wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2026 – 06:27 AM JST

PDB ID	:	8GN1 / pdb_00008gn1
Title	:	Crystal structure of DBBQ-bound photosystem II complex
Authors	:	Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on	:	2022-08-22
Resolution	:	2.10 Å(reported)

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

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

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

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

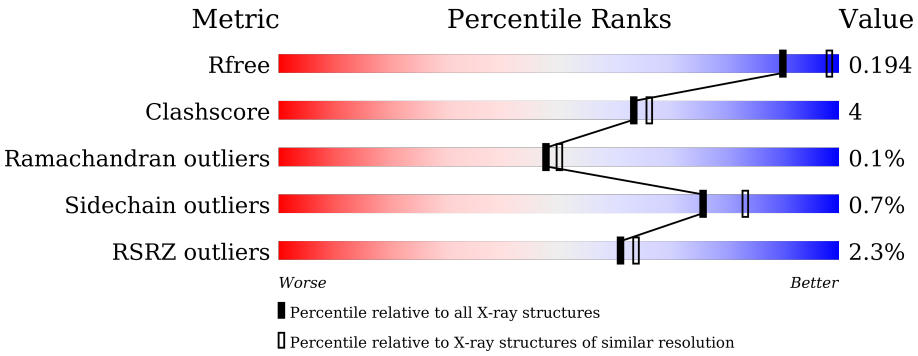
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



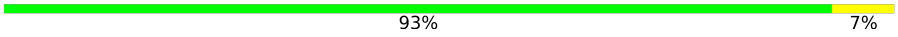
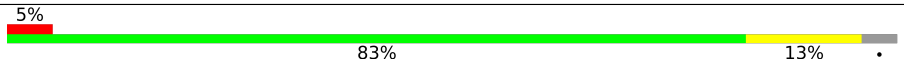
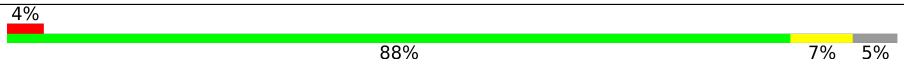
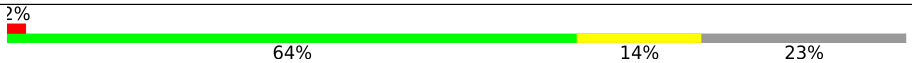
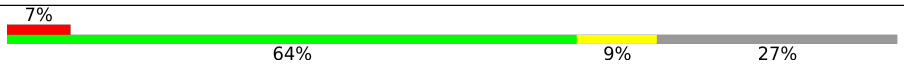
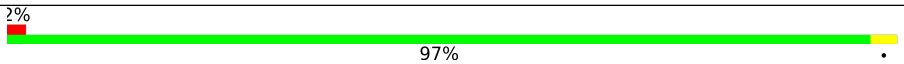
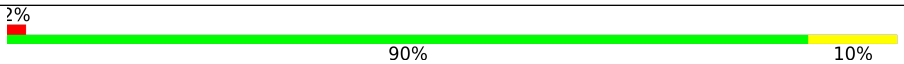
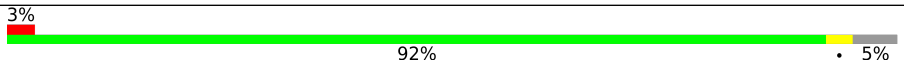
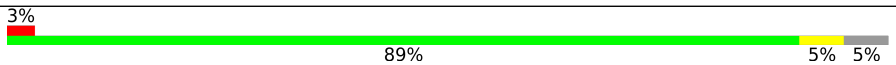
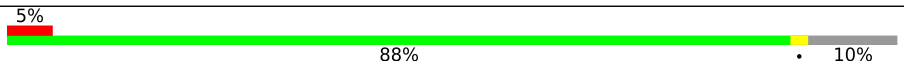
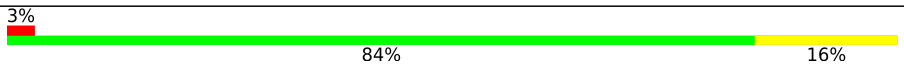
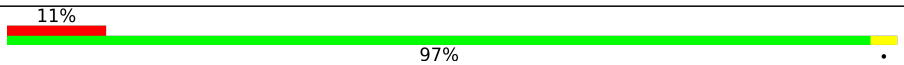
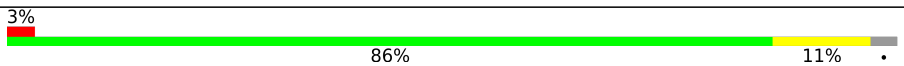
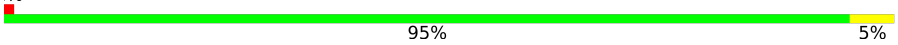
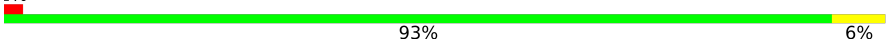
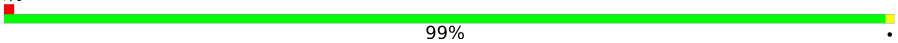
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	89% 8%
1	a	344	90% 8%
2	B	505	94% 6%
2	b	505	91% 9%
3	C	455	91% 7%
3	c	455	93% 7%

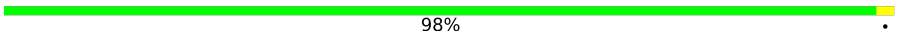
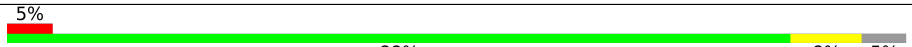
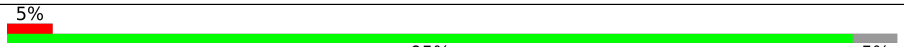
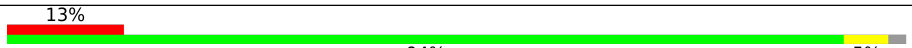
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	41	

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
43	HEC	V	201	X	-	-	-
43	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 54282 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	3	0
			2610	1713	428	454	15			
1	a	334	Total	C	N	O	S	0	3	0
			2620	1717	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	5	0
			3997	2623	667	694	13			
2	b	503	Total	C	N	O	S	0	8	0
			3962	2601	660	688	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	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	0	0
			3518	2303	589	613	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	342	Total	C	N	O	S	0	4	0
			2743	1819	447	464	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			649	425	103	121			
5	e	79	Total	C	N	O	0	0	0
			629	414	99	116			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			293	198	45	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	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	1	0
			293	205	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			298	202	45	51			
11	l	36	Total	C	N	O	0	2	0
			301	204	47	50			

- 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
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			270	182	39	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1864	1167	313	379	5			
13	o	243	Total	C	N	O	S	0	3	0
			1865	1169	311	379	6			

- 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
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			778	494	132	152			
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	1	0
			1059	675	177	203	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			220	146	35	36	3			
17	y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			275	185	44	46			
18	x	38	Total	C	N	O	0	1	0
			278	188	44	46			

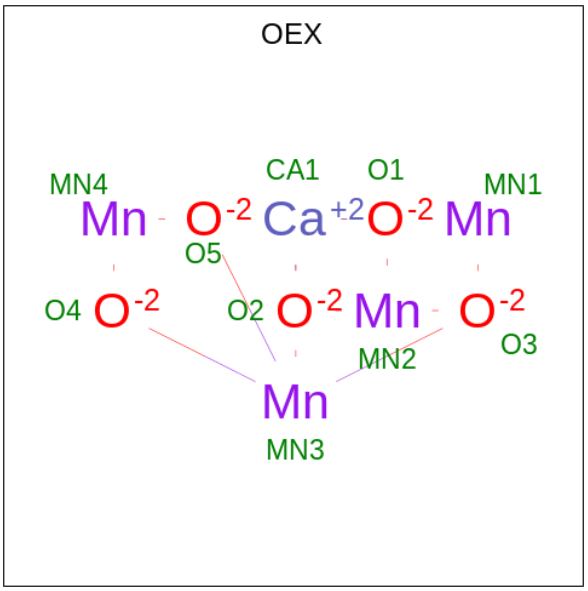
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			458	315	67	74	2			
19	z	61	Total	C	N	O	S	0	0	0
			453	309	70	72	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			207	133	39	35			

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

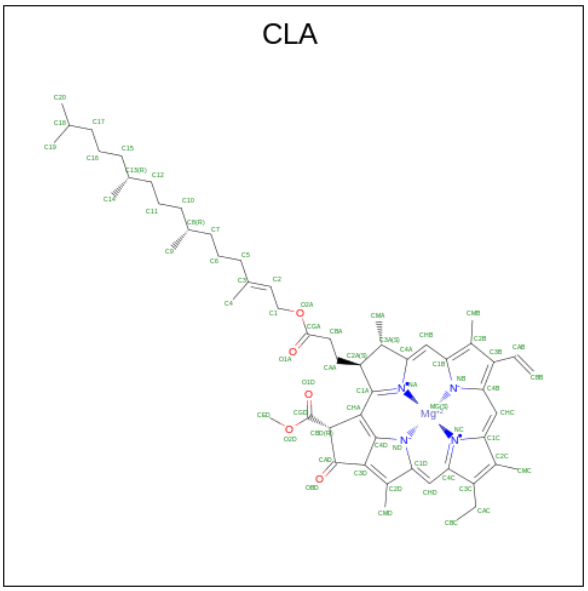
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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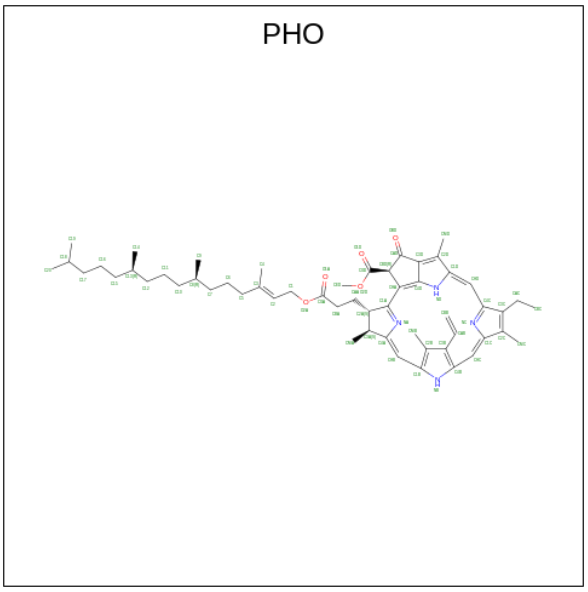
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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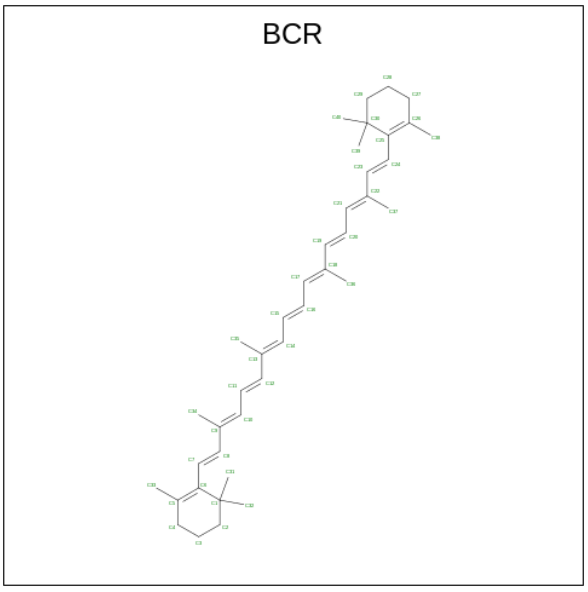
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



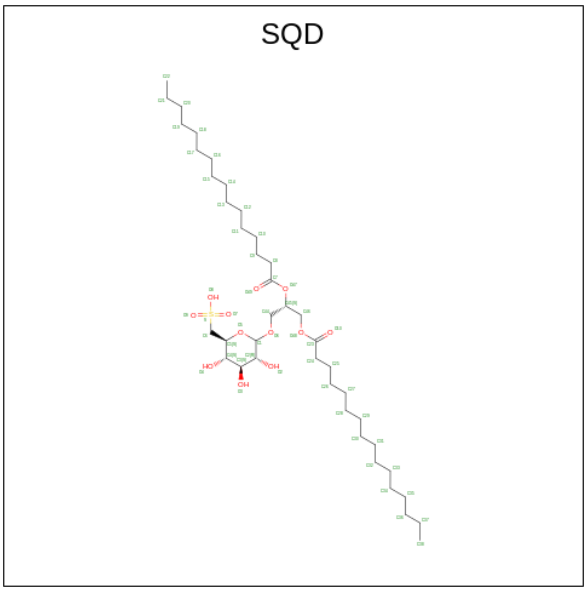
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



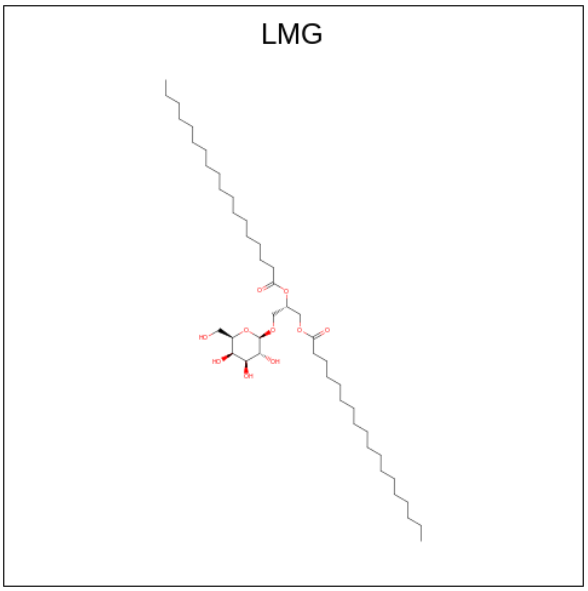
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total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

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



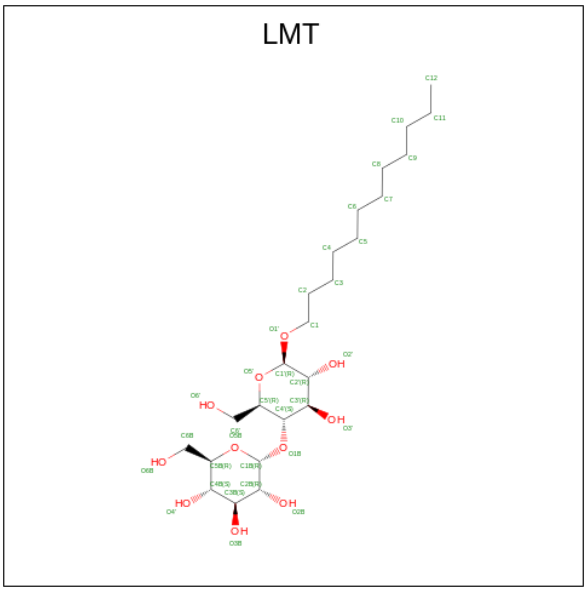
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			49	36	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			45	32	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			53	40	12	1		
27	a	1	Total	C	O	S	0	0
			47	34	12	1		
27	f	1	Total	C	O	S	0	0
			37	27	9	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 51 41 10	0	0
28	B	1	Total C O 51 41 10	0	0
28	C	1	Total C O 51 41 10	0	0
28	C	1	Total C O 48 38 10	0	0
28	D	1	Total C O 44 34 10	0	0
28	b	1	Total C O 51 41 10	0	0
28	c	1	Total C O 49 39 10	0	0
28	c	1	Total C O 48 38 10	0	0
28	d	1	Total C O 48 38 10	0	0
28	i	1	Total C O 51 41 10	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 34 23 11	0	0
29	A	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 24 18 6	0	0
29	E	1	Total C O 24 18 6	0	0
29	I	1	Total C O 24 18 6	0	0
29	J	1	Total C O 24 18 6	0	0
29	M	1	Total C O 35 24 11	0	0
29	T	1	Total C O 24 18 6	0	0
29	Z	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	b	1	Total C O 25 19 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	f	1	Total C O 24 18 6	0	0
29	i	1	Total C O 24 18 6	0	0
29	j	1	Total C O 23 17 6	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	z	1	Total C O 33 22 11	0	0

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

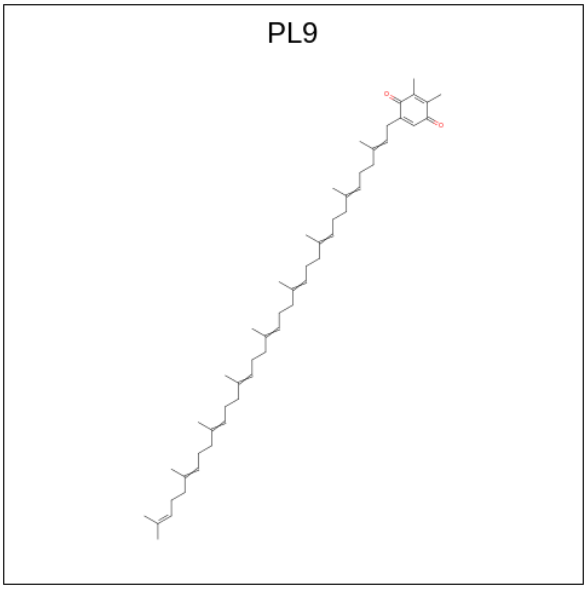
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	2	Total C O 55 50 5	0	0
30	B	5	Total C O 74 68 6	0	0
30	C	2	Total C O 50 45 5	0	0
30	D	3	Total C O 65 60 5	0	0
30	E	4	Total C 43 43	0	0
30	I	2	Total C 29 29	0	0
30	J	1	Total C 15 15	0	0
30	M	1	Total C O 15 13 2	0	0
30	T	1	Total C 9 9	0	0
30	Y	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	a	2	Total C O 26 22 4	0	0
30	b	4	Total C O 56 52 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	2	Total C O 48 43 5	0	0
30	d	4	Total C O 82 75 7	0	0
30	e	1	Total C 15 15	0	0
30	h	2	Total C 23 23	0	0
30	i	2	Total C O 29 25 4	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C 12 12	0	0
30	m	1	Total C 13 13	0	0
30	t	1	Total C 8 8	0	0

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



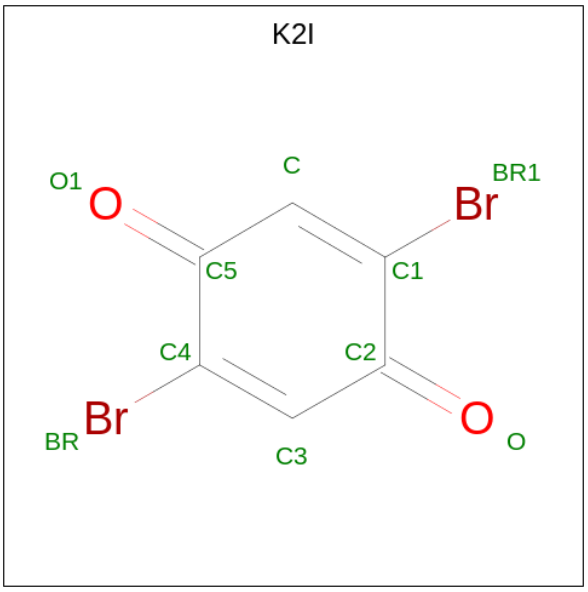
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C 39 39	0	0

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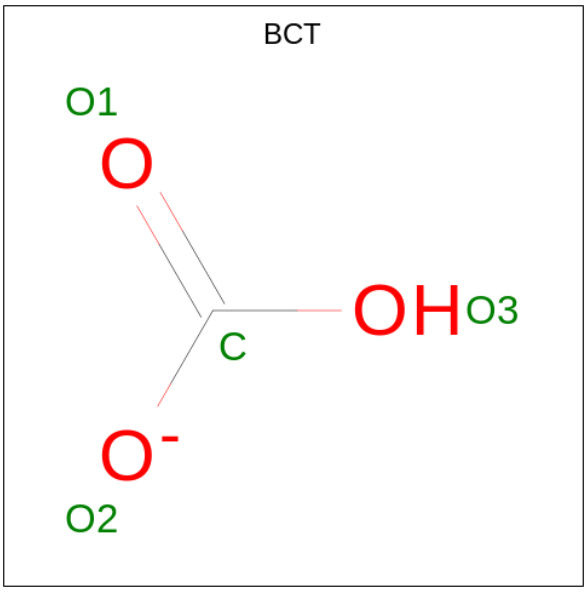
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	D	1	Total C O 55 53 2	0	0
31	d	1	Total C O 55 53 2	0	0
31	x	1	Total C 39 39	0	0

- Molecule 32 is 2,5-bis(bromanyl)cyclohexa-2,5-diene-1,4-dione (CCD ID: K2I) (formula: $C_6H_2Br_2O_2$) (labeled as "Ligand of Interest" by depositor).



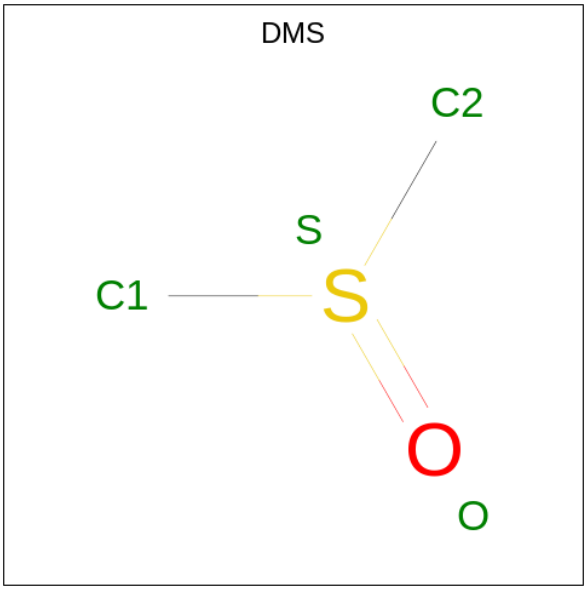
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Br C O 20 4 12 4	0	1
32	A	1	Total Br C O 10 2 6 2	0	0
32	a	1	Total Br C O 20 4 12 4	0	1
32	a	1	Total Br C O 10 2 6 2	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 4 1 3	0	0
33	a	1	Total C O 4 1 3	0	0

- Molecule 34 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	E	1	Total	C	O	S	0	0
			4	2	1	1		
34	E	1	Total	C	O	S	0	0
			4	2	1	1		
34	F	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		
34	a	1	Total	C	O	S	0	0
			4	2	1	1		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	c	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	d	1	Total	C	O	S	0	0
			4	2	1	1		
34	e	1	Total	C	O	S	0	0
			4	2	1	1		
34	i	1	Total	C	O	S	0	0
			4	2	1	1		
34	j	1	Total	C	O	S	0	0
			4	2	1	1		
34	k	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		

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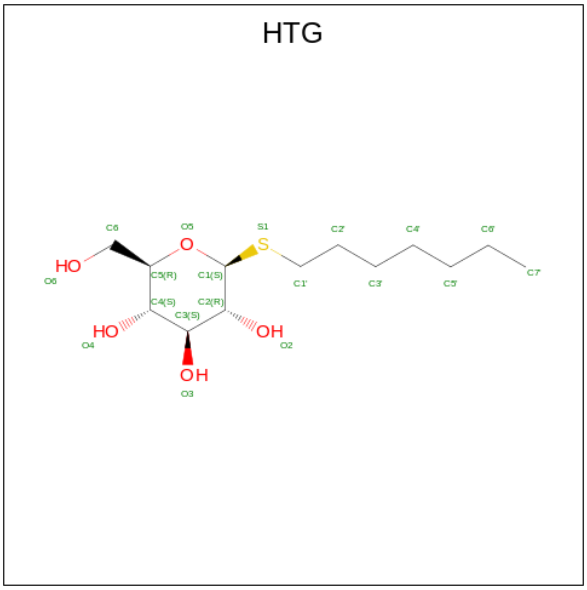
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	t	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	x	1	Total	C	O	S	0	0
			4	2	1	1		
34	z	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



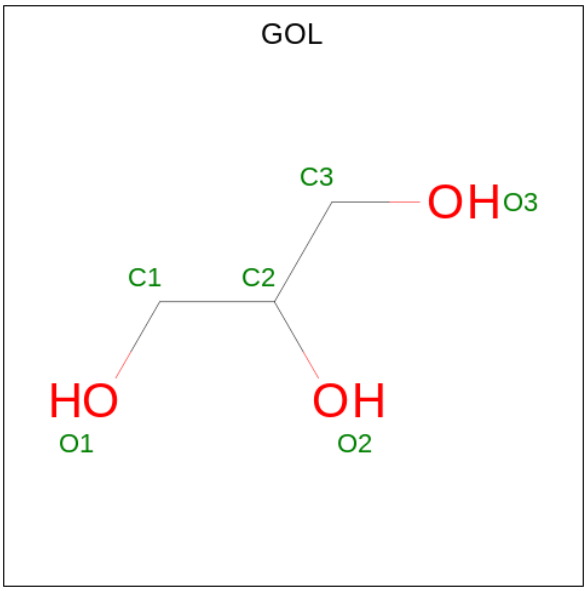
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 38 26 10 2	0	1
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 37 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



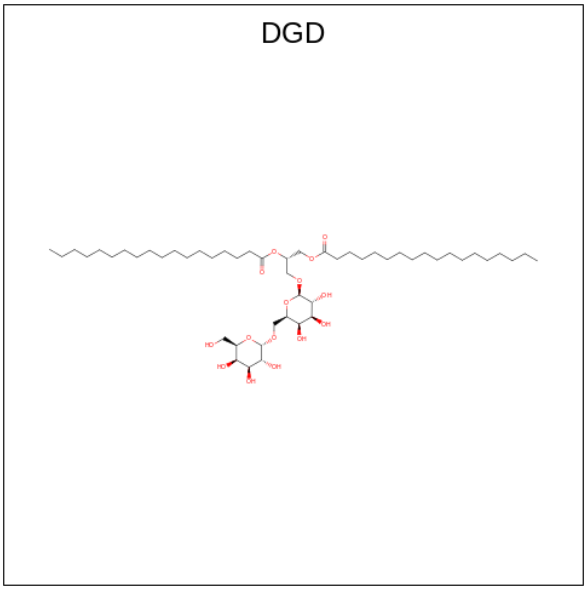
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	B	1	Total C O 6 3 3	0	0
37	B	1	Total C O 6 3 3	0	0
37	C	1	Total C O 6 3 3	0	0
37	C	1	Total C O 6 3 3	0	0
37	D	1	Total C O 6 3 3	0	0
37	H	1	Total C O 6 3 3	0	0
37	O	1	Total C O 6 3 3	0	0
37	U	1	Total C O 6 3 3	0	0
37	U	1	Total C O 6 3 3	0	0
37	V	1	Total C O 6 3 3	0	0
37	Z	1	Total C O 6 3 3	0	0
37	a	1	Total C O 6 3 3	0	0
37	b	1	Total C O 6 3 3	0	0
37	c	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	d	1	Total C O 6 3 3	0	0
37	k	1	Total C O 6 3 3	0	0
37	o	1	Total C O 6 3 3	0	0
37	o	1	Total C O 6 3 3	0	0
37	v	1	Total C O 6 3 3	0	0
37	v	1	Total C O 6 3 3	0	0
37	v	1	Total C O 6 3 3	0	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



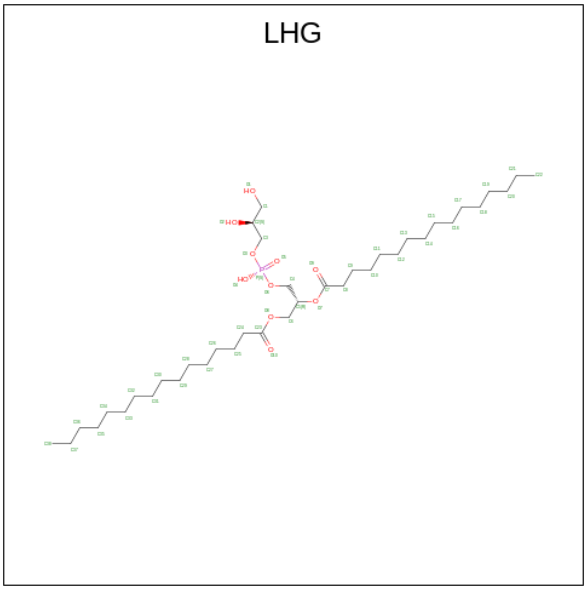
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	C	1	Total C O 62 47 15	0	0
38	C	1	Total C O 62 47 15	0	0
38	C	1	Total C O 62 47 15	0	0
38	D	1	Total C O 46 35 11	0	0

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

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



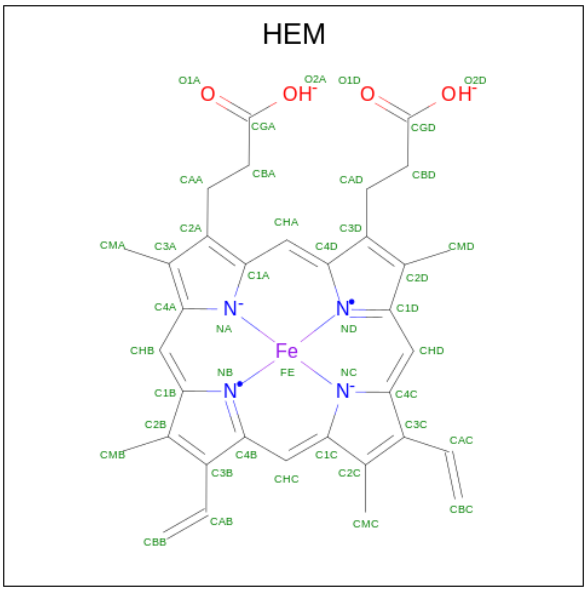
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	D	1	Total C O P 49 38 10 1	0	0
39	D	1	Total C O P 49 38 10 1	0	0
39	D	1	Total C O P 44 33 10 1	0	0
39	E	1	Total C O P 49 38 10 1	0	0
39	L	1	Total C O P 49 38 10 1	0	0
39	d	1	Total C O P 49 38 10 1	0	0

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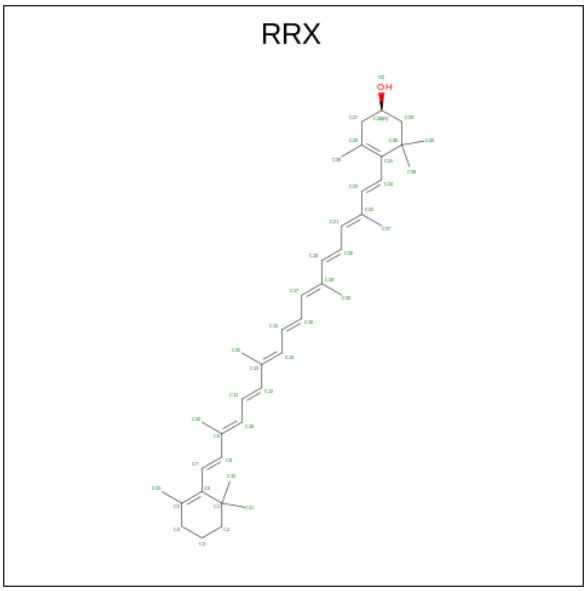
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	d	1	Total C O P 49 38 10 1	0	0
39	d	1	Total C O P 36 25 10 1	0	0
39	e	1	Total C O P 32 22 9 1	0	0
39	l	1	Total C O P 49 38 10 1	0	0

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 41 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

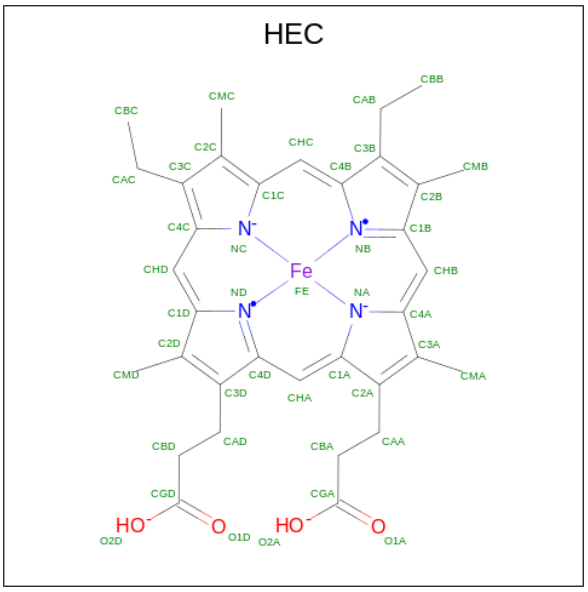


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	H	1	Total C O 41 40 1	0	0
41	h	1	Total C O 41 40 1	0	0

- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 43 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	A	142	Total	O	0	0
			142	142		
44	B	291	Total	O	0	0
			291	291		
44	C	231	Total	O	0	0
			231	231		
44	D	140	Total	O	0	2
			142	142		
44	E	34	Total	O	0	0
			34	34		
44	F	6	Total	O	0	0
			6	6		
44	H	47	Total	O	0	0
			47	47		
44	I	11	Total	O	0	0
			11	11		
44	J	13	Total	O	0	0
			13	13		
44	K	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	L	19	Total O 19 19	0	0
44	M	6	Total O 6 6	0	0
44	O	148	Total O 148 148	0	0
44	T	13	Total O 13 13	0	0
44	U	80	Total O 80 80	0	0
44	V	121	Total O 121 121	0	0
44	Y	5	Total O 5 5	0	0
44	X	14	Total O 14 14	0	0
44	Z	1	Total O 1 1	0	0
44	a	135	Total O 135 135	0	0
44	b	265	Total O 268 268	0	3
44	c	229	Total O 229 229	0	0
44	d	135	Total O 135 135	0	0
44	e	23	Total O 23 23	0	0
44	f	9	Total O 9 9	0	0
44	h	32	Total O 32 32	0	0
44	i	12	Total O 12 12	0	0
44	j	15	Total O 15 15	0	0
44	k	8	Total O 8 8	0	0
44	l	13	Total O 14 14	0	1
44	m	9	Total O 9 9	0	0

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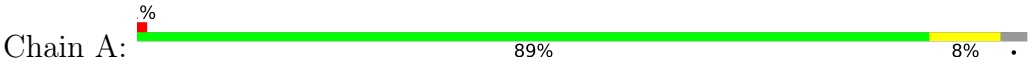
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	o	130	Total O 131 131	0	1
44	t	11	Total O 11 11	0	0
44	u	90	Total O 91 91	0	1
44	v	98	Total O 100 100	0	2
44	y	8	Total O 8 8	0	0
44	x	12	Total O 12 12	0	0
44	z	4	Total O 4 4	0	0
44	R	1	Total O 1 1	0	0

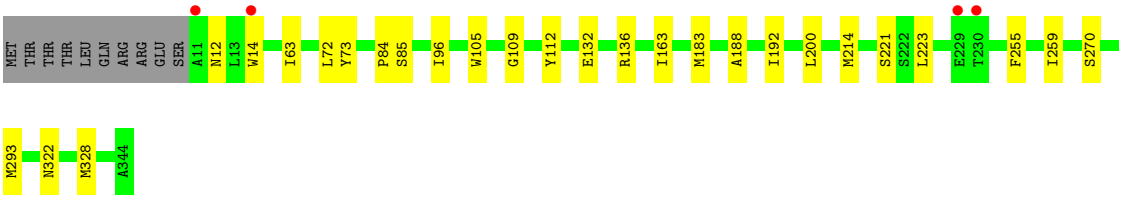
3 Residue-property plots (i)

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

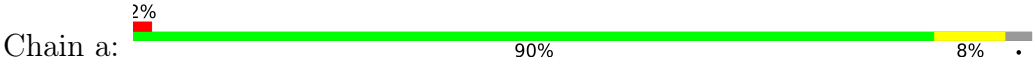
Chain A:

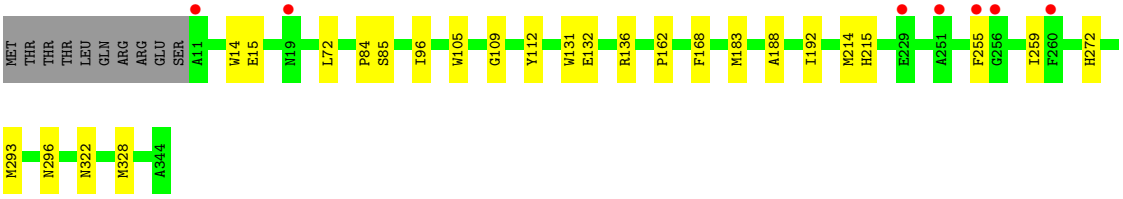




• Molecule 1: Photosystem II protein D1

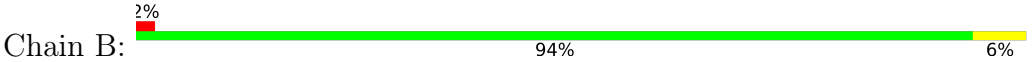
Chain a:

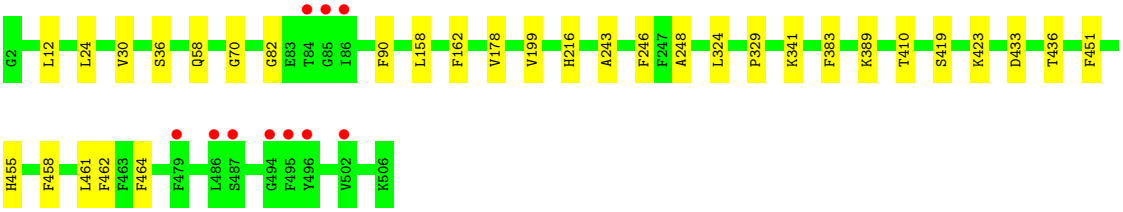




• Molecule 2: Photosystem II CP47 reaction center protein

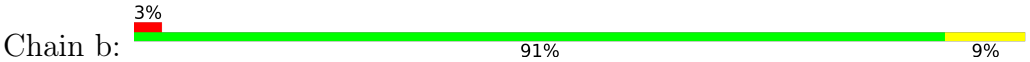
Chain B:

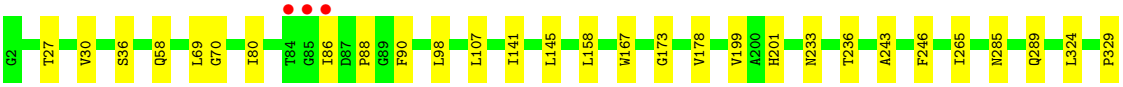


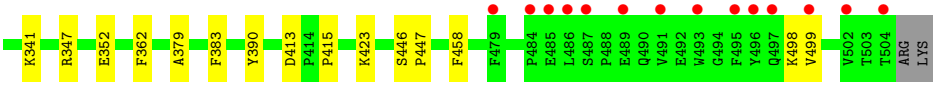


• Molecule 2: Photosystem II CP47 reaction center protein

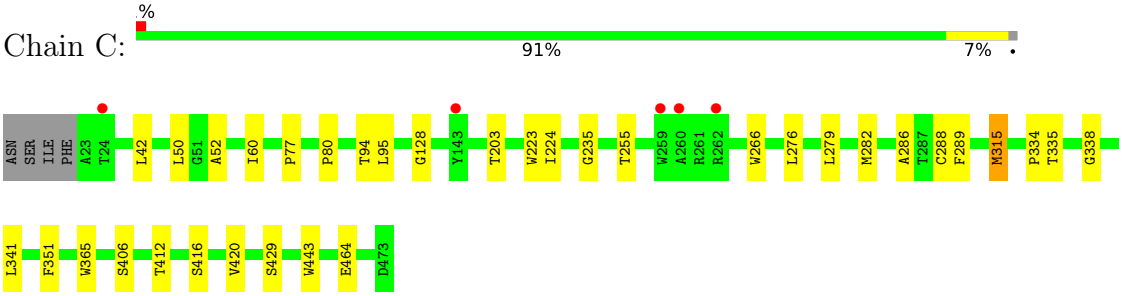
Chain b:



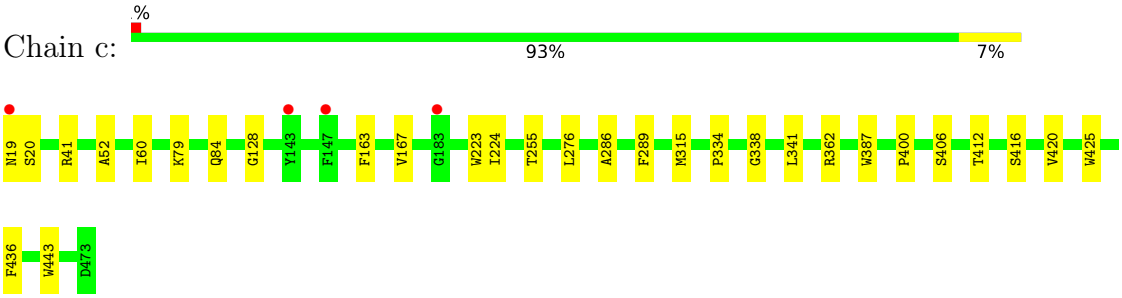




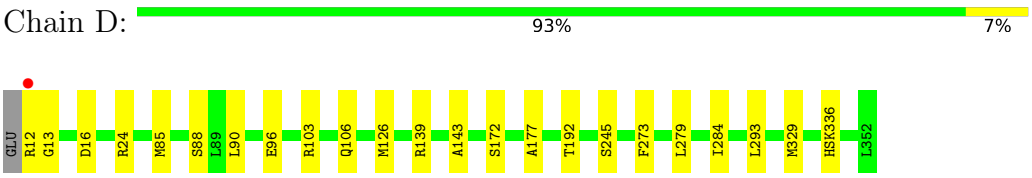
• Molecule 3: Photosystem II CP43 reaction center protein



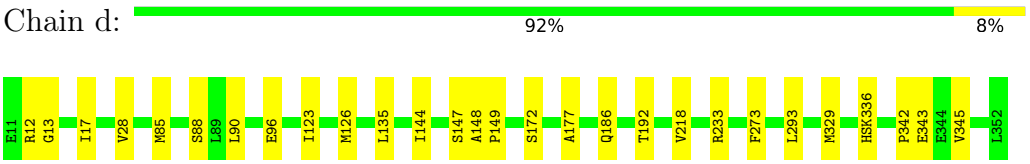
• Molecule 3: Photosystem II CP43 reaction center protein



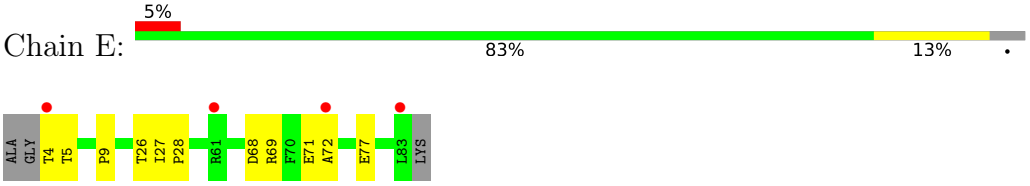
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



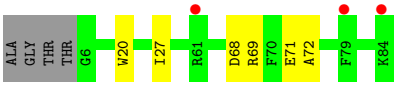
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

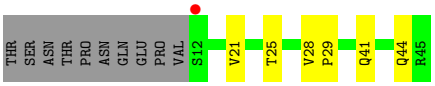




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

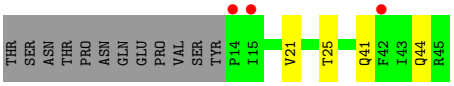




• Molecule 6: Cytochrome b559 subunit beta

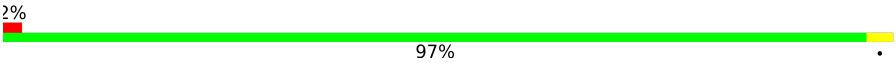
Chain f:





• Molecule 7: Photosystem II reaction center protein H

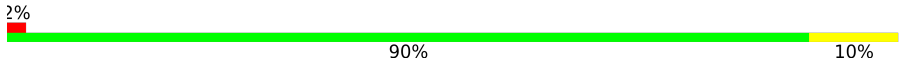
Chain H:

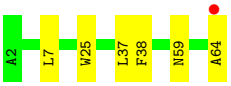




• Molecule 7: Photosystem II reaction center protein H

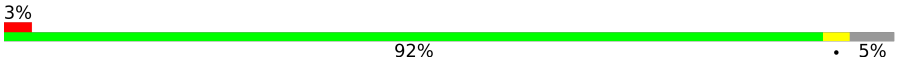
Chain h:

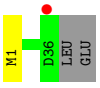




• Molecule 8: Photosystem II reaction center protein I

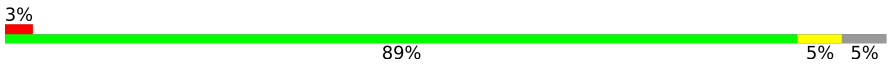
Chain I:

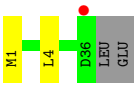




• Molecule 8: Photosystem II reaction center protein I

Chain i:

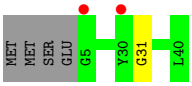




• Molecule 9: Photosystem II reaction center protein J

Chain J:

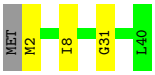




• Molecule 9: Photosystem II reaction center protein J

Chain j:

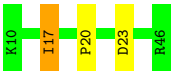




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

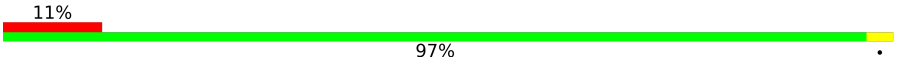
Chain k:

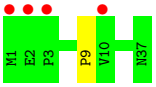




• Molecule 11: Photosystem II reaction center protein L

Chain L:

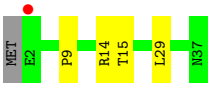




• Molecule 11: Photosystem II reaction center protein L

Chain l:

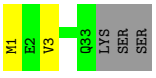




• Molecule 12: Photosystem II reaction center protein M

Chain M:

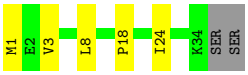




• Molecule 12: Photosystem II reaction center protein M

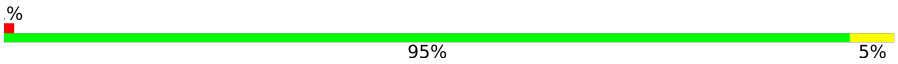
Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

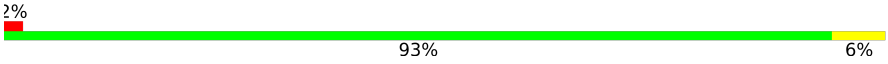
Chain O:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

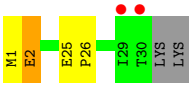




• Molecule 14: Photosystem II reaction center protein T

Chain T:

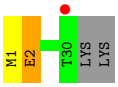




• Molecule 14: Photosystem II reaction center protein T

Chain t:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

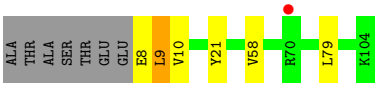




• Molecule 15: Photosystem II 12 kDa extrinsic protein

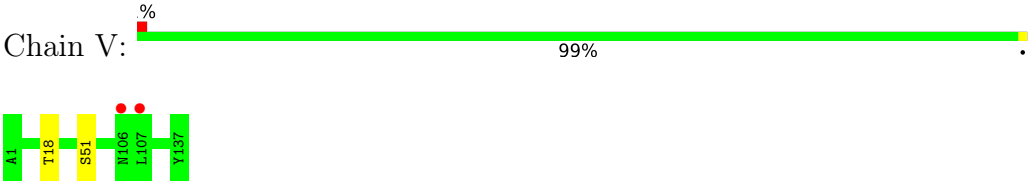
Chain u:





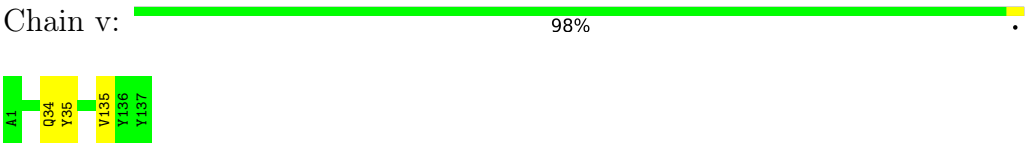
• Molecule 16: Cytochrome c-550

Chain V:



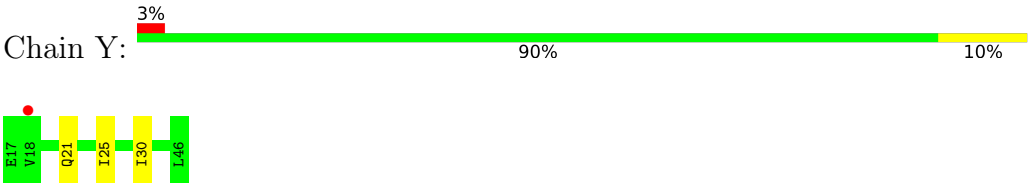
• Molecule 16: Cytochrome c-550

Chain v:



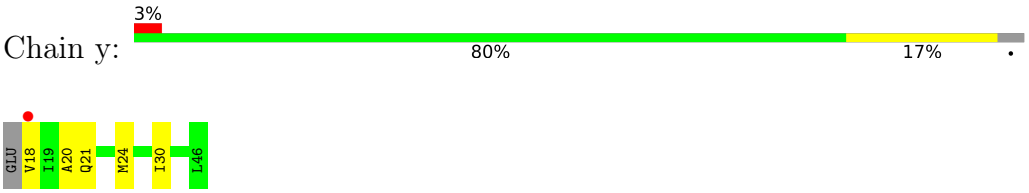
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



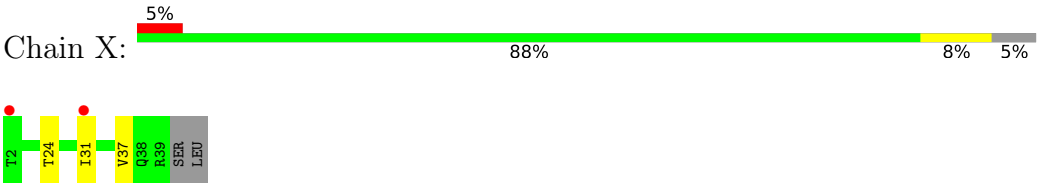
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



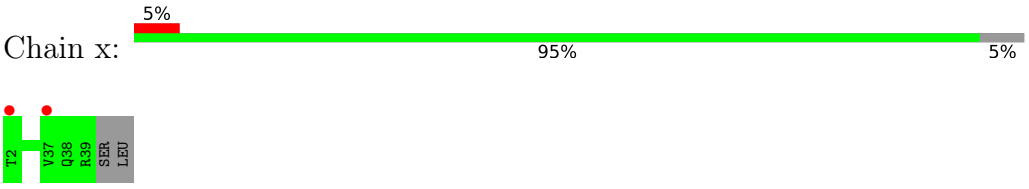
• Molecule 18: Photosystem II reaction center protein X

Chain X:



• Molecule 18: Photosystem II reaction center protein X

Chain x:



• Molecule 19: Photosystem II reaction center protein Z

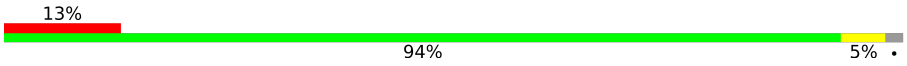
Chain Z:

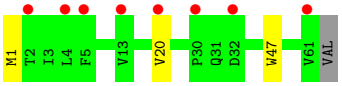




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

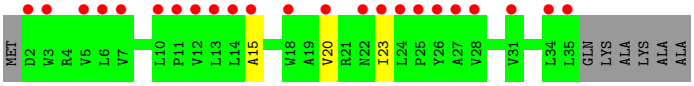




• Molecule 20: Photosystem II protein Y

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.19Å 228.46Å 286.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.10 49.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.02-2.10) 88.1 (49.02-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.157 , 0.191 0.163 , 0.194	Depositor DCC
R_{free} test set	22959 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54282	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, HTG, LMT, BCR, SQD, LMG, LHG, PL9, RRX, CL, DMS, FE2, UNL, HEM, BCT, CLA, HSK, HEC, CA, K2I, FME, PHO, GOL, MG, OEX

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	0.35	0/2704	0.53	0/3690
1	a	0.34	0/2713	0.52	0/3700
2	B	0.33	0/4149	0.49	0/5652
2	b	0.32	0/4123	0.47	0/5619
3	C	0.30	0/3613	0.46	0/4919
3	c	0.28	0/3632	0.46	0/4945
4	D	0.36	0/2804	0.50	0/3820
4	d	0.34	0/2827	0.48	0/3850
5	E	0.27	0/671	0.45	0/918
5	e	0.24	0/648	0.44	0/887
6	F	0.24	0/284	0.43	0/387
6	f	0.25	0/265	0.45	0/360
7	H	0.28	0/511	0.42	0/697
7	h	0.26	0/511	0.43	0/697
8	I	0.21	0/290	0.40	0/393
8	i	0.25	0/293	0.43	0/396
9	J	0.23	0/257	0.40	0/349
9	j	0.22	0/277	0.36	0/376
10	K	0.25	0/306	0.45	0/422
10	k	0.24	0/296	0.42	0/408
11	L	0.39	0/308	0.43	0/420
11	l	0.35	0/314	0.44	0/428
12	M	0.30	0/257	0.52	0/352
12	m	0.32	0/266	0.46	0/363
13	O	0.31	0/1901	0.50	0/2579
13	o	0.28	0/1905	0.49	0/2583
14	T	0.34	0/255	0.42	0/346
14	t	0.33	0/255	0.40	0/346
15	U	0.32	0/792	0.49	0/1073
15	u	0.31	0/785	0.47	0/1064
16	V	0.32	0/1083	0.46	0/1470

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.26	0/1073	0.44	0/1461
17	Y	0.22	0/221	0.37	0/296
17	y	0.24	0/213	0.40	0/285
18	X	0.21	0/278	0.34	0/376
18	x	0.20	0/284	0.35	0/384
19	Z	0.20	0/459	0.38	0/630
19	z	0.17	0/454	0.35	0/622
20	R	0.16	0/209	0.33	0/290
All	All	0.31	0/42486	0.47	0/57853

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2610	0	2506	20	0
1	a	2620	0	2527	18	0
2	B	3997	0	3860	31	0
2	b	3962	0	3813	30	0
3	C	3494	0	3418	27	0
3	c	3518	0	3434	23	0
4	D	2726	0	2629	19	0
4	d	2743	0	2652	21	0
5	E	649	0	627	8	0
5	e	629	0	600	6	0
6	F	275	0	282	3	0
6	f	257	0	269	2	0
7	H	498	0	518	3	0
7	h	498	0	518	5	0
8	I	293	0	302	0	0
8	i	296	0	311	1	0
9	J	251	0	257	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	271	0	270	4	0
10	K	293	0	303	3	0
10	k	286	0	285	4	0
11	L	298	0	309	1	0
11	l	301	0	320	4	0
12	M	261	0	280	1	0
12	m	270	0	293	4	0
13	O	1864	0	1835	9	0
13	o	1865	0	1842	10	0
14	T	256	0	256	2	0
14	t	256	0	256	1	0
15	U	778	0	782	6	0
15	u	774	0	773	3	0
16	V	1059	0	1074	2	0
16	v	1052	0	1040	3	0
17	Y	220	0	245	3	0
17	y	212	0	237	4	0
18	X	275	0	301	3	0
18	x	278	0	305	0	0
19	Z	458	0	472	0	0
19	z	453	0	459	3	0
20	R	207	0	157	2	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	4	0
24	B	1040	0	1152	25	0
24	C	845	0	936	29	0
24	D	195	0	216	5	0
24	a	195	0	216	6	0
24	b	1040	0	1152	27	0
24	c	845	0	936	28	0
24	d	195	0	216	7	0
25	A	128	0	148	2	0
25	a	128	0	148	1	0
26	A	40	0	56	1	0
26	B	120	0	168	6	0
26	C	80	0	112	7	0
26	D	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	K	40	0	56	1	0
26	T	40	0	56	5	0
26	Y	40	0	56	3	0
26	a	40	0	56	1	0
26	b	120	0	168	6	0
26	c	120	0	168	6	0
26	d	40	0	56	1	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
27	A	103	0	143	2	0
27	B	54	0	78	3	0
27	F	45	0	57	2	0
27	L	54	0	78	1	0
27	a	100	0	131	2	0
27	f	37	0	45	1	0
28	A	51	0	72	1	0
28	B	51	0	72	2	0
28	C	99	0	138	2	0
28	D	44	0	58	0	0
28	b	51	0	72	1	0
28	c	97	0	134	1	0
28	d	48	0	66	0	0
28	i	51	0	72	2	0
29	A	69	0	87	3	0
29	B	94	0	127	2	0
29	E	24	0	35	0	0
29	I	24	0	35	0	0
29	J	24	0	35	1	0
29	M	35	0	46	2	0
29	T	24	0	35	0	0
29	Z	35	0	46	0	0
29	a	70	0	92	4	0
29	b	25	0	35	0	0
29	f	24	0	35	0	0
29	i	24	0	35	1	0
29	j	23	0	22	0	0
29	m	70	0	92	2	0
29	z	33	0	35	2	0
30	A	55	0	0	0	0
30	B	74	0	0	0	0
30	C	50	0	0	0	0
30	D	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	E	43	0	0	0	0
30	I	29	0	0	0	0
30	J	15	0	0	0	0
30	M	15	0	0	0	0
30	T	9	0	0	0	0
30	X	18	0	0	0	0
30	Y	10	0	0	0	0
30	a	26	0	0	0	0
30	b	56	0	0	0	0
30	c	48	0	0	0	0
30	d	82	0	0	0	0
30	e	15	0	0	0	0
30	h	23	0	0	0	0
30	i	29	0	0	0	0
30	j	16	0	0	0	0
30	k	12	0	0	0	0
30	m	13	0	0	0	0
30	t	8	0	0	0	0
31	A	39	0	59	2	0
31	D	55	0	80	0	0
31	d	55	0	80	1	0
31	x	39	0	59	1	0
32	A	30	0	0	3	0
32	a	30	0	0	3	0
33	A	4	0	0	0	0
33	a	4	0	0	0	0
34	A	20	0	30	0	0
34	B	52	0	78	2	0
34	C	52	0	78	3	0
34	D	20	0	30	0	0
34	E	8	0	12	0	0
34	F	4	0	6	0	0
34	O	44	0	66	2	0
34	T	12	0	18	0	0
34	U	4	0	6	2	0
34	V	28	0	42	1	0
34	a	16	0	24	0	0
34	b	48	0	72	2	0
34	c	56	0	84	2	0
34	d	28	0	42	3	0
34	e	4	0	6	0	0
34	i	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	j	4	0	6	0	0
34	k	4	0	6	0	0
34	o	36	0	54	1	0
34	t	4	0	6	0	0
34	u	16	0	24	0	0
34	v	40	0	60	1	0
34	x	4	0	6	0	0
34	z	4	0	6	0	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	o	1	0	0	0	0
36	B	114	0	156	8	0
36	C	38	0	52	0	0
36	D	19	0	26	3	0
36	I	19	0	26	1	0
36	O	19	0	26	1	0
36	V	19	0	26	0	0
36	b	76	0	104	7	0
36	c	57	0	78	0	0
36	d	38	0	52	2	0
36	i	19	0	26	0	0
37	B	12	0	16	2	0
37	C	12	0	16	0	0
37	D	6	0	8	1	0
37	H	6	0	8	0	0
37	O	6	0	8	0	0
37	U	12	0	16	0	0
37	V	6	0	8	0	0
37	Z	6	0	8	0	0
37	a	6	0	8	0	0
37	b	6	0	8	0	0
37	c	6	0	8	2	0
37	d	6	0	8	0	0
37	k	6	0	8	0	0
37	o	12	0	16	2	0
37	v	18	0	24	0	0
38	C	186	0	246	9	0
38	D	46	0	57	0	0
38	H	62	0	82	0	0
38	c	186	0	246	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	62	0	82	1	0
39	D	142	0	209	5	0
39	E	49	0	74	5	0
39	L	49	0	74	2	0
39	d	134	0	190	3	0
39	e	32	0	43	1	0
39	l	49	0	74	1	0
40	F	43	0	30	1	0
40	e	43	0	30	2	0
41	H	41	0	56	3	0
41	h	41	0	56	3	0
42	J	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	0	0
43	v	43	0	30	0	0
44	A	142	0	0	0	0
44	B	291	0	0	2	0
44	C	231	0	0	1	0
44	D	142	0	0	0	0
44	E	34	0	0	0	0
44	F	6	0	0	0	0
44	H	47	0	0	0	0
44	I	11	0	0	0	0
44	J	13	0	0	0	0
44	K	12	0	0	0	0
44	L	19	0	0	0	0
44	M	6	0	0	0	0
44	O	148	0	0	1	0
44	R	1	0	0	0	0
44	T	13	0	0	0	0
44	U	80	0	0	4	0
44	V	121	0	0	0	0
44	X	14	0	0	0	0
44	Y	5	0	0	0	0
44	Z	1	0	0	0	0
44	a	135	0	0	0	0
44	b	268	0	0	4	0
44	c	229	0	0	0	0
44	d	135	0	0	0	0
44	e	23	0	0	0	0
44	f	9	0	0	0	0
44	h	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	12	0	0	0	0
44	j	15	0	0	1	0
44	k	8	0	0	0	0
44	l	14	0	0	0	0
44	m	9	0	0	0	0
44	o	131	0	0	3	0
44	t	11	0	0	0	0
44	u	91	0	0	0	0
44	v	100	0	0	1	0
44	x	12	0	0	0	0
44	y	8	0	0	0	0
44	z	4	0	0	0	0
All	All	54282	0	52476	414	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 4.

