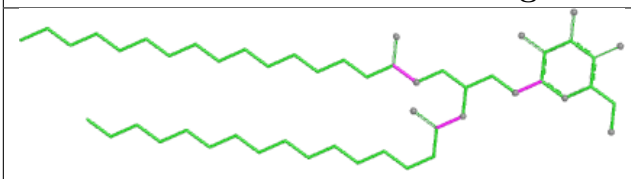


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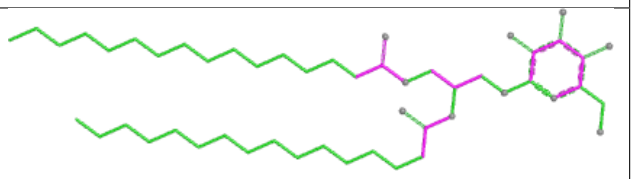


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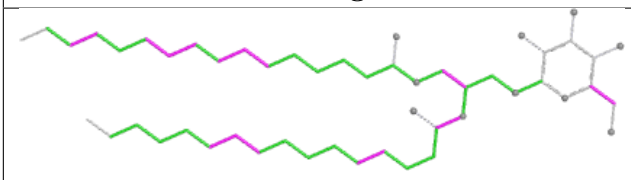
Ligand LMG C 521



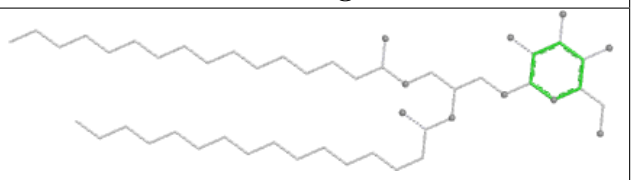
Bond lengths



Bond angles

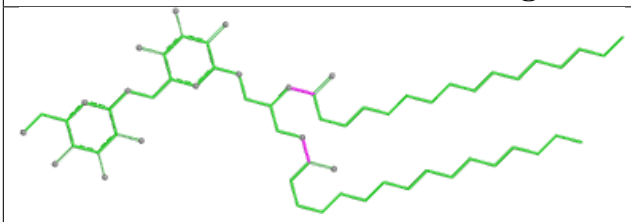


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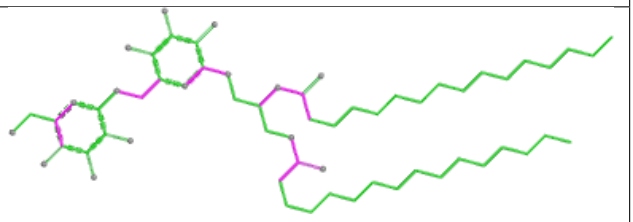


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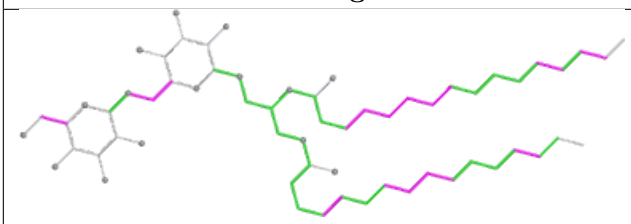
Ligand DGD C 517



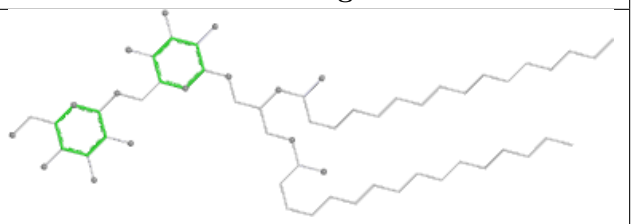
Bond lengths



Bond angles

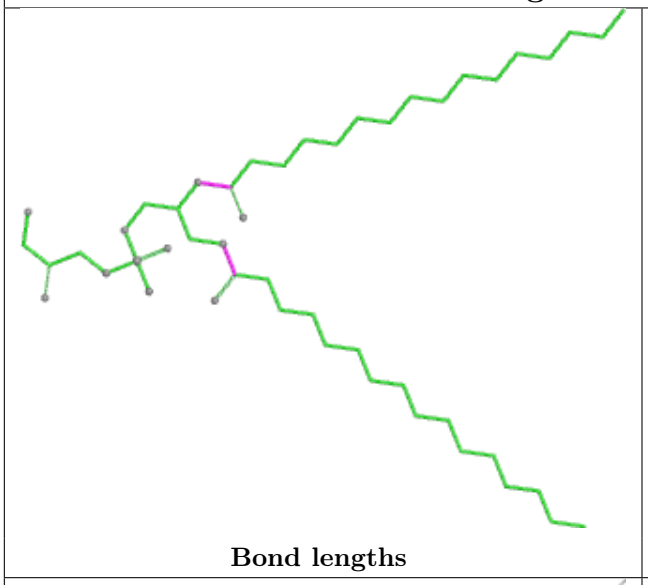


Torsions

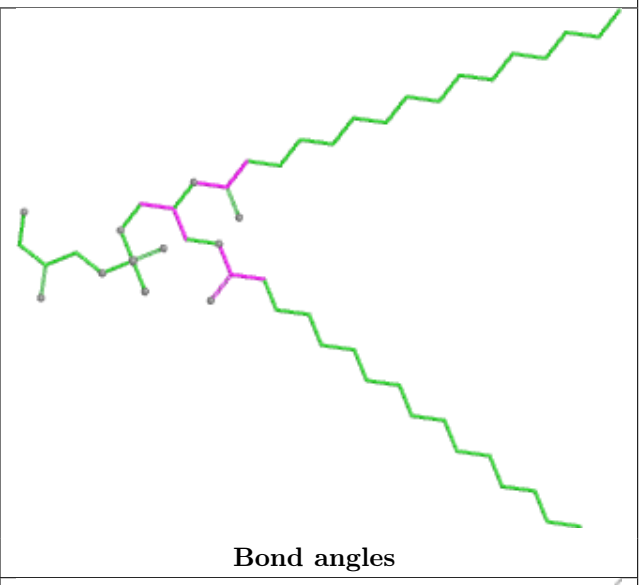


Rings

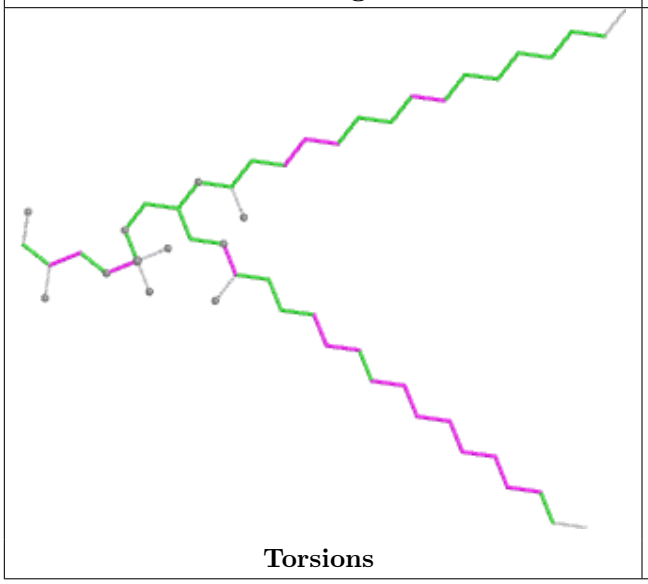
Ligand LHG d 408



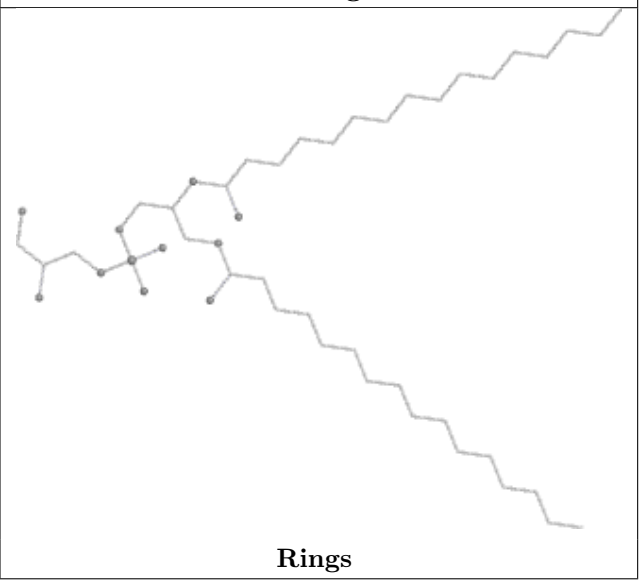
Bond lengths



Bond angles

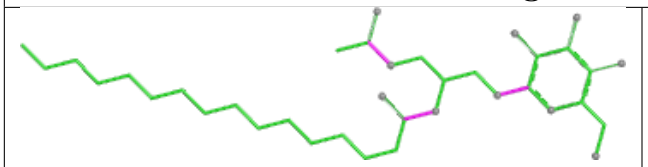


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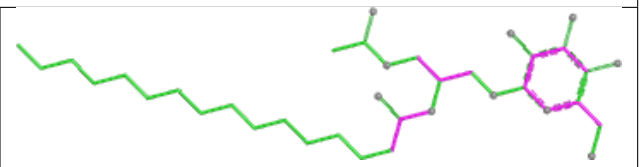


Rings

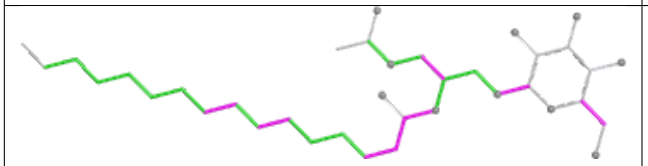
Ligand LMG Z 101



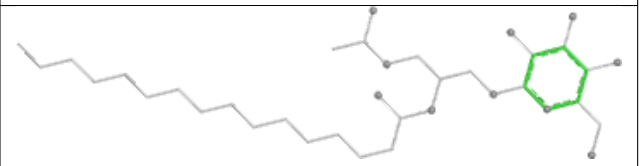
Bond lengths



Bond angles

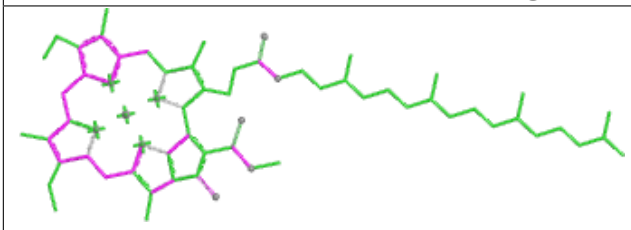


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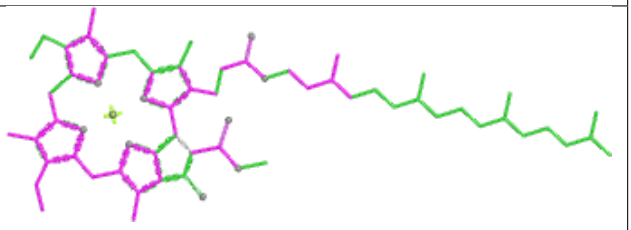


Rings

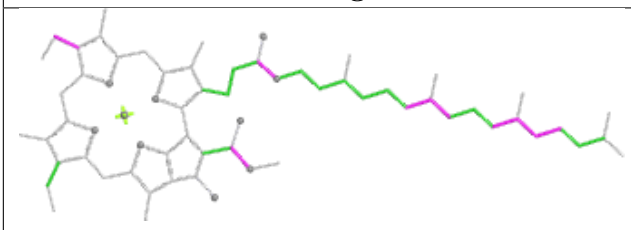
Ligand CLA C 514



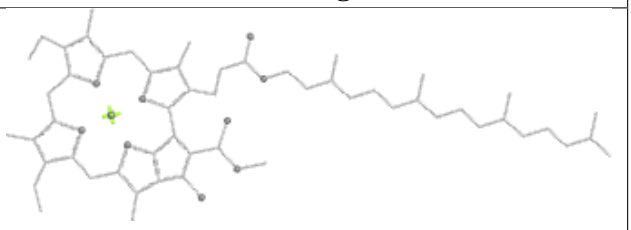
Bond lengths



Bond angles

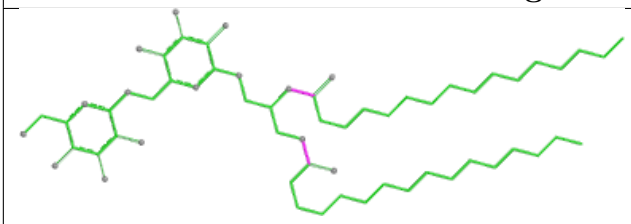


Torsions

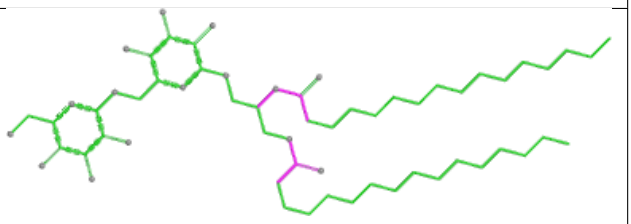


Rings

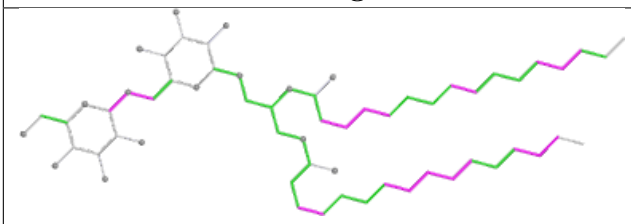
Ligand DGD c 518



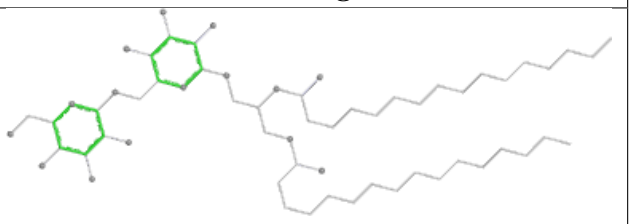
Bond lengths



Bond angles

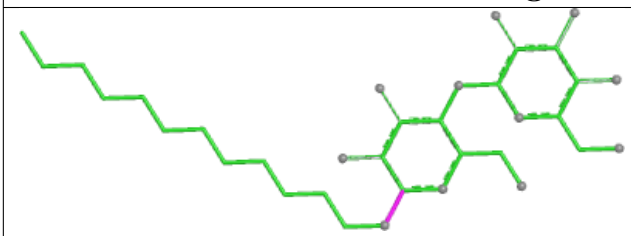


Torsions

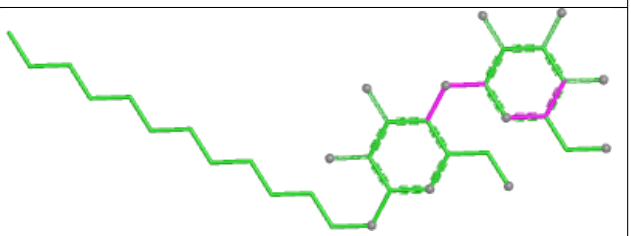


Rings

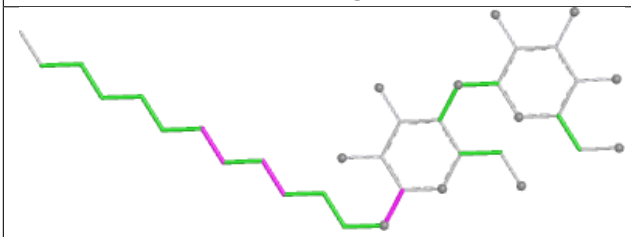
Ligand LMT a 418



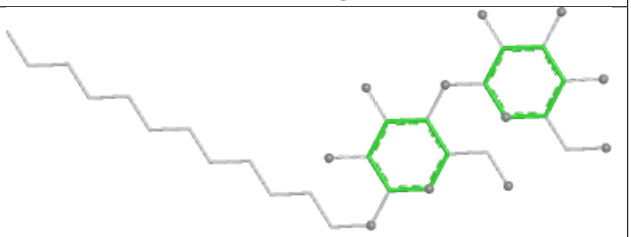
Bond lengths



Bond angles

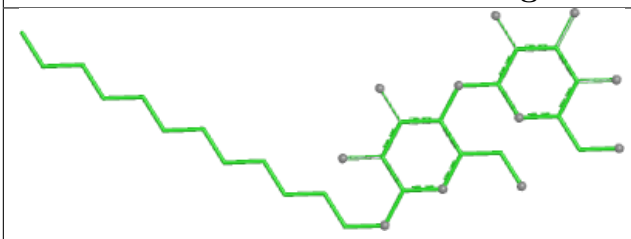


Torsions

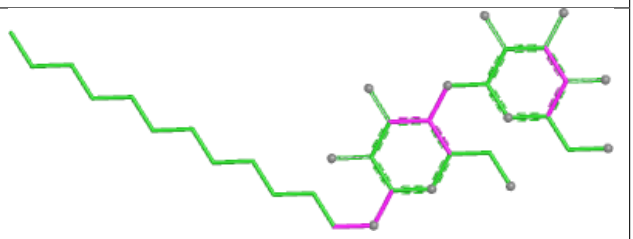


Rings

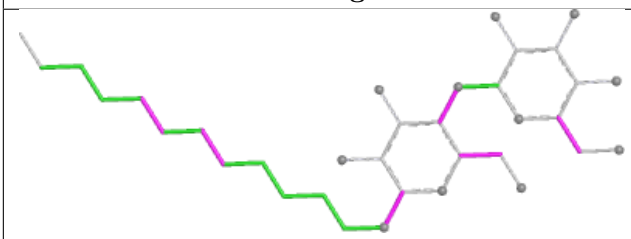
Ligand LMT D 404



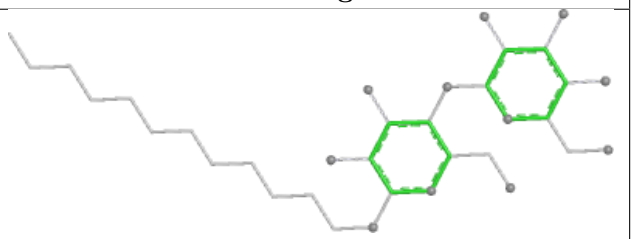
Bond lengths



Bond angles

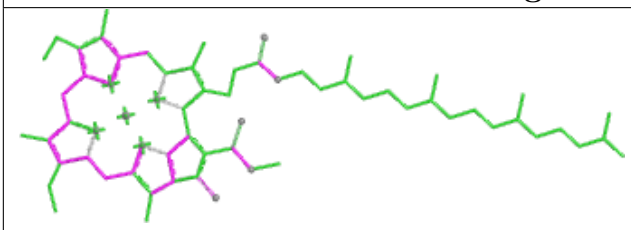


Torsions

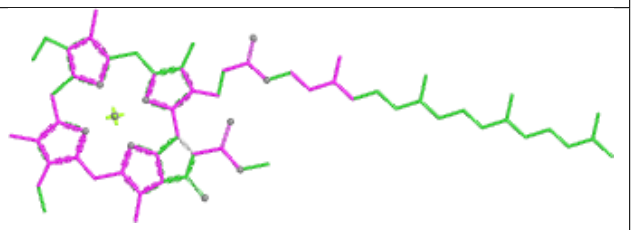


Rings

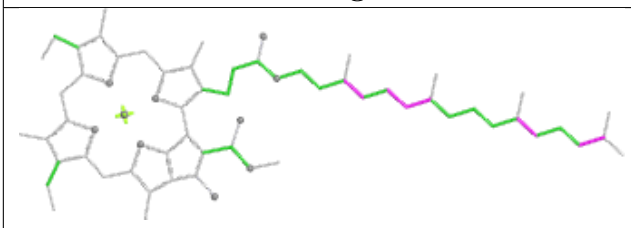
Ligand CLA B 605



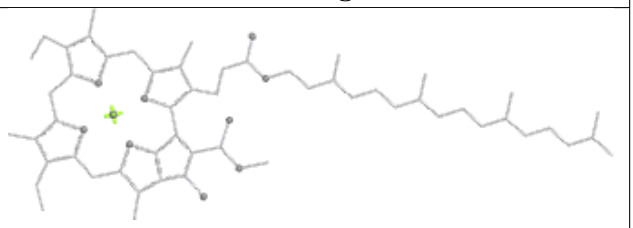
Bond lengths



Bond angles

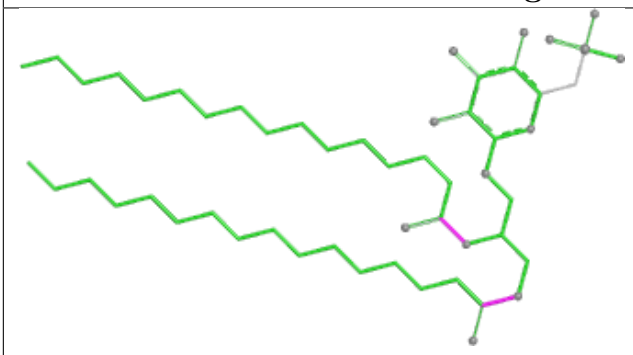


Torsions

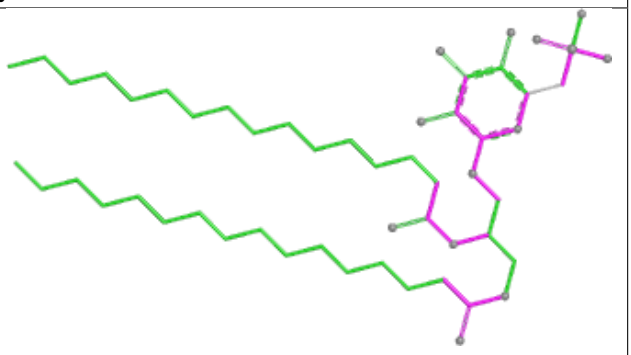


Rings

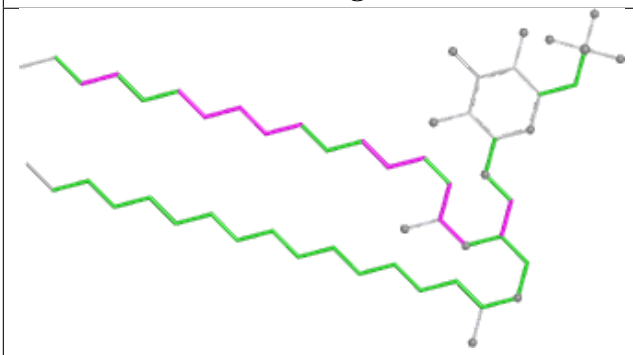
Ligand SQD C 501



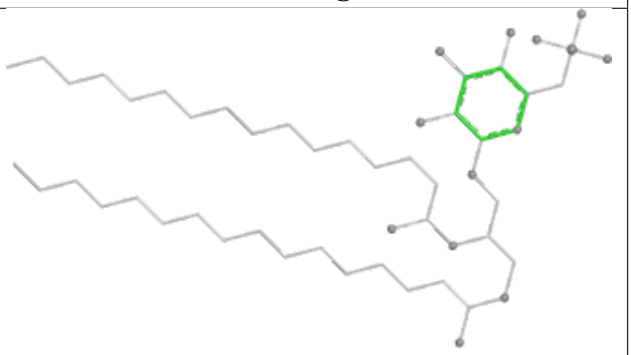
Bond lengths



Bond angles

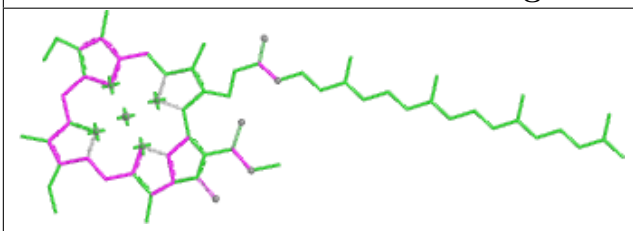


Torsions

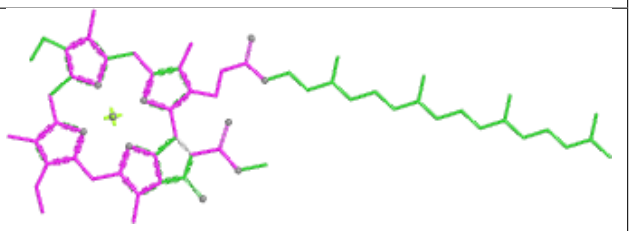


Rings

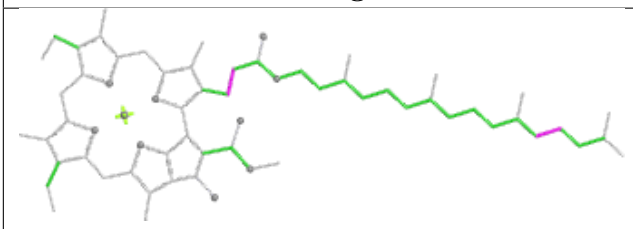
Ligand CLA A 404



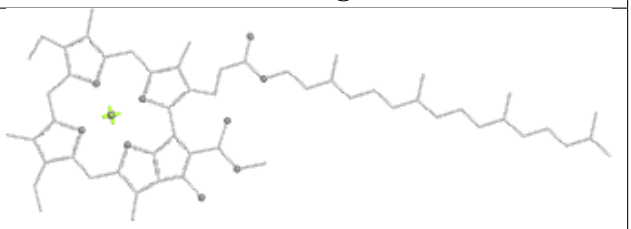
Bond lengths



Bond angles

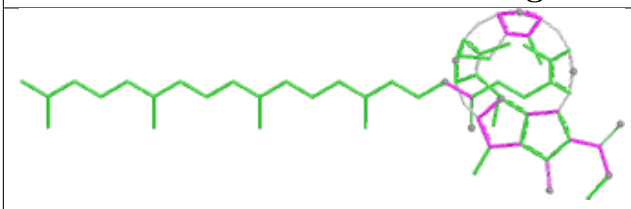


Torsions

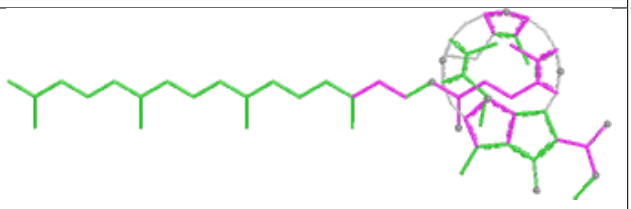


Rings

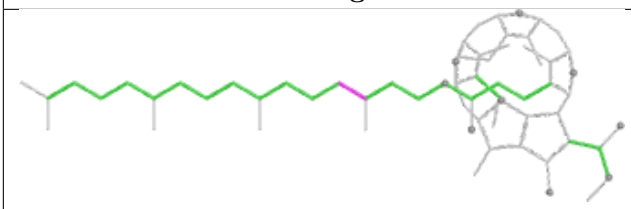
Ligand PHO a 406



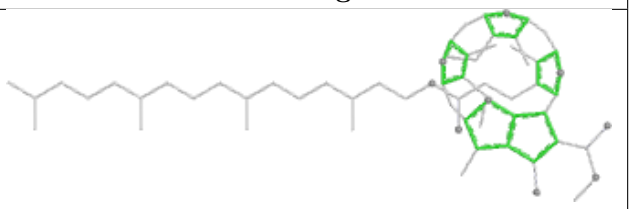
Bond lengths



Bond angles

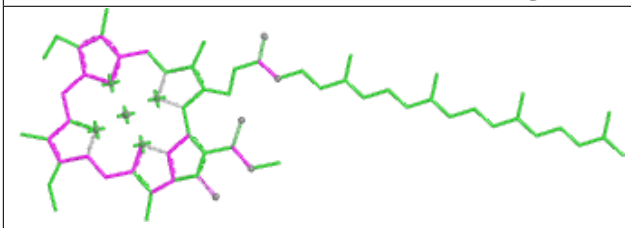


Torsions

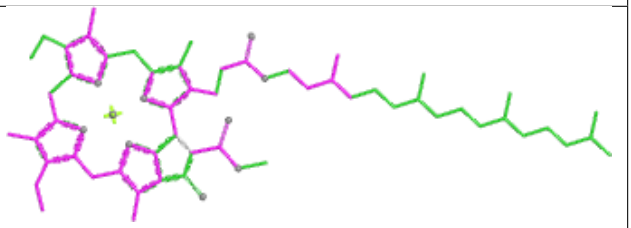


Rings

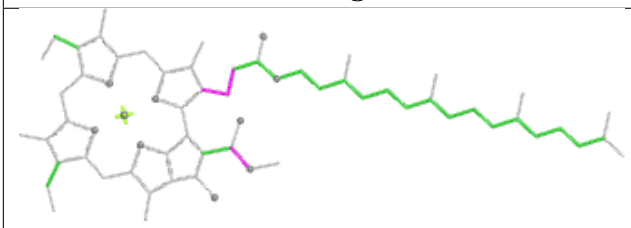
Ligand CLA C 502



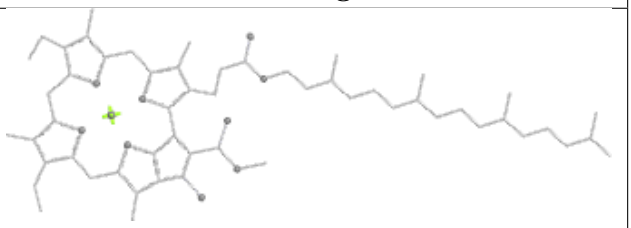
Bond lengths



Bond angles

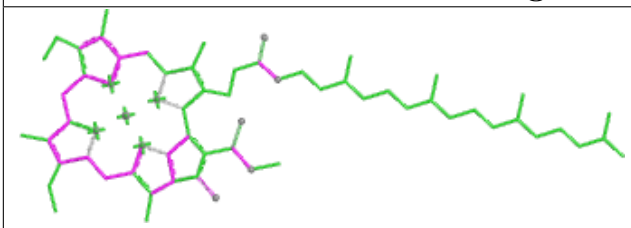


Torsions

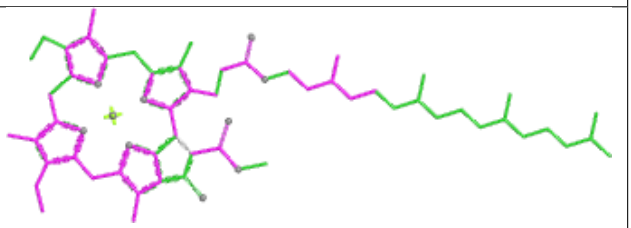


Rings

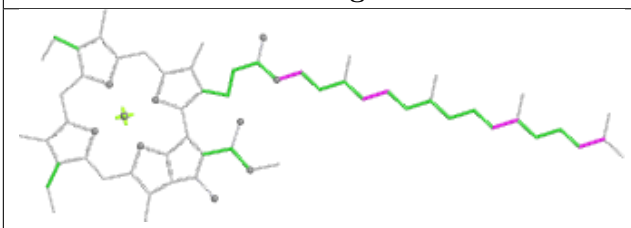
Ligand CLA d 403



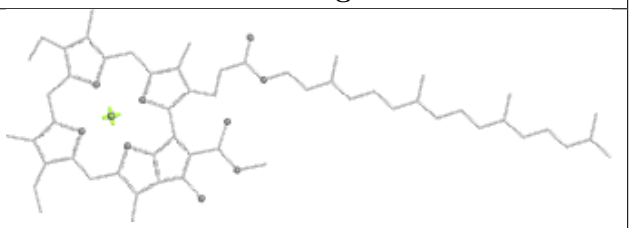
Bond lengths



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.48	1 (0%) 90 92	25, 48, 72, 137	2 (0%)
1	a	334/344 (97%)	-0.48	3 (0%) 81 84	25, 52, 80, 120	3 (0%)
2	B	504/505 (99%)	-0.42	0 100 100	21, 52, 84, 142	10 (1%)
2	b	504/505 (99%)	-0.30	7 (1%) 73 78	25, 56, 94, 158	4 (0%)
3	C	451/455 (99%)	-0.25	1 (0%) 91 92	26, 61, 86, 159	4 (0%)
3	c	455/455 (100%)	-0.27	2 (0%) 88 91	33, 68, 90, 125	2 (0%)
4	D	342/342 (100%)	-0.46	0 100 100	39, 49, 71, 145	0
4	d	341/342 (99%)	-0.53	0 100 100	41, 54, 76, 139	0
5	E	81/84 (96%)	-0.07	1 (1%) 76 81	36, 73, 102, 146	1 (1%)
5	e	79/84 (94%)	-0.07	1 (1%) 75 79	63, 77, 119, 148	0
6	F	34/44 (77%)	0.02	1 (2%) 53 60	55, 66, 90, 118	0
6	f	31/44 (70%)	-0.03	1 (3%) 50 57	62, 71, 101, 153	0
7	H	64/65 (98%)	0.02	3 (4%) 36 42	31, 64, 82, 136	1 (1%)
7	h	64/65 (98%)	0.03	1 (1%) 70 76	56, 68, 92, 108	0
8	I	37/38 (97%)	-0.07	0 100 100	52, 64, 128, 151	0
8	i	37/38 (97%)	-0.15	1 (2%) 56 63	56, 64, 127, 156	0
9	J	38/39 (97%)	-0.13	0 100 100	52, 74, 136, 177	0
9	j	39/39 (100%)	0.06	0 100 100	61, 79, 134, 165	0
10	K	37/37 (100%)	-0.29	0 100 100	61, 73, 94, 116	0
10	k	37/37 (100%)	-0.22	0 100 100	70, 77, 99, 117	0
11	L	36/37 (97%)	-0.13	1 (2%) 55 61	21, 44, 100, 144	1 (2%)
11	l	36/37 (97%)	-0.20	1 (2%) 55 61	21, 45, 103, 123	1 (2%)
12	M	32/36 (88%)	-0.35	0 100 100	22, 47, 74, 151	1 (3%)
12	m	33/36 (91%)	-0.44	0 100 100	42, 48, 83, 138	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%)	-0.32	0 100 100	26, 62, 117, 181	3 (1%)
13	o	243/244 (99%)	-0.22	0 100 100	27, 65, 125, 174	2 (0%)
14	T	29/32 (90%)	-0.44	1 (3%) 48 55	40, 45, 85, 116	0
14	t	29/32 (90%)	-0.44	1 (3%) 48 55	41, 48, 76, 139	0
15	U	96/104 (92%)	-0.48	0 100 100	48, 59, 90, 98	0
15	u	97/104 (93%)	-0.43	0 100 100	52, 65, 85, 127	0
16	V	137/137 (100%)	-0.40	0 100 100	45, 59, 86, 117	0
16	v	137/137 (100%)	-0.32	0 100 100	53, 74, 106, 131	0
17	X	38/40 (95%)	0.06	0 100 100	62, 75, 100, 117	0
17	x	38/40 (95%)	0.06	0 100 100	64, 80, 116, 164	0
18	Y	29/30 (96%)	0.31	2 (6%) 23 26	73, 92, 147, 178	0
18	y	29/30 (96%)	0.15	0 100 100	80, 94, 124, 126	0
19	Z	62/62 (100%)	-0.03	0 100 100	75, 90, 136, 185	0
19	z	62/62 (100%)	0.31	1 (1%) 70 76	82, 101, 140, 175	0
20	R	34/34 (100%)	1.14	5 (14%) 6 7	91, 113, 146, 149	0
All	All	5283/5384 (98%)	-0.30	35 (0%) 84 87	21, 59, 103, 185	35 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	6.0
7	h	65	LEU	3.7
1	a	264	SER	3.6
3	C	23	ALA	3.5
14	t	30	THR	3.4

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
8	FME	I	1	10/11	0.95	0.08	56,66,73,76	0
8	FME	i	1	10/11	0.96	0.06	54,67,72,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.96	0.07	39,46,70,75	0
12	FME	M	1	10/11	0.97	0.10	38,58,80,89	0
12	FME	m	1	10/11	0.97	0.06	40,57,77,93	0
14	FME	T	1	10/11	0.97	0.07	44,46,68,71	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
34	LMT	C	525	35/35	0.65	0.17	97,149,164,168	0
34	LMT	E	102	35/35	0.66	0.19	117,161,175,176	0
34	LMT	e	101	35/35	0.68	0.17	114,176,180,181	0
30	UNL	j	101	10/-	0.69	0.26	86,94,101,102	0
34	LMT	a	412	35/35	0.70	0.19	70,139,150,152	0
30	UNL	A	414	28/-	0.71	0.20	93,105,126,127	0
34	LMT	D	403	35/35	0.73	0.21	70,135,146,152	0
33	HTG	b	622	19/19	0.74	0.15	90,147,155,155	0
30	UNL	J	101	10/-	0.75	0.30	76,91,99,100	0
34	LMT	a	418	35/35	0.76	0.15	119,152,162,163	0
33	HTG	D	413	16/19	0.76	0.14	91,119,132,136	0
27	SQD	f	102	43/54	0.79	0.16	119,138,168,171	0
33	HTG	B	622	19/19	0.79	0.19	76,96,106,106	0
36	CA	F	101	1/1	0.79	0.14	129,129,129,129	0
33	HTG	c	522	19/19	0.80	0.14	118,141,149,151	0
30	UNL	m	102	10/-	0.80	0.22	65,72,99,100	0
34	LMT	m	103	35/35	0.81	0.14	68,104,116,119	0
30	UNL	i	101	40/-	0.81	0.19	75,103,153,163	0
30	UNL	a	415	30/-	0.82	0.15	102,114,136,145	0
32	LHG	a	419	42/49	0.82	0.14	98,142,173,177	0
33	HTG	C	522	19/19	0.83	0.14	114,127,137,138	0
30	UNL	C	526	34/-	0.83	0.16	90,120,133,134	0
31	LMG	C	521	51/55	0.83	0.17	77,131,166,170	0
31	LMG	Z	101	37/55	0.83	0.16	79,133,167,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	I	101	40/-	0.83	0.19	73,109,155,156	0
26	GOL	O	302	6/6	0.83	0.09	84,85,88,89	0
30	UNL	c	525	32/-	0.84	0.17	90,115,132,135	0
30	UNL	b	625	33/-	0.84	0.16	67,101,152,154	0
34	LMT	D	404	35/35	0.85	0.13	73,118,133,134	0
31	LMG	c	521	51/55	0.85	0.15	78,133,158,163	0
34	LMT	M	104	35/35	0.85	0.14	80,152,175,176	0
33	HTG	V	202	11/19	0.85	0.12	117,124,127,128	0
30	UNL	M	103	10/-	0.86	0.20	66,78,91,94	0
33	HTG	h	101	16/19	0.86	0.11	99,136,147,148	0
33	HTG	b	621	19/19	0.86	0.16	68,82,114,118	0
32	LHG	E	101	42/49	0.86	0.16	80,126,141,143	0
34	LMT	b	620	25/35	0.87	0.15	92,128,152,154	0
34	LMT	b	626	25/35	0.87	0.15	52,77,134,137	0
29	PL9	A	413	55/55	0.87	0.21	80,108,117,118	0
30	UNL	D	412	40/-	0.87	0.18	61,93,130,131	0
33	HTG	B	621	19/19	0.87	0.16	65,82,115,116	0
27	SQD	A	411	54/54	0.88	0.14	67,87,125,127	0
27	SQD	a	411	54/54	0.88	0.12	69,96,137,142	0
26	GOL	B	626	6/6	0.88	0.18	91,105,106,108	0
23	CLA	b	601	65/65	0.88	0.12	65,83,126,136	0
29	PL9	a	414	55/55	0.88	0.22	90,117,133,138	0
26	GOL	c	501	6/6	0.88	0.16	62,73,78,81	0
30	UNL	B	625	33/-	0.88	0.14	59,113,154,157	0
34	LMT	B	628	25/35	0.88	0.14	54,82,139,141	0
30	UNL	d	411	36/-	0.88	0.16	75,100,133,136	0
26	GOL	c	526	6/6	0.88	0.18	117,120,128,129	0
31	LMG	z	101	39/55	0.89	0.15	86,136,147,149	0
34	LMT	M	102	35/35	0.89	0.11	58,107,138,142	0
26	GOL	v	202	6/6	0.89	0.21	62,91,95,95	0
26	GOL	B	627	6/6	0.89	0.17	109,114,117,119	0
34	LMT	t	101	26/35	0.89	0.14	80,119,138,141	0
27	SQD	D	415	43/54	0.89	0.13	76,114,135,142	0
23	CLA	B	601	65/65	0.90	0.11	57,78,119,129	0
27	SQD	L	102	54/54	0.90	0.12	64,92,116,121	0
26	GOL	b	623	6/6	0.90	0.17	89,99,105,112	0
27	SQD	B	620	54/54	0.90	0.12	62,94,126,130	0
31	LMG	C	520	51/55	0.90	0.14	61,92,114,119	0
26	GOL	A	410	6/6	0.91	0.13	71,74,79,88	0
33	HTG	b	624	19/19	0.92	0.10	68,80,100,107	0
31	LMG	a	417	51/55	0.92	0.13	62,96,110,122	0
23	CLA	C	514	65/65	0.92	0.12	69,80,114,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	h	102	40/40	0.93	0.10	56,67,80,84	0
30	UNL	x	101	18/-	0.93	0.13	71,80,124,127	0
31	LMG	A	415	51/55	0.93	0.12	63,90,109,114	0
30	UNL	d	410	17/-	0.93	0.13	69,82,99,100	0
23	CLA	C	505	65/65	0.93	0.11	49,57,95,109	0
31	LMG	D	414	51/55	0.93	0.12	51,74,116,126	0
33	HTG	B	624	19/19	0.93	0.10	68,83,91,99	0
26	GOL	a	410	6/6	0.93	0.12	66,73,88,94	0
25	BCR	T	101	40/40	0.93	0.08	43,54,64,64	0
35	DGD	C	518	62/66	0.93	0.11	51,67,124,134	0
31	LMG	c	520	51/55	0.93	0.12	69,96,133,136	0
36	CA	O	301	1/1	0.93	0.08	116,116,116,116	0
32	LHG	A	416	49/49	0.94	0.13	44,63,85,88	0
25	BCR	t	102	40/40	0.94	0.08	42,59,74,75	0
30	UNL	D	411	17/-	0.94	0.15	64,81,117,117	0
32	LHG	b	628	49/49	0.94	0.10	43,59,69,83	0
23	CLA	C	507	65/65	0.94	0.12	58,72,128,137	0
27	SQD	C	501	54/54	0.94	0.12	58,86,115,118	0
23	CLA	b	616	65/65	0.94	0.10	47,61,122,124	0
23	CLA	c	508	65/65	0.94	0.11	58,70,81,90	0
23	CLA	c	514	65/65	0.94	0.10	71,91,124,127	0
31	LMG	M	101	51/55	0.94	0.11	53,72,94,115	0
25	BCR	C	515	40/40	0.94	0.10	67,80,90,93	0
25	BCR	D	407	40/40	0.94	0.11	52,63,101,108	0
25	BCR	H	101	40/40	0.94	0.10	50,69,79,81	0
23	CLA	C	513	65/65	0.94	0.11	63,73,122,125	0
31	LMG	m	101	51/55	0.94	0.11	52,72,99,103	0
23	CLA	B	614	65/65	0.94	0.10	38,48,100,107	0
36	CA	v	201	1/1	0.94	0.09	117,117,117,117	0
25	BCR	Y	101	40/40	0.95	0.08	61,70,82,89	0
25	BCR	a	408	40/40	0.95	0.07	42,50,58,61	0
25	BCR	c	515	40/40	0.95	0.10	75,86,94,95	0
25	BCR	d	405	40/40	0.95	0.10	58,69,91,104	0
27	SQD	a	409	54/54	0.95	0.10	71,87,124,125	0
23	CLA	c	507	65/65	0.95	0.10	61,74,127,135	0
25	BCR	k	102	40/40	0.95	0.09	64,75,91,97	0
23	CLA	B	616	65/65	0.95	0.10	47,58,137,141	0
29	PL9	D	408	55/55	0.95	0.09	39,49,61,70	0
23	CLA	c	513	65/65	0.95	0.11	70,88,122,129	0
26	GOL	B	623	6/6	0.95	0.10	73,86,93,97	0
23	CLA	D	406	65/65	0.95	0.10	50,59,132,135	0
23	CLA	d	404	65/65	0.95	0.09	54,64,120,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	GOL	C	523	6/6	0.95	0.17	60,63,69,69	0
25	BCR	B	618	40/40	0.95	0.07	43,54,71,76	0
25	BCR	B	619	40/40	0.95	0.09	48,59,76,80	0
23	CLA	C	508	65/65	0.95	0.09	55,64,78,87	0
32	LHG	D	410	49/49	0.95	0.12	50,64,123,134	0
26	GOL	b	627	6/6	0.95	0.15	99,99,102,103	0
32	LHG	L	101	49/49	0.95	0.10	42,56,69,95	0
30	UNL	X	101	18/-	0.95	0.11	63,76,94,95	0
23	CLA	b	614	65/65	0.95	0.09	40,48,112,114	0
32	LHG	d	409	49/49	0.95	0.12	60,69,125,134	0
35	DGD	C	519	62/66	0.95	0.10	47,62,104,119	0
35	DGD	c	518	62/66	0.95	0.10	56,76,120,133	0
23	CLA	B	606	65/65	0.95	0.09	44,53,102,110	0
25	BCR	K	101	40/40	0.95	0.10	63,74,77,80	0
36	CA	o	301	1/1	0.95	0.05	104,104,104,104	0
23	CLA	c	505	65/65	0.95	0.10	56,65,106,116	0
37	BCT	D	401	4/4	0.95	0.08	59,64,65,66	0
37	BCT	d	401	4/4	0.95	0.07	57,58,64,67	0
32	LHG	d	407	49/49	0.96	0.11	48,66,80,86	0
32	LHG	d	408	49/49	0.96	0.09	43,54,73,84	0
23	CLA	b	609	65/65	0.96	0.08	53,62,76,93	0
25	BCR	c	516	40/40	0.96	0.09	57,69,76,79	0
23	CLA	b	610	65/65	0.96	0.09	50,56,70,78	0
23	CLA	b	612	65/65	0.96	0.08	44,52,64,73	0
25	BCR	k	101	40/40	0.96	0.09	65,77,87,88	0
23	CLA	C	504	65/65	0.96	0.08	55,63,74,79	0
23	CLA	A	408	65/65	0.96	0.09	44,51,115,124	0
23	CLA	c	504	65/65	0.96	0.08	58,69,78,82	0
23	CLA	B	607	65/65	0.96	0.08	37,46,67,75	0
23	CLA	c	506	65/65	0.96	0.09	50,62,85,89	0
23	CLA	B	610	65/65	0.96	0.09	47,53,67,83	0
23	CLA	C	509	65/65	0.96	0.09	50,58,123,136	0
23	CLA	c	509	65/65	0.96	0.09	53,63,127,129	0
23	CLA	c	511	65/65	0.96	0.08	58,66,75,79	0
23	CLA	c	512	65/65	0.96	0.08	60,72,86,94	0
23	CLA	C	510	65/65	0.96	0.09	56,64,85,88	0
23	CLA	C	511	65/65	0.96	0.08	53,62,85,92	0
23	CLA	C	512	65/65	0.96	0.09	58,68,84,91	0
24	PHO	D	402	64/64	0.96	0.07	41,51,56,57	0
25	BCR	A	409	40/40	0.96	0.07	40,50,59,61	0
23	CLA	B	611	65/65	0.96	0.07	40,45,64,75	0
23	CLA	A	406	65/65	0.96	0.08	40,48,104,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	602	65/65	0.96	0.08	46,55,75,83	0
23	CLA	a	404	65/65	0.96	0.07	43,46,67,80	0
23	CLA	a	407	65/65	0.96	0.10	46,55,130,131	0
31	LMG	d	412	51/55	0.96	0.10	57,72,117,133	0
35	DGD	C	517	62/66	0.96	0.10	48,58,103,108	0
23	CLA	C	502	65/65	0.96	0.09	53,60,73,81	0
23	CLA	b	605	65/65	0.96	0.08	42,49,69,75	0
35	DGD	H	102	62/66	0.96	0.08	45,60,78,83	0
23	CLA	b	606	65/65	0.96	0.08	46,55,120,127	0
35	DGD	c	519	62/66	0.96	0.09	55,64,105,112	0
35	DGD	h	103	62/66	0.96	0.09	52,65,73,75	0
32	LHG	D	409	49/49	0.96	0.09	44,53,73,86	0
23	CLA	b	607	65/65	0.96	0.08	38,45,78,87	0
25	BCR	b	617	40/40	0.96	0.07	41,48,59,64	0
29	PL9	d	406	55/55	0.96	0.08	40,48,59,67	0
25	BCR	b	618	40/40	0.96	0.07	39,55,72,77	0
25	BCR	b	619	40/40	0.96	0.07	49,59,85,92	0
23	CLA	a	405	65/65	0.97	0.09	45,53,124,126	0
23	CLA	B	612	65/65	0.97	0.07	42,50,61,66	0
23	CLA	B	613	65/65	0.97	0.07	39,47,87,92	0
23	CLA	b	602	65/65	0.97	0.08	49,59,75,86	0
23	CLA	b	603	65/65	0.97	0.07	47,54,76,85	0
23	CLA	c	510	65/65	0.97	0.08	60,66,87,92	0
23	CLA	b	604	65/65	0.97	0.08	40,48,108,117	0
23	CLA	B	603	65/65	0.97	0.07	44,52,68,73	0
23	CLA	B	615	65/65	0.97	0.07	46,52,78,89	0
23	CLA	B	608	65/65	0.97	0.07	45,53,70,73	0
23	CLA	d	402	65/65	0.97	0.07	40,46,62,68	0
23	CLA	b	608	65/65	0.97	0.07	50,57,73,78	0
24	PHO	A	407	64/64	0.97	0.06	38,43,53,62	0
23	CLA	B	609	65/65	0.97	0.07	50,59,74,85	0
24	PHO	a	406	64/64	0.97	0.06	40,47,52,55	0
24	PHO	a	416	64/64	0.97	0.06	45,52,58,65	0
23	CLA	C	503	65/65	0.97	0.08	50,59,82,93	0
25	BCR	B	617	40/40	0.97	0.06	40,50,60,62	0
23	CLA	b	611	65/65	0.97	0.07	43,50,70,82	0
35	DGD	c	517	62/66	0.97	0.09	51,65,96,104	0
23	CLA	B	605	65/65	0.97	0.07	40,46,61,72	0
23	CLA	b	613	65/65	0.97	0.07	40,48,81,86	0
25	BCR	C	516	40/40	0.97	0.08	54,64,79,83	0
23	CLA	D	405	65/65	0.97	0.07	38,44,62,70	0
23	CLA	b	615	65/65	0.97	0.07	47,56,78,82	0