The worst 5 of 414 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:14:TRP:HD1	29:a:2120:LMT:H6B	0.98	0.91
1:a:14:TRP:CD1	29:a:2120:LMT:H6B	1.91	0.86
4:D:13:GLY:HA3	36:D:413:HTG:H62	1.62	0.82
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.68	0.76
24:b:618:CLA:H2	24:b:619:CLA:HBB2	1.71	0.73

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	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36	36
1	a	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36	36
2	B	508/505 (101%)	502 (99%)	6 (1%)	0	100	100
2	b	509/505 (101%)	503 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	442 (98%)	8 (2%)	1 (0%)	43	44
3	c	453/455 (100%)	443 (98%)	9 (2%)	1 (0%)	43	44
4	D	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
4	d	342/342 (100%)	335 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	77/83 (93%)	77 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
7	h	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
13	o	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5244/5387 (97%)	5155 (98%)	85 (2%)	4 (0%)	48	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	416	SER
3	C	416	SER
1	A	259	ILE
1	a	259	ILE

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	267/279 (96%)	266 (100%)	1 (0%)	84	89
1	a	270/279 (97%)	269 (100%)	1 (0%)	84	89
2	B	405/403 (100%)	405 (100%)	0	100	100
2	b	398/403 (99%)	395 (99%)	3 (1%)	73	81
3	C	354/356 (99%)	351 (99%)	3 (1%)	73	81
3	c	355/356 (100%)	352 (99%)	3 (1%)	73	81
4	D	275/276 (100%)	273 (99%)	2 (1%)	76	83
4	d	278/276 (101%)	275 (99%)	3 (1%)	65	74
5	E	70/72 (97%)	68 (97%)	2 (3%)	37	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	66/72 (92%)	66 (100%)	0	100	100
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	34
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	32
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	37
10	k	28/30 (93%)	28 (100%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	205/207 (99%)	205 (100%)	0	100	100
13	o	206/207 (100%)	203 (98%)	3 (2%)	57	65
14	T	25/28 (89%)	24 (96%)	1 (4%)	28	29
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	49
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	49
16	V	115/117 (98%)	115 (100%)	0	100	100
16	v	114/117 (97%)	114 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	25
17	y	21/23 (91%)	20 (95%)	1 (5%)	23	23
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	45/51 (88%)	45 (100%)	0	100	100
19	z	43/51 (84%)	43 (100%)	0	100	100
20	R	11/33 (33%)	11 (100%)	0	100	100
All	All	4252/4401 (97%)	4220 (99%)	32 (1%)	76	81

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	t	2	GLU
15	u	9	LEU
15	U	70[B]	ARG
15	U	70[A]	ARG
15	u	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	296	ASN
2	b	331	ASN
2	b	289	GLN
3	c	385	GLN
4	D	186	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
4	HSK	D	336[A]	-	9,10,12	10.51	2 (22%)	6,12,16	2.12	2 (33%)
8	FME	I	1	8	8,9,10	0.60	0	7,9,11	1.56	2 (28%)
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.66	2 (28%)
4	HSK	D	336[B]	-	9,11,12	1.84	2 (22%)	6,14,16	3.92	4 (66%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.32	1 (14%)
19	FME	Z	1	19	8,9,10	0.63	0	7,9,11	1.81	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HSK	d	336[A]	-	9,10,12	5.62	1 (11%)	6,12,16	1.85	3 (50%)
8	FME	i	1	8	8,9,10	0.58	0	7,9,11	1.59	2 (28%)
19	FME	z	1	19	8,9,10	0.62	0	7,9,11	1.63	4 (57%)
4	HSK	d	336[B]	-	9,11,12	1.78	2 (22%)	6,14,16	3.96	4 (66%)
12	FME	M	1	12	8,9,10	0.73	0	7,9,11	1.33	1 (14%)
14	FME	t	1	14	8,9,10	0.66	0	7,9,11	1.79	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	m	1	12	-	1/7/9/11	-
19	FME	Z	1	19	-	3/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
19	FME	z	1	19	-	4/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-31.36	0.97	1.38
4	d	336[A]	HSK	OM-ND1	-16.46	1.17	1.38
4	D	336[B]	HSK	OM-ND1	4.06	1.44	1.38
4	d	336[B]	HSK	OM-ND1	3.70	1.43	1.38
4	D	336[B]	HSK	CE1-ND1	-2.44	1.33	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	336[B]	HSK	ND1-CE1-NE2	-6.13	104.08	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	336[B]	HSK	ND1-CE1-NE2	-6.04	104.20	111.75
4	d	336[B]	HSK	CE1-ND1-CG	5.87	114.88	107.37
4	D	336[B]	HSK	CE1-ND1-CG	5.66	114.61	107.37
4	d	336[B]	HSK	CD2-NE2-CE1	3.62	109.63	105.22

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Z	1	FME	CA-CB-CG-SD
12	m	1	FME	O1-CN-N-CA
14	t	1	FME	N-CA-CB-CG
19	z	1	FME	N-CA-CB-CG
19	z	1	FME	C-CA-CB-CG

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 399 ligands modelled in this entry, 13 are monoatomic and 44 are unknown - leaving 342 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	$\#\|Z\| > 2$
34	DMS	a	2123	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
36	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.07	2 (8%)
24	CLA	B	604	2	69,73,73	2.48	24 (34%)	83,113,113	2.49	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	OEX	A	401	1,44,3	0,14,14	-	-	-		
33	BCT	a	2108	22	2,3,3	0.57	0	2,3,3	1.08	0
34	DMS	B	648	-	3,3,3	2.66	1 (33%)	3,3,3	0.36	0
27	SQD	F	101	-	44,45,54	1.10	3 (6%)	53,56,65	1.57	10 (18%)
34	DMS	T	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
39	LHG	D	410	-	48,48,48	0.89	2 (4%)	51,54,54	0.92	3 (5%)
25	PHO	A	407	-	58,69,69	2.67	13 (22%)	56,99,99	2.91	16 (28%)
34	DMS	b	642	-	3,3,3	2.71	1 (33%)	3,3,3	0.59	0
29	LMT	Z	101	-	36,36,36	0.40	0	47,47,47	0.83	0
26	BCR	d	406	-	41,41,41	0.86	1 (2%)	56,56,56	1.70	8 (14%)
24	CLA	B	606	2	69,73,73	2.35	22 (31%)	83,113,113	2.51	24 (28%)
34	DMS	V	207	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
34	DMS	B	639	-	3,3,3	2.60	1 (33%)	3,3,3	0.60	0
34	DMS	D	420	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	CLA	B	608	44	69,73,73	2.50	22 (31%)	83,113,113	2.40	30 (36%)
34	DMS	b	632	-	3,3,3	2.45	1 (33%)	3,3,3	0.57	0
29	LMT	A	414	-	35,35,36	0.44	0	46,46,47	1.13	4 (8%)
28	LMG	b	623	-	51,51,55	0.93	2 (3%)	59,59,63	1.01	2 (3%)
36	HTG	B	625[A]	-	19,19,19	1.01	1 (5%)	23,24,24	1.23	1 (4%)
34	DMS	B	643	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
34	DMS	c	538	-	3,3,3	2.71	1 (33%)	3,3,3	0.62	0
29	LMT	E	105	-	24,24,36	0.51	1 (4%)	29,29,47	0.88	1 (3%)
34	DMS	T	106	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
34	DMS	C	539	-	3,3,3	2.76	1 (33%)	3,3,3	0.70	0
24	CLA	C	511	3	69,73,73	2.58	25 (36%)	83,113,113	2.42	29 (34%)
34	DMS	O	311	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
34	DMS	v	208	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
37	GOL	a	2101	-	5,5,5	1.02	0	5,5,5	1.12	0
34	DMS	d	419	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
24	CLA	a	2110	44	69,73,73	2.34	22 (31%)	83,113,113	2.73	30 (36%)
34	DMS	c	529	-	3,3,3	2.61	1 (33%)	3,3,3	0.34	0
34	DMS	V	210	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
38	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.18	8 (10%)
24	CLA	c	510	3	69,73,73	2.52	23 (33%)	83,113,113	2.51	24 (28%)
24	CLA	C	504	3	69,73,73	2.56	22 (31%)	83,113,113	2.38	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	607	2	69,73,73	2.87	24 (34%)	83,113,113	2.50	30 (36%)
24	CLA	B	613	2	69,73,73	2.31	25 (36%)	83,113,113	2.56	24 (28%)
24	CLA	B	605	2	69,73,73	2.54	23 (33%)	83,113,113	2.36	25 (30%)
24	CLA	b	604	44	69,73,73	2.49	25 (36%)	83,113,113	2.42	24 (28%)
34	DMS	E	107	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
24	CLA	D	401	44	69,73,73	2.27	23 (33%)	83,113,113	2.75	29 (34%)
26	BCR	T	101	-	41,41,41	0.72	0	56,56,56	1.67	14 (25%)
24	CLA	b	610	44	69,73,73	2.69	24 (34%)	83,113,113	2.44	30 (36%)
36	HTG	b	625	-	19,19,19	0.91	1 (5%)	23,24,24	1.80	6 (26%)
37	GOL	v	204	-	5,5,5	0.80	0	5,5,5	0.94	0
34	DMS	U	503	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
29	LMT	i	104	-	24,24,36	0.54	1 (4%)	29,29,47	1.38	3 (10%)
34	DMS	O	308	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	T	105	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	B	642	-	3,3,3	2.66	1 (33%)	3,3,3	0.40	0
24	CLA	c	507	3	69,73,73	2.58	24 (34%)	83,113,113	2.42	25 (30%)
29	LMT	B	636	-	36,36,36	0.49	0	47,47,47	1.06	4 (8%)
36	HTG	b	601	-	19,19,19	1.04	2 (10%)	23,24,24	1.57	4 (17%)
34	DMS	O	312	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	C	533	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
24	CLA	D	404	4	69,73,73	2.23	22 (31%)	83,113,113	2.74	30 (36%)
43	HEC	V	201	16	50,50,50	1.95	7 (14%)	68,82,82	1.56	9 (13%)
43	HEC	v	201	16	50,50,50	1.95	10 (20%)	68,82,82	1.58	12 (17%)
34	DMS	d	420	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
36	HTG	D	413	-	19,19,19	1.06	2 (10%)	23,24,24	1.24	3 (13%)
34	DMS	b	633	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
34	DMS	a	2124	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	v	207	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
24	CLA	C	506	3	69,73,73	2.68	24 (34%)	83,113,113	2.27	26 (31%)
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	1.09	4 (8%)
34	DMS	B	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
24	CLA	C	510	3	69,73,73	2.61	25 (36%)	83,113,113	2.51	27 (32%)
36	HTG	d	414	-	19,19,19	1.01	2 (10%)	23,24,24	1.26	1 (4%)
38	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	5 (6%)
32	K2I	A	418[A]	-	8,10,10	1.34	0	10,14,14	2.63	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	c	532	-	3,3,3	2.58	1 (33%)	3,3,3	0.34	0
27	SQD	A	411	-	48,49,54	1.03	3 (6%)	57,60,65	1.71	10 (17%)
27	SQD	a	2115	-	46,47,54	1.03	3 (6%)	55,58,65	1.78	11 (20%)
37	GOL	o	2603	-	5,5,5	0.83	0	5,5,5	1.08	0
34	DMS	B	641	-	3,3,3	2.55	1 (33%)	3,3,3	0.43	0
24	CLA	B	615	2	69,73,73	2.32	22 (31%)	83,113,113	2.68	27 (32%)
24	CLA	b	608	2	69,73,73	2.24	24 (34%)	83,113,113	2.66	25 (30%)
26	BCR	c	517	-	41,41,41	0.77	0	56,56,56	1.53	10 (17%)
34	DMS	a	2122	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
34	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
34	DMS	A	422	-	3,3,3	2.53	1 (33%)	3,3,3	0.65	0
34	DMS	u	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.59	0
32	K2I	a	2118[B]	-	8,10,10	1.37	1 (12%)	10,14,14	2.26	3 (30%)
37	GOL	U	502	-	5,5,5	0.85	0	5,5,5	0.97	0
26	BCR	c	528	-	41,41,41	0.72	0	56,56,56	1.45	9 (16%)
28	LMG	D	412	42	44,44,55	0.93	2 (4%)	52,52,63	0.90	4 (7%)
34	DMS	C	531	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
34	DMS	O	314	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
28	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.16	5 (8%)
29	LMT	a	2120	-	36,36,36	0.48	0	47,47,47	1.20	6 (12%)
25	PHO	A	408	-	58,69,69	2.80	14 (24%)	56,99,99	2.89	14 (25%)
24	CLA	d	404	4	69,73,73	2.41	24 (34%)	83,113,113	2.42	28 (33%)
34	DMS	B	638	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
34	DMS	i	106	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
34	DMS	c	536	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
24	CLA	c	511	3	69,73,73	2.75	24 (34%)	83,113,113	2.37	26 (31%)
34	DMS	v	214	-	3,3,3	2.76	1 (33%)	3,3,3	0.77	0
24	CLA	d	401	44	69,73,73	2.42	21 (30%)	83,113,113	2.69	32 (38%)
37	GOL	C	525	-	5,5,5	0.93	0	5,5,5	0.95	0
24	CLA	c	509	44	69,73,73	2.52	24 (34%)	83,113,113	2.59	30 (36%)
32	K2I	A	418[B]	-	8,10,10	1.35	1 (12%)	10,14,14	2.12	4 (40%)
34	DMS	B	649	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
34	DMS	F	103	-	3,3,3	2.67	1 (33%)	3,3,3	0.71	0
34	DMS	e	104	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
24	CLA	C	509	3	69,73,73	2.62	24 (34%)	83,113,113	2.41	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	GOL	U	501	-	5,5,5	1.12	0	5,5,5	0.89	0
24	CLA	B	609	2	69,73,73	2.50	25 (36%)	83,113,113	2.42	27 (32%)
24	CLA	C	512	3	69,73,73	2.78	25 (36%)	83,113,113	2.43	29 (34%)
29	LMT	b	624	-	25,25,36	0.44	0	30,30,47	1.15	3 (10%)
34	DMS	u	202	-	3,3,3	2.68	1 (33%)	3,3,3	0.71	0
24	CLA	C	514	3	69,73,73	2.58	24 (34%)	83,113,113	2.45	27 (32%)
37	GOL	v	202	-	5,5,5	0.97	0	5,5,5	0.93	0
34	DMS	o	2612	-	3,3,3	2.72	1 (33%)	3,3,3	0.65	0
34	DMS	C	535	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
34	DMS	o	2611	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
34	DMS	B	647	-	3,3,3	2.69	1 (33%)	3,3,3	0.46	0
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
34	DMS	o	2606	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
37	GOL	H	103	-	5,5,5	0.95	0	5,5,5	0.86	0
40	HEM	e	103	6,5	50,50,50	1.94	10 (20%)	66,82,82	1.41	8 (12%)
26	BCR	C	516	-	41,41,41	0.73	0	56,56,56	1.54	10 (17%)
31	PL9	D	407	-	55,55,55	0.72	2 (3%)	68,69,69	1.58	15 (22%)
32	K2I	a	2119	-	8,10,10	1.37	2 (25%)	10,14,14	1.56	3 (30%)
34	DMS	o	2608	-	3,3,3	2.65	1 (33%)	3,3,3	0.42	0
26	BCR	K	101	-	41,41,41	0.73	0	56,56,56	1.35	8 (14%)
36	HTG	c	526	-	19,19,19	1.08	2 (10%)	23,24,24	1.17	1 (4%)
38	DGD	h	703	-	63,63,67	0.92	3 (4%)	77,77,81	1.06	6 (7%)
34	DMS	c	535	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
37	GOL	D	403	-	5,5,5	1.15	0	5,5,5	0.87	0
34	DMS	B	650	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	O	305	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
34	DMS	o	2604	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
37	GOL	Z	102	-	5,5,5	0.97	0	5,5,5	0.83	0
24	CLA	b	614	2	69,73,73	2.62	25 (36%)	83,113,113	2.49	30 (36%)
36	HTG	c	524	-	19,19,19	1.08	2 (10%)	23,24,24	1.58	2 (8%)
24	CLA	C	505	44	69,73,73	2.54	24 (34%)	83,113,113	2.41	25 (30%)
34	DMS	u	201	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
37	GOL	d	415	-	5,5,5	0.90	0	5,5,5	0.99	0
34	DMS	V	208	-	3,3,3	2.67	1 (33%)	3,3,3	0.60	0
26	BCR	A	410	-	41,41,41	0.82	0	56,56,56	1.43	8 (14%)
34	DMS	E	108	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	PL9	d	407	-	55,55,55	0.74	1 (1%)	68,69,69	1.58	15 (22%)
34	DMS	d	422	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
29	LMT	j	1601	-	22,22,36	0.64	1 (4%)	26,26,47	1.18	2 (7%)
26	BCR	t	102	-	41,41,41	0.72	0	56,56,56	1.55	17 (30%)
34	DMS	d	418	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
38	DGD	C	517	-	63,63,67	0.84	3 (4%)	77,77,81	1.07	6 (7%)
34	DMS	C	534	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0
24	CLA	B	617	2	69,73,73	2.35	23 (33%)	83,113,113	2.61	26 (31%)
34	DMS	o	2607	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
34	DMS	C	537	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
32	K2I	a	2118[A]	-	8,10,10	1.38	1 (12%)	10,14,14	2.37	4 (40%)
34	DMS	V	202	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	0
36	HTG	O	302	-	19,19,19	0.99	1 (5%)	23,24,24	0.96	2 (8%)
41	RRX	H	101	-	42,42,42	0.74	0	57,58,58	1.33	8 (14%)
39	LHG	D	411	-	43,43,48	0.93	2 (4%)	46,49,54	1.00	3 (6%)
26	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.39	6 (10%)
36	HTG	b	602	-	19,19,19	1.13	2 (10%)	23,24,24	1.81	4 (17%)
34	DMS	v	211	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
39	LHG	D	409	-	48,48,48	0.88	2 (4%)	51,54,54	1.16	6 (11%)
24	CLA	b	605	2	69,73,73	2.51	24 (34%)	83,113,113	2.44	29 (34%)
37	GOL	B	635	-	5,5,5	1.08	0	5,5,5	0.90	0
24	CLA	B	612	2	69,73,73	2.66	24 (34%)	83,113,113	2.55	28 (33%)
38	DGD	D	408	-	46,46,67	1.03	2 (4%)	53,54,81	1.16	4 (7%)
29	LMT	a	2103	-	36,36,36	0.39	0	47,47,47	1.22	5 (10%)
24	CLA	b	612	2	69,73,73	2.56	24 (34%)	83,113,113	2.47	30 (36%)
36	HTG	C	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.77	4 (17%)
24	CLA	b	618	2	69,73,73	2.38	21 (30%)	83,113,113	2.37	28 (33%)
28	LMG	B	622	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	4 (6%)
26	BCR	k	2003	-	41,41,41	0.66	0	56,56,56	1.48	11 (19%)
24	CLA	B	614	2	69,73,73	2.30	23 (33%)	83,113,113	2.48	28 (33%)
37	GOL	k	2001	-	5,5,5	0.93	0	5,5,5	0.92	0
24	CLA	B	607	2	69,73,73	2.49	24 (34%)	83,113,113	2.52	27 (32%)
27	SQD	B	621	-	53,54,54	1.07	4 (7%)	62,65,65	1.52	8 (12%)
24	CLA	b	619	2	69,73,73	2.47	23 (33%)	83,113,113	2.51	26 (31%)
34	DMS	k	2004	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	513	3	69,73,73	2.53	22 (31%)	83,113,113	2.56	30 (36%)
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	1.03	4 (8%)
34	DMS	c	531	-	3,3,3	2.65	1 (33%)	3,3,3	0.41	0
24	CLA	B	611	44	69,73,73	2.39	24 (34%)	83,113,113	2.52	29 (34%)
24	CLA	b	616	2	69,73,73	2.57	24 (34%)	83,113,113	2.48	29 (34%)
34	DMS	B	644	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
34	DMS	O	306	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
37	GOL	O	303	-	5,5,5	0.94	0	5,5,5	0.92	0
29	LMT	B	623	-	36,36,36	0.39	0	47,47,47	1.33	7 (14%)
24	CLA	C	508	44	69,73,73	2.62	24 (34%)	83,113,113	2.48	29 (34%)
28	LMG	d	411	42	48,48,55	0.95	2 (4%)	56,56,63	1.04	2 (3%)
26	BCR	D	406	-	41,41,41	0.82	1 (2%)	56,56,56	1.60	8 (14%)
34	DMS	u	204	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
37	GOL	o	2601	-	5,5,5	1.01	0	5,5,5	0.85	0
33	BCT	A	421	22	2,3,3	0.60	0	2,3,3	0.98	0
34	DMS	x	802	-	3,3,3	2.71	1 (33%)	3,3,3	0.65	0
37	GOL	C	524	-	5,5,5	0.90	0	5,5,5	0.97	0
39	LHG	e	101	-	31,31,48	0.89	1 (3%)	33,36,54	1.07	1 (3%)
29	LMT	A	420	-	36,36,36	0.56	1 (2%)	47,47,47	1.35	5 (10%)
37	GOL	v	203	-	5,5,5	1.05	0	5,5,5	1.19	1 (20%)
34	DMS	C	536	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
34	DMS	o	2605	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
36	HTG	V	204	-	19,19,19	0.97	2 (10%)	23,24,24	1.88	5 (21%)
34	DMS	O	304	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	A	425	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
34	DMS	v	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.62	0
34	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
24	CLA	C	502	3	69,73,73	2.48	24 (34%)	83,113,113	2.32	22 (26%)
37	GOL	V	203	-	5,5,5	0.96	0	5,5,5	0.89	0
37	GOL	b	631	-	5,5,5	0.87	0	5,5,5	0.99	0
34	DMS	V	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.57	0
39	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
21	OEX	a	2104	1,44,3	0,14,14	-	-	-		
27	SQD	a	2102	-	52,53,54	1.02	3 (5%)	61,64,65	1.22	5 (8%)
36	HTG	B	627	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
28	LMG	C	526	-	48,48,55	0.98	2 (4%)	56,56,63	1.26	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
37	GOL	B	632	-	5,5,5	0.98	0	5,5,5	0.81	0
24	CLA	c	505	3	69,73,73	2.83	23 (33%)	83,113,113	2.33	29 (34%)
24	CLA	D	405	4	69,73,73	2.47	25 (36%)	83,113,113	2.47	28 (33%)
36	HTG	d	403	-	19,19,19	1.10	2 (10%)	23,24,24	1.06	2 (8%)
24	CLA	C	503	3	69,73,73	2.66	24 (34%)	83,113,113	2.51	27 (32%)
31	PL9	x	801	-	38,38,55	0.40	0	45,45,69	1.77	15 (33%)
34	DMS	D	418	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
34	DMS	C	527	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
24	CLA	b	613	44	69,73,73	2.43	24 (34%)	83,113,113	2.49	28 (33%)
34	DMS	C	532	-	3,3,3	2.64	1 (33%)	3,3,3	0.38	0
34	DMS	b	639	-	3,3,3	2.63	1 (33%)	3,3,3	0.42	0
29	LMT	I	1201	-	24,24,36	0.44	0	29,29,47	1.14	3 (10%)
34	DMS	v	213	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
37	GOL	c	527	-	5,5,5	0.76	0	5,5,5	1.03	0
24	CLA	c	515	3	69,73,73	2.58	25 (36%)	83,113,113	2.37	25 (30%)
29	LMT	T	102	-	24,24,36	0.40	0	29,29,47	0.97	1 (3%)
36	HTG	I	1202	-	19,19,19	1.15	2 (10%)	23,24,24	1.95	4 (17%)
34	DMS	C	530	-	3,3,3	2.69	1 (33%)	3,3,3	0.63	0
41	RRX	h	702	-	42,42,42	0.71	0	57,58,58	1.37	9 (15%)
34	DMS	A	424	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
34	DMS	t	103	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
26	BCR	b	622	-	41,41,41	0.79	1 (2%)	56,56,56	1.40	6 (10%)
26	BCR	a	2114	-	41,41,41	0.75	0	56,56,56	1.32	6 (10%)
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	c	542	-	3,3,3	2.64	1 (33%)	3,3,3	0.56	0
36	HTG	B	624	-	19,19,19	1.10	1 (5%)	23,24,24	1.27	2 (8%)
29	LMT	z	1801	-	33,33,36	0.43	0	43,43,47	0.97	2 (4%)
34	DMS	b	636	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
24	CLA	b	615	2	69,73,73	2.32	22 (31%)	83,113,113	2.62	25 (30%)
34	DMS	o	2609	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
38	DGD	c	518	-	63,63,67	0.81	2 (3%)	77,77,81	1.20	6 (7%)
39	LHG	d	410	-	35,35,48	1.10	2 (5%)	38,41,54	1.01	3 (7%)
29	LMT	m	102	-	36,36,36	0.50	0	47,47,47	1.16	5 (10%)
34	DMS	v	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.54	0
36	HTG	B	628	-	19,19,19	1.02	2 (10%)	23,24,24	1.58	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	K2I	A	419	-	8,10,10	1.30	1 (12%)	10,14,14	1.44	3 (30%)
34	DMS	b	635	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
24	CLA	B	616	2	69,73,73	2.47	22 (31%)	83,113,113	2.57	30 (36%)
26	BCR	b	621	-	41,41,41	0.84	0	56,56,56	1.20	6 (10%)
28	LMG	i	101	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	4 (6%)
34	DMS	V	205	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
34	DMS	C	538	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
24	CLA	c	513	3	69,73,73	2.48	22 (31%)	83,113,113	2.42	31 (37%)
24	CLA	C	507	3	69,73,73	2.73	22 (31%)	83,113,113	2.57	28 (33%)
25	PHO	a	2112	-	58,69,69	2.74	13 (22%)	56,99,99	2.86	14 (25%)
38	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	4 (5%)
40	HEM	F	102	6,5	50,50,50	1.87	8 (16%)	66,82,82	1.47	9 (13%)
28	LMG	c	522	-	48,48,55	1.00	2 (4%)	56,56,63	1.25	6 (10%)
34	DMS	O	310	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
34	DMS	c	541	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
24	CLA	d	405	4	69,73,73	2.52	24 (34%)	83,113,113	2.47	29 (34%)
34	DMS	o	2610	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
29	LMT	J	102	-	24,24,36	0.51	0	29,29,47	1.05	2 (6%)
36	HTG	B	626	-	19,19,19	1.08	2 (10%)	23,24,24	1.57	3 (13%)
34	DMS	c	537	-	3,3,3	2.69	1 (33%)	3,3,3	0.63	0
24	CLA	B	602	44	69,73,73	2.48	25 (36%)	83,113,113	2.46	24 (28%)
28	LMG	c	521	-	49,49,55	0.93	2 (4%)	57,57,63	1.12	5 (8%)
34	DMS	C	528	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
24	CLA	b	606	2	69,73,73	2.51	23 (33%)	83,113,113	2.51	33 (39%)
28	LMG	A	412	-	51,51,55	0.97	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	c	503	3	69,73,73	2.43	23 (33%)	83,113,113	2.62	25 (30%)
34	DMS	A	423	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
36	HTG	B	625[B]	-	19,19,19	1.00	1 (5%)	23,24,24	1.47	4 (17%)
24	CLA	a	2113	1	69,73,73	2.26	22 (31%)	83,113,113	2.59	28 (33%)
26	BCR	B	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.13	4 (7%)
34	DMS	v	206	-	3,3,3	2.70	1 (33%)	3,3,3	0.63	0
24	CLA	b	609	2	69,73,73	2.45	25 (36%)	83,113,113	2.39	25 (30%)
34	DMS	b	634	-	3,3,3	2.72	1 (33%)	3,3,3	0.63	0
34	DMS	c	533	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
24	CLA	A	405	1	69,73,73	2.40	23 (33%)	83,113,113	2.43	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	504	3	69,73,73	2.38	23 (33%)	83,113,113	2.42	25 (30%)
34	DMS	C	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	c	530	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
34	DMS	B	646	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
24	CLA	A	409	1	69,73,73	2.35	23 (33%)	83,113,113	2.56	31 (37%)
34	DMS	b	641	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
34	DMS	A	426	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
34	DMS	O	313	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	v	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
31	PL9	A	417	-	38,38,55	0.52	0	45,45,69	1.67	9 (20%)
26	BCR	B	620	-	41,41,41	0.75	0	56,56,56	1.24	7 (12%)
34	DMS	O	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
24	CLA	B	603	2	69,73,73	2.46	23 (33%)	83,113,113	2.47	28 (33%)
39	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
25	PHO	a	2111	-	58,69,69	2.56	11 (18%)	56,99,99	2.79	12 (21%)
34	DMS	V	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	z	1802	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
26	BCR	c	516	-	41,41,41	0.75	0	56,56,56	1.56	9 (16%)
24	CLA	b	617	2	69,73,73	2.46	24 (34%)	83,113,113	2.53	29 (34%)
34	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.65	0
27	SQD	A	413	-	53,54,54	1.04	3 (5%)	62,65,65	1.29	6 (9%)
34	DMS	c	540	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
34	DMS	D	419	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	9 (14%)
29	LMT	f	101	-	24,24,36	0.55	1 (4%)	29,29,47	0.89	1 (3%)
24	CLA	a	2109	1	69,73,73	2.62	24 (34%)	83,113,113	2.50	27 (32%)
39	LHG	E	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.06	3 (5%)
26	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.45	7 (12%)
34	DMS	d	421	-	3,3,3	2.69	1 (33%)	3,3,3	0.66	0
34	DMS	c	539	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
34	DMS	b	638	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
36	HTG	b	626	-	19,19,19	1.09	2 (10%)	23,24,24	1.33	2 (8%)
34	DMS	d	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
38	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.02	5 (6%)
24	CLA	c	506	44	69,73,73	2.35	22 (31%)	83,113,113	2.60	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	512	3	69,73,73	2.43	23 (33%)	83,113,113	2.37	26 (31%)
24	CLA	B	610	2	69,73,73	2.59	23 (33%)	83,113,113	2.44	28 (33%)
24	CLA	c	514	3	69,73,73	2.63	24 (34%)	83,113,113	2.55	29 (34%)
34	DMS	v	212	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
27	SQD	f	102	-	35,36,54	1.65	3 (8%)	40,41,65	1.40	5 (12%)
39	LHG	d	409	-	48,48,48	0.80	2 (4%)	51,54,54	0.97	3 (5%)
29	LMT	B	637	-	24,24,36	0.51	0	29,29,47	0.71	0
24	CLA	c	508	3	69,73,73	2.49	24 (34%)	83,113,113	2.51	29 (34%)
34	DMS	D	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
36	HTG	i	103	-	19,19,19	0.97	2 (10%)	23,24,24	1.25	1 (4%)
34	DMS	j	1604	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
39	LHG	l	101	-	48,48,48	0.87	2 (4%)	51,54,54	1.13	3 (5%)
34	DMS	c	534	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
26	BCR	Y	302	-	41,41,41	0.77	0	56,56,56	1.62	10 (17%)
34	DMS	a	2121	-	3,3,3	2.51	1 (33%)	3,3,3	0.17	0
34	DMS	D	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.48	0
38	DGD	c	520	-	63,63,67	0.84	3 (4%)	77,77,81	0.97	5 (6%)
26	BCR	b	620	-	41,41,41	0.78	0	56,56,56	1.38	4 (7%)
24	CLA	A	406	44	69,73,73	2.25	23 (33%)	83,113,113	2.50	31 (37%)
36	HTG	c	523	-	19,19,19	1.00	2 (10%)	23,24,24	1.68	4 (17%)
24	CLA	b	611	2	69,73,73	2.52	24 (34%)	83,113,113	2.49	29 (34%)
34	DMS	d	423	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	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
32	K2I	A	419	-	-	-	0/1/1/1
24	CLA	b	612	2	-	3/39/115/115	-
36	HTG	C	521	-	-	3/10/30/30	0/1/1/1
24	CLA	B	604	2	-	3/39/115/115	-
24	CLA	b	618	2	-	6/39/115/115	-
36	HTG	C	522	-	-	3/10/30/30	0/1/1/1
28	LMG	B	622	-	-	12/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	616	2	-	11/39/115/115	-
26	BCR	b	621	-	-	1/29/63/63	0/2/2/2
28	LMG	i	101	-	-	12/46/66/70	0/1/1/1
26	BCR	k	2003	-	-	0/29/63/63	0/2/2/2
28	LMG	C	520	-	-	14/46/66/70	0/1/1/1
27	SQD	F	101	-	-	15/40/60/69	0/1/1/1
39	LHG	D	410	-	-	9/53/53/53	-
29	LMT	a	2120	-	-	12/21/61/61	0/2/2/2
25	PHO	A	407	-	-	5/37/103/103	0/5/6/6
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	d	404	4	-	4/39/115/115	-
24	CLA	c	513	3	-	3/39/115/115	-
29	LMT	Z	101	-	-	10/21/61/61	0/2/2/2
26	BCR	d	406	-	-	6/29/63/63	0/2/2/2
24	CLA	B	614	2	-	3/39/115/115	-
37	GOL	k	2001	-	-	2/4/4/4	-
24	CLA	B	607	2	-	10/39/115/115	-
24	CLA	C	507	3	-	14/39/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	B	606	2	-	5/39/115/115	-
24	CLA	b	619	2	-	8/39/115/115	-
25	PHO	a	2112	-	-	2/37/103/103	0/5/6/6
38	DGD	c	519	-	-	19/51/91/95	0/2/2/2
28	LMG	c	522	-	-	9/43/63/70	0/1/1/1
40	HEM	F	102	6,5	-	3/14/54/54	-
24	CLA	c	511	3	-	8/39/115/115	-
24	CLA	d	405	4	-	4/39/115/115	-
24	CLA	C	513	3	-	7/39/115/115	-
24	CLA	d	401	44	-	4/39/115/115	-
24	CLA	B	608	44	-	3/39/115/115	-
29	LMT	m	103	-	-	1/21/61/61	0/2/2/2
24	CLA	B	611	44	-	9/39/115/115	-
24	CLA	b	616	2	-	4/39/115/115	-
28	LMG	b	623	-	-	12/46/66/70	0/1/1/1
29	LMT	A	414	-	-	6/20/60/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	B	625[A]	-	-	4/10/30/30	0/1/1/1
37	GOL	C	525	-	-	2/4/4/4	-
24	CLA	c	509	44	-	8/39/115/115	-
29	LMT	J	102	-	-	6/15/35/61	0/1/1/2
32	K2I	A	418[B]	-	-	-	0/1/1/1
29	LMT	E	105	-	-	7/15/35/61	0/1/1/2
36	HTG	B	626	-	-	4/10/30/30	0/1/1/1
24	CLA	B	602	44	-	12/39/115/115	-
37	GOL	O	303	-	-	4/4/4/4	-
29	LMT	B	623	-	-	10/21/61/61	0/2/2/2
28	LMG	c	521	-	-	13/44/64/70	0/1/1/1
24	CLA	C	508	44	-	7/39/115/115	-
28	LMG	d	411	42	-	7/43/63/70	0/1/1/1
24	CLA	C	511	3	-	6/39/115/115	-
37	GOL	a	2101	-	-	2/4/4/4	-
24	CLA	b	606	2	-	2/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
37	GOL	o	2601	-	-	3/4/4/4	-
24	CLA	a	2110	44	-	7/39/115/115	-
28	LMG	A	412	-	-	16/46/66/70	0/1/1/1
24	CLA	c	503	3	-	1/39/115/115	-
38	DGD	C	519	-	-	6/51/91/95	0/2/2/2
24	CLA	C	509	3	-	7/39/115/115	-
36	HTG	B	625[B]	-	-	3/10/30/30	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
37	GOL	C	524	-	-	0/4/4/4	-
37	GOL	U	501	-	-	2/4/4/4	-
24	CLA	a	2113	1	-	7/39/115/115	-
24	CLA	c	510	3	-	5/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
39	LHG	e	101	-	-	16/35/35/53	-
24	CLA	C	504	3	-	5/39/115/115	-
24	CLA	C	512	3	-	5/39/115/115	-
24	CLA	b	607	2	-	6/39/115/115	-
24	CLA	B	613	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	A	420	-	-	6/21/61/61	0/2/2/2
24	CLA	b	609	2	-	5/39/115/115	-
29	LMT	b	624	-	-	4/17/37/61	0/1/1/2
37	GOL	v	203	-	-	1/4/4/4	-
24	CLA	C	514	3	-	2/39/115/115	-
24	CLA	A	405	1	-	6/39/115/115	-
24	CLA	c	504	3	-	6/39/115/115	-
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
37	GOL	v	202	-	-	2/4/4/4	-
24	CLA	B	605	2	-	7/39/115/115	-
24	CLA	b	604	44	-	12/39/115/115	-
24	CLA	A	409	1	-	9/39/115/115	-
24	CLA	D	401	44	-	5/39/115/115	-
26	BCR	T	101	-	-	3/29/63/63	0/2/2/2
24	CLA	b	610	44	-	1/39/115/115	-
36	HTG	b	625	-	-	0/10/30/30	0/1/1/1
31	PL9	A	417	-	-	11/42/42/73	-
37	GOL	v	204	-	-	4/4/4/4	-
24	CLA	C	502	3	-	6/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
37	GOL	H	103	-	-	2/4/4/4	-
24	CLA	B	603	2	-	5/39/115/115	-
37	GOL	V	203	-	-	4/4/4/4	-
39	LHG	d	408	-	-	11/53/53/53	-
40	HEM	e	103	6,5	-	4/14/54/54	-
25	PHO	a	2111	-	-	4/37/103/103	0/5/6/6
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
29	LMT	i	104	-	-	11/15/35/61	0/1/1/2
31	PL9	D	407	-	-	3/53/73/73	0/1/1/1
37	GOL	b	631	-	-	2/4/4/4	-
26	BCR	c	516	-	-	2/29/63/63	0/2/2/2
32	K2I	a	2119	-	-	-	0/1/1/1
39	LHG	L	101	-	-	14/53/53/53	-
24	CLA	c	507	3	-	5/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	617	2	-	12/39/115/115	-
29	LMT	B	636	-	-	8/21/61/61	0/2/2/2
27	SQD	A	413	-	-	12/49/69/69	0/1/1/1
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
36	HTG	b	601	-	-	2/10/30/30	0/1/1/1
27	SQD	a	2102	-	-	12/48/68/69	0/1/1/1
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
29	LMT	f	101	-	-	6/15/35/61	0/1/1/2
38	DGD	h	703	-	-	8/51/91/95	0/2/2/2
24	CLA	D	404	4	-	3/39/115/115	-
24	CLA	a	2109	1	-	3/39/115/115	-
37	GOL	D	403	-	-	0/4/4/4	-
28	LMG	C	526	-	-	11/43/63/70	0/1/1/1
39	LHG	E	101	-	-	19/53/53/53	-
37	GOL	B	632	-	-	0/4/4/4	-
43	HEC	V	201	16	1/1/3/7	6/14/54/54	-
26	BCR	C	515	-	-	3/29/63/63	0/2/2/2
43	HEC	v	201	16	1/1/3/7	6/14/54/54	-
24	CLA	c	505	3	-	1/39/115/115	-
37	GOL	Z	102	-	-	2/4/4/4	-
24	CLA	b	614	2	-	3/39/115/115	-
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
24	CLA	D	405	4	-	6/39/115/115	-
36	HTG	D	413	-	-	2/10/30/30	0/1/1/1
24	CLA	C	503	3	-	5/39/115/115	-
31	PL9	x	801	-	-	9/42/42/73	-
36	HTG	d	403	-	-	4/10/30/30	0/1/1/1
24	CLA	C	505	44	-	6/39/115/115	-
24	CLA	C	506	3	-	4/39/115/115	-
24	CLA	b	613	44	-	6/39/115/115	-
36	HTG	b	626	-	-	5/10/30/30	0/1/1/1
37	GOL	d	415	-	-	2/4/4/4	-
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
29	LMT	I	1201	-	-	7/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	DGD	H	102	-	-	9/51/91/95	0/2/2/2
29	LMT	M	101	-	-	5/21/61/61	0/2/2/2
37	GOL	c	527	-	-	1/4/4/4	-
24	CLA	c	506	44	-	8/39/115/115	-
24	CLA	c	515	3	-	6/39/115/115	-
24	CLA	c	512	3	-	9/39/115/115	-
24	CLA	C	510	3	-	6/39/115/115	-
29	LMT	T	102	-	-	7/15/35/61	0/1/1/2
31	PL9	d	407	-	-	4/53/73/73	0/1/1/1
24	CLA	B	610	2	-	5/39/115/115	-
36	HTG	I	1202	-	-	3/10/30/30	0/1/1/1
29	LMT	j	1601	-	-	5/11/31/61	0/1/1/2
24	CLA	c	514	3	-	6/39/115/115	-
26	BCR	t	102	-	-	3/29/63/63	0/2/2/2
38	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	B	617	2	-	11/39/115/115	-
27	SQD	f	102	-	-	13/38/38/69	-
41	RRX	h	702	-	-	1/29/65/65	0/2/2/2
36	HTG	d	414	-	-	1/10/30/30	0/1/1/1
38	DGD	C	518	-	-	19/51/91/95	0/2/2/2
39	LHG	d	409	-	-	12/53/53/53	-
32	K2I	A	418[A]	-	-	-	0/1/1/1
32	K2I	a	2118[A]	-	-	-	0/1/1/1
29	LMT	B	637	-	-	9/15/35/61	0/1/1/2
24	CLA	c	508	3	-	8/39/115/115	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
27	SQD	A	411	-	-	9/44/64/69	0/1/1/1
27	SQD	a	2115	-	-	12/42/62/69	0/1/1/1
36	HTG	i	103	-	-	1/10/30/30	0/1/1/1
36	HTG	O	302	-	-	5/10/30/30	0/1/1/1
41	RRX	H	101	-	-	1/29/65/65	0/2/2/2
26	BCR	a	2114	-	-	2/29/63/63	0/2/2/2
39	LHG	D	411	-	-	11/48/48/53	-
37	GOL	o	2603	-	-	3/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
36	HTG	B	624	-	-	3/10/30/30	0/1/1/1
29	LMT	z	1801	-	-	8/16/56/61	0/2/2/2
39	LHG	l	101	-	-	16/53/53/53	-
24	CLA	B	615	2	-	12/39/115/115	-
24	CLA	b	608	2	-	5/39/115/115	-
39	LHG	D	409	-	-	16/53/53/53	-
24	CLA	b	615	2	-	3/39/115/115	-
26	BCR	Y	302	-	-	4/29/63/63	0/2/2/2
24	CLA	b	605	2	-	1/39/115/115	-
26	BCR	c	517	-	-	2/29/63/63	0/2/2/2
38	DGD	c	520	-	-	10/51/91/95	0/2/2/2
26	BCR	b	620	-	-	2/29/63/63	0/2/2/2
24	CLA	A	406	44	-	7/39/115/115	-
38	DGD	c	518	-	-	17/51/91/95	0/2/2/2
39	LHG	d	410	-	-	6/40/40/53	-
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
37	GOL	B	635	-	-	0/4/4/4	-
32	K2I	a	2118[B]	-	-	-	0/1/1/1
24	CLA	B	612	2	-	5/39/115/115	-
38	DGD	D	408	-	-	17/40/61/95	0/1/1/2
37	GOL	U	502	-	-	2/4/4/4	-
29	LMT	a	2103	-	-	11/21/61/61	0/2/2/2
24	CLA	b	611	2	-	1/39/115/115	-
36	HTG	B	628	-	-	1/10/30/30	0/1/1/1
26	BCR	c	528	-	-	4/29/63/63	0/2/2/2
28	LMG	D	412	42	-	10/39/59/70	0/1/1/1

The worst 5 of 1999 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	MG-NA	11.53	2.33	2.06
24	C	512	CLA	MG-NA	11.41	2.33	2.06
24	C	508	CLA	MG-NA	10.32	2.30	2.06
24	C	506	CLA	MG-NA	9.69	2.29	2.06
24	C	504	CLA	MG-NA	9.53	2.28	2.06

The worst 5 of 2600 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	407	PHO	C2D-C1D-ND	12.52	118.17	109.53
25	A	408	PHO	C2D-C1D-ND	12.48	118.14	109.53
25	a	2111	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	c	503	CLA	C1D-ND-C4D	-10.88	98.61	106.33
24	D	404	CLA	C1D-ND-C4D	-10.56	98.83	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	V	201	HEC	NA
43	v	201	HEC	NA

5 of 1230 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

170 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	604	CLA	1	0
27	F	101	SQD	2	0
26	d	406	BCR	1	0
24	B	606	CLA	4	0
29	A	414	LMT	2	0
28	b	623	LMG	1	0
36	B	625[A]	HTG	3	0
34	B	643	DMS	1	0
24	C	511	CLA	1	0
24	a	2110	CLA	2	0
38	C	519	DGD	1	0
24	c	510	CLA	3	0
24	C	504	CLA	5	0
24	b	607	CLA	3	0
24	B	613	CLA	1	0
24	B	605	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	604	CLA	4	0
24	D	401	CLA	2	0
26	T	101	BCR	5	0
24	b	610	CLA	1	0
36	b	625	HTG	3	0
34	U	503	DMS	2	0
29	i	104	LMT	1	0
24	c	507	CLA	2	0
29	B	636	LMT	1	0
36	b	601	HTG	1	0
24	D	404	CLA	2	0
36	D	413	HTG	3	0
34	b	633	DMS	1	0
24	C	506	CLA	1	0
29	M	101	LMT	2	0
24	C	510	CLA	4	0
38	C	518	DGD	6	0
34	c	532	DMS	1	0
27	A	411	SQD	2	0
27	a	2115	SQD	1	0
37	o	2603	GOL	1	0
24	B	615	CLA	2	0
24	b	608	CLA	6	0
26	c	517	BCR	2	0
32	a	2118[B]	K2I	2	0
26	c	528	BCR	1	0
28	C	520	LMG	1	0
29	a	2120	LMT	2	0
25	A	408	PHO	2	0
24	d	404	CLA	2	0
24	c	511	CLA	2	0
24	d	401	CLA	4	0
24	c	509	CLA	2	0
32	A	418[B]	K2I	2	0
24	C	509	CLA	2	0
24	C	512	CLA	2	0
24	C	514	CLA	6	0
34	B	647	DMS	1	0
34	o	2606	DMS	1	0
40	e	103	HEM	2	0
26	C	516	BCR	3	0
32	a	2119	K2I	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	K	101	BCR	1	0
38	h	703	DGD	1	0
37	D	403	GOL	1	0
24	b	614	CLA	1	0
24	C	505	CLA	1	0
26	A	410	BCR	1	0
31	d	407	PL9	1	0
26	t	102	BCR	6	0
38	C	517	DGD	2	0
34	C	534	DMS	1	0
24	B	617	CLA	3	0
36	O	302	HTG	1	0
41	H	101	RRX	3	0
39	D	411	LHG	2	0
26	B	618	BCR	2	0
36	b	602	HTG	3	0
39	D	409	LHG	3	0
24	b	605	CLA	1	0
37	B	635	GOL	2	0
24	B	612	CLA	1	0
29	a	2103	LMT	2	0
24	b	612	CLA	1	0
24	b	618	CLA	4	0
28	B	622	LMG	2	0
26	k	2003	BCR	1	0
24	B	614	CLA	1	0
24	B	607	CLA	1	0
27	B	621	SQD	3	0
24	b	619	CLA	4	0
24	C	513	CLA	4	0
34	c	531	DMS	1	0
24	B	611	CLA	2	0
24	b	616	CLA	2	0
29	B	623	LMT	1	0
24	C	508	CLA	2	0
37	o	2601	GOL	1	0
39	e	101	LHG	1	0
29	A	420	LMT	1	0
34	b	643	DMS	1	0
24	C	502	CLA	4	0
39	L	101	LHG	2	0
27	a	2102	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	526	LMG	1	0
24	c	505	CLA	4	0
24	D	405	CLA	1	0
36	d	403	HTG	2	0
24	C	503	CLA	2	0
31	x	801	PL9	1	0
24	b	613	CLA	1	0
37	c	527	GOL	2	0
24	c	515	CLA	1	0
36	I	1202	HTG	1	0
41	h	702	RRX	3	0
26	b	622	BCR	2	0
26	a	2114	BCR	1	0
36	B	624	HTG	1	0
29	z	1801	LMT	2	0
38	c	518	DGD	1	0
29	m	102	LMT	2	0
34	v	205	DMS	1	0
36	B	628	HTG	1	0
32	A	419	K2I	1	0
24	B	616	CLA	2	0
26	b	621	BCR	3	0
28	i	101	LMG	2	0
24	c	513	CLA	4	0
24	C	507	CLA	1	0
25	a	2112	PHO	1	0
38	c	519	DGD	3	0
40	F	102	HEM	1	0
34	O	310	DMS	1	0
24	d	405	CLA	1	0
29	J	102	LMT	1	0
24	B	602	CLA	1	0
28	c	521	LMG	1	0
34	C	528	DMS	2	0
28	A	412	LMG	1	0
24	c	503	CLA	3	0
36	B	625[B]	HTG	3	0
24	a	2113	CLA	2	0
26	B	619	BCR	2	0
24	b	609	CLA	2	0
24	A	405	CLA	2	0
24	c	504	CLA	3	0

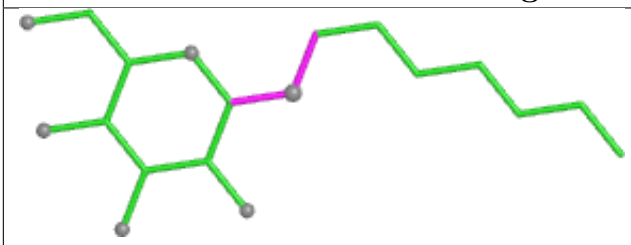
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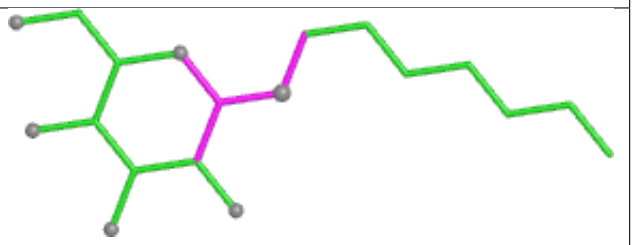
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	529	DMS	1	0
24	A	409	CLA	1	0
31	A	417	PL9	2	0
26	B	620	BCR	2	0
24	B	603	CLA	2	0
39	d	408	LHG	2	0
34	V	206	DMS	1	0
26	c	516	BCR	3	0
34	O	309	DMS	1	0
27	L	102	SQD	1	0
24	a	2109	CLA	2	0
39	E	101	LHG	5	0
26	C	515	BCR	4	0
36	b	626	HTG	1	0
34	d	417	DMS	2	0
24	c	506	CLA	5	0
24	c	512	CLA	1	0
24	B	610	CLA	4	0
24	c	514	CLA	4	0
27	f	102	SQD	1	0
39	d	409	LHG	1	0
24	c	508	CLA	2	0
39	l	101	LHG	1	0
26	Y	302	BCR	3	0
38	c	520	DGD	3	0
26	b	620	BCR	1	0
24	A	406	CLA	1	0
34	d	423	DMS	1	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.

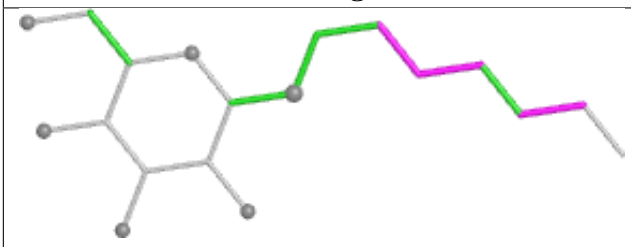
Ligand HTG C 521



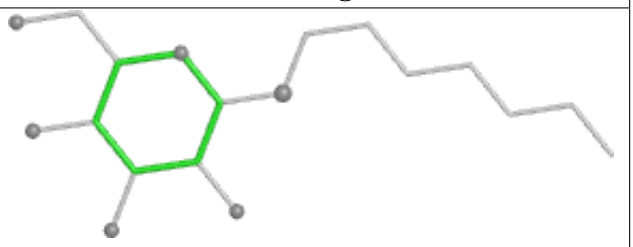
Bond lengths



Bond angles

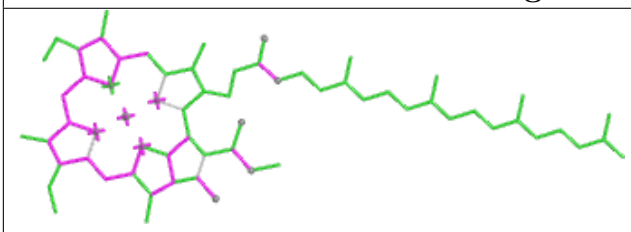


Torsions

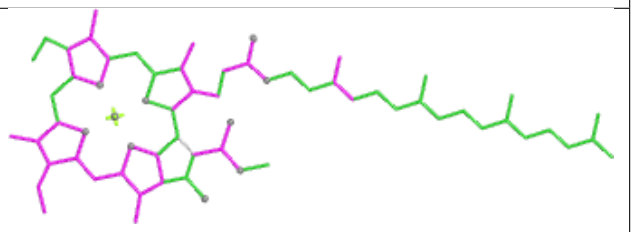


Rings

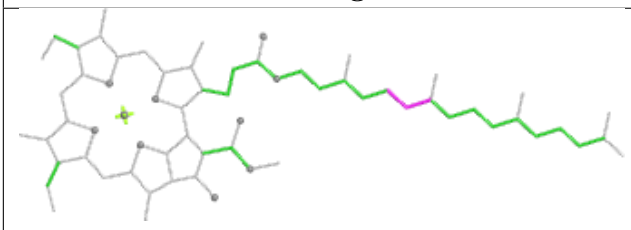
Ligand CLA B 604



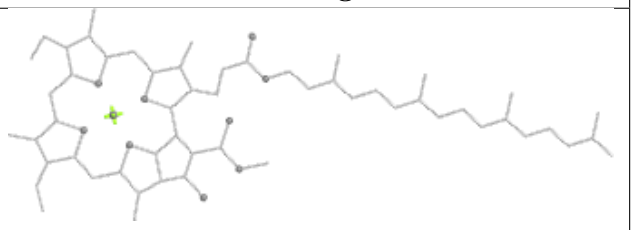
Bond lengths



Bond angles

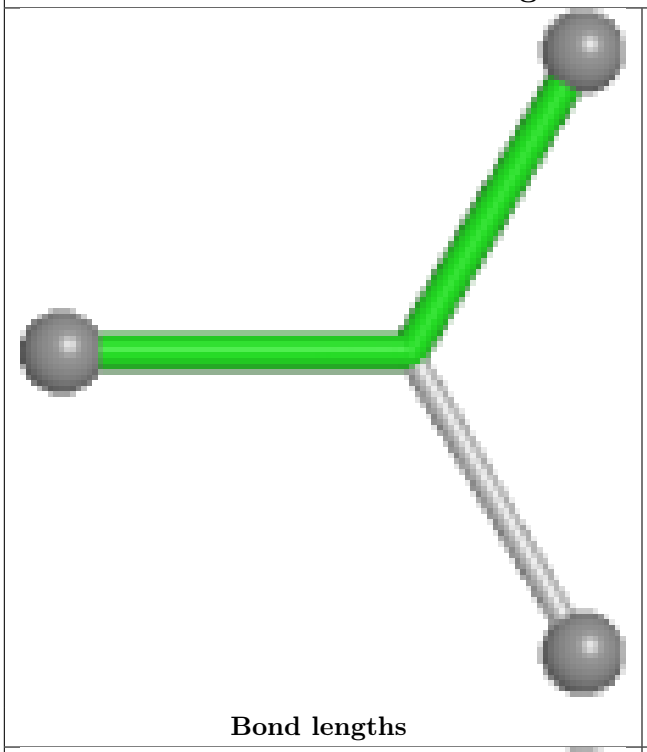


Torsions

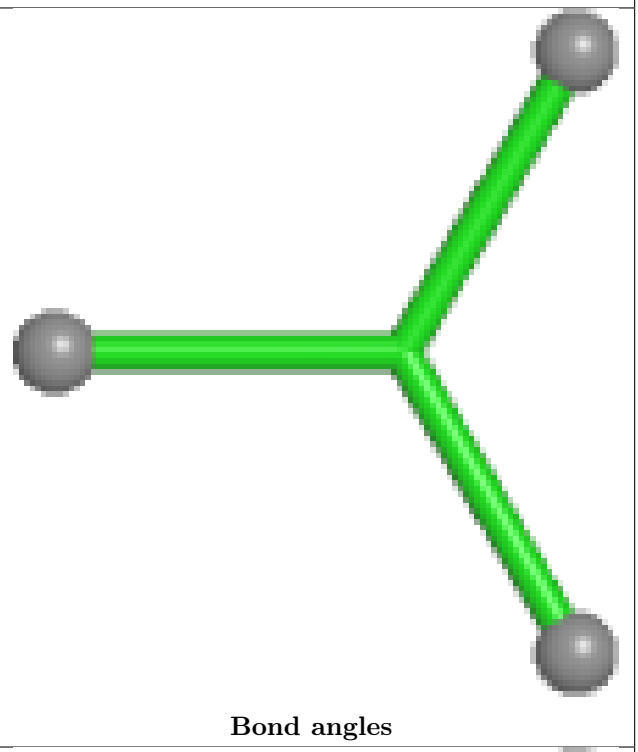


Rings

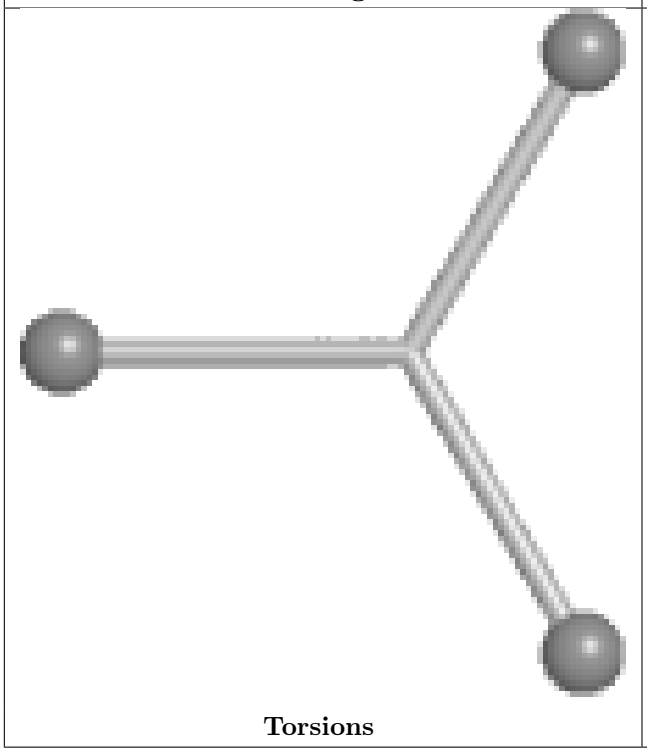
Ligand BCT a 2108



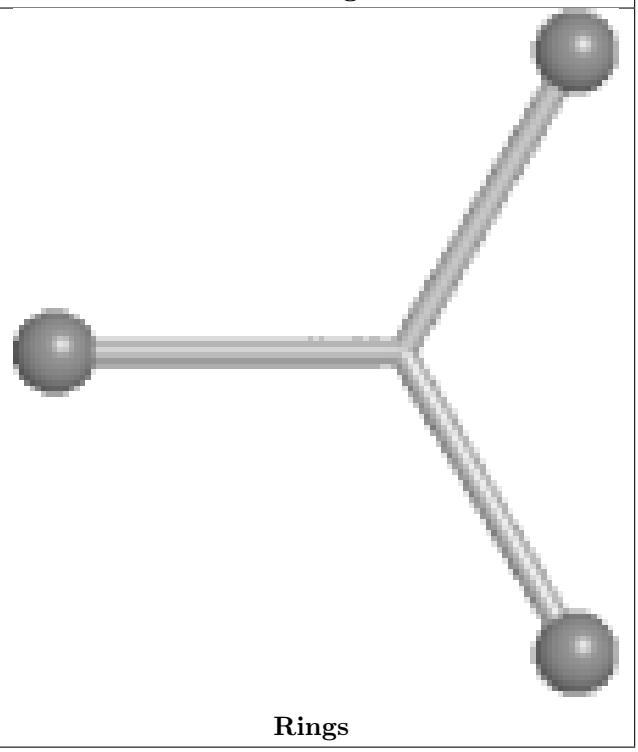
Bond lengths



Bond angles

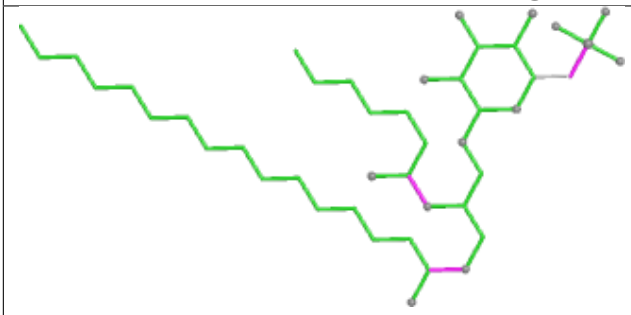


Torsions

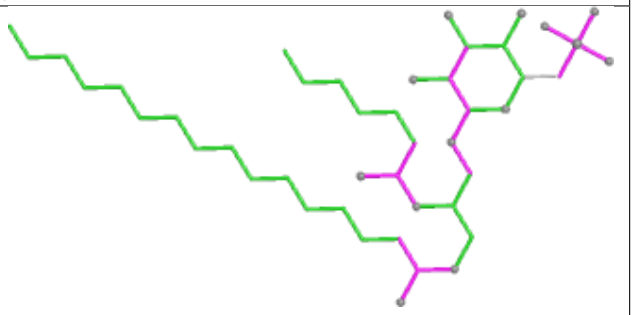


Rings

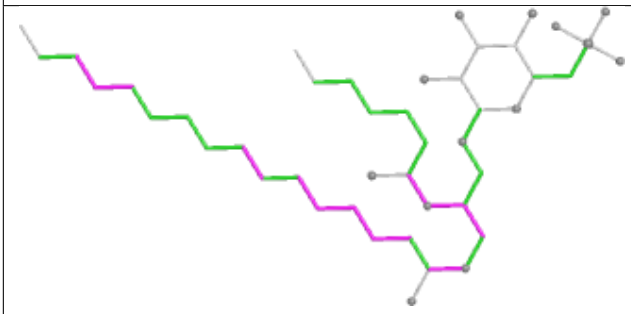
Ligand SQD F 101



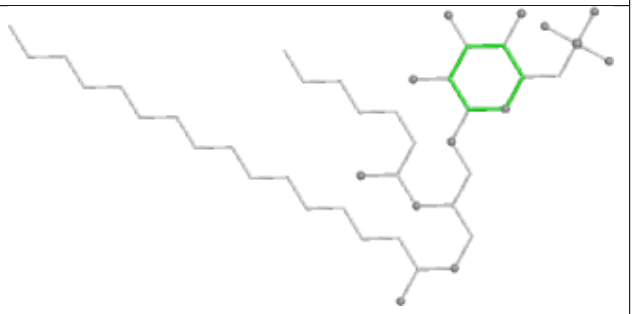
Bond lengths



Bond angles

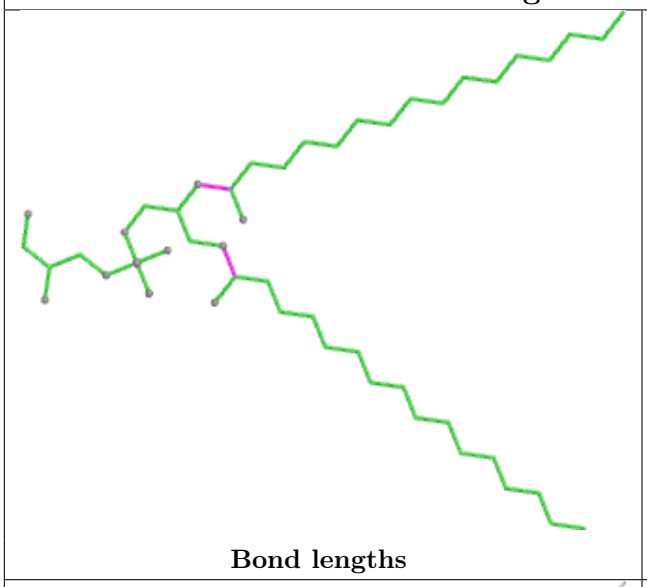


Torsions

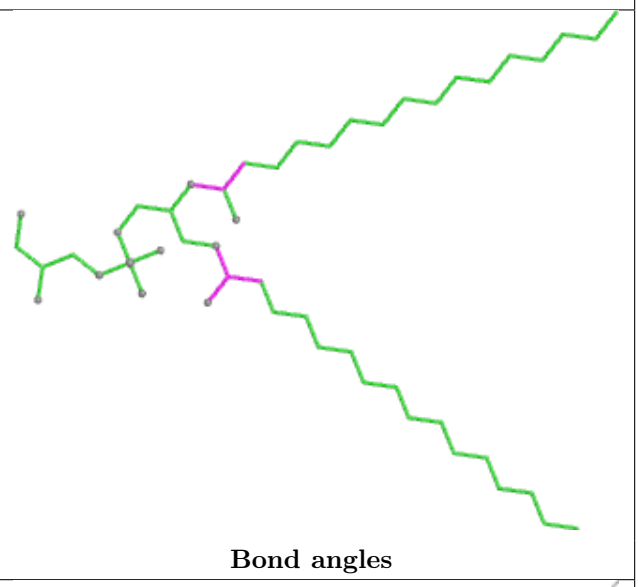


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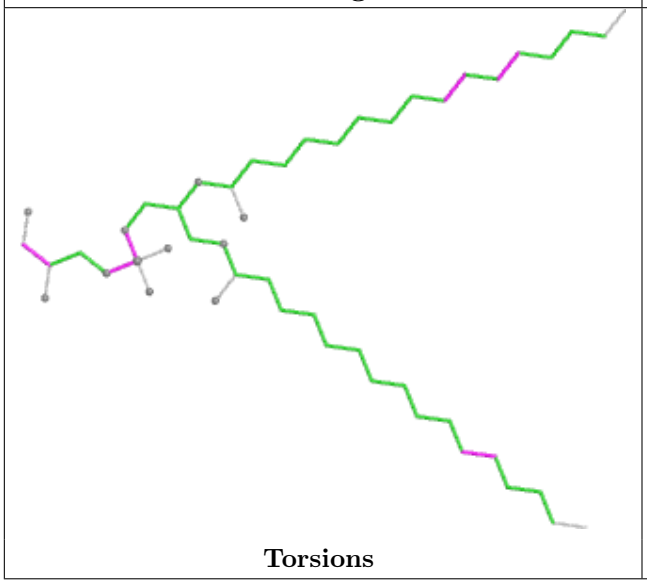
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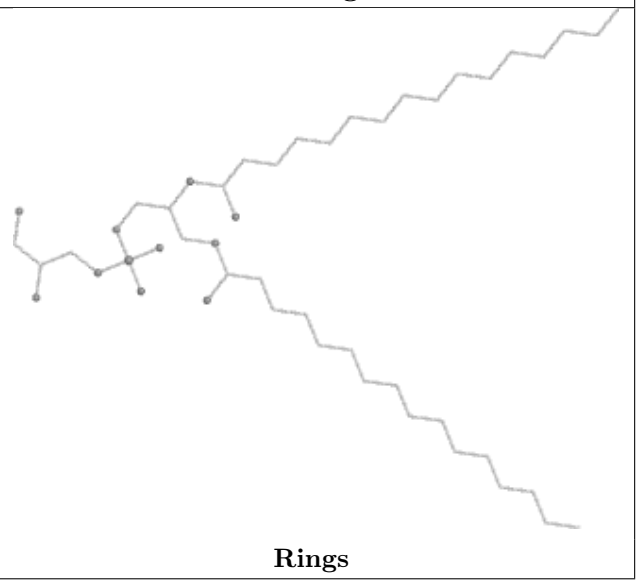
Bond lengths



Bond angles



Torsions

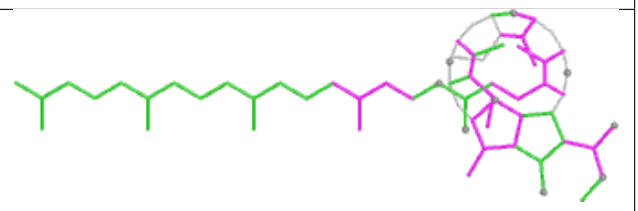


Rings

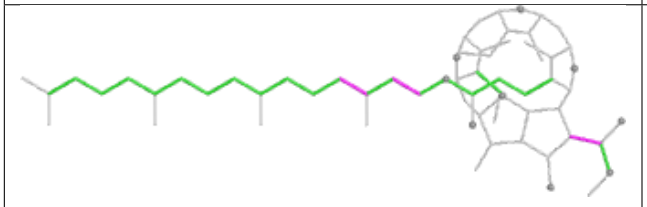
Ligand PHO A 407



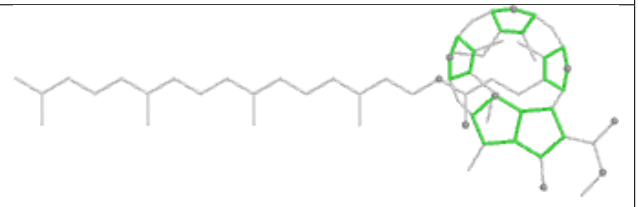
Bond lengths



Bond angles

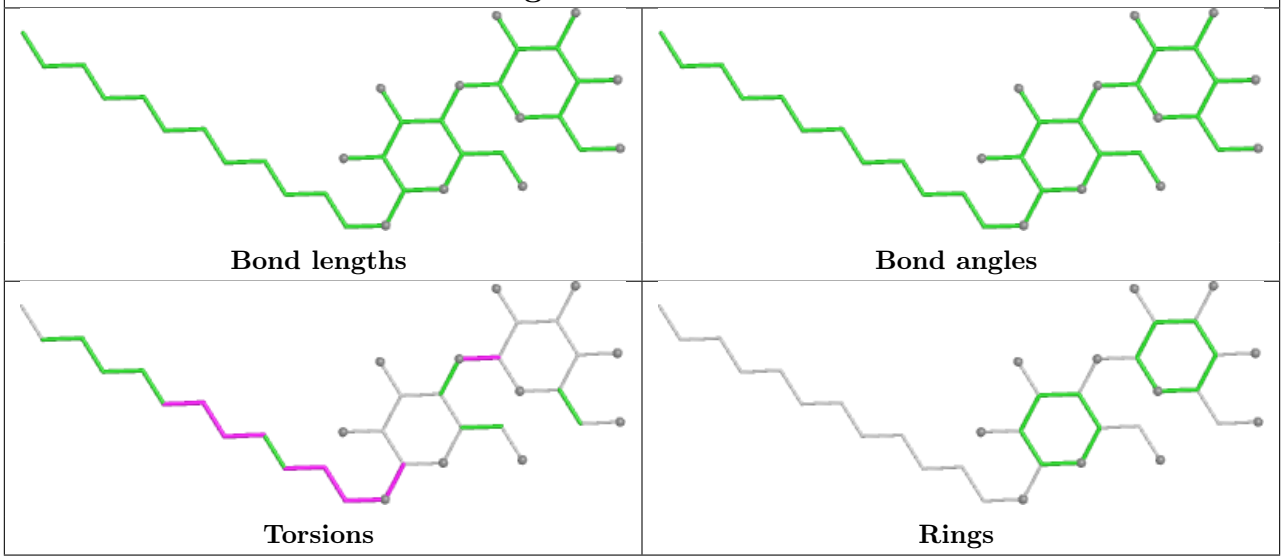


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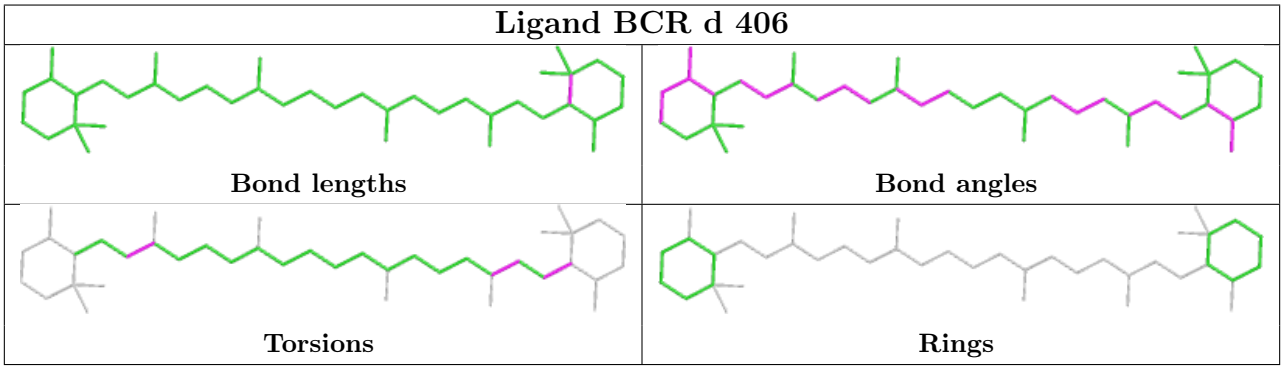


Rings

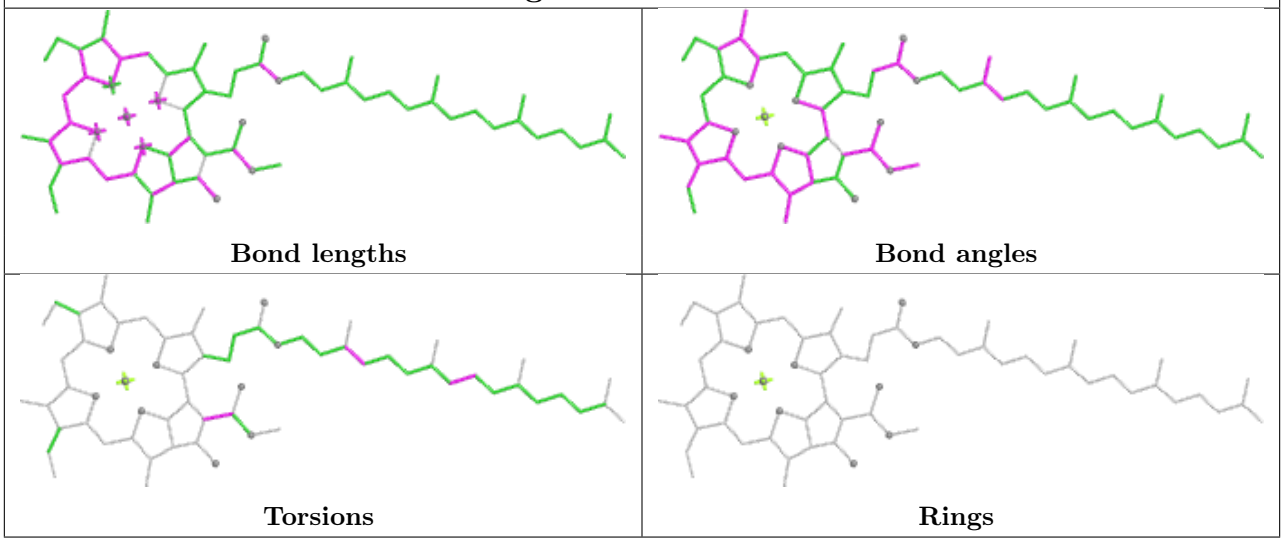
Ligand LMT Z 101



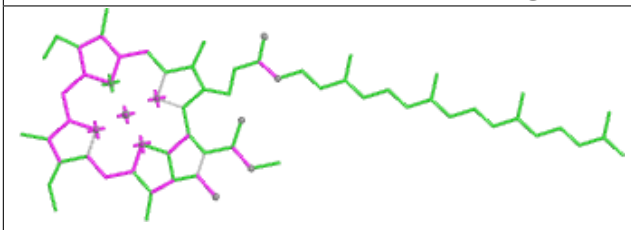
Ligand BCR d 406



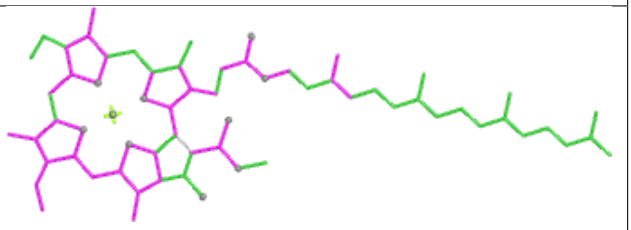
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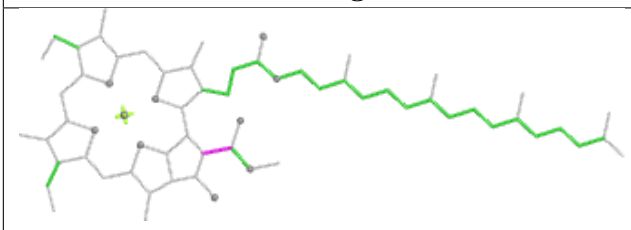
Ligand CLA B 608



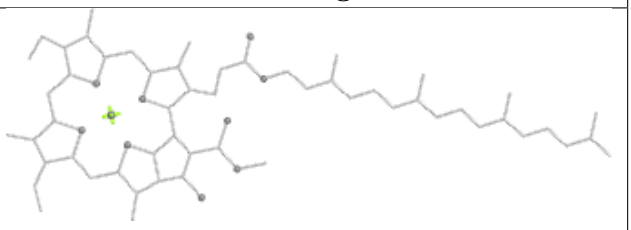
Bond lengths



Bond angles

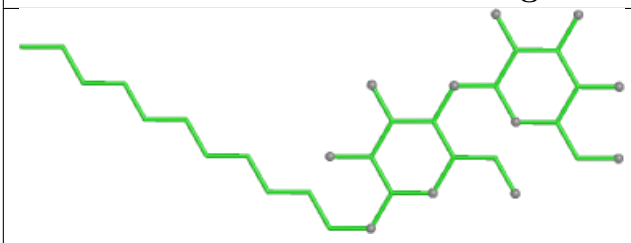


Torsions



Rings

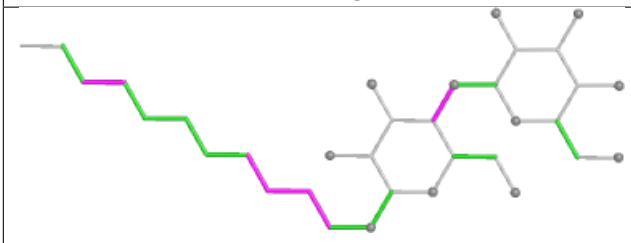
Ligand LMT A 414



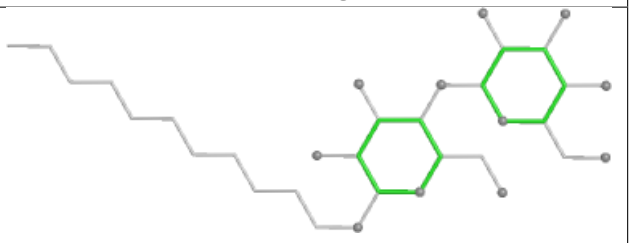
Bond lengths



Bond angles



Torsions

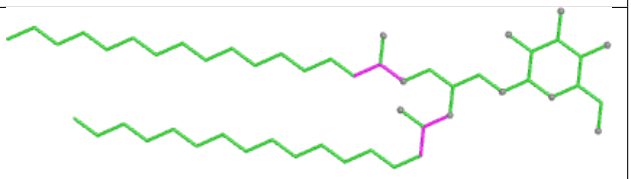


Rings

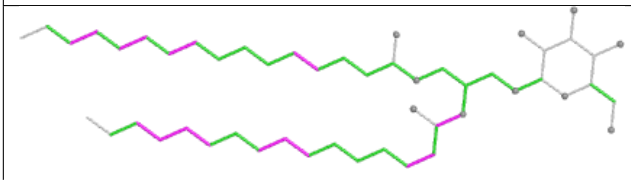
Ligand LMG b 623



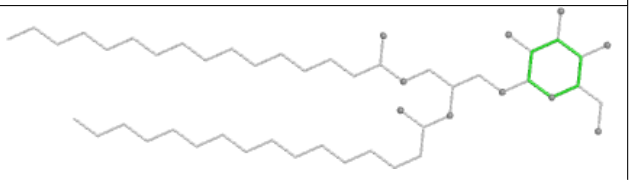
Bond lengths



Bond angles

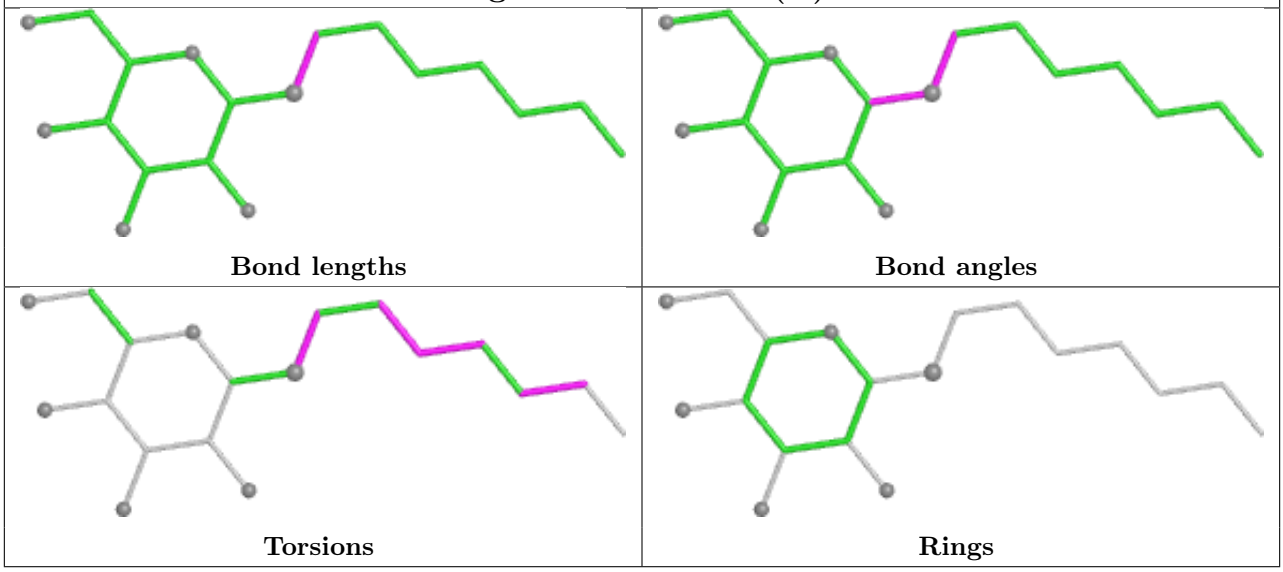


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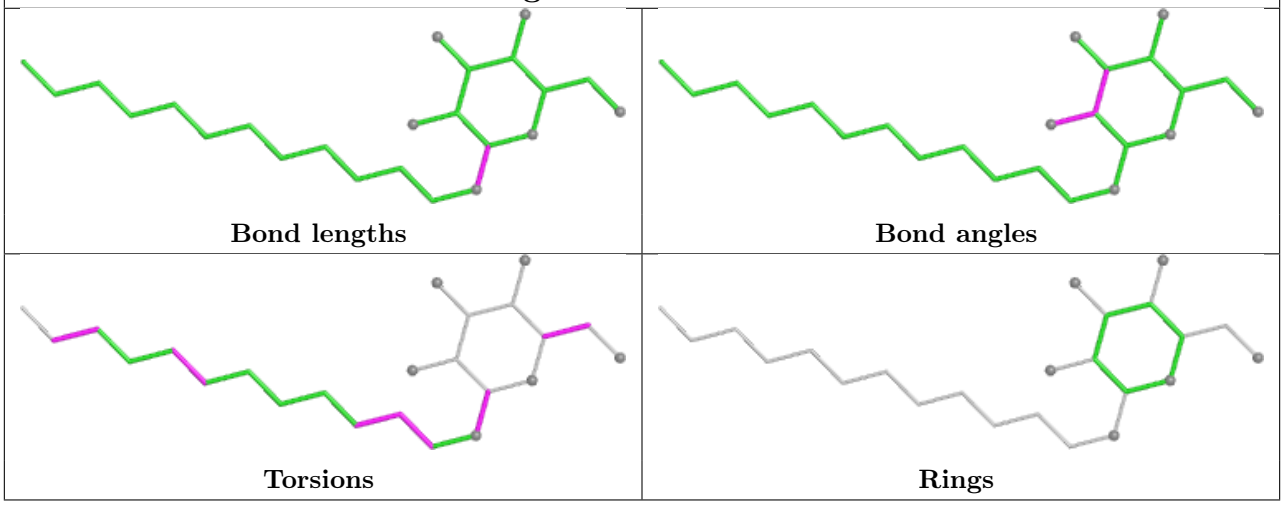


Rings

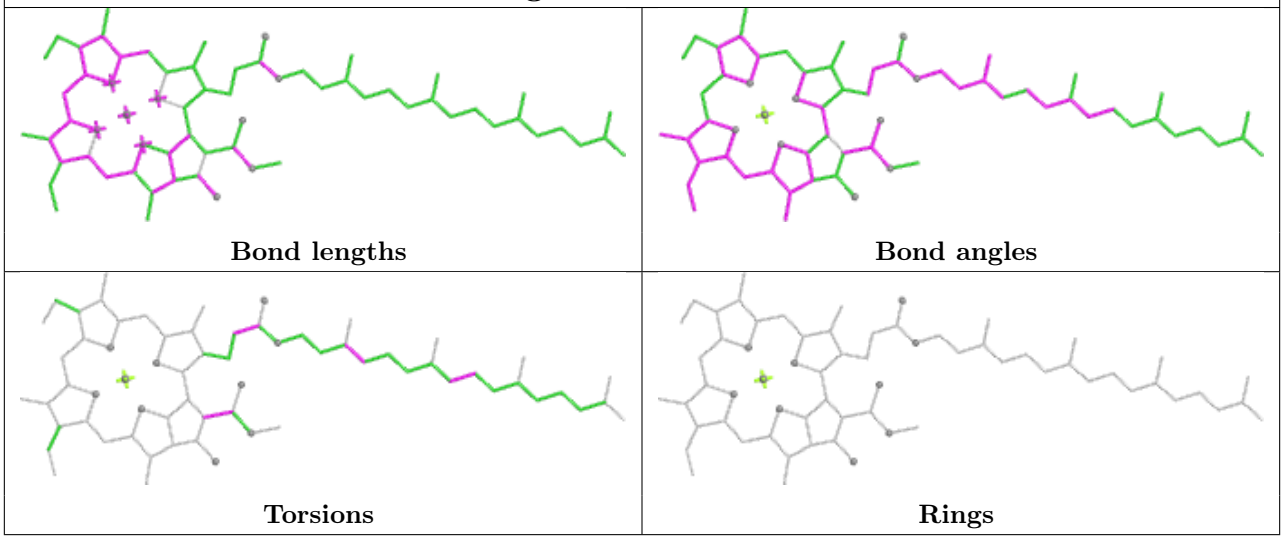
Ligand HTG B 625 (A)



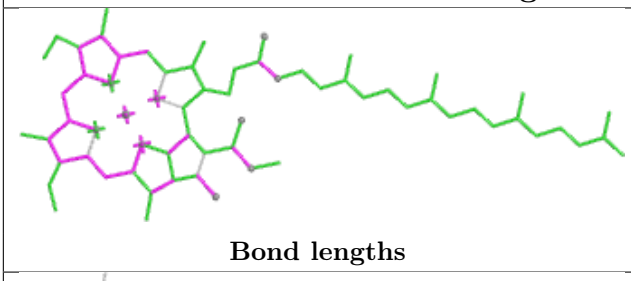
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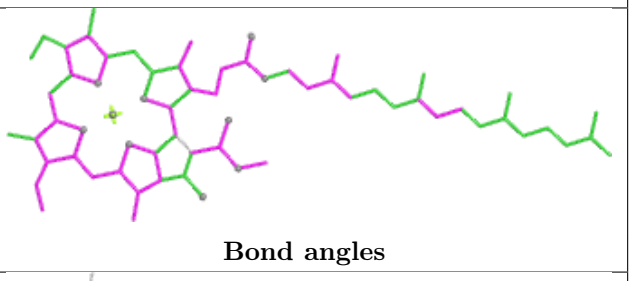
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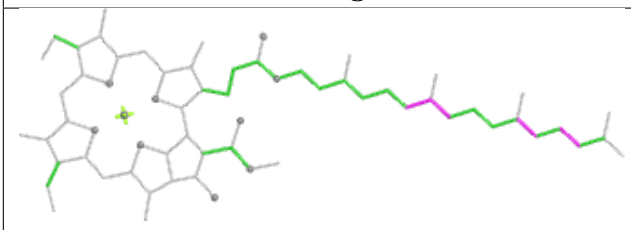
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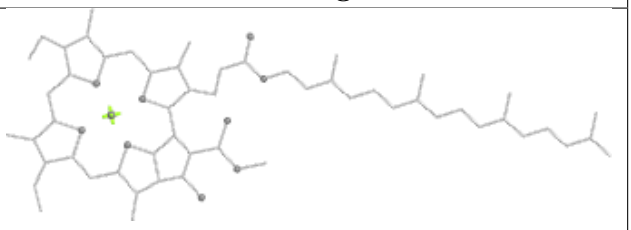
Bond lengths



Bond angles

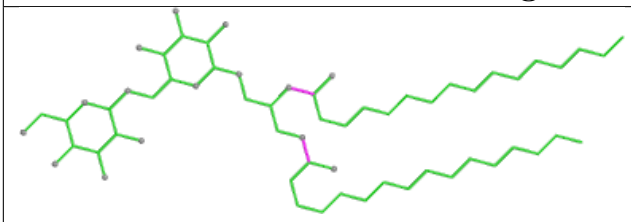


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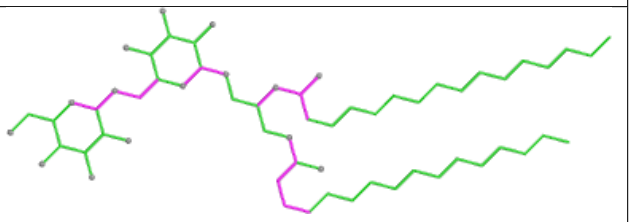


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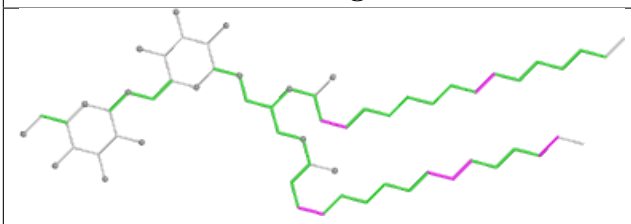
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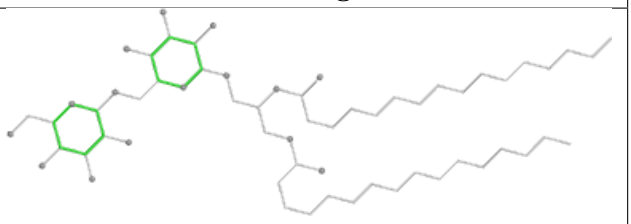
Bond lengths



Bond angles

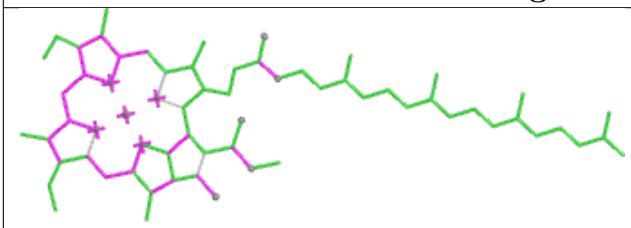


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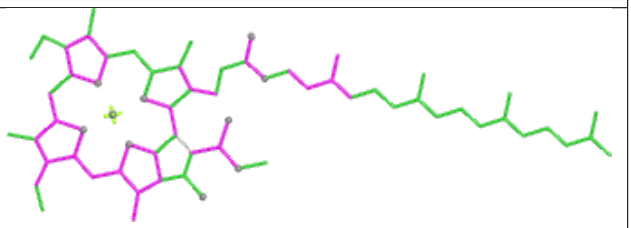


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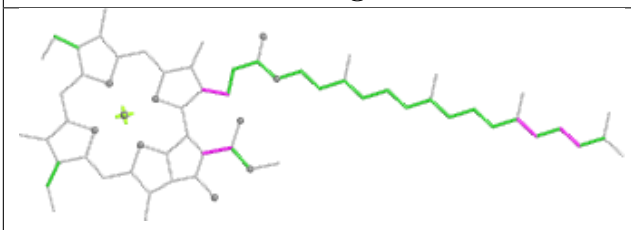
Ligand CLA c 510



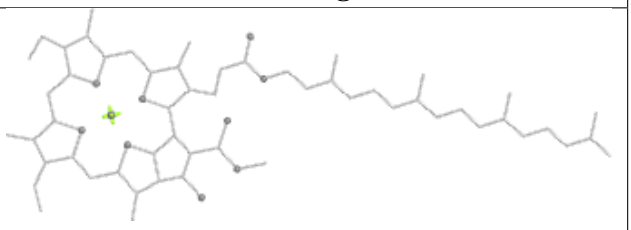
Bond lengths



Bond angles

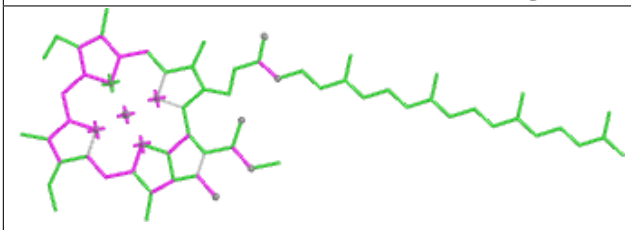


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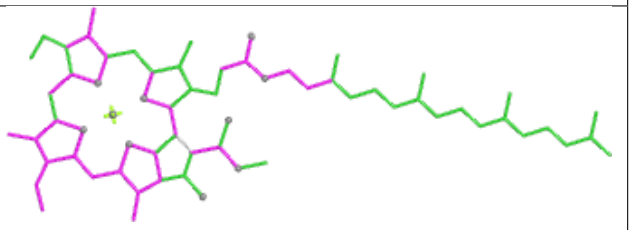


Rings

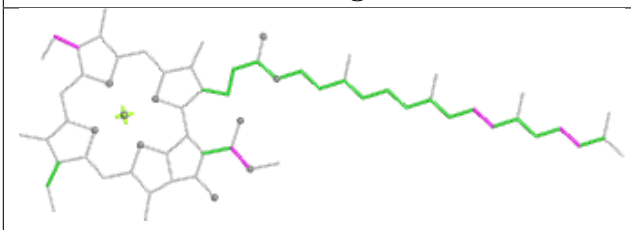
Ligand CLA C 504



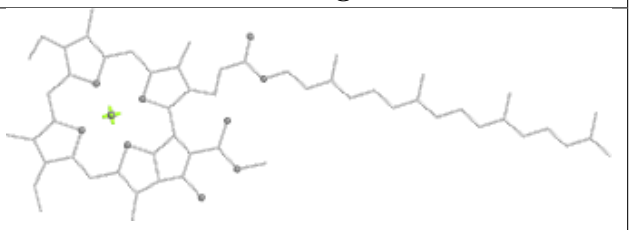
Bond lengths



Bond angles

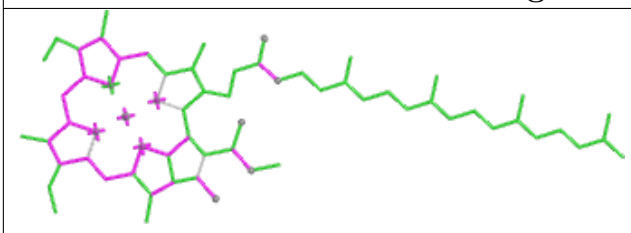


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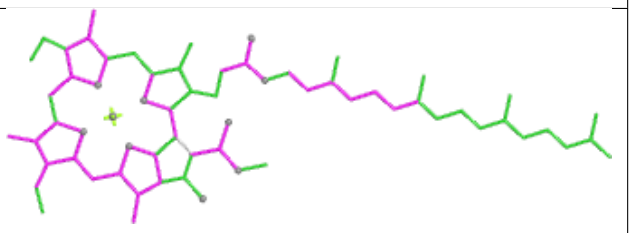


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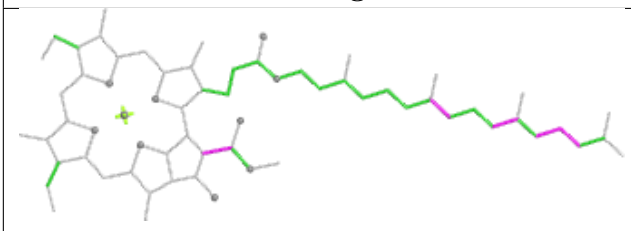
Ligand CLA b 607



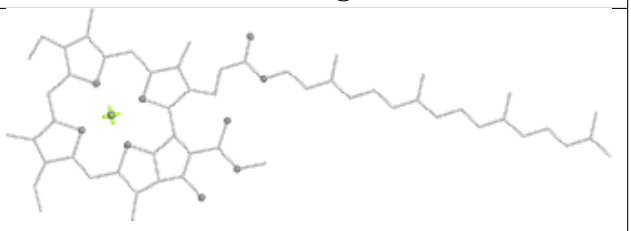
Bond lengths



Bond angles

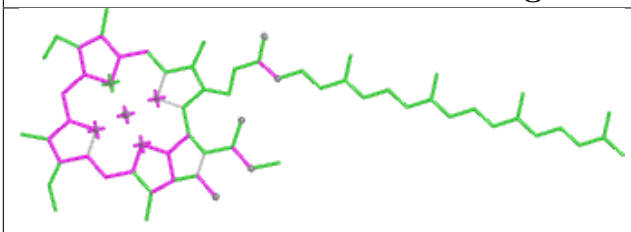


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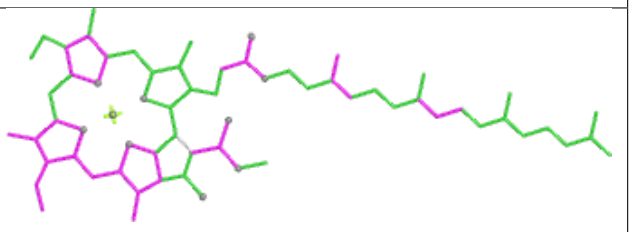


Rings

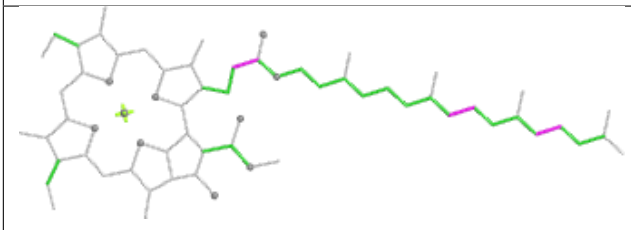
Ligand CLA B 613



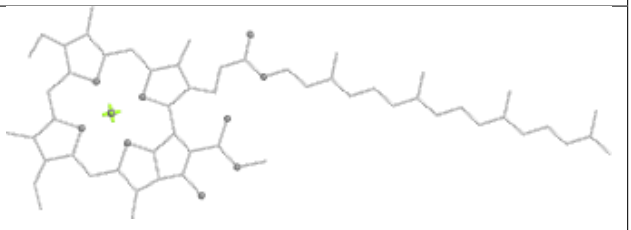
Bond lengths



Bond angles

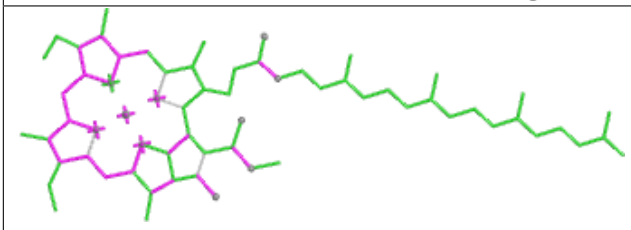


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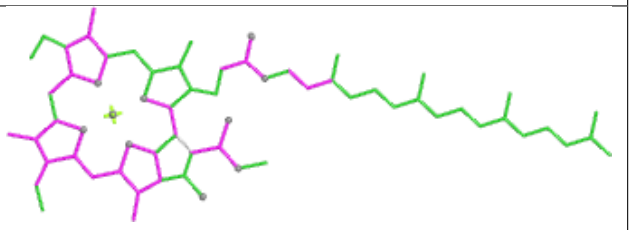


Rings

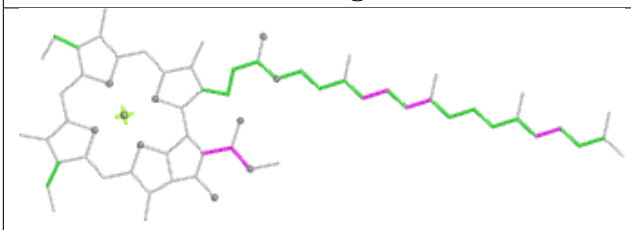
Ligand CLA B 605



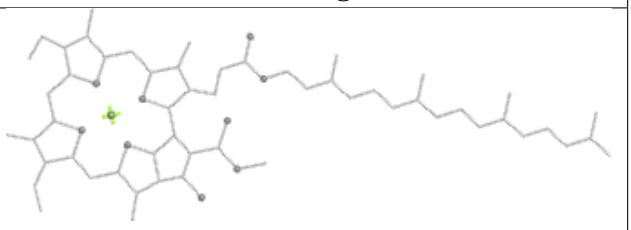
Bond lengths



Bond angles

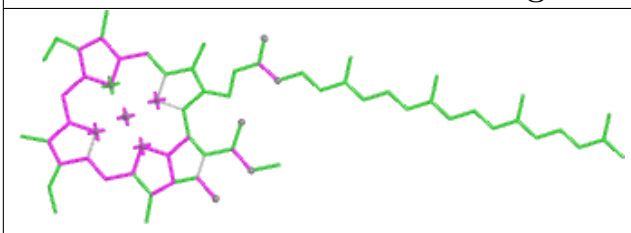


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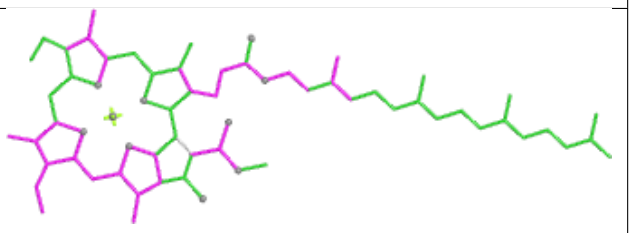


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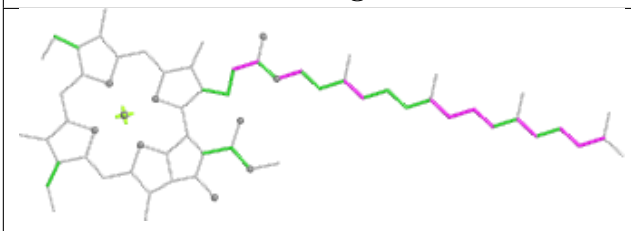
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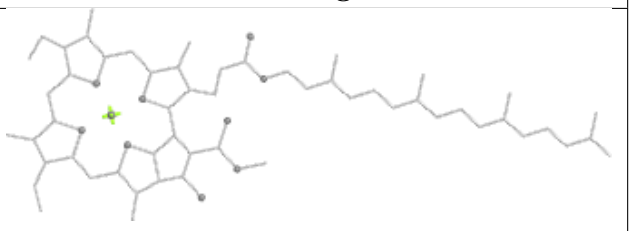
Bond lengths



Bond angles

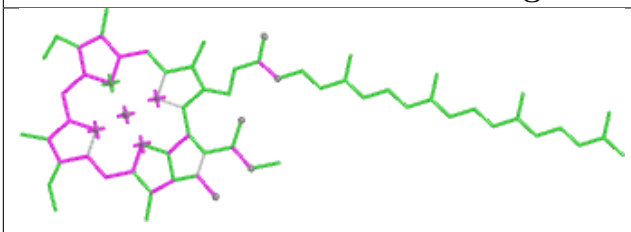


Torsions

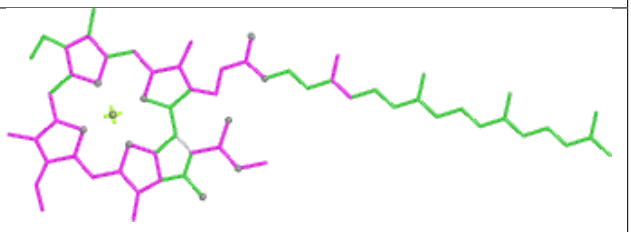


Rings

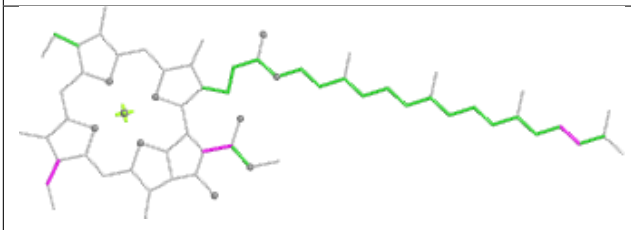
Ligand CLA D 401



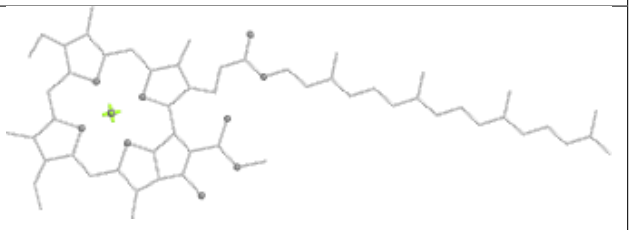
Bond lengths



Bond angles

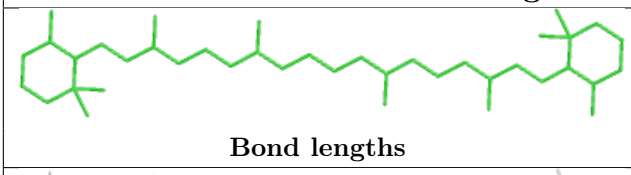


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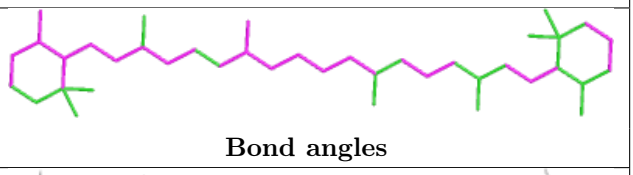


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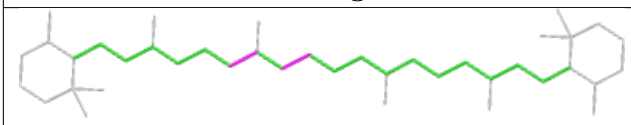
Ligand BCR T 101



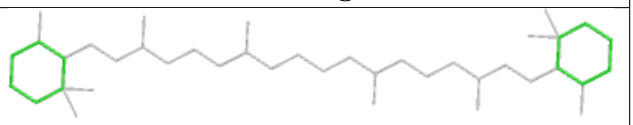
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Bond angles

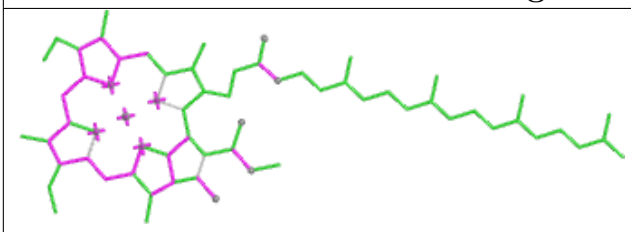


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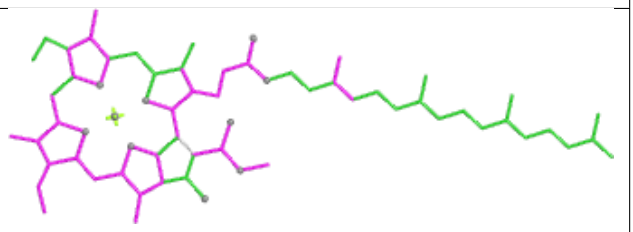


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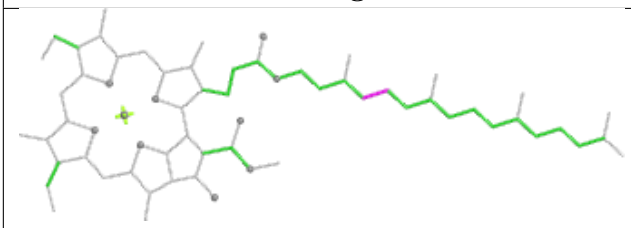
Ligand CLA b 610



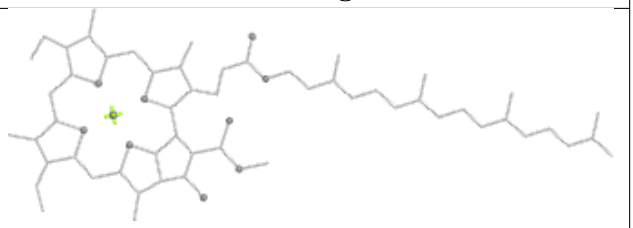
Bond lengths



Bond angles

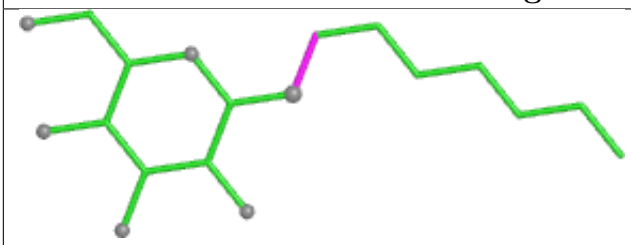


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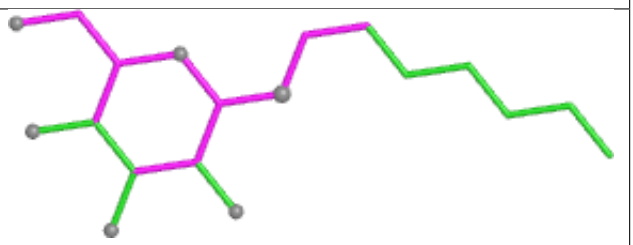


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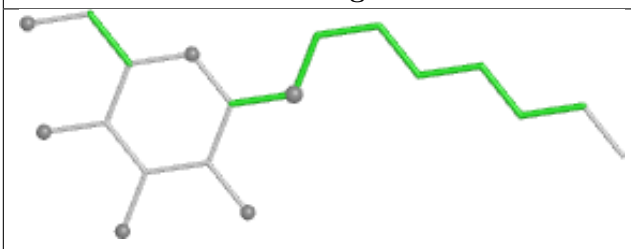
Ligand HTG b 625



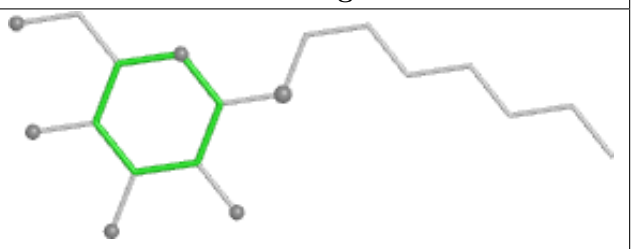
Bond lengths



Bond angles

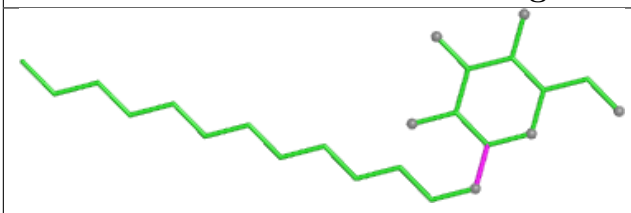


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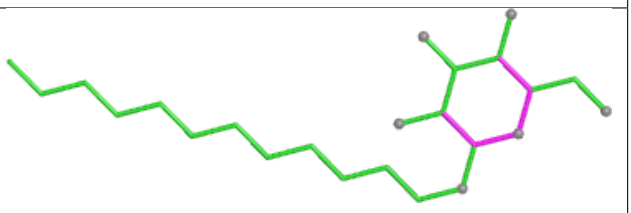


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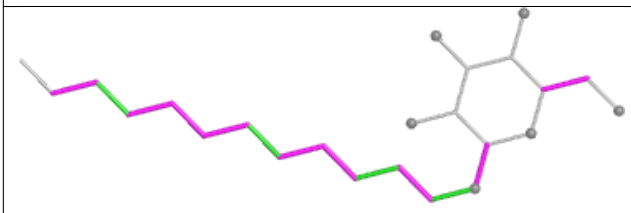
Ligand LMT i 104



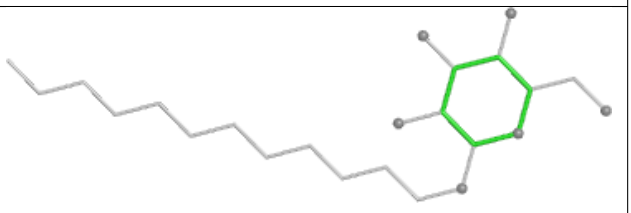
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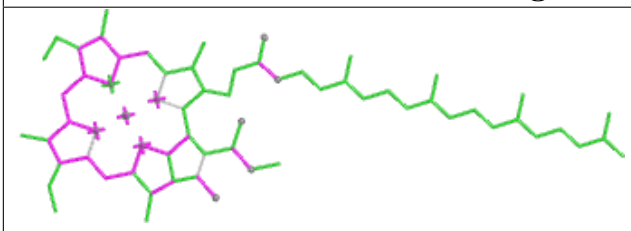


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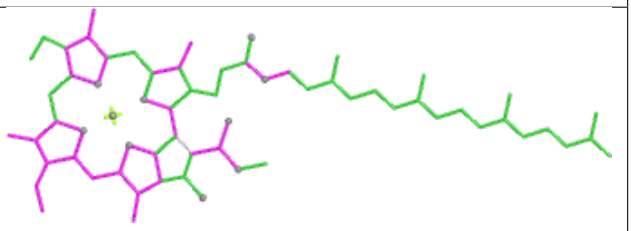


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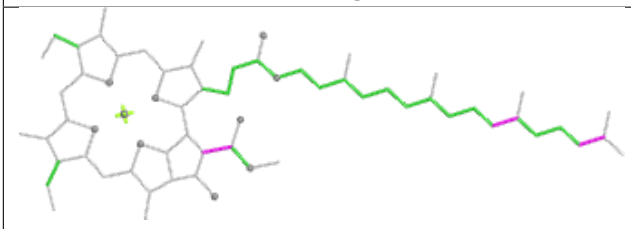
Ligand CLA c 507



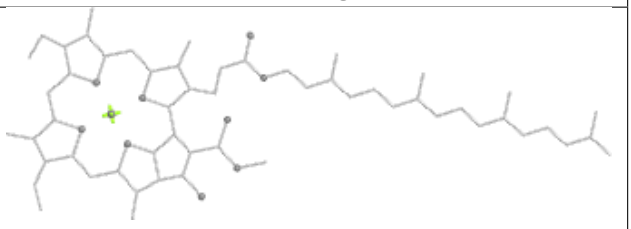
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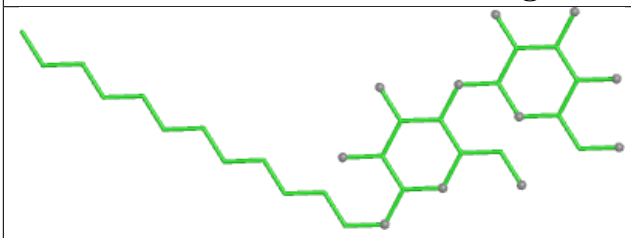


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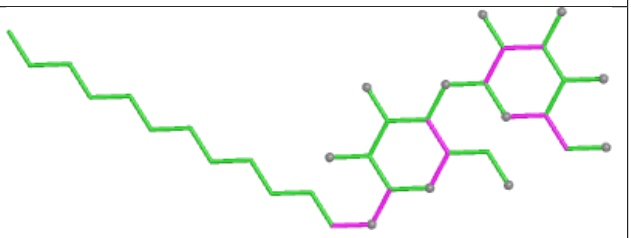


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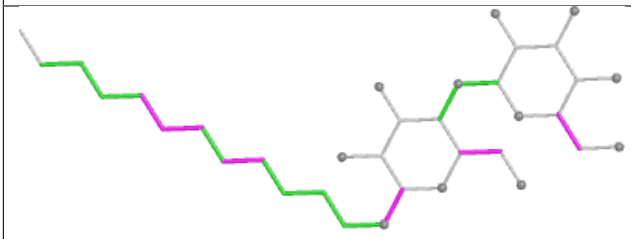
Ligand LMT B 636



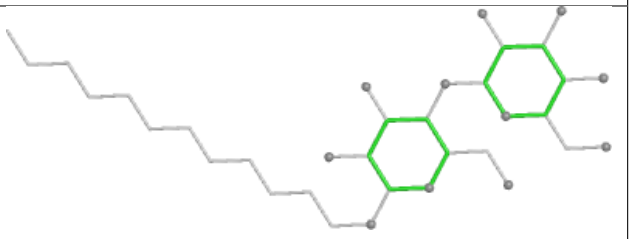
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Bond angles

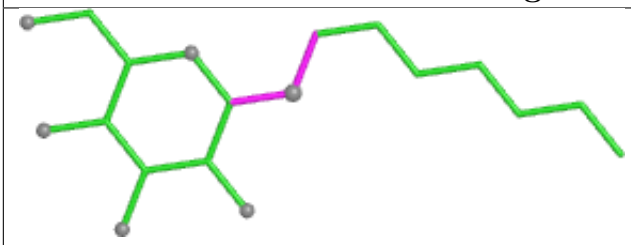


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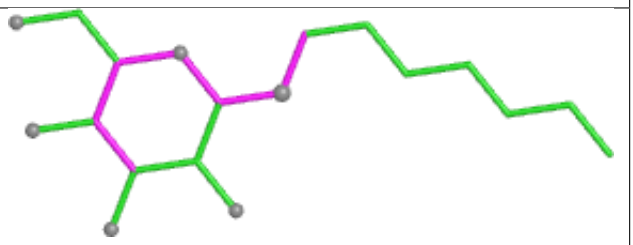


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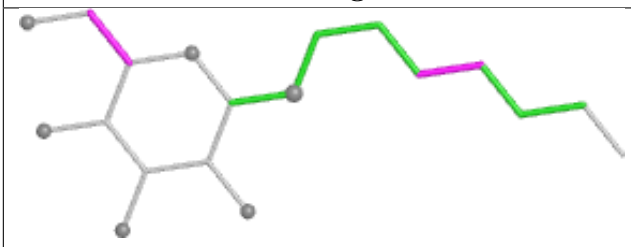
Ligand HTG b 601



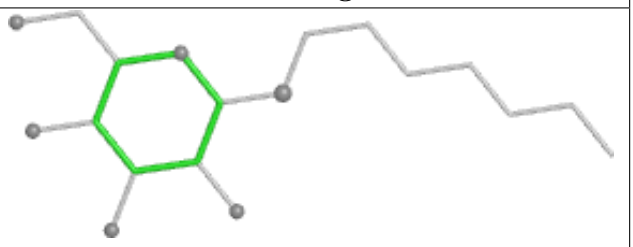
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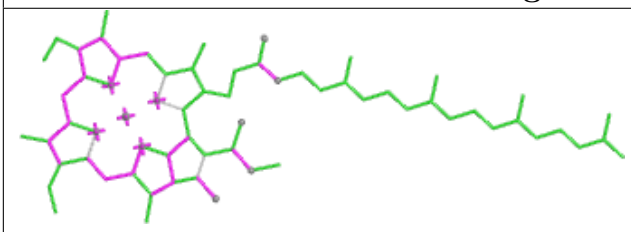


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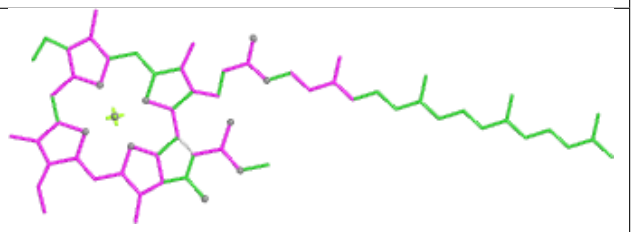


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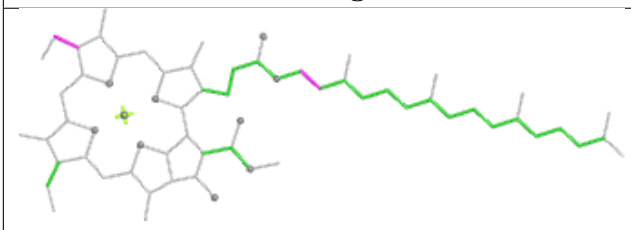
Ligand CLA D 404



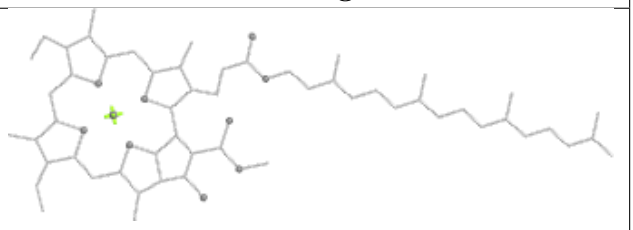
Bond lengths



Bond angles

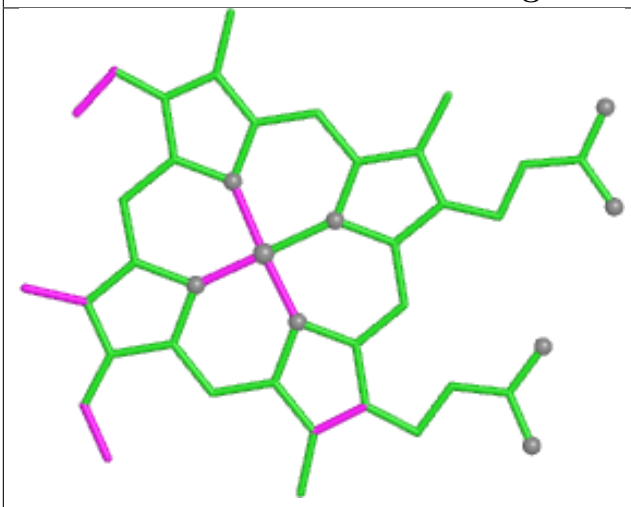


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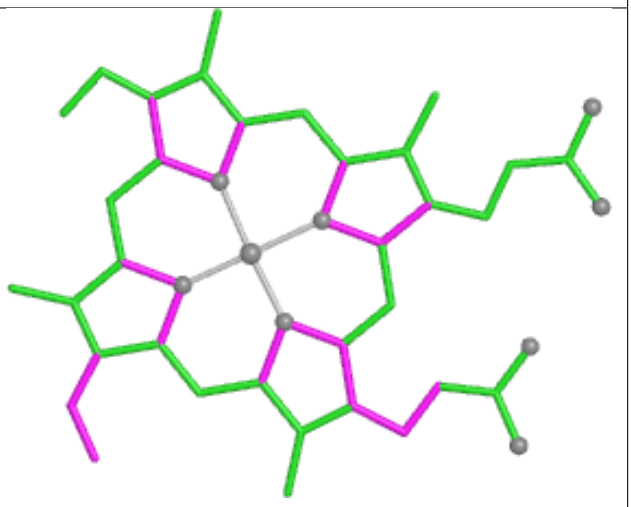


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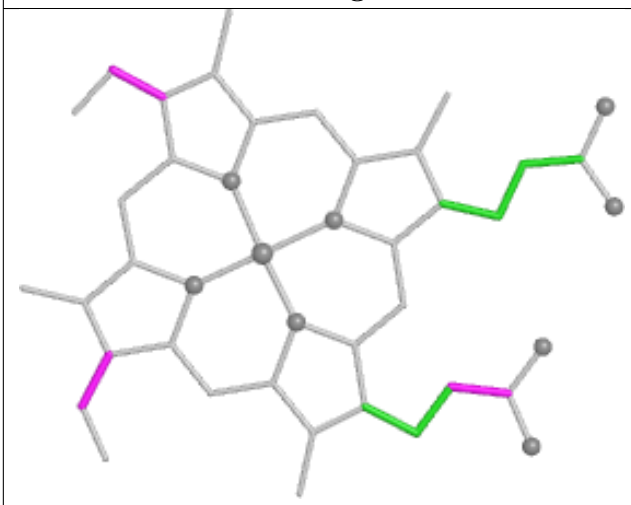
Ligand HEC V 201



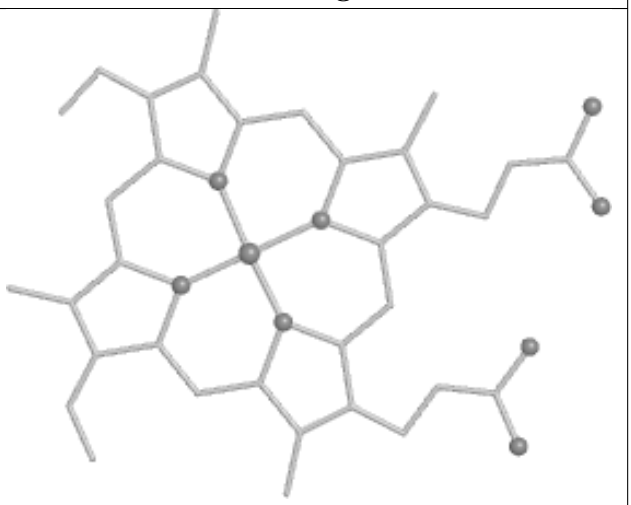
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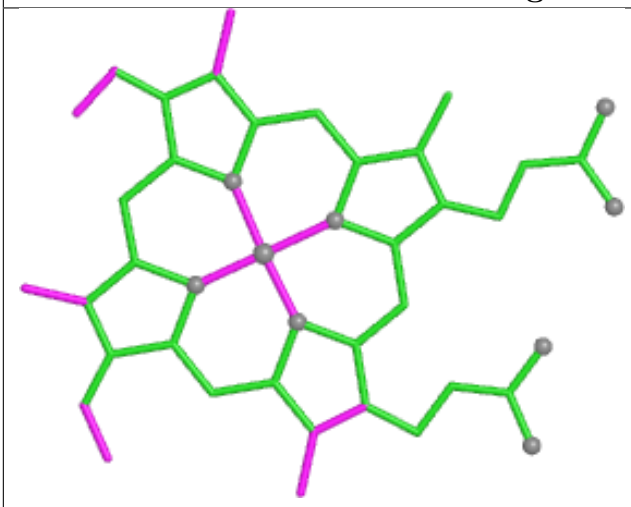


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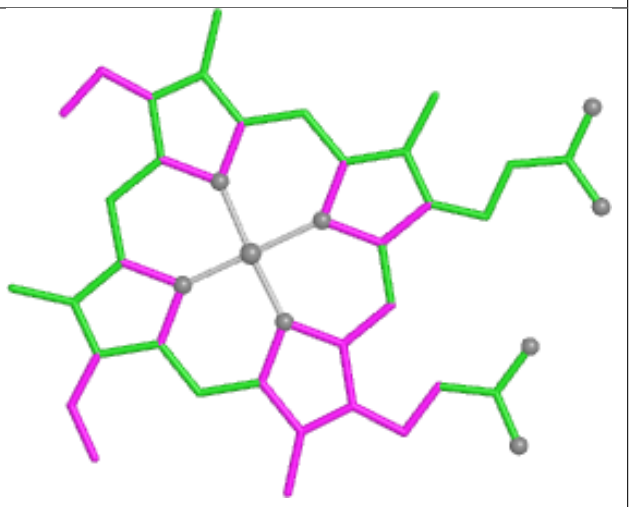