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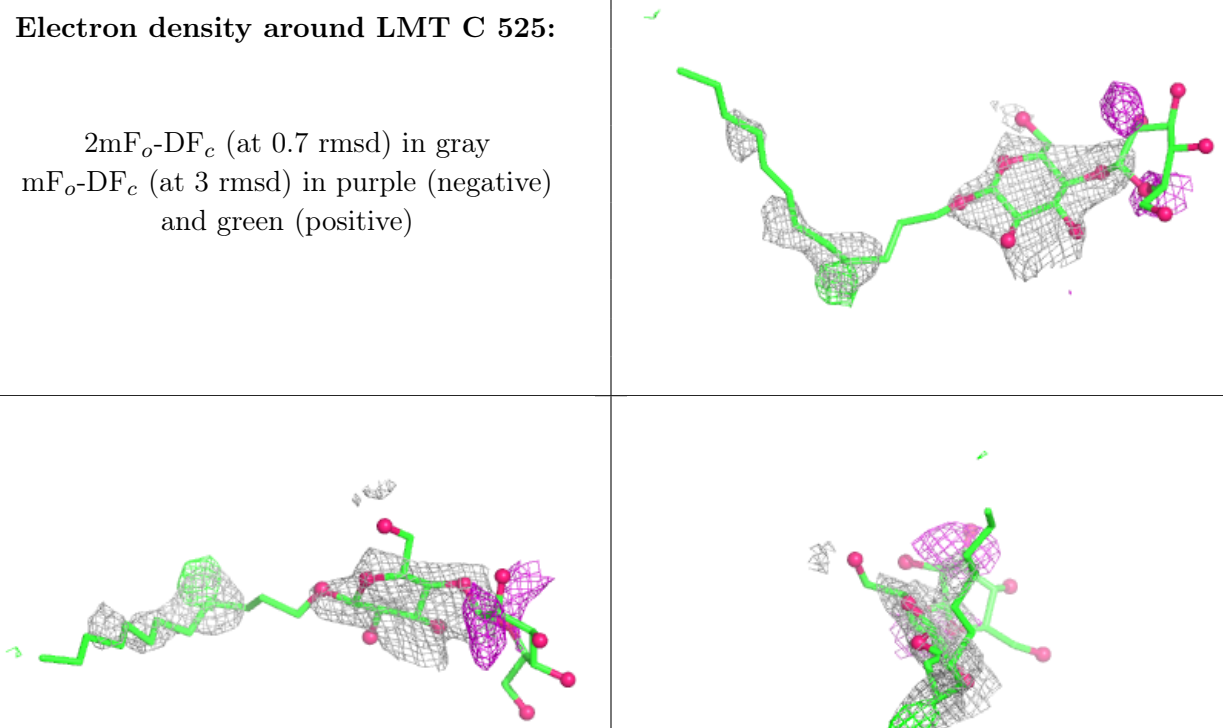
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	A	404	65/65	0.97	0.07	39,42,67,72	0
23	CLA	c	502	65/65	0.97	0.08	57,66,80,84	0
23	CLA	c	503	65/65	0.97	0.07	55,62,77,89	0
23	CLA	C	506	65/65	0.97	0.07	50,57,90,94	0
38	HEM	E	103	43/43	0.97	0.07	62,71,86,98	0
38	HEM	f	101	43/43	0.97	0.08	70,83,119,127	0
39	MG	J	102	1/1	0.97	0.08	61,61,61,61	0
40	HEC	v	203	43/43	0.97	0.07	59,65,70,75	0
23	CLA	B	604	65/65	0.98	0.07	38,45,105,110	0
23	CLA	d	403	65/65	0.98	0.06	42,47,71,80	0
36	CA	c	523	1/1	0.98	0.06	81,81,81,81	0
36	CA	c	524	1/1	0.98	0.04	90,90,90,90	0
23	CLA	A	405	65/65	0.98	0.06	38,44,54,56	0
40	HEC	V	201	43/43	0.98	0.07	50,53,58,62	0
36	CA	C	524	1/1	0.98	0.11	72,72,72,72	0
21	FE2	a	401	1/1	0.99	0.03	61,61,61,61	0
22	CL	A	403	1/1	0.99	0.03	45,45,45,45	0
28	OEX	A	412	10/10	0.99	0.04	44,49,53,56	0
39	MG	j	102	1/1	0.99	0.04	68,68,68,68	0
28	OEX	a	413	10/10	0.99	0.03	45,54,55,56	0
22	CL	a	403	1/1	0.99	0.06	49,49,49,49	0
21	FE2	A	401	1/1	1.00	0.03	61,61,61,61	0
22	CL	a	402	1/1	1.00	0.05	48,48,48,48	0
22	CL	A	402	1/1	1.00	0.05	40,40,40,40	0

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

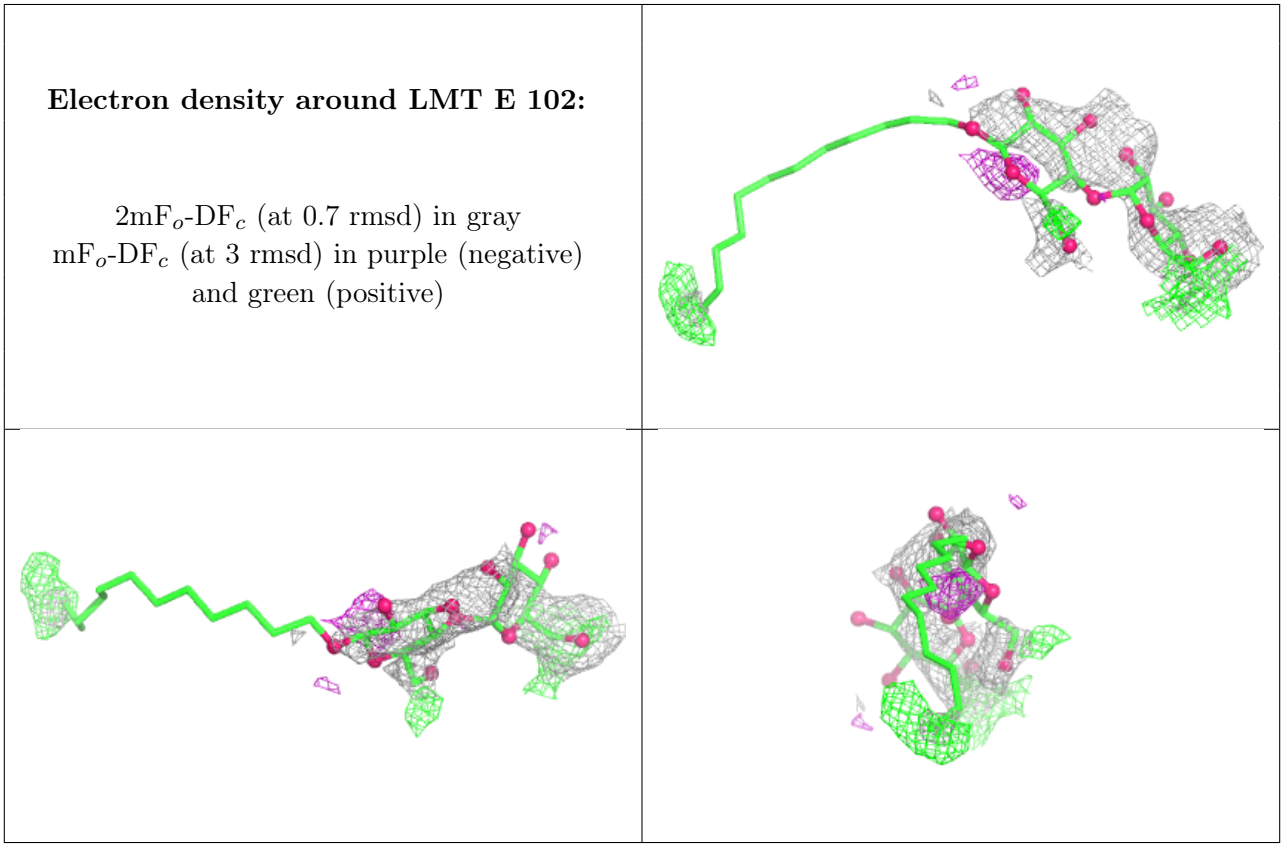
Electron density around LMT C 525:

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



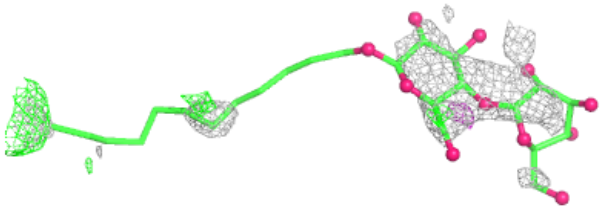
Electron density around LMT E 102:

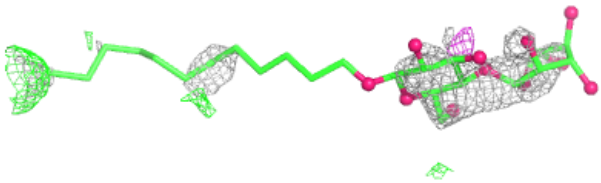
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

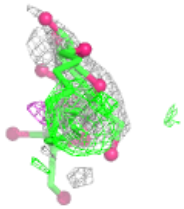


Electron density around LMT e 101:

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

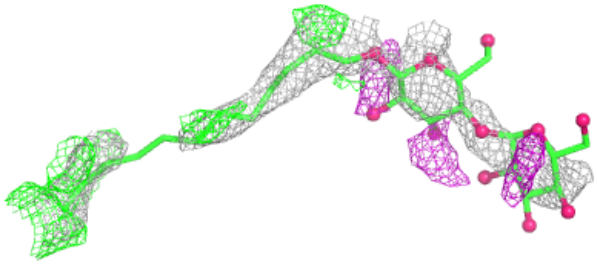


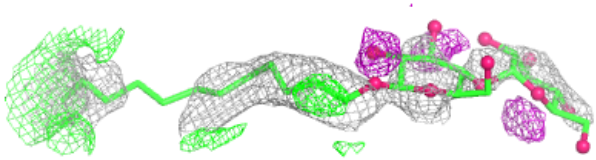


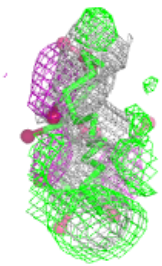


Electron density around LMT a 412:

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

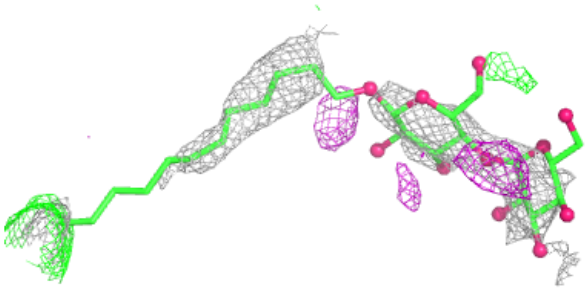


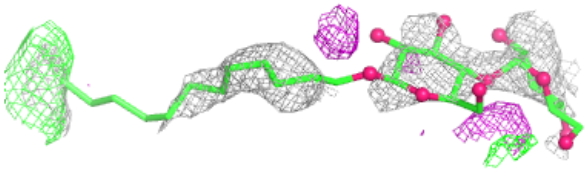


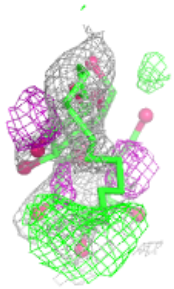


Electron density around LMT D 403:

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

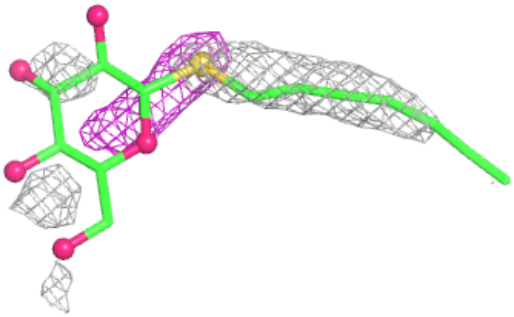


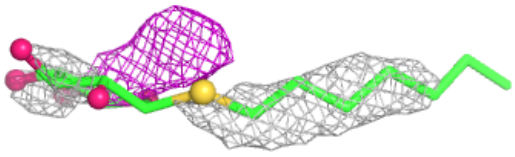


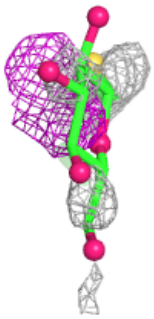


Electron density around HTG b 622:

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

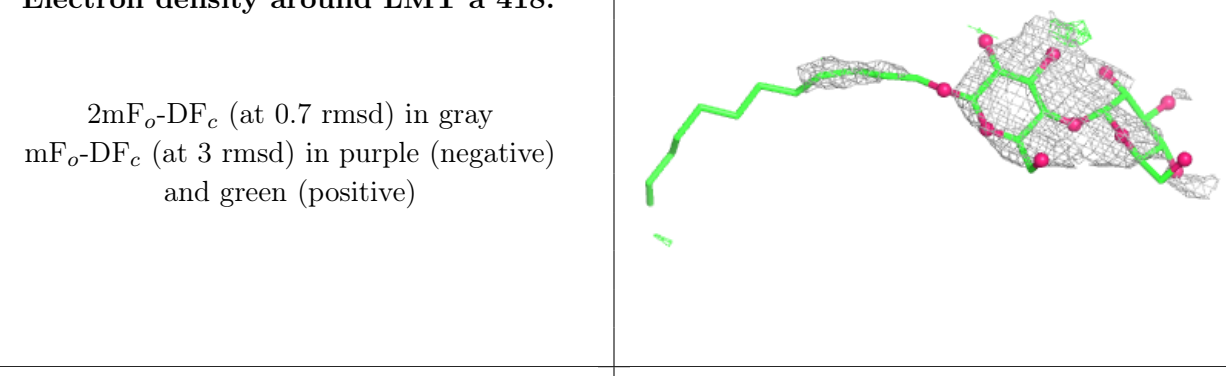


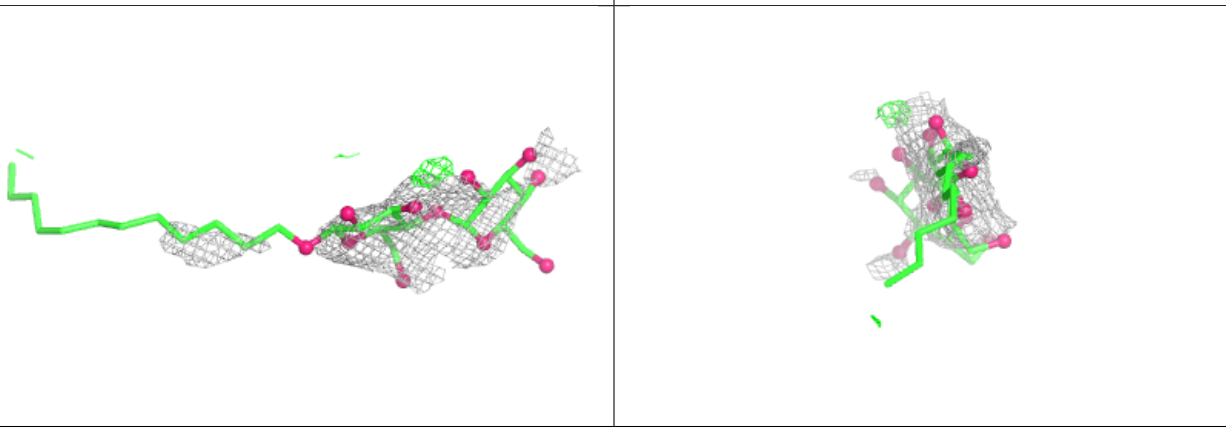




Electron density around LMT a 418:

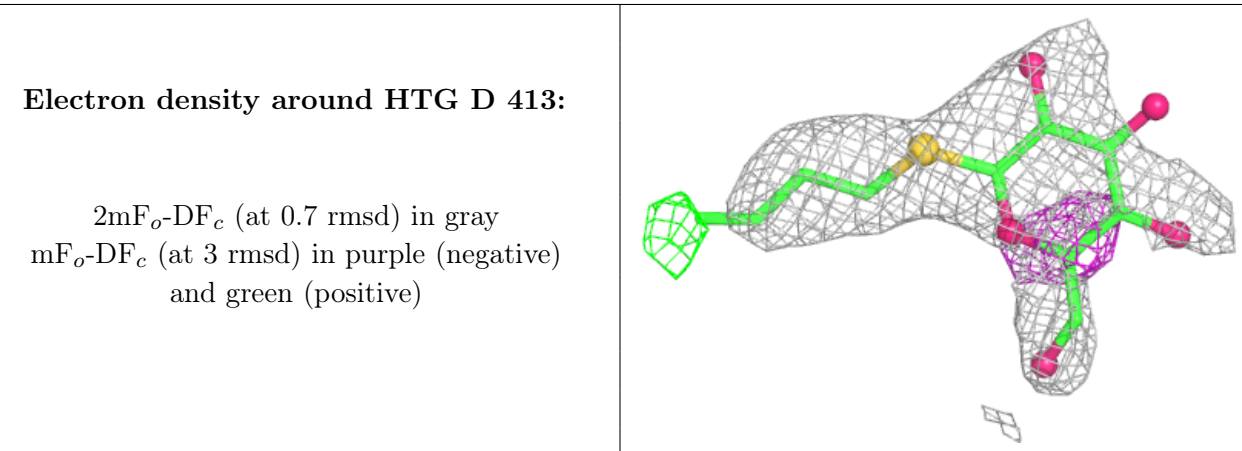
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

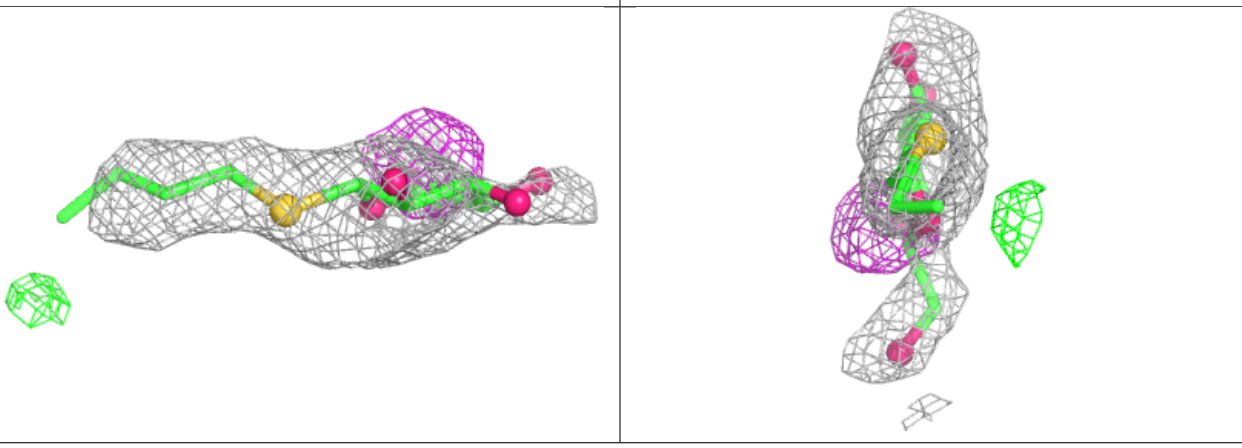




Electron density around HTG D 413:

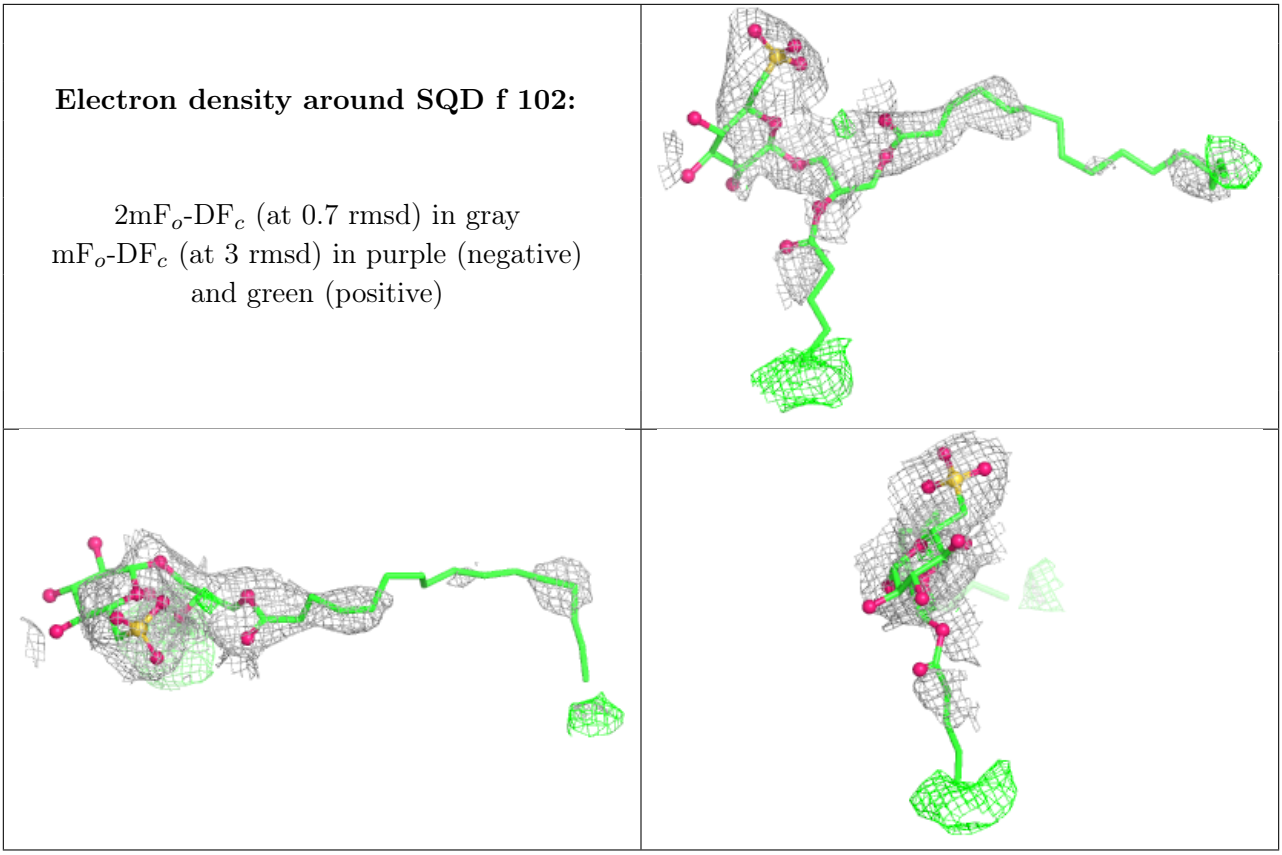
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





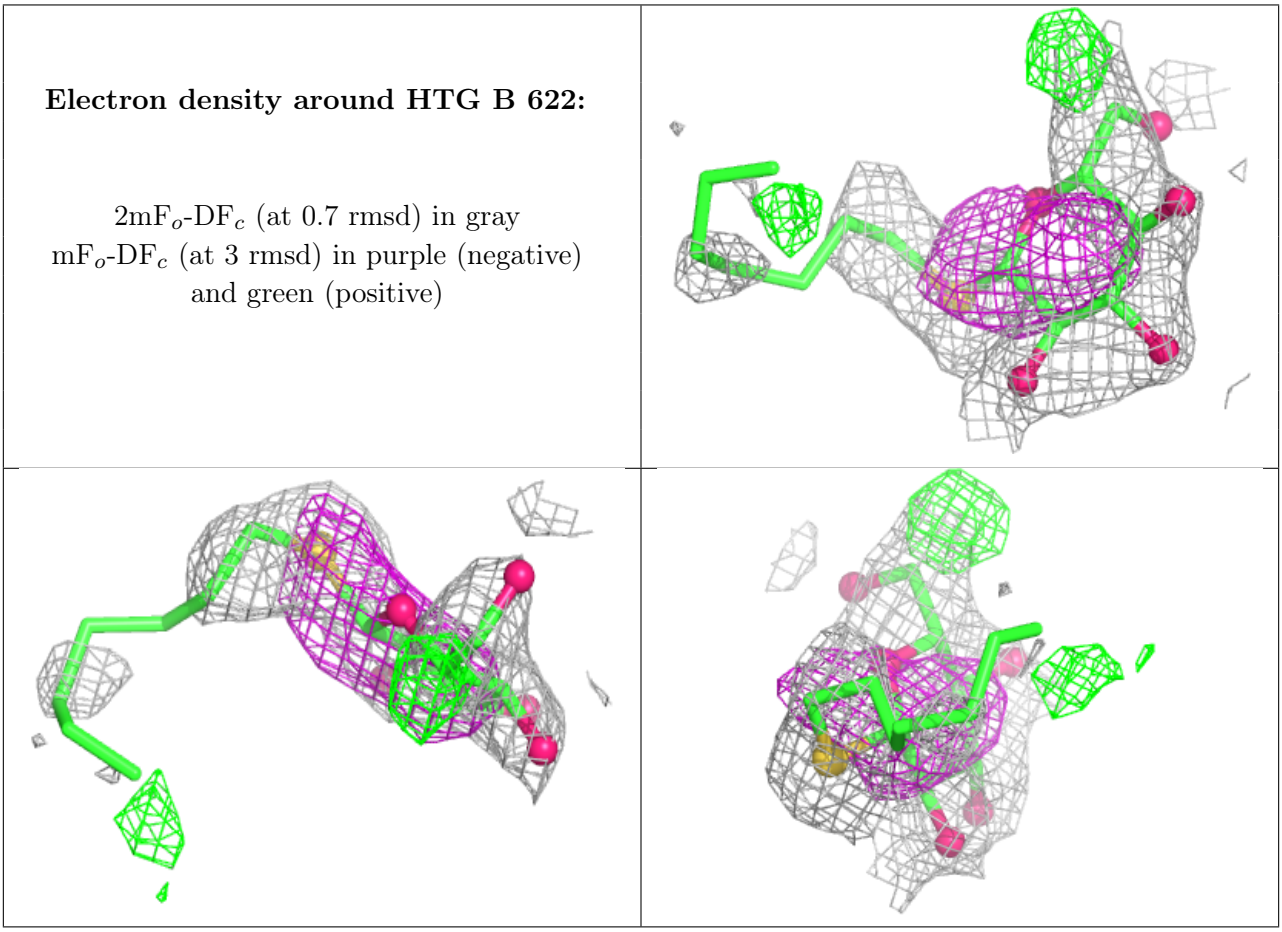
Electron density around SQD f 102:

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



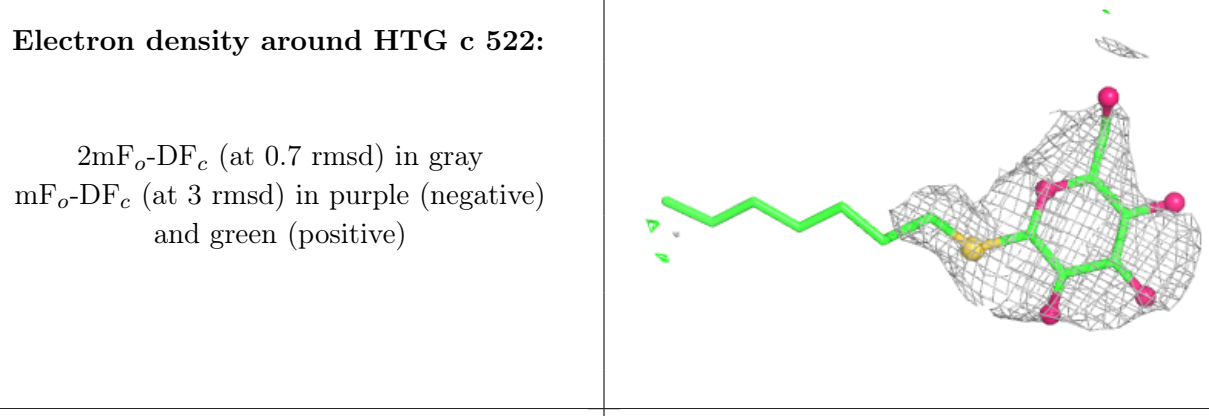
Electron density around HTG B 622:

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



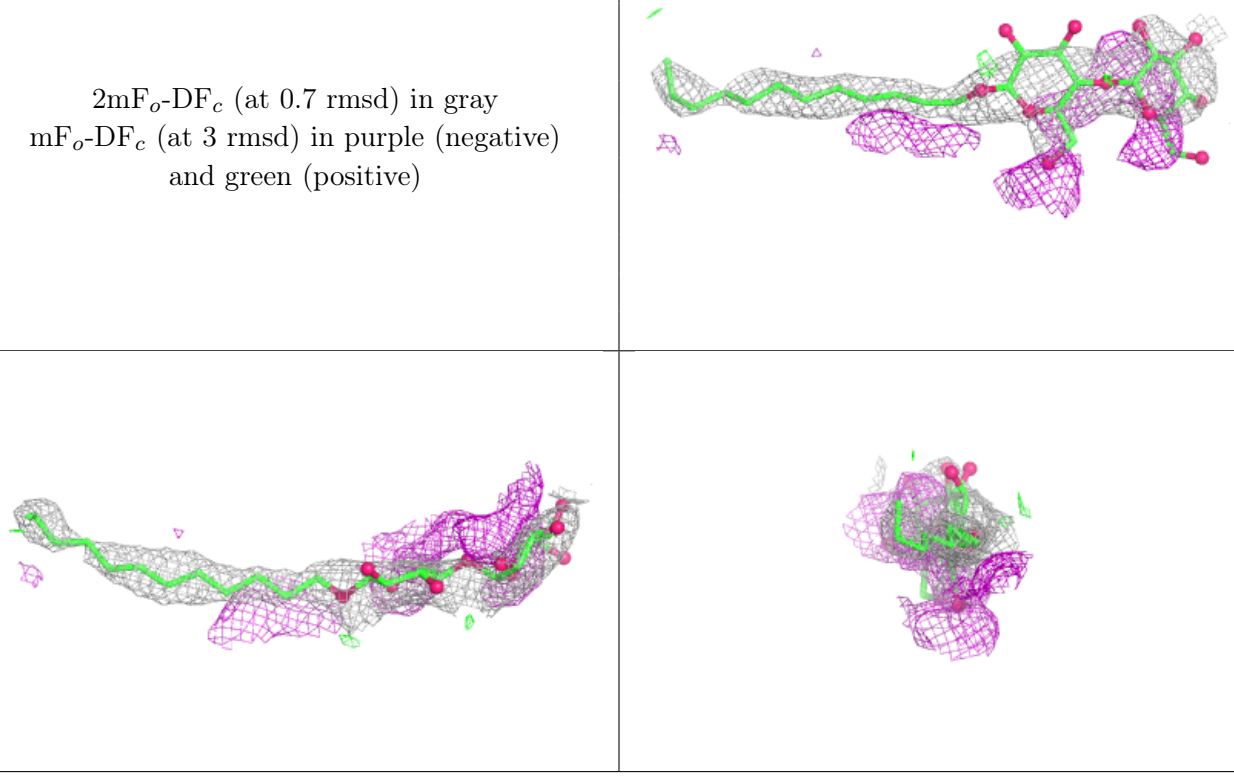
Electron density around HTG c 522:

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



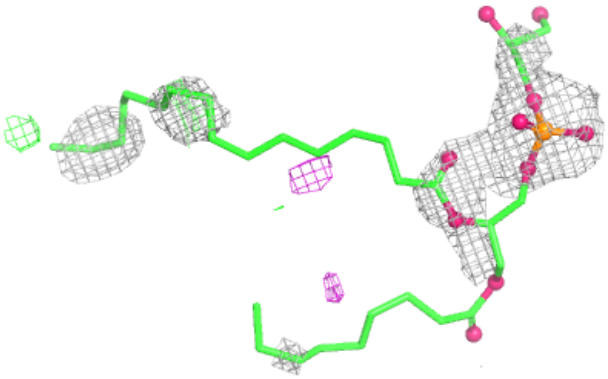
Electron density around LMT m 103:

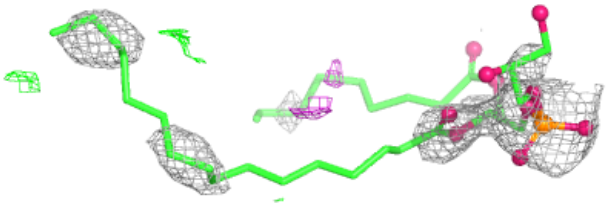
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

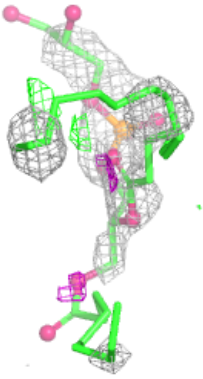


Electron density around LHG a 419:

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

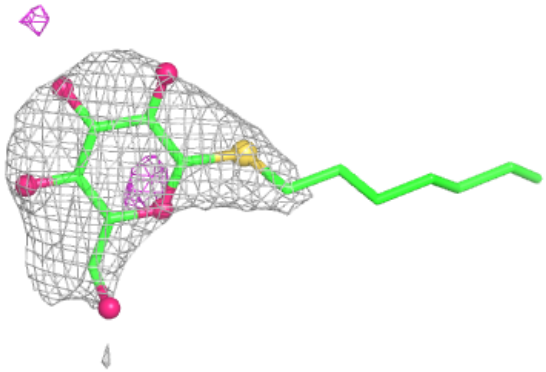


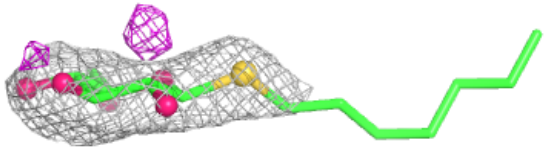


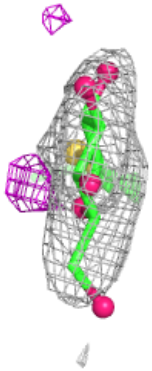


Electron density around HTG C 522:

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

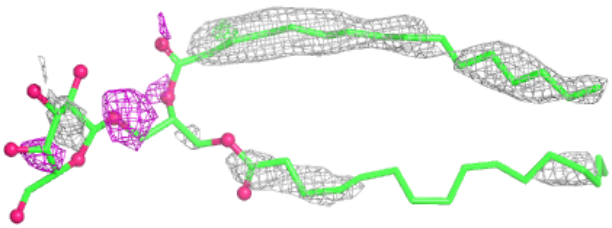


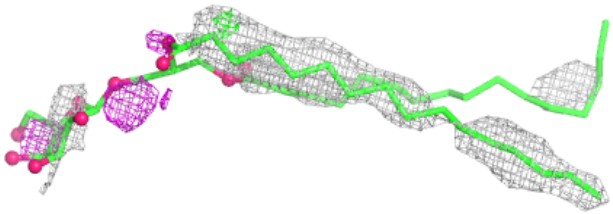


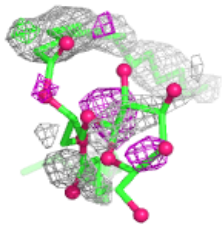


Electron density around LMG C 521:

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

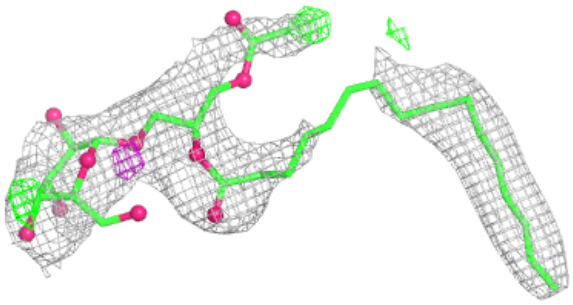


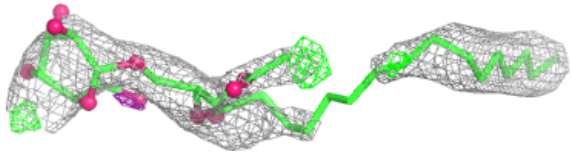


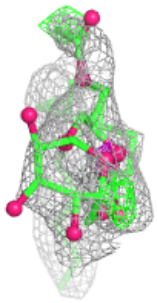


Electron density around LMG Z 101:

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

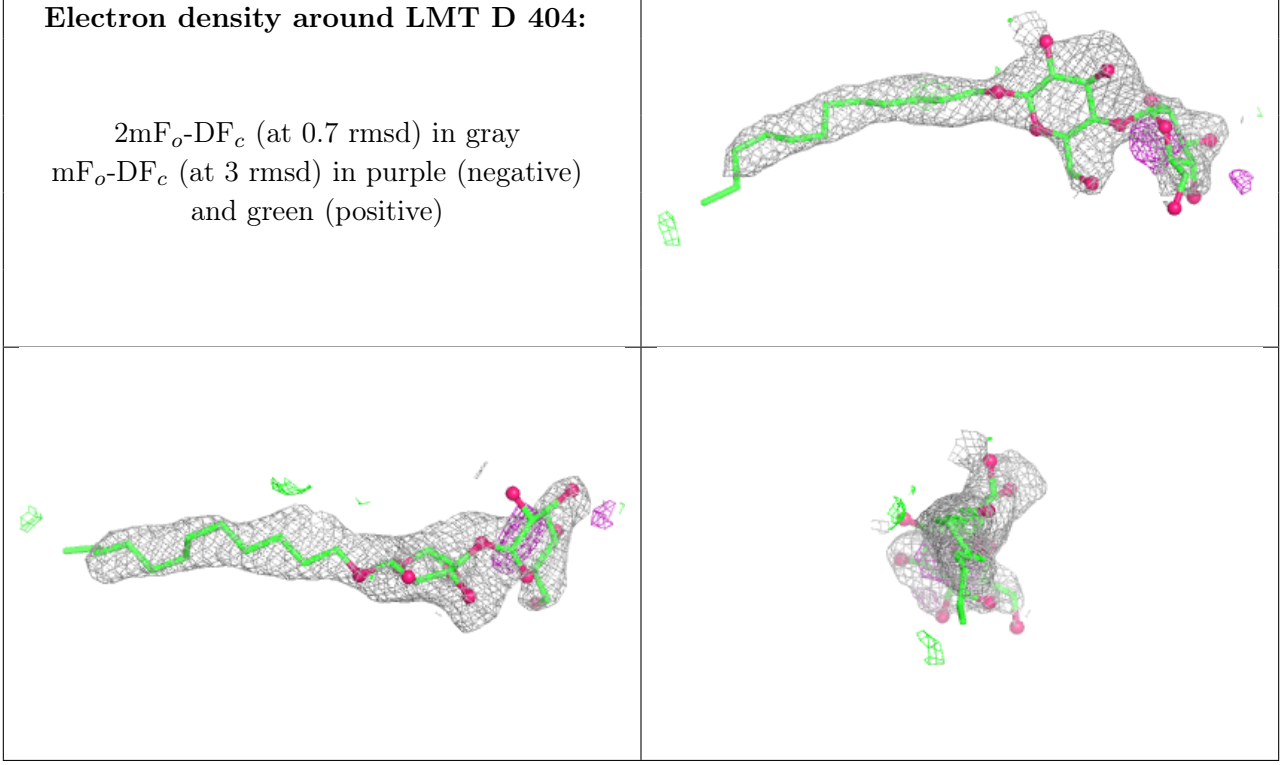






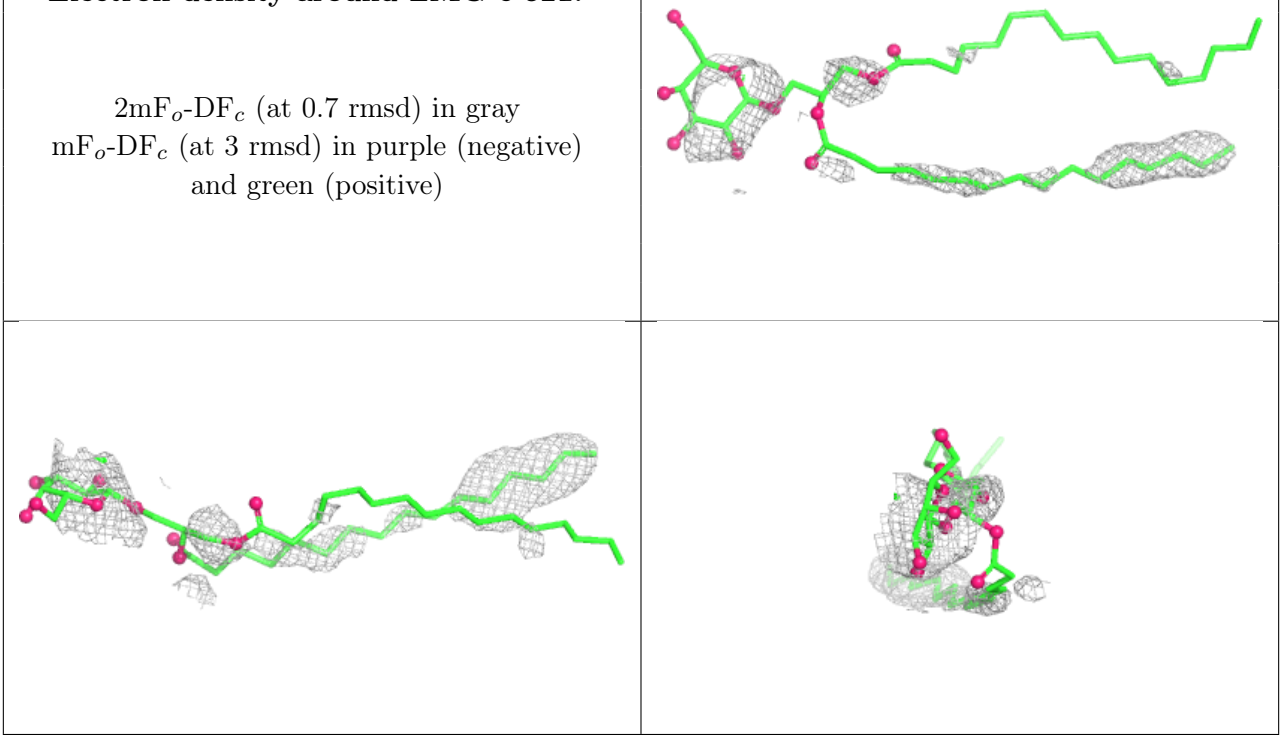
Electron density around LMT D 404:

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



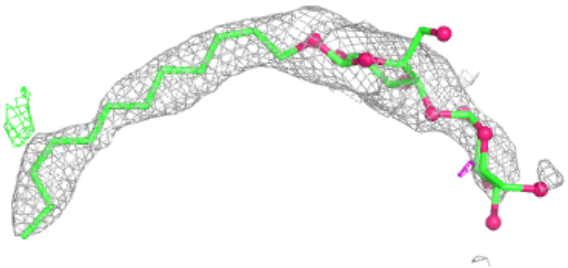
Electron density around LMG c 521:

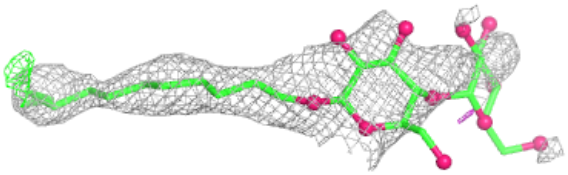
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

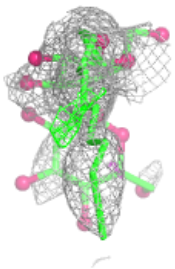


Electron density around LMT M 104:

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

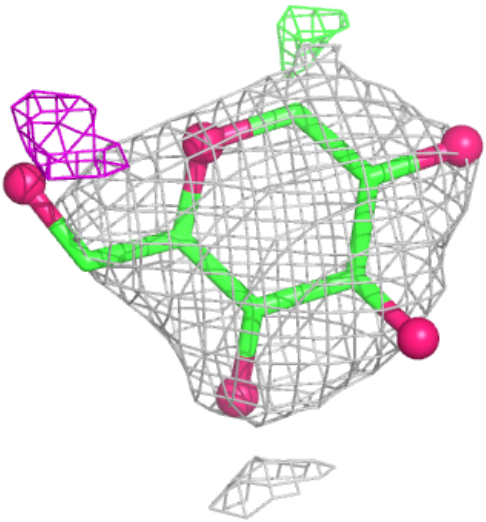


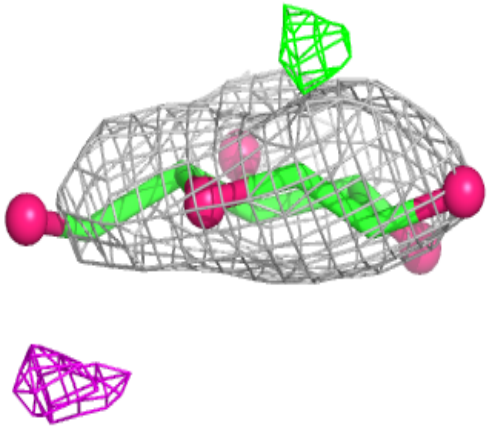


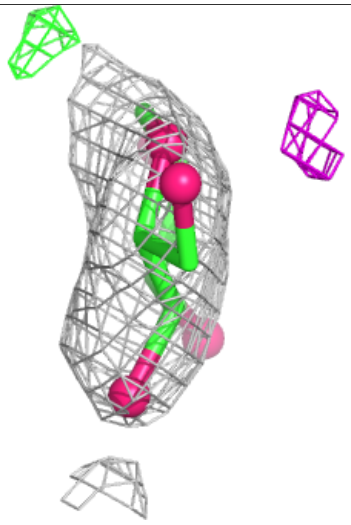


Electron density around HTG V 202:

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

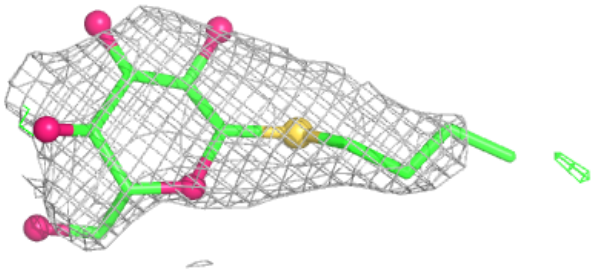


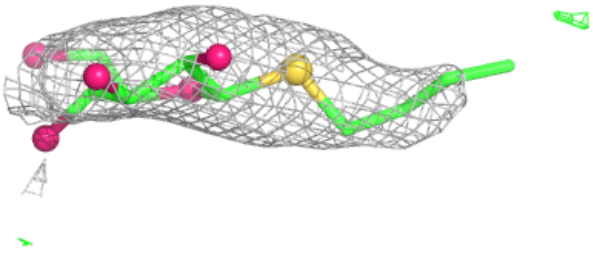


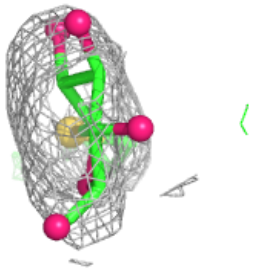


Electron density around HTG h 101:

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

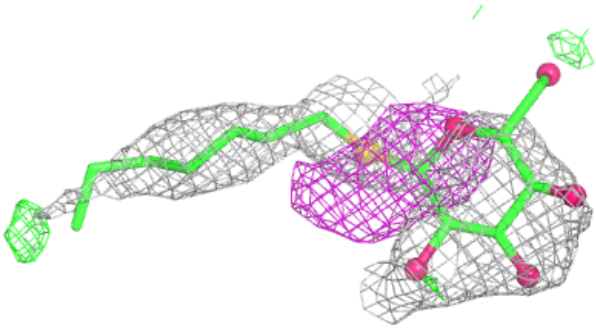


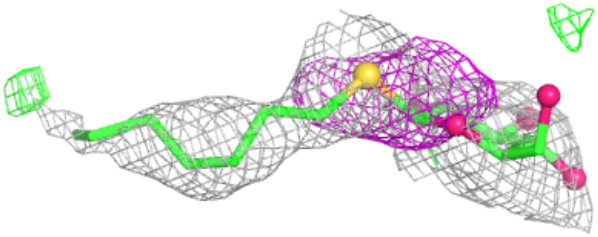


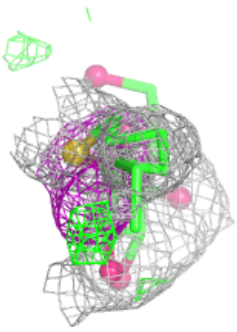


Electron density around HTG b 621:

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

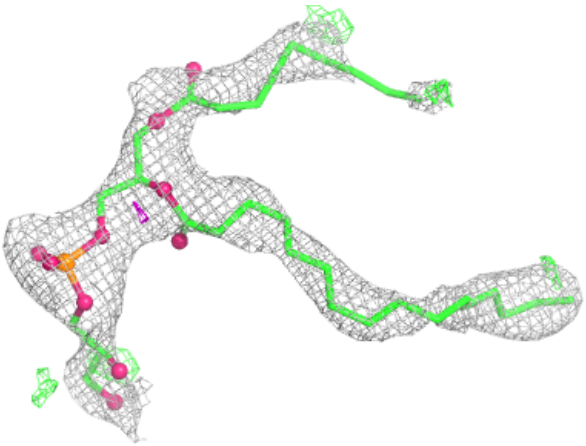


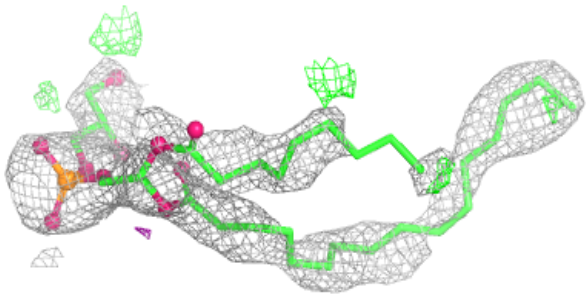


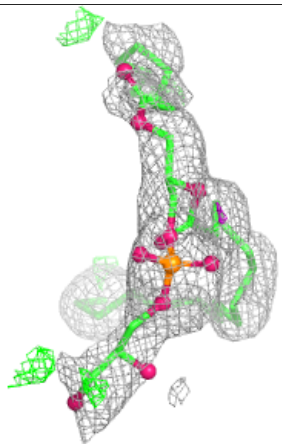


Electron density around LHG E 101:

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

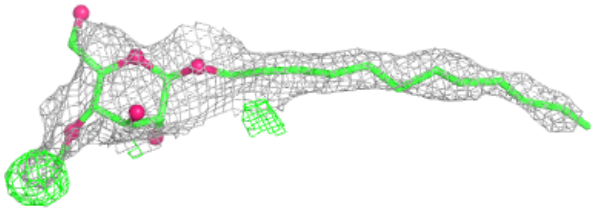


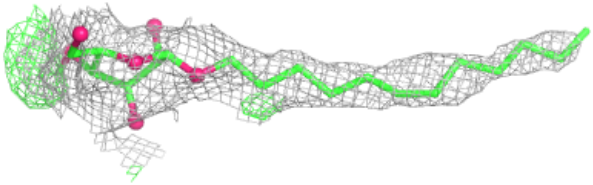


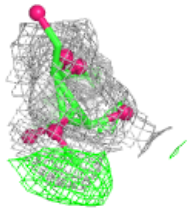


Electron density around LMT b 620:

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

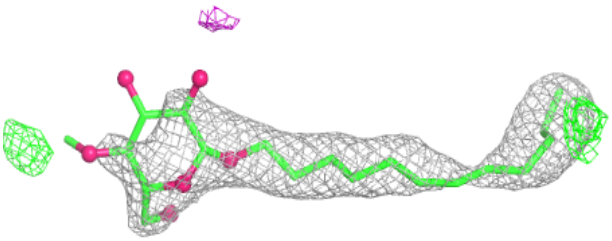


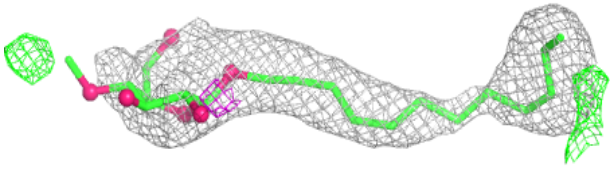


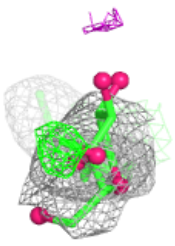


Electron density around LMT b 626:

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

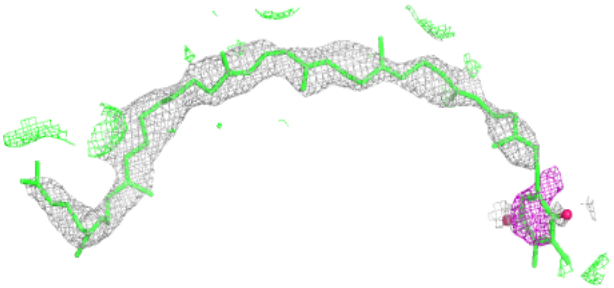


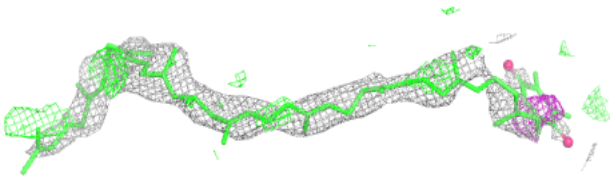


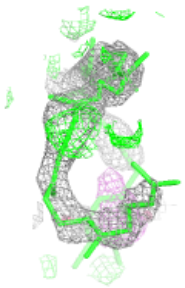


Electron density around PL9 A 413:

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

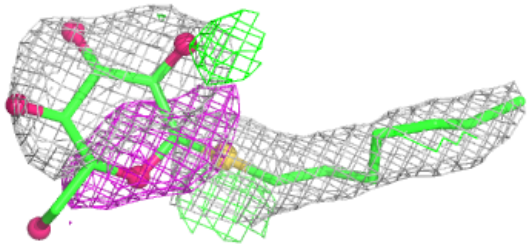


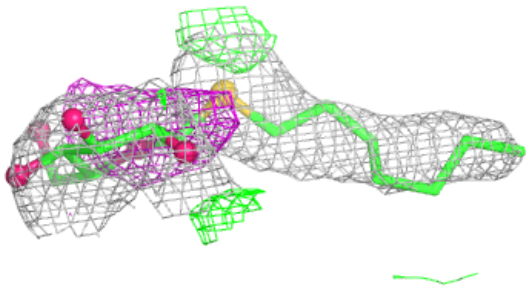


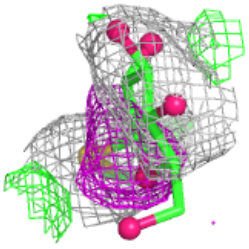


Electron density around HTG B 621:

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

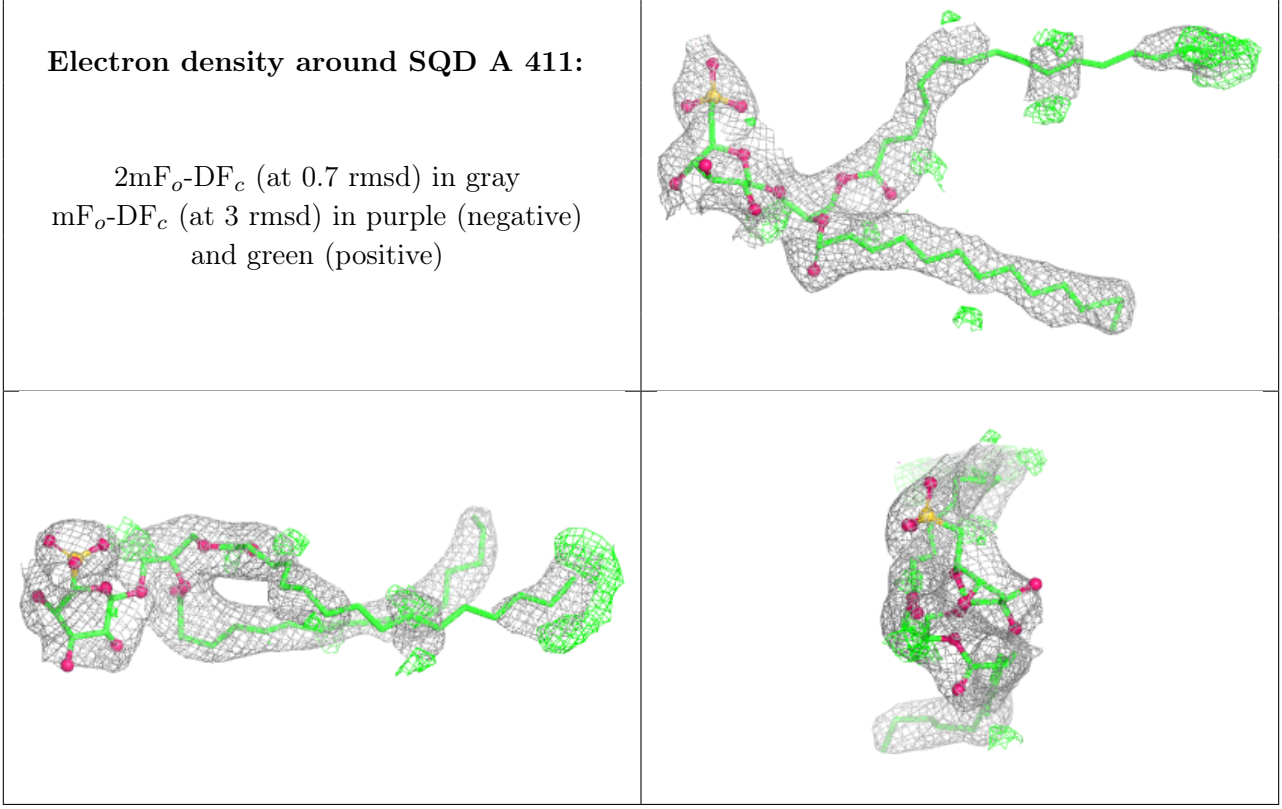






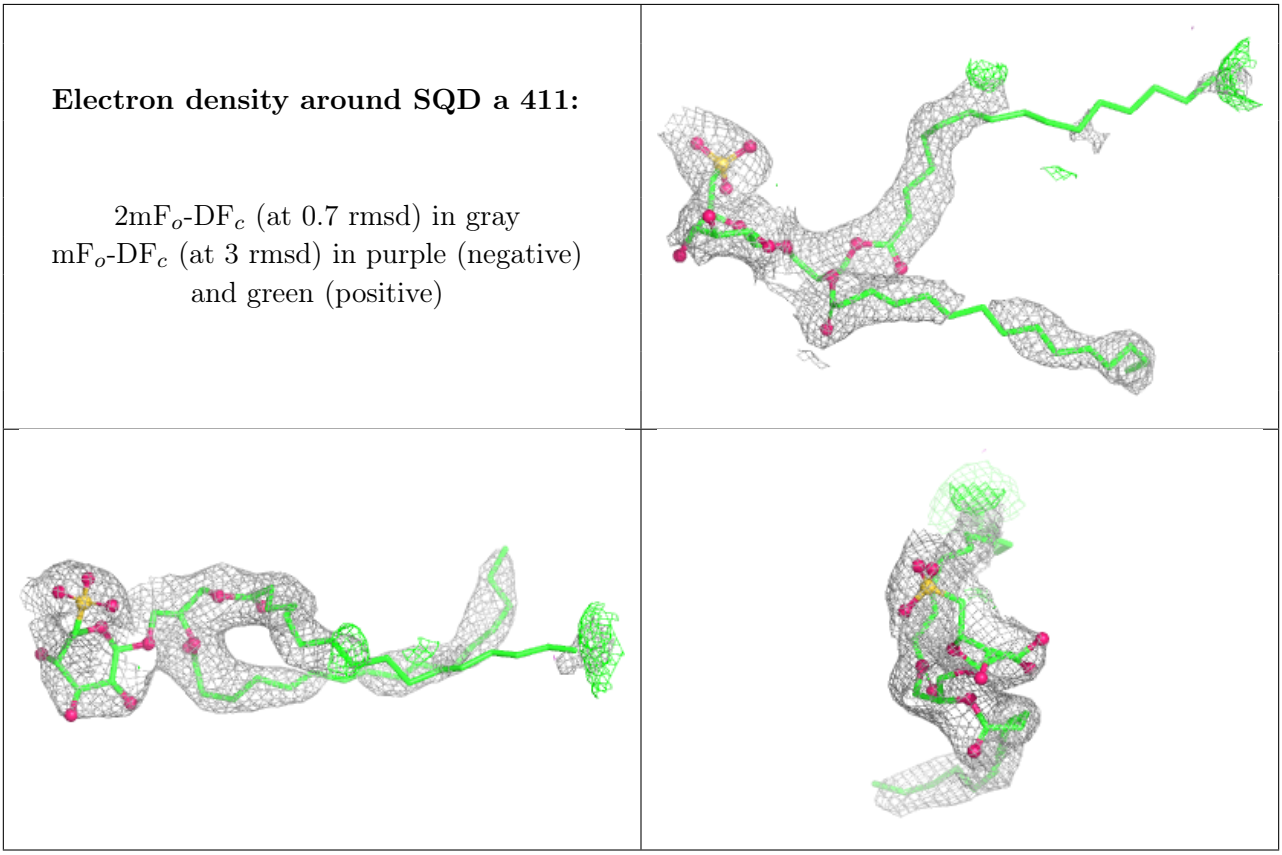
Electron density around SQD A 411:

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



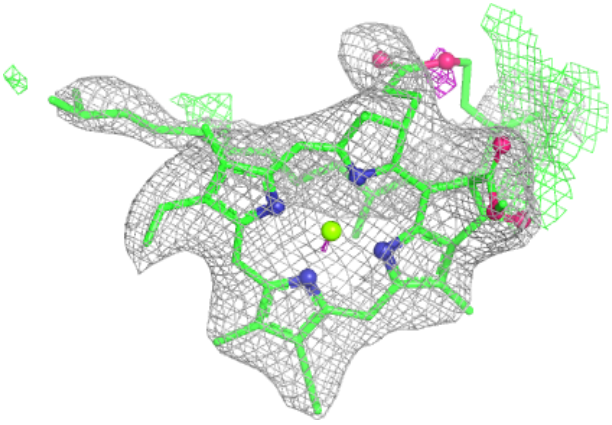
Electron density around SQD a 411:

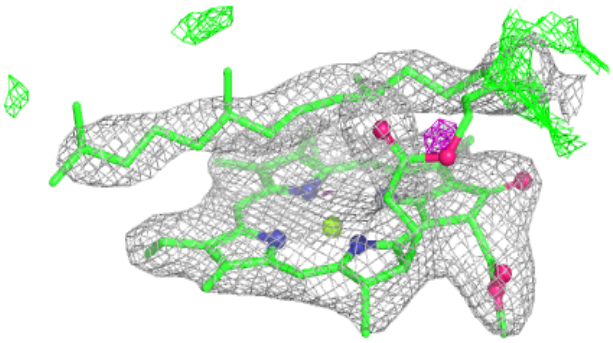
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

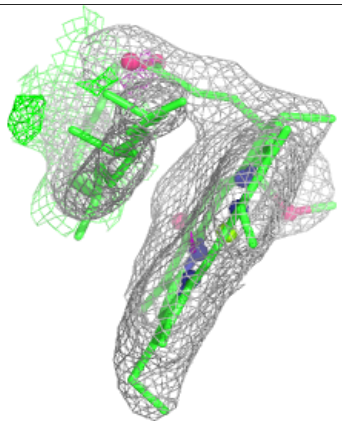


Electron density around CLA b 601:

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

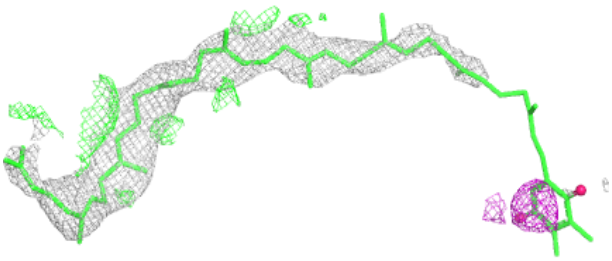


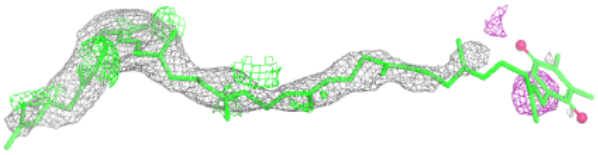


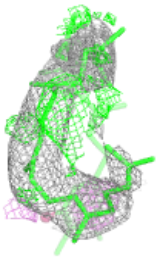


Electron density around PL9 a 414:

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

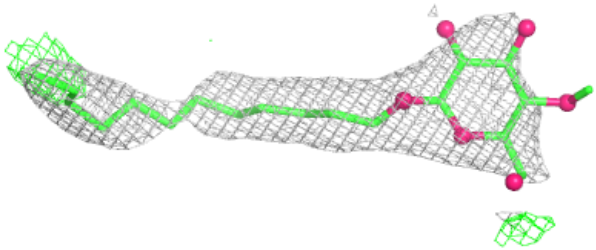


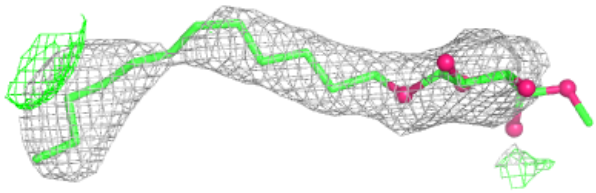


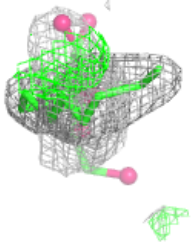


Electron density around LMT B 628:

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

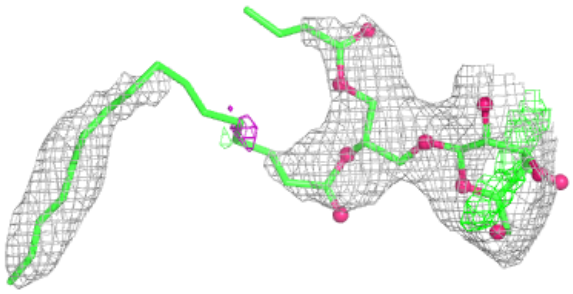


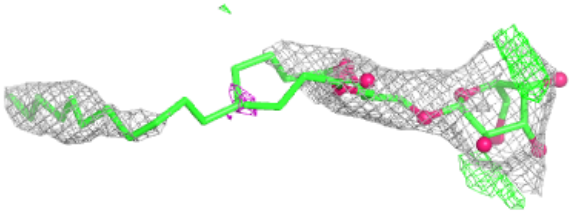


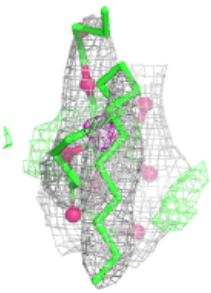


Electron density around LMG z 101:

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

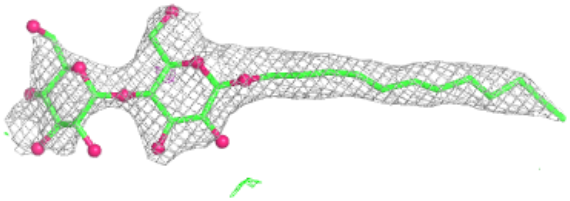


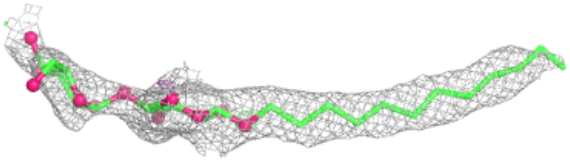


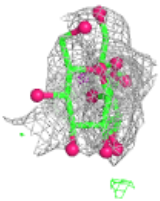


Electron density around LMT M 102:

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

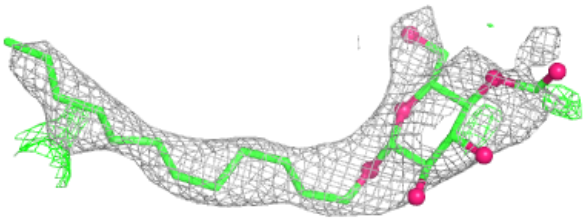


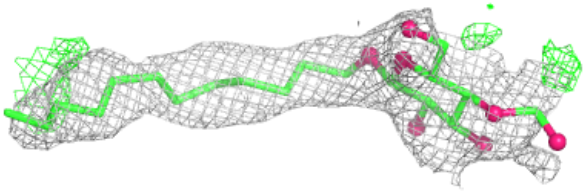


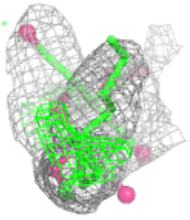


Electron density around LMT t 101:

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

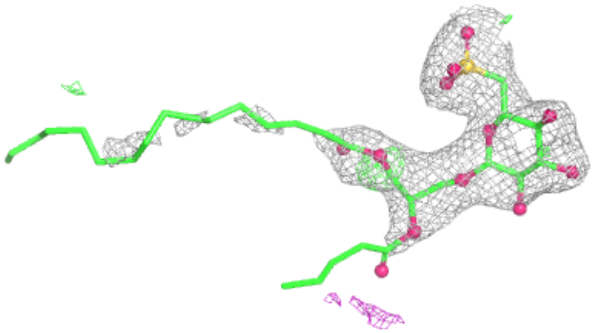


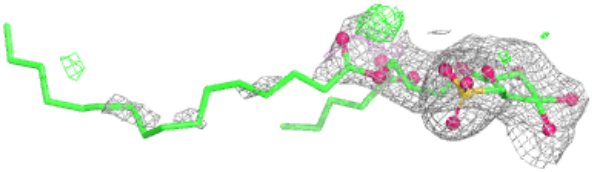


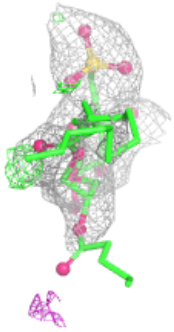


Electron density around SQD D 415:

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

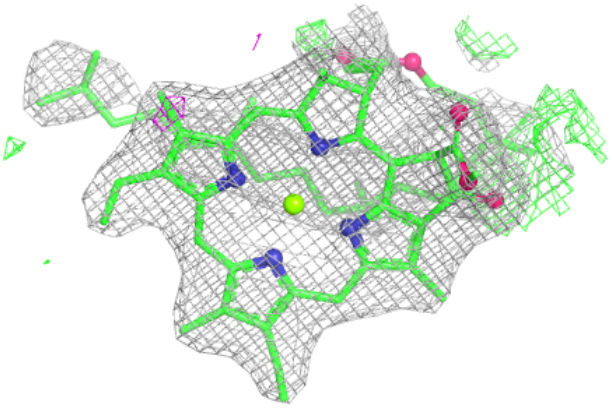


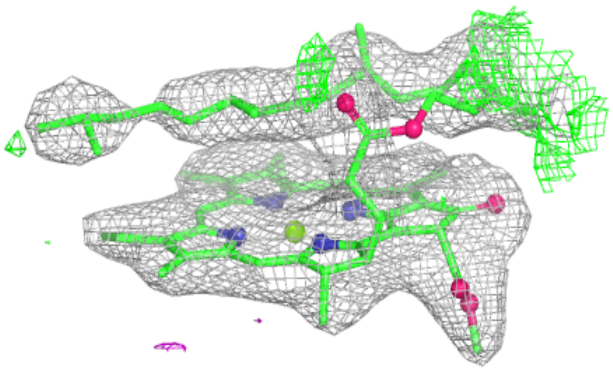


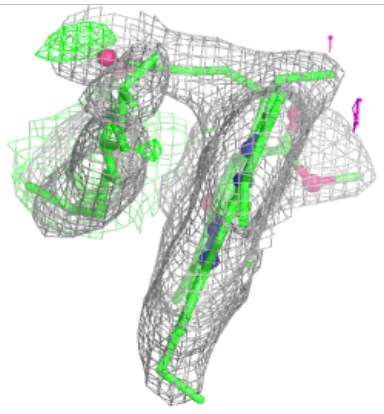


Electron density around CLA B 601:

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

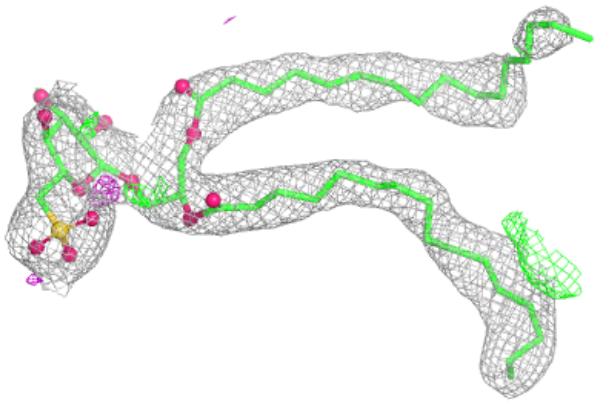


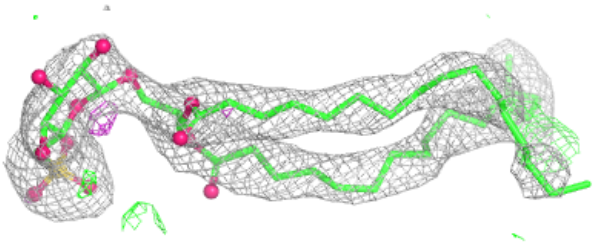


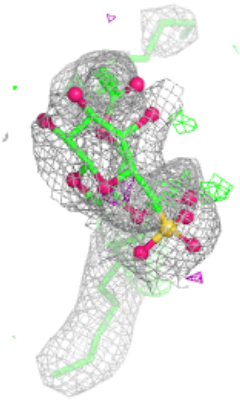


Electron density around SQD L 102:

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

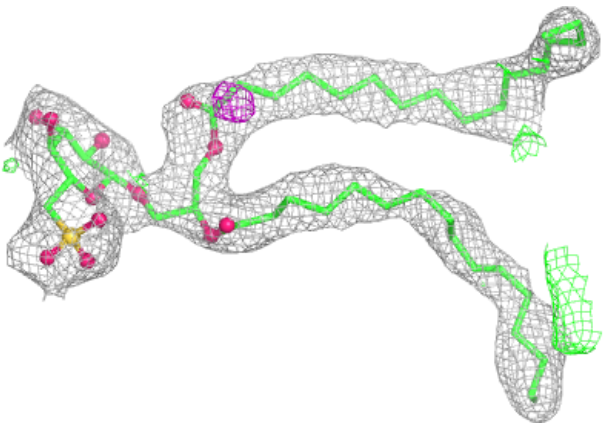


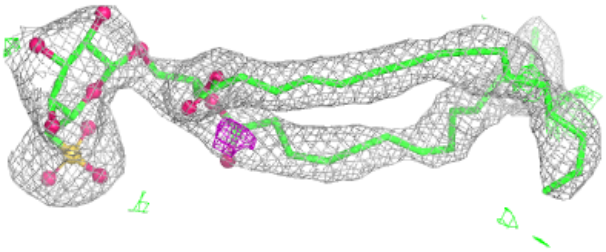


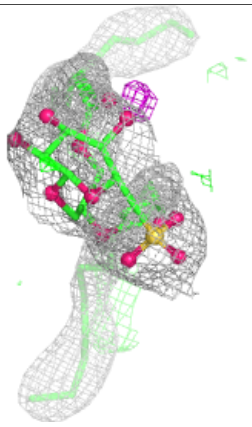


Electron density around SQD B 620:

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

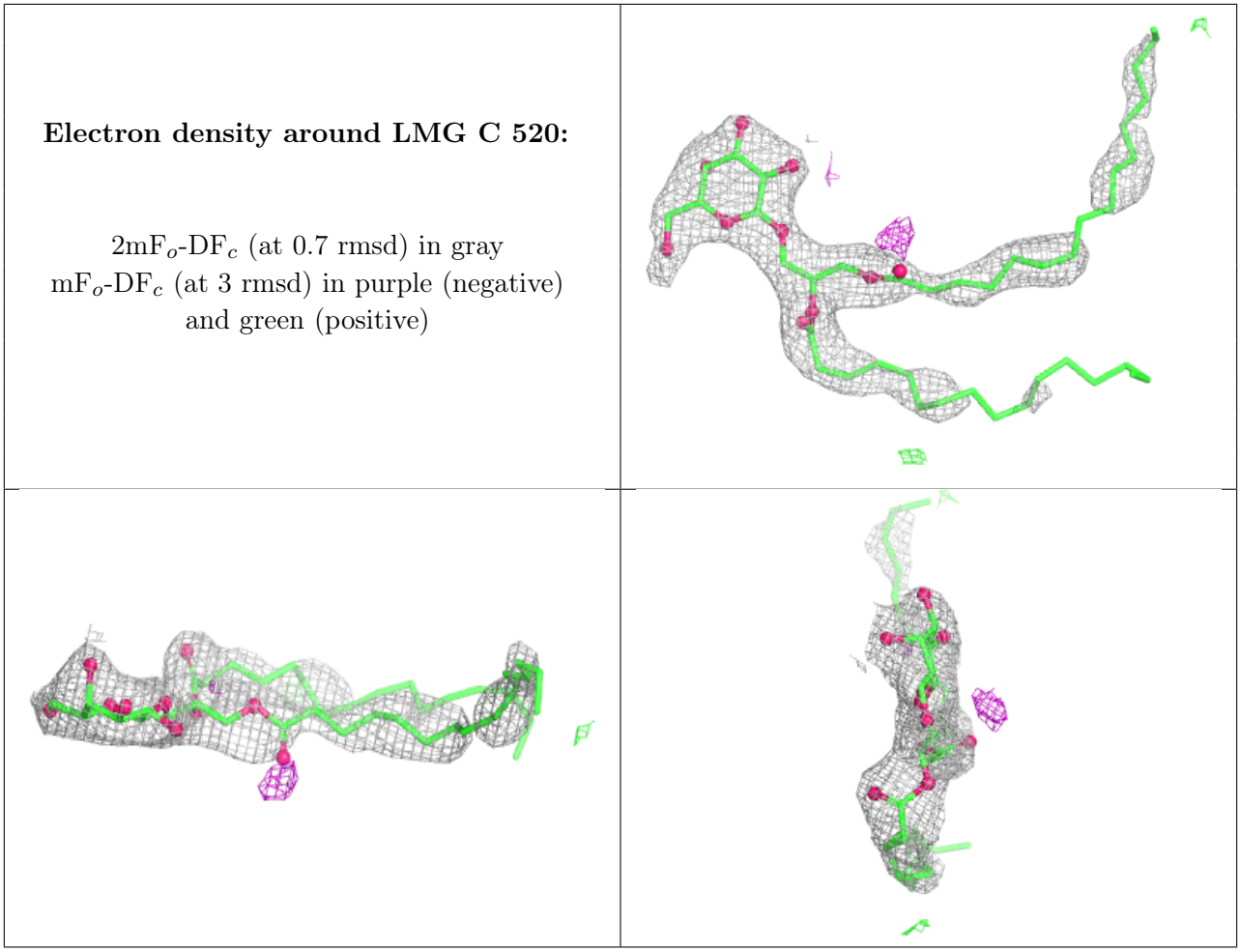






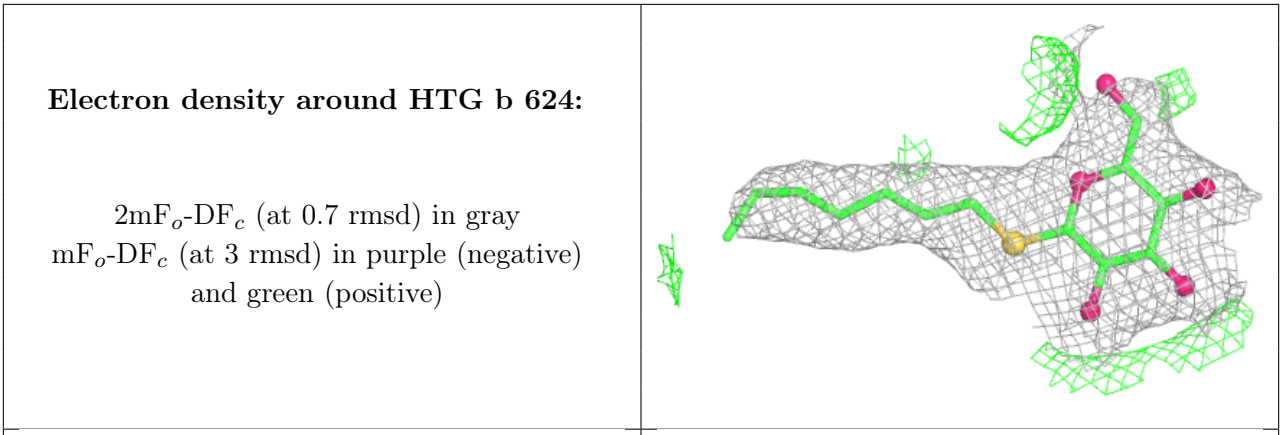
Electron density around LMG C 520:

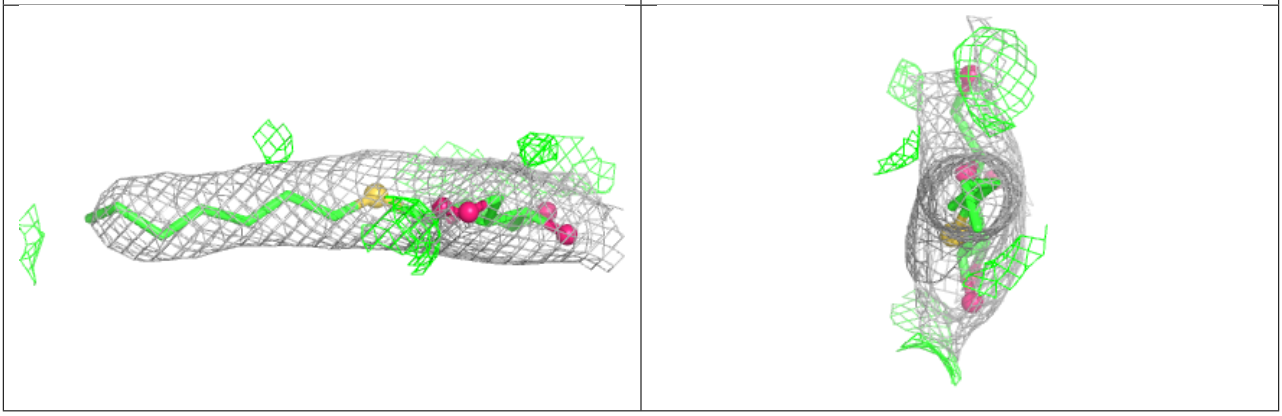
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HTG b 624:

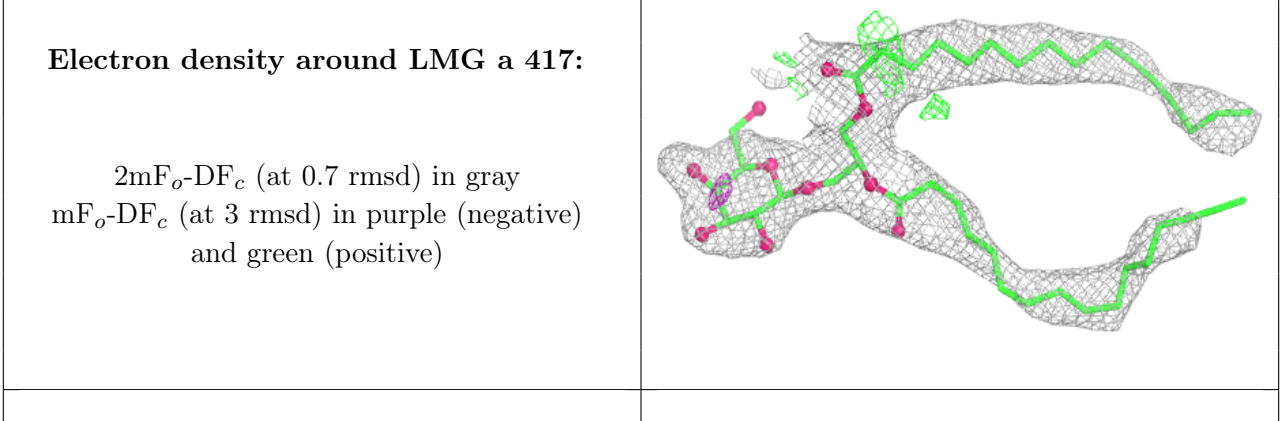
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

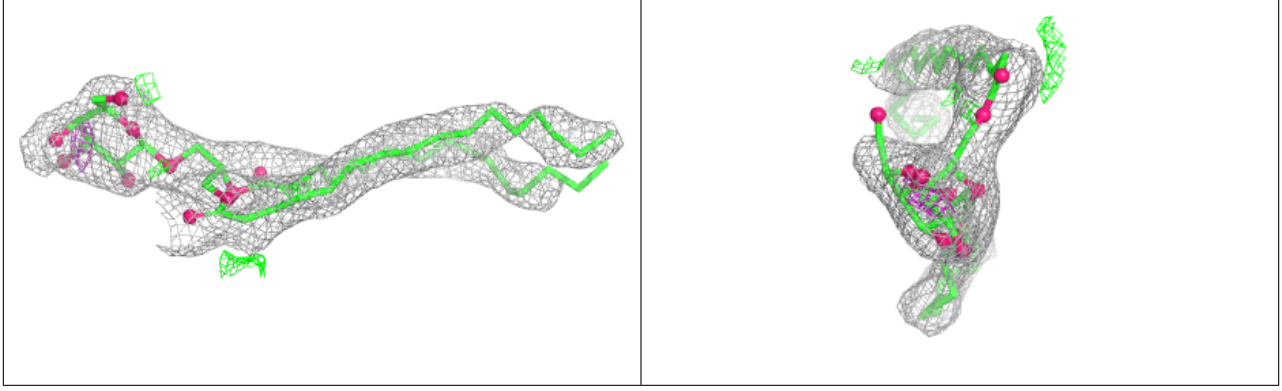




Electron density around LMG a 417:

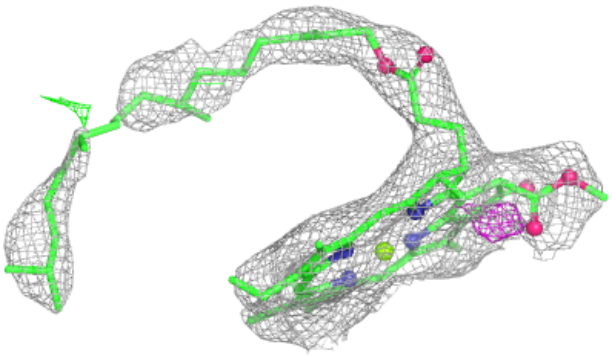
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

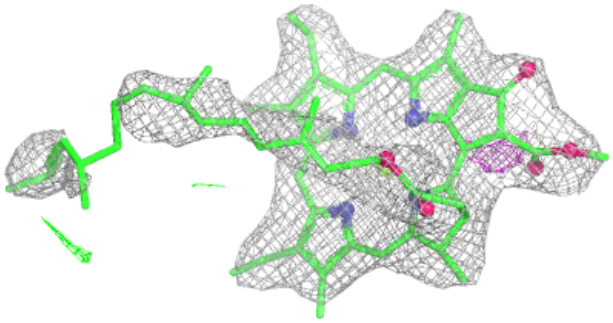


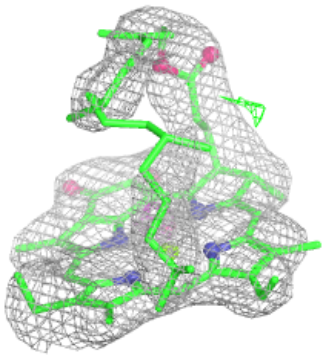


Electron density around CLA C 514:

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

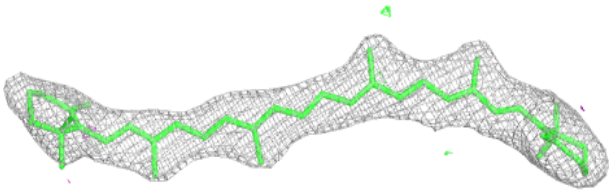


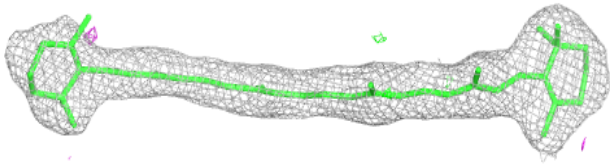


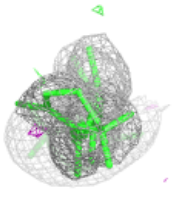


Electron density around BCR h 102:

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

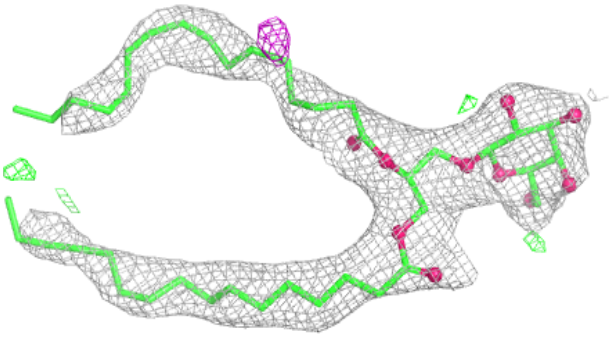


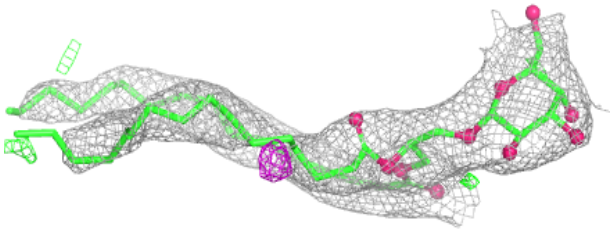


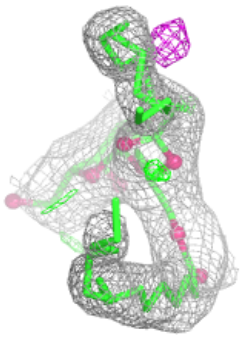


Electron density around LMG A 415:

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

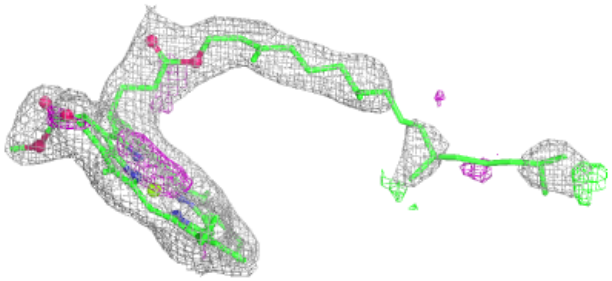


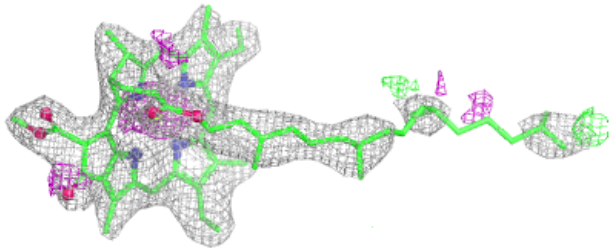


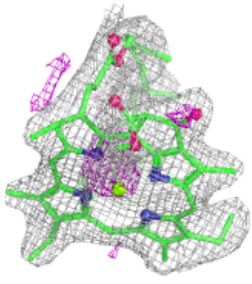


Electron density around CLA C 505:

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

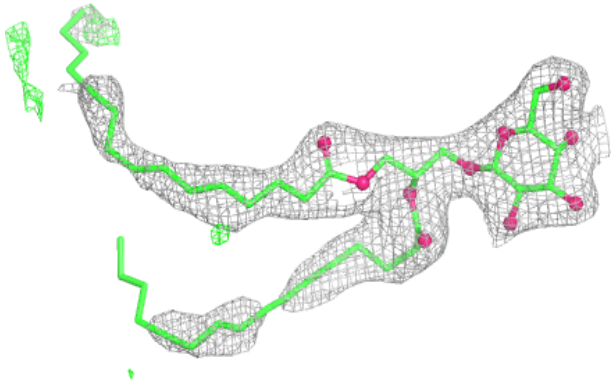




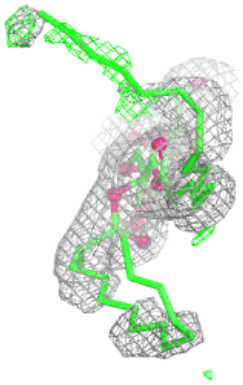


Electron density around LMG D 414:

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

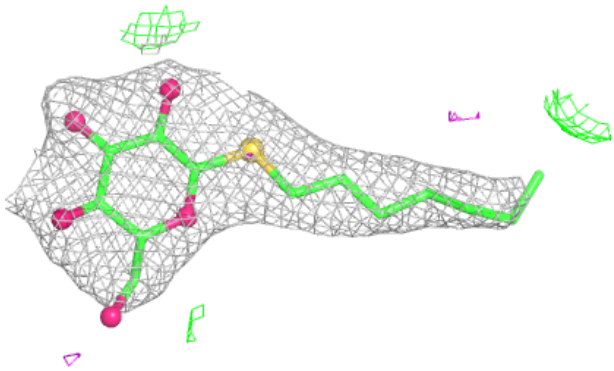


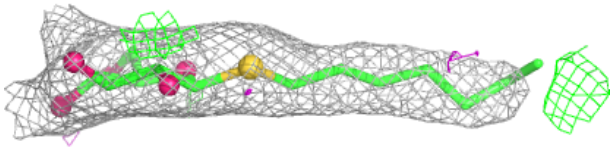


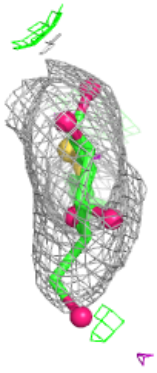


Electron density around HTG B 624:

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

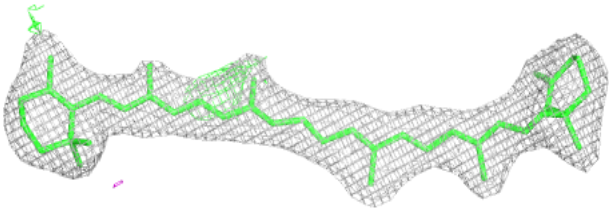


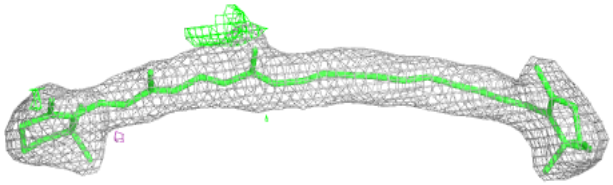


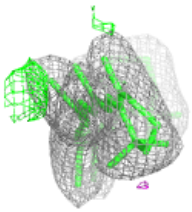


Electron density around BCR T 101:

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

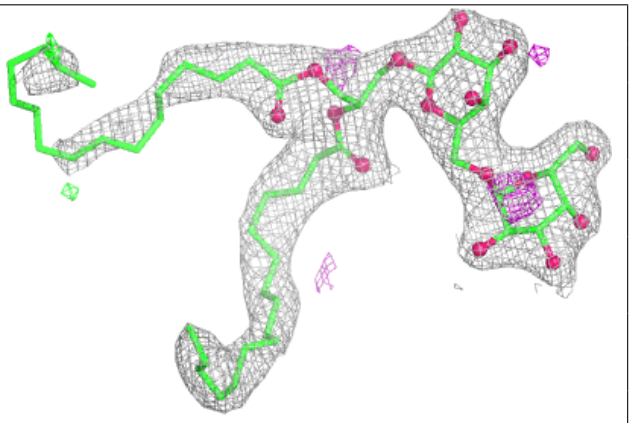


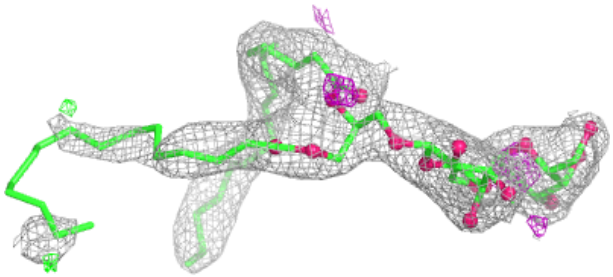




Electron density around DGD C 518:

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

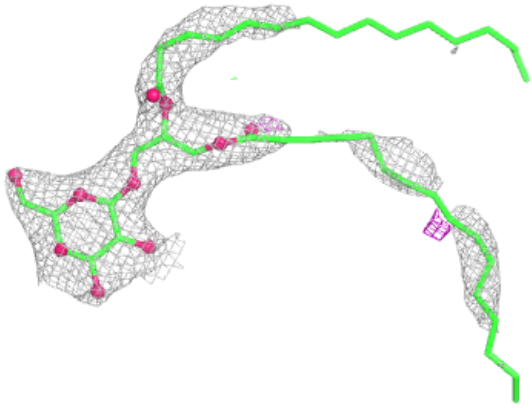


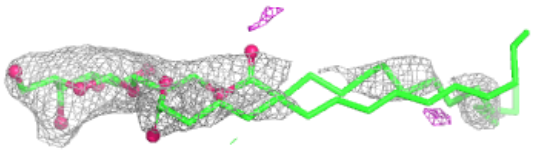


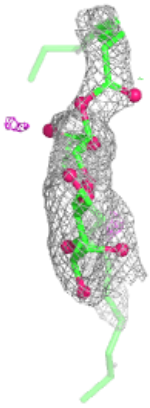


Electron density around LMG c 520:

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

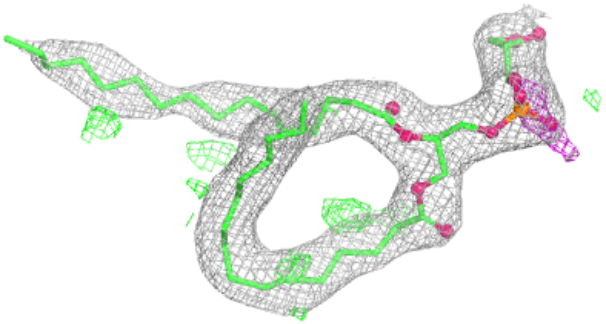


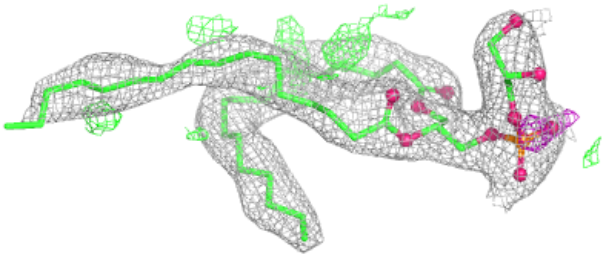


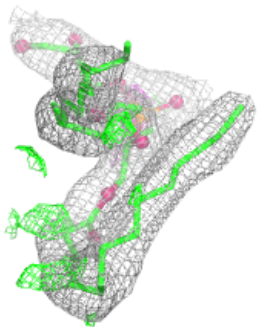


Electron density around LHG A 416:

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

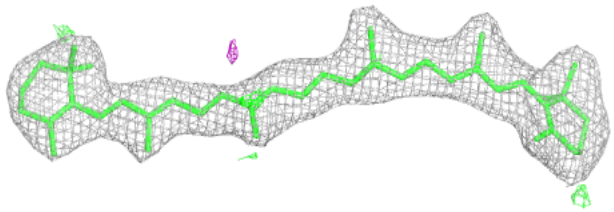


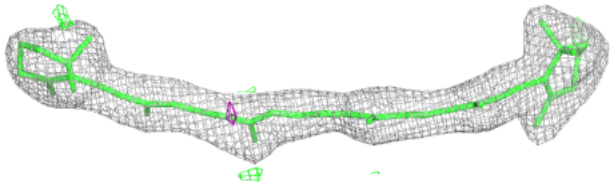


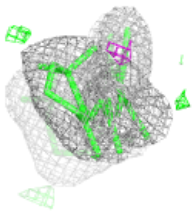


Electron density around BCR t 102:

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

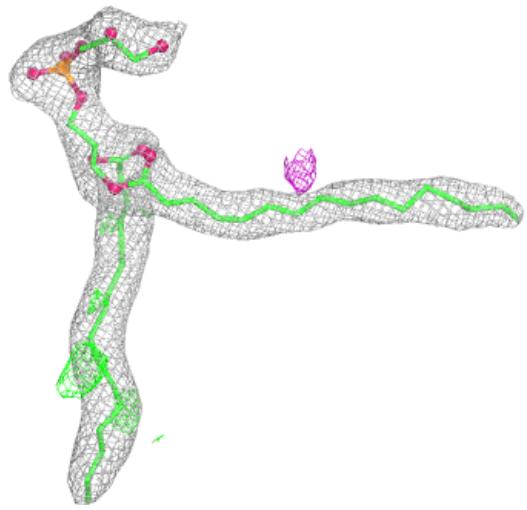


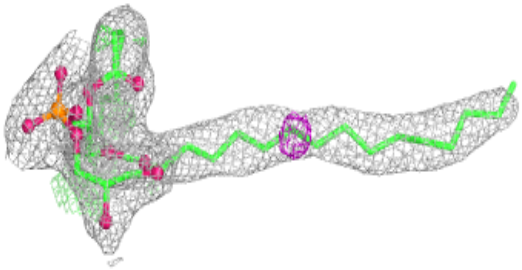


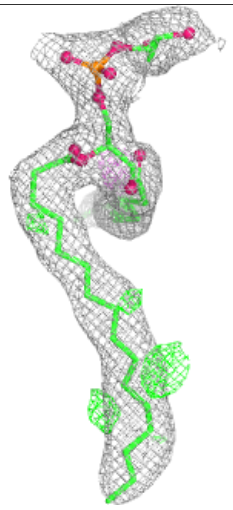


Electron density around LHG b 628:

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

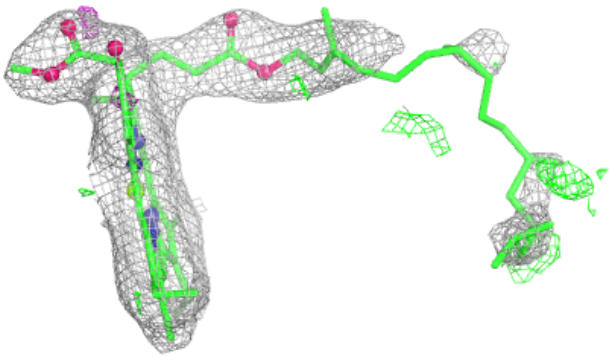


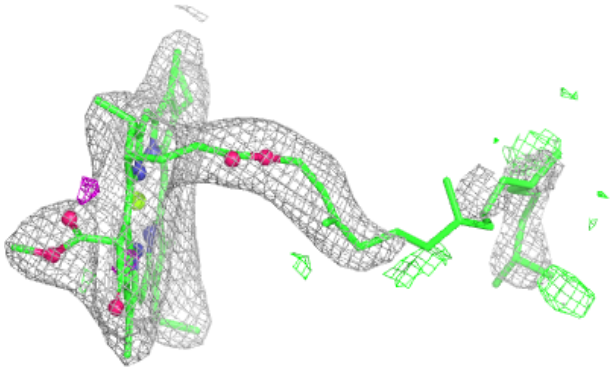


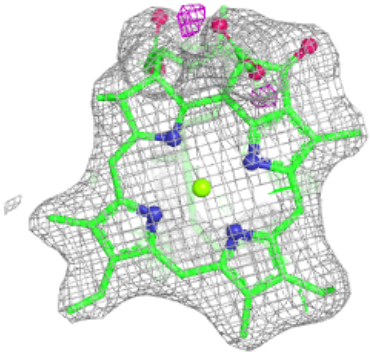


Electron density around CLA C 507:

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

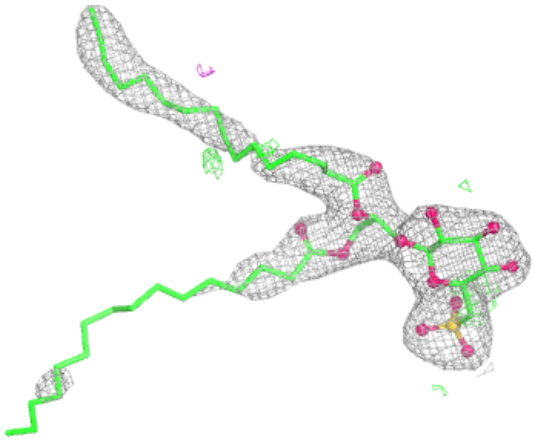


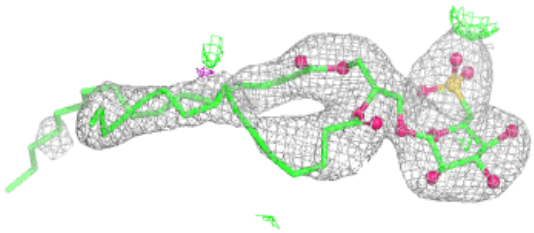


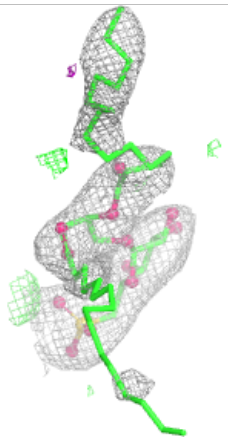


Electron density around SQD C 501:

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

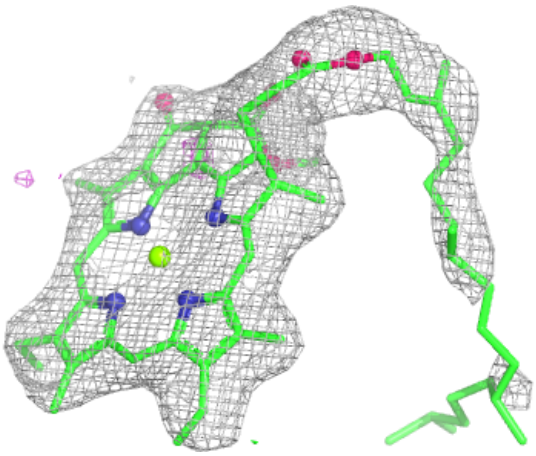


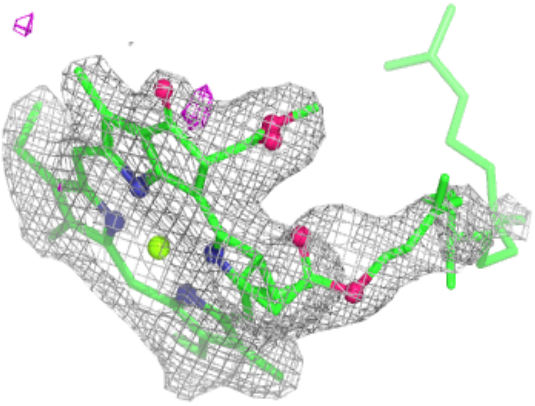


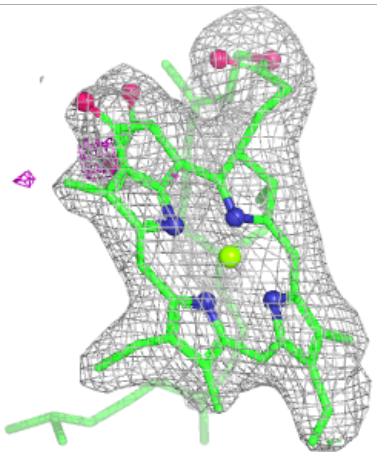


Electron density around CLA b 616:

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

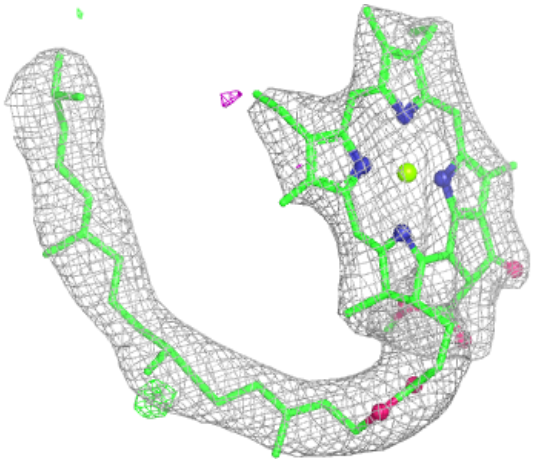


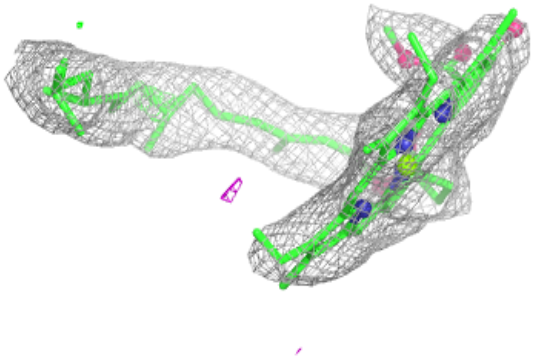


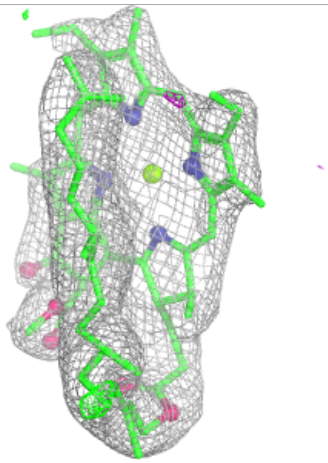


Electron density around CLA c 508:

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

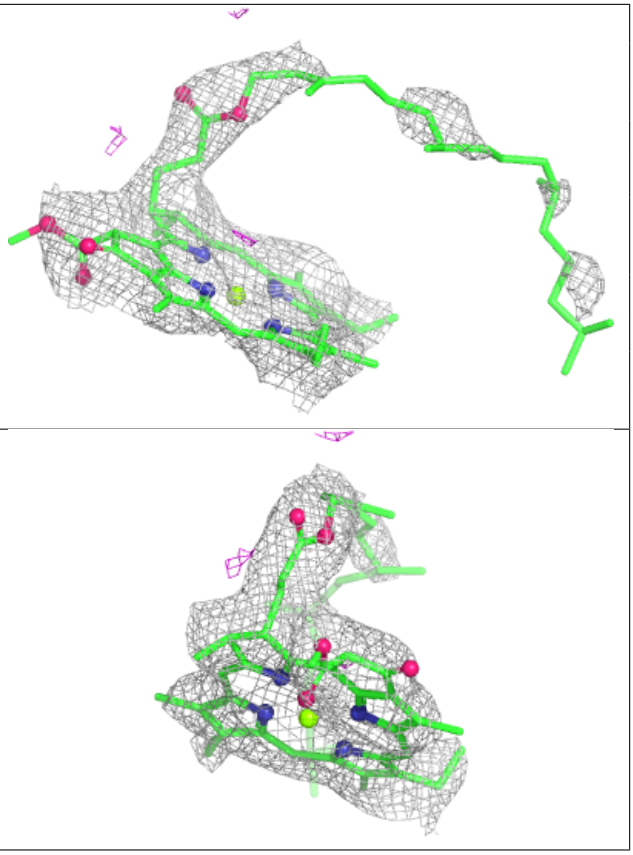






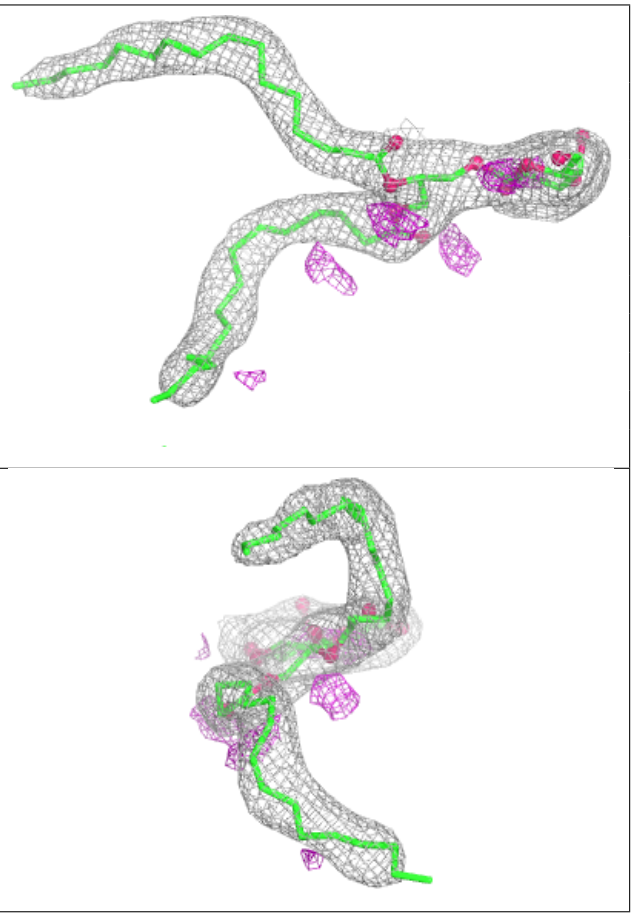
Electron density around CLA c 514:

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



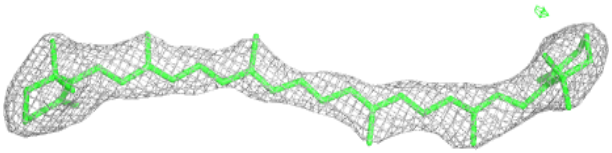
Electron density around LMG M 101:

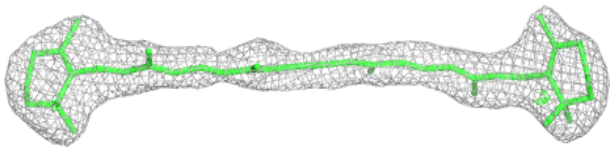
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

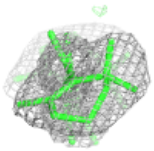


Electron density around BCR C 515:

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

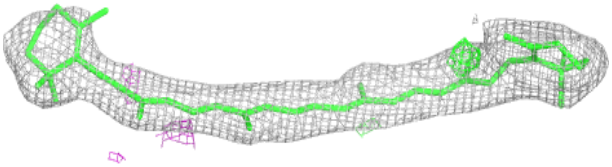


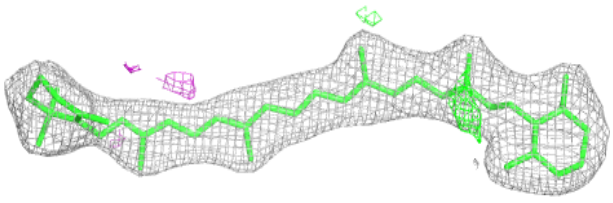


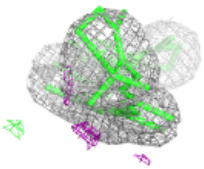


Electron density around BCR D 407:

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

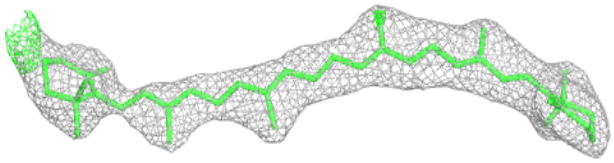


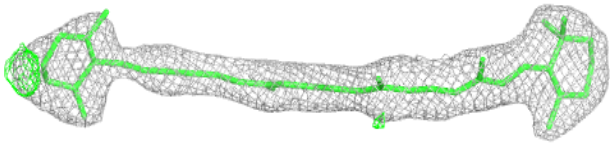


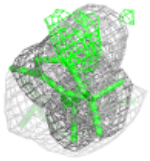


Electron density around BCR H 101:

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

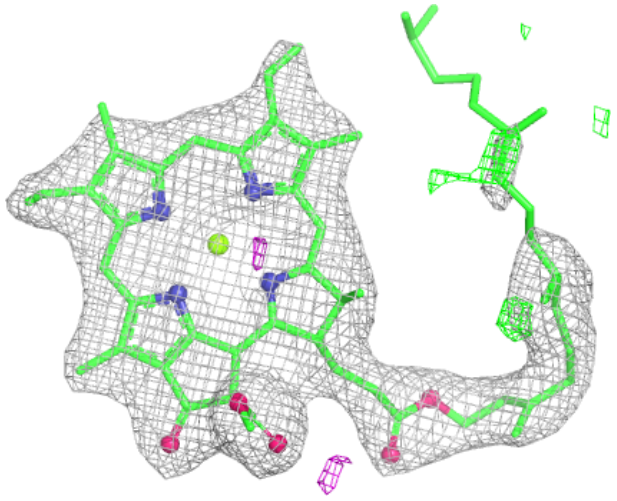


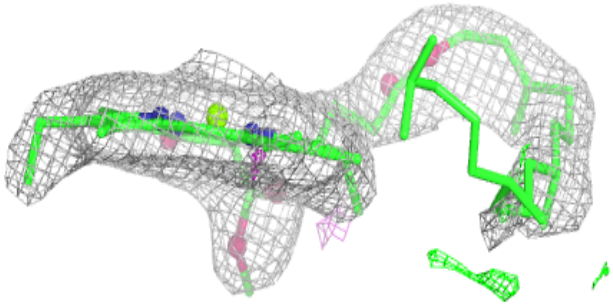


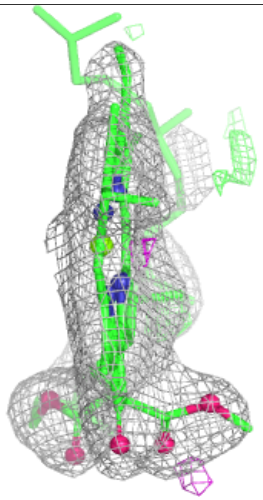


Electron density around CLA C 513:

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

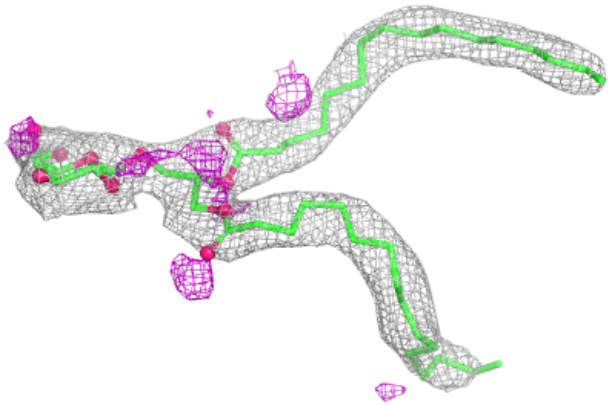


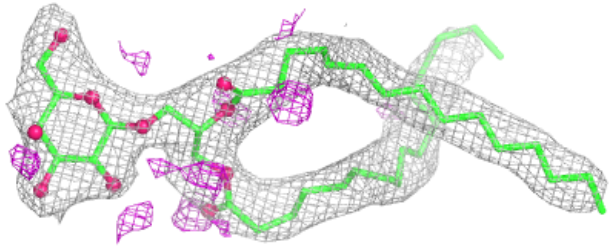


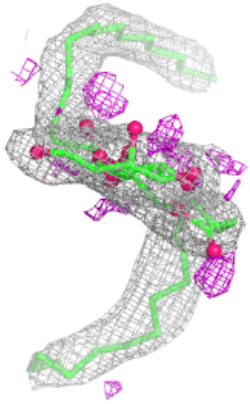


Electron density around LMG m 101:

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

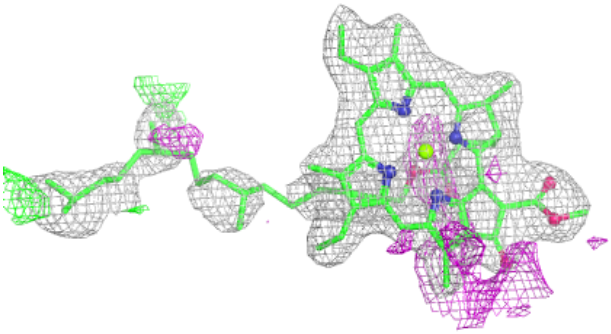


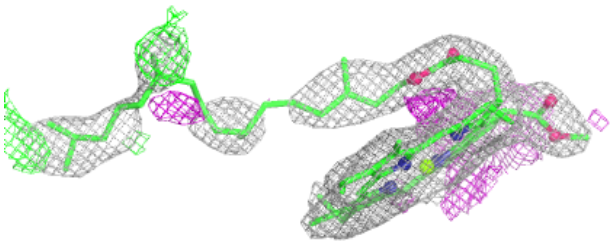


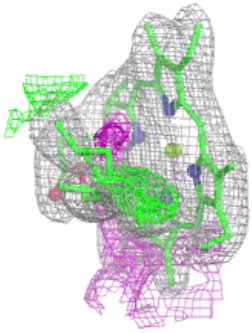


Electron density around CLA B 614:

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

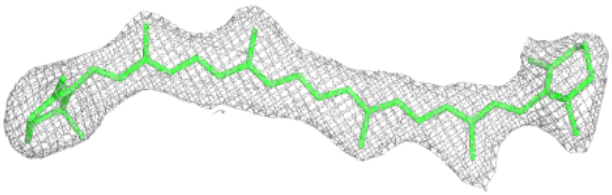


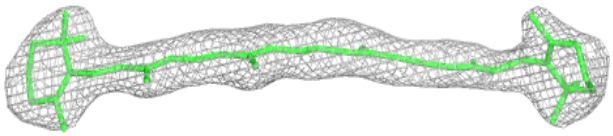


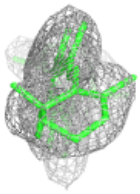


Electron density around BCR Y 101:

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

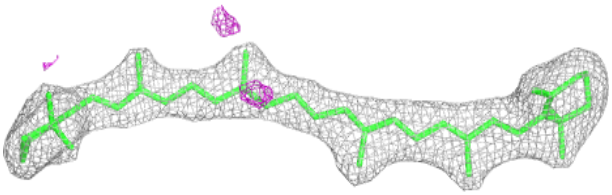


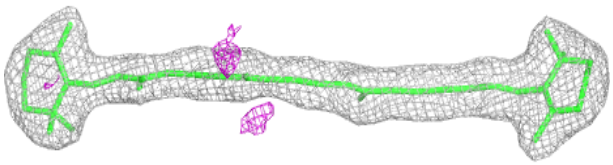


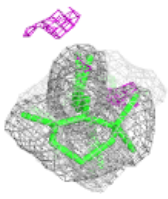


Electron density around BCR a 408:

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

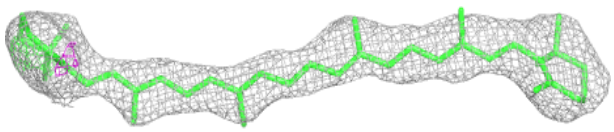


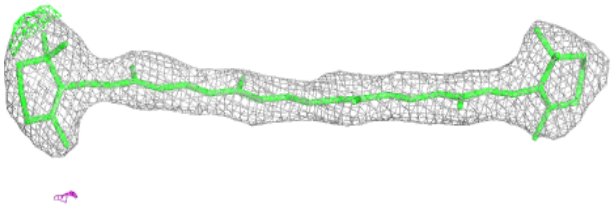


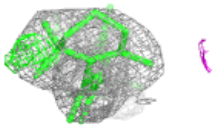


Electron density around BCR c 515:

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

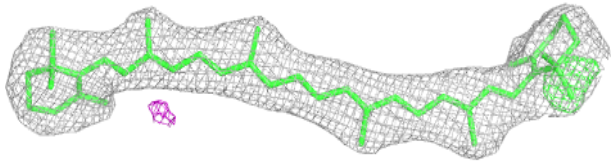


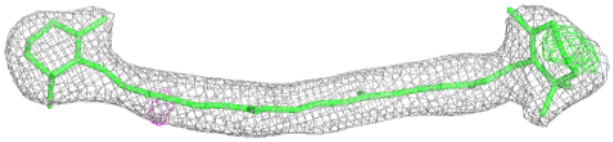


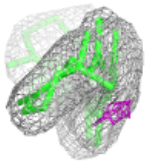


Electron density around BCR d 405:

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

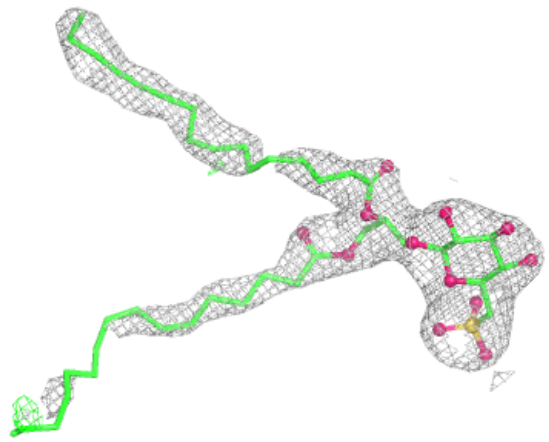


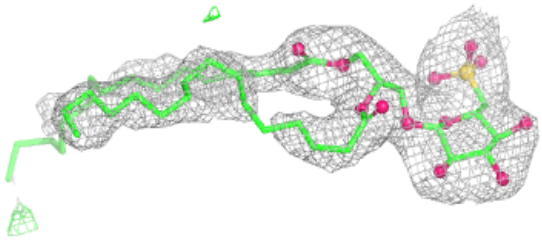


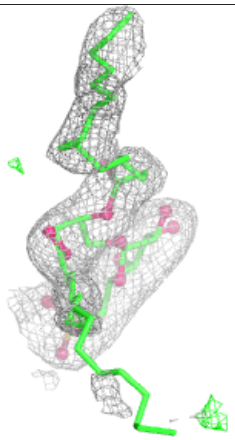


Electron density around SQD a 409:

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

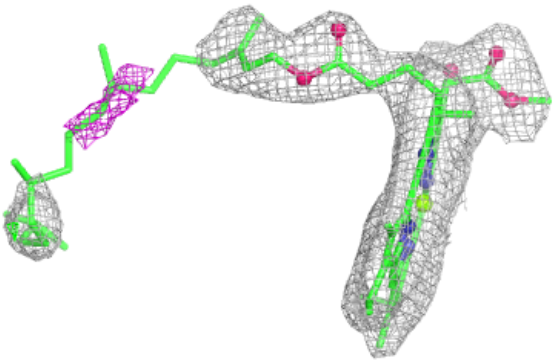


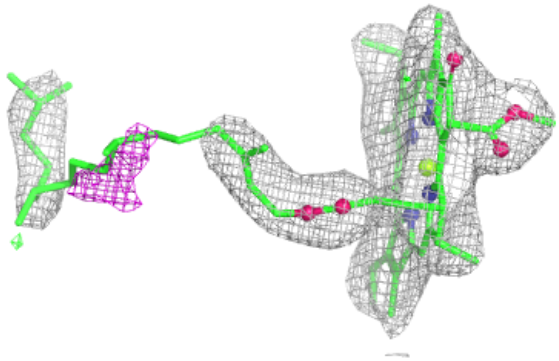


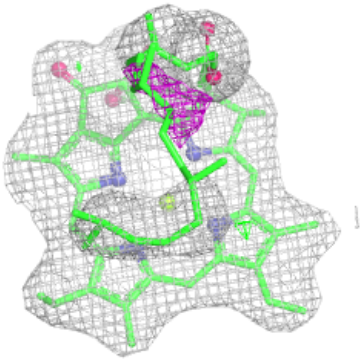


Electron density around CLA c 507:

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

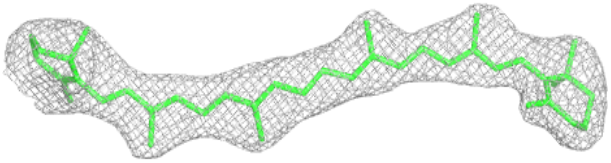


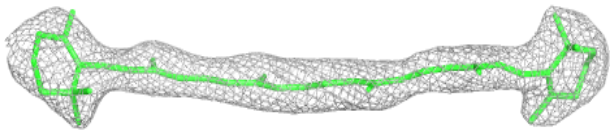


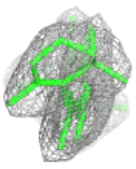


Electron density around BCR k 102:

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

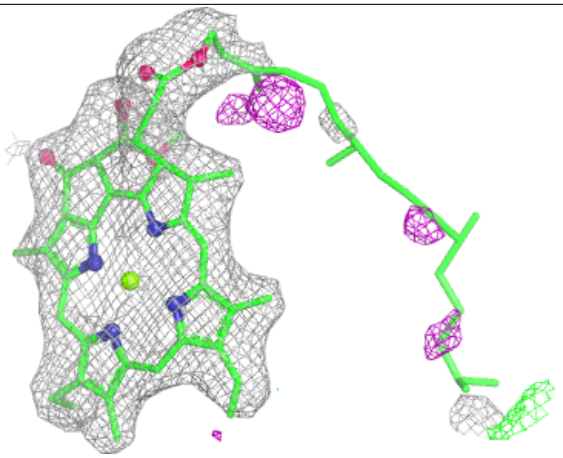


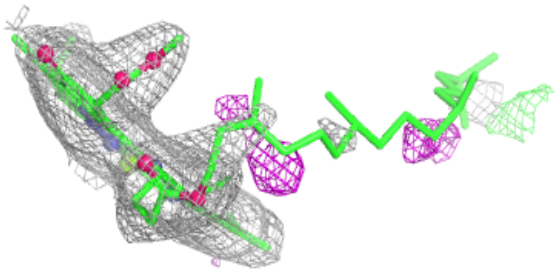


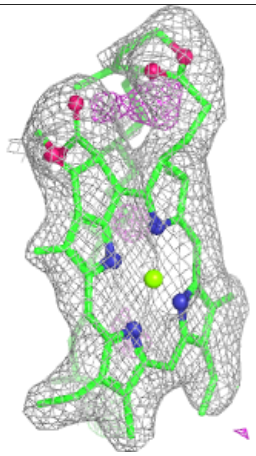


Electron density around CLA B 616:

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

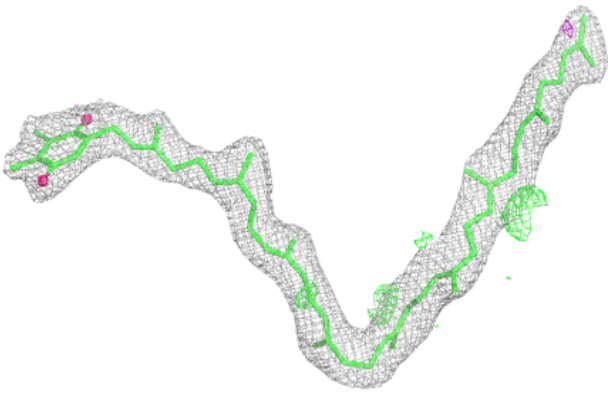


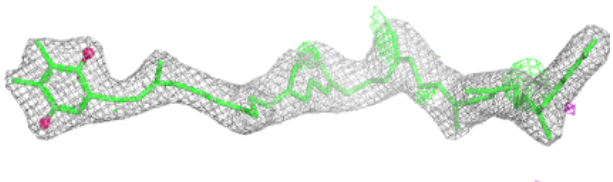


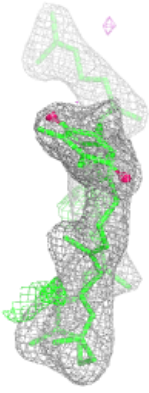


Electron density around PL9 D 408:

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

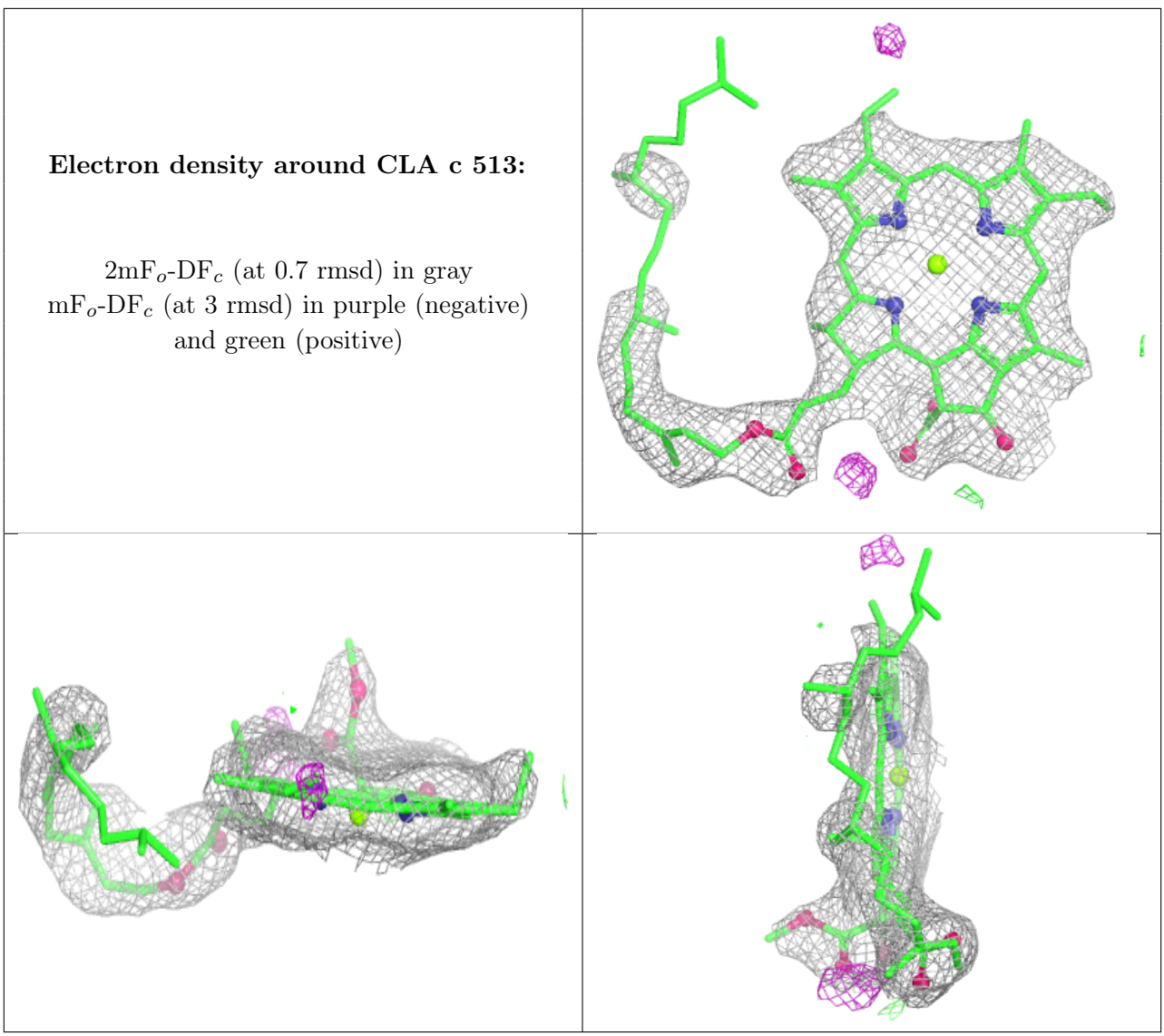






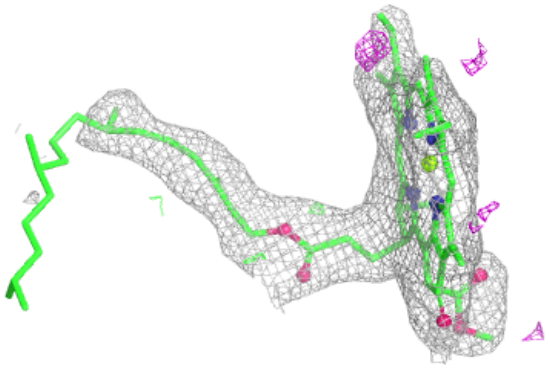
Electron density around CLA c 513:

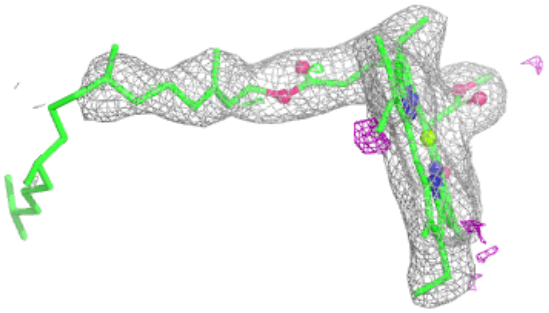
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

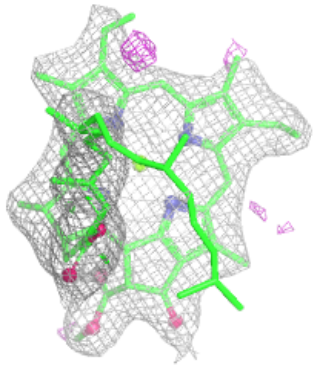


Electron density around CLA D 406:

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

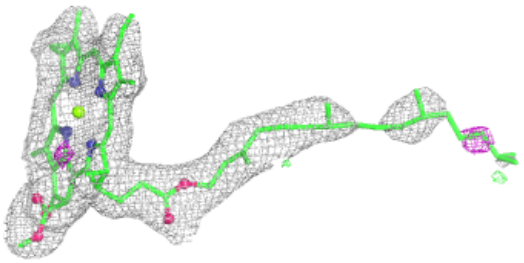


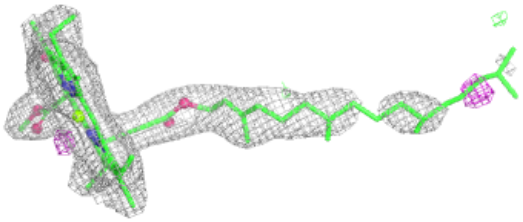


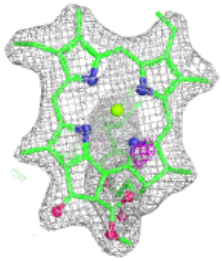


Electron density around CLA d 404:

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

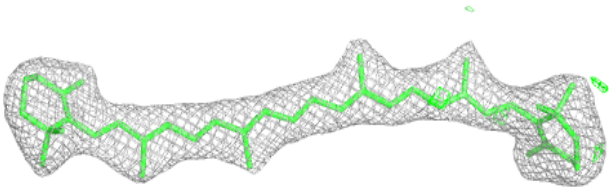


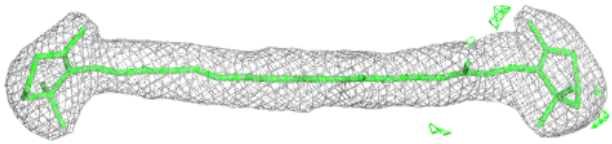


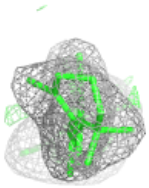


Electron density around BCR B 618:

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

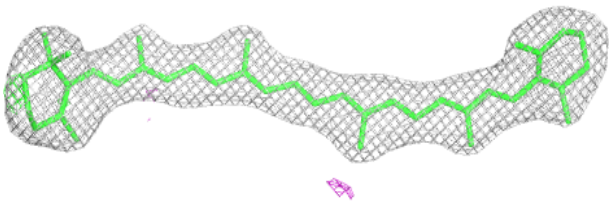


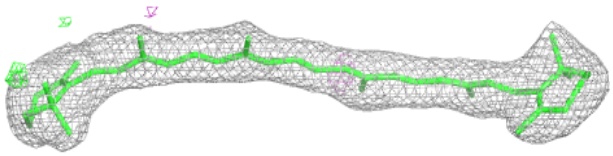


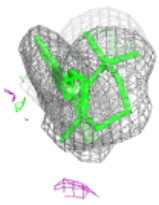


Electron density around BCR B 619:

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

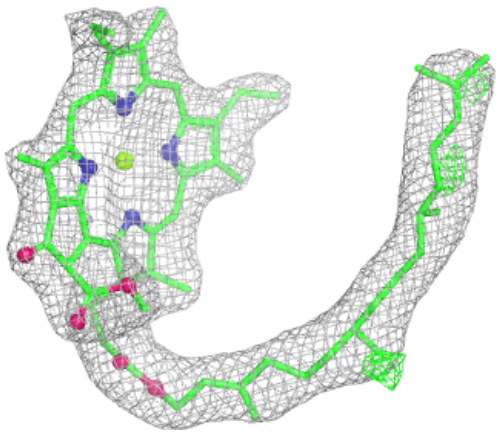


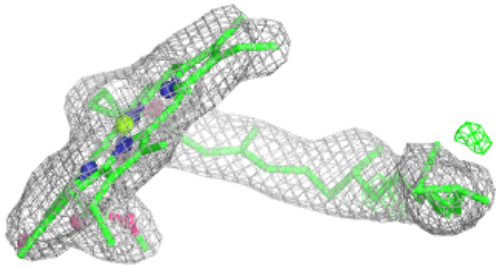


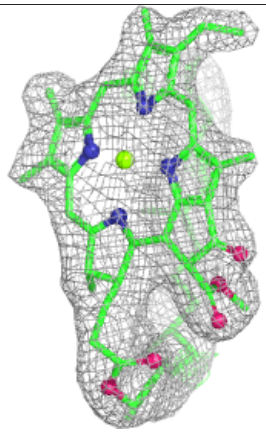


Electron density around CLA C 508:

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

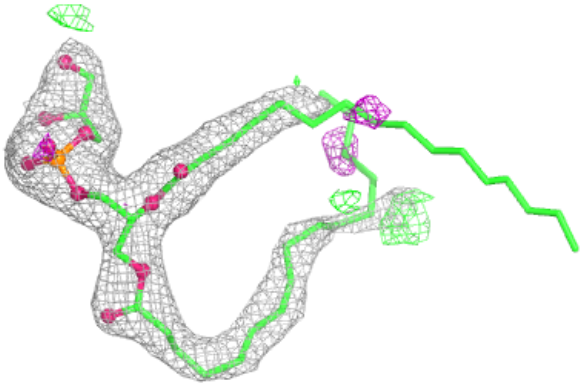


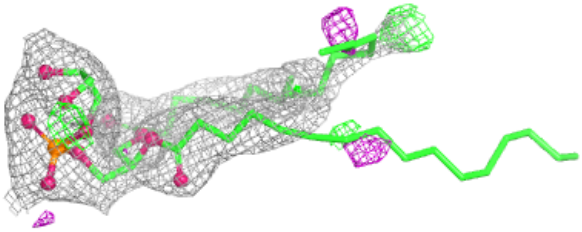


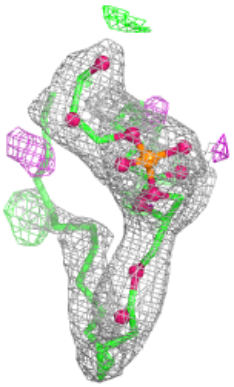


Electron density around LHG D 410:

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

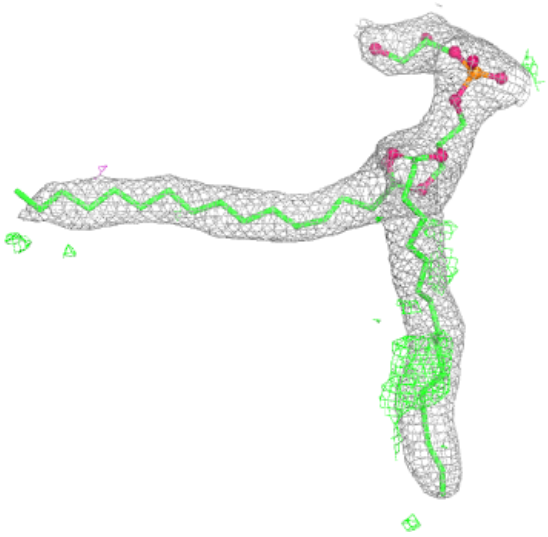


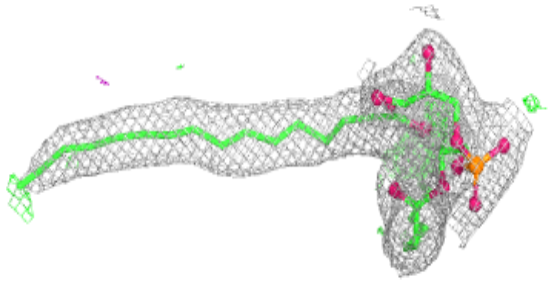


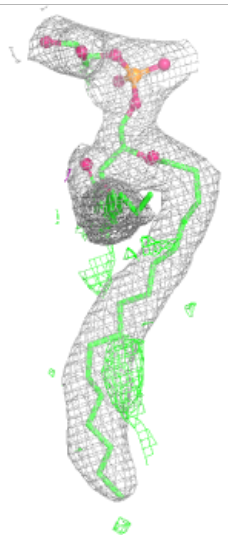


Electron density around LHG L 101:

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

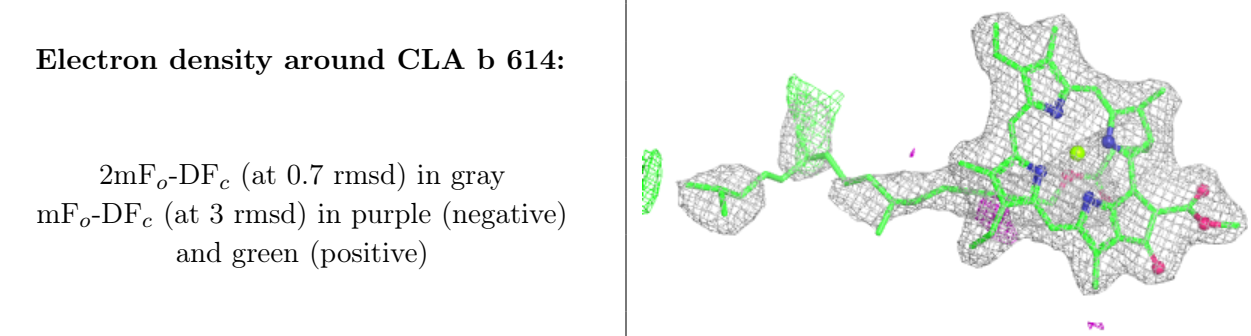


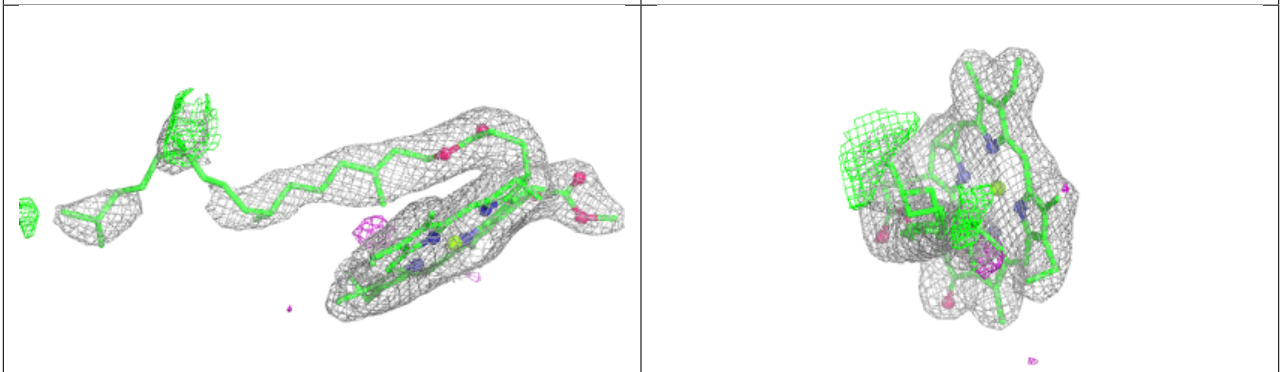




Electron density around CLA b 614:

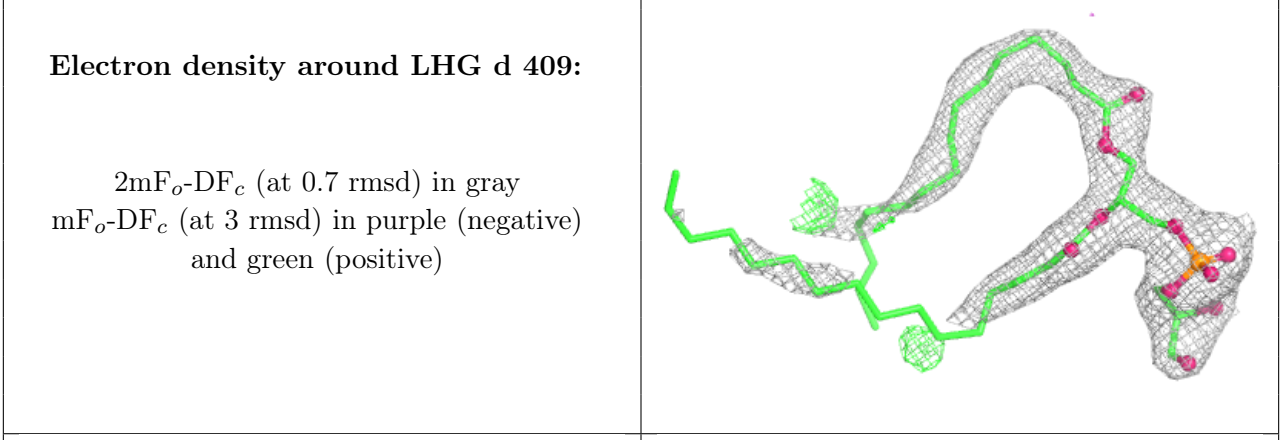
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

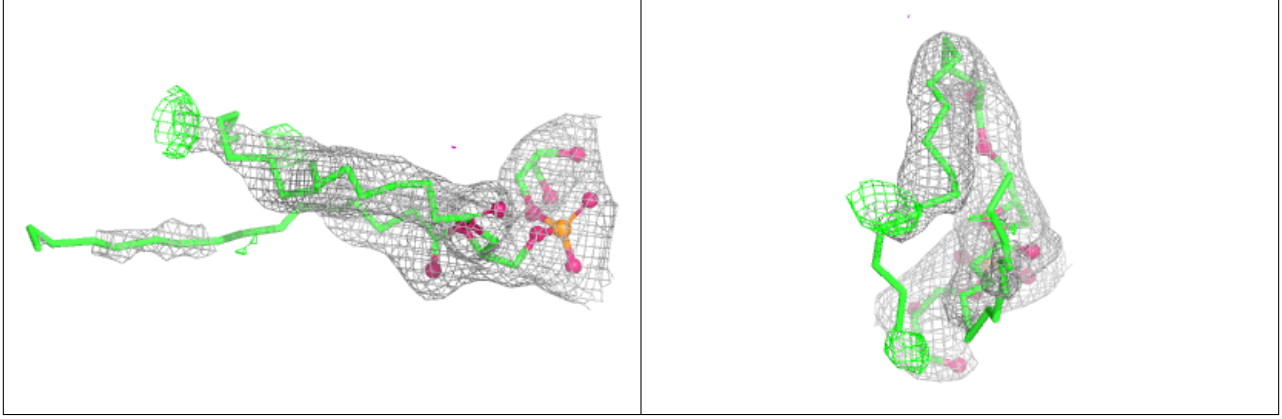




Electron density around LHG d 409:

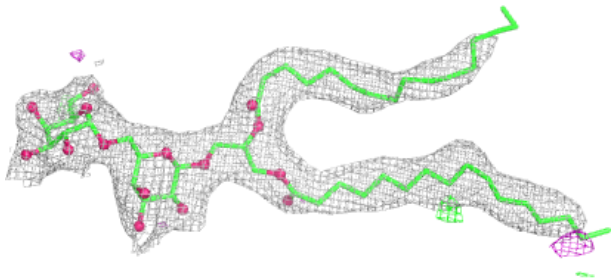
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

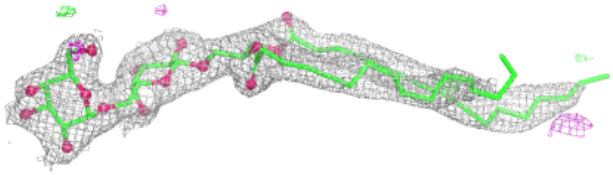




Electron density around DGD C 519:

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

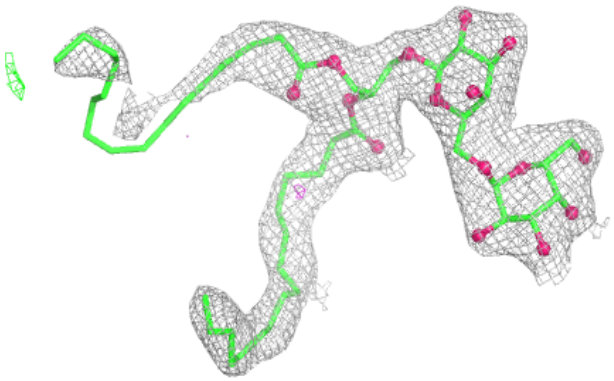


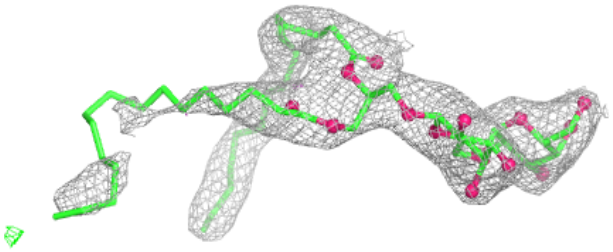


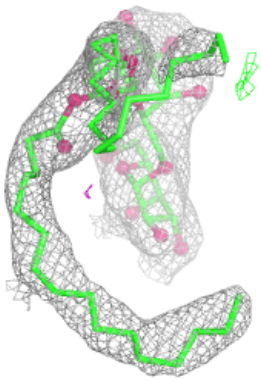


Electron density around DGD c 518:

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

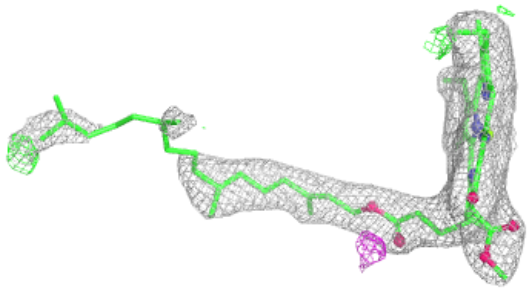


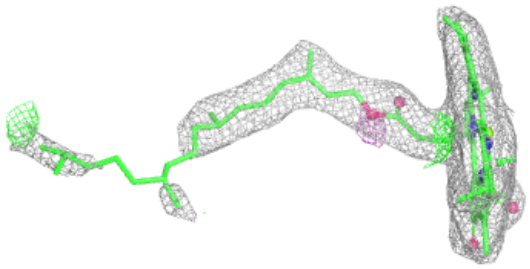


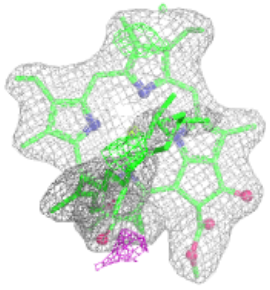


Electron density around CLA B 606:

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

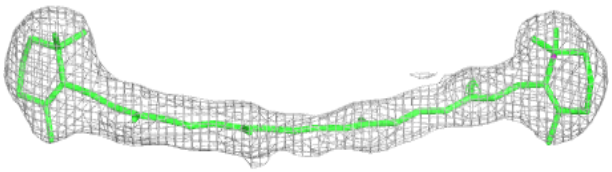


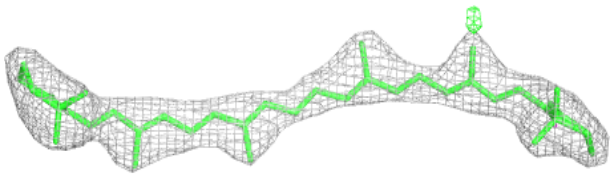


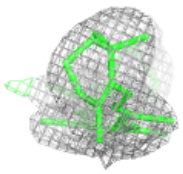


Electron density around BCR K 101:

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

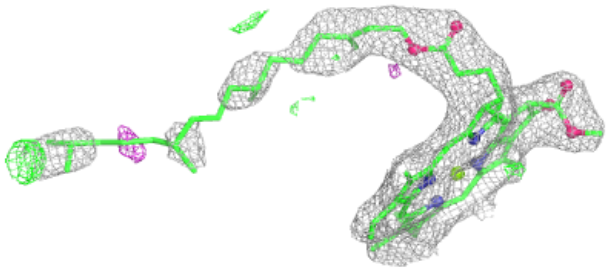


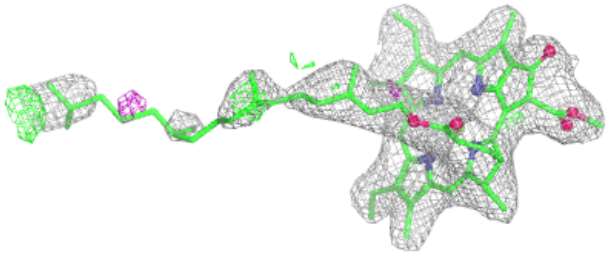


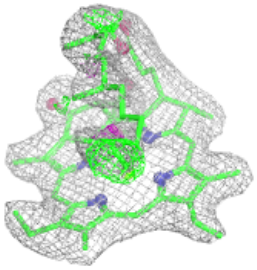


Electron density around CLA c 505:

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

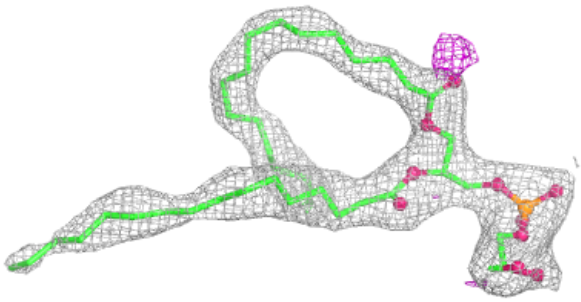


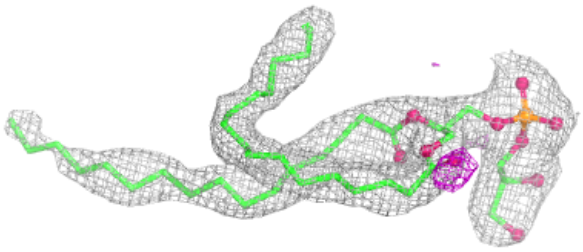


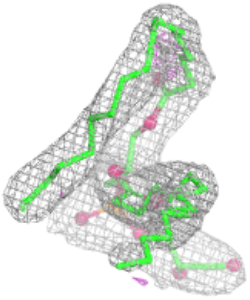


Electron density around LHG d 407:

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

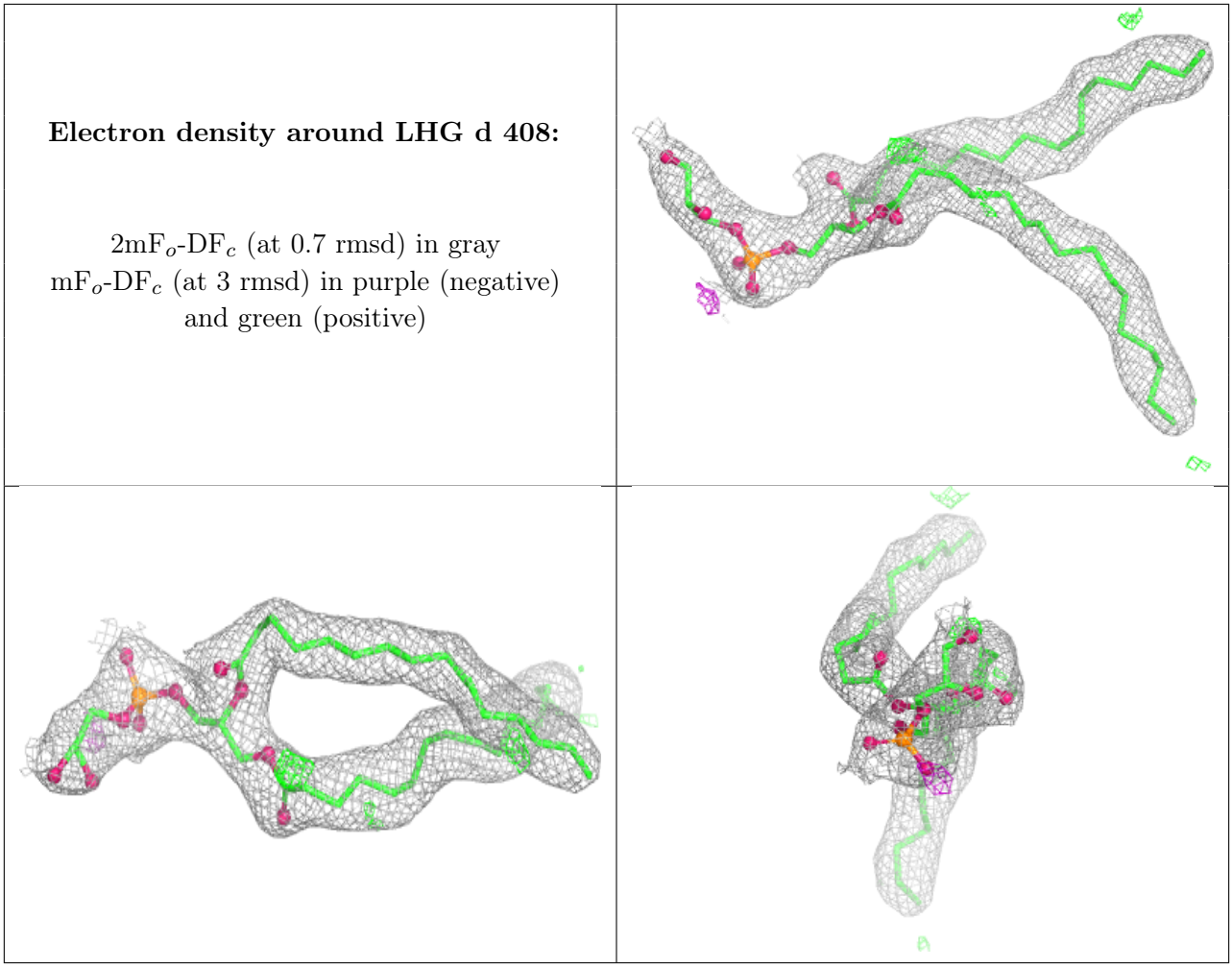






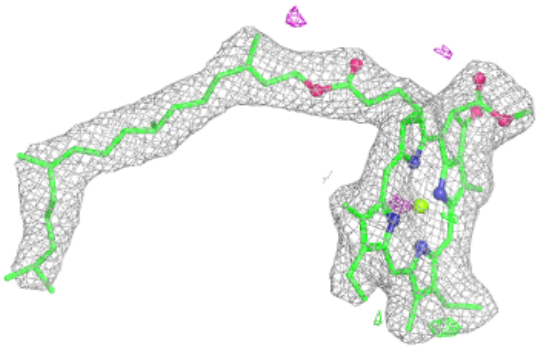
Electron density around LHG d 408:

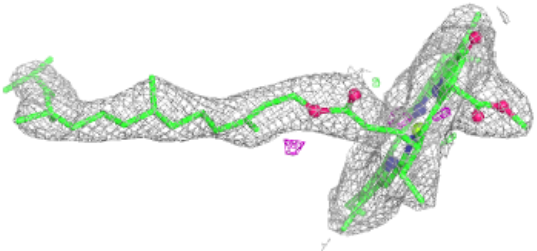
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

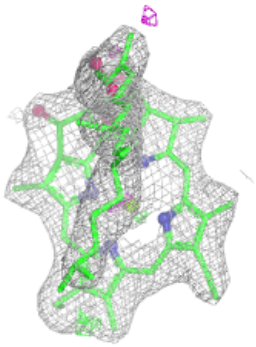


Electron density around CLA b 609:

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

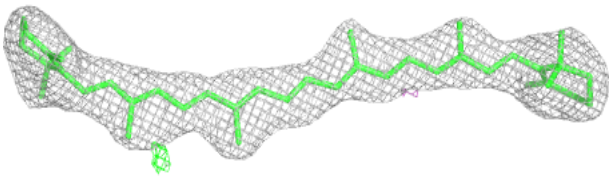


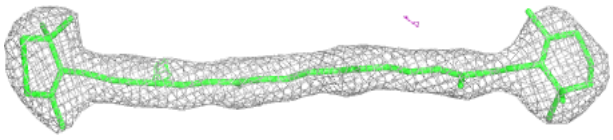


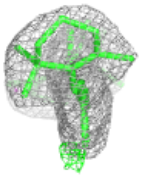


Electron density around BCR c 516:

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

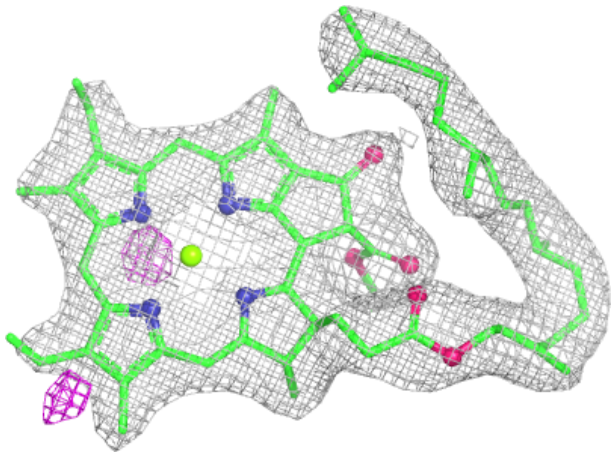


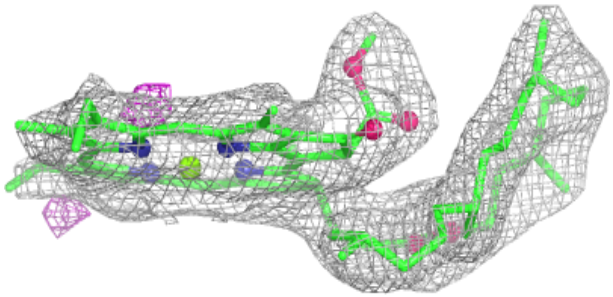


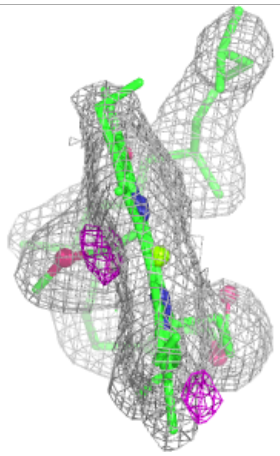


Electron density around CLA b 610:

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

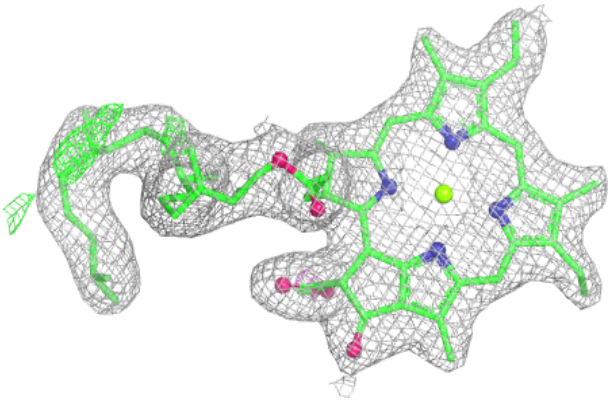


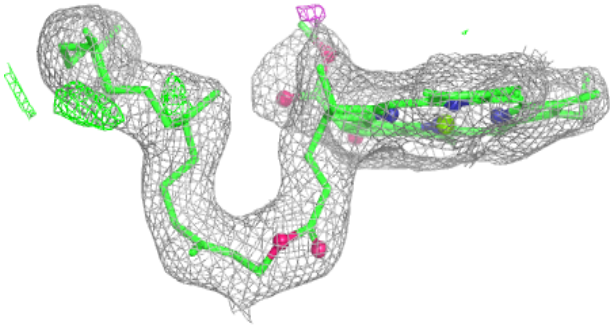


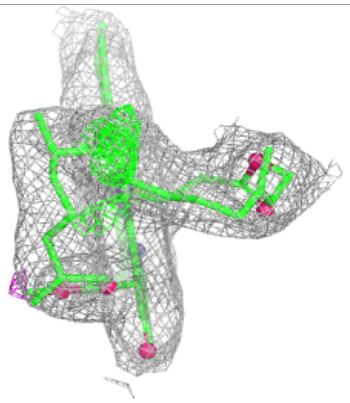


Electron density around CLA b 612:

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

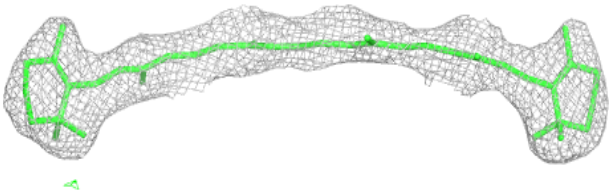


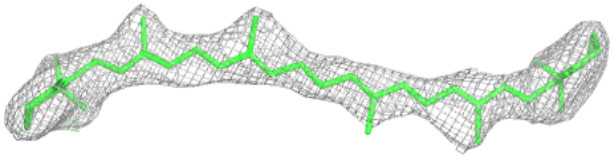


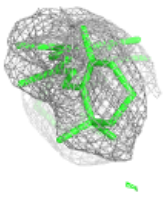


Electron density around BCR k 101:

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

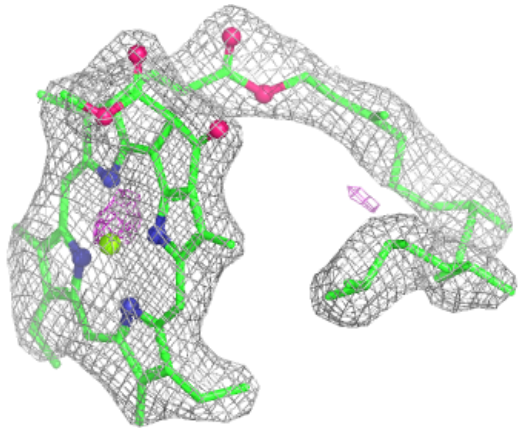


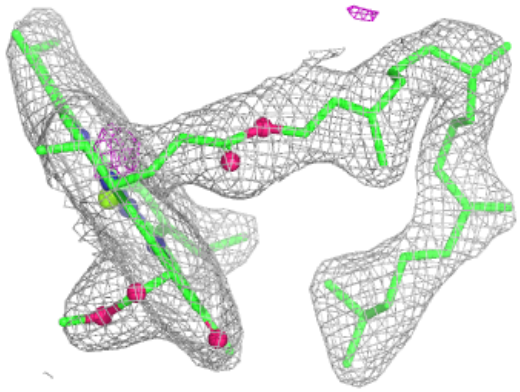


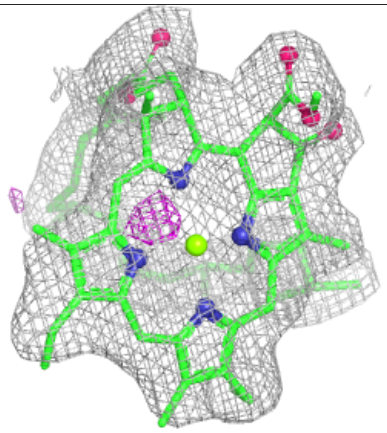


Electron density around CLA C 504:

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

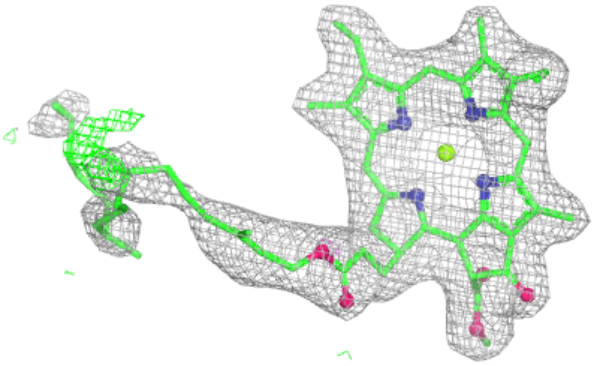


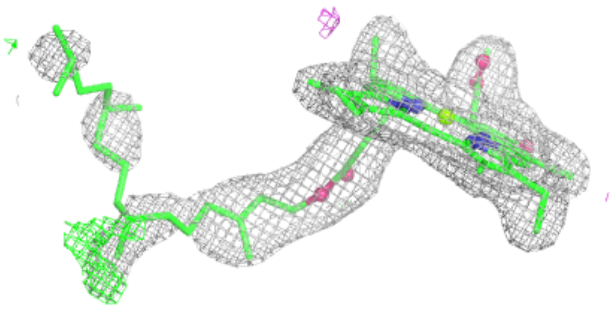


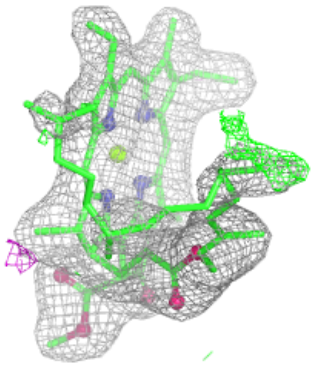


Electron density around CLA A 408:

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

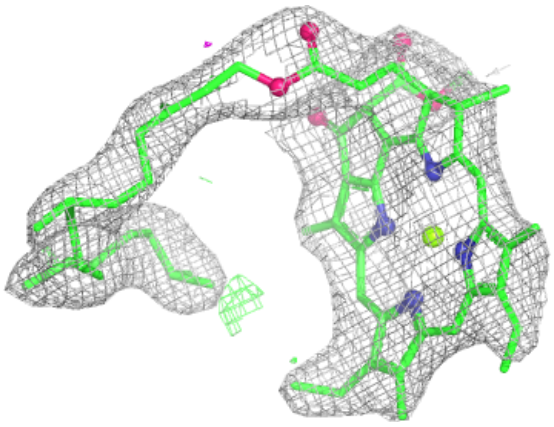


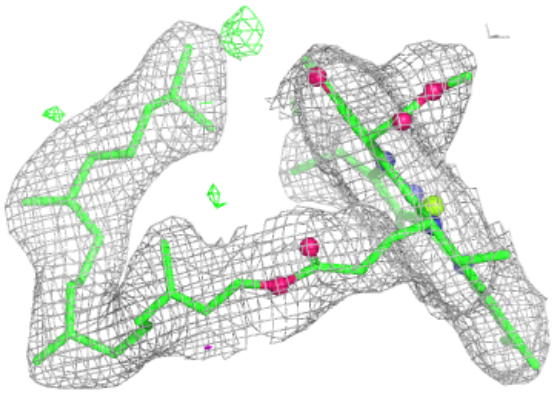


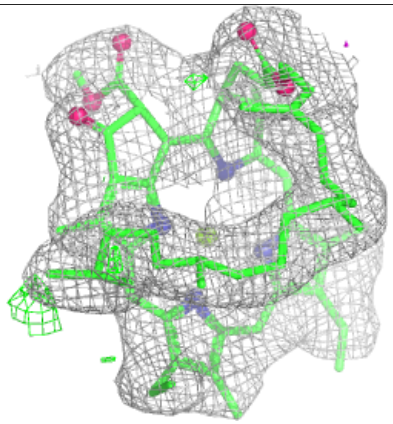


Electron density around CLA c 504:

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

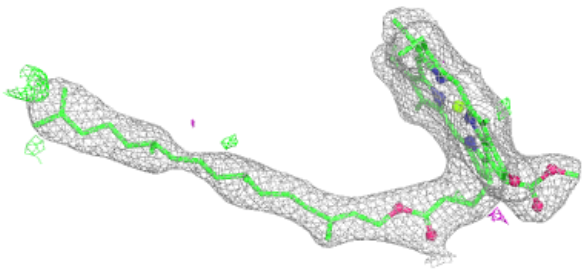


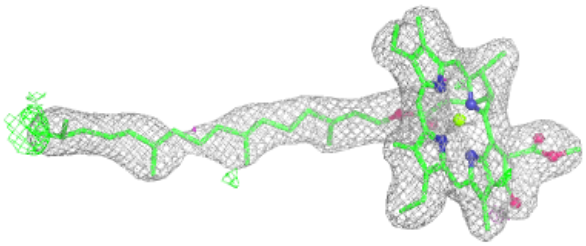


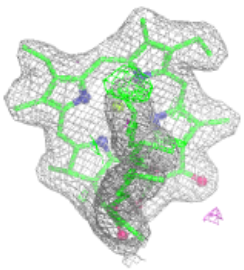


Electron density around CLA B 607:

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

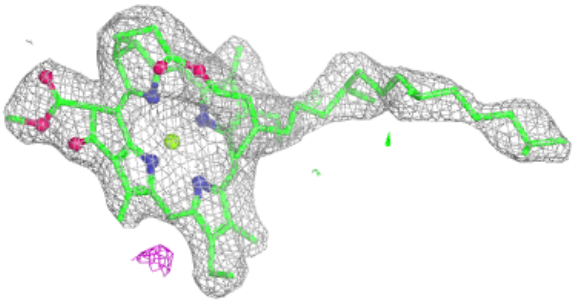


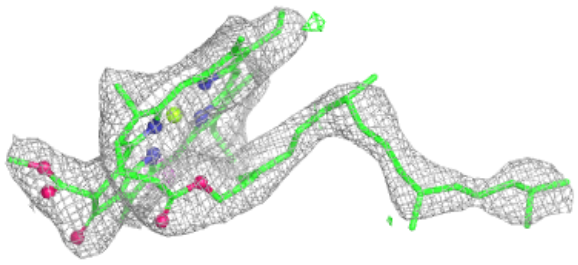


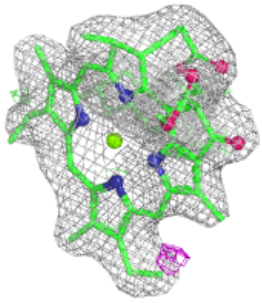


Electron density around CLA c 506:

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

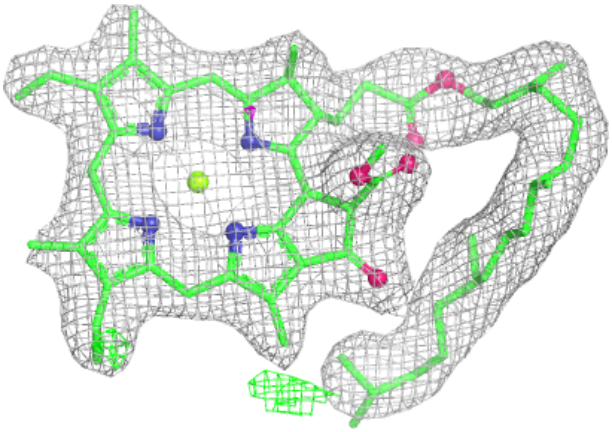


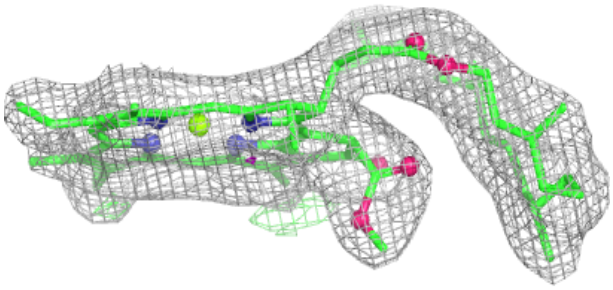


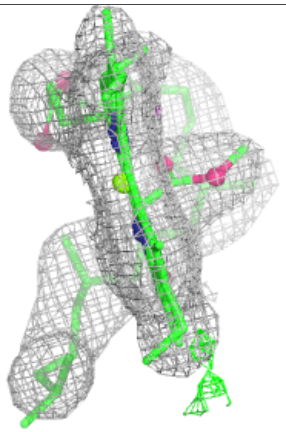


Electron density around CLA B 610:

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

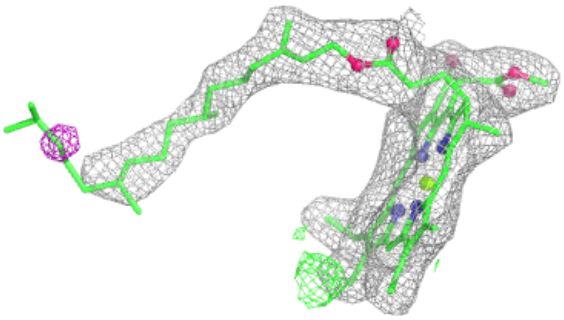


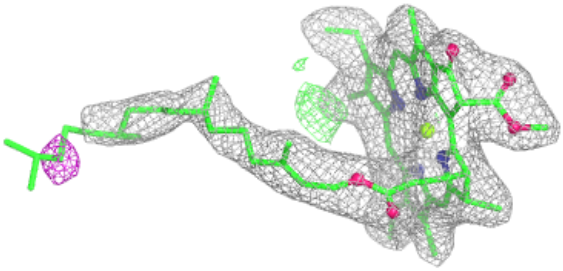


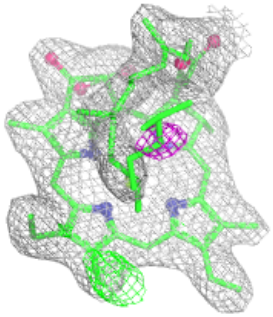


Electron density around CLA C 509:

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

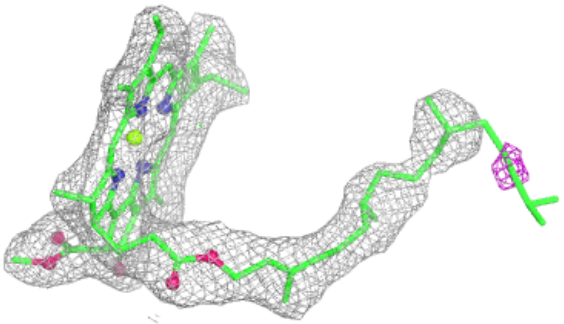


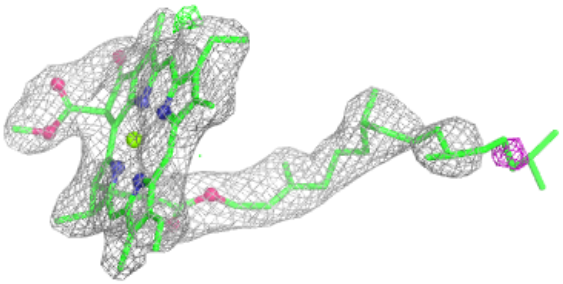


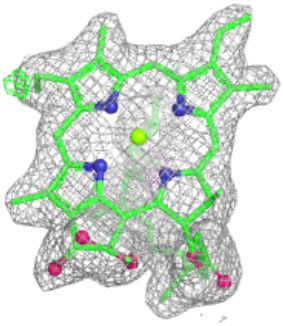


Electron density around CLA c 509:

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

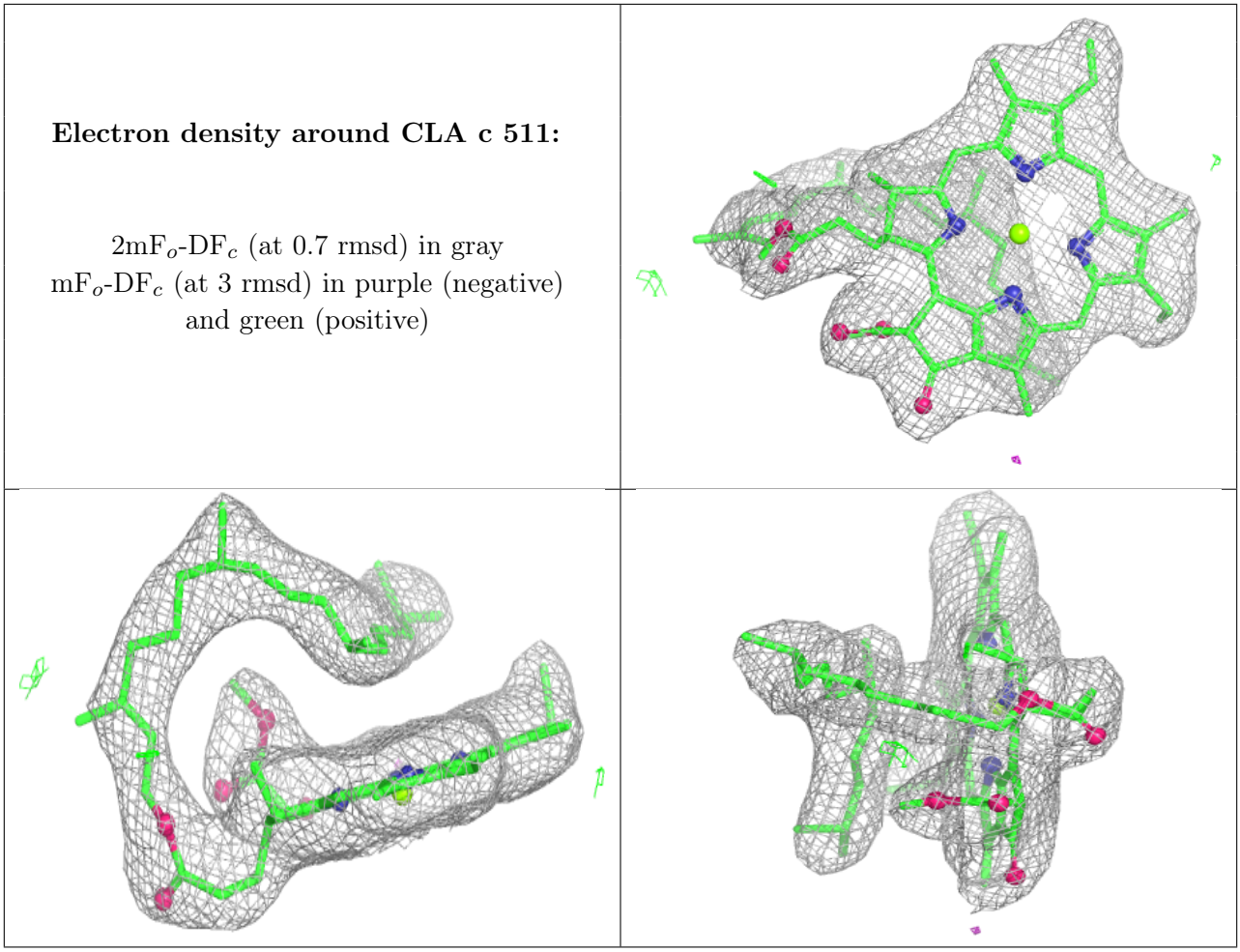






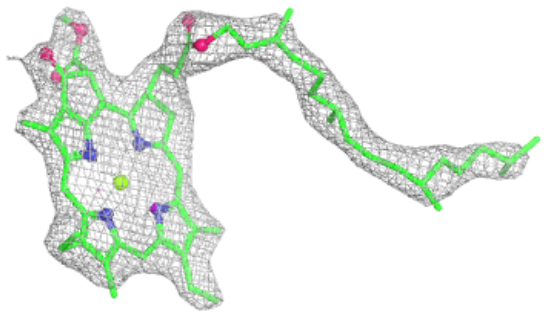
Electron density around CLA c 511:

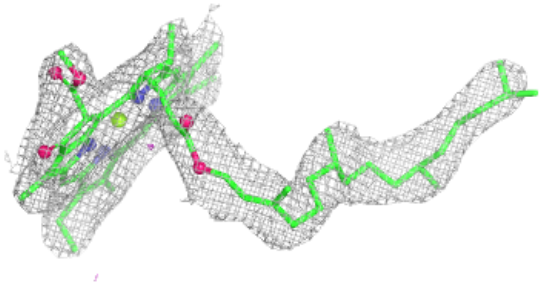
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

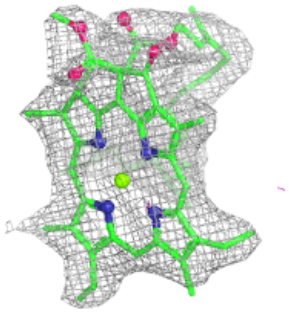


Electron density around CLA c 512:

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

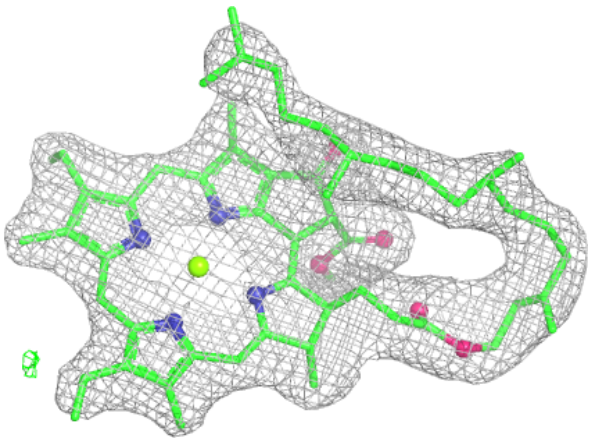


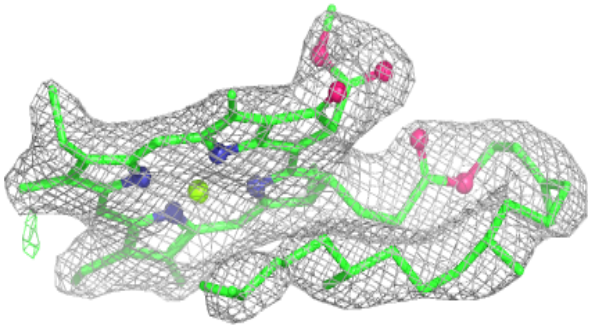


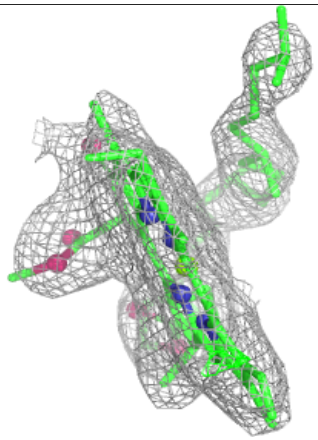


Electron density around CLA C 510:

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

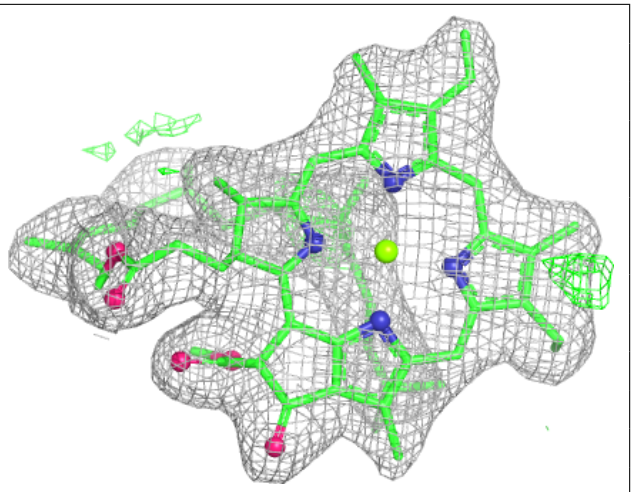


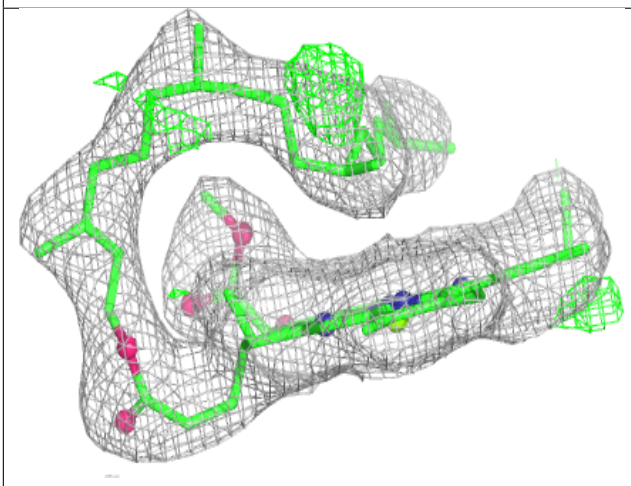


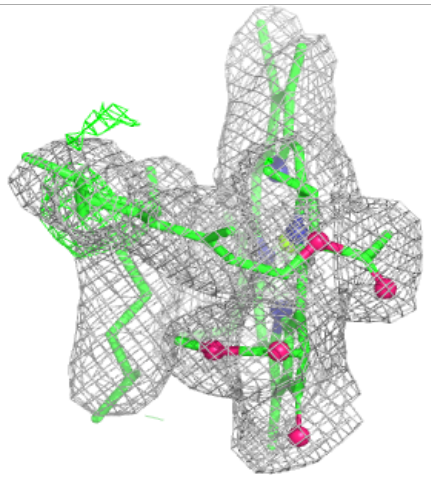


Electron density around CLA C 511:

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

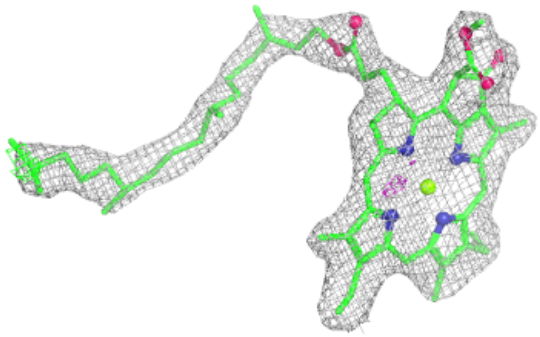


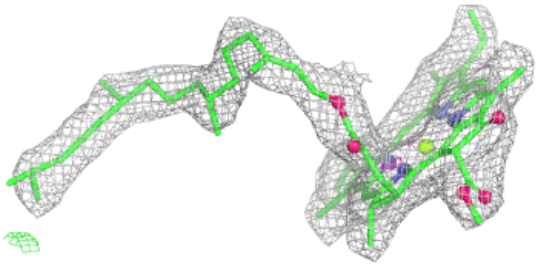


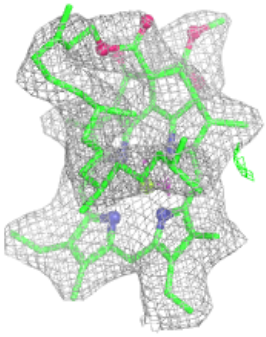


Electron density around CLA C 512:

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

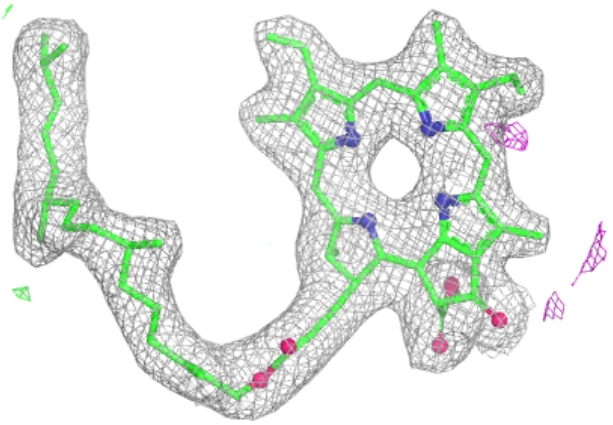


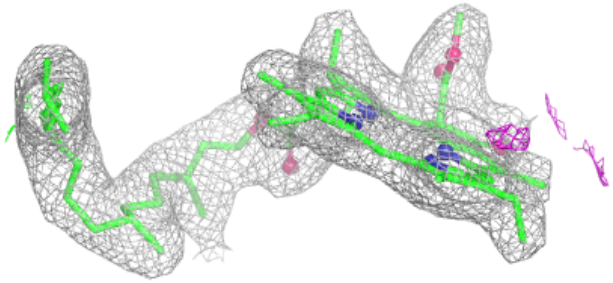


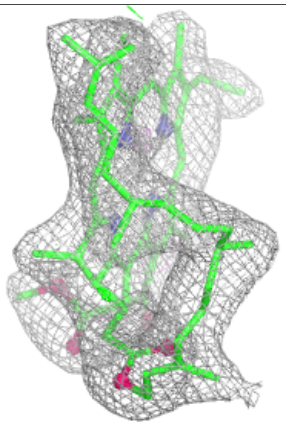


Electron density around PHO D 402:

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

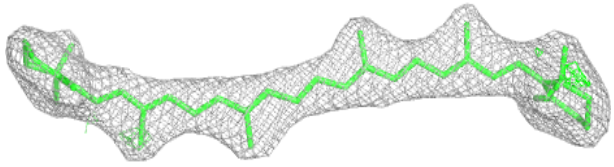


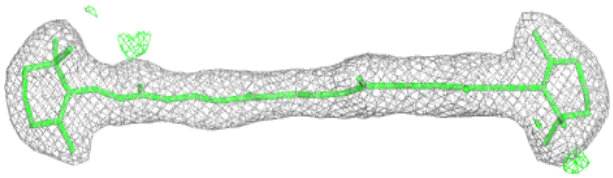


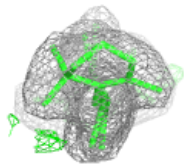


Electron density around BCR A 409:

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

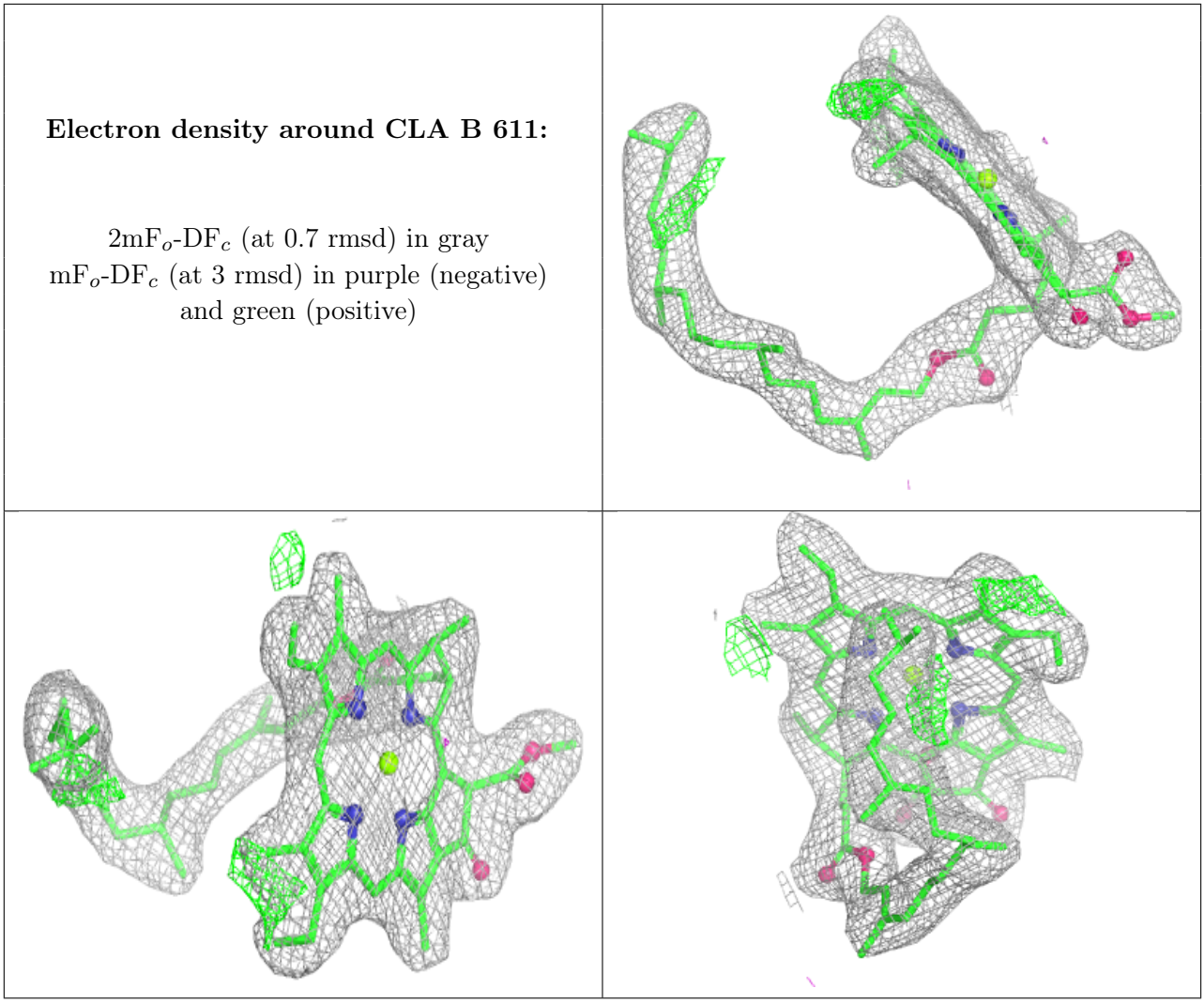






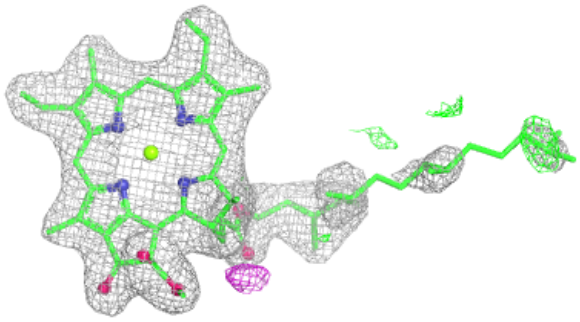
Electron density around CLA B 611:

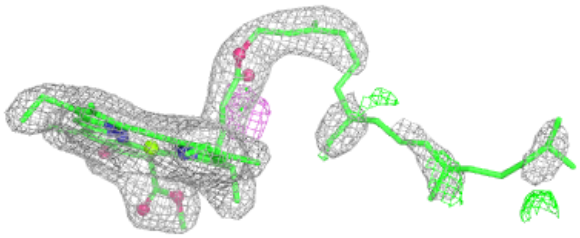
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 406:

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

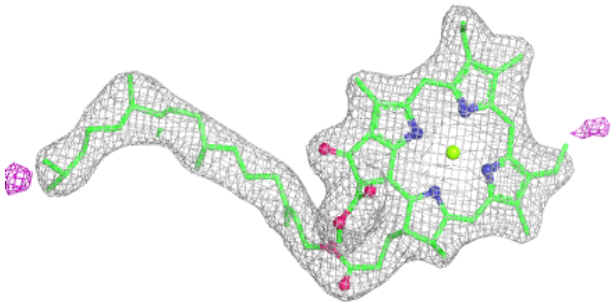


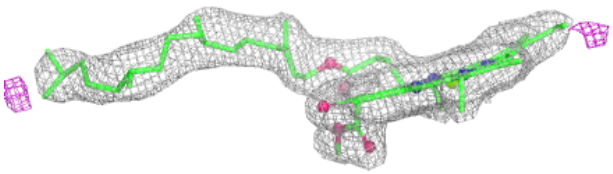


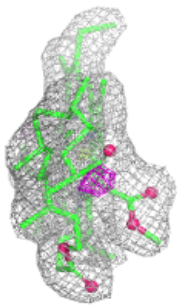


Electron density around CLA B 602:

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

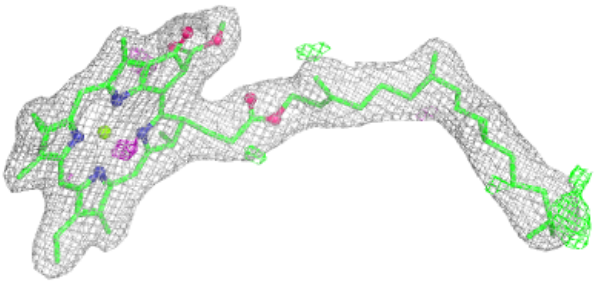


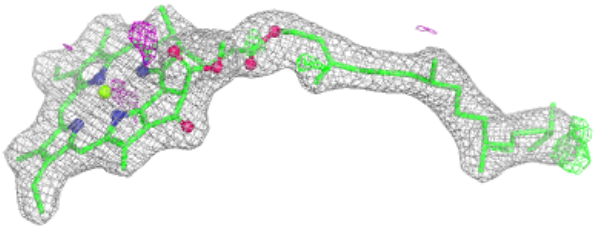


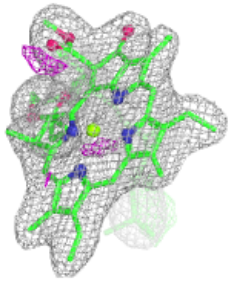


Electron density around CLA a 404:

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

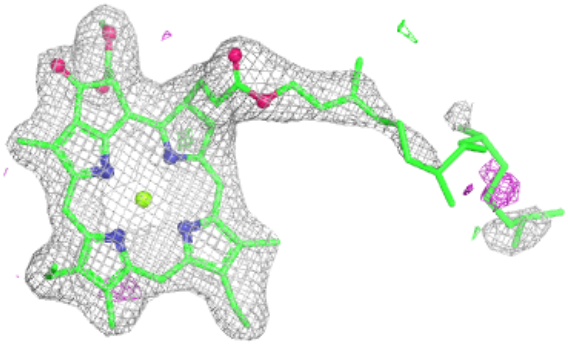


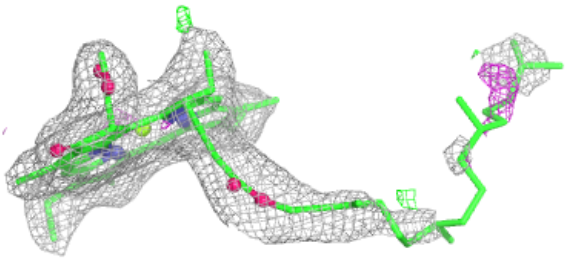




Electron density around CLA a 407:

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

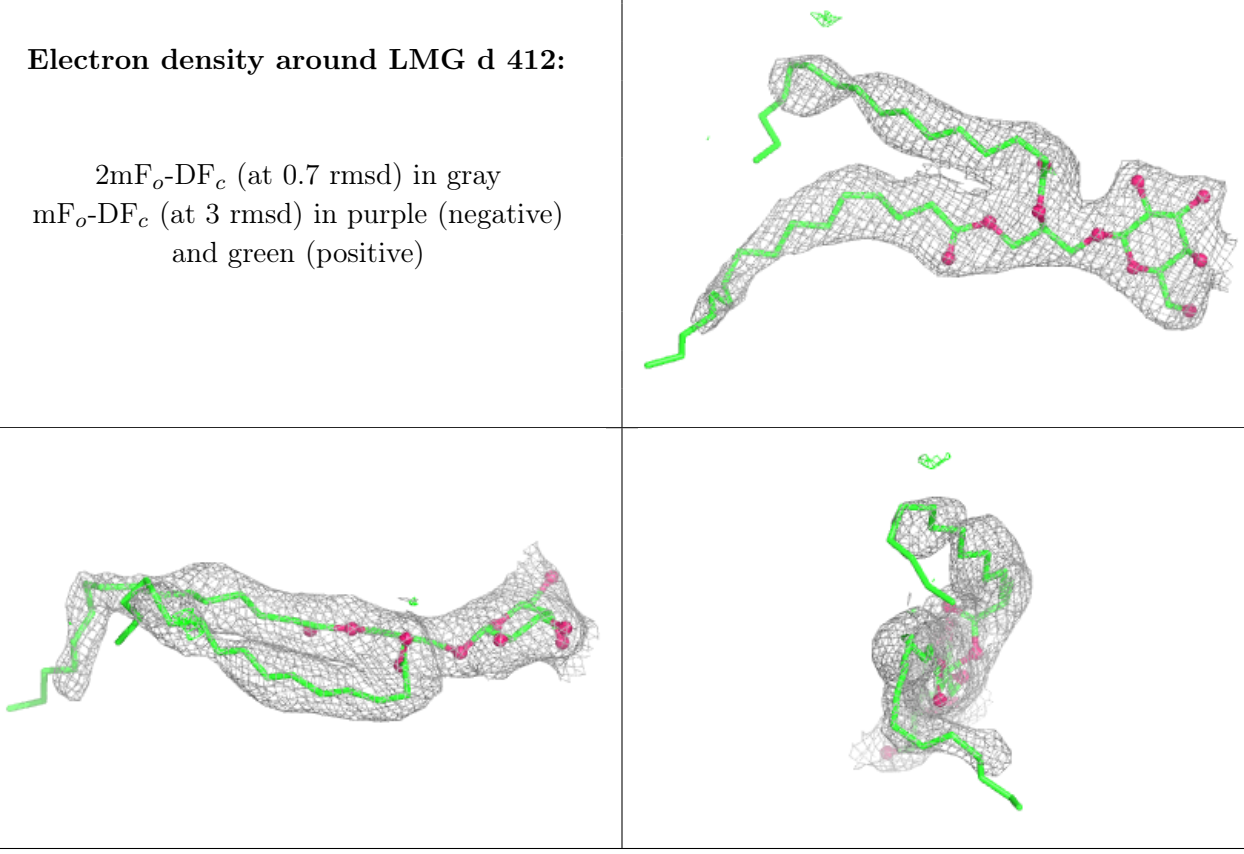






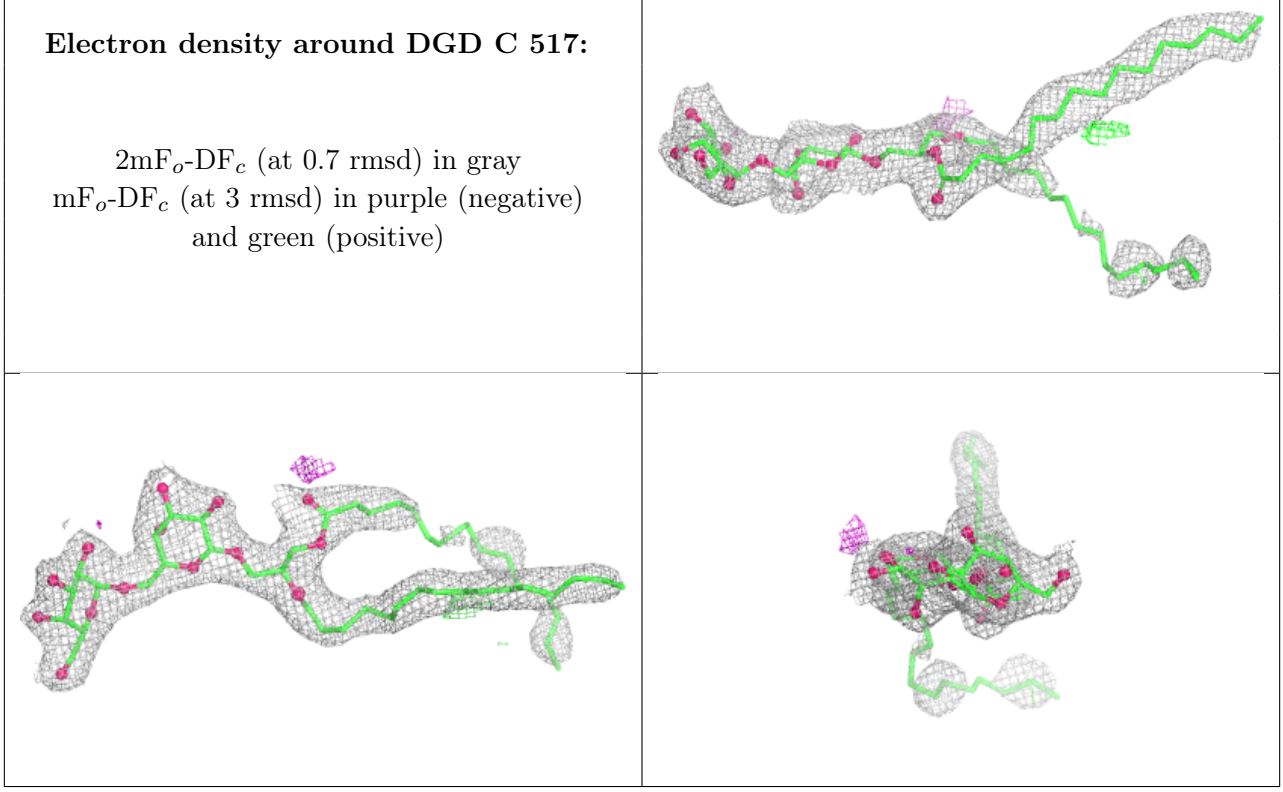
Electron density around LMG d 412:

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



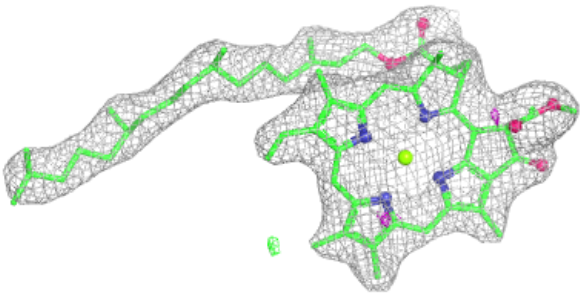
Electron density around DGD C 517:

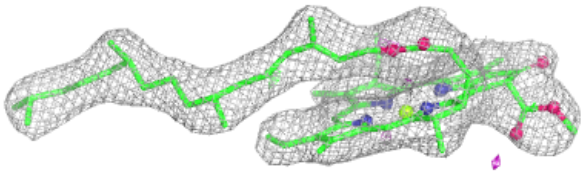
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

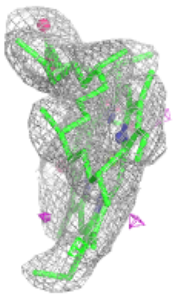


Electron density around CLA C 502:

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

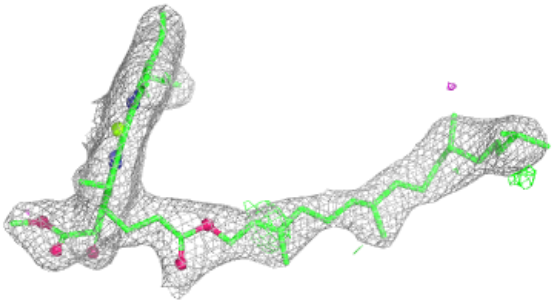


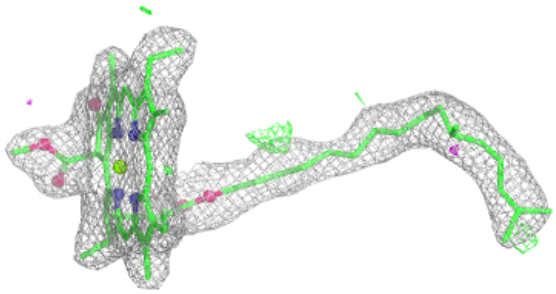


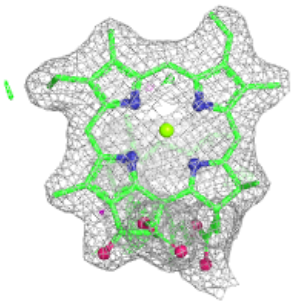


Electron density around CLA b 605:

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

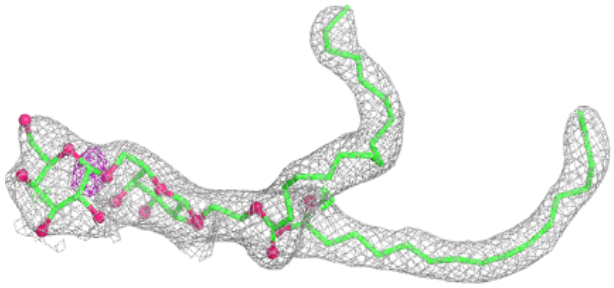


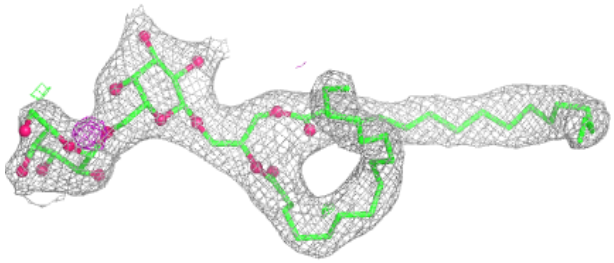


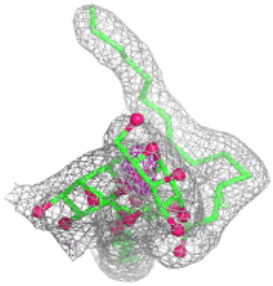


Electron density around DGD H 102:

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

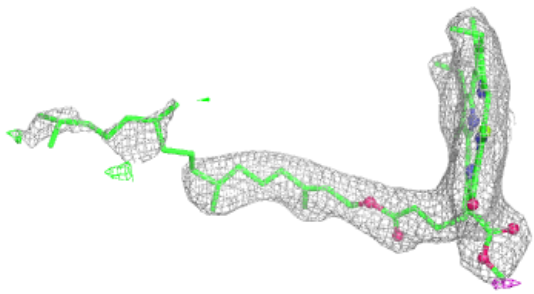


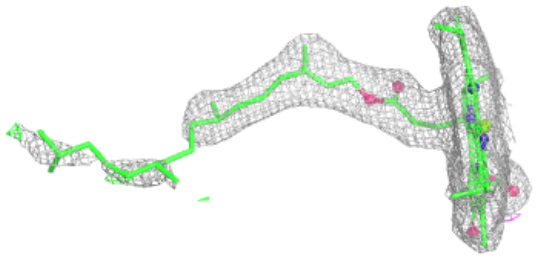


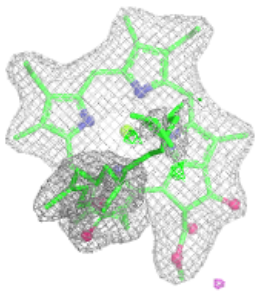


Electron density around CLA b 606:

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

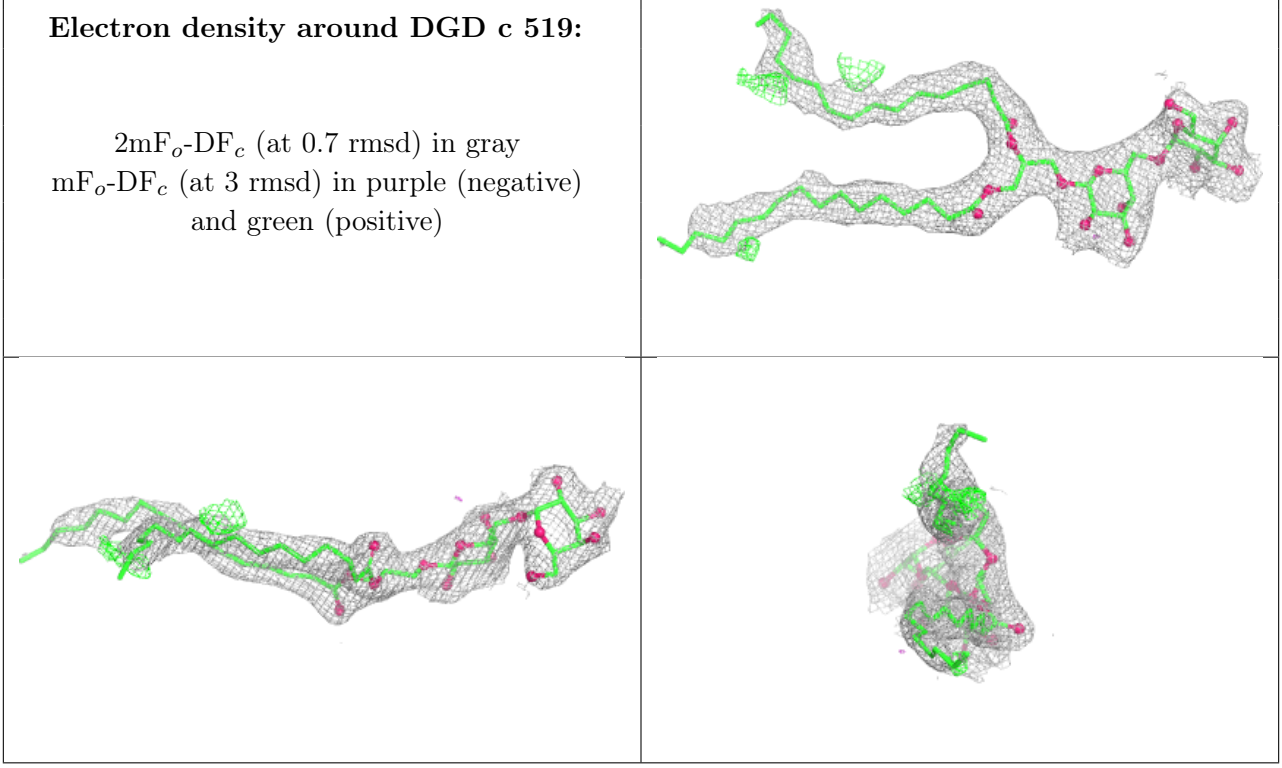






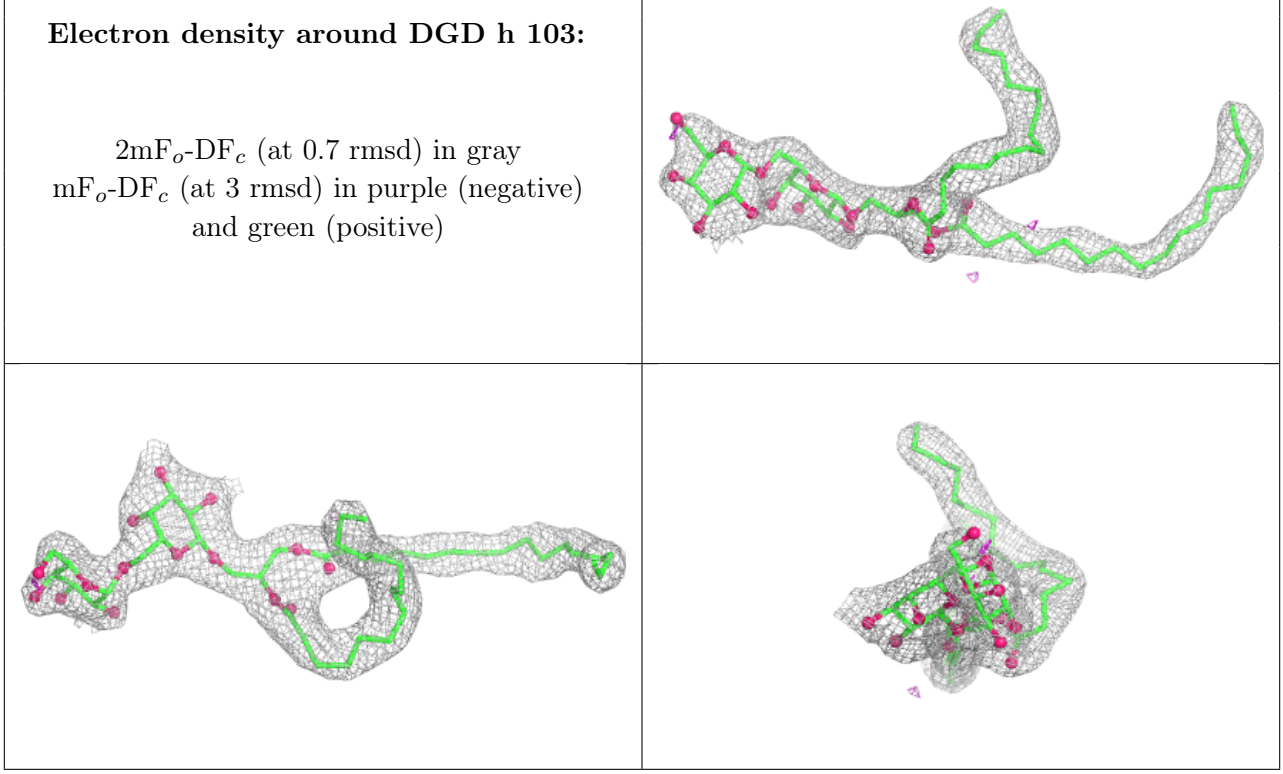
Electron density around DGD c 519:

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



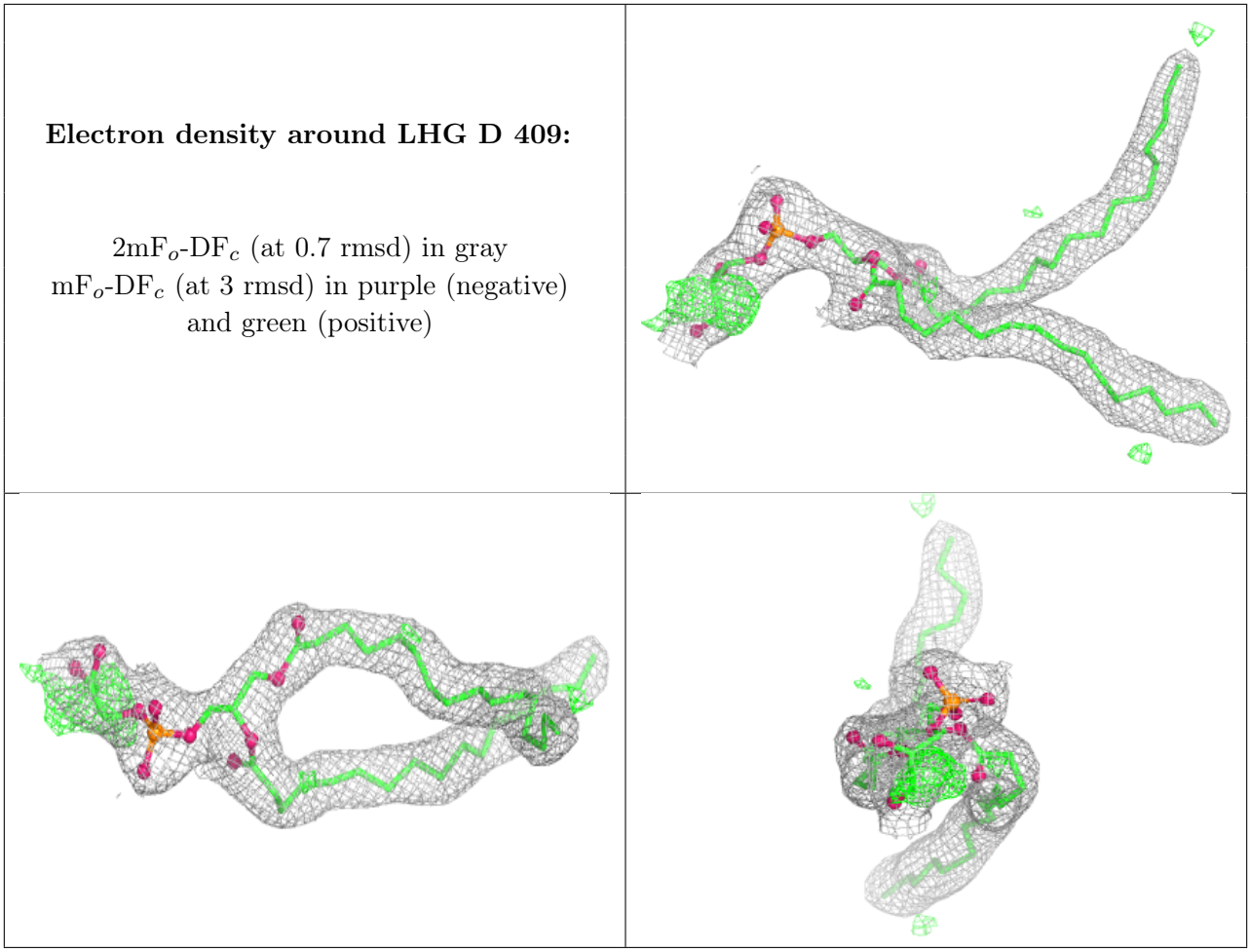
Electron density around DGD h 103:

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



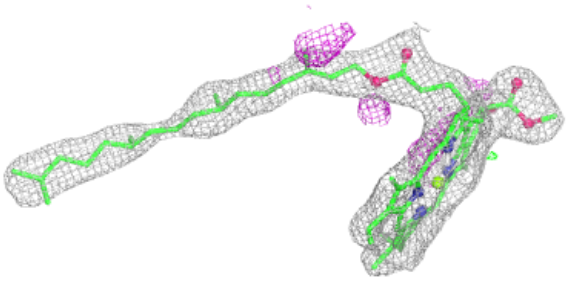
Electron density around LHG D 409:

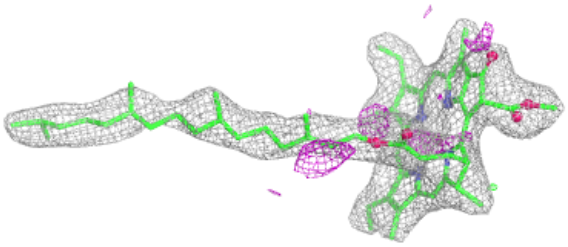
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

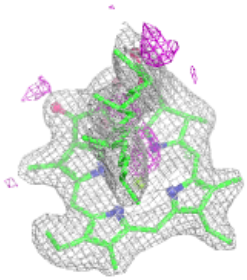


Electron density around CLA b 607:

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

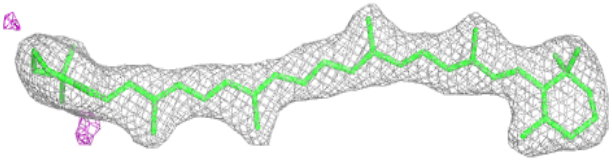


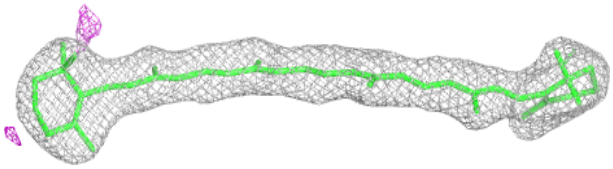


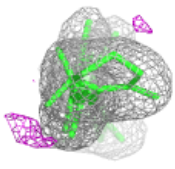


Electron density around BCR b 617:

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

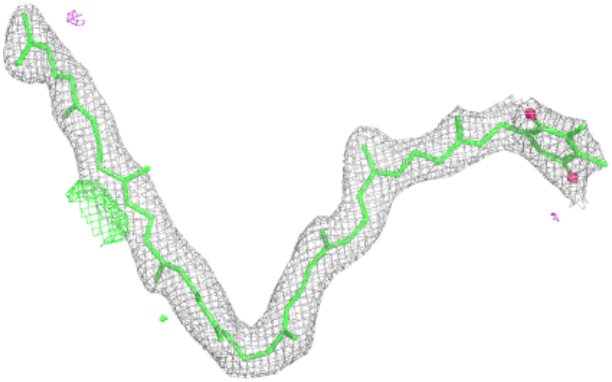


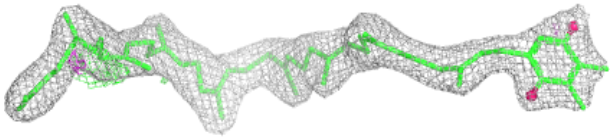


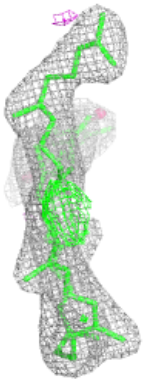


Electron density around PL9 d 406:

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

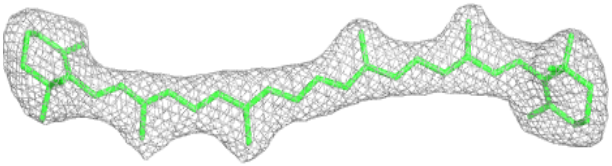


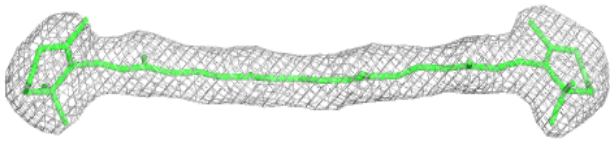


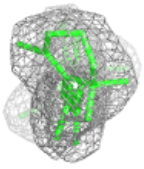


Electron density around BCR b 618:

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

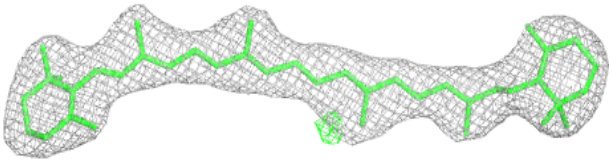


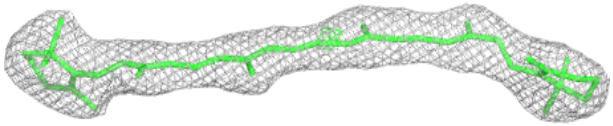


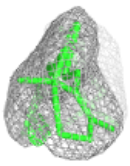


Electron density around BCR b 619:

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

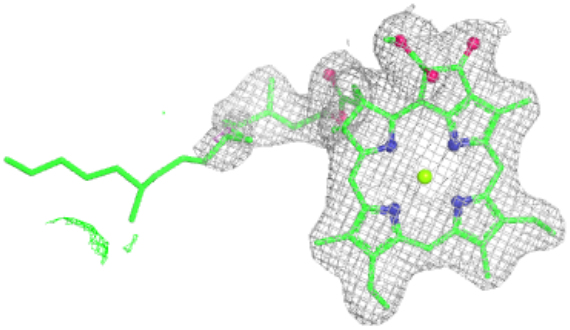


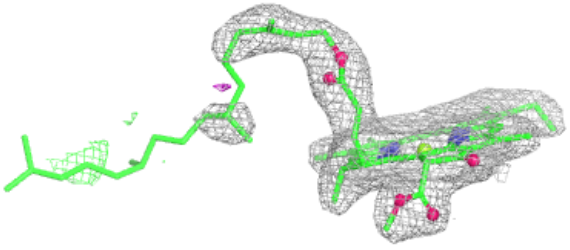


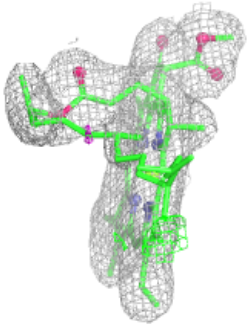


Electron density around CLA a 405:

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

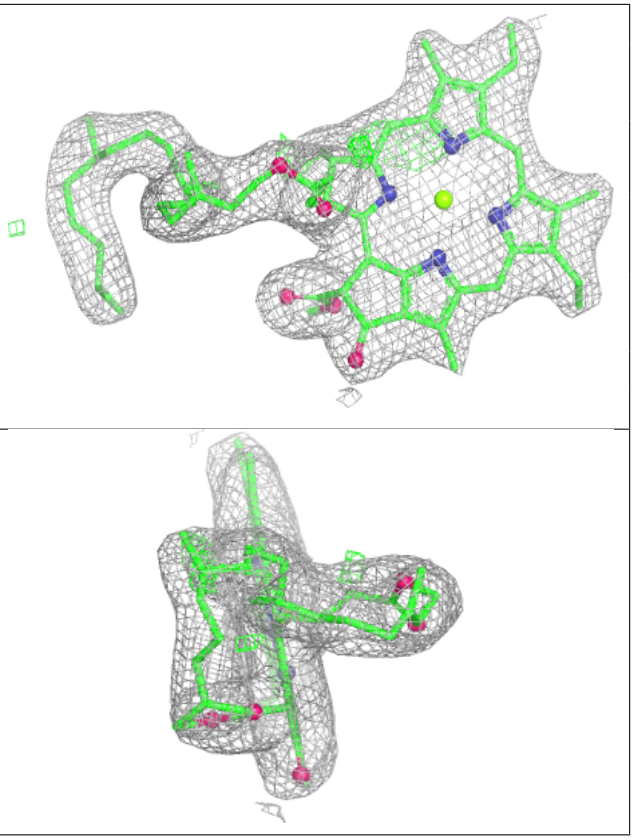


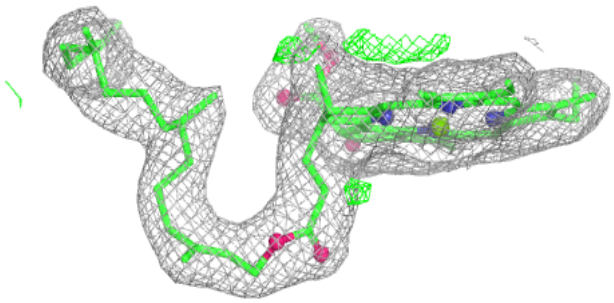




Electron density around CLA B 612:

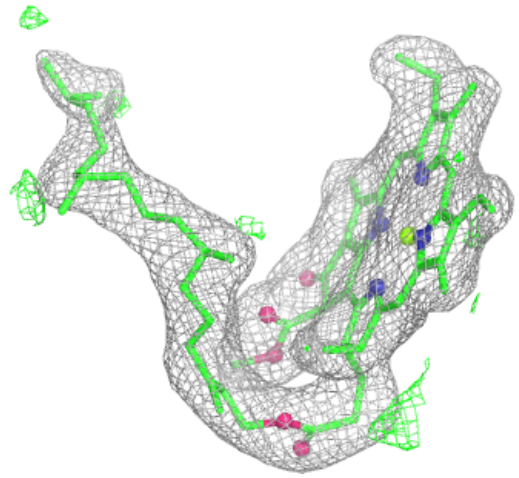
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

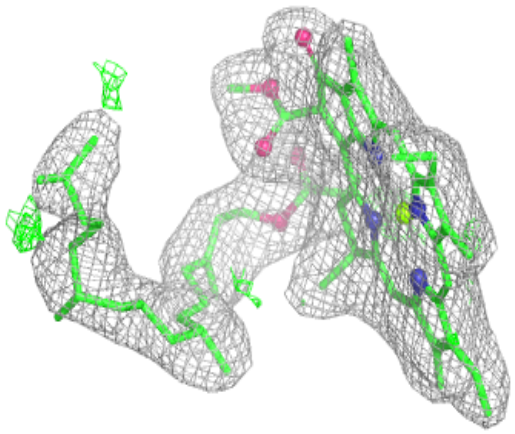


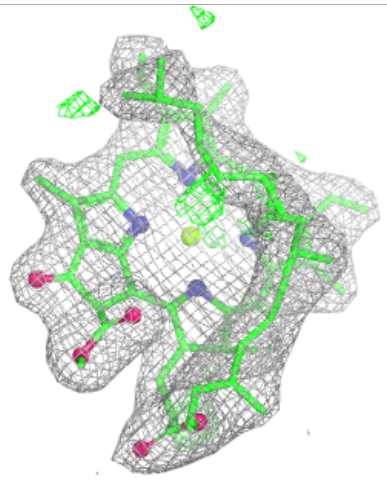


Electron density around CLA B 613:

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

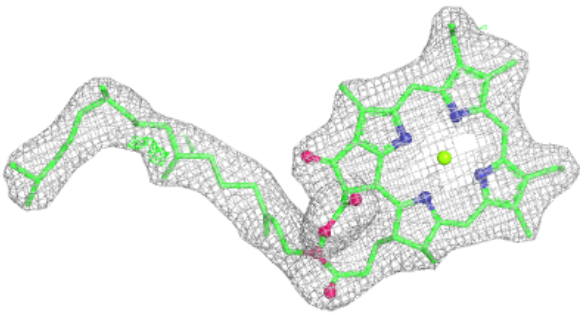


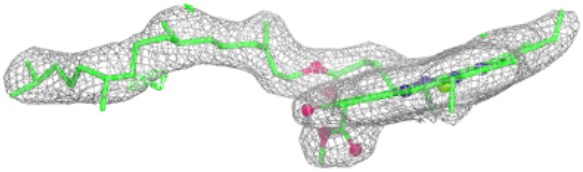


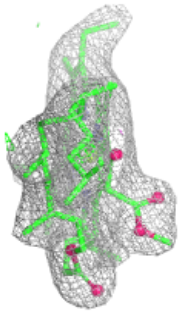


Electron density around CLA b 602:

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

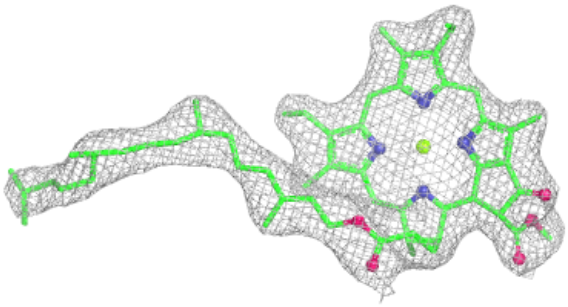


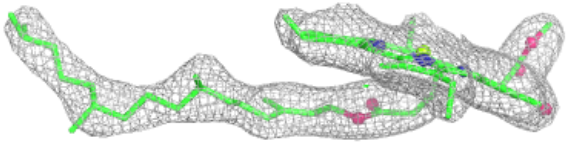


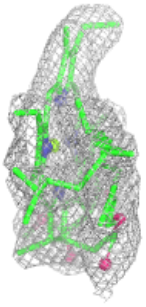


Electron density around CLA b 603:

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

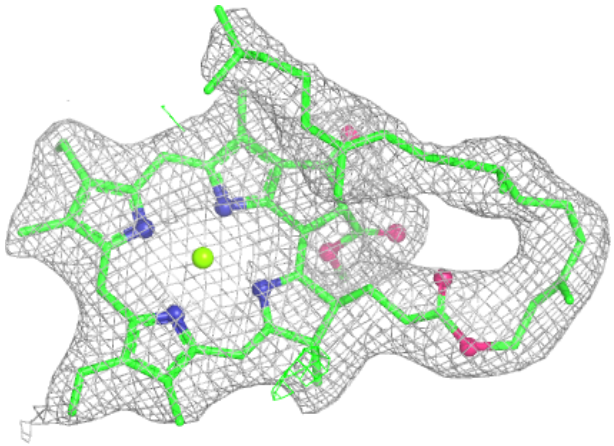


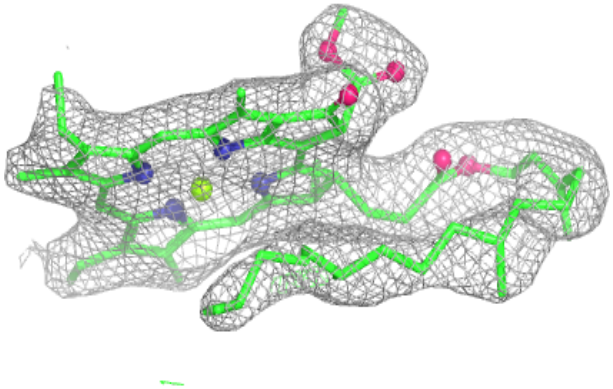


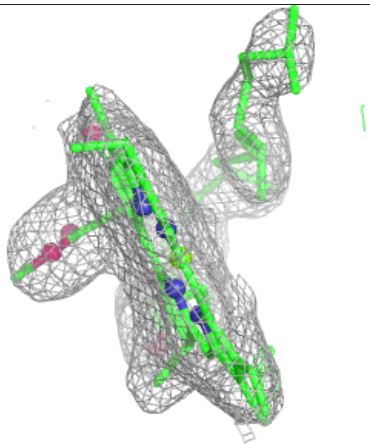


Electron density around CLA c 510:

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

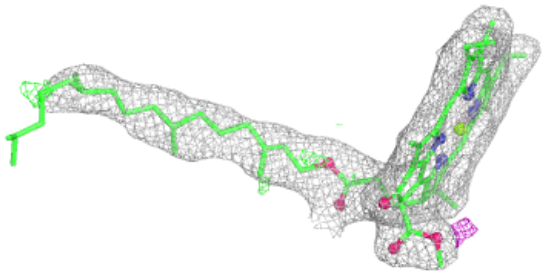


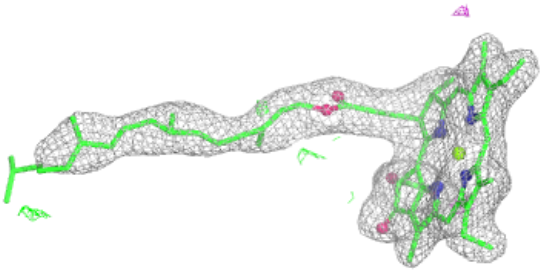


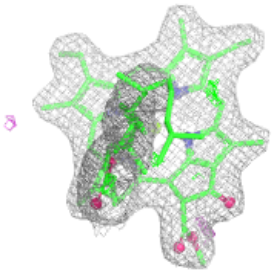


Electron density around CLA b 604:

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

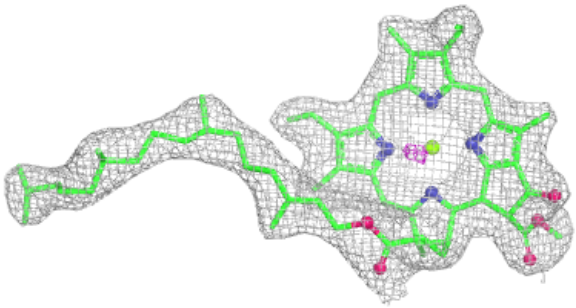


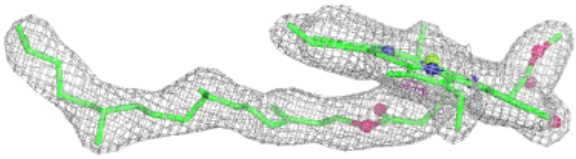




Electron density around CLA B 603:

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

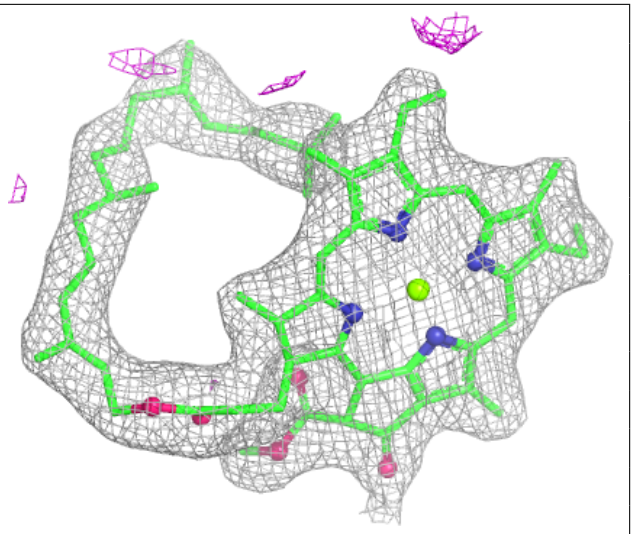


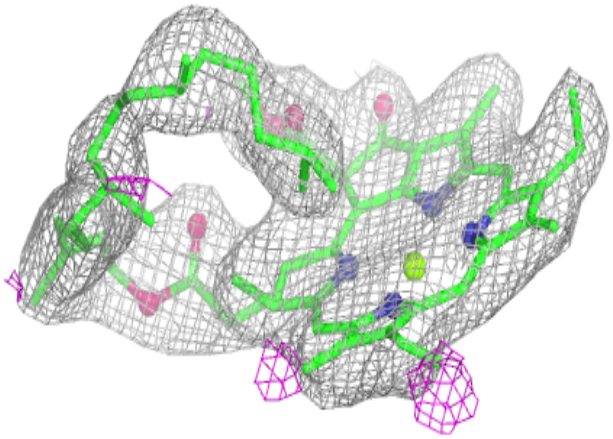


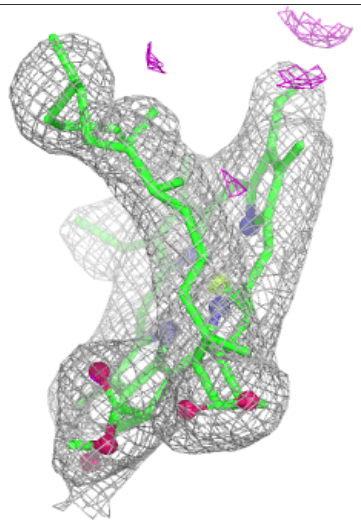


Electron density around CLA B 615:

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

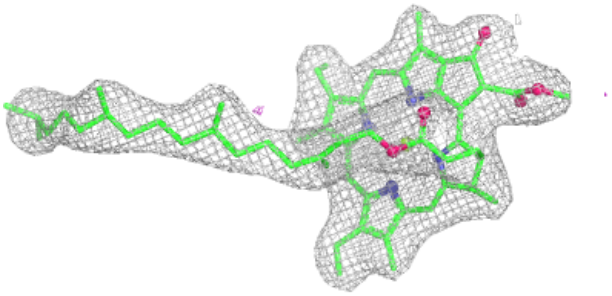


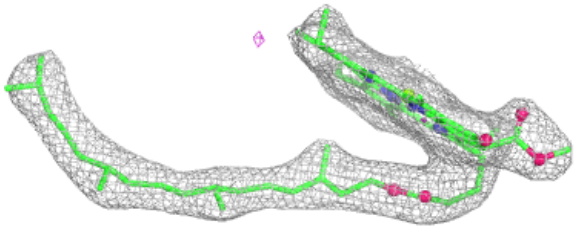


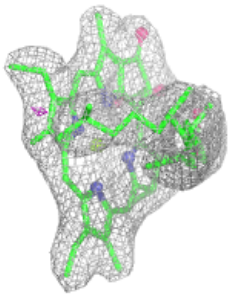


Electron density around CLA B 608:

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

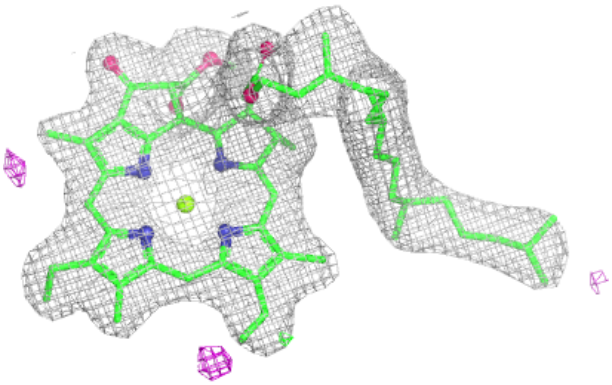


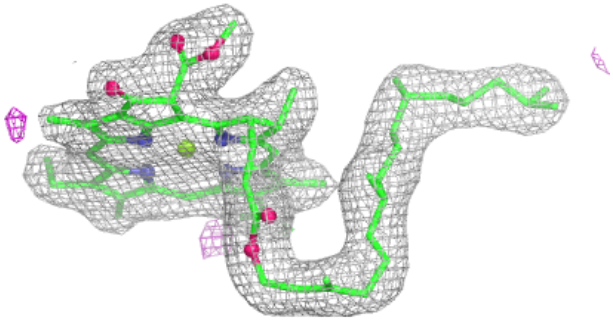


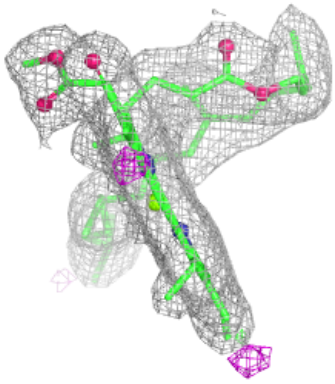


Electron density around CLA d 402:

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

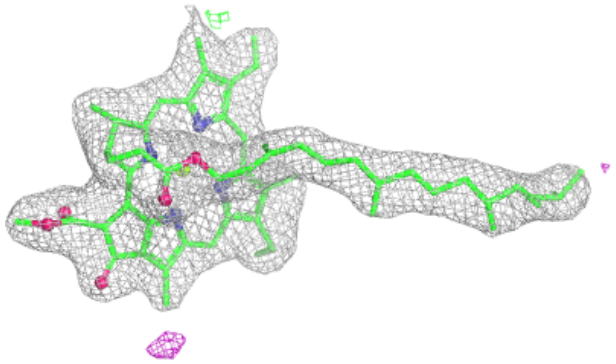


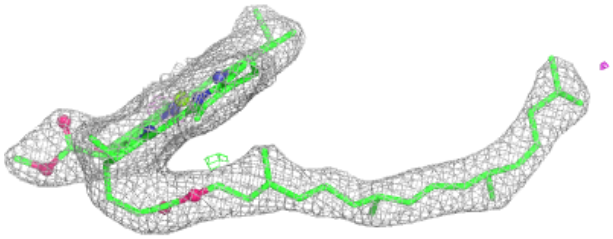


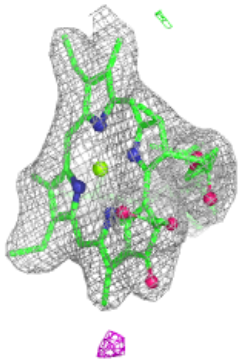


Electron density around CLA b 608:

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

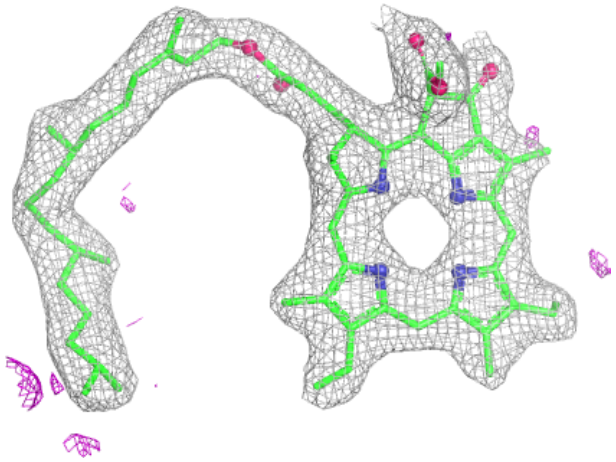


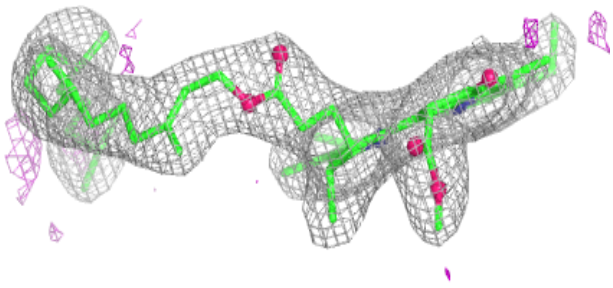


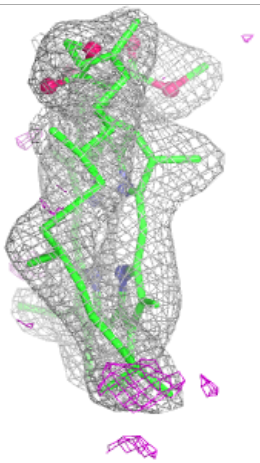


Electron density around PHO A 407:

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

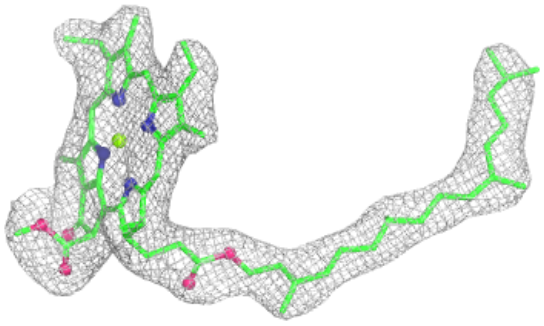


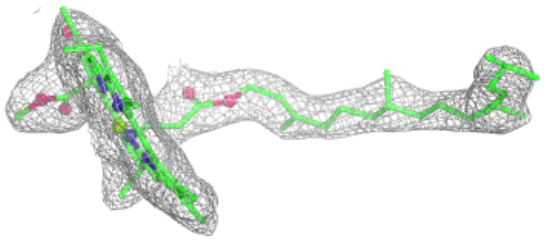


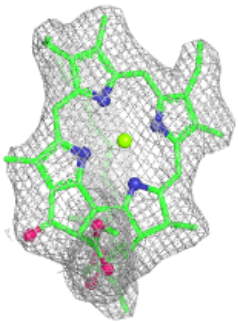


Electron density around CLA B 609:

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

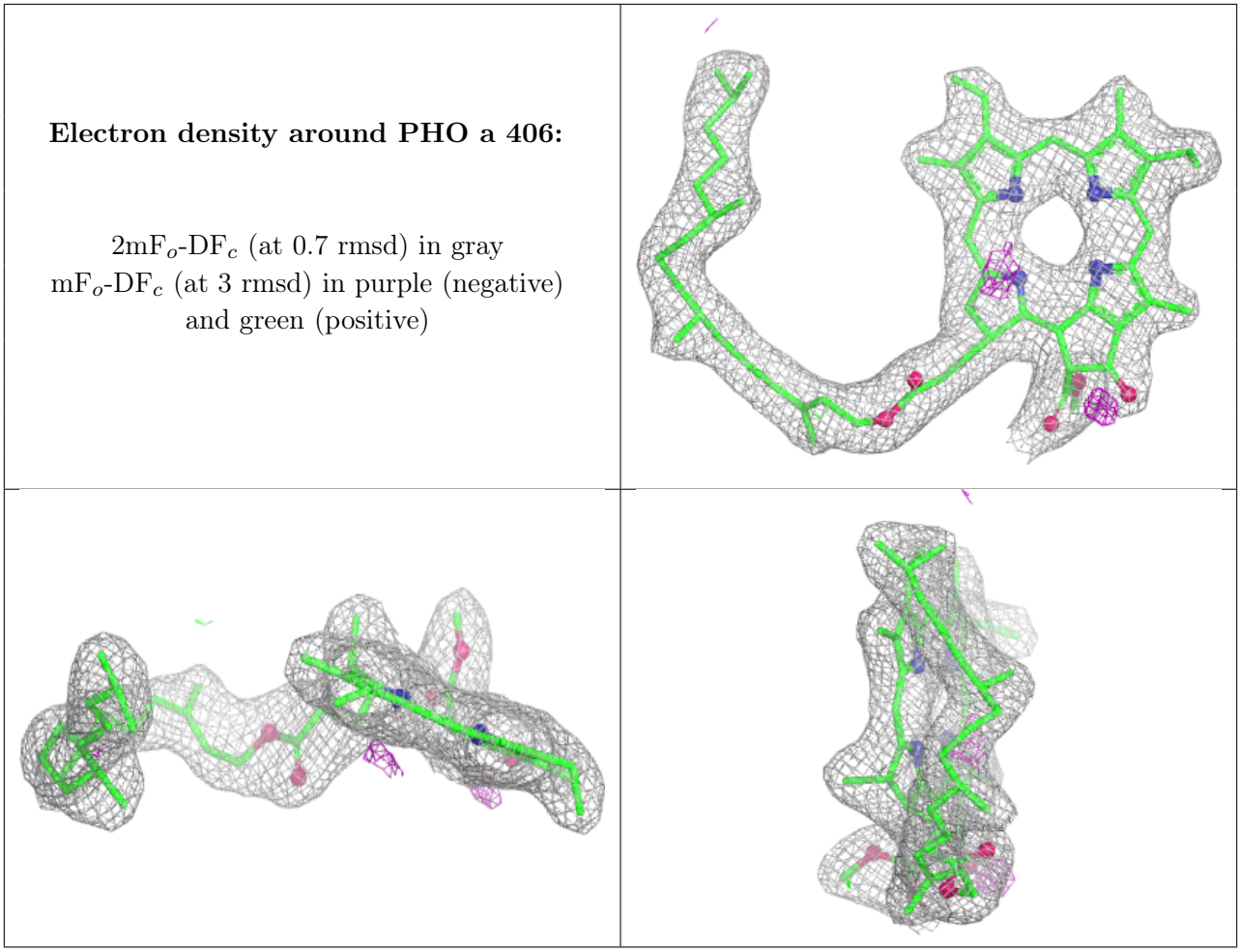






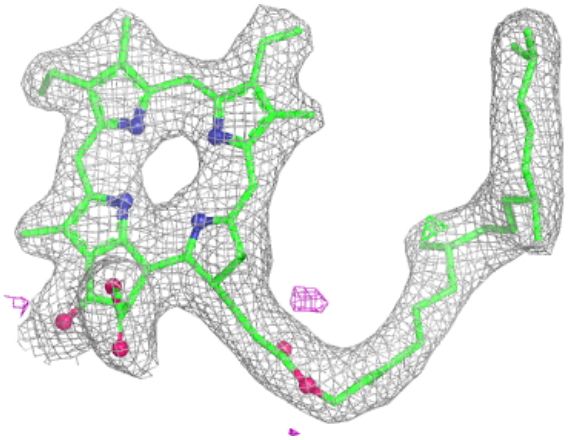
Electron density around PHO a 406:

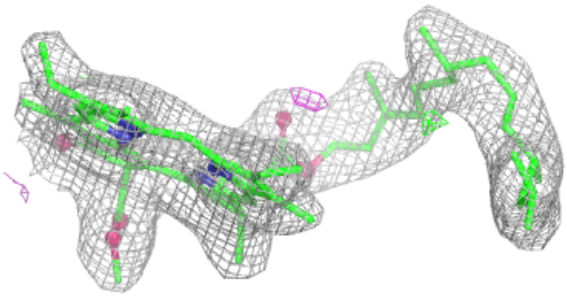
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

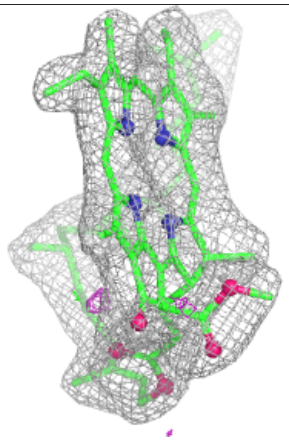


Electron density around PHO a 416:

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

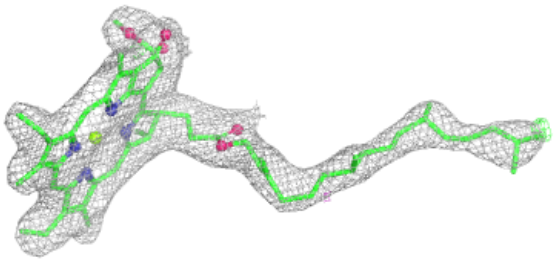


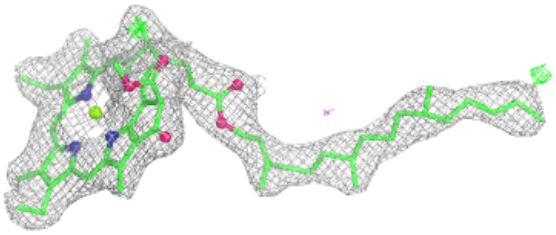


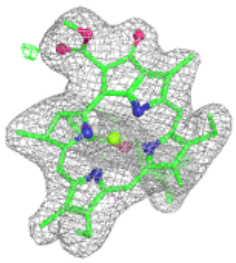


Electron density around CLA C 503:

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

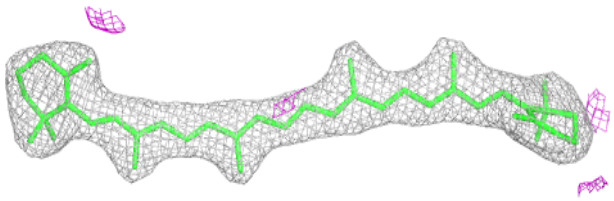


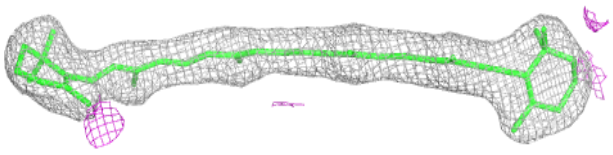


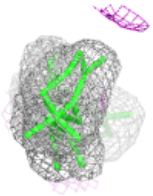


Electron density around BCR B 617:

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

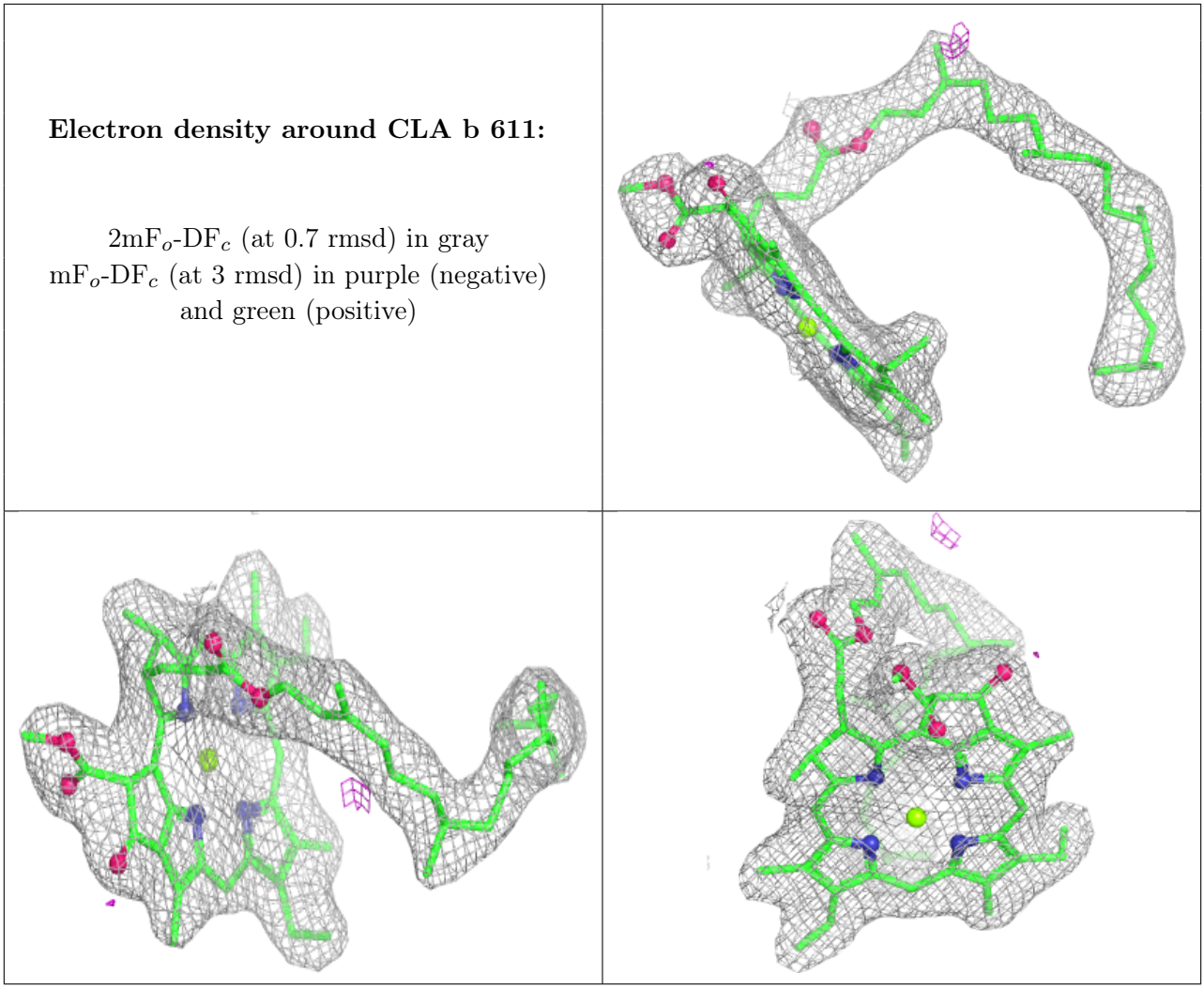






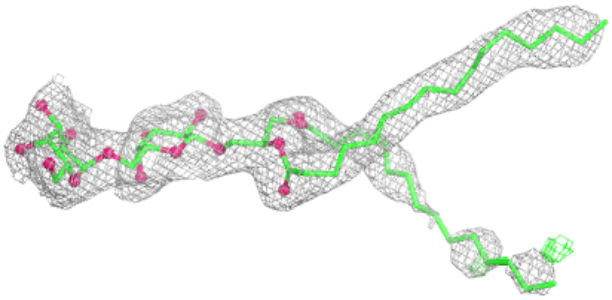
Electron density around CLA b 611:

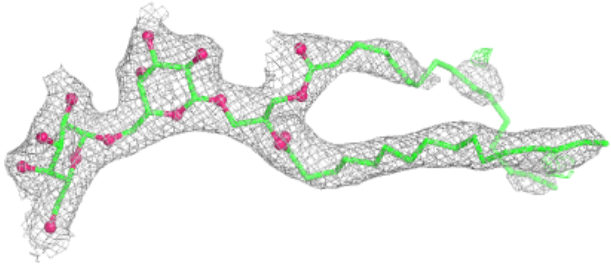
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

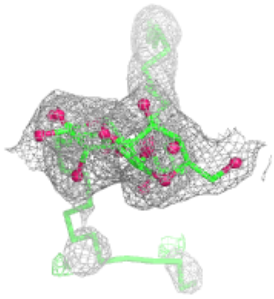


Electron density around DGD c 517:

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

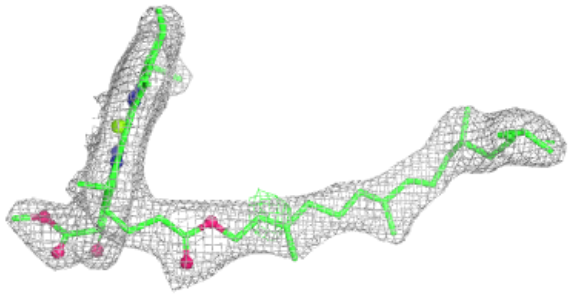


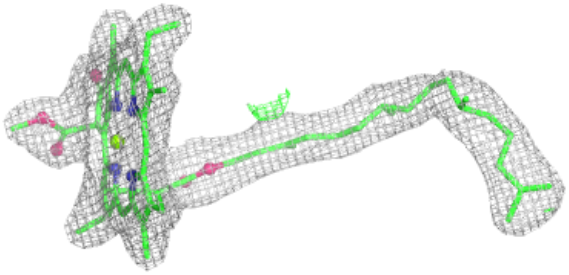


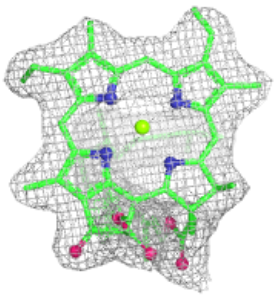


Electron density around CLA B 605:

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

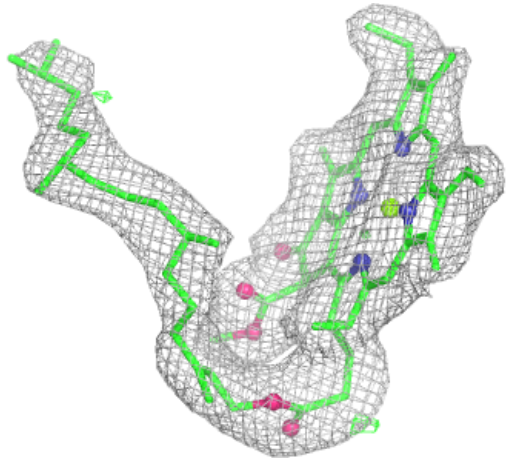


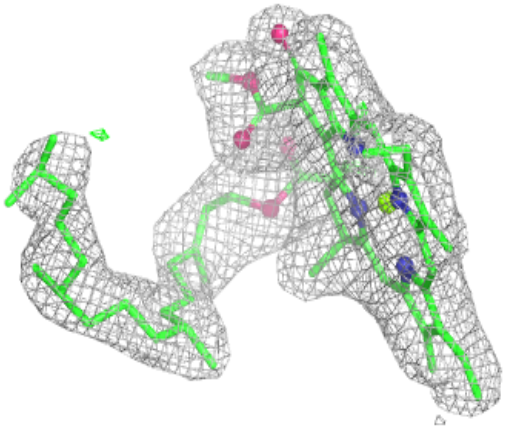


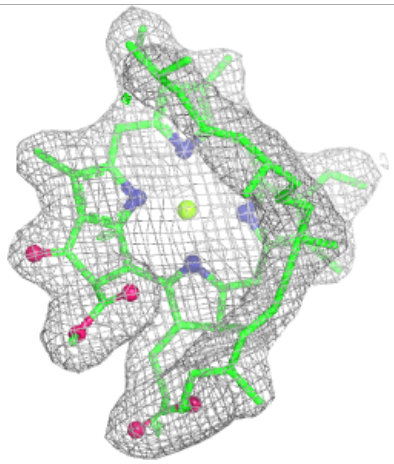


Electron density around CLA b 613:

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

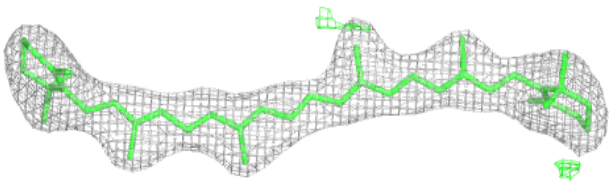


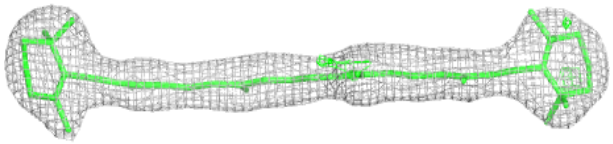


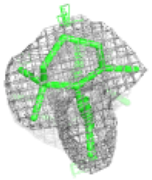


Electron density around BCR C 516:

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

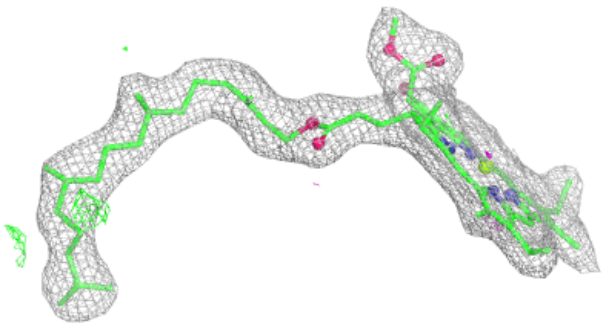


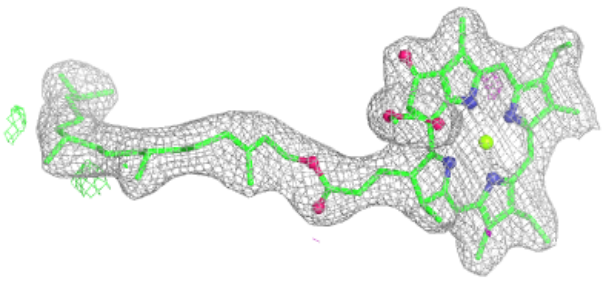


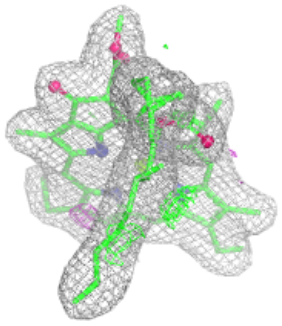


Electron density around CLA D 405:

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

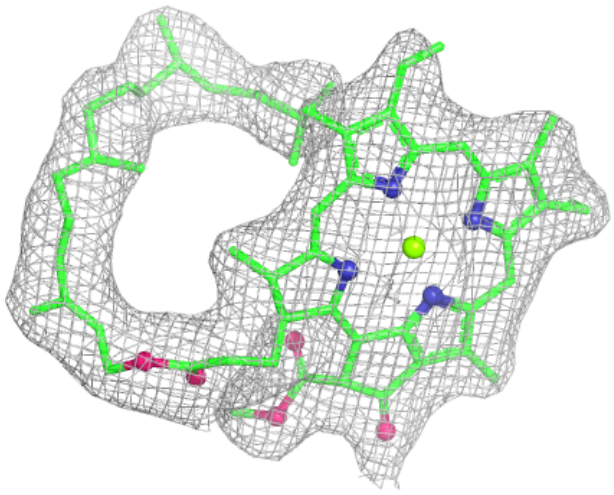


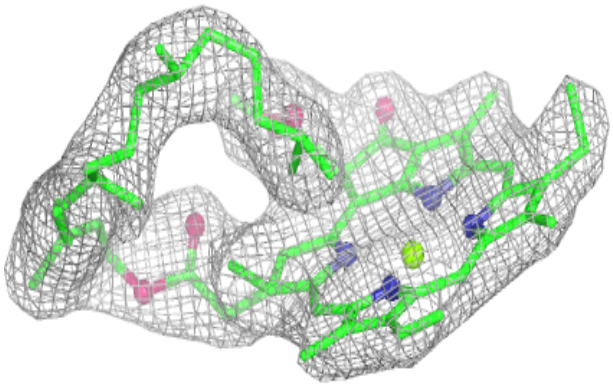


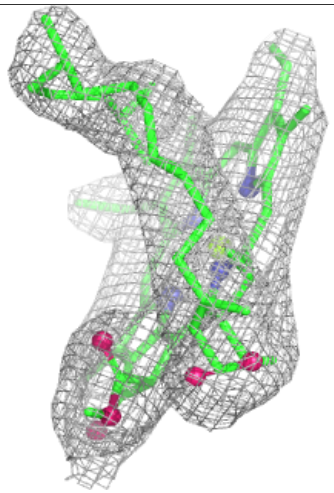


Electron density around CLA b 615:

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

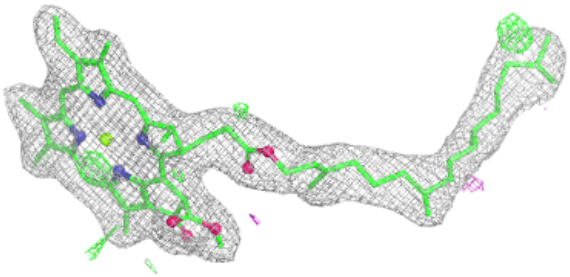


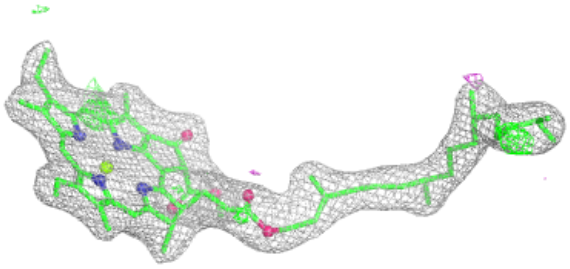


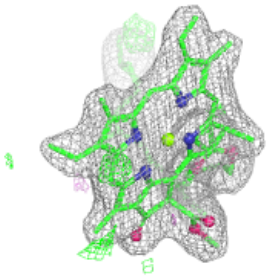


Electron density around CLA A 404:

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

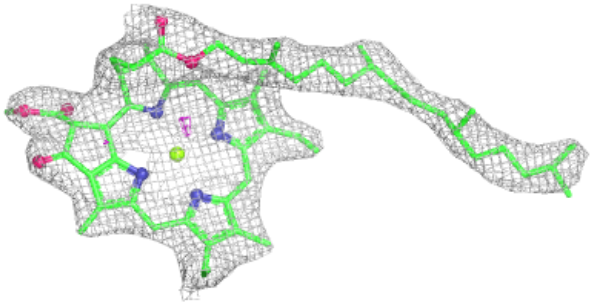


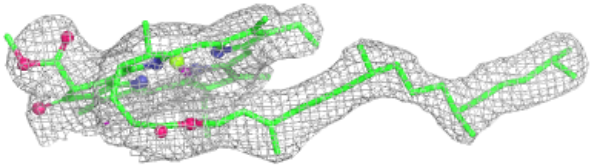


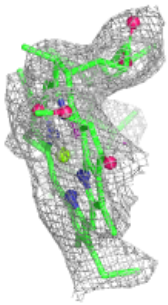


Electron density around CLA c 502:

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

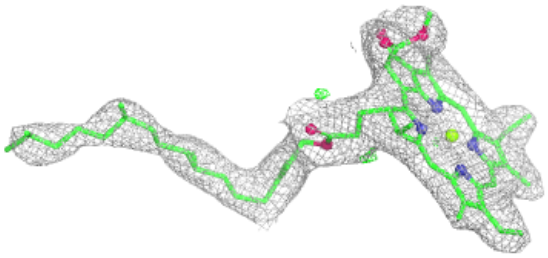


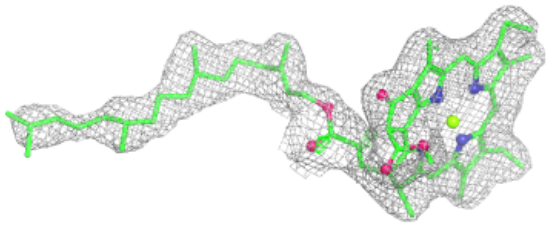


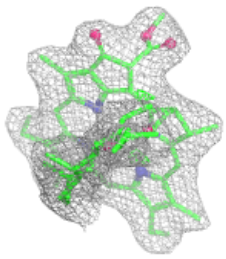


Electron density around CLA c 503:

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

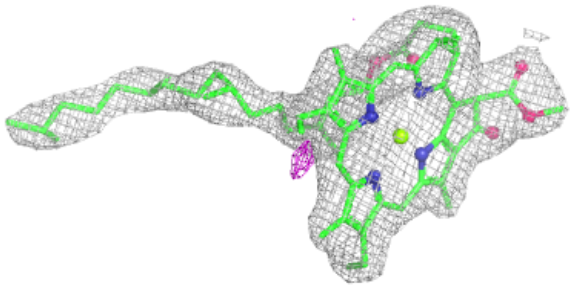


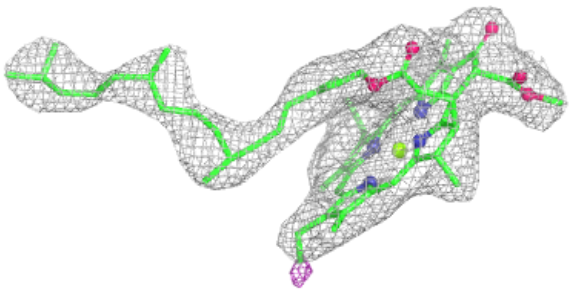


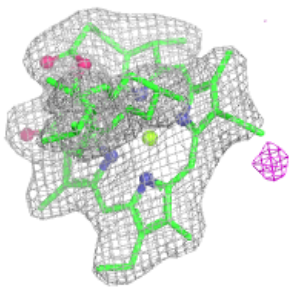


Electron density around CLA C 506:

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

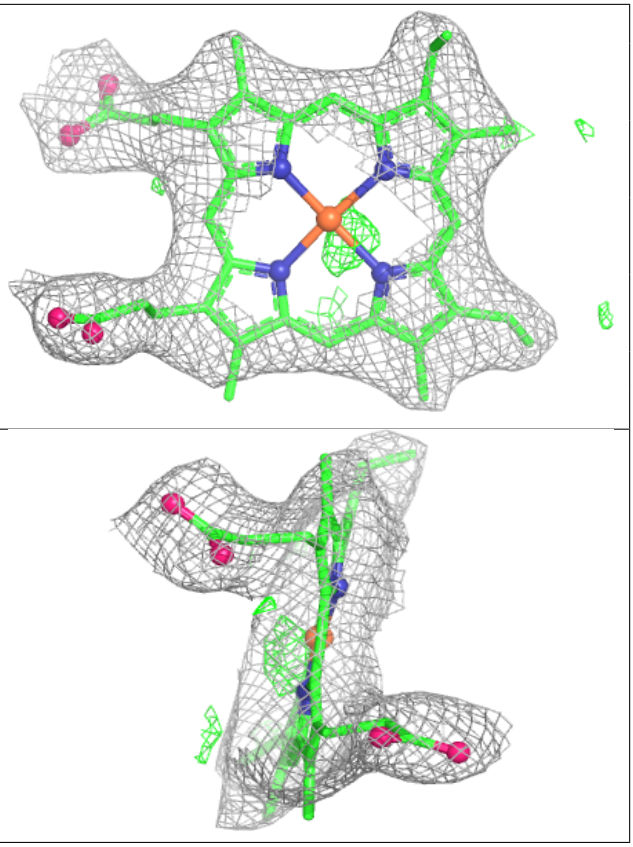






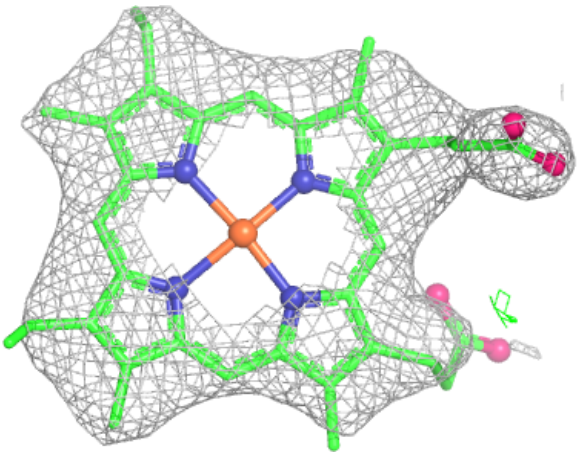
Electron density around HEM E 103:

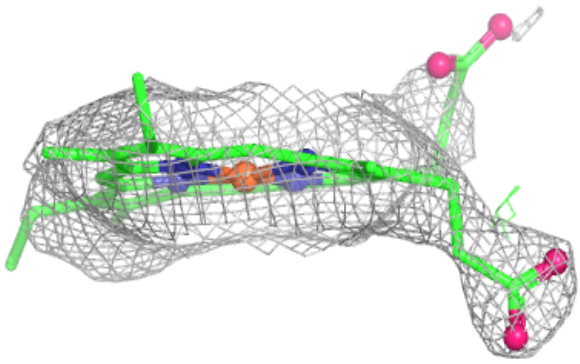
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

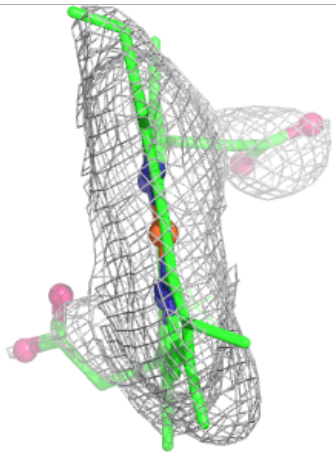


Electron density around HEM f 101:

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

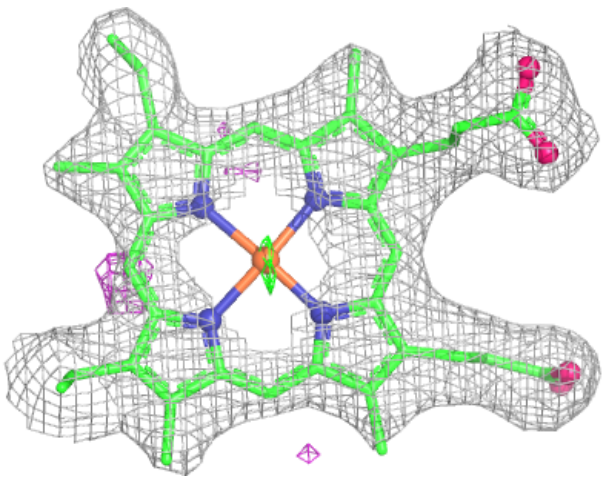


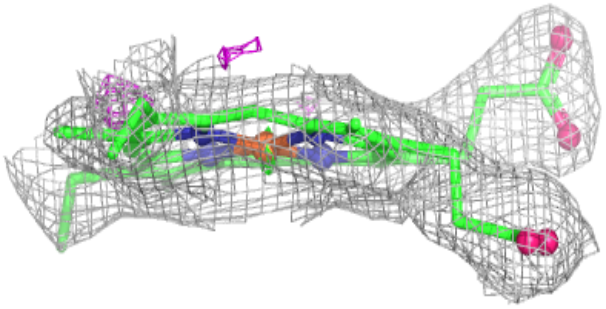


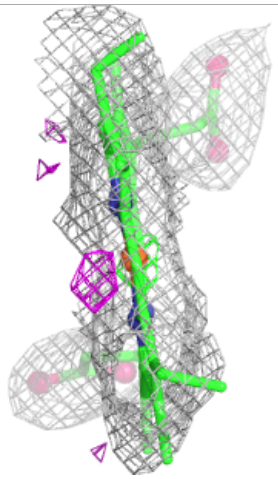


Electron density around HEC v 203:

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

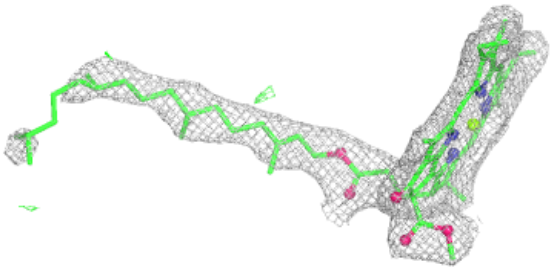


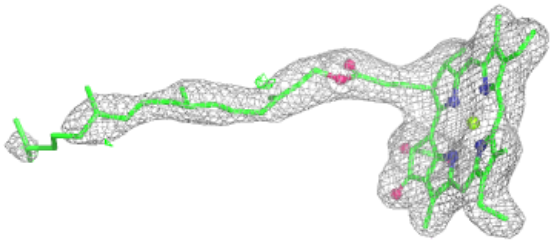


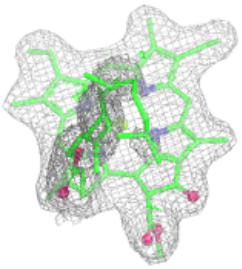


Electron density around CLA B 604:

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

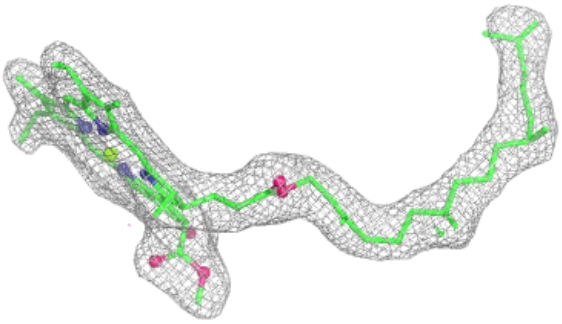


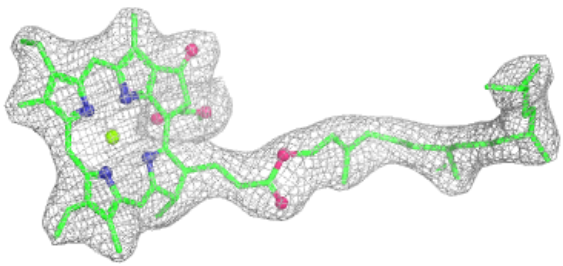


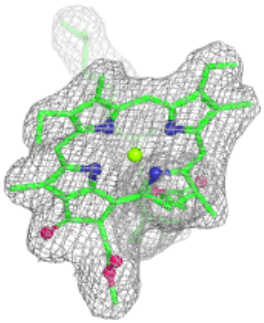


Electron density around CLA d 403:

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

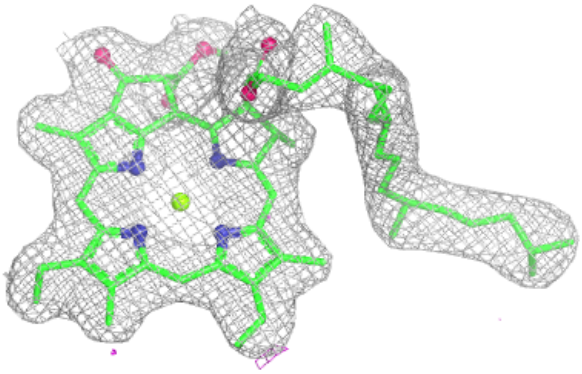


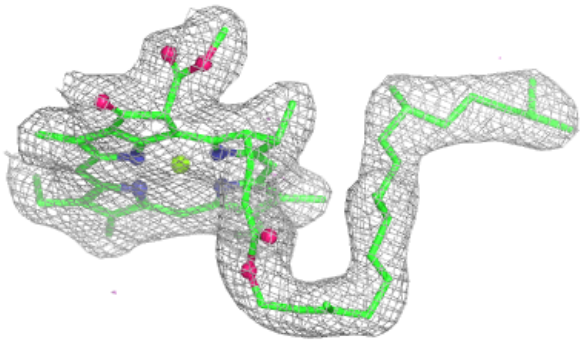


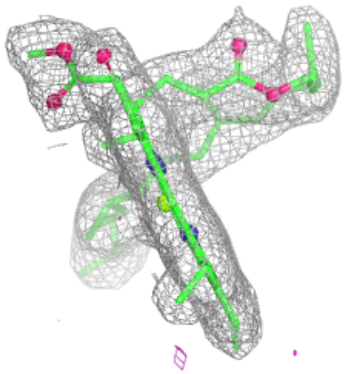


Electron density around CLA A 405:

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

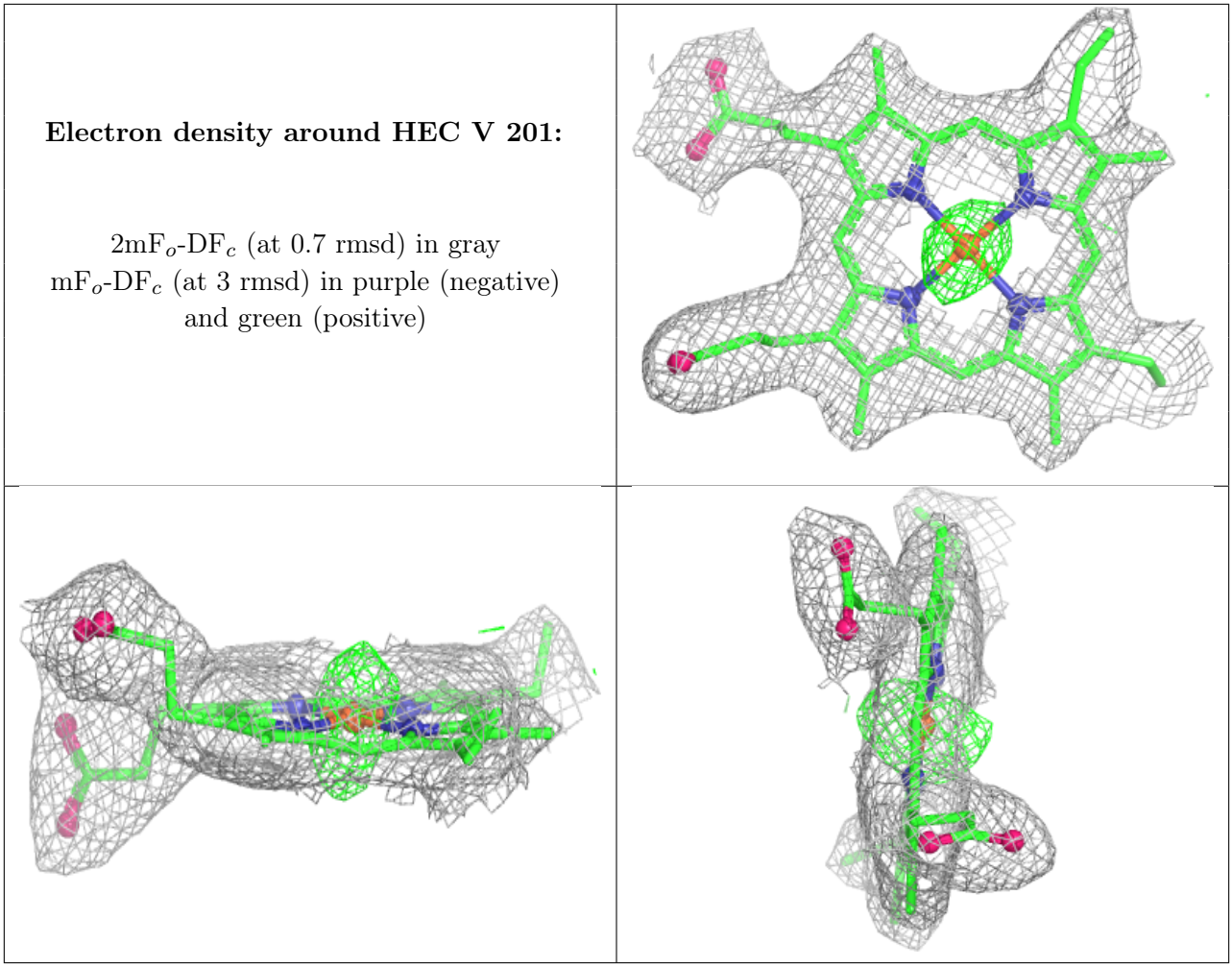






Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.