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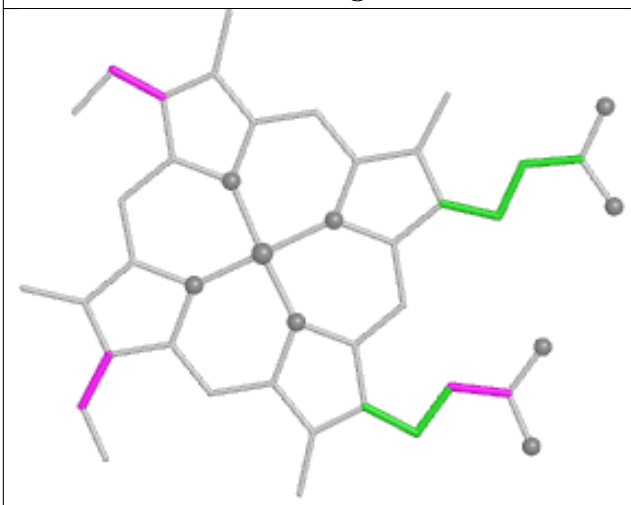
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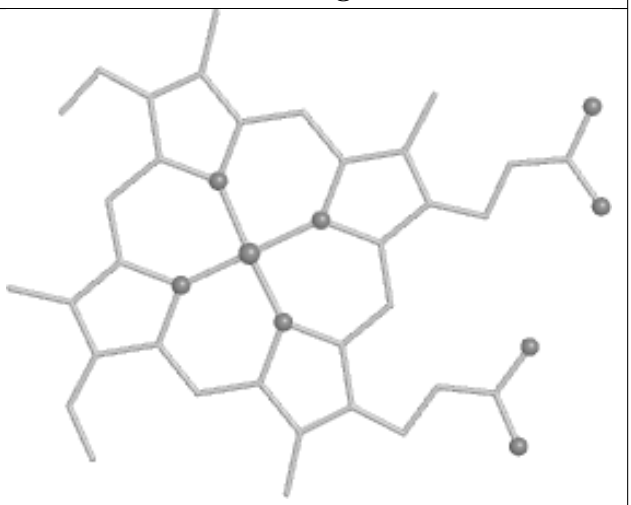
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Bond angles

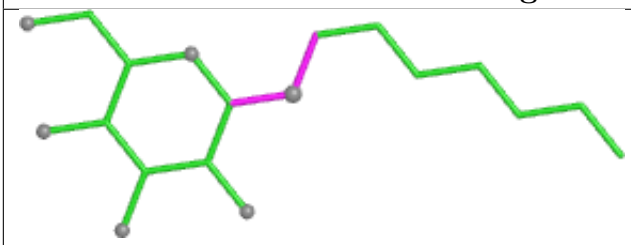


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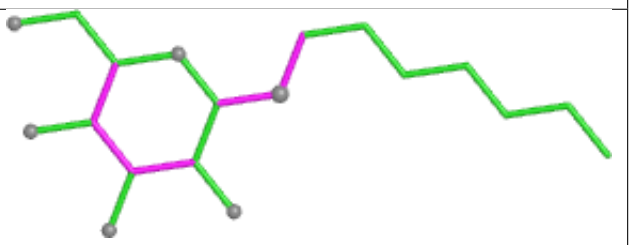


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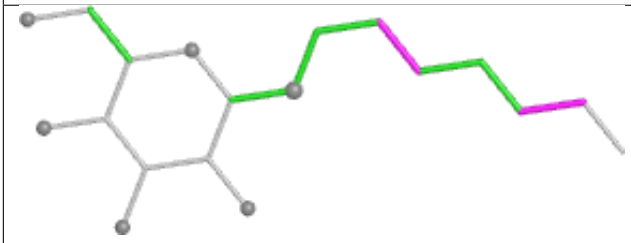
Ligand HTG D 413



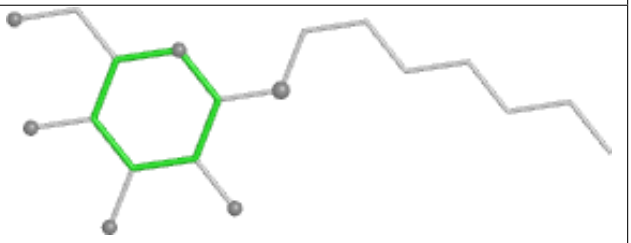
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Bond angles

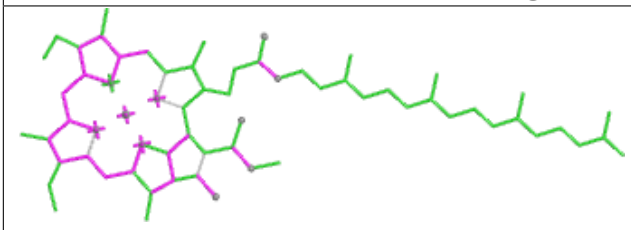


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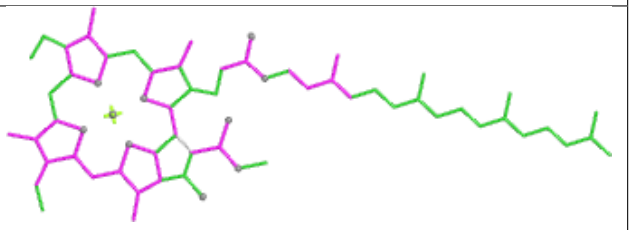


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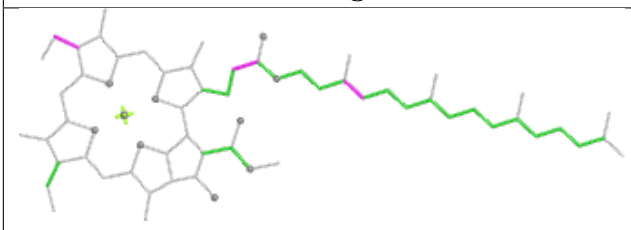
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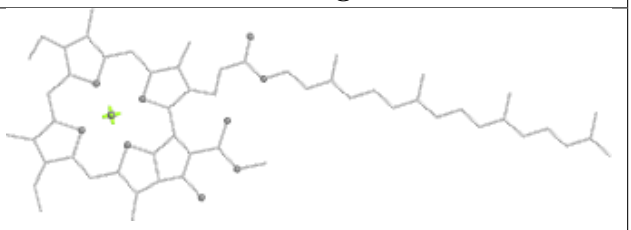
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Bond angles

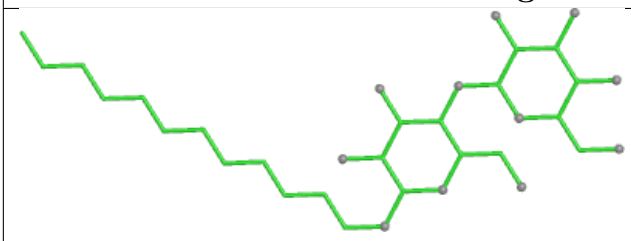


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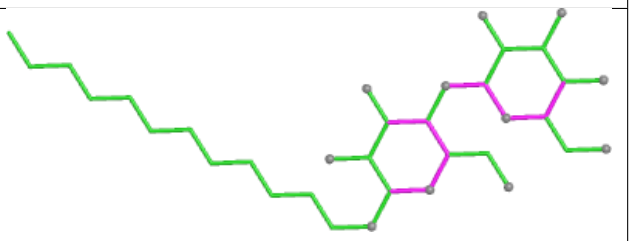


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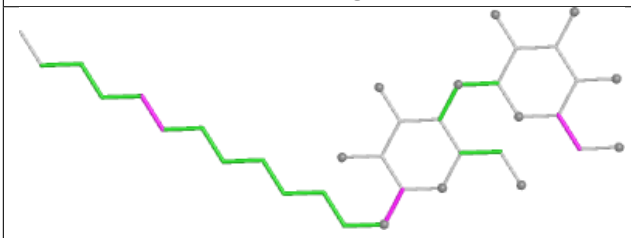
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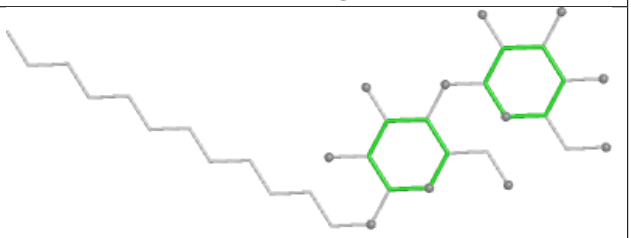
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Bond angles

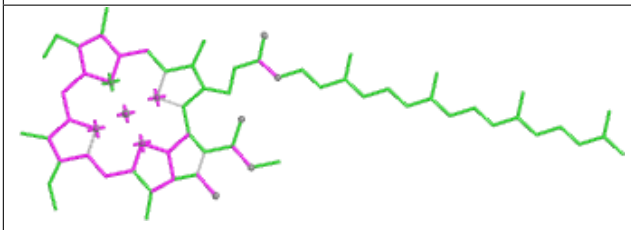


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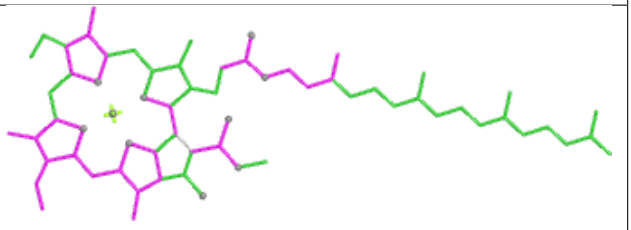


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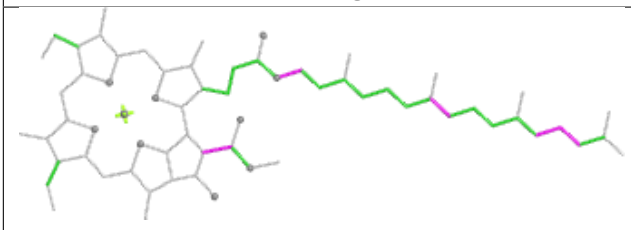
Ligand CLA C 510



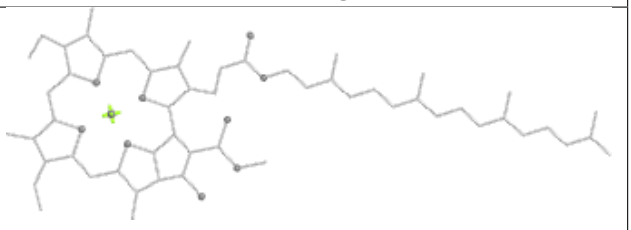
Bond lengths



Bond angles

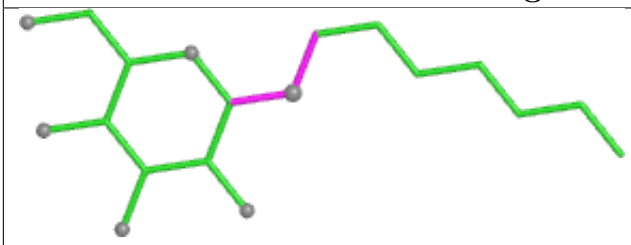


Torsions

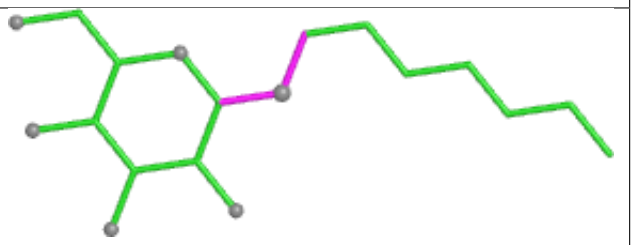


Rings

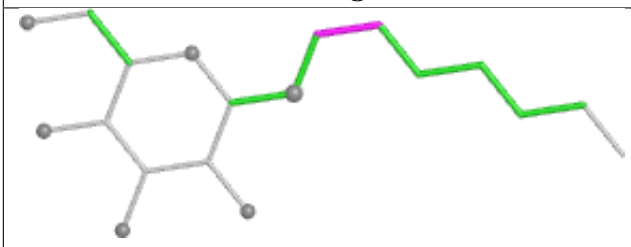
Ligand HTG d 414



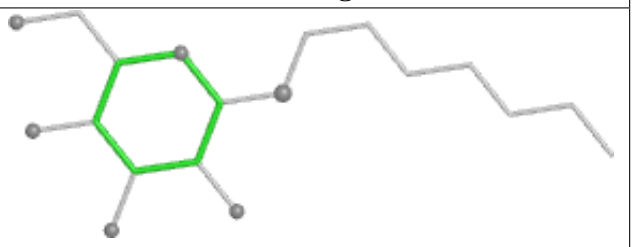
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Bond angles

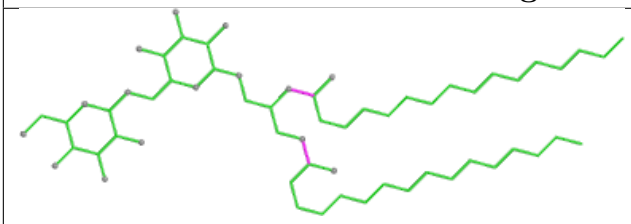


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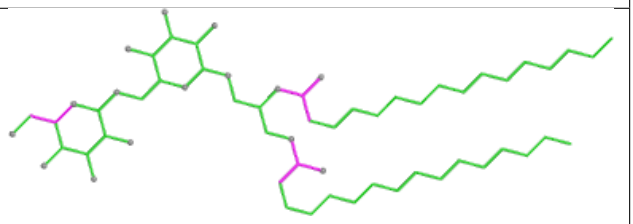


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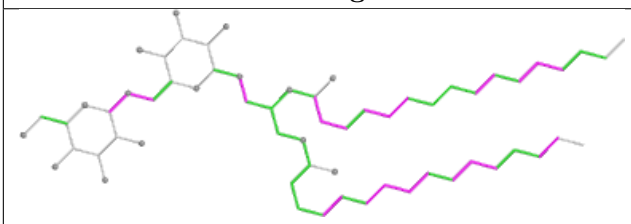
Ligand DGD C 518



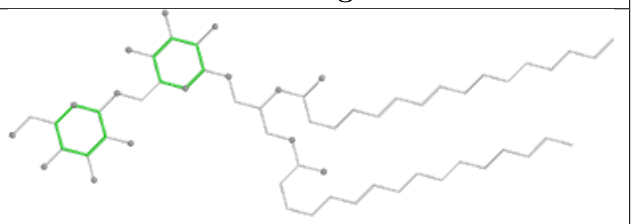
Bond lengths



Bond angles

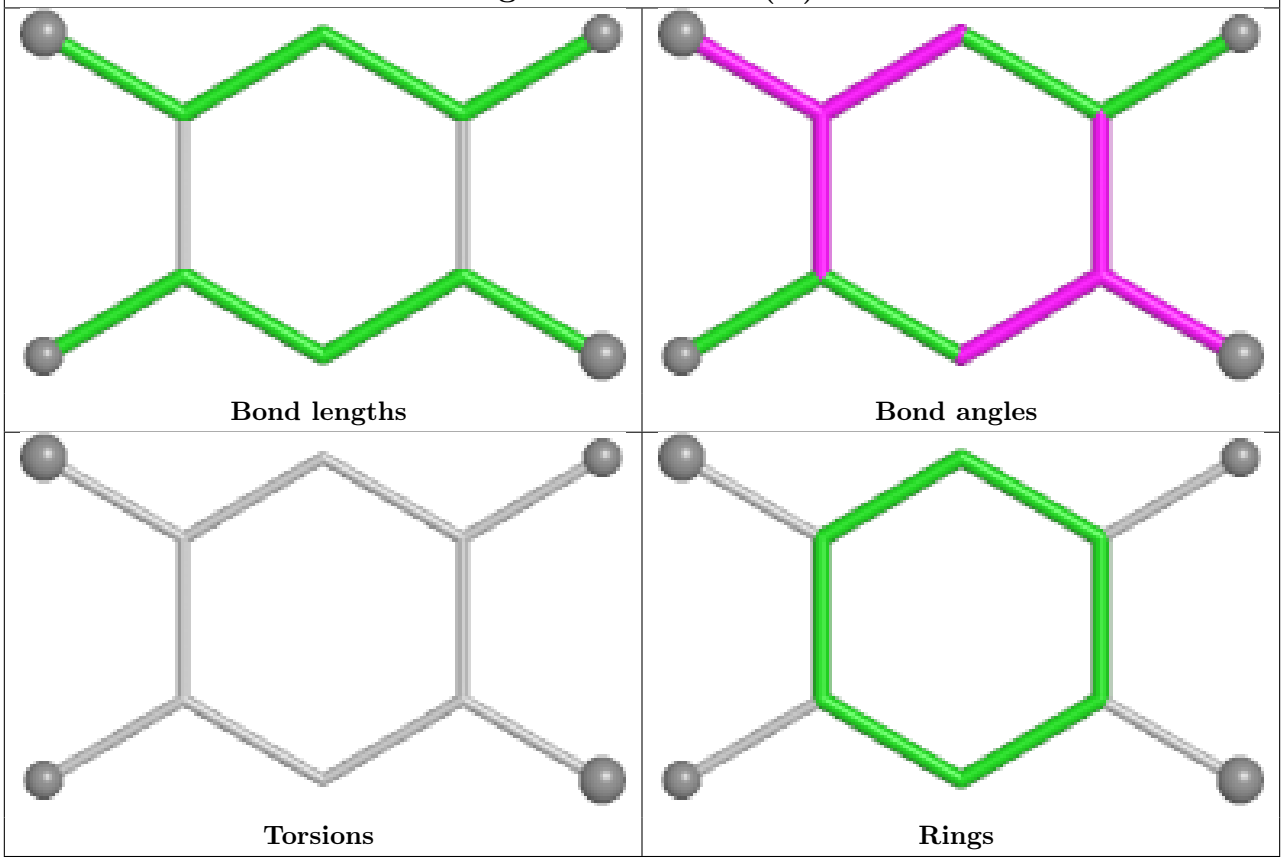


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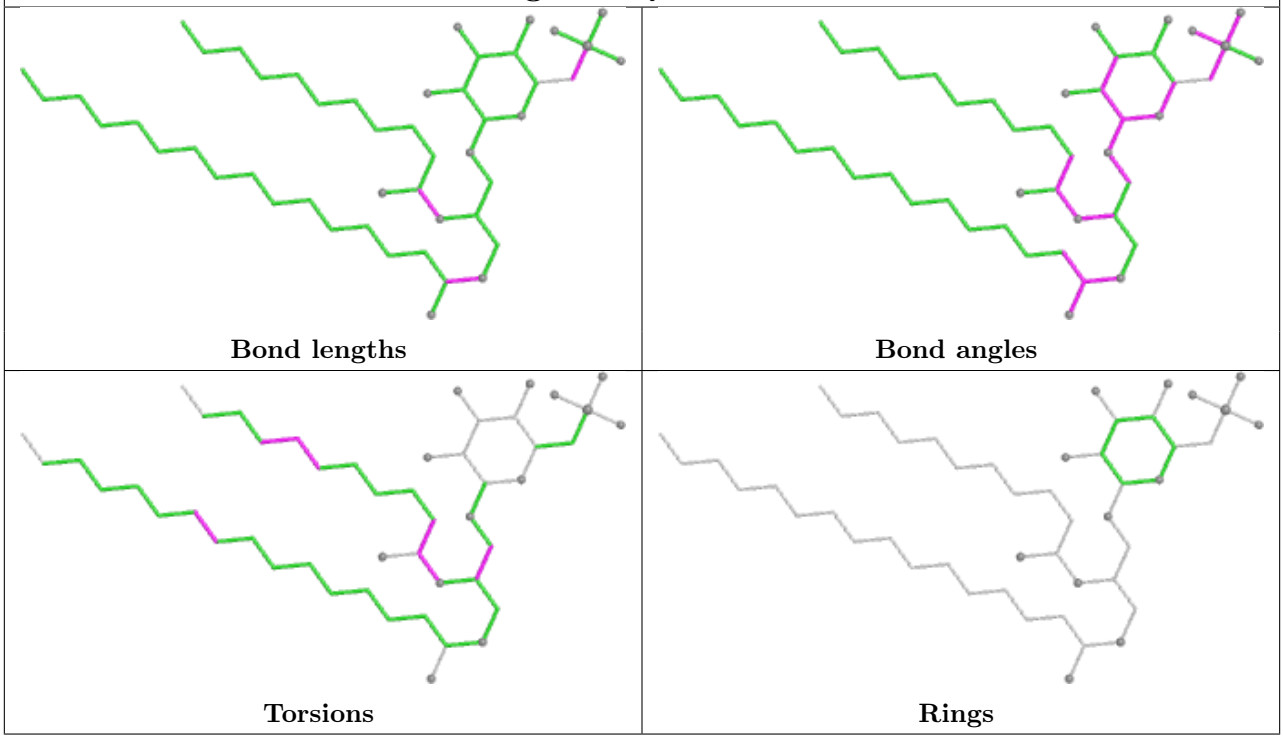


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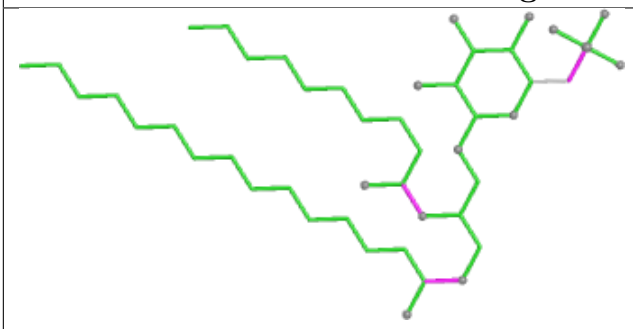
Ligand K2I A 418 (A)



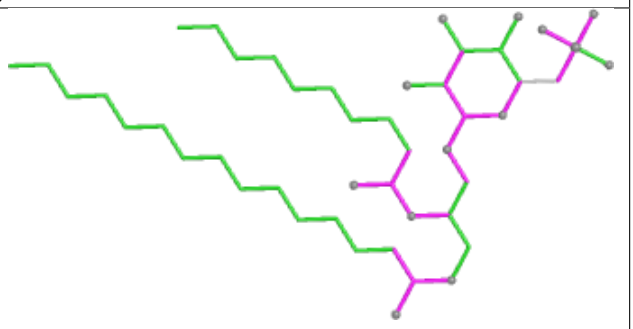
Ligand SQD A 411



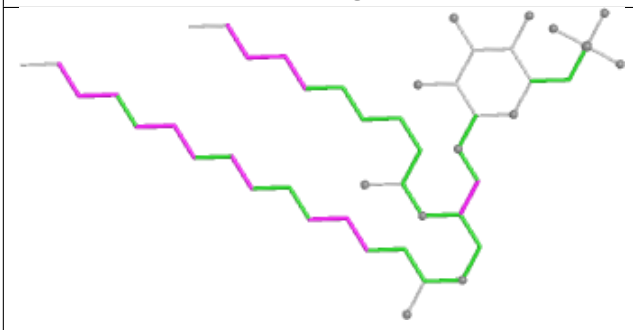
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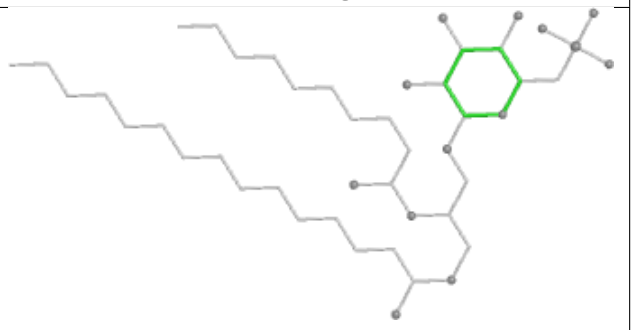
Bond lengths



Bond angles

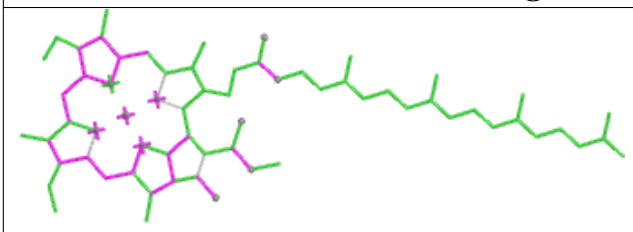


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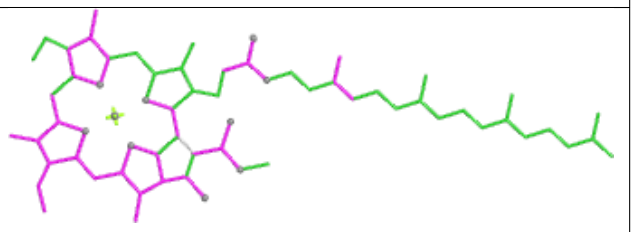


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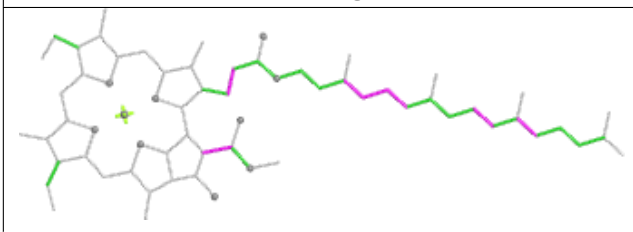
Ligand CLA B 615



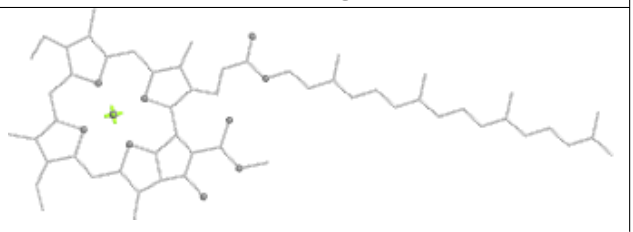
Bond lengths



Bond angles

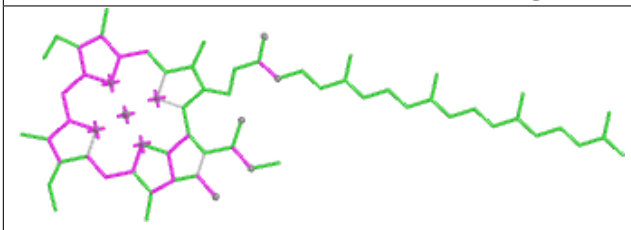


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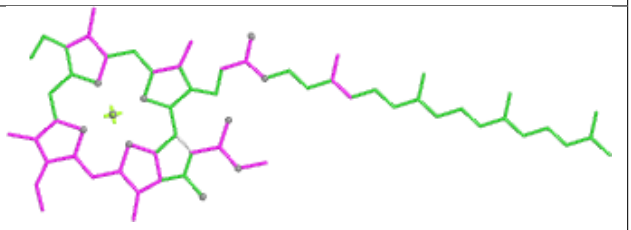


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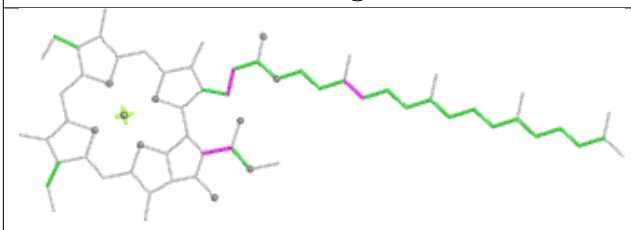
Ligand CLA b 608



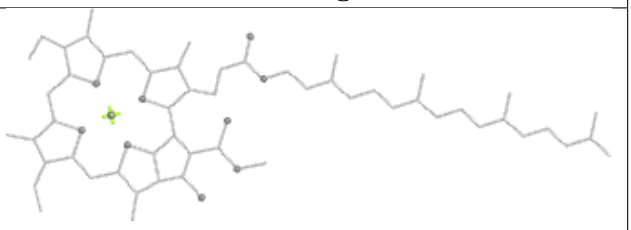
Bond lengths



Bond angles



Torsions

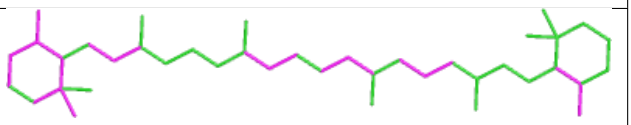


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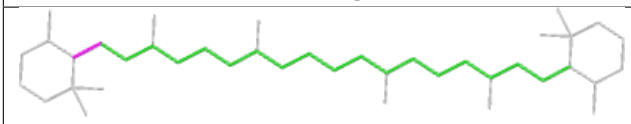
Ligand BCR c 517



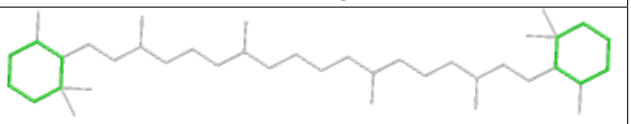
Bond lengths



Bond angles

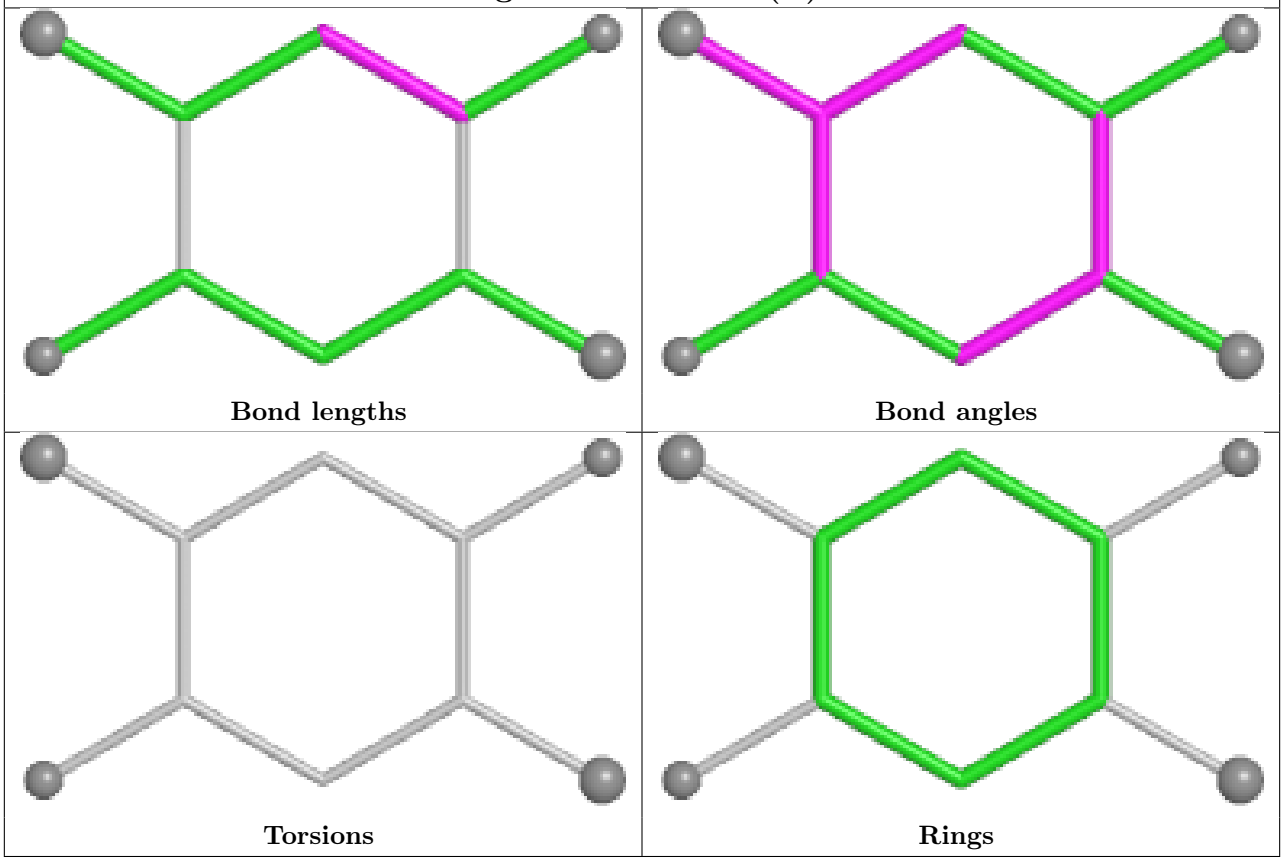


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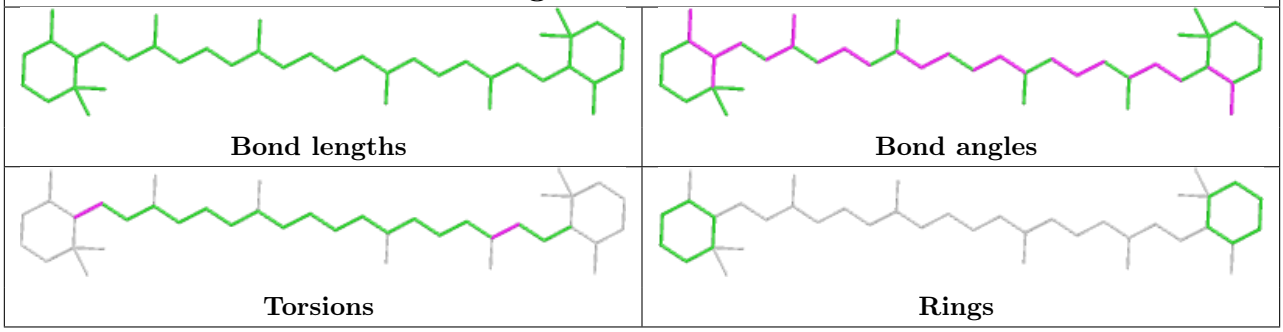


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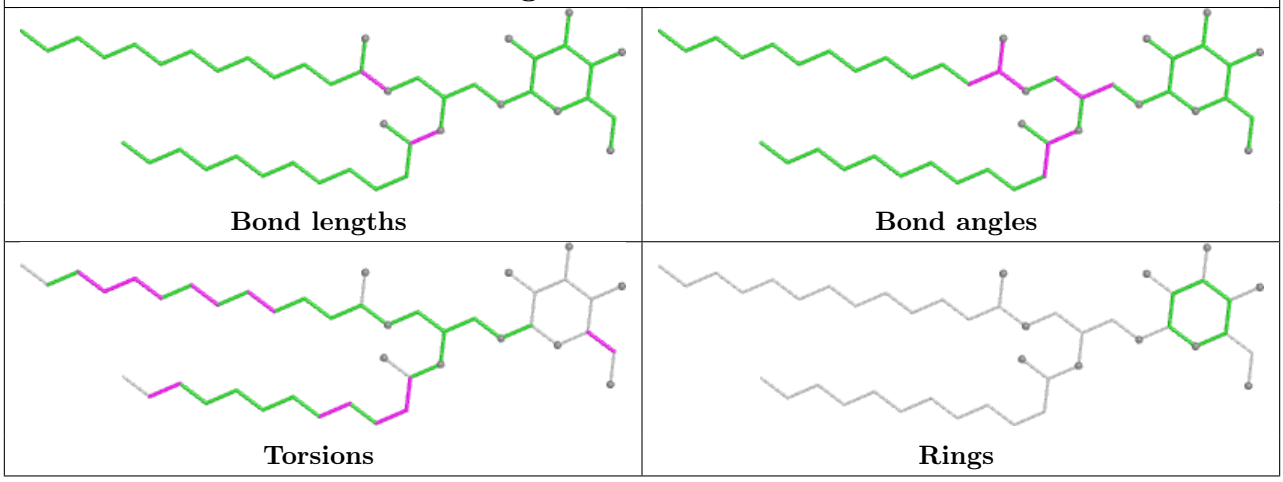
Ligand K2I a 2118 (B)



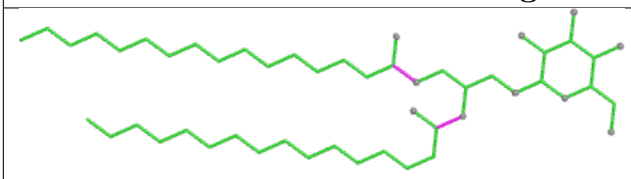
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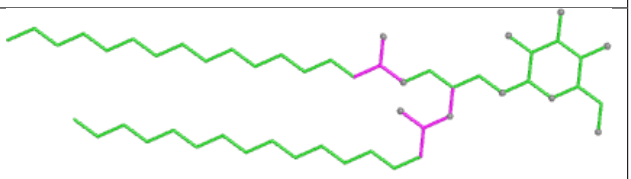
Ligand LMG D 412



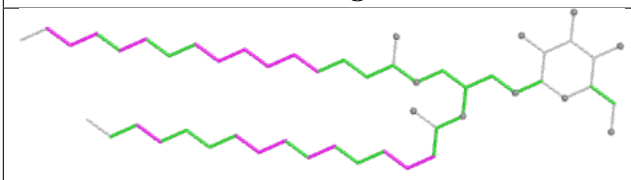
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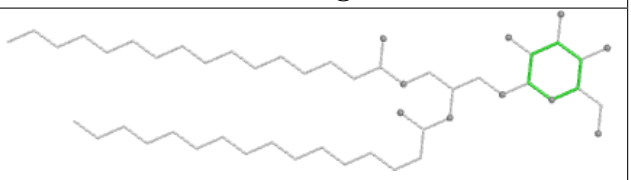
Bond lengths



Bond angles

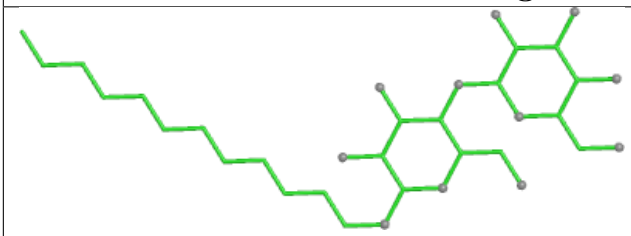


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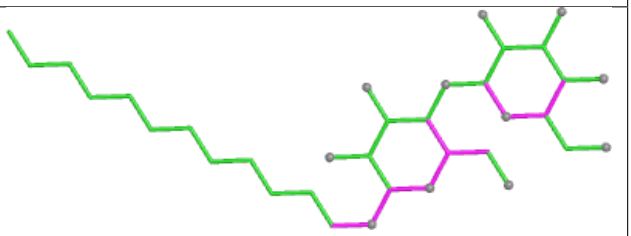


Rings

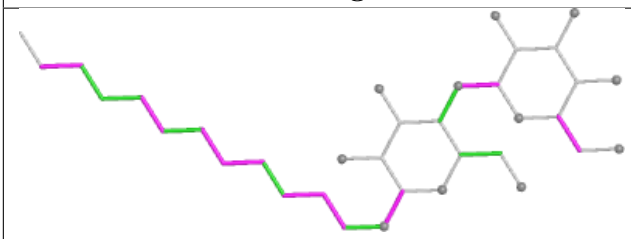
Ligand LMT a 2120



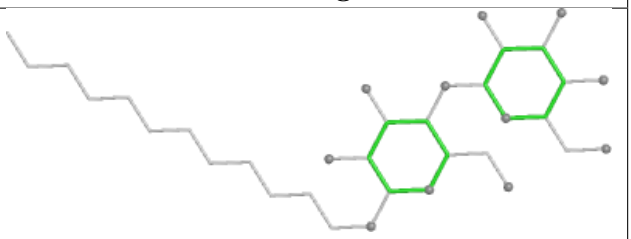
Bond lengths



Bond angles

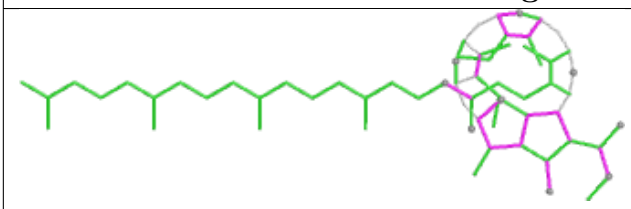


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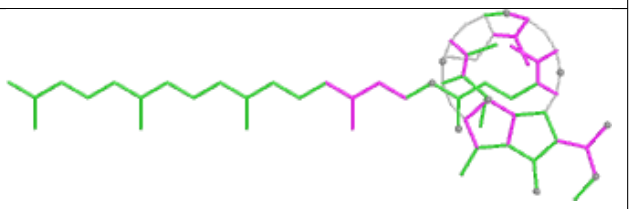


Rings

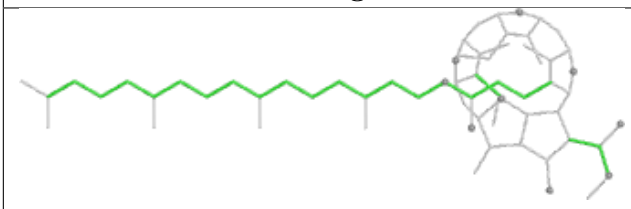
Ligand PHO A 408



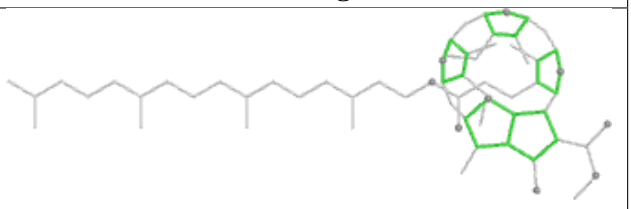
Bond lengths



Bond angles

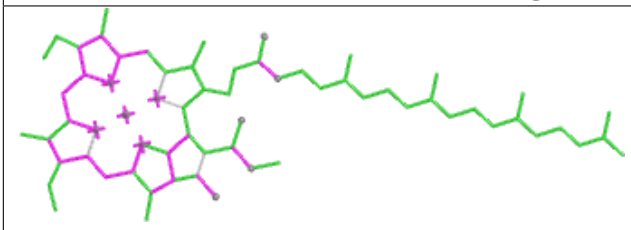


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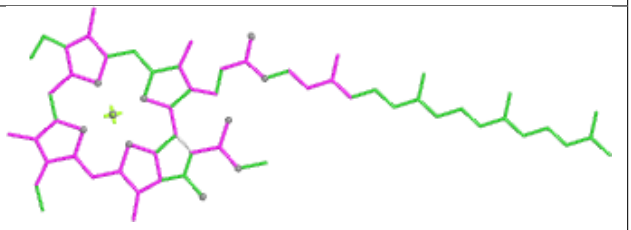


Rings

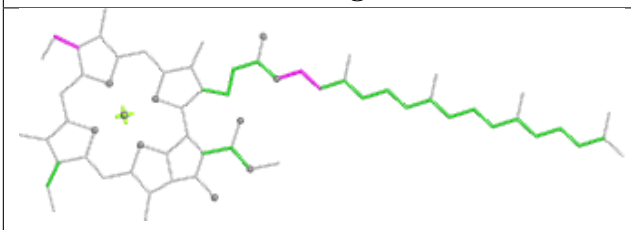
Ligand CLA d 404



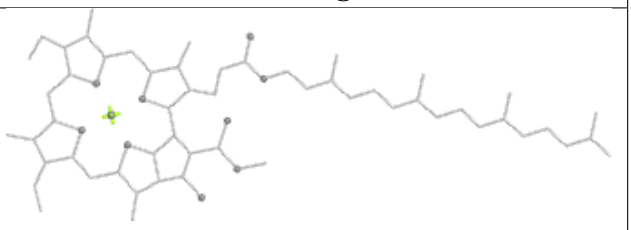
Bond lengths



Bond angles

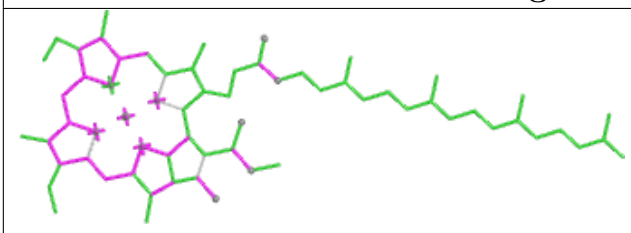


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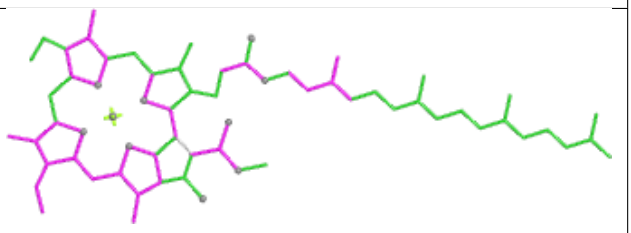


Rings

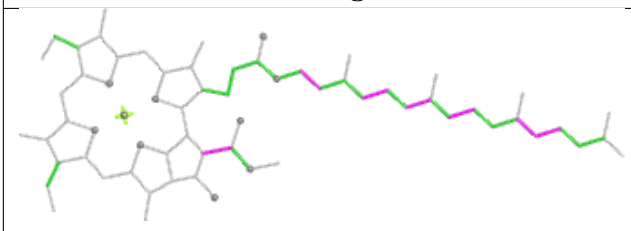
Ligand CLA c 511



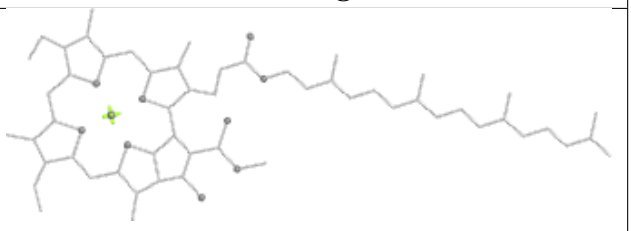
Bond lengths



Bond angles

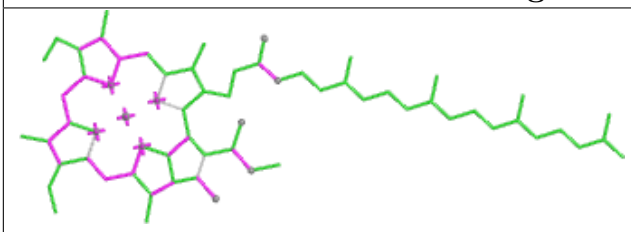


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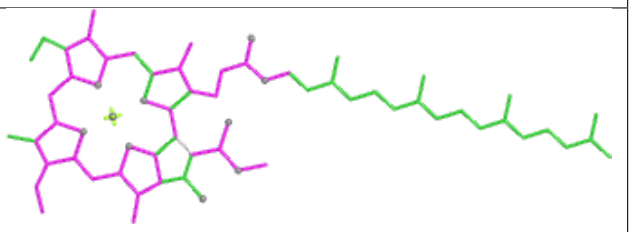


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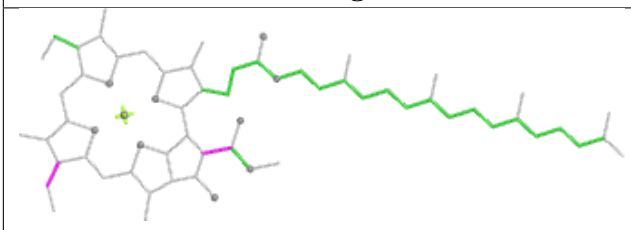
Ligand CLA d 401



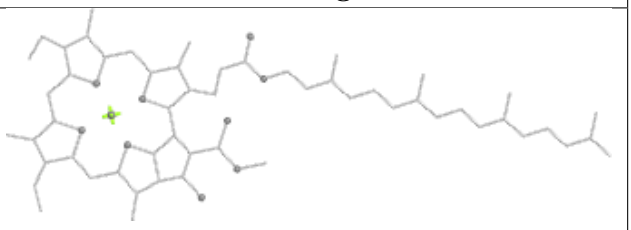
Bond lengths



Bond angles

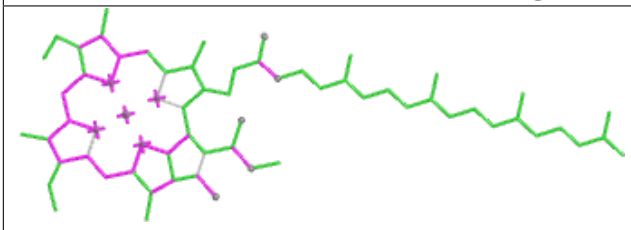


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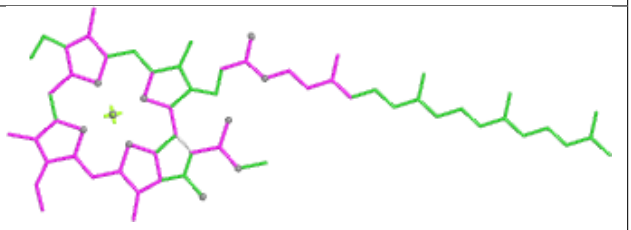


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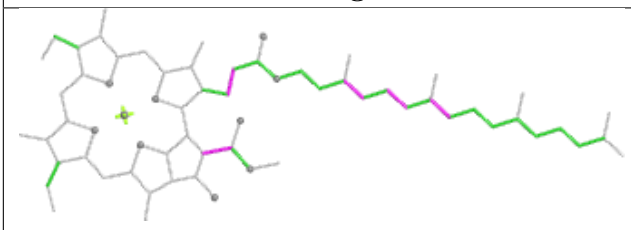
Ligand CLA c 509



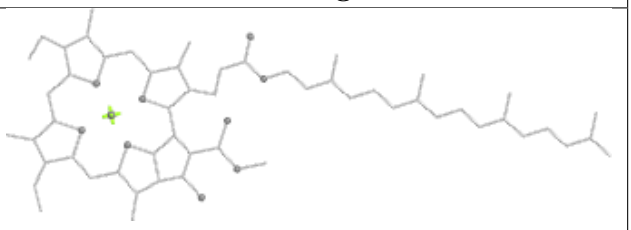
Bond lengths



Bond angles

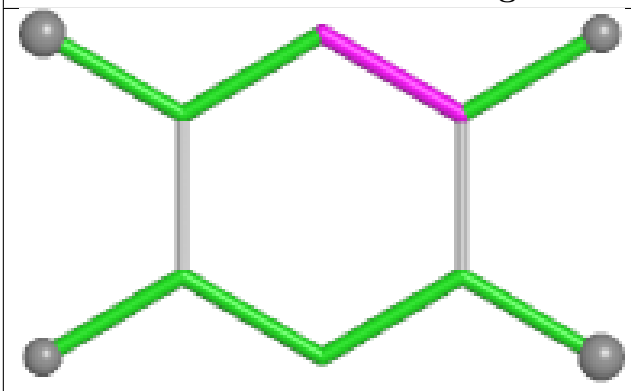


Torsions

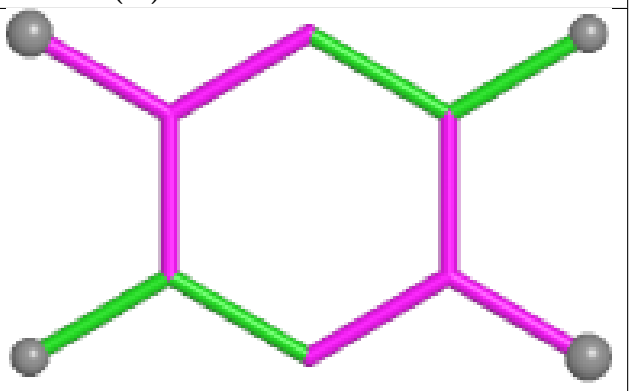


Rings

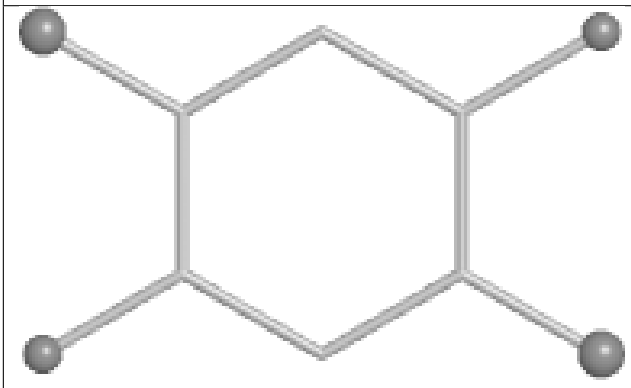
Ligand K2I A 418 (B)



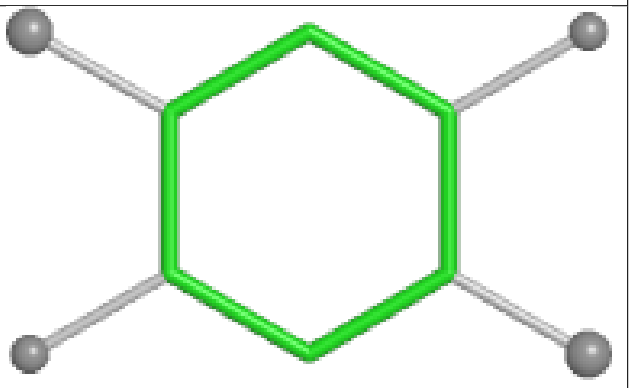
Bond lengths



Bond angles

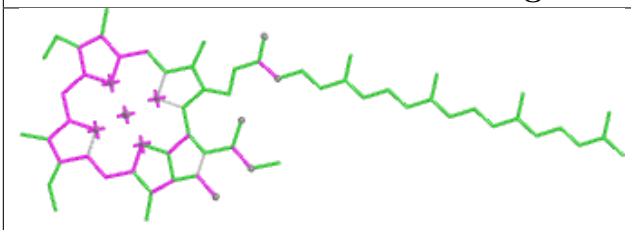


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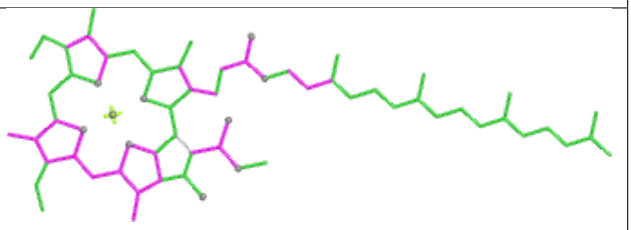


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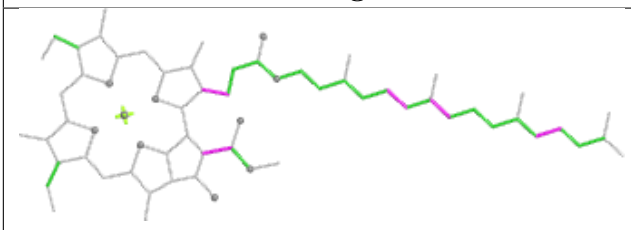
Ligand CLA C 509



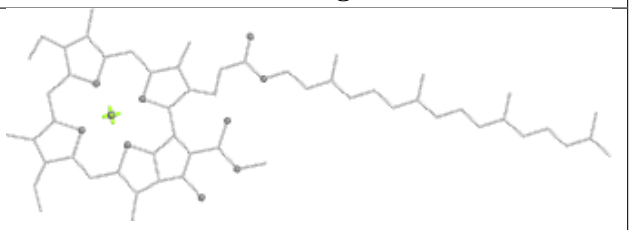
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Bond angles

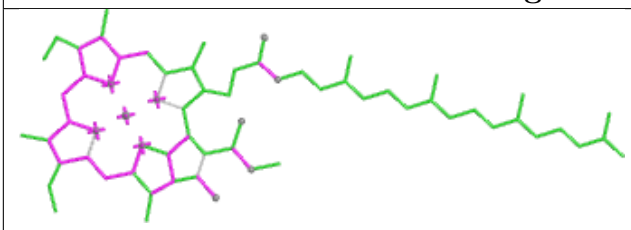


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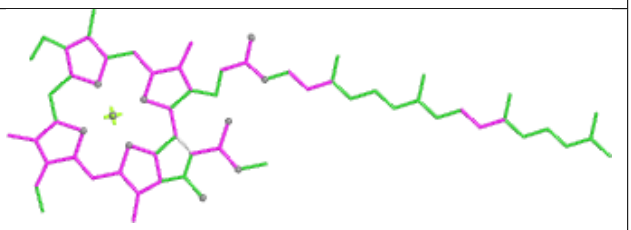


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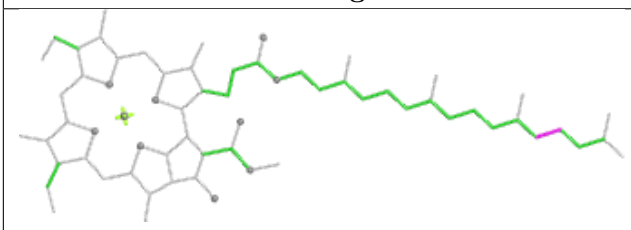
Ligand CLA B 609



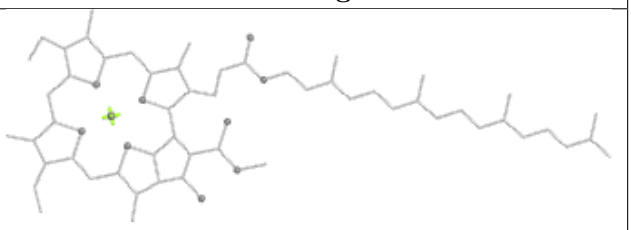
Bond lengths



Bond angles

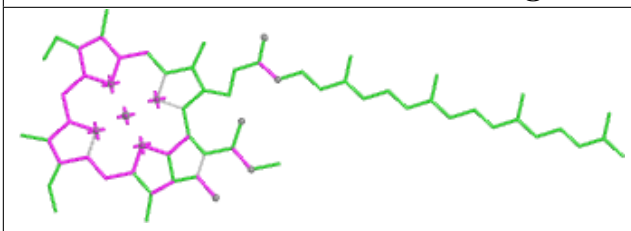


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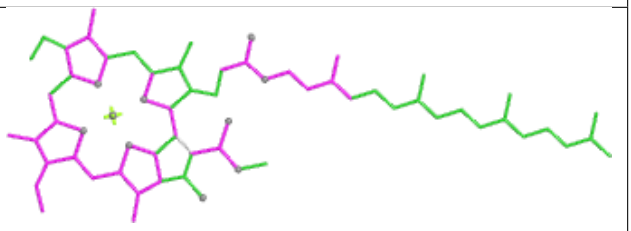


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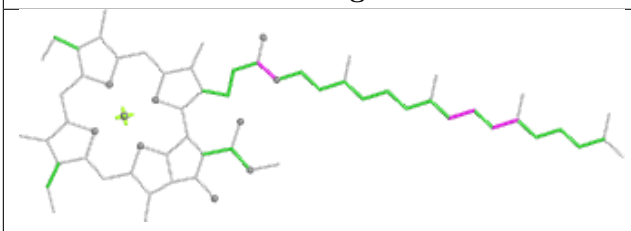
Ligand CLA C 512



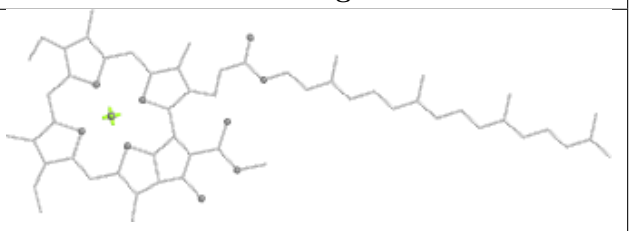
Bond lengths



Bond angles

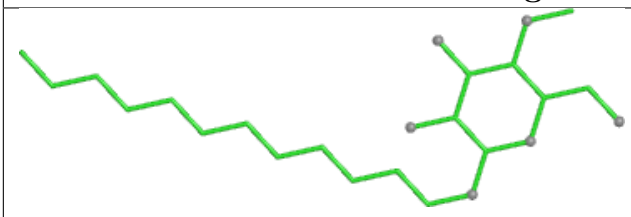


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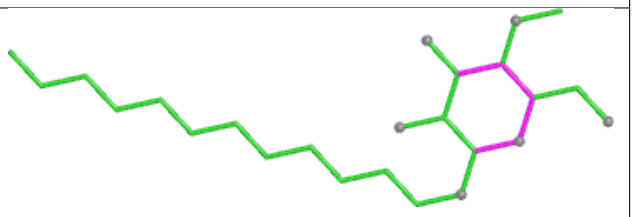


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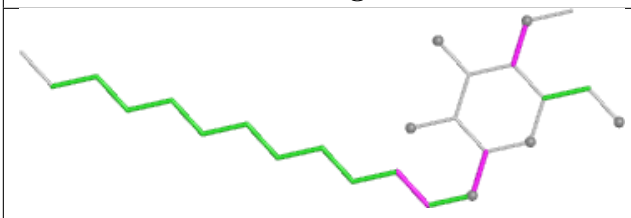
Ligand LMT b 624



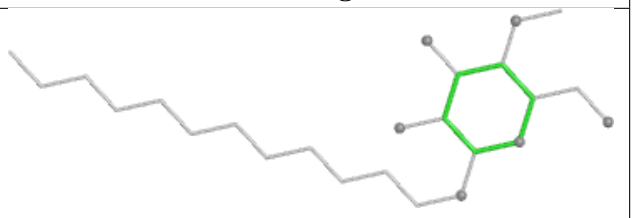
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Bond angles

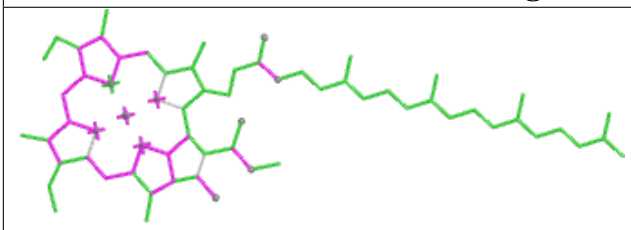


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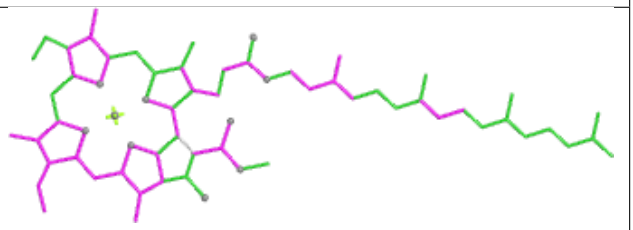


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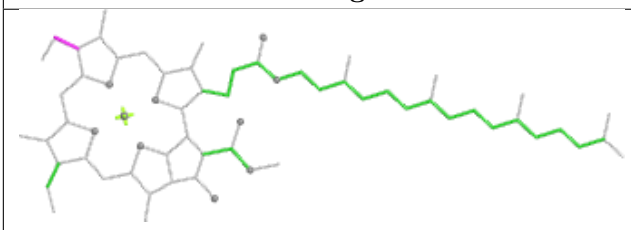
Ligand CLA C 514



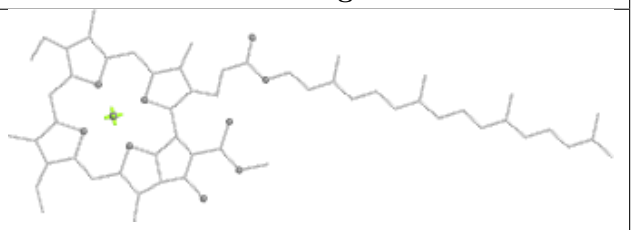
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Bond angles

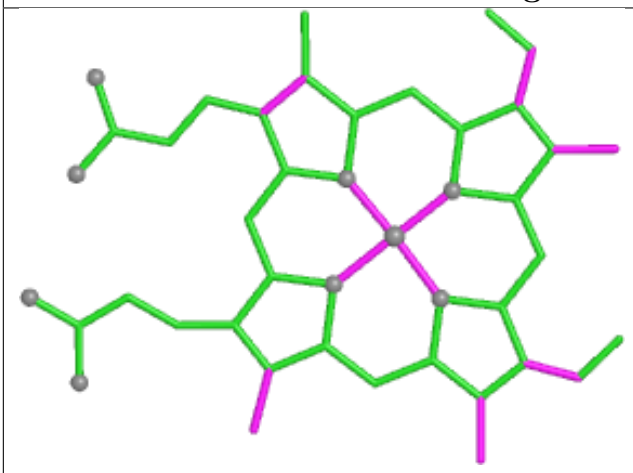


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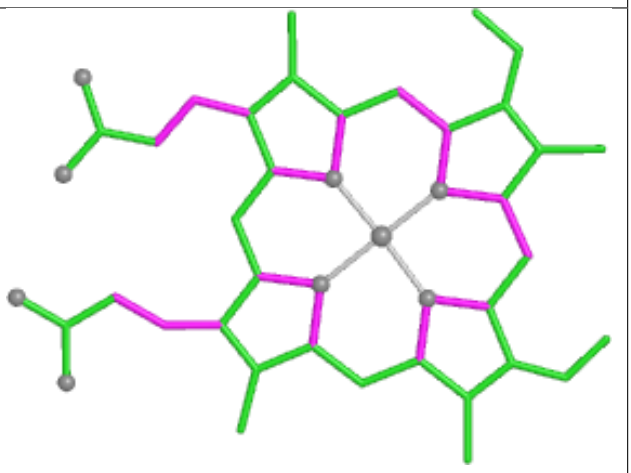


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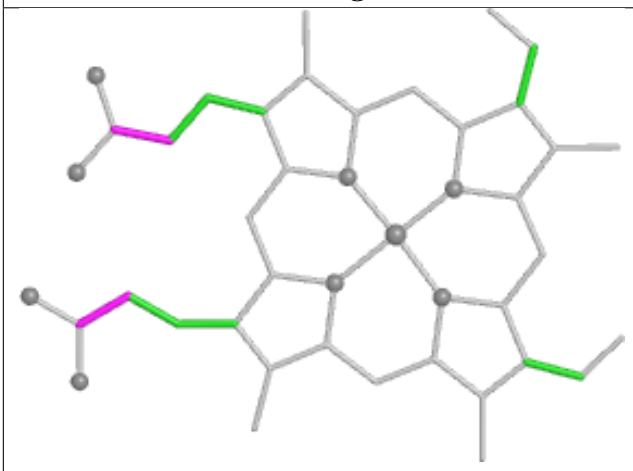
Ligand HEM e 103



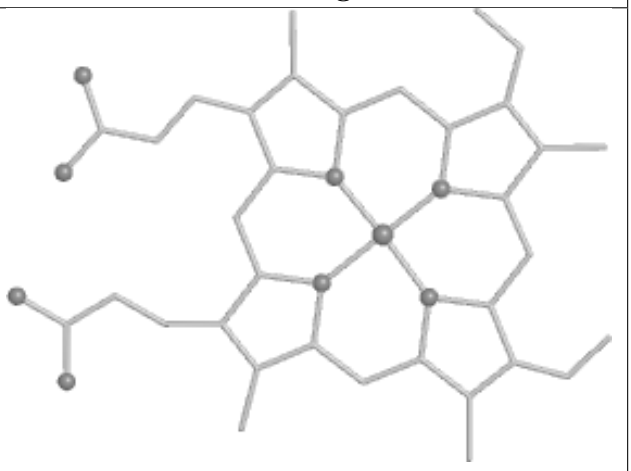
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Bond angles

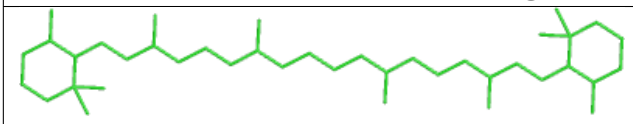


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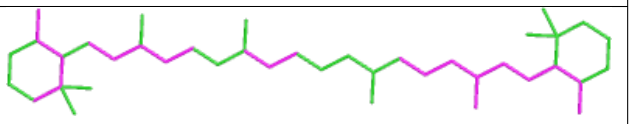


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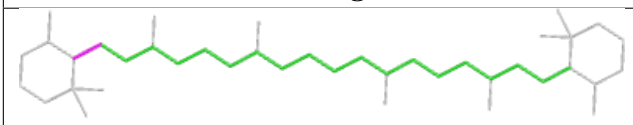
Ligand BCR C 516



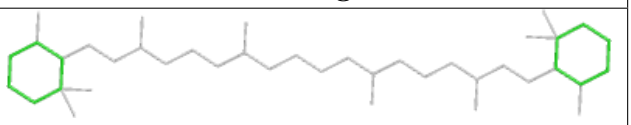
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Bond angles

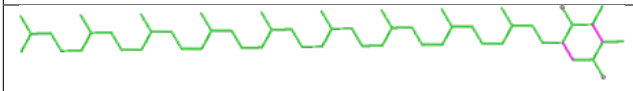


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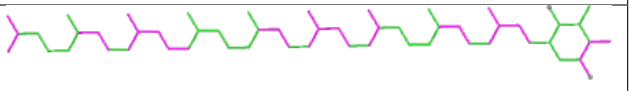


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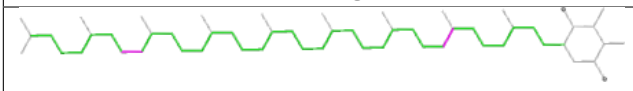
Ligand PL9 D 407



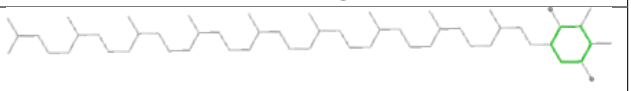
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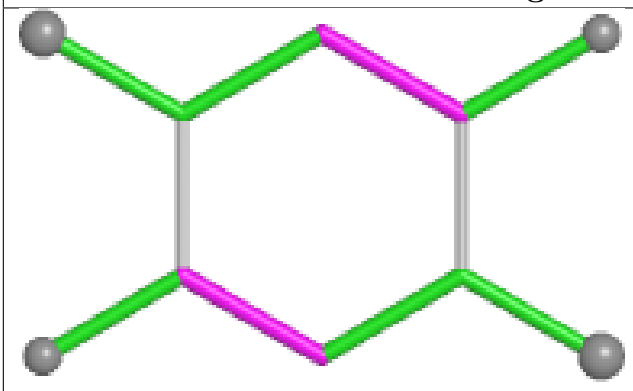


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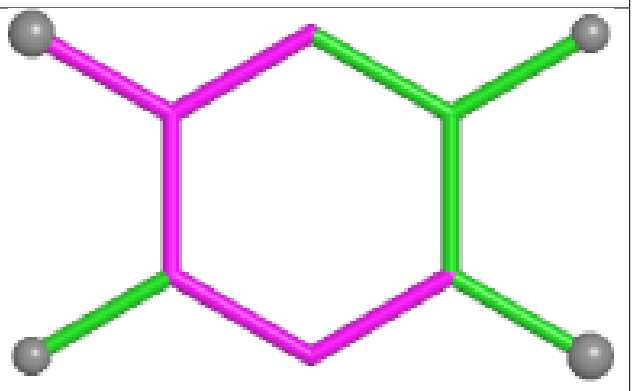


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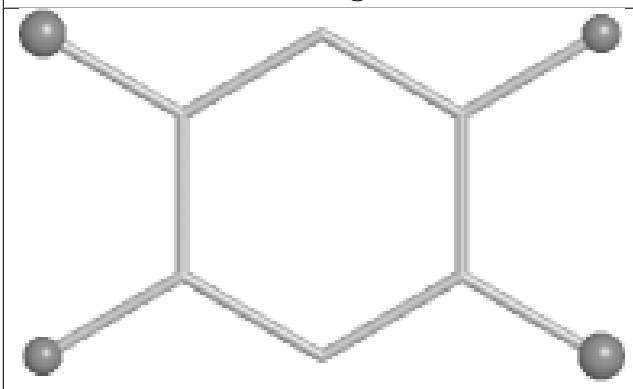
Ligand K2I a 2119



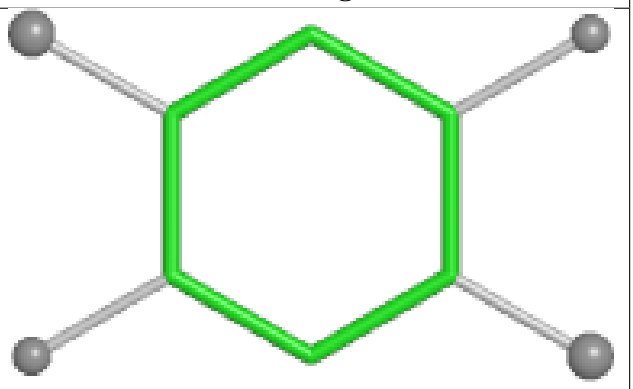
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Bond angles

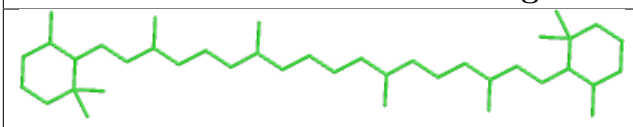


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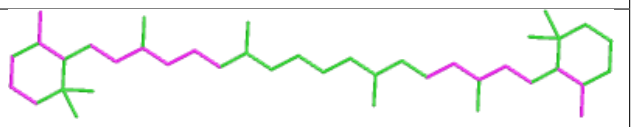


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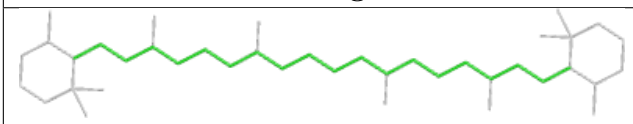
Ligand BCR K 101



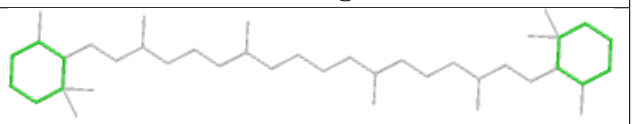
Bond lengths



Bond angles

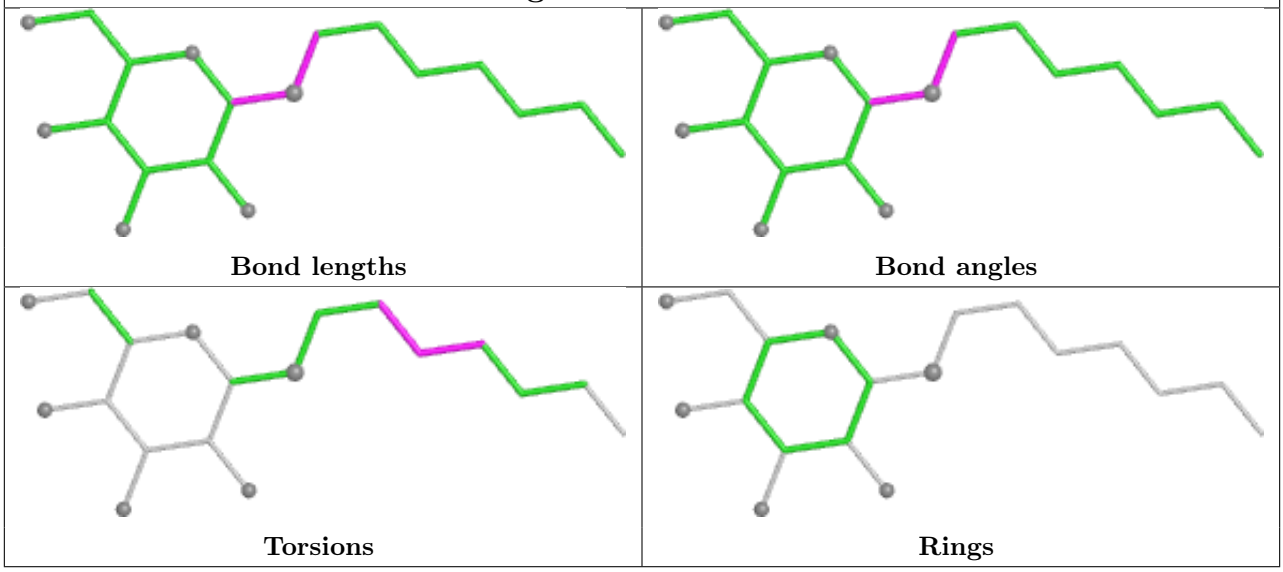


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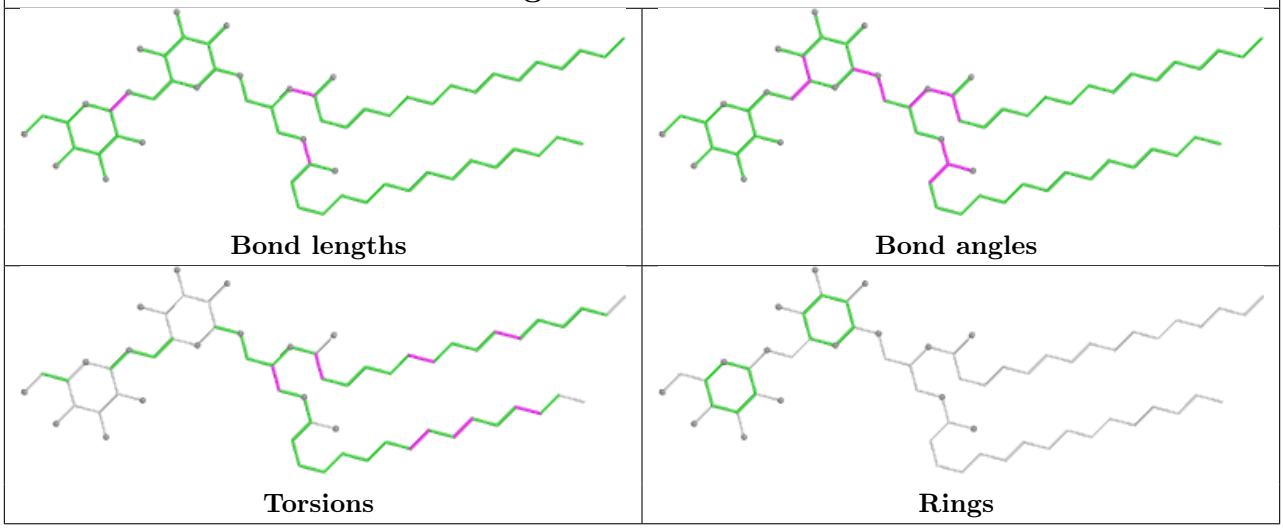


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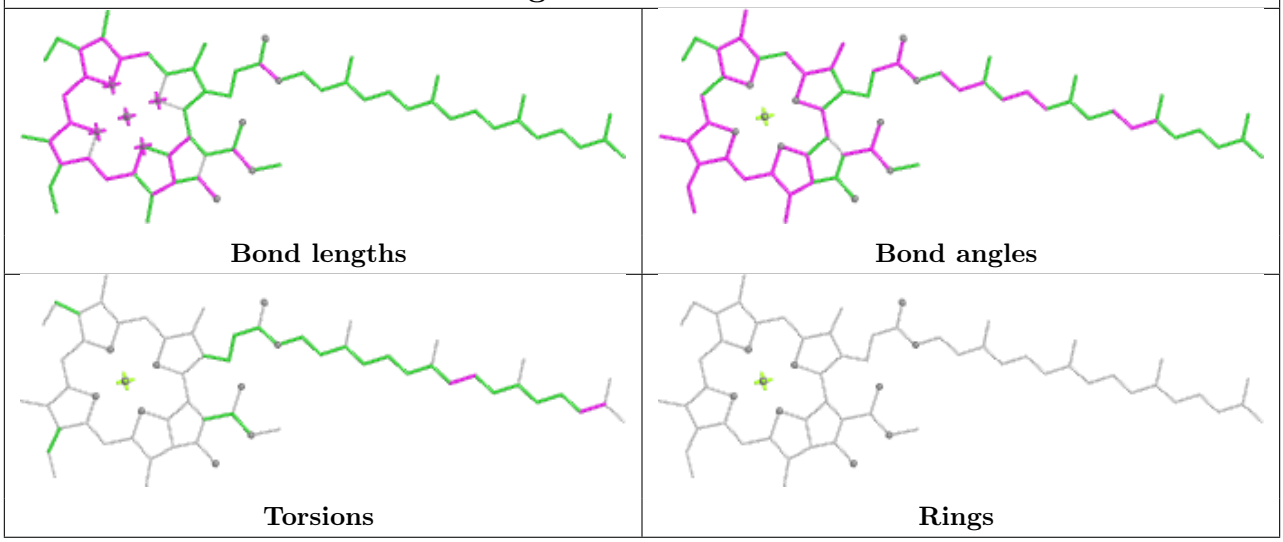
Ligand HTG c 526



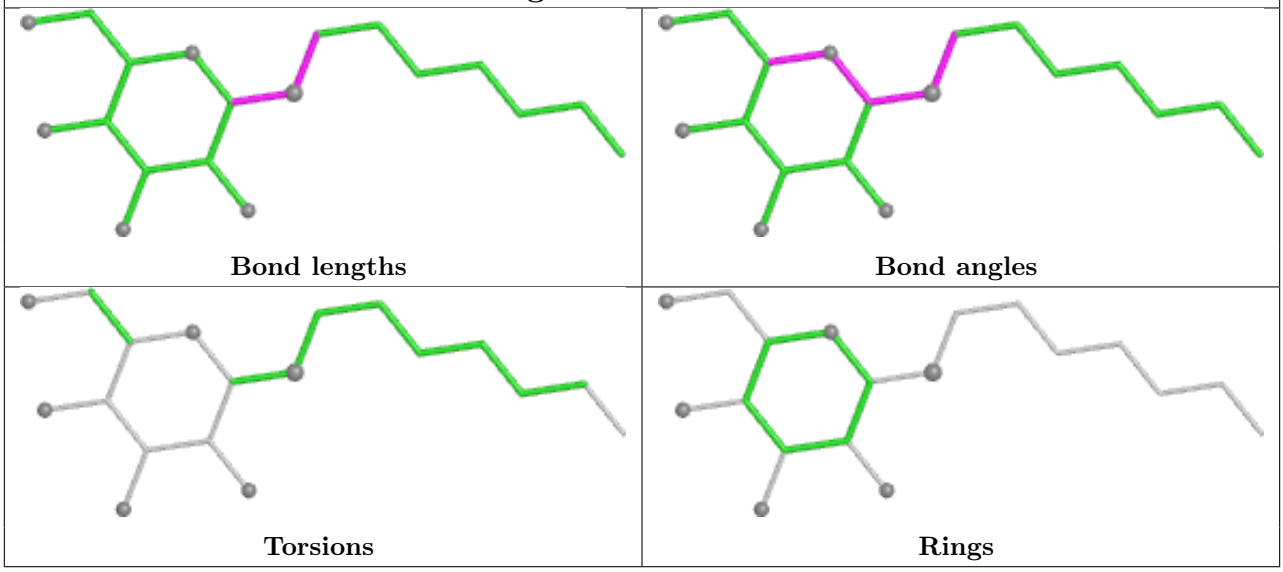
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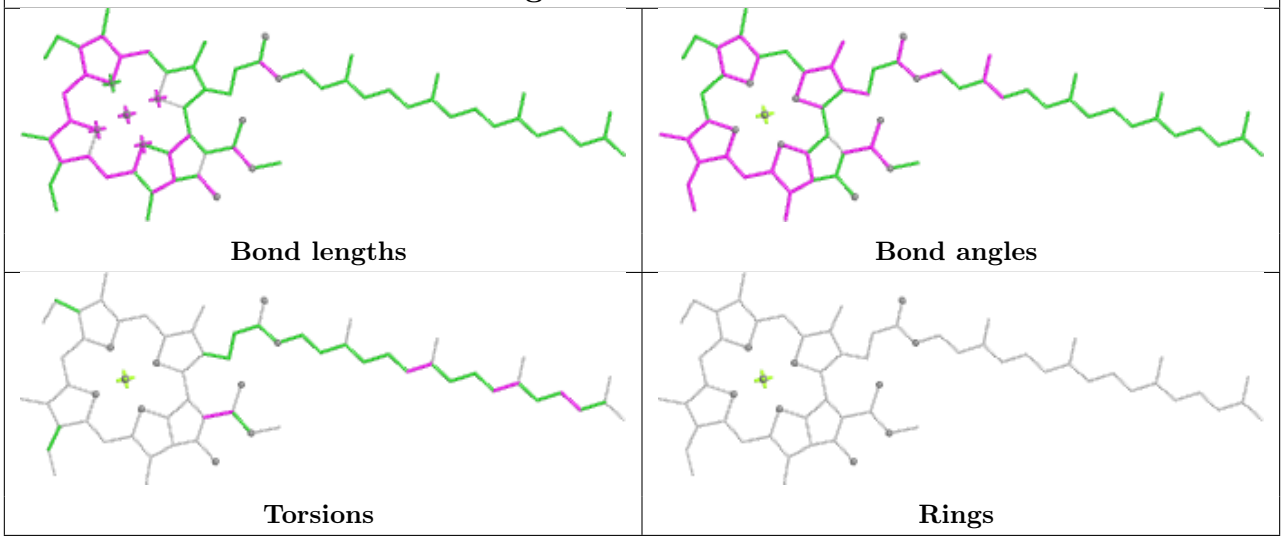
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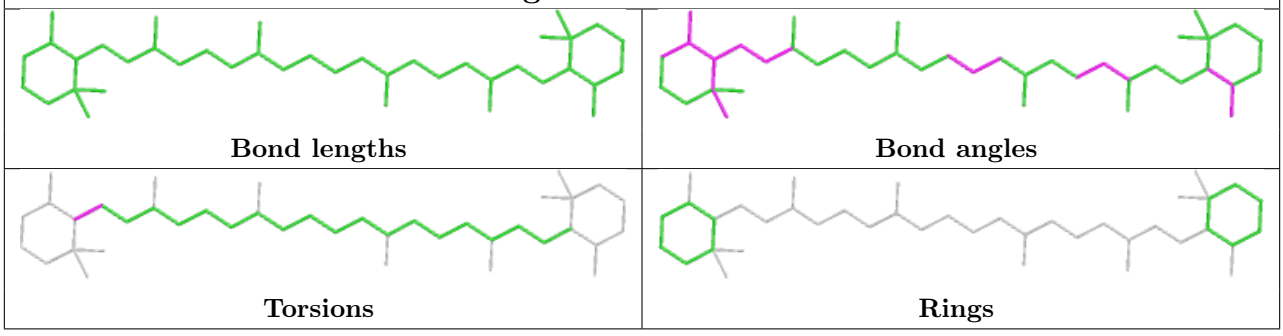
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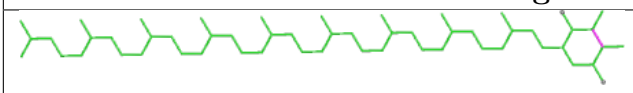
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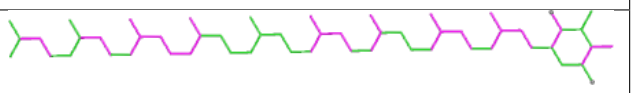
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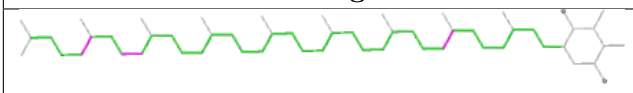
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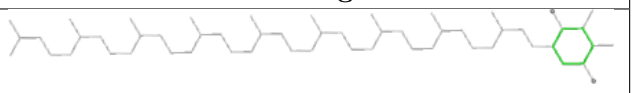
Bond lengths



Bond angles

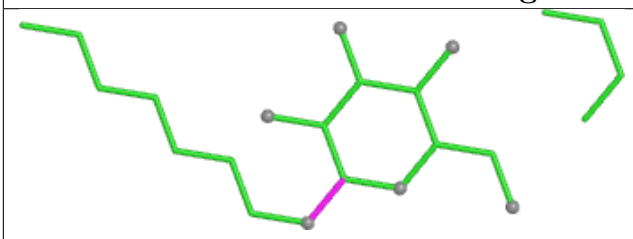


Torsions

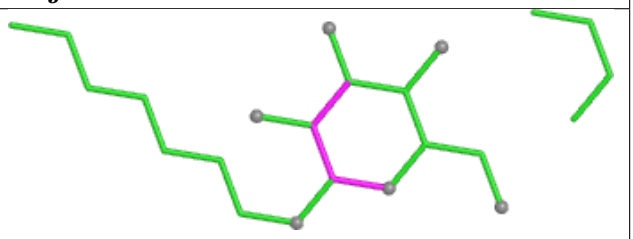


Rings

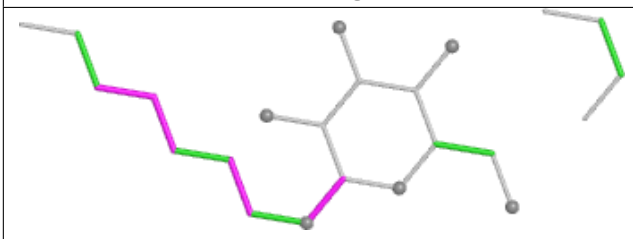
Ligand LMT j 1601



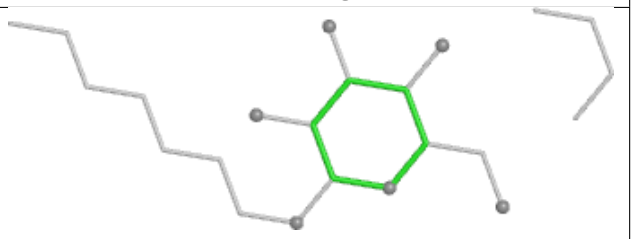
Bond lengths



Bond angles

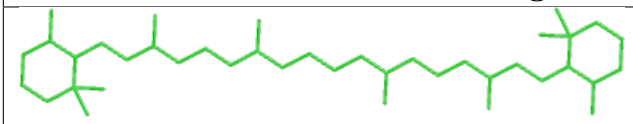


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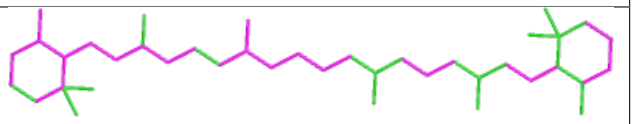


Rings

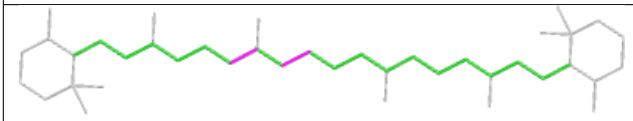
Ligand BCR t 102



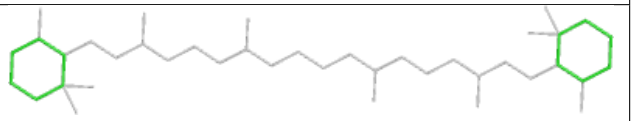
Bond lengths



Bond angles

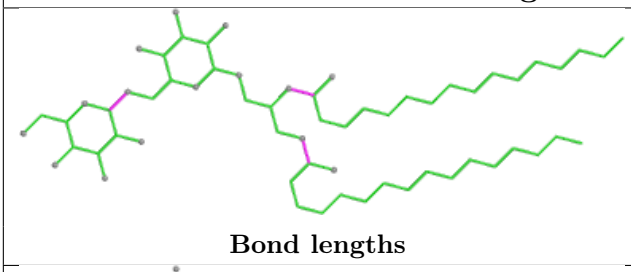


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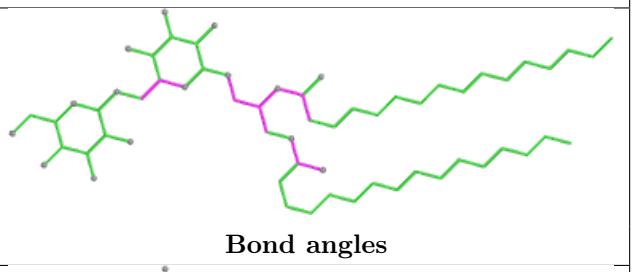


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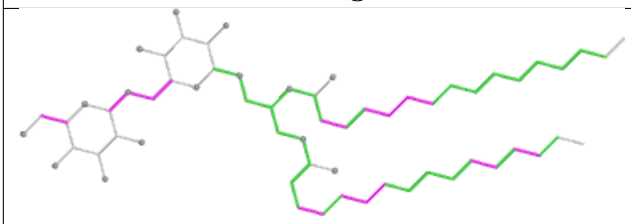
Ligand DGD C 517



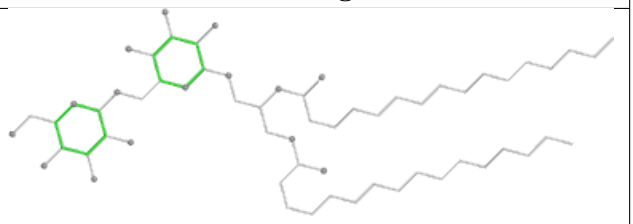
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Bond angles

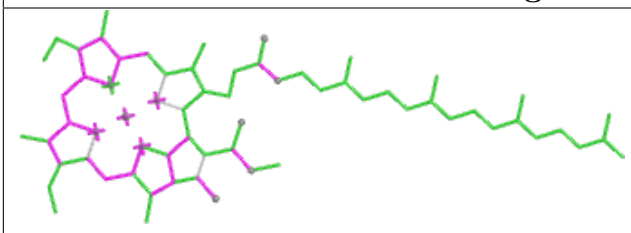


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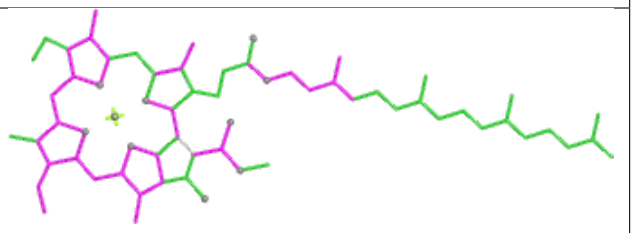


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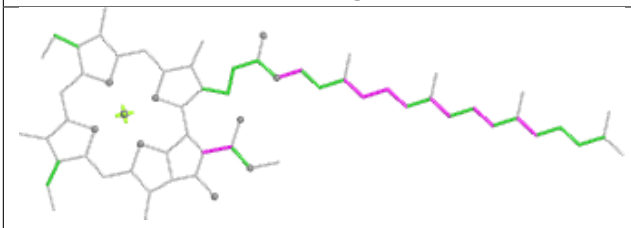
Ligand CLA B 617



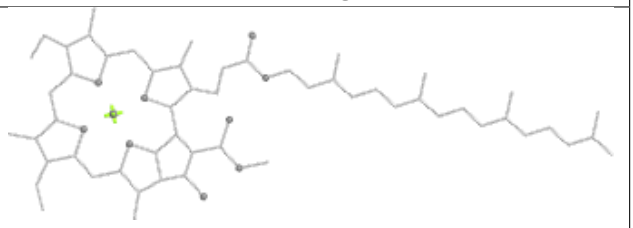
Bond lengths



Bond angles

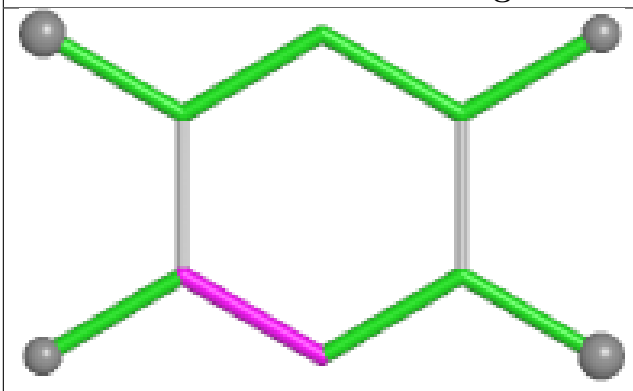


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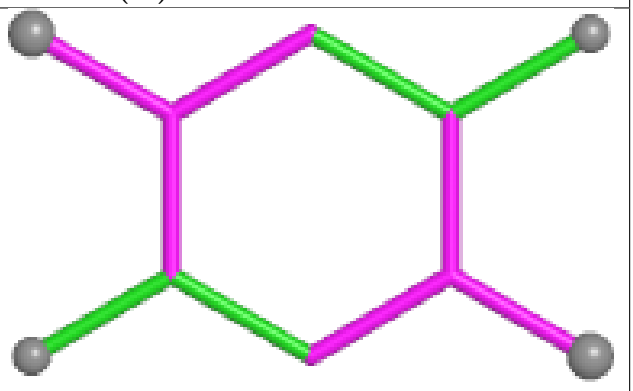


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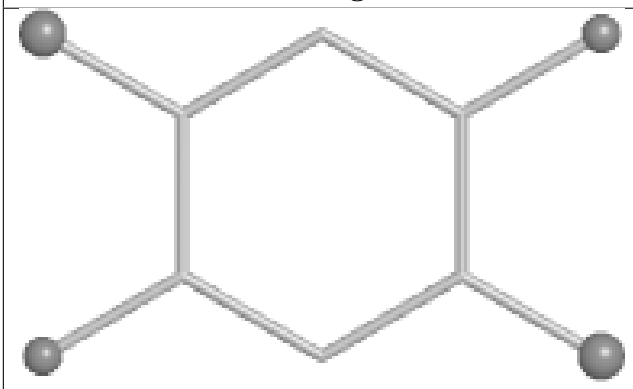
Ligand K2I a 2118 (A)



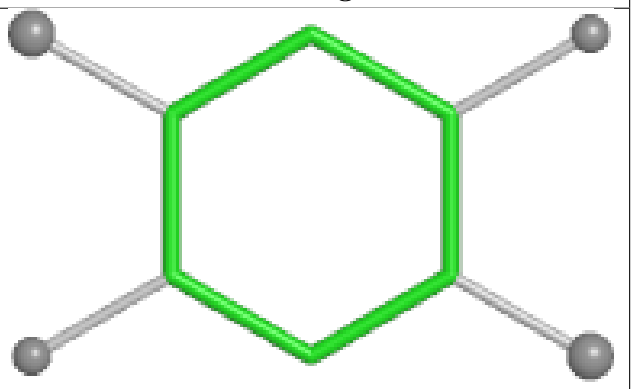
Bond lengths



Bond angles

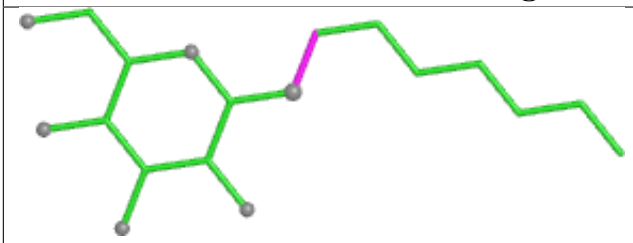


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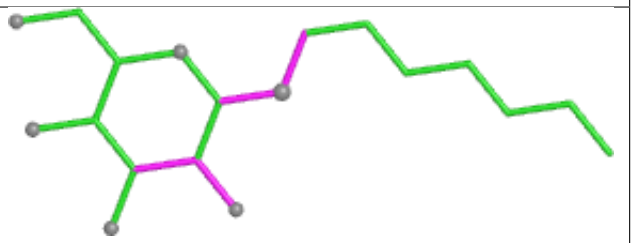


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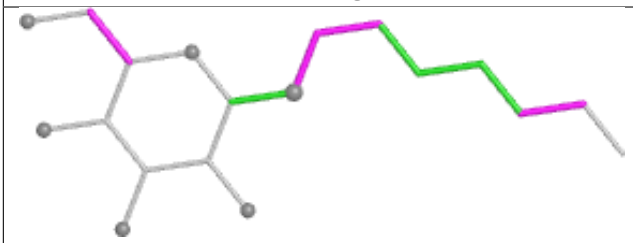
Ligand HTG O 302



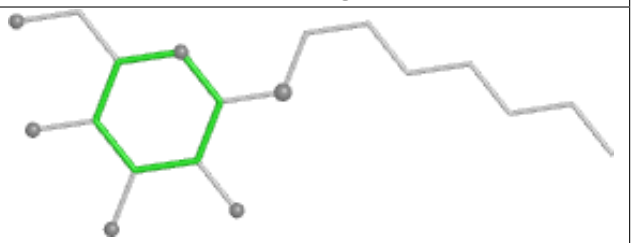
Bond lengths



Bond angles

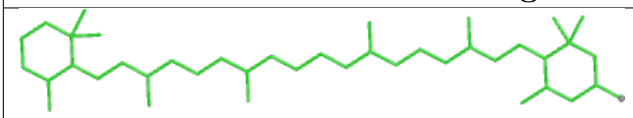


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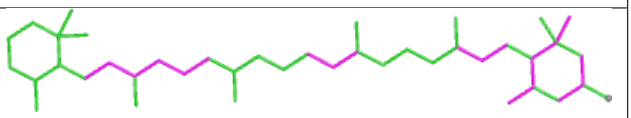


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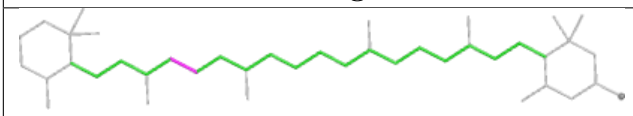
Ligand RRX H 101



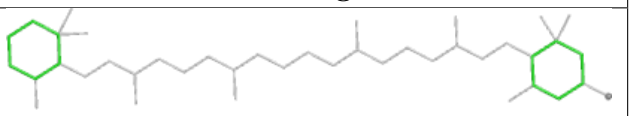
Bond lengths



Bond angles

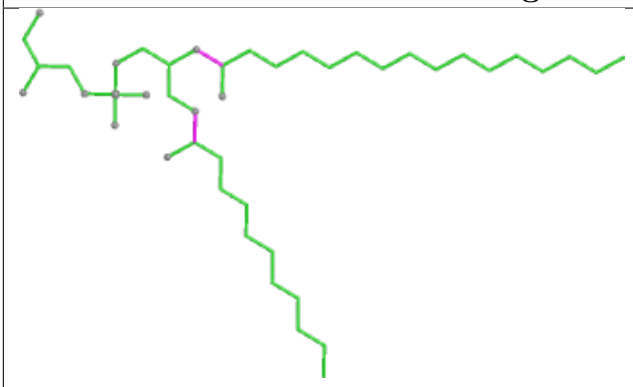


Torsions



Rings

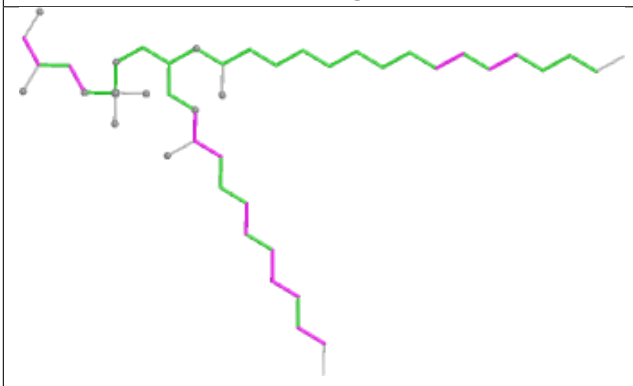
Ligand LHG D 411



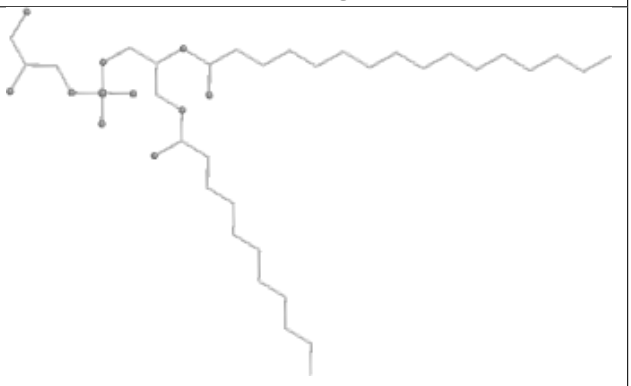
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Bond angles

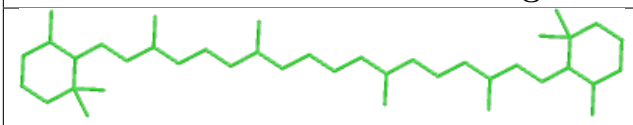


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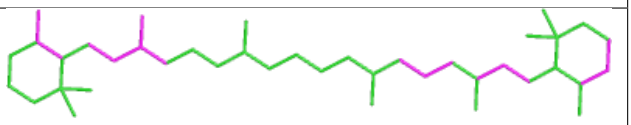


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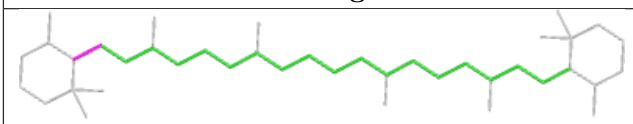
Ligand BCR B 618



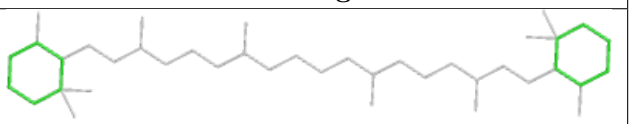
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Bond angles

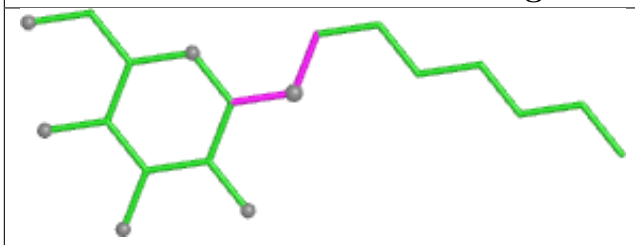


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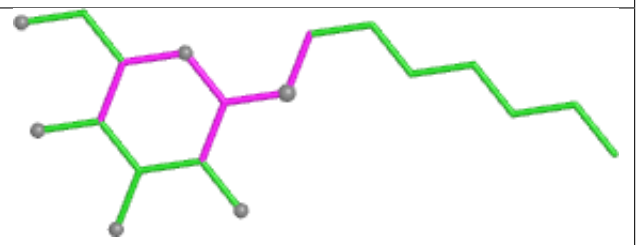


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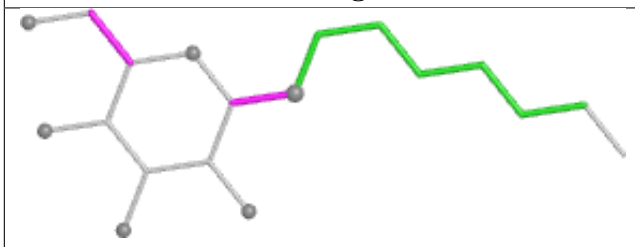
Ligand HTG b 602



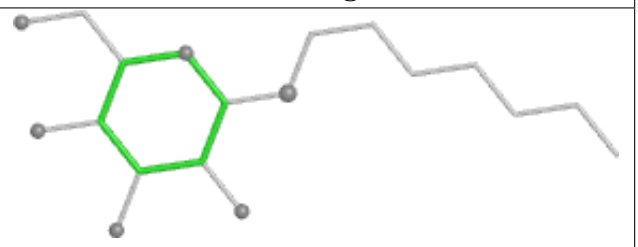
Bond lengths



Bond angles

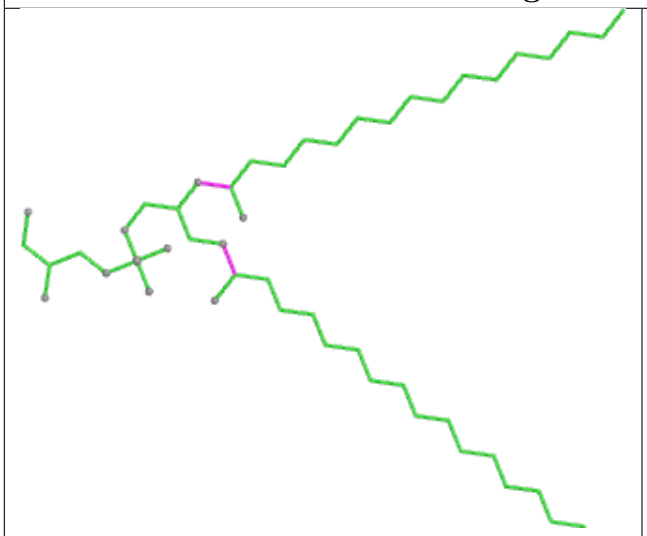


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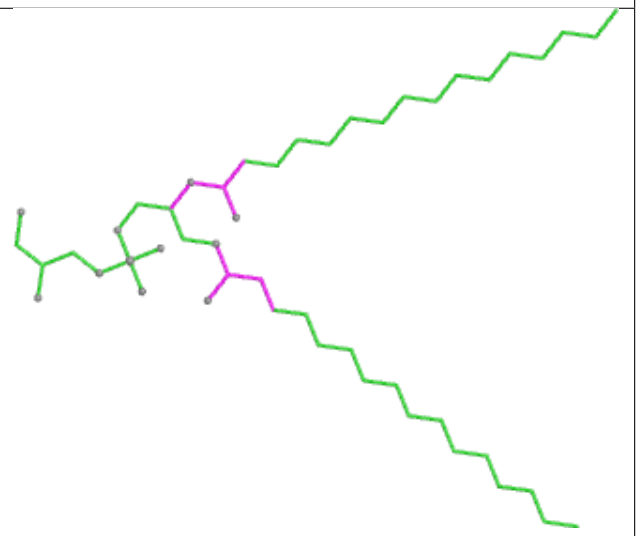


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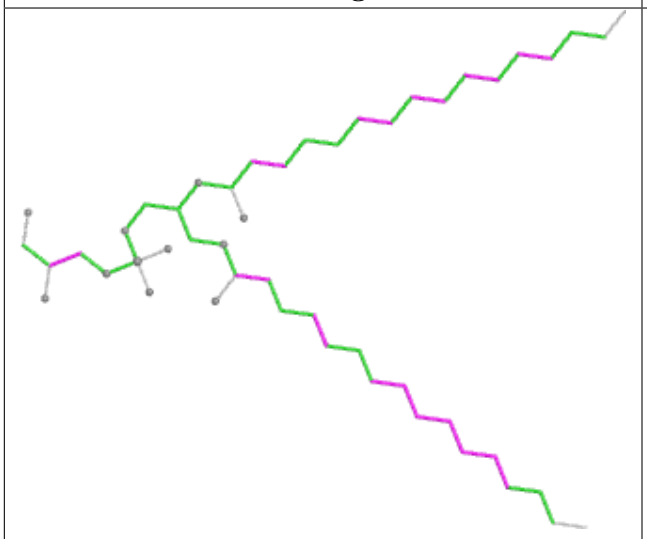
Ligand LHG D 409



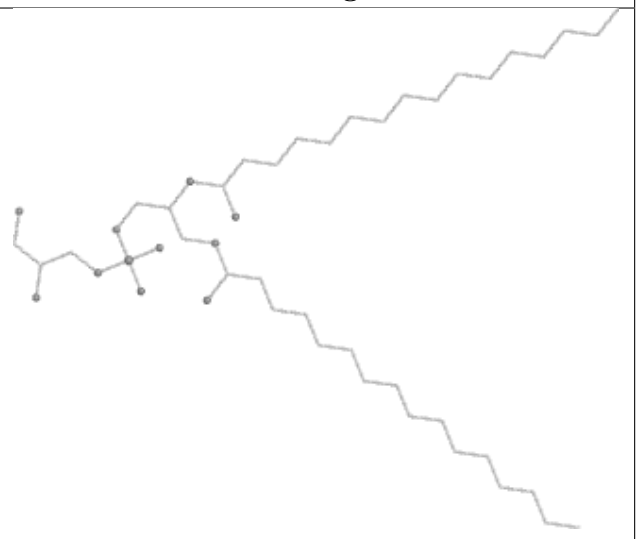
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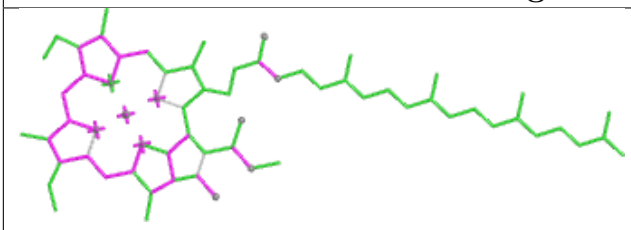


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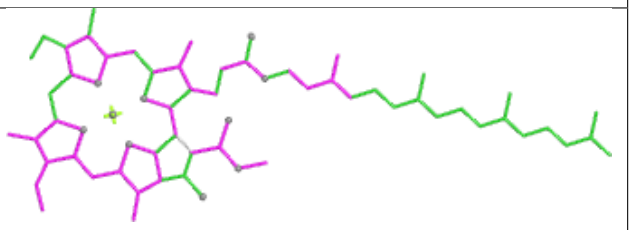


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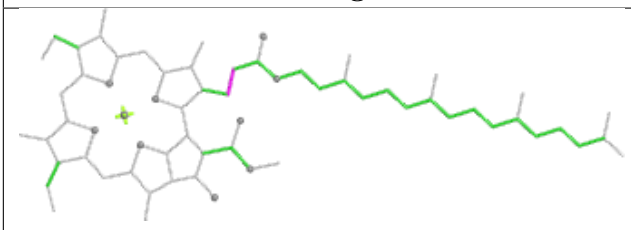
Ligand CLA b 605



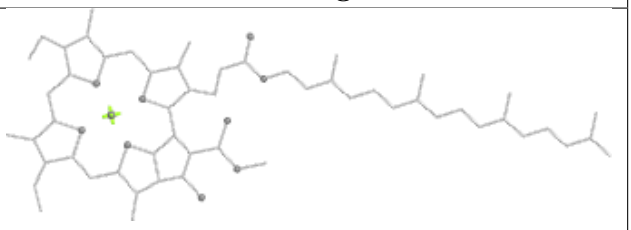
Bond lengths



Bond angles

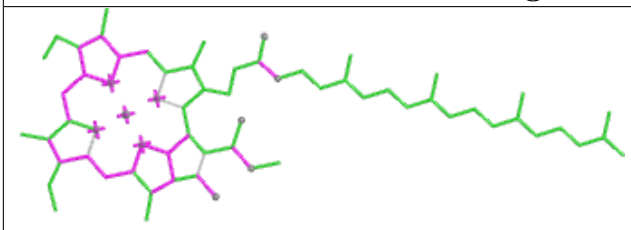


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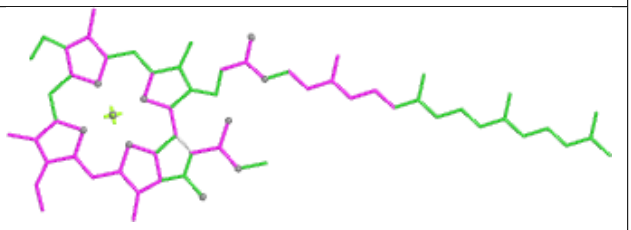


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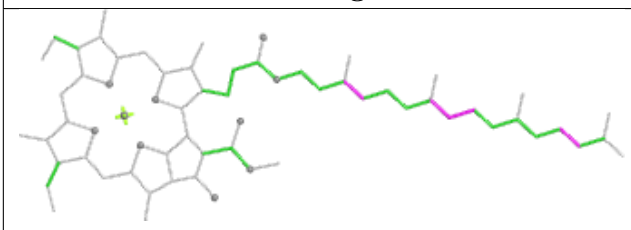
Ligand CLA B 612



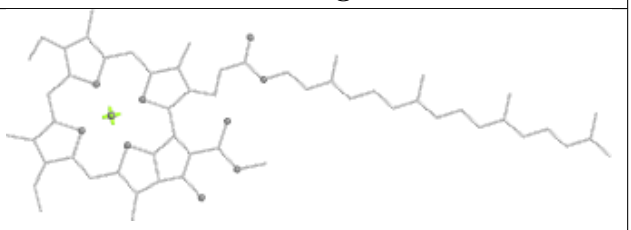
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Bond angles

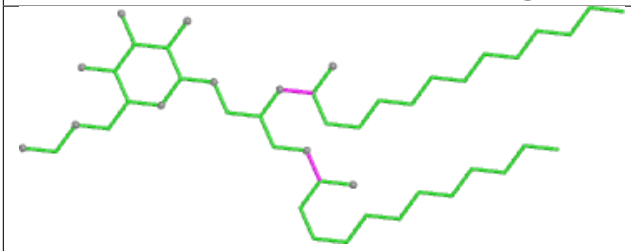


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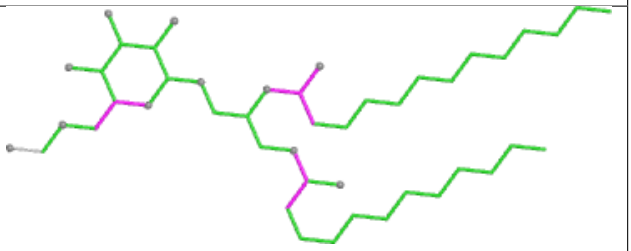


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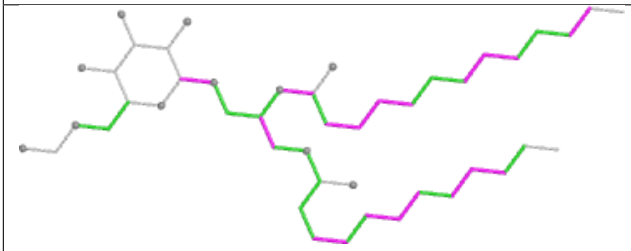
Ligand DGD D 408



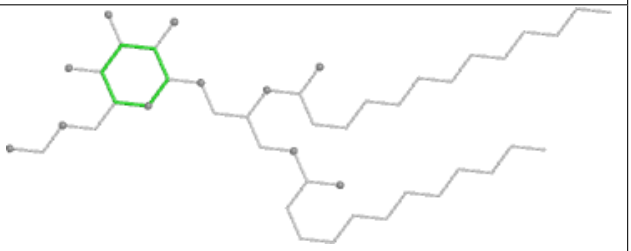
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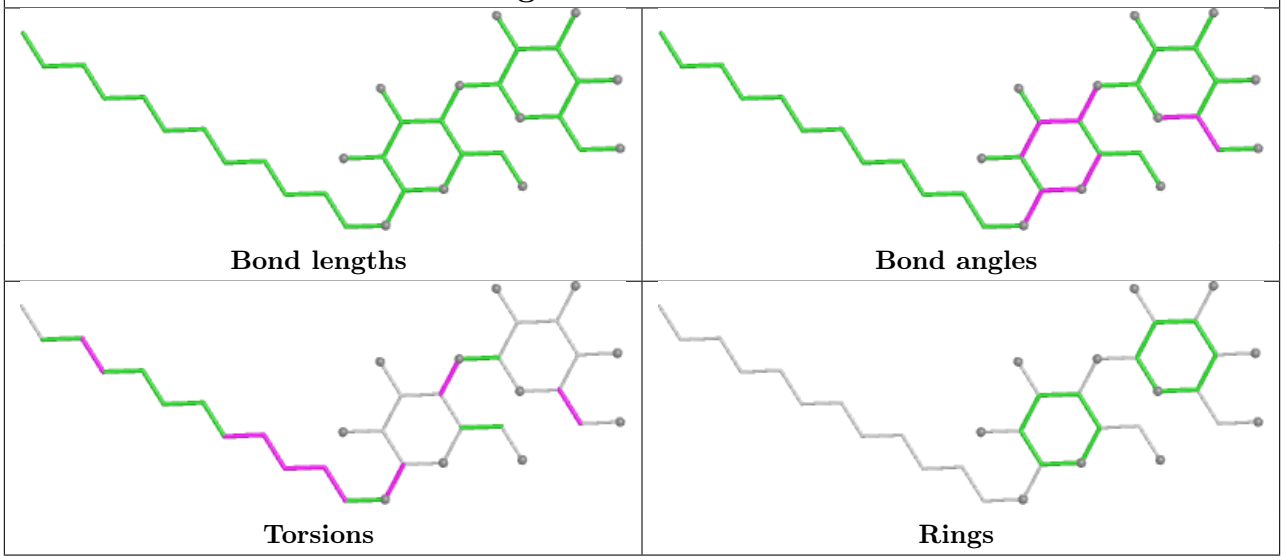


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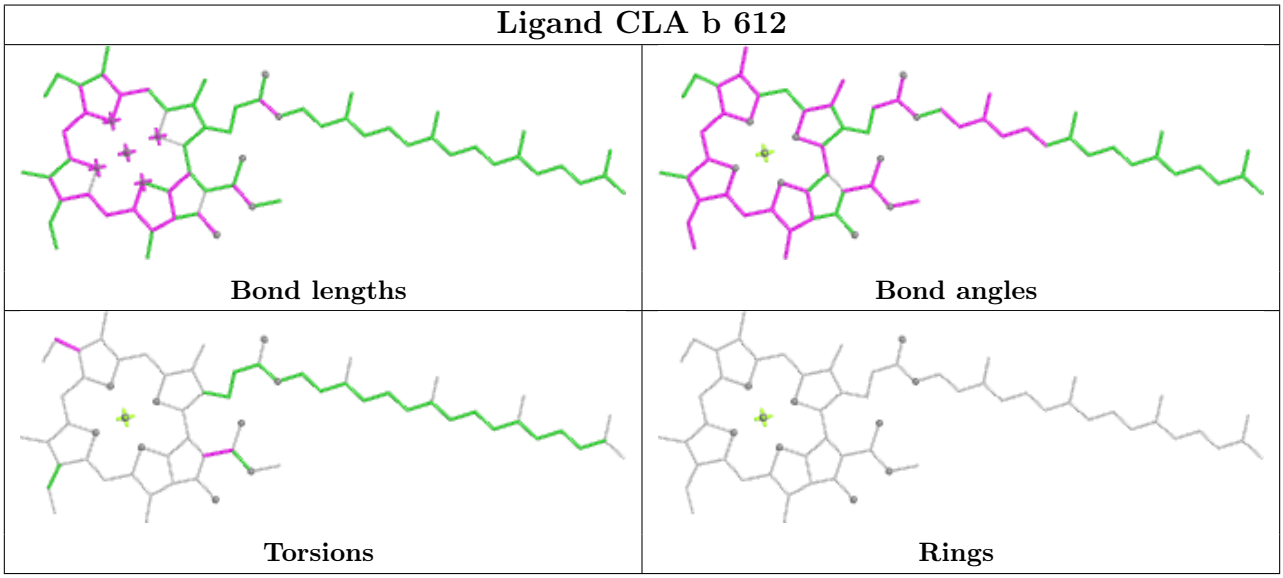


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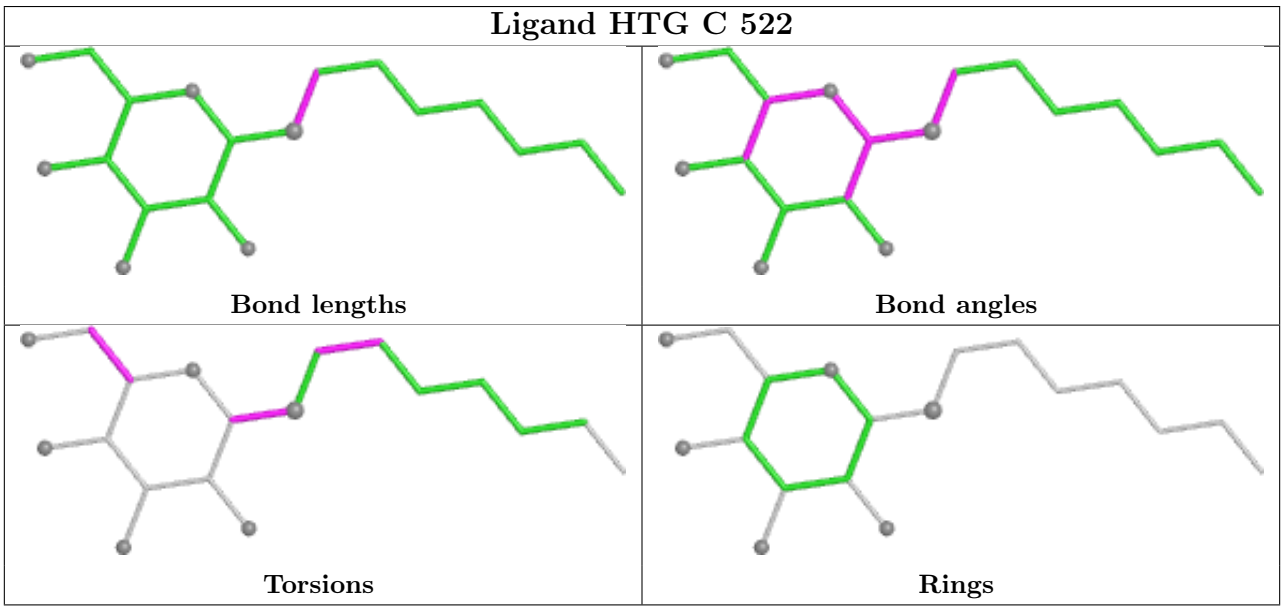
Ligand LMT a 2103



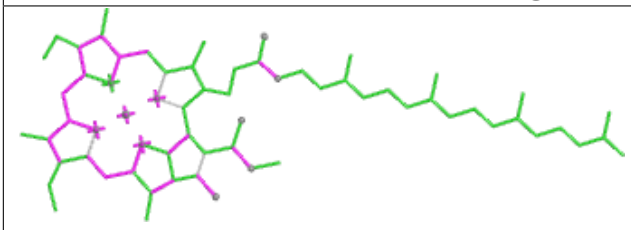
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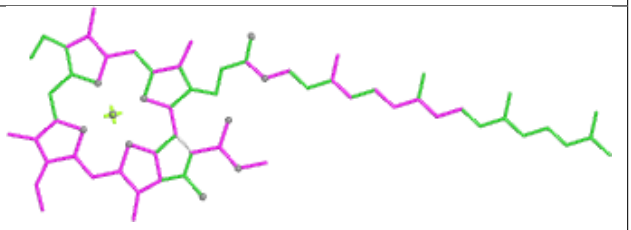
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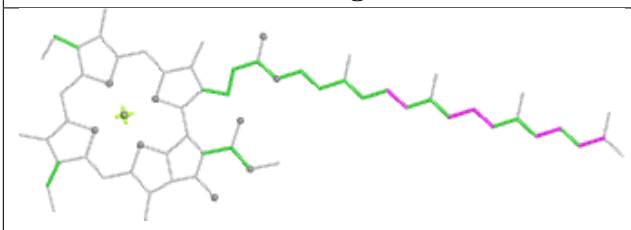
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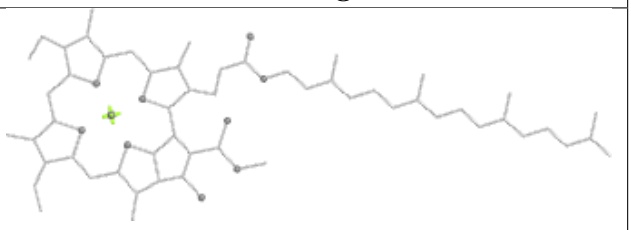
Bond lengths



Bond angles

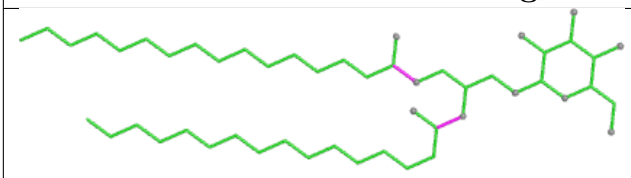


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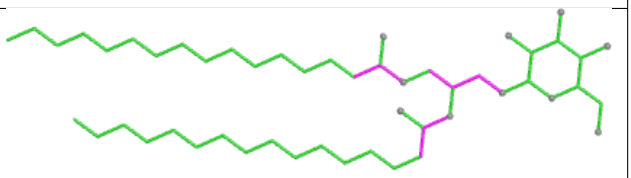


Rings

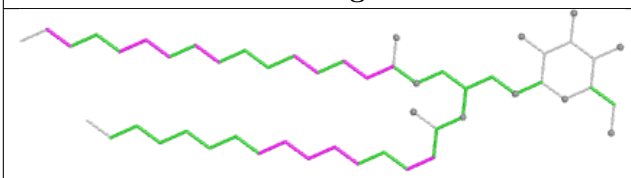
Ligand LMG B 622



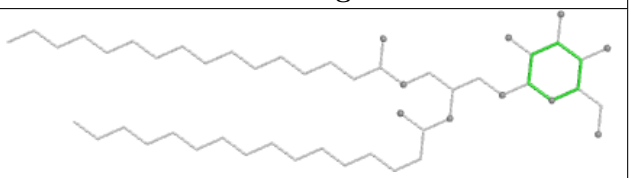
Bond lengths



Bond angles



Torsions

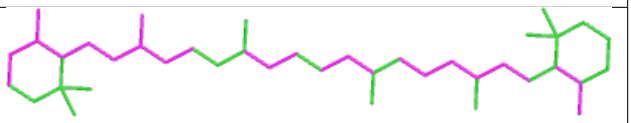


Rings

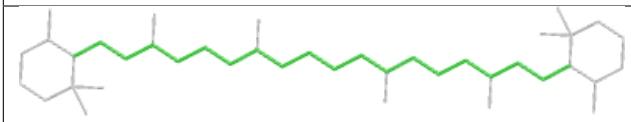
Ligand BCR k 2003



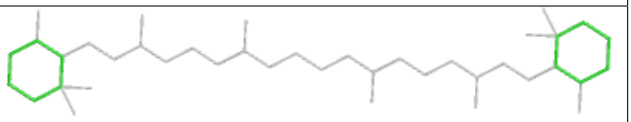
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Bond angles

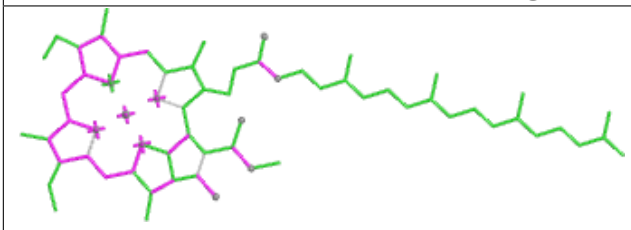


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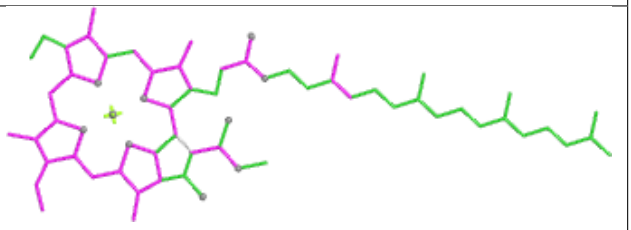


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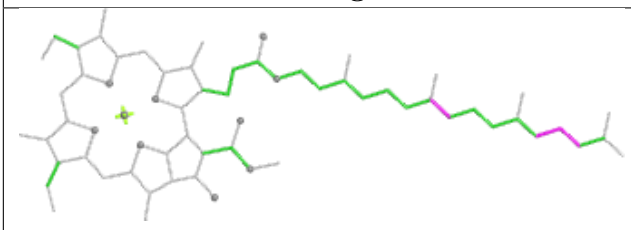
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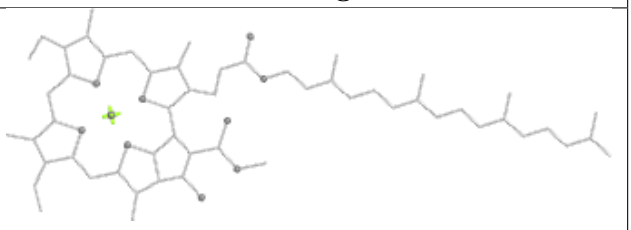
Bond lengths



Bond angles

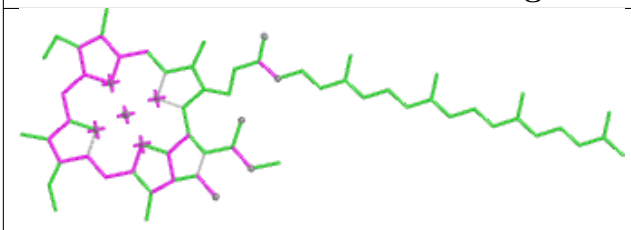


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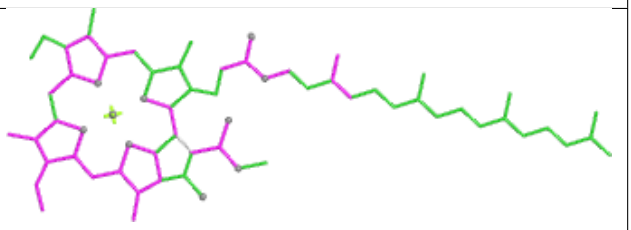


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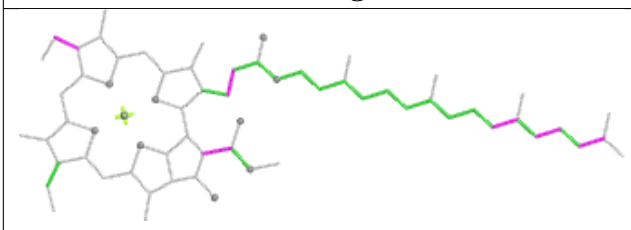
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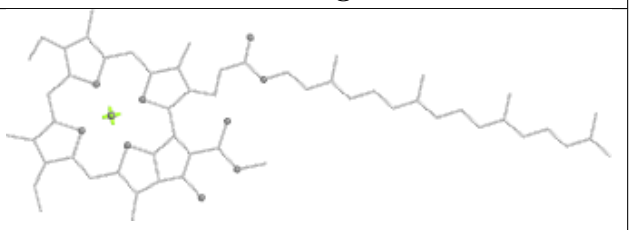
Bond lengths



Bond angles

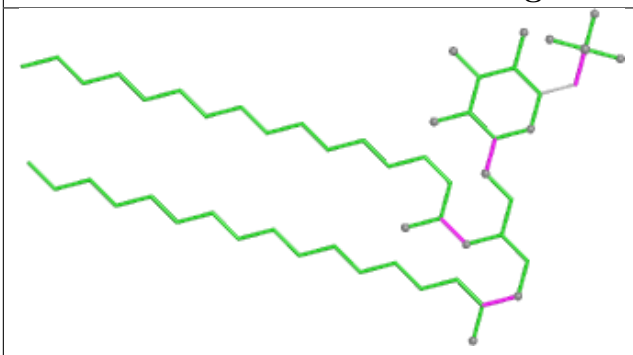


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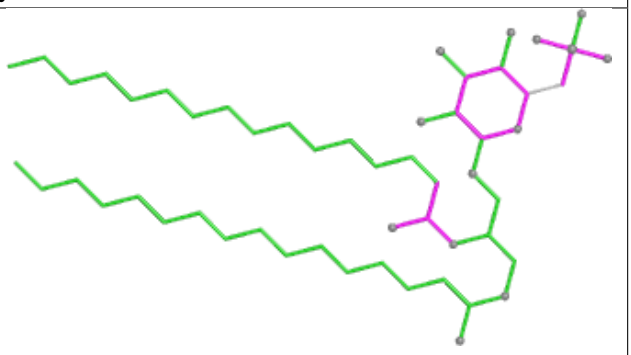


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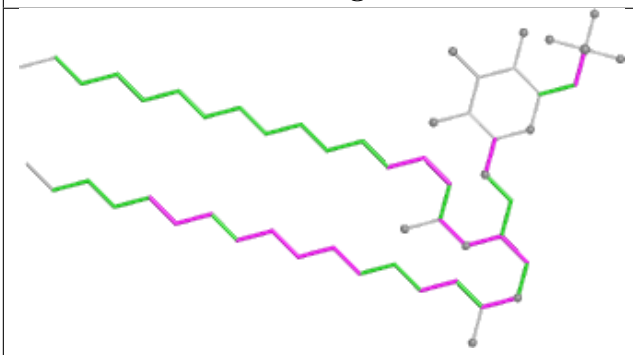
Ligand SQD B 621



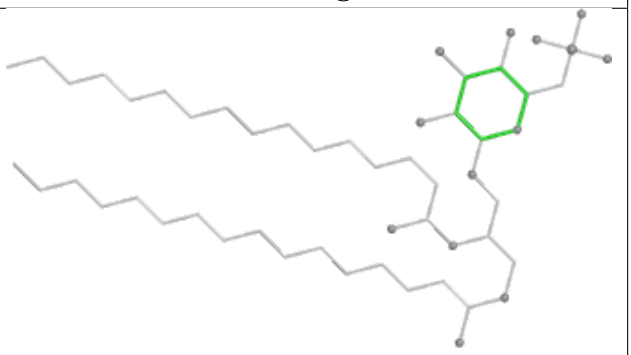
Bond lengths



Bond angles

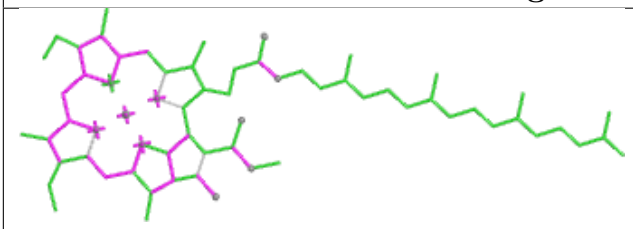


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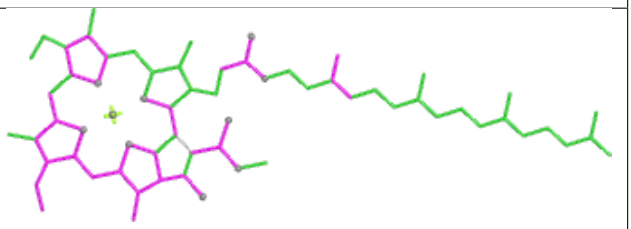


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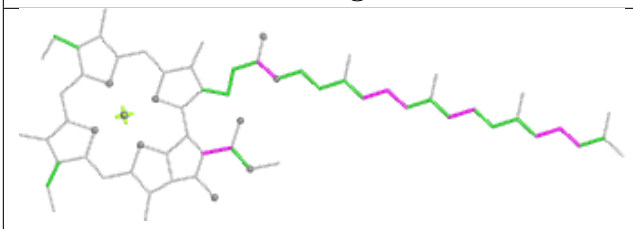
Ligand CLA b 619



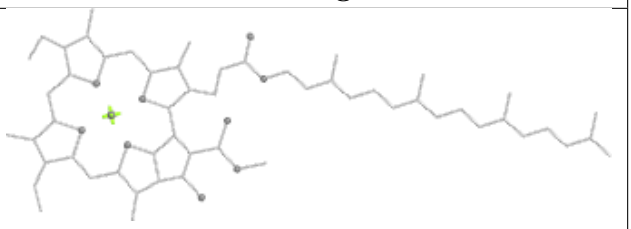
Bond lengths



Bond angles

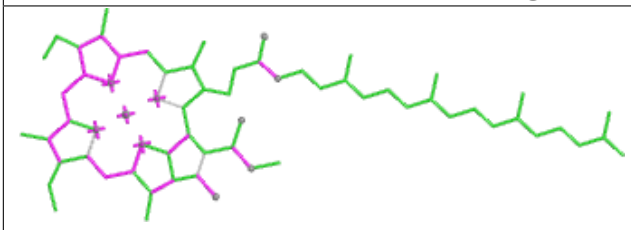


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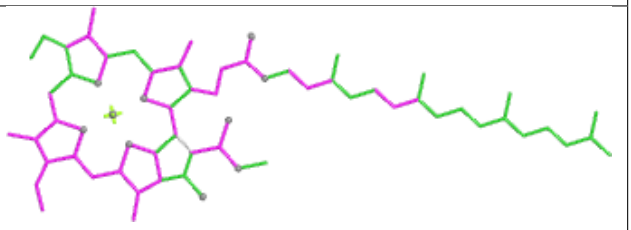


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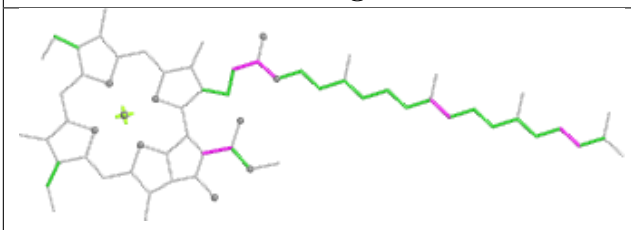
Ligand CLA C 513



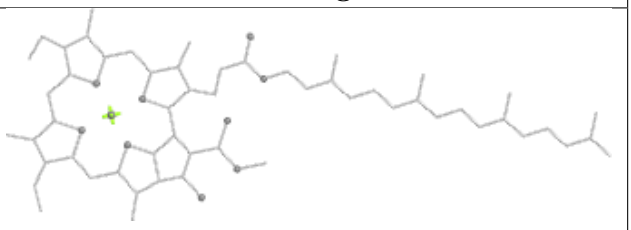
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Bond angles

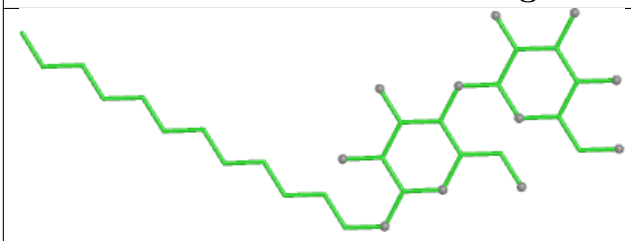


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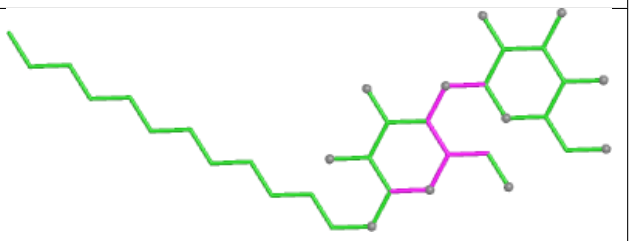


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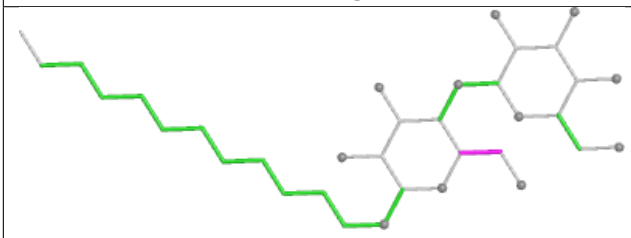
Ligand LMT m 103



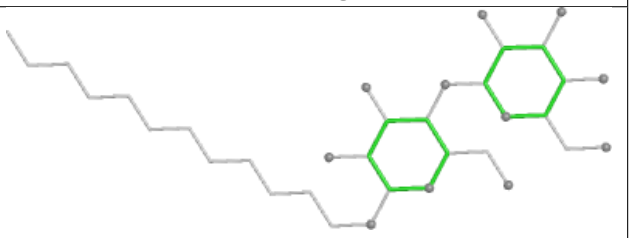
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Bond angles

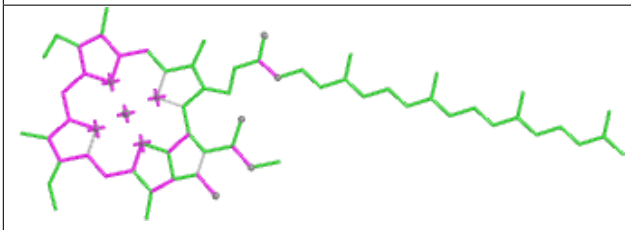


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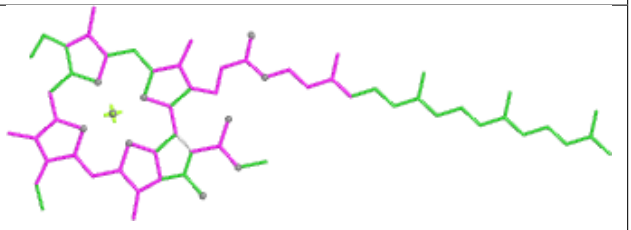


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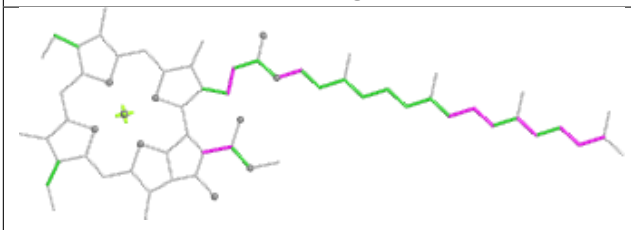
Ligand CLA B 611



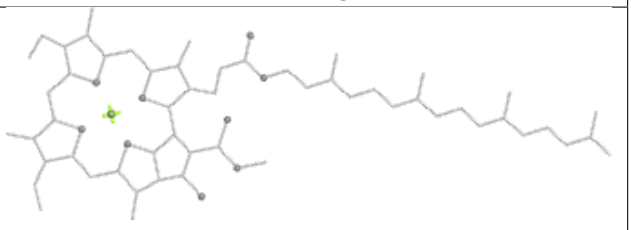
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Bond angles

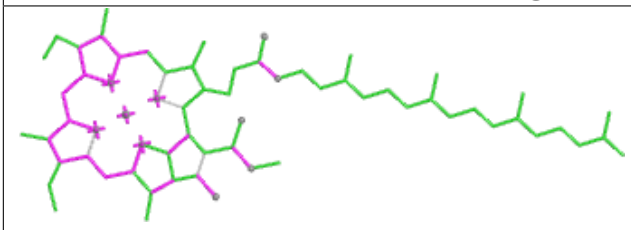


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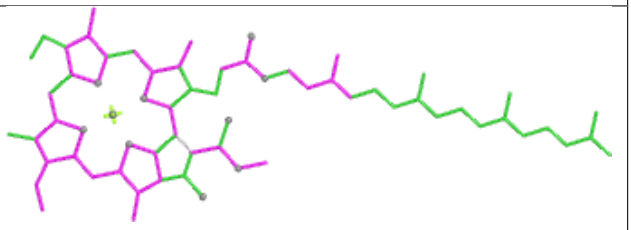


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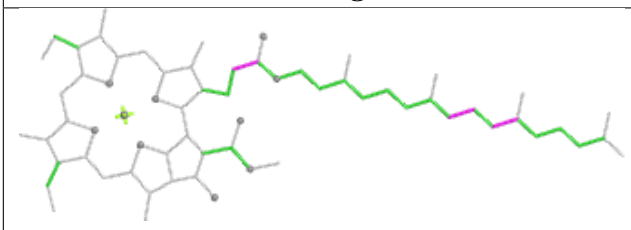
Ligand CLA b 616



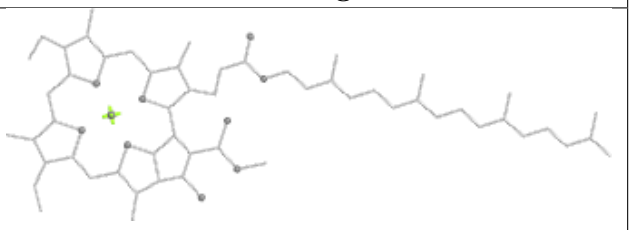
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Bond angles

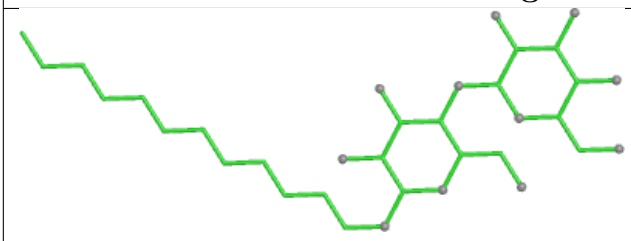


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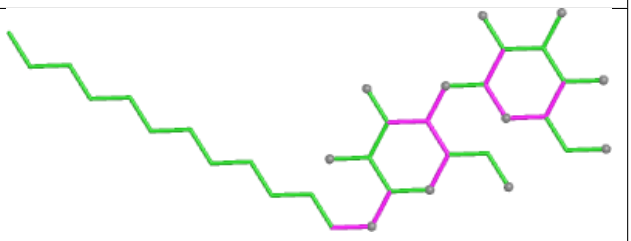


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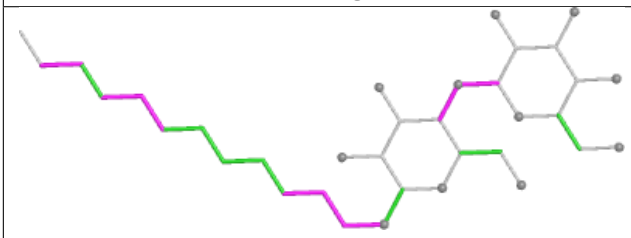
Ligand LMT B 623



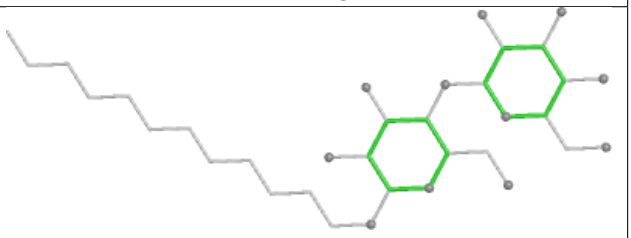
Bond lengths



Bond angles

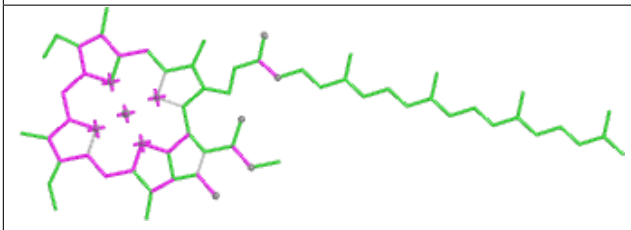


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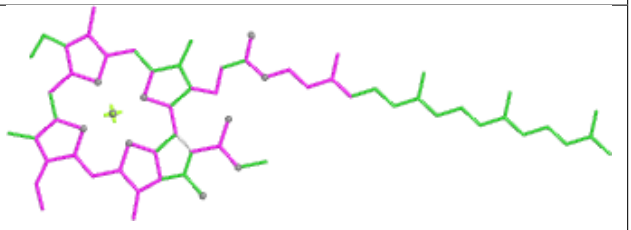


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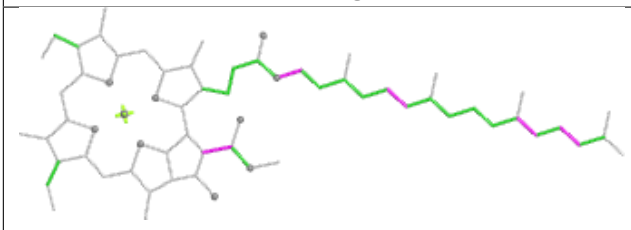
Ligand CLA C 508



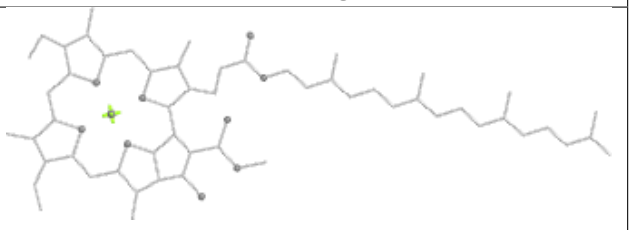
Bond lengths



Bond angles

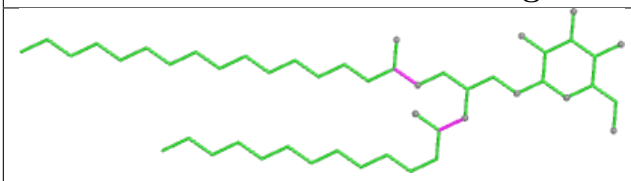


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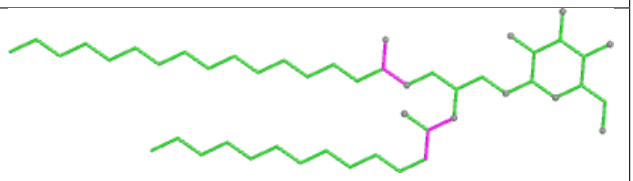


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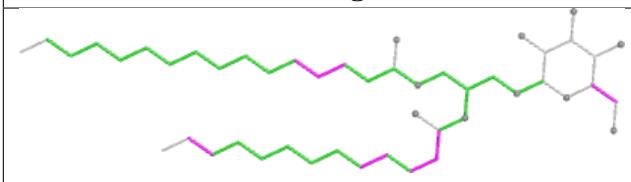
Ligand LMG d 411



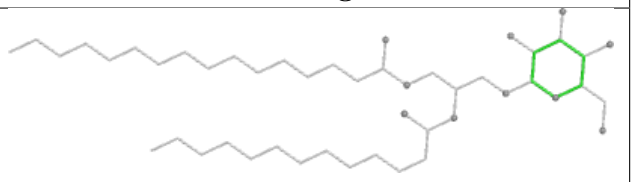
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Bond angles

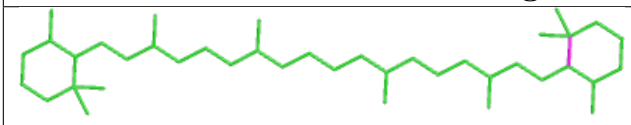


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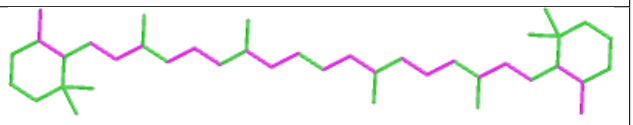


Rings

Ligand BCR D 406



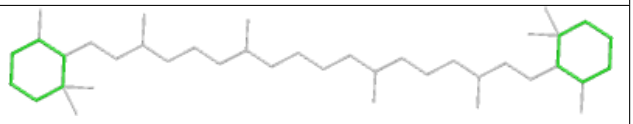
Bond lengths



Bond angles

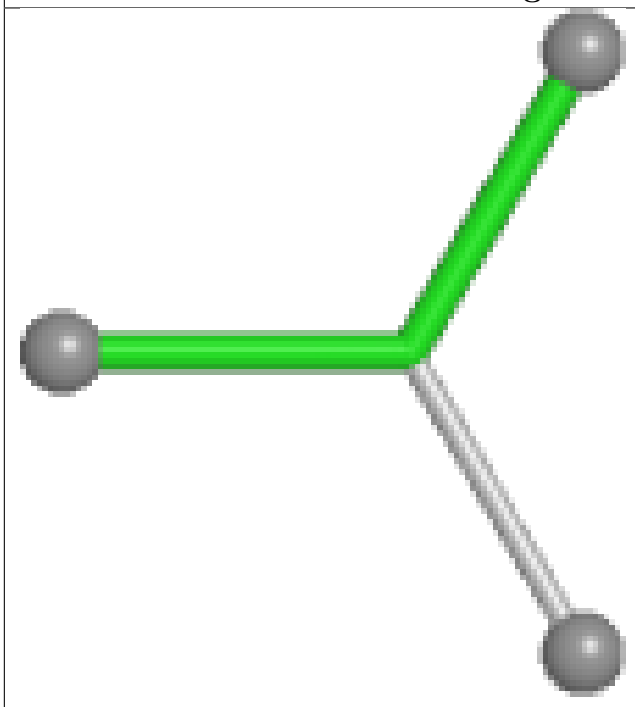


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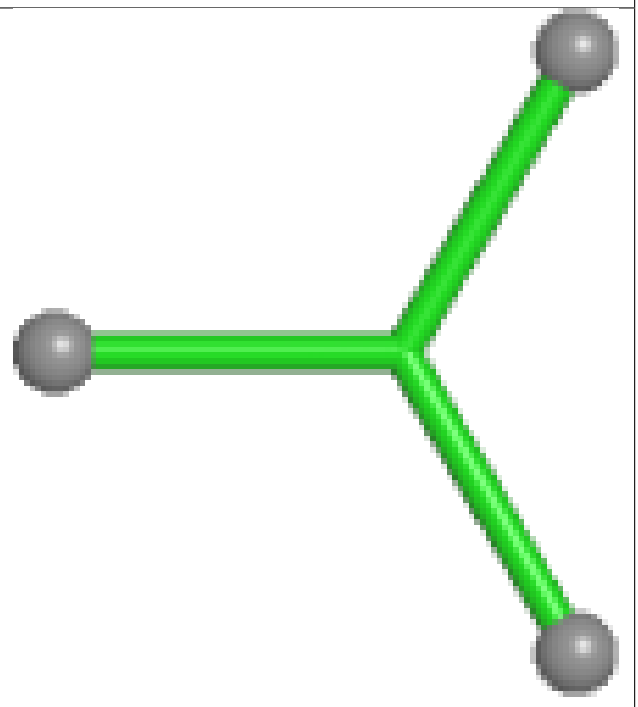


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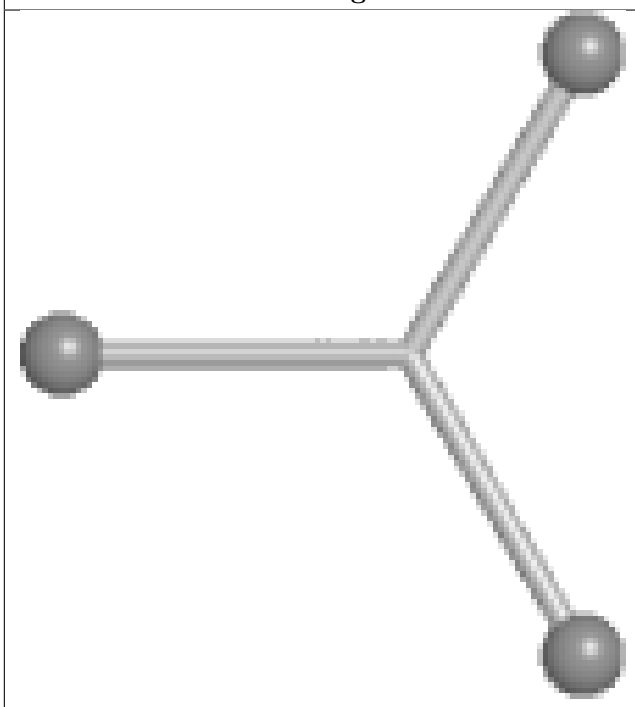
Ligand BCT A 421



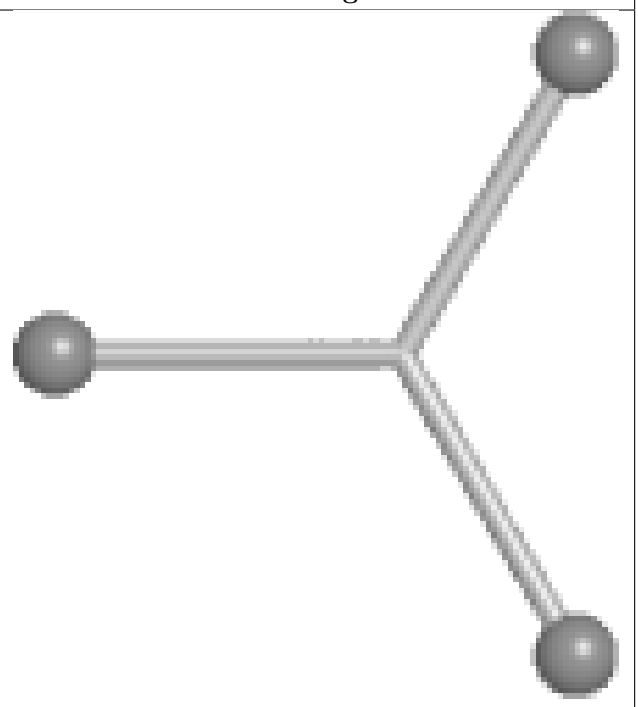
Bond lengths



Bond angles

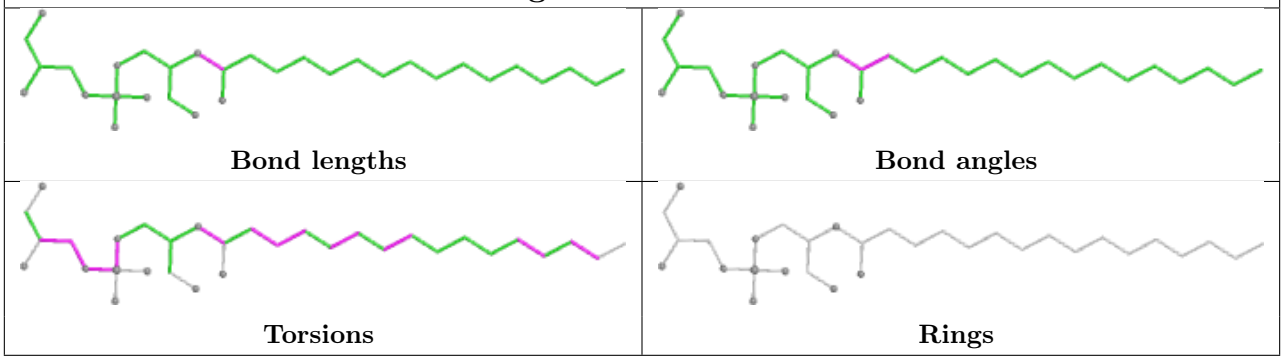


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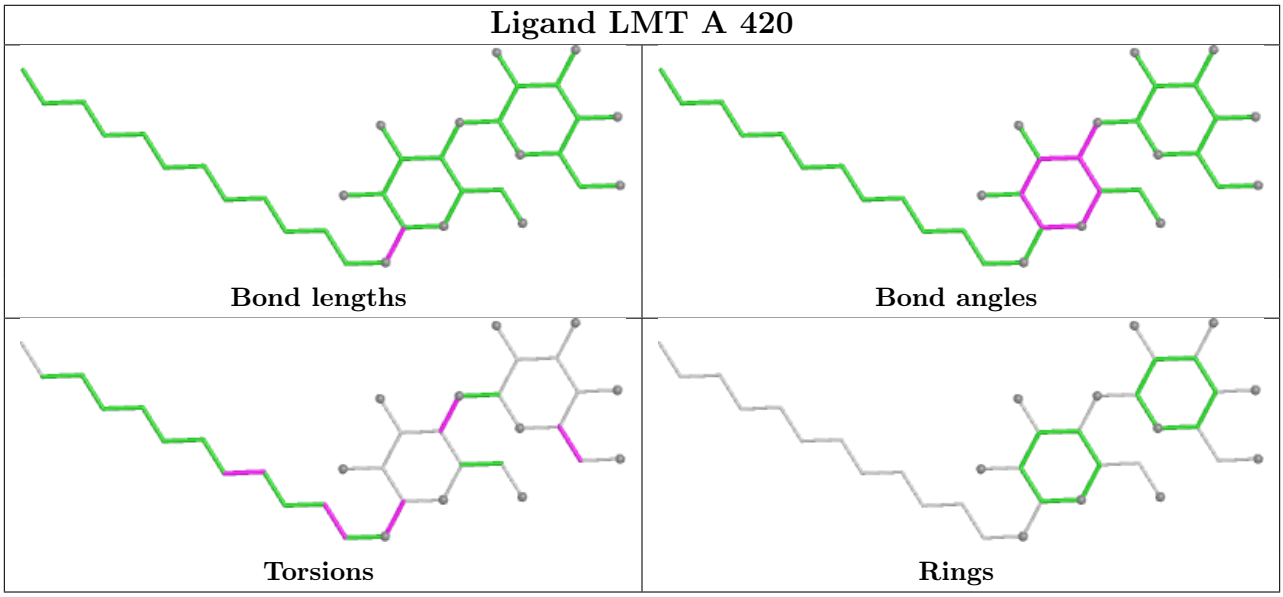


Rings

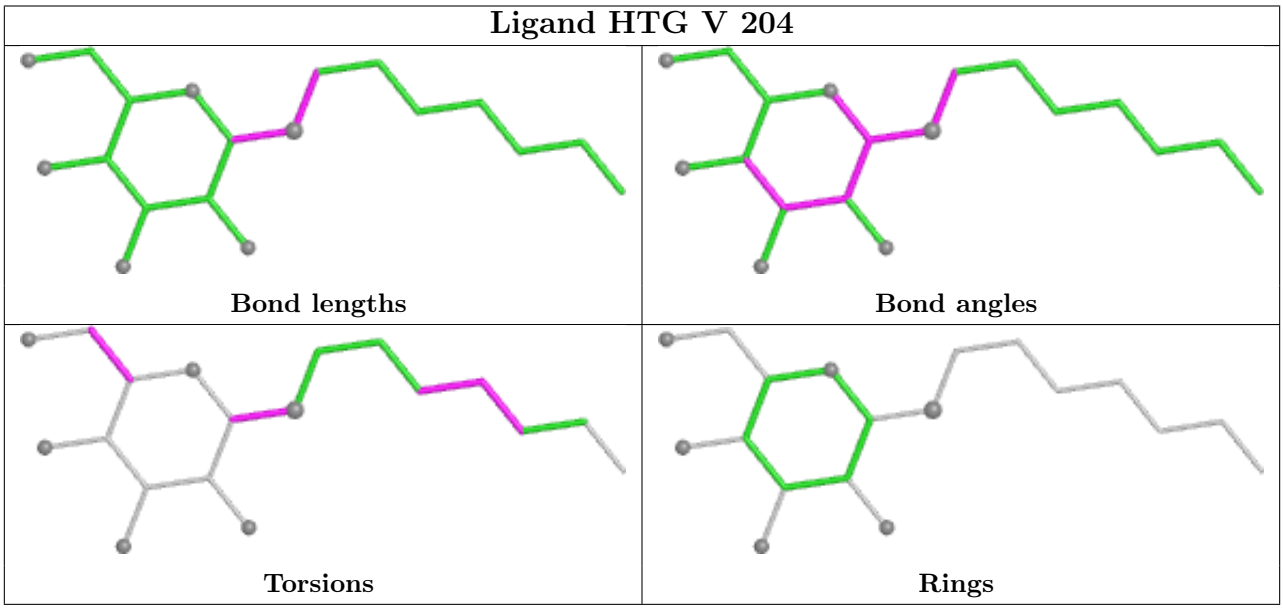
Ligand LHG e 101



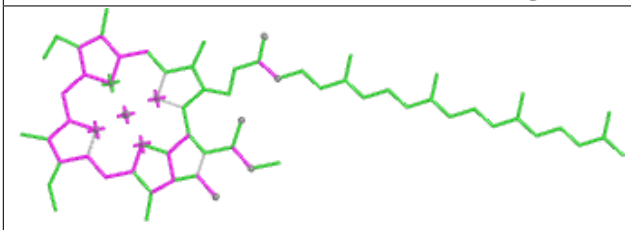
Ligand LMT A 420



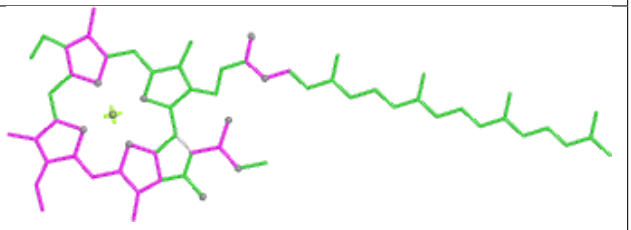
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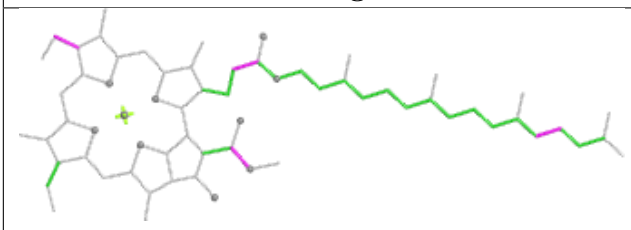
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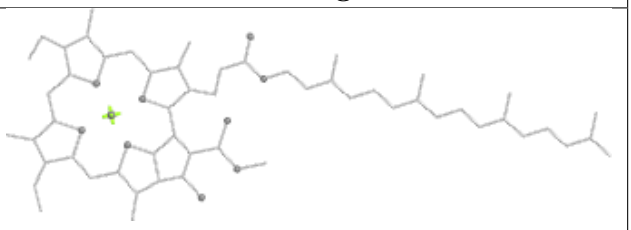
Bond lengths



Bond angles

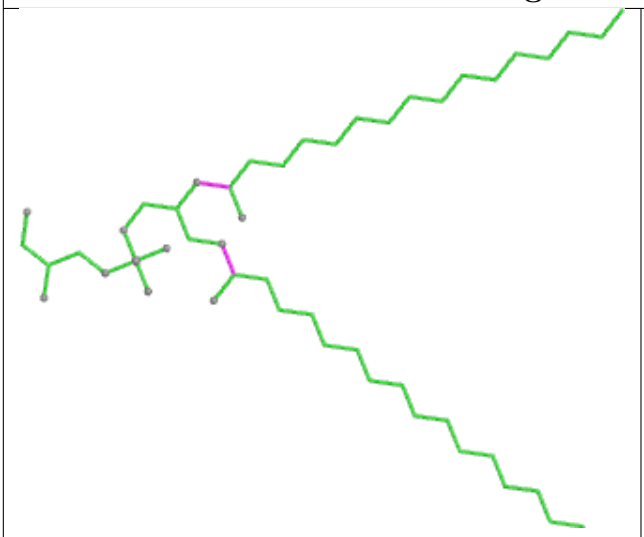


Torsions

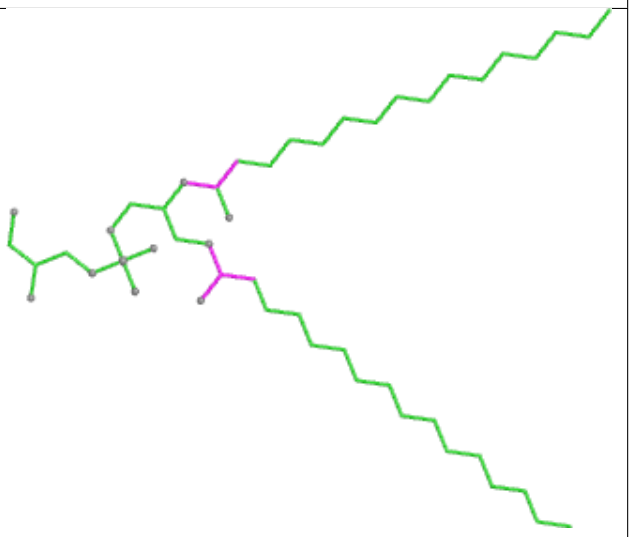


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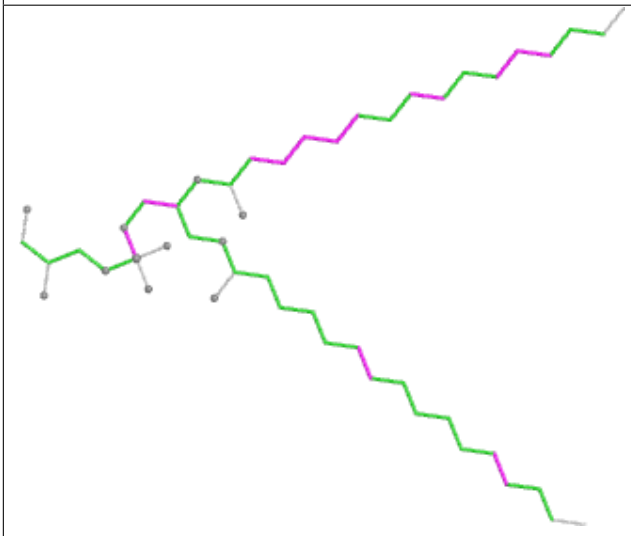
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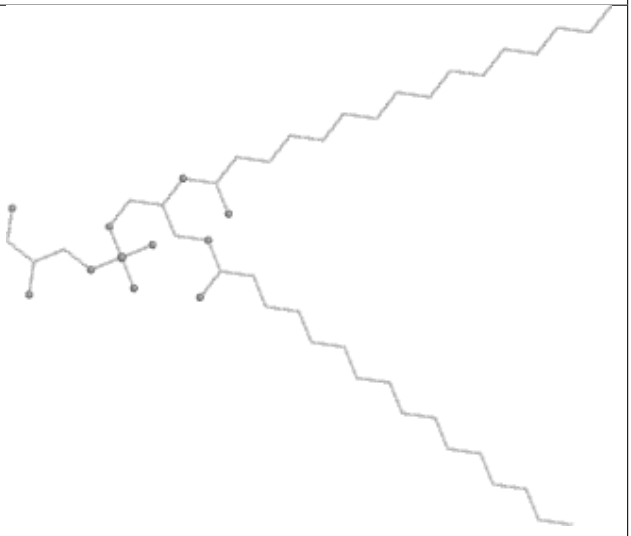
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Bond angles

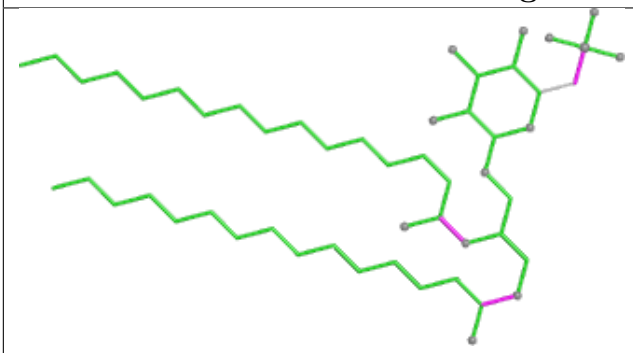


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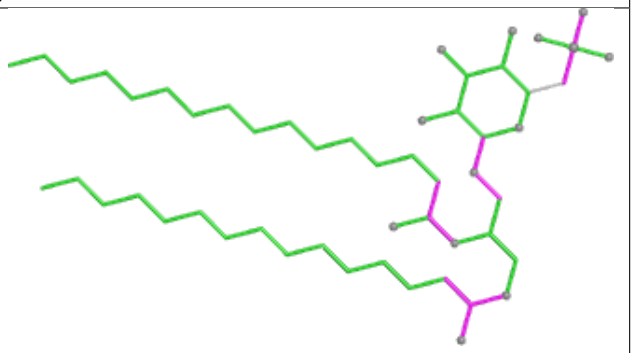


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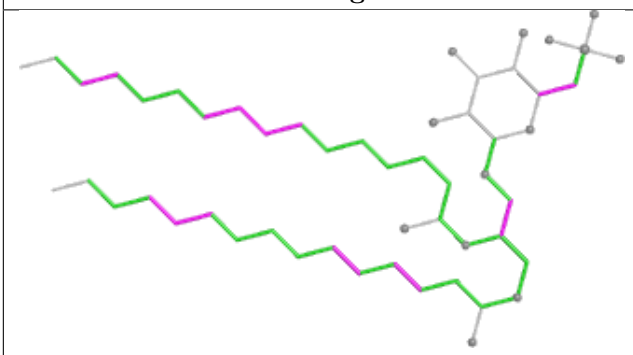
Ligand SQD a 2102



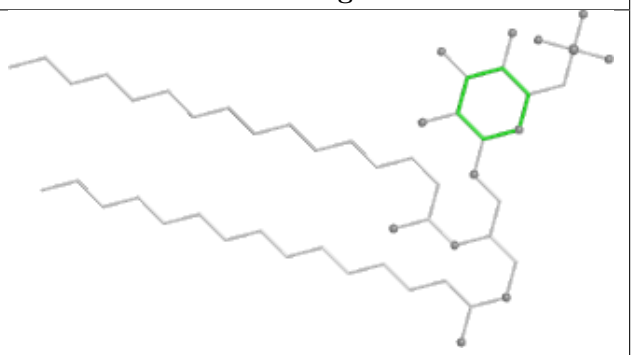
Bond lengths



Bond angles

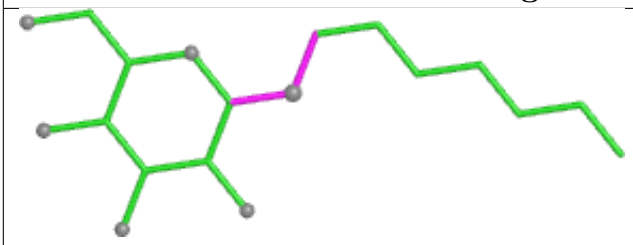


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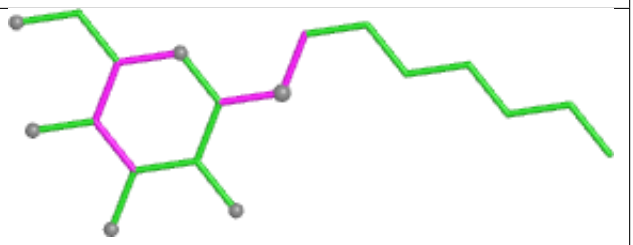


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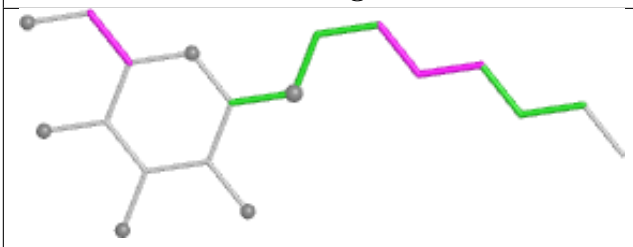
Ligand HTG B 627



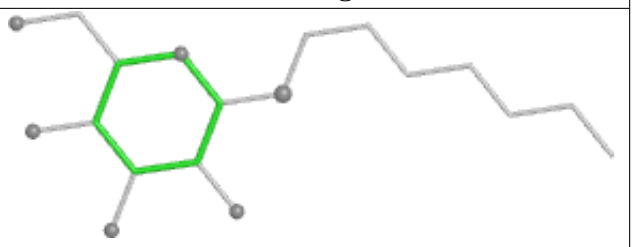
Bond lengths



Bond angles

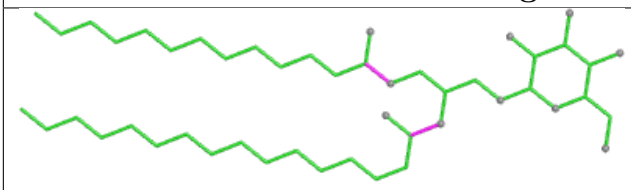


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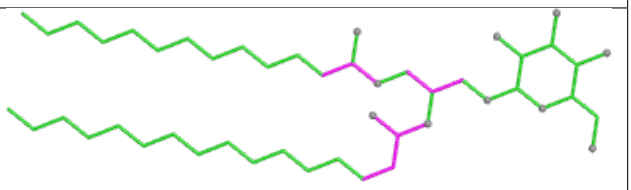


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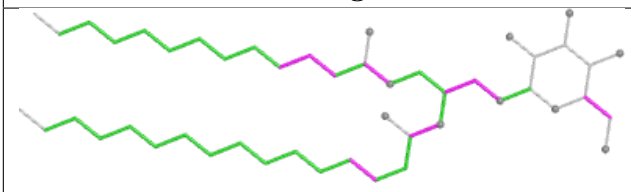
Ligand LMG C 526



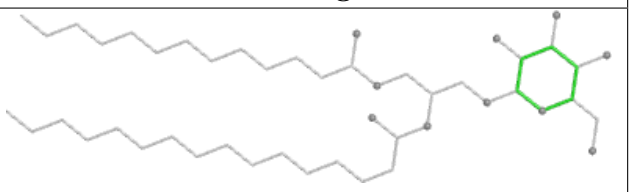
Bond lengths



Bond angles

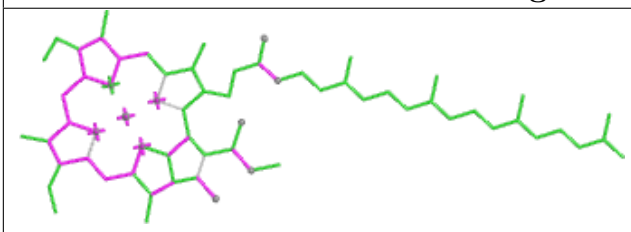


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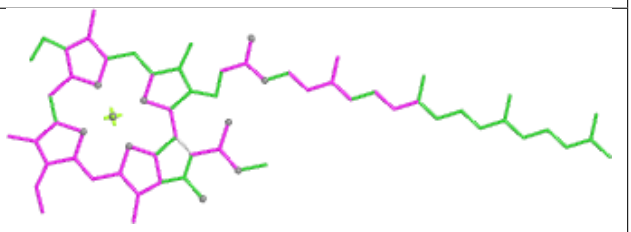


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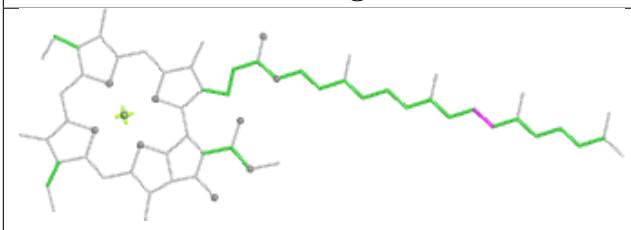
Ligand CLA c 505



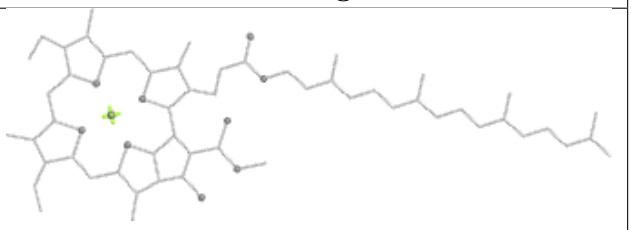
Bond lengths



Bond angles

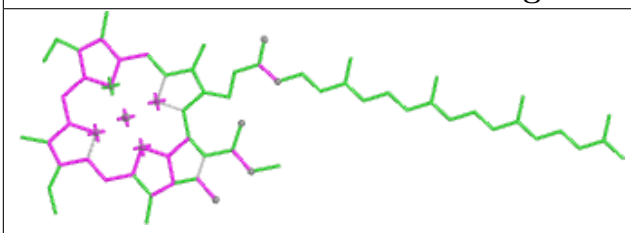


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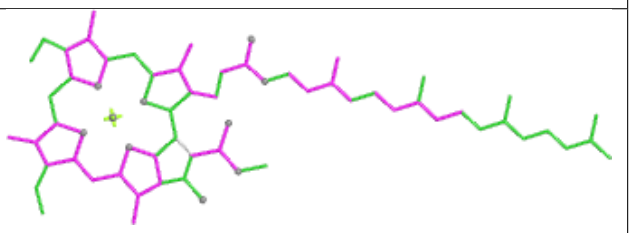


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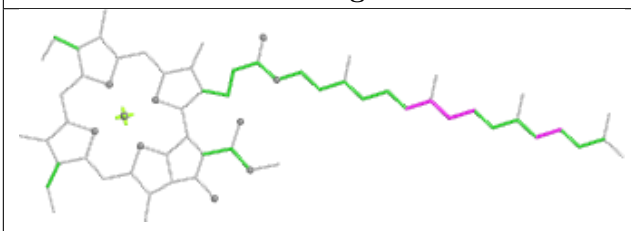
Ligand CLA D 405



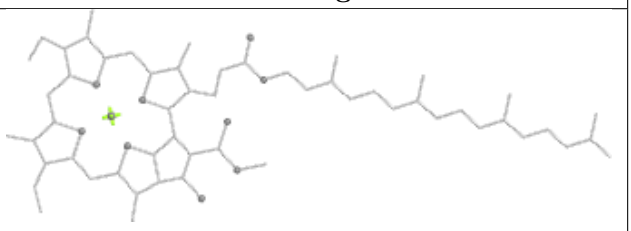
Bond lengths



Bond angles

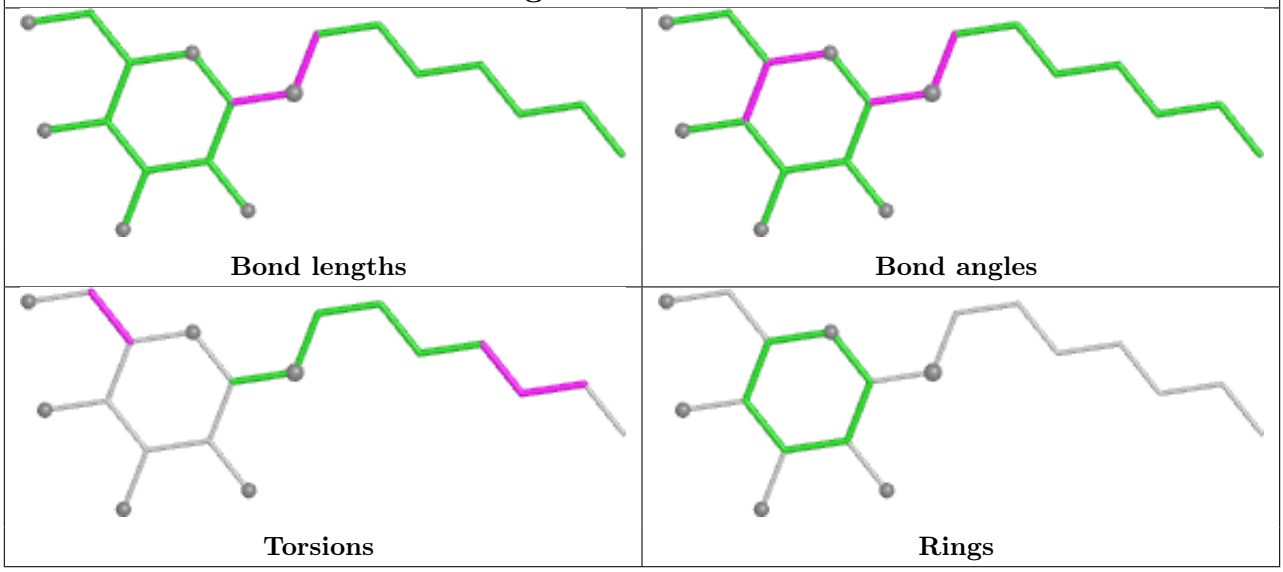


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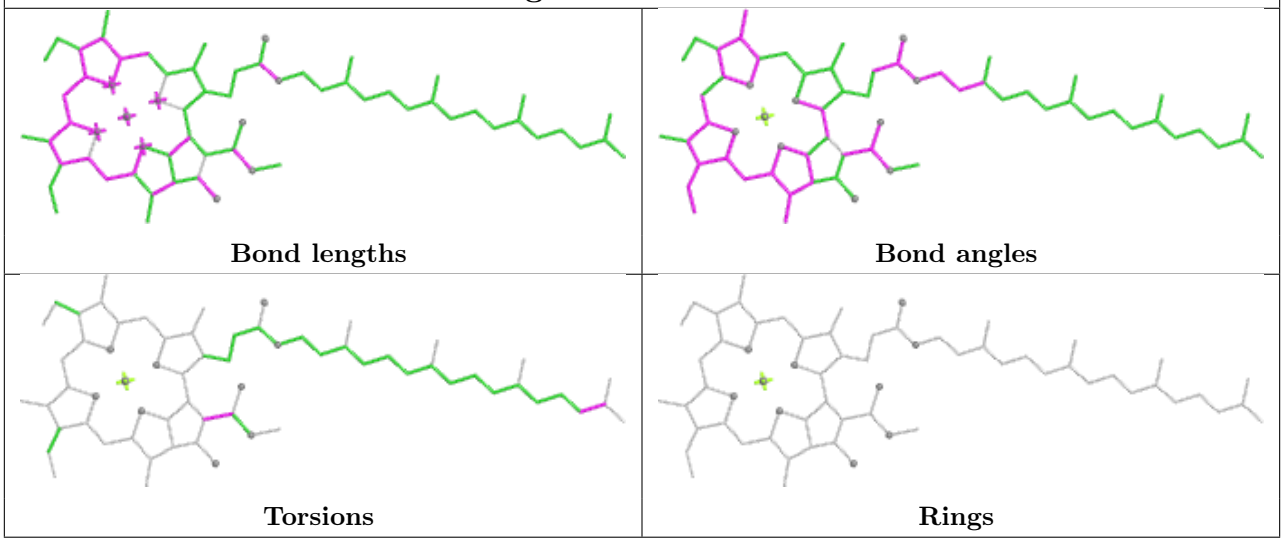


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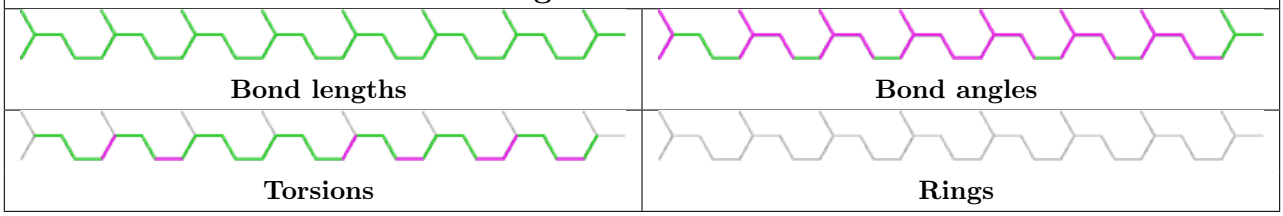
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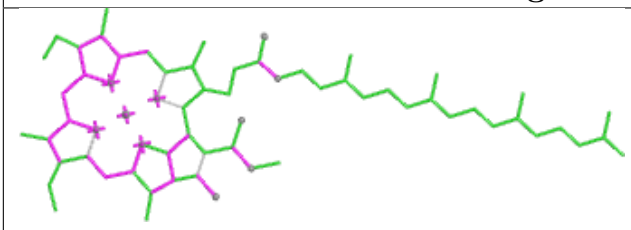
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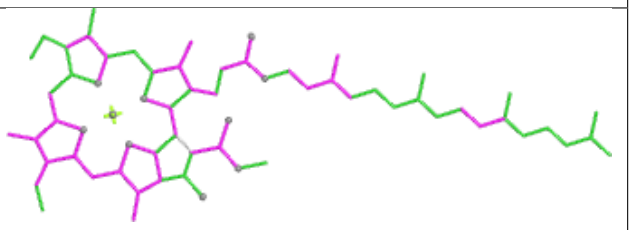
Ligand PL9 x 801



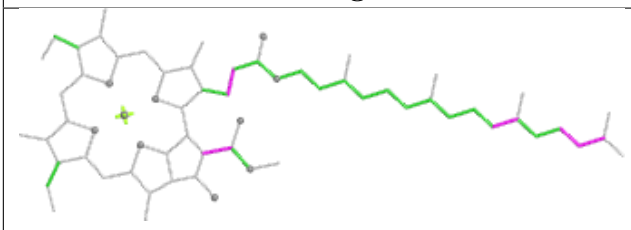
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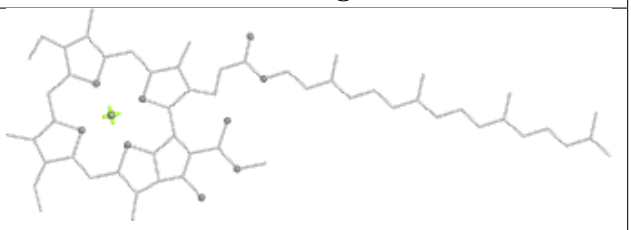
Bond lengths



Bond angles

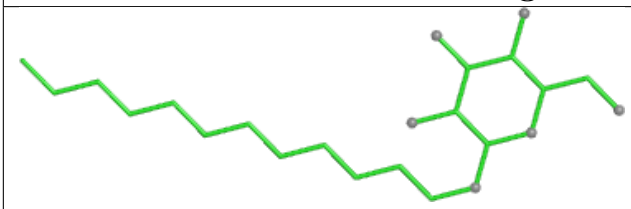


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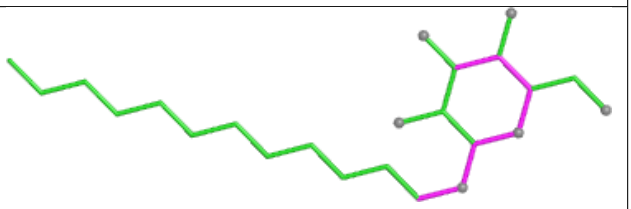


Rings

Ligand LMT I 1201



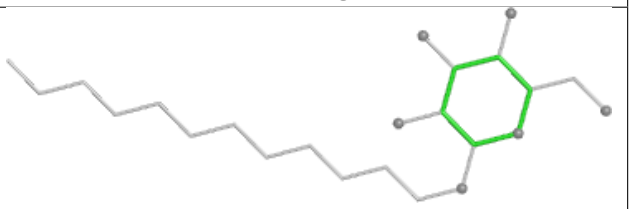
Bond lengths



Bond angles

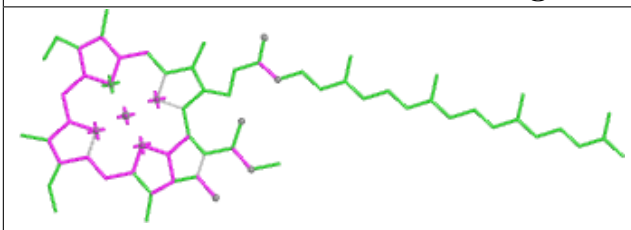


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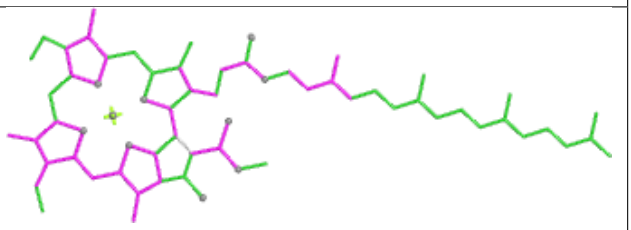


Rings

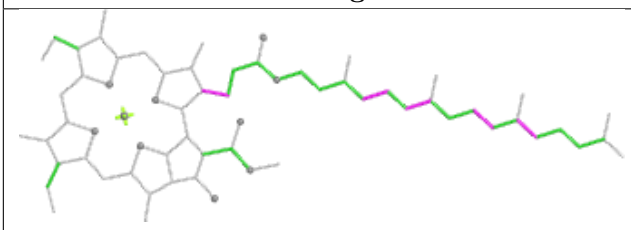
Ligand CLA c 515



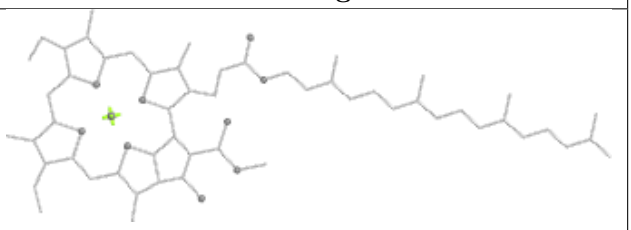
Bond lengths



Bond angles

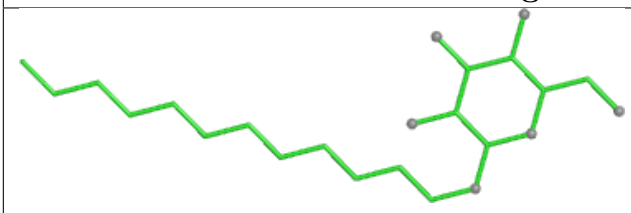


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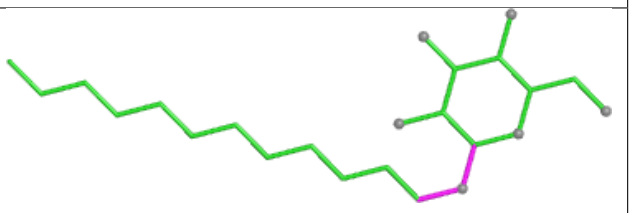


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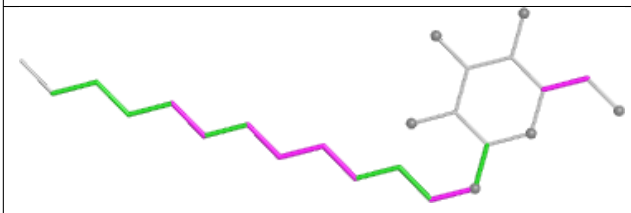
Ligand LMT T 102



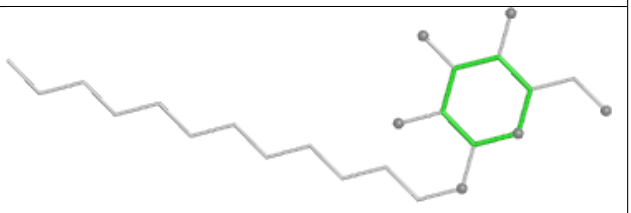
Bond lengths



Bond angles

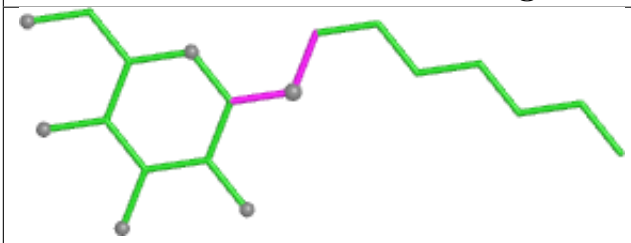


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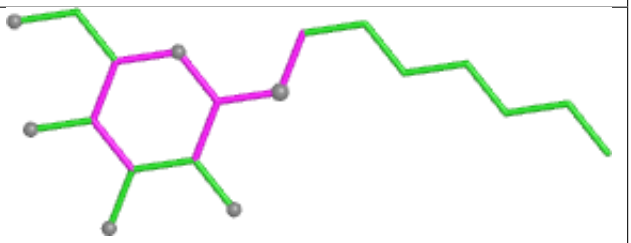


Rings

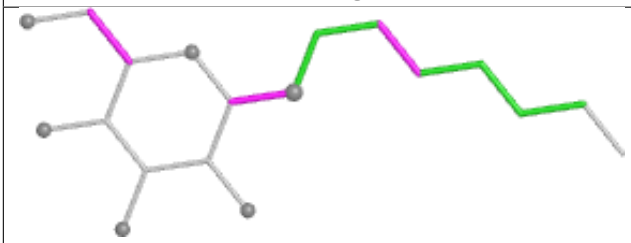
Ligand HTG I 1202



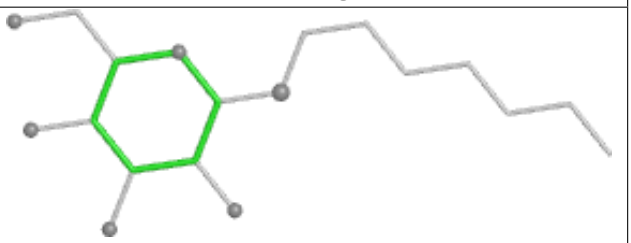
Bond lengths



Bond angles

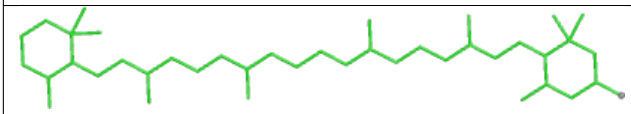


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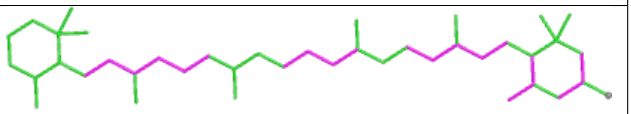


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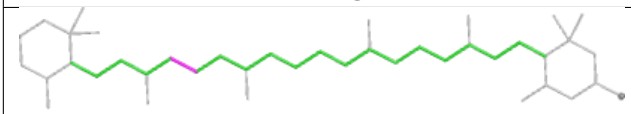
Ligand RRX h 702



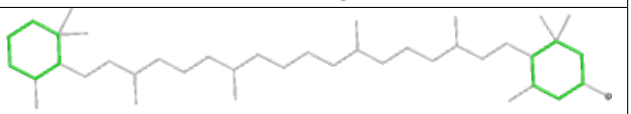
Bond lengths



Bond angles

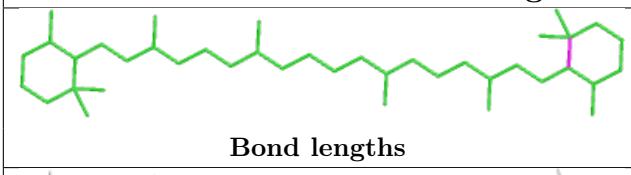


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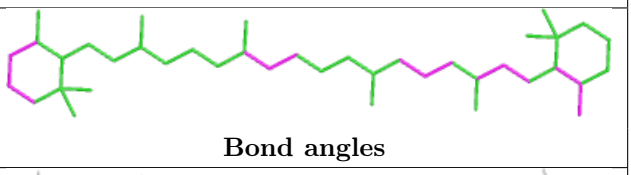


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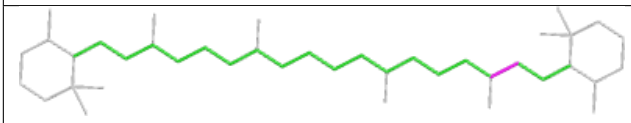
Ligand BCR b 622



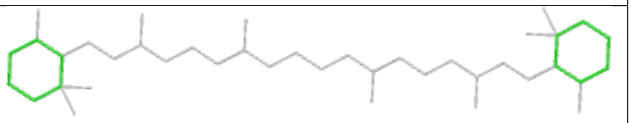
Bond lengths



Bond angles



Torsions

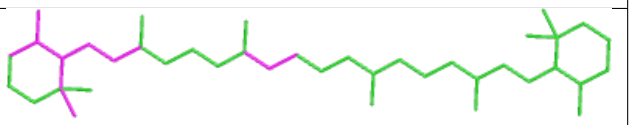


Rings

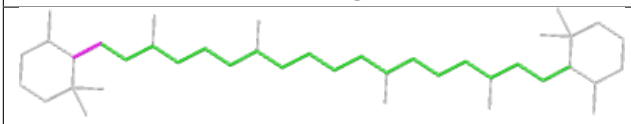
Ligand BCR a 2114



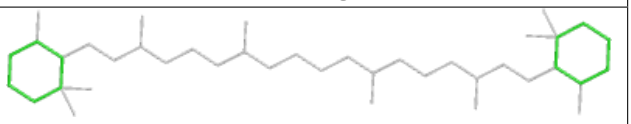
Bond lengths



Bond angles

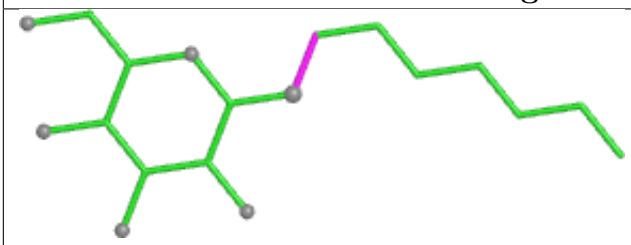


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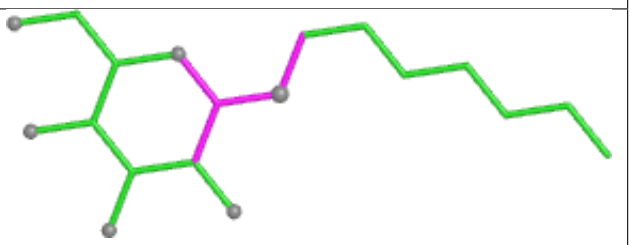


Rings

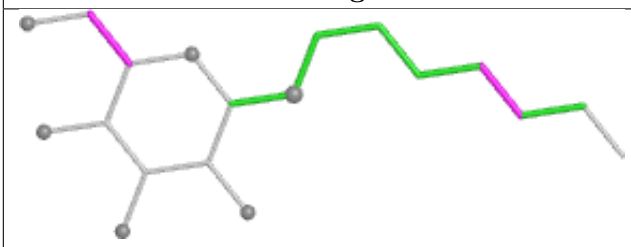
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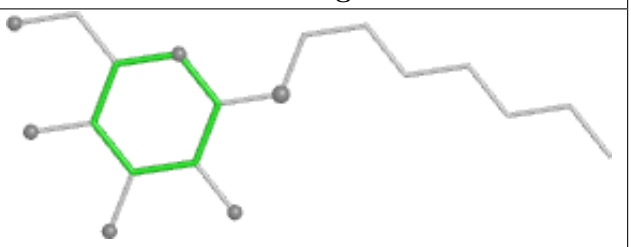
Bond lengths



Bond angles

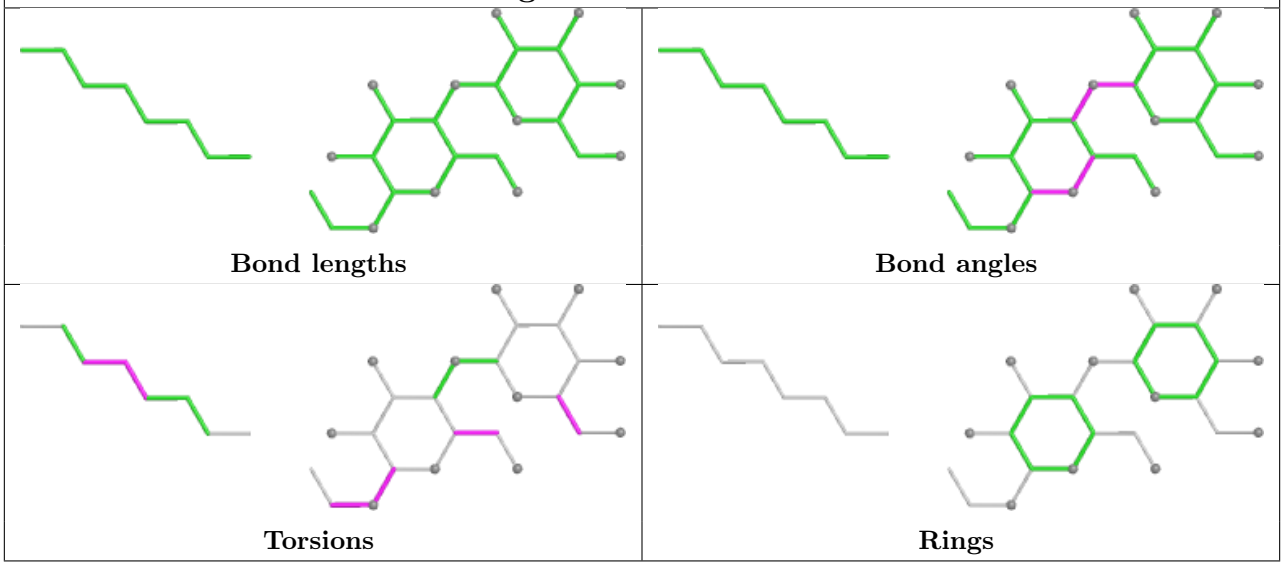


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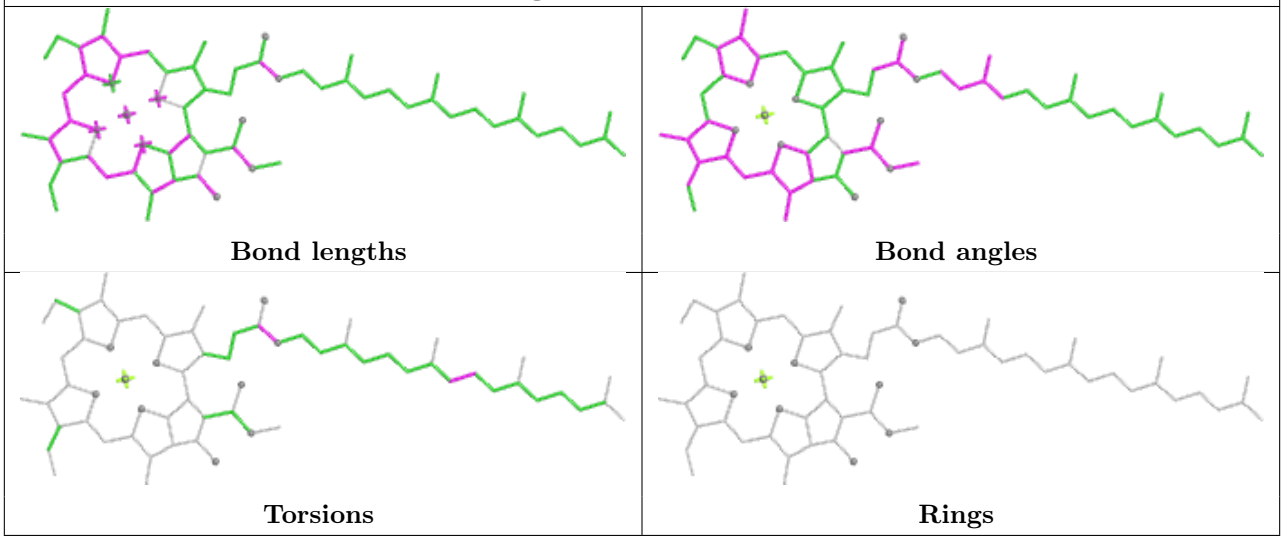


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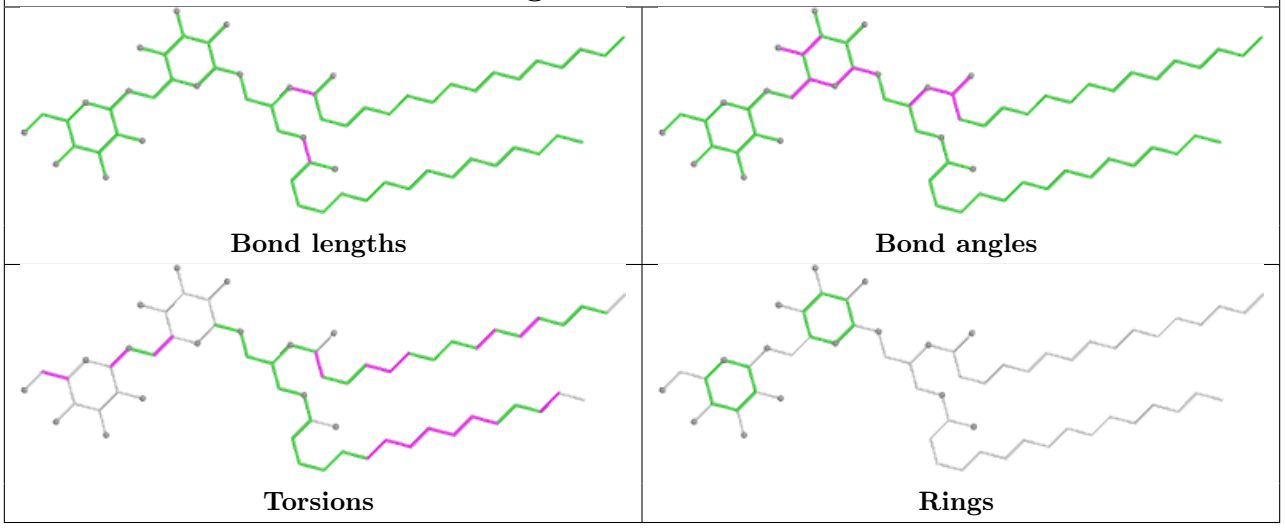
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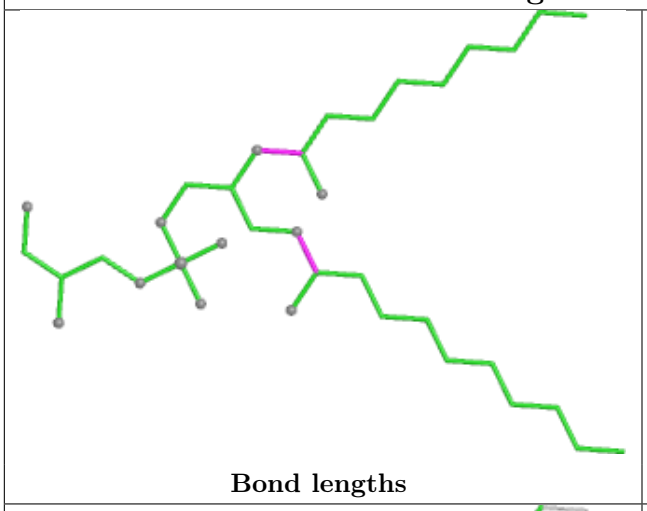
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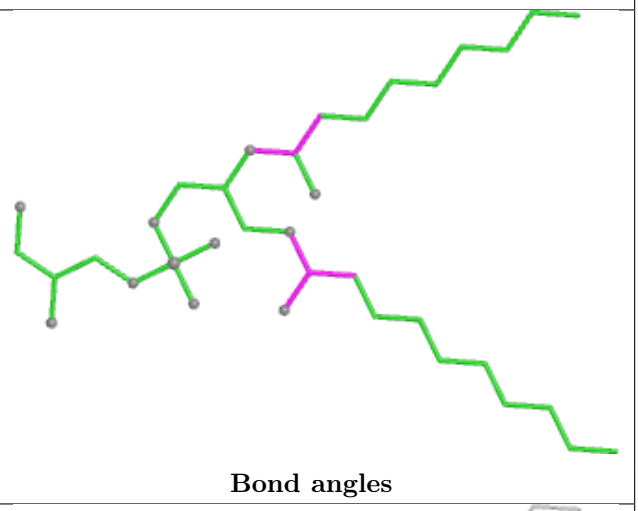
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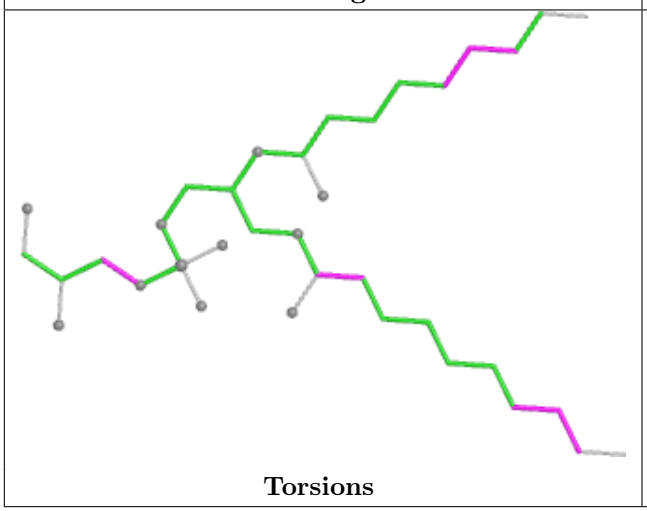
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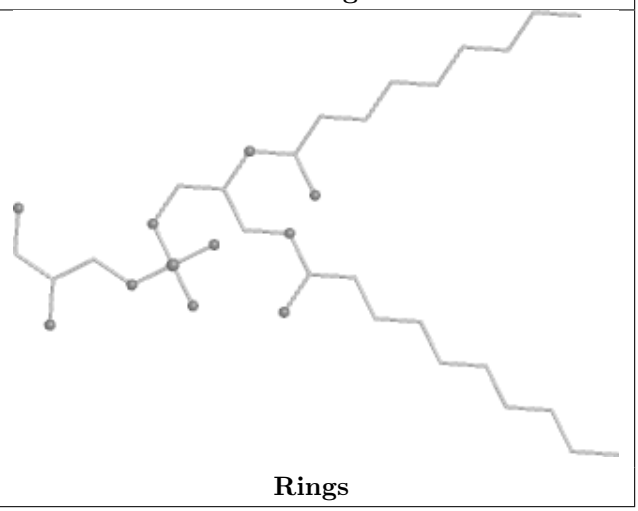
Bond lengths



Bond angles

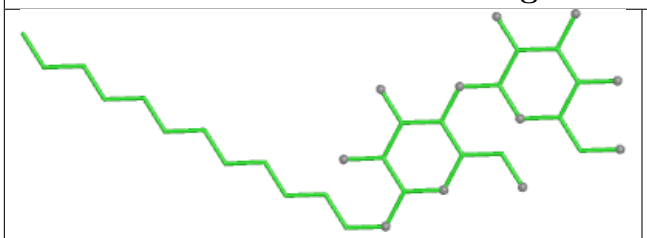


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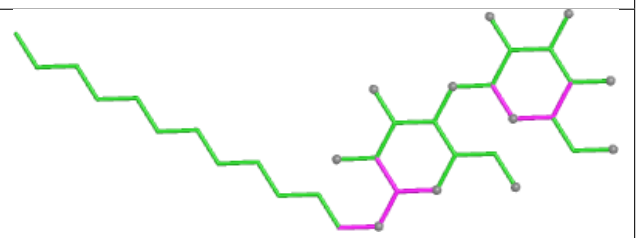


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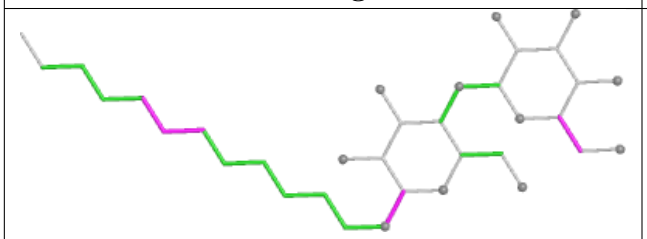
Ligand LMT m 102



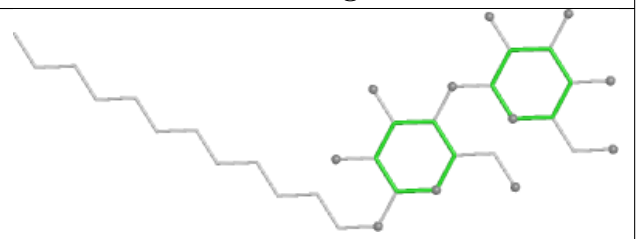
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Bond angles

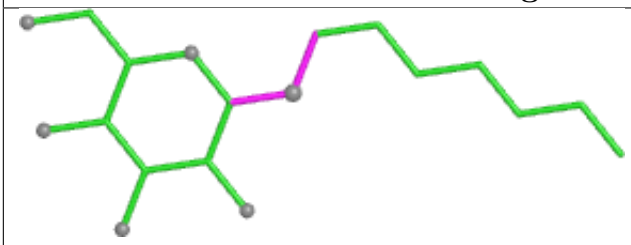


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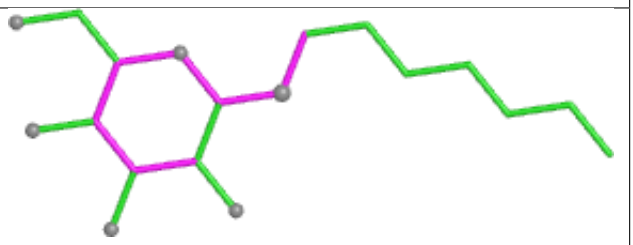


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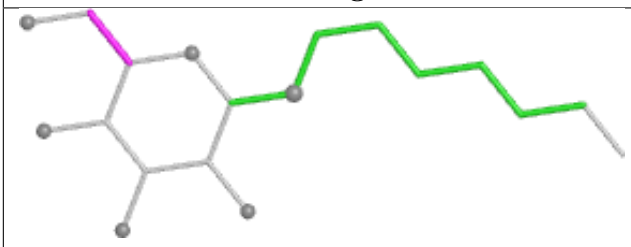
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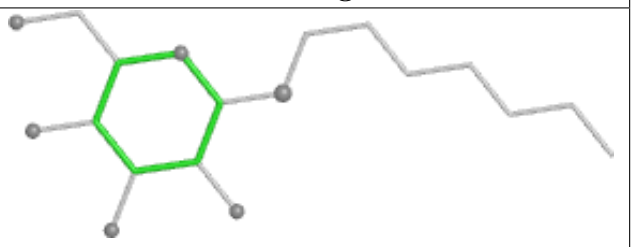
Bond lengths



Bond angles

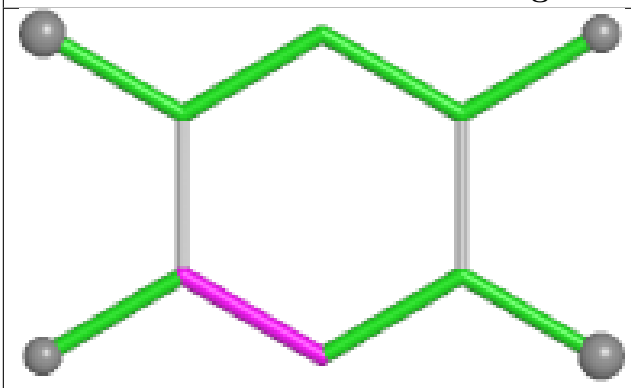


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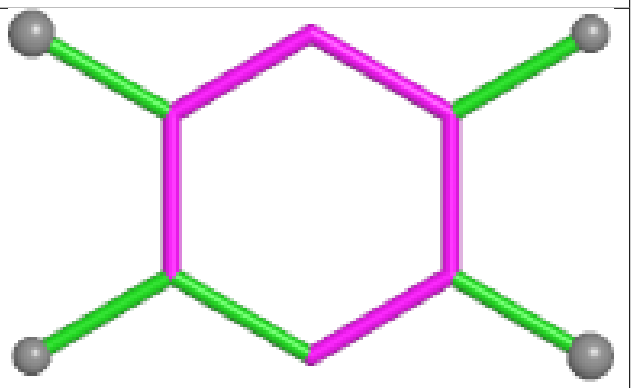


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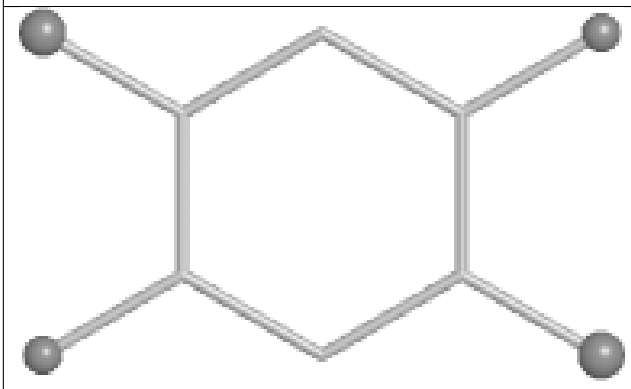
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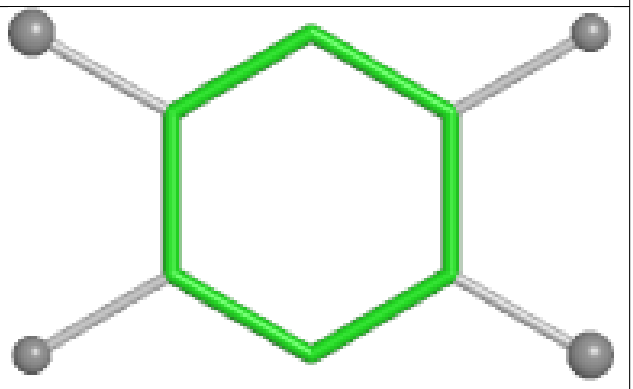
Bond lengths



Bond angles

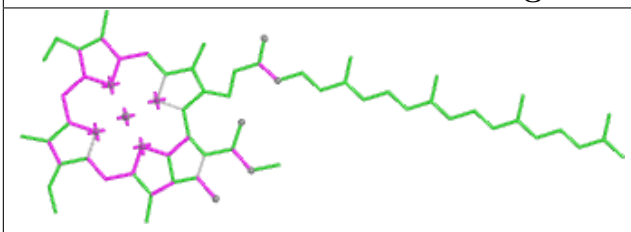


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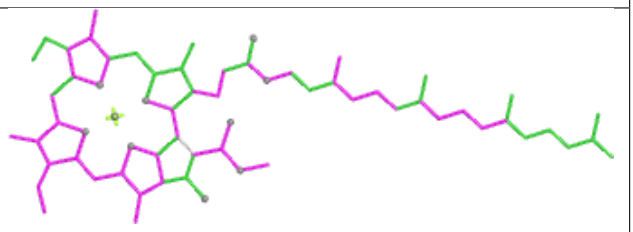


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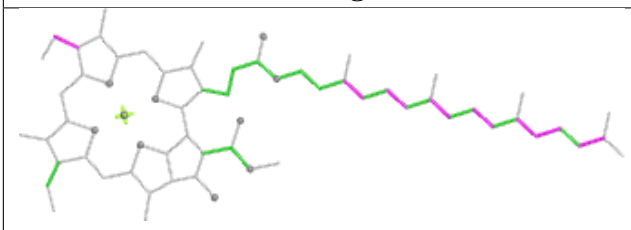
Ligand CLA B 616



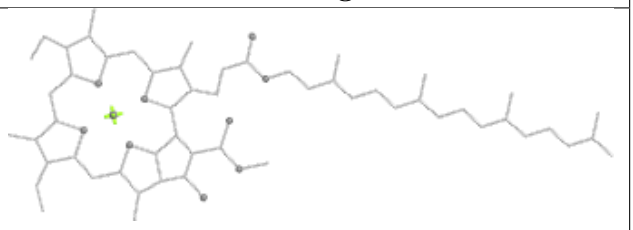
Bond lengths



Bond angles



Torsions



Rings

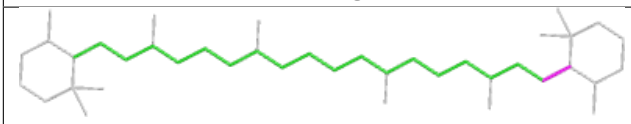
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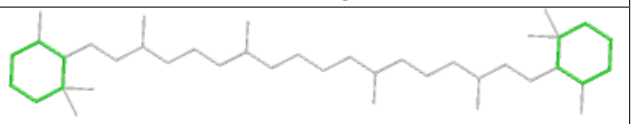
Bond lengths



Bond angles

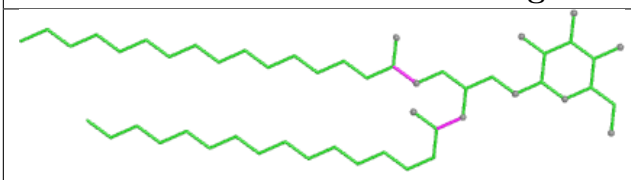


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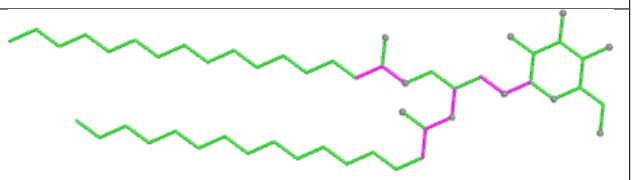


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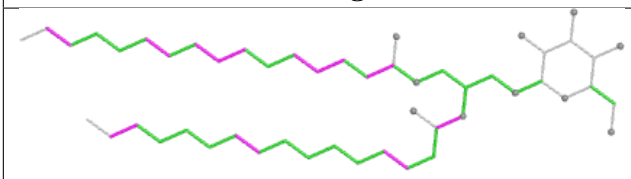
Ligand LMG i 101



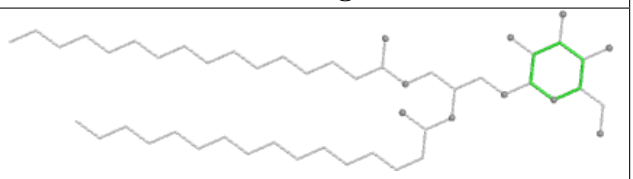
Bond lengths



Bond angles

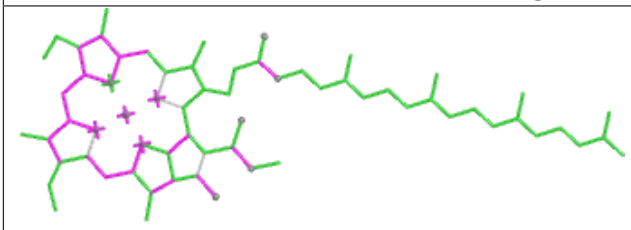


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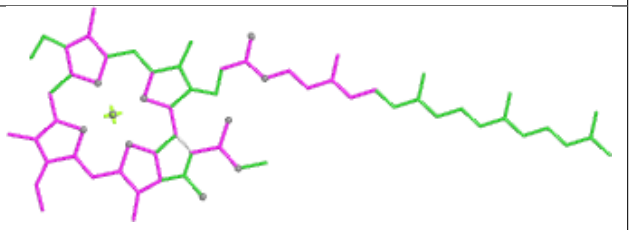


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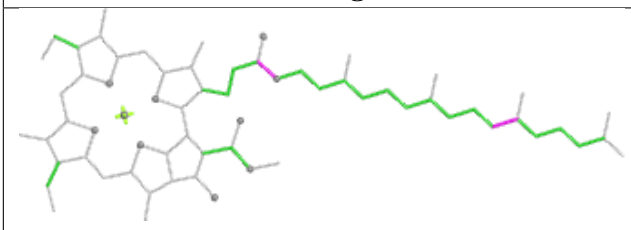
Ligand CLA c 513



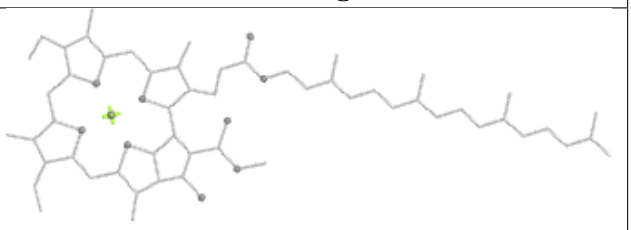
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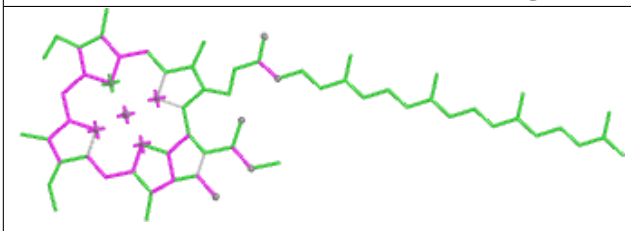


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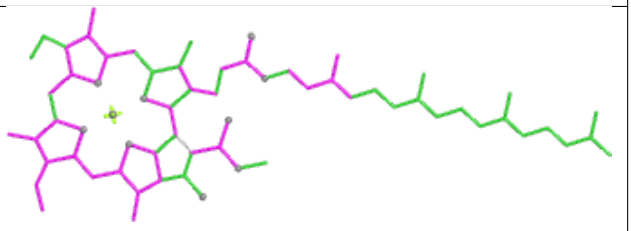


Rings

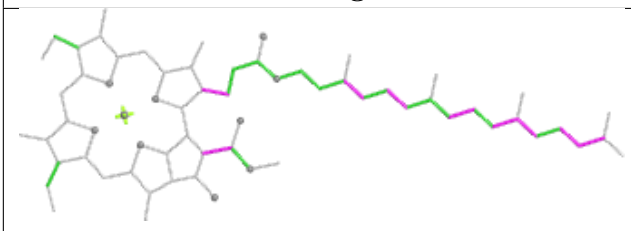
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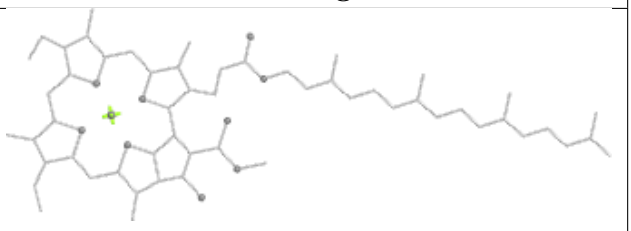
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Bond angles

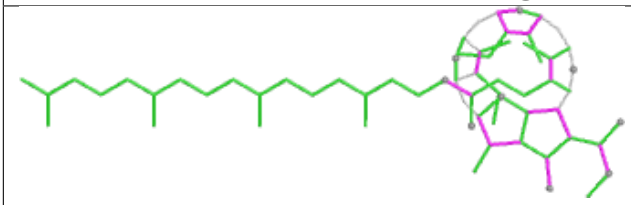


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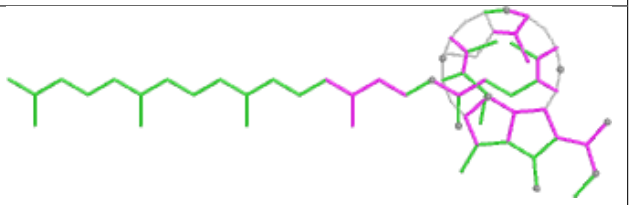


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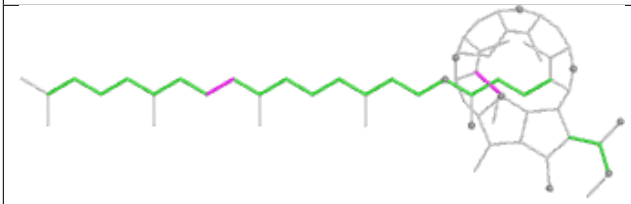
Ligand PHO a 2112



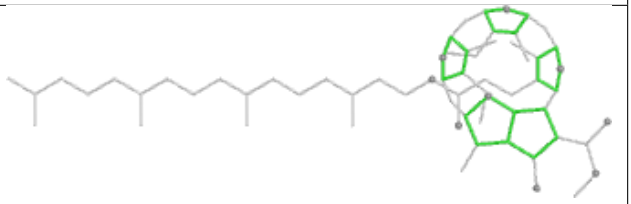
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Bond angles

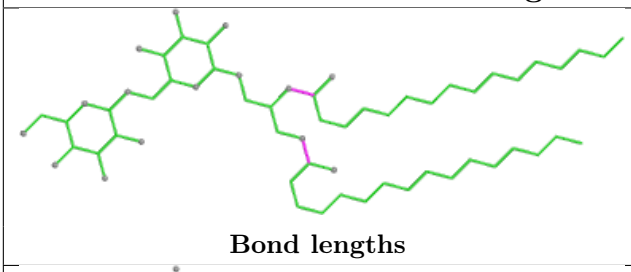


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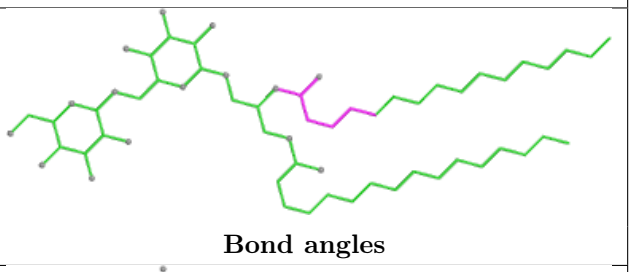


Rings

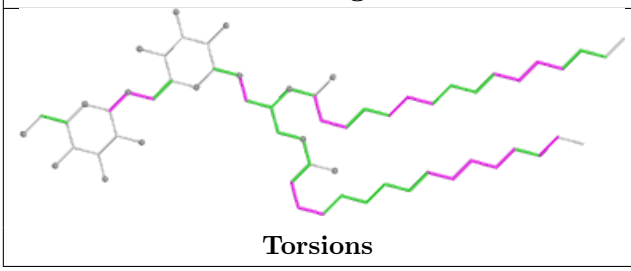
Ligand DGD c 519



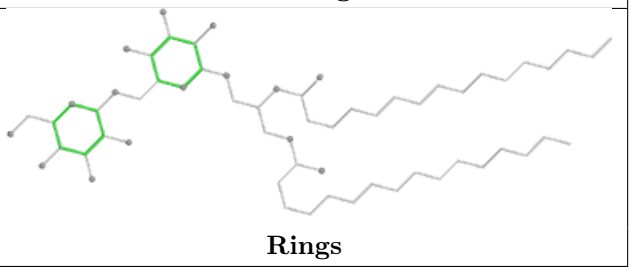
Bond lengths



Bond angles

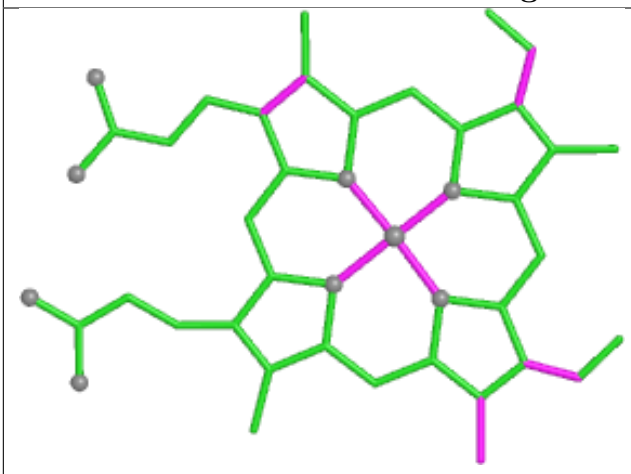


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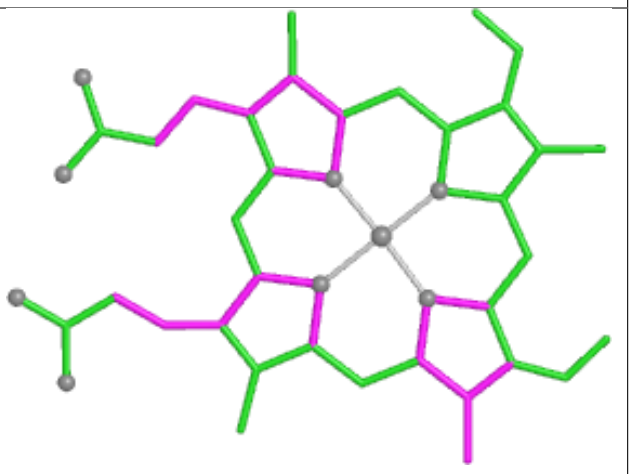


Rings

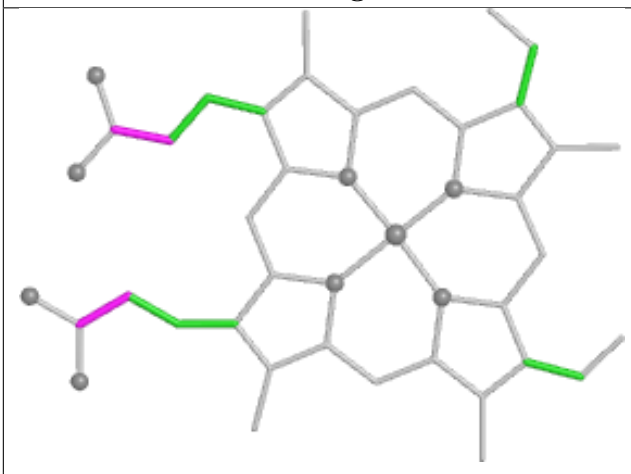
Ligand HEM F 102



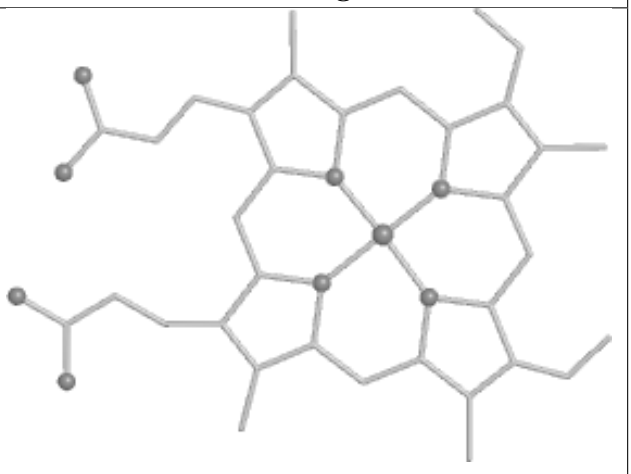
Bond lengths



Bond angles

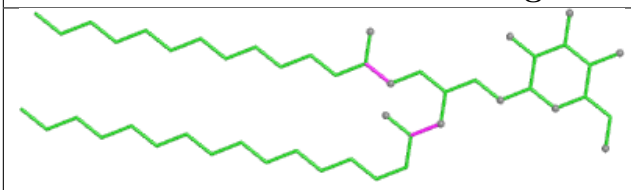


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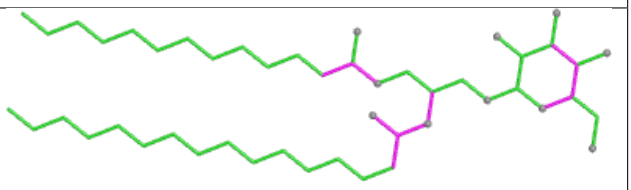


Rings

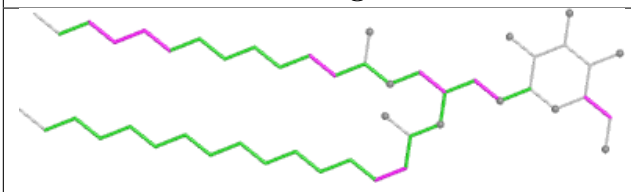
Ligand LMG c 522



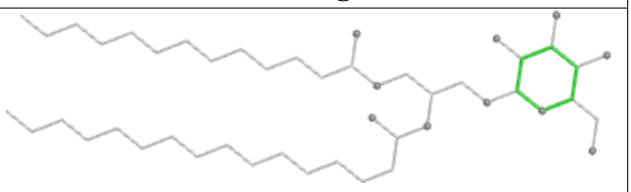
Bond lengths



Bond angles

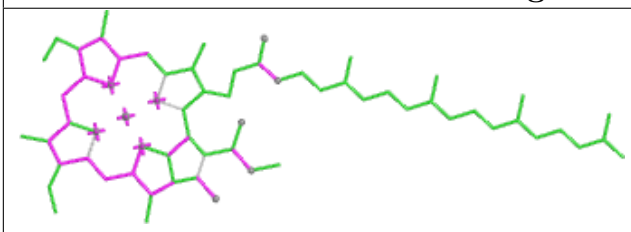


Torsions

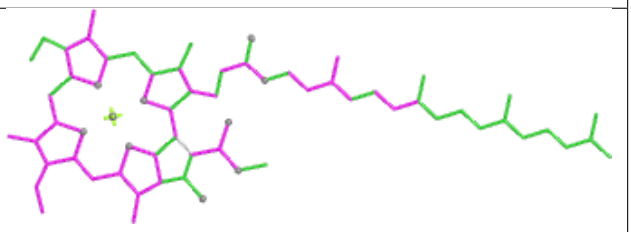


Rings

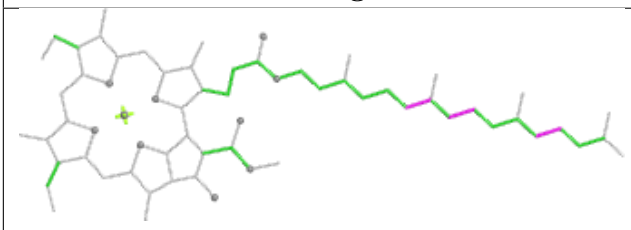
Ligand CLA d 405



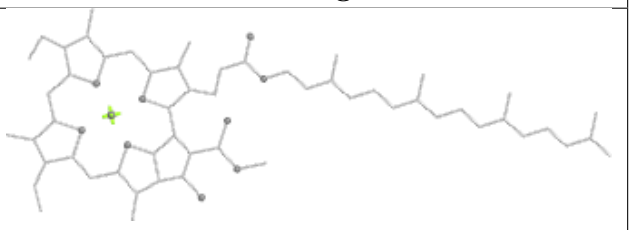
Bond lengths



Bond angles

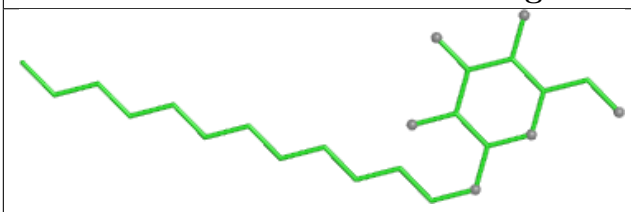


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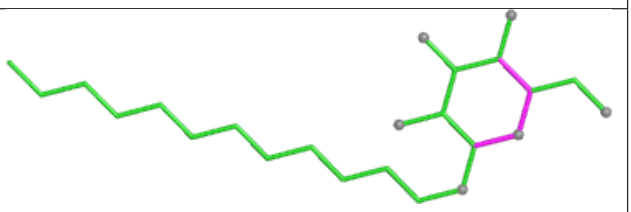


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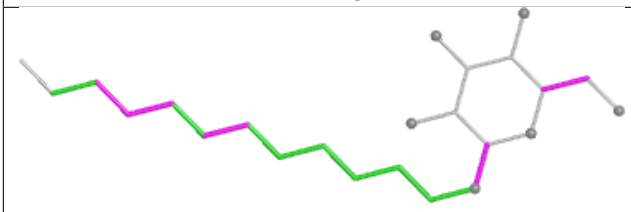
Ligand LMT J 102



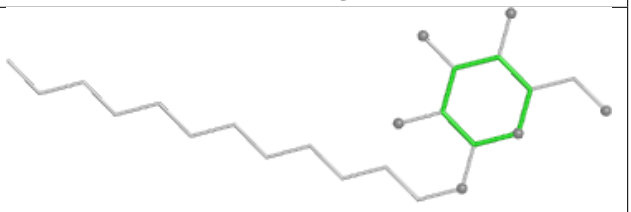
Bond lengths



Bond angles

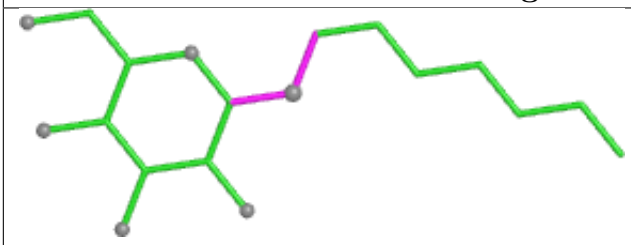


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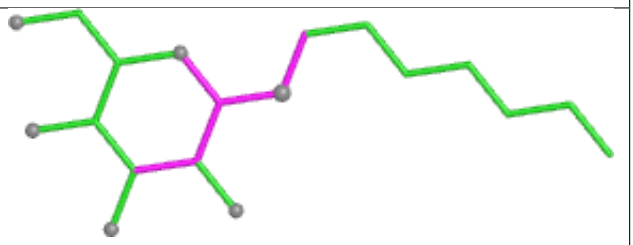


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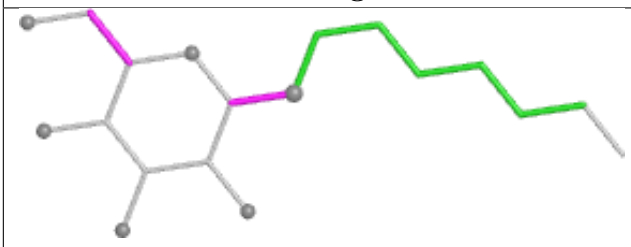
Ligand HTG B 626



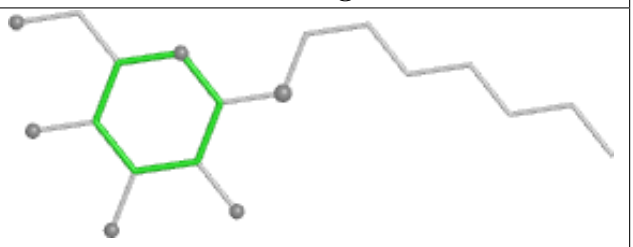
Bond lengths



Bond angles

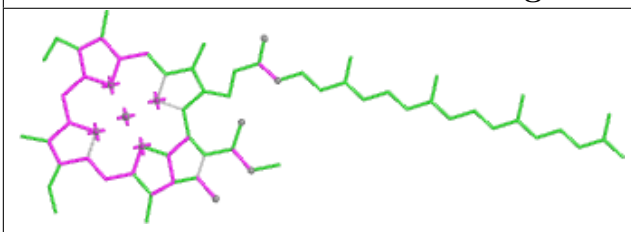


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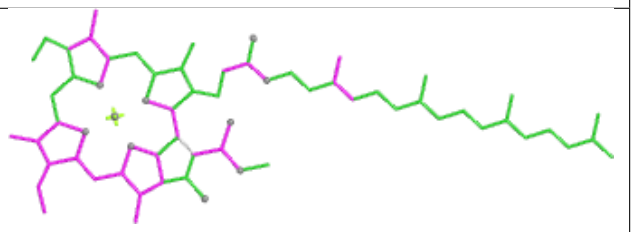


Rings

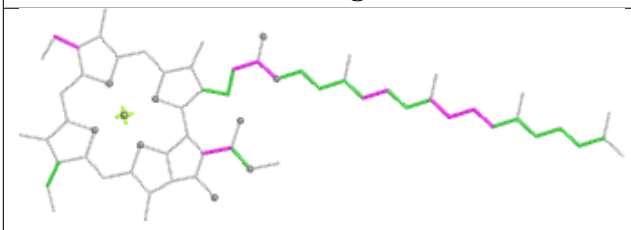
Ligand CLA B 602



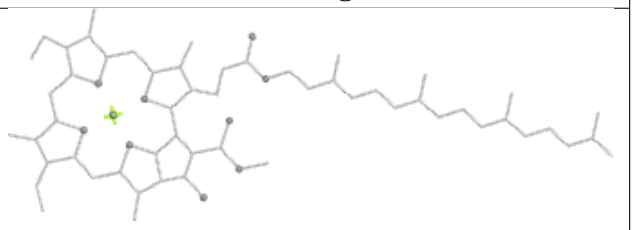
Bond lengths



Bond angles

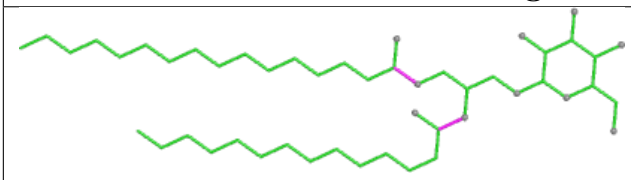


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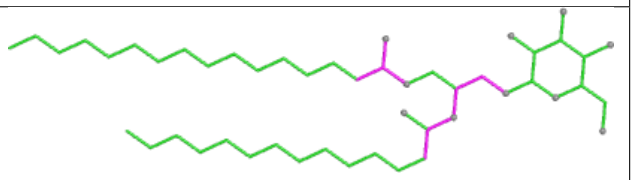


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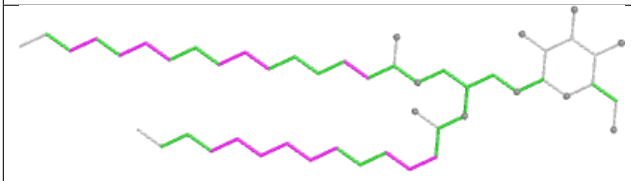
Ligand LMG c 521



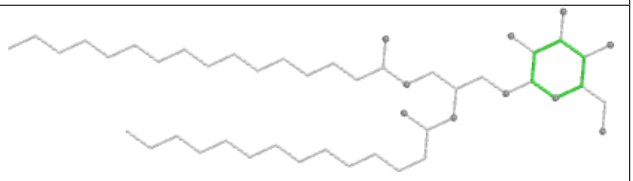
Bond lengths



Bond angles

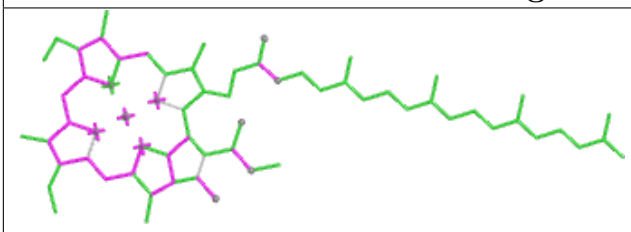


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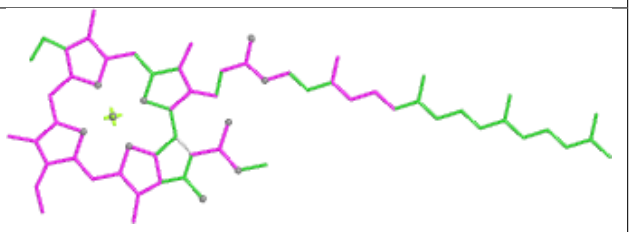


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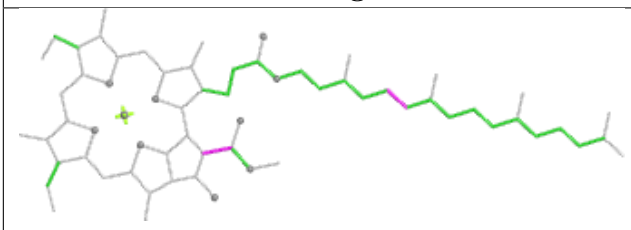
Ligand CLA b 606



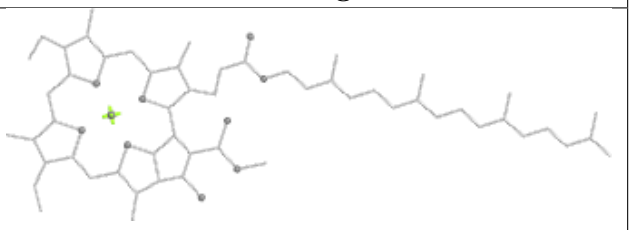
Bond lengths



Bond angles

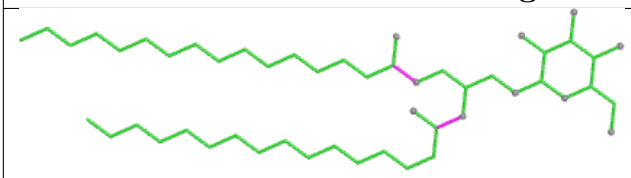


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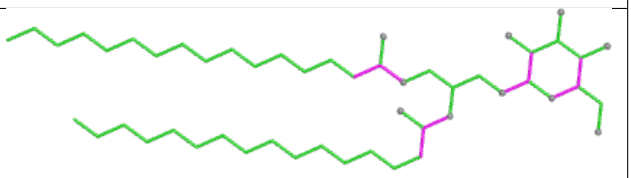


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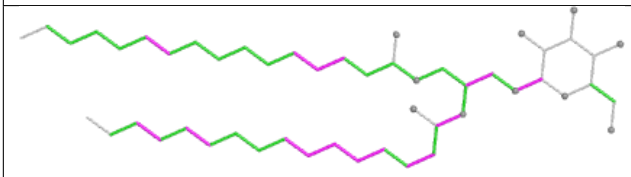
Ligand LMG A 412



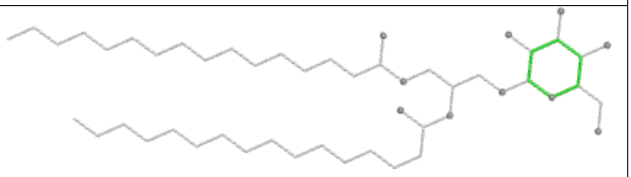
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Bond angles

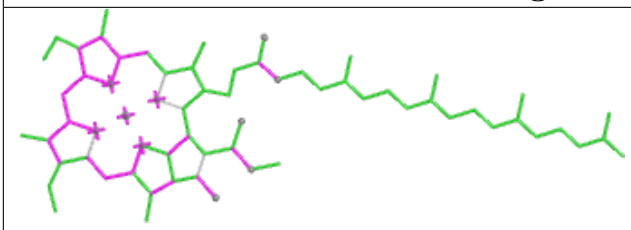


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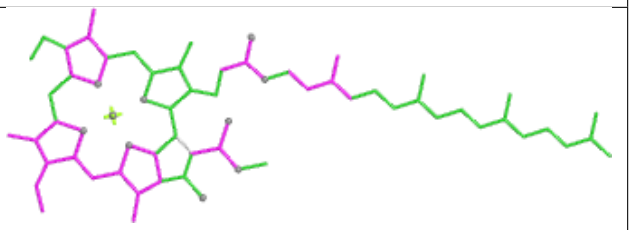


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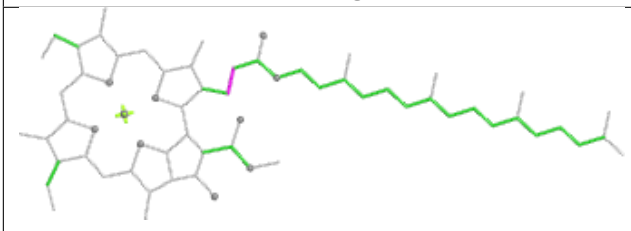
Ligand CLA c 503



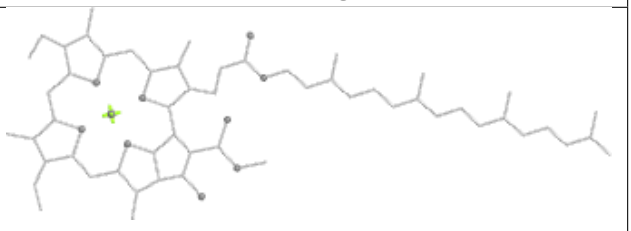
Bond lengths



Bond angles

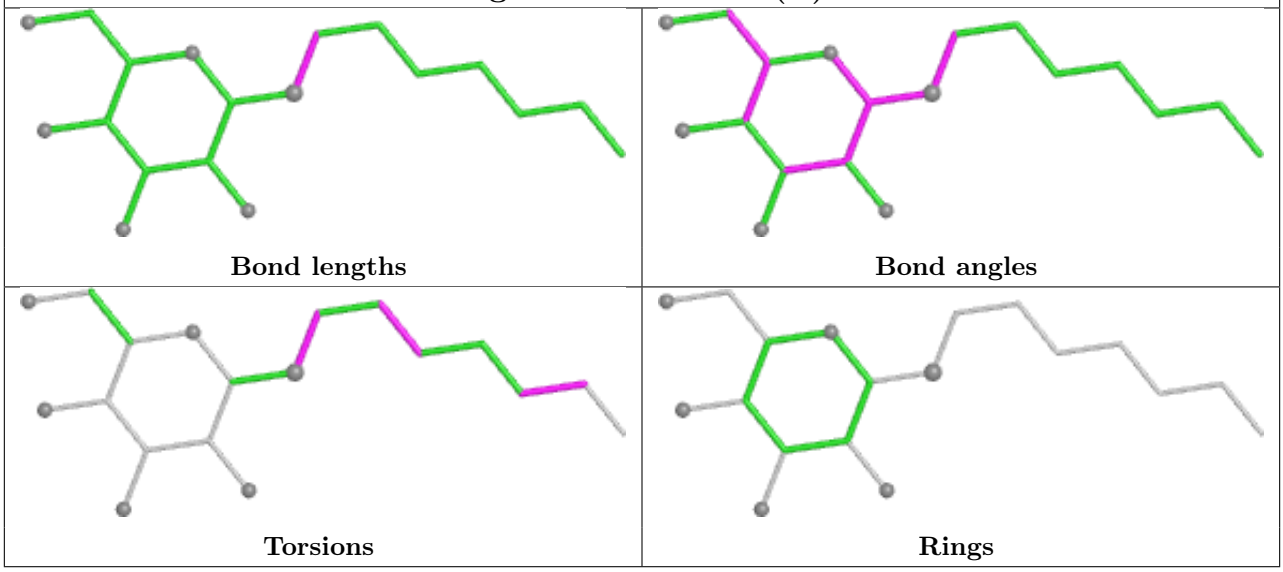


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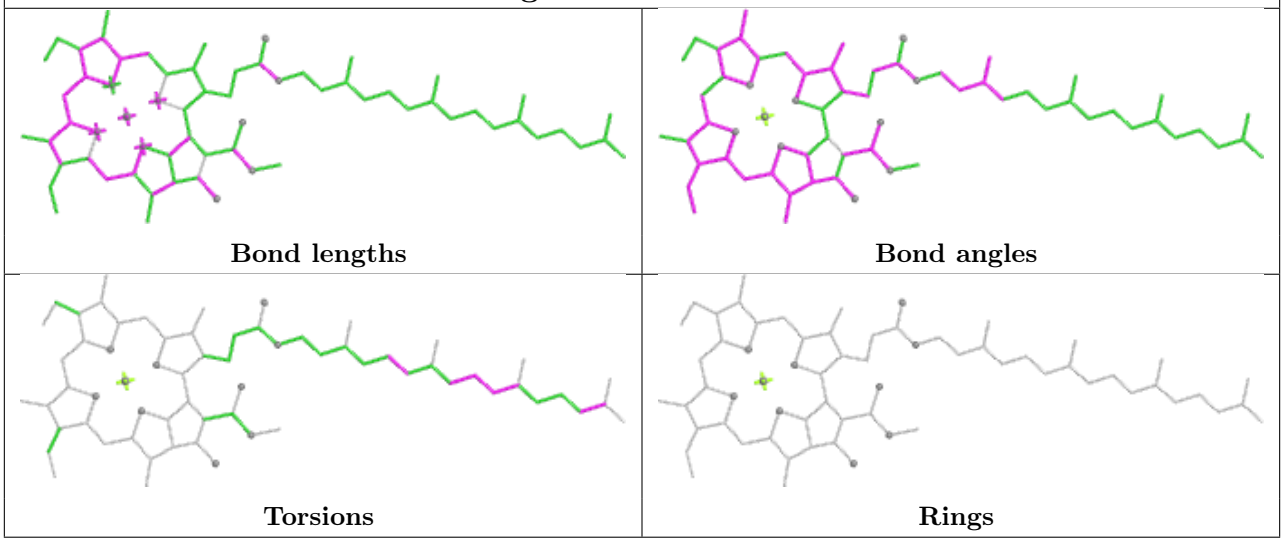


Rings

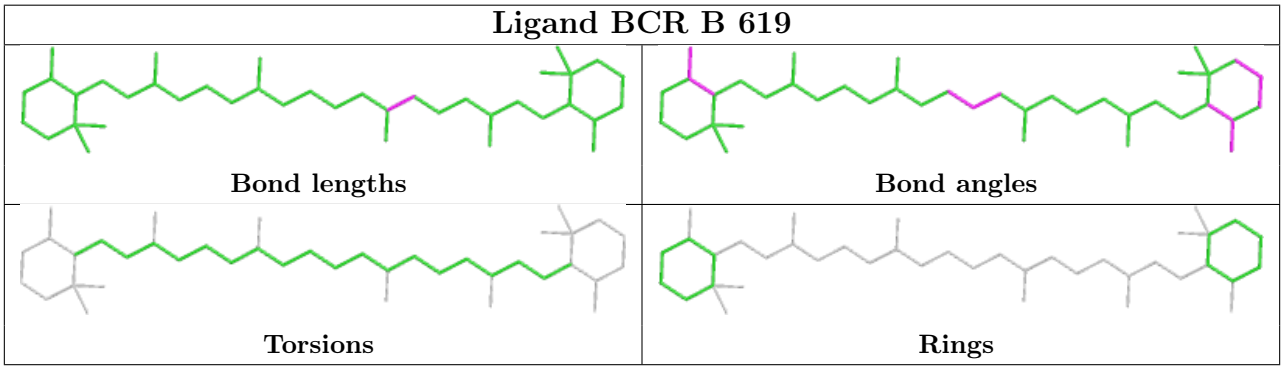
Ligand HTG B 625 (B)



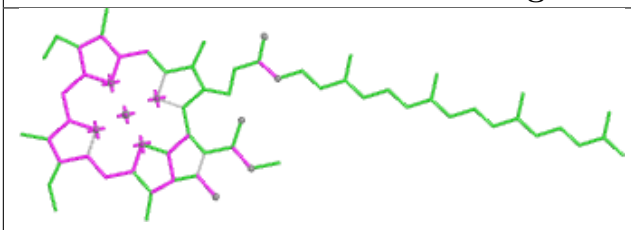
Ligand CLA a 2113



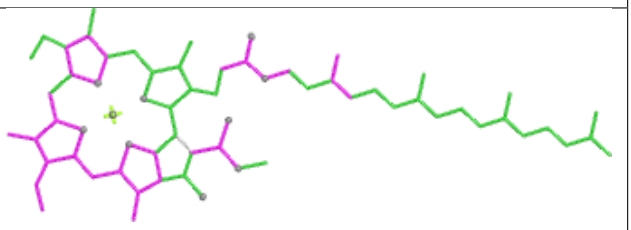
Ligand BCR B 619



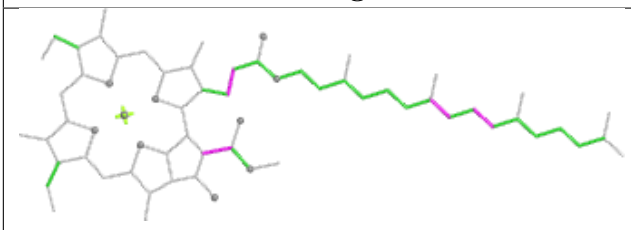
Ligand CLA b 609



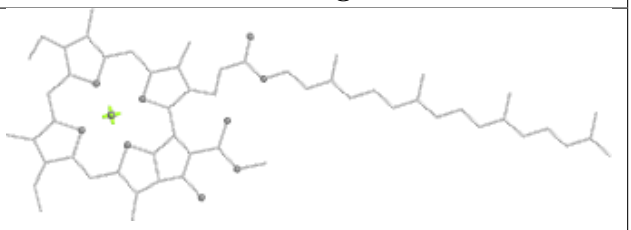
Bond lengths



Bond angles

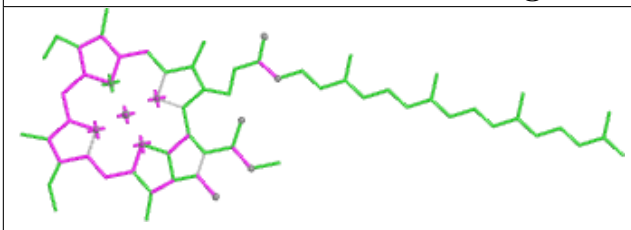


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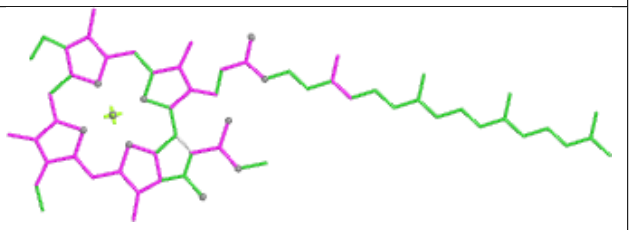


Rings

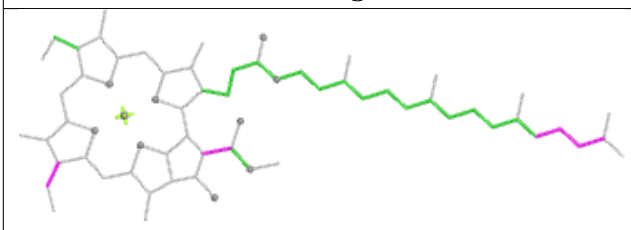
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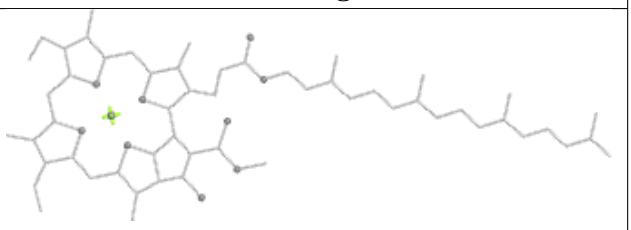
Bond lengths



Bond angles

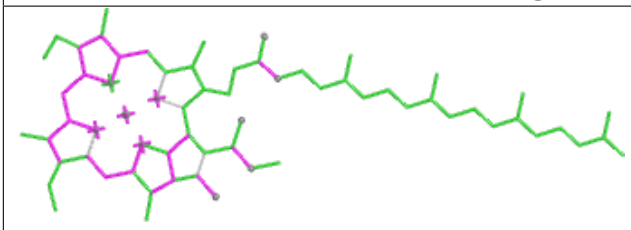


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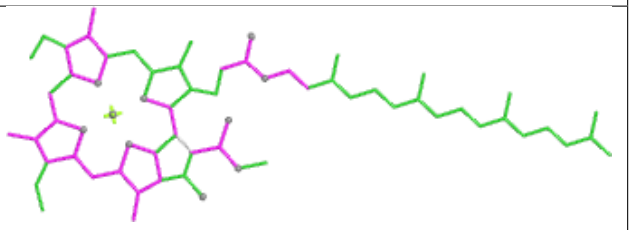


Rings

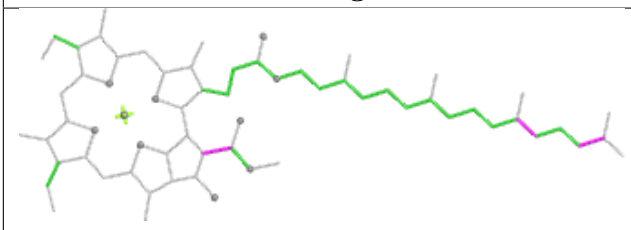
Ligand CLA c 504



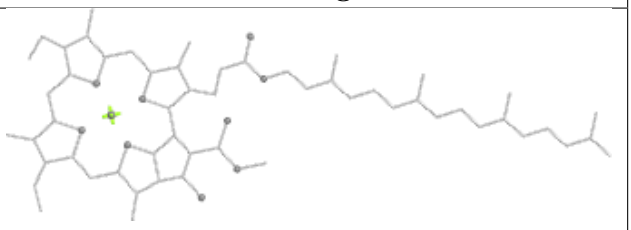
Bond lengths



Bond angles

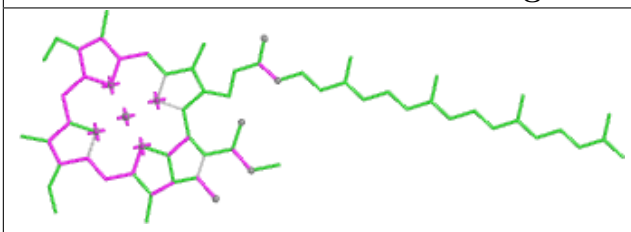


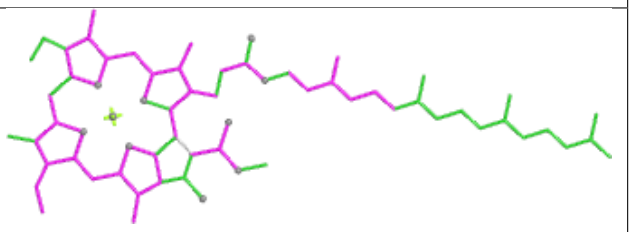
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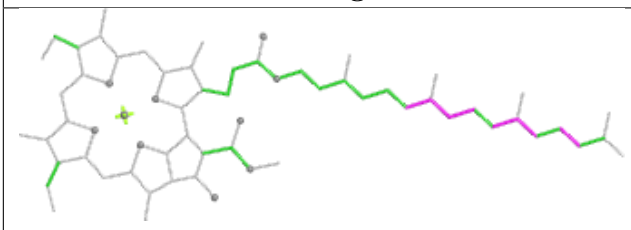


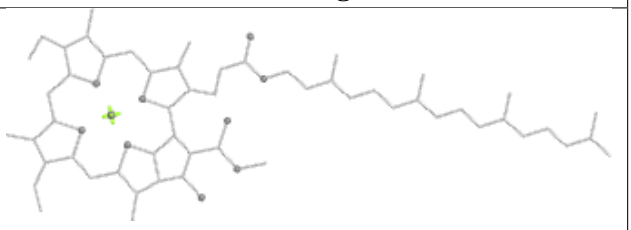
Rings

Ligand CLA A 409


Bond lengths


Bond angles


Torsions


Rings

Ligand PL9 A 417

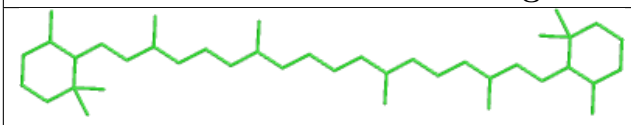

Bond lengths

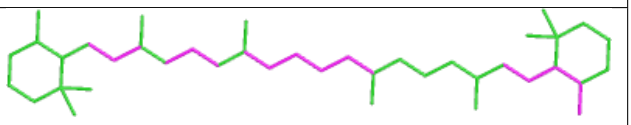

Bond angles


Torsions

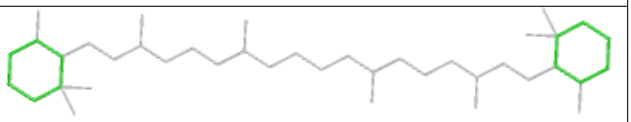

Rings

Ligand BCR B 620

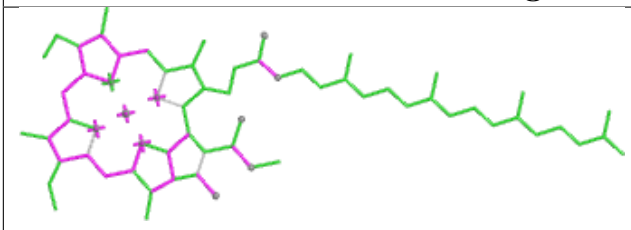

Bond lengths

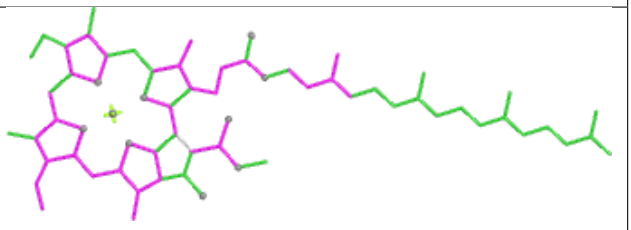

Bond angles

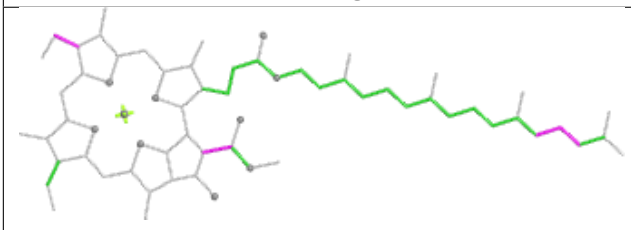

Torsions

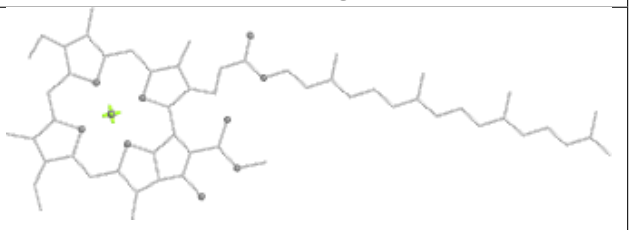

Rings

Ligand CLA B 603

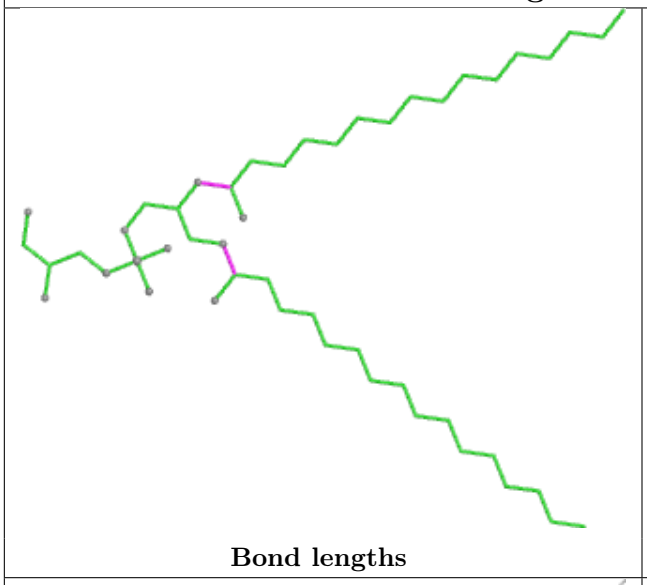

Bond lengths


Bond angles

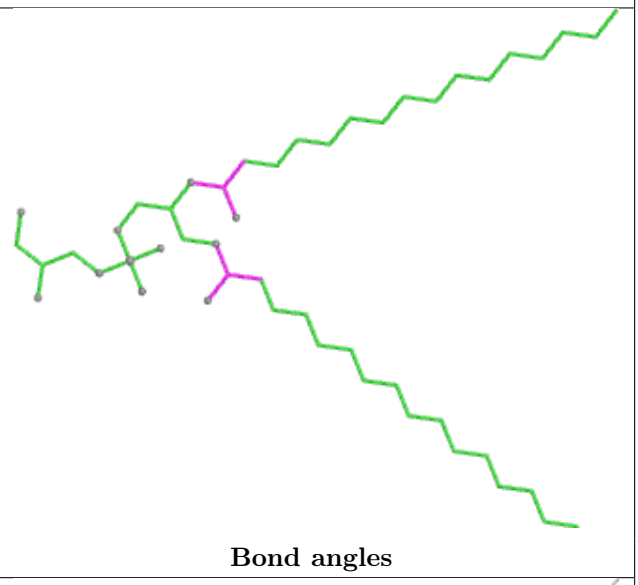

Torsions


Rings

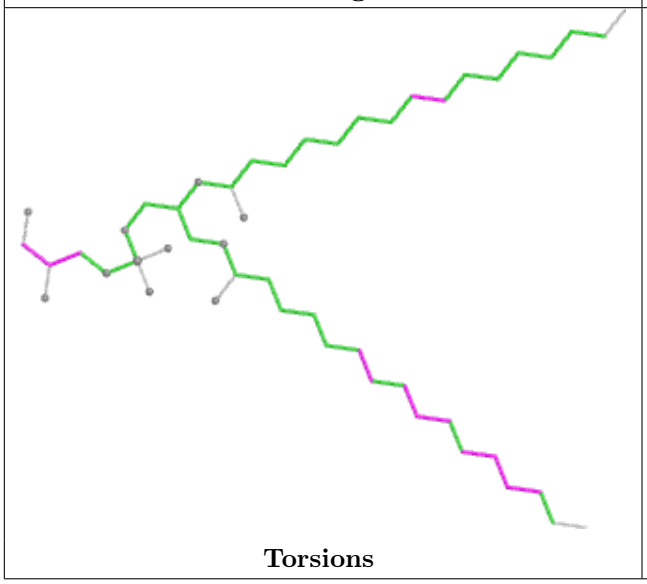
Ligand LHG d 408



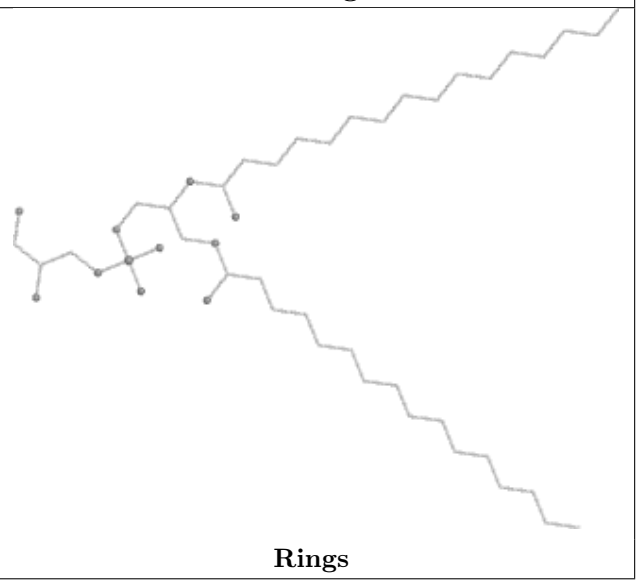
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Bond angles

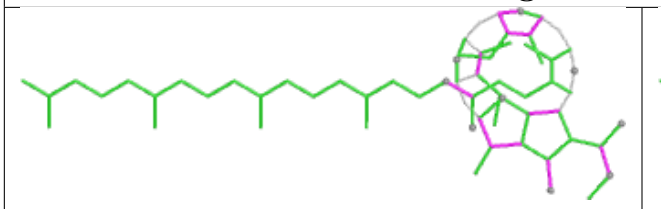


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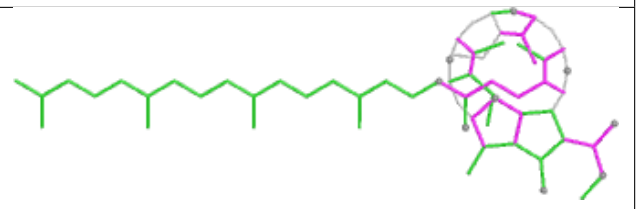


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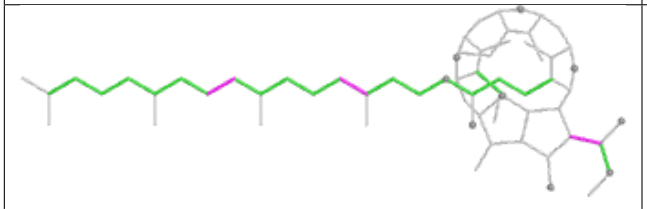
Ligand PHO a 2111



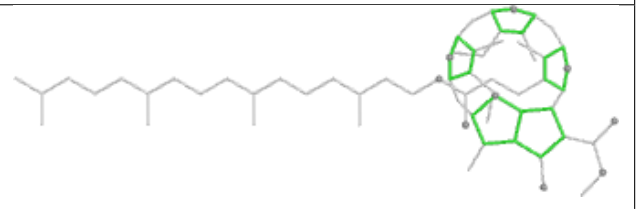
Bond lengths



Bond angles

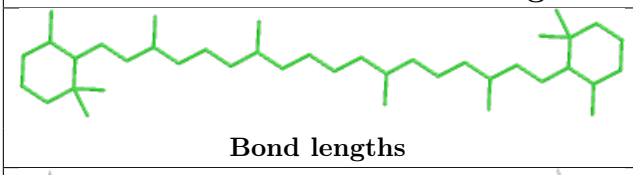


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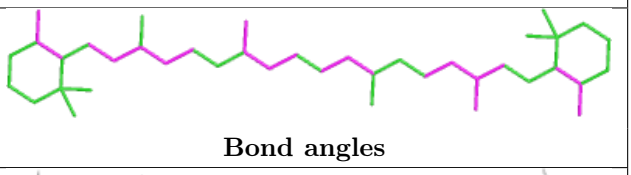


Rings

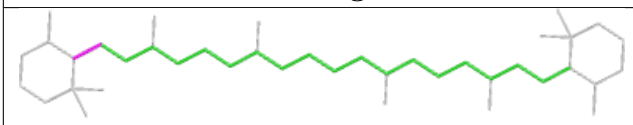
Ligand BCR c 516



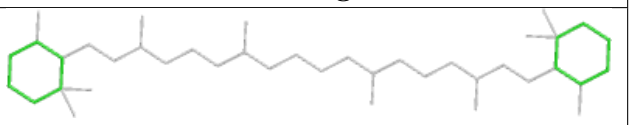
Bond lengths



Bond angles

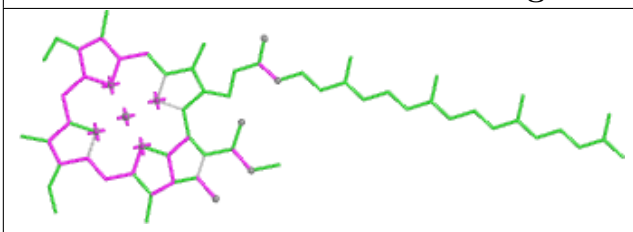


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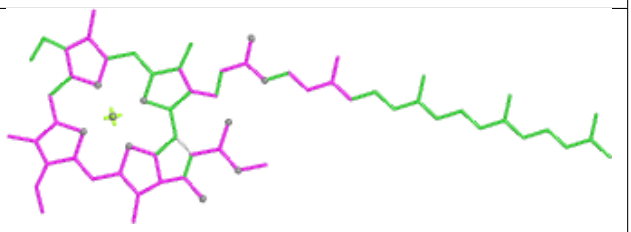


Rings

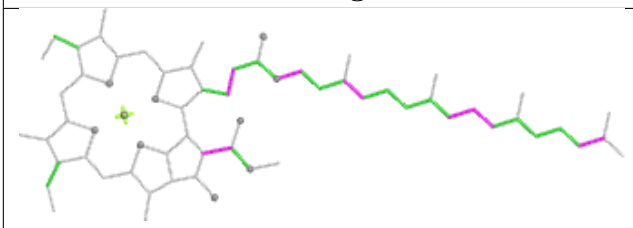
Ligand CLA b 617



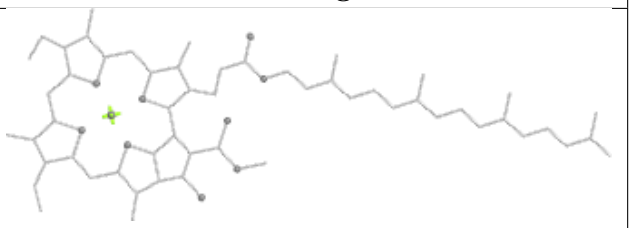
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Bond angles

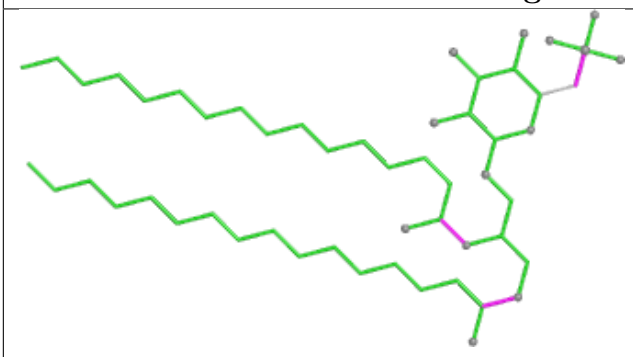


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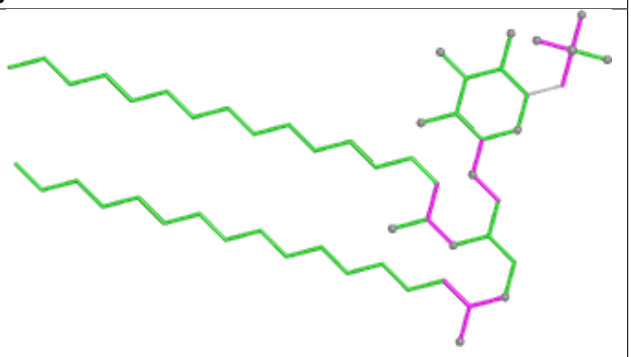


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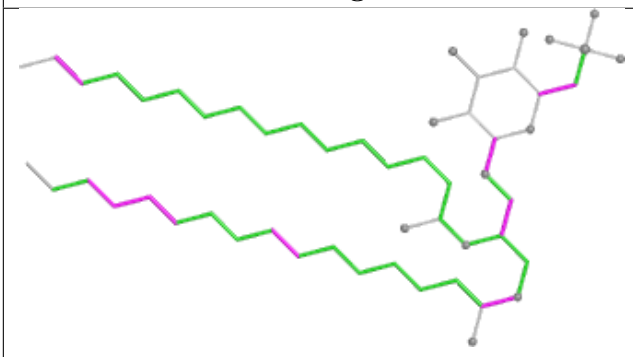
Ligand SQD A 413



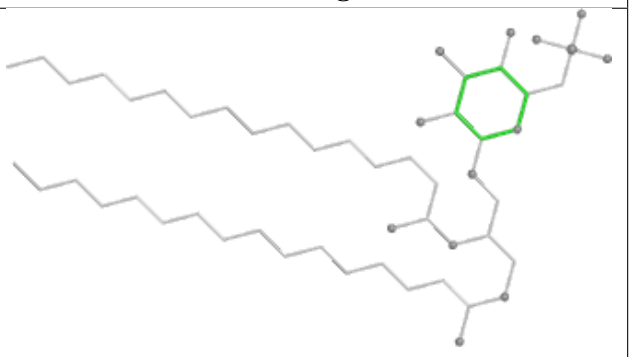
Bond lengths



Bond angles

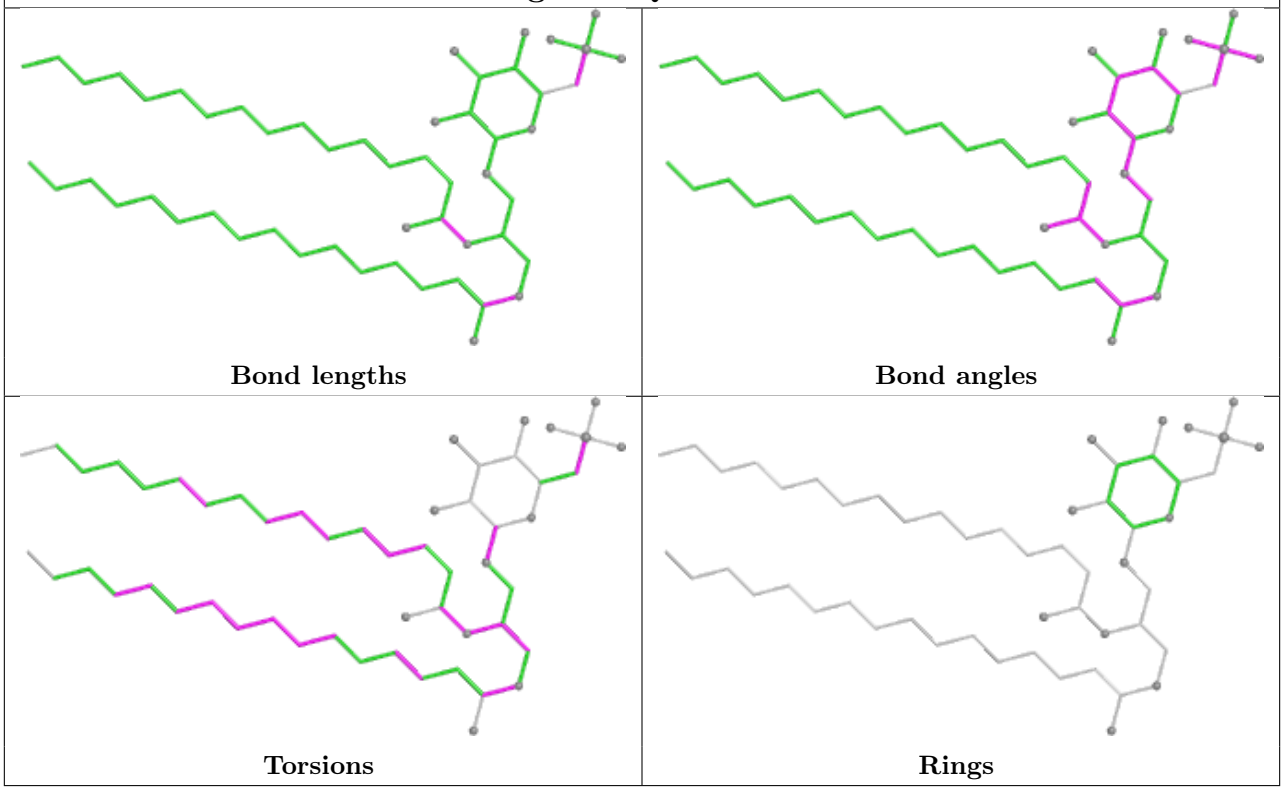


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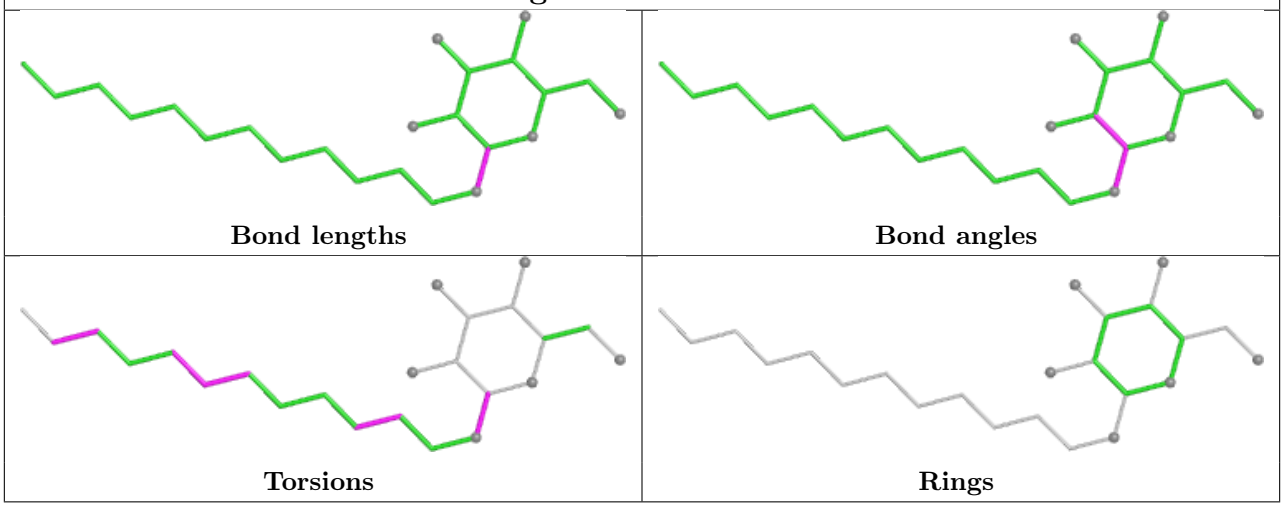


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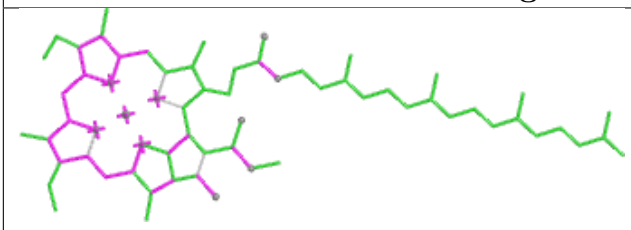
Ligand SQD L 102



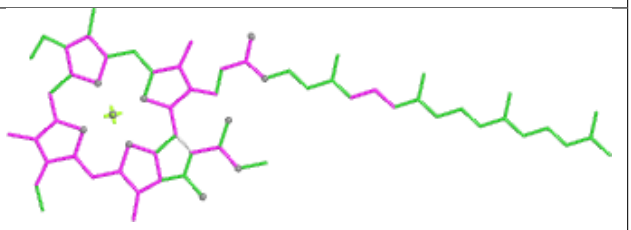
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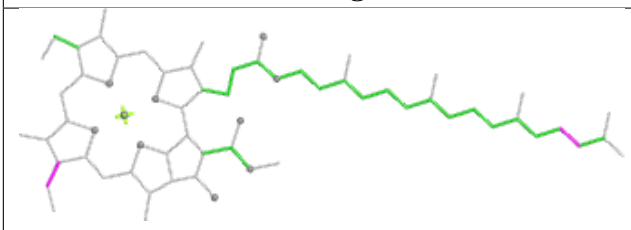
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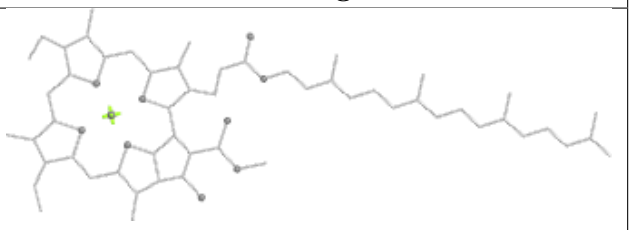
Bond lengths



Bond angles

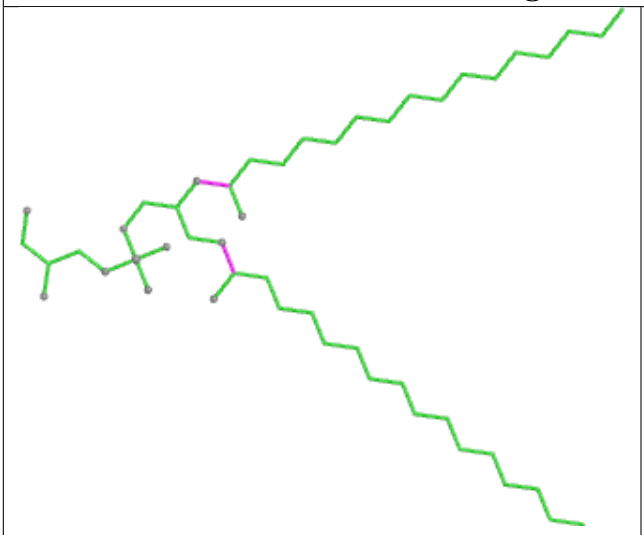


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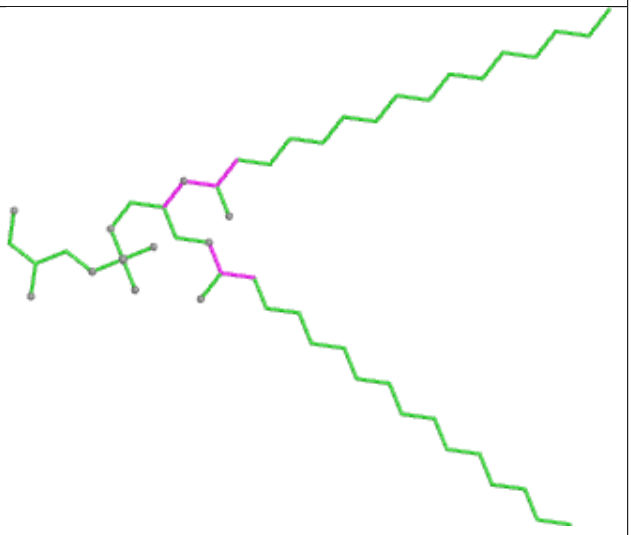


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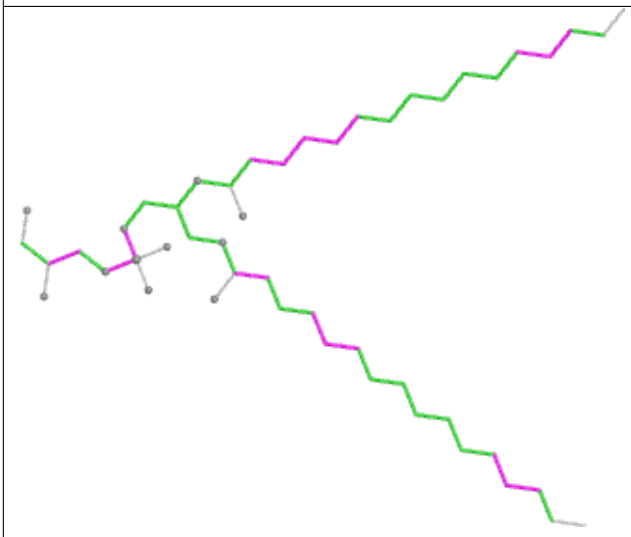
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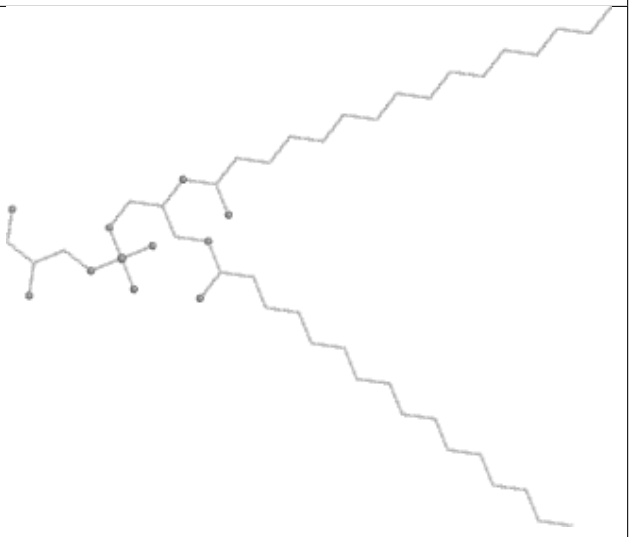
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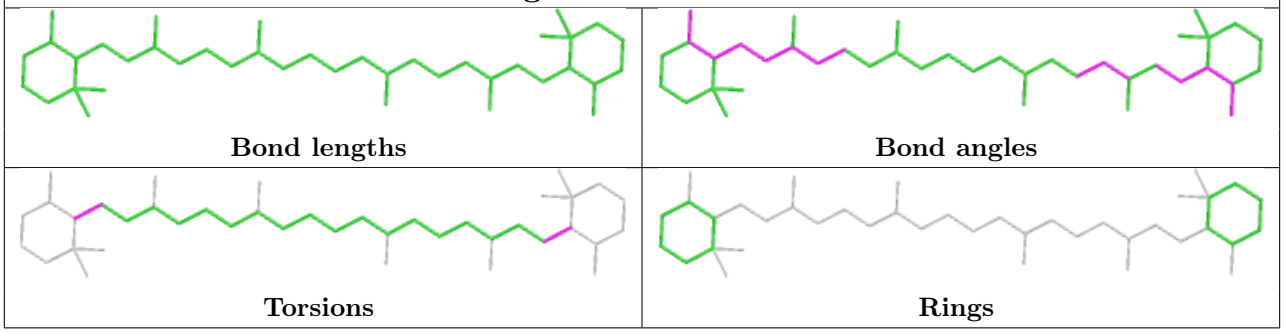


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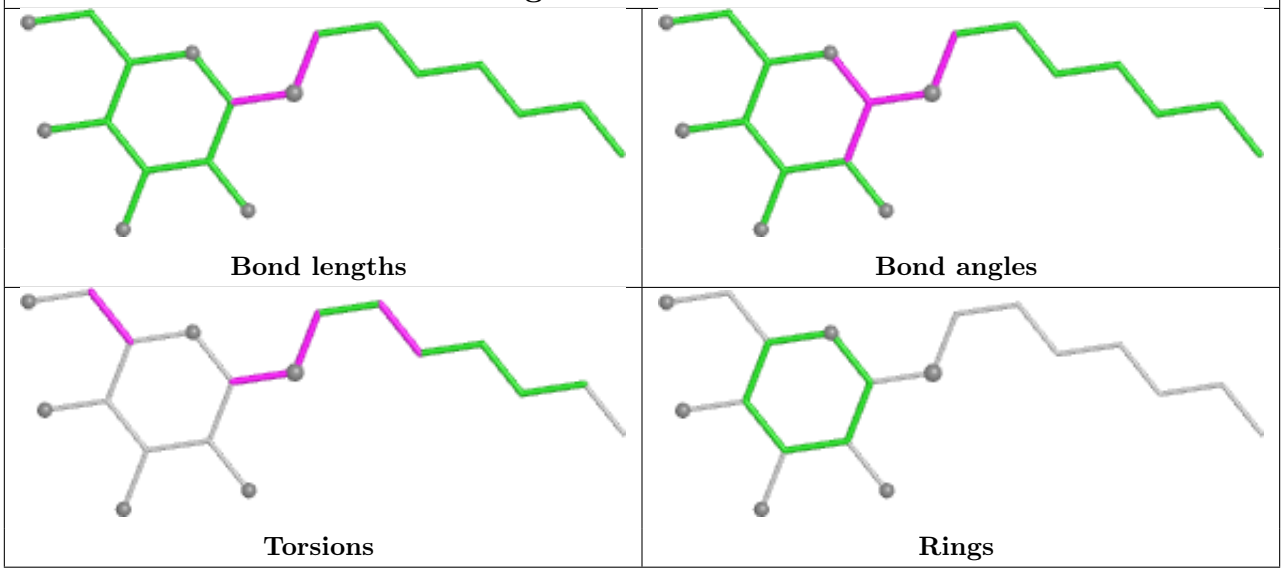


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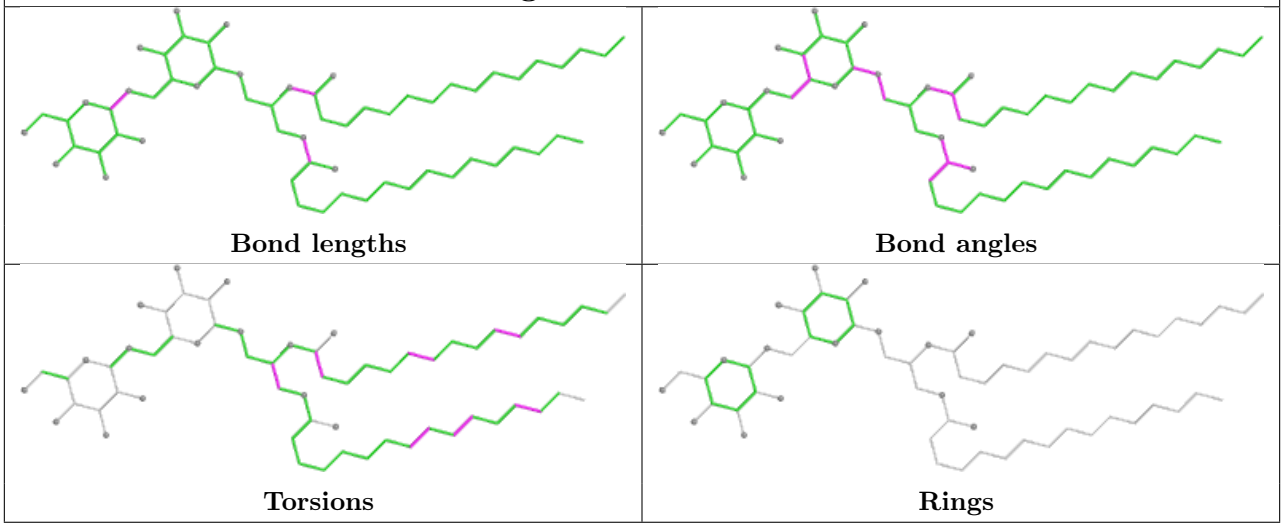
Ligand BCR C 515



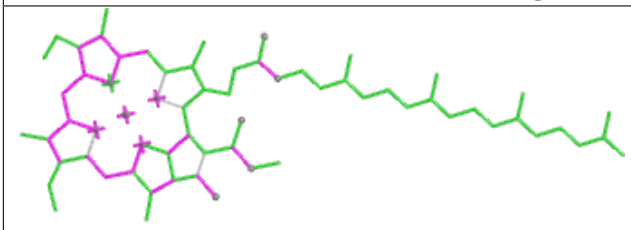
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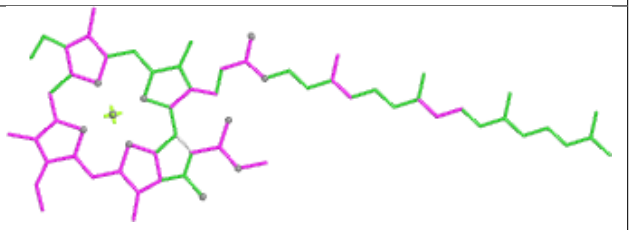
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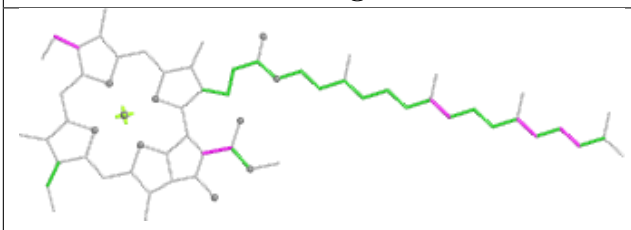
Ligand CLA c 506



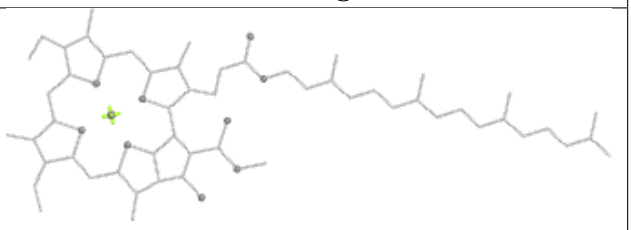
Bond lengths



Bond angles

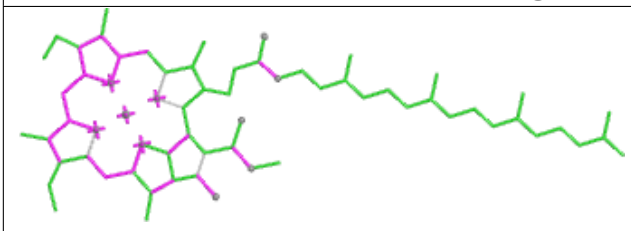


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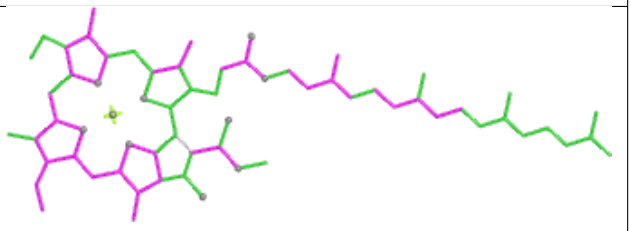


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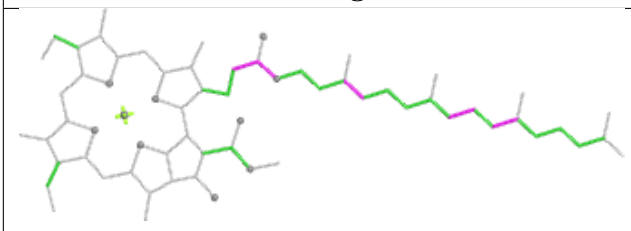
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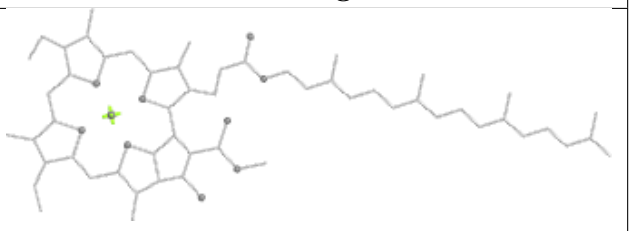
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Bond angles

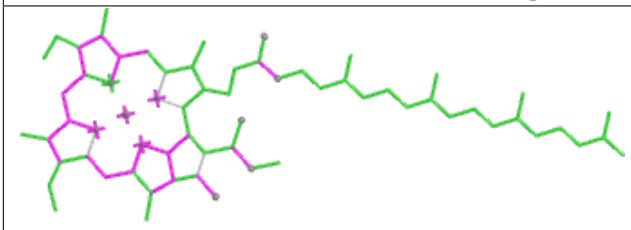


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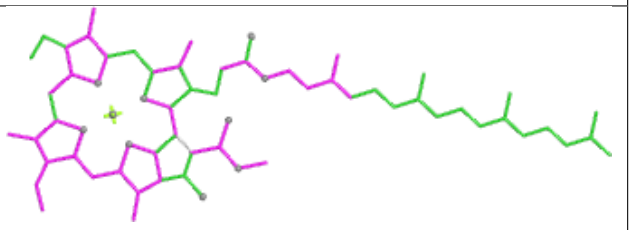


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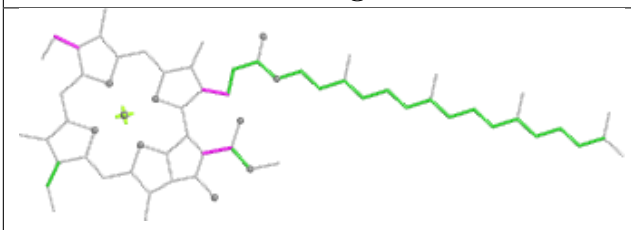
Ligand CLA B 610



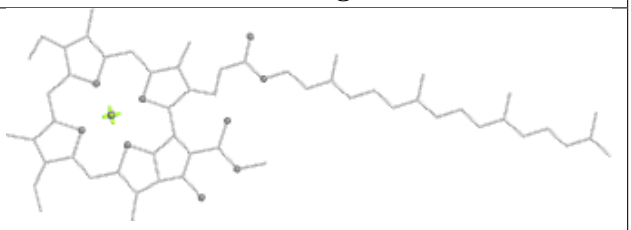
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Bond angles

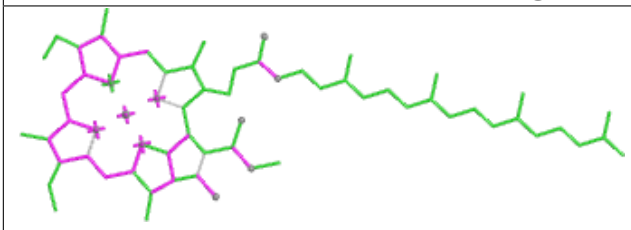


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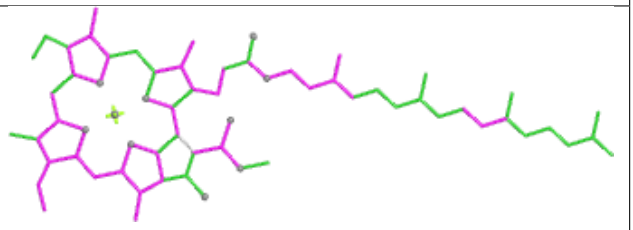


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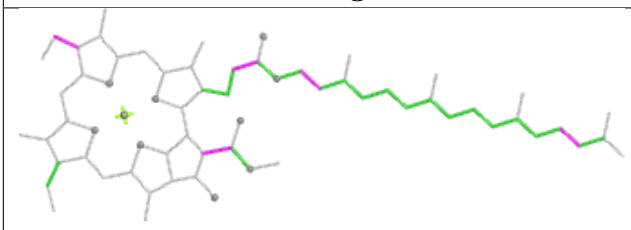
Ligand CLA c 514



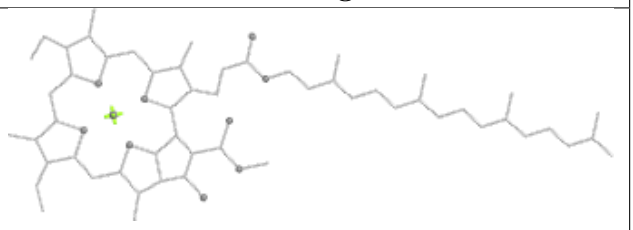
Bond lengths



Bond angles

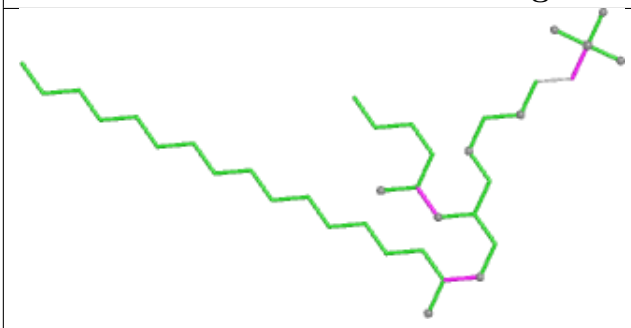


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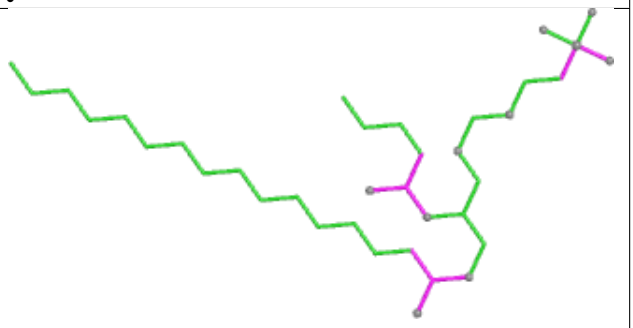


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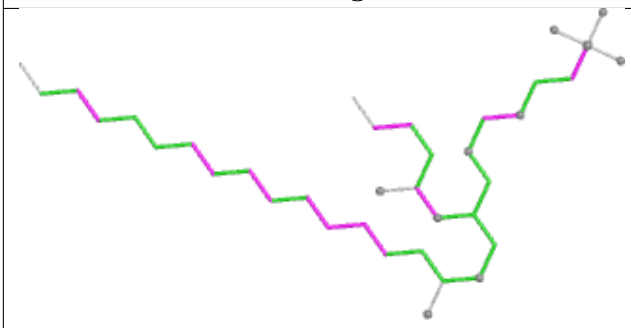
Ligand SQD f 102



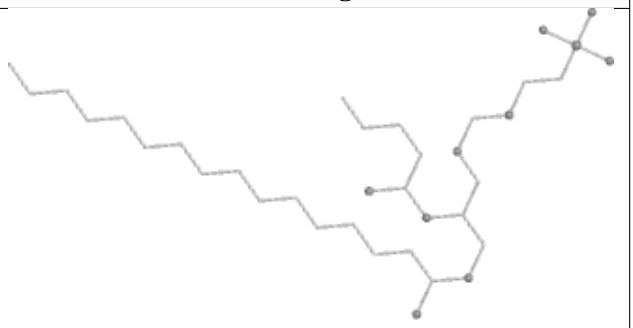
Bond lengths



Bond angles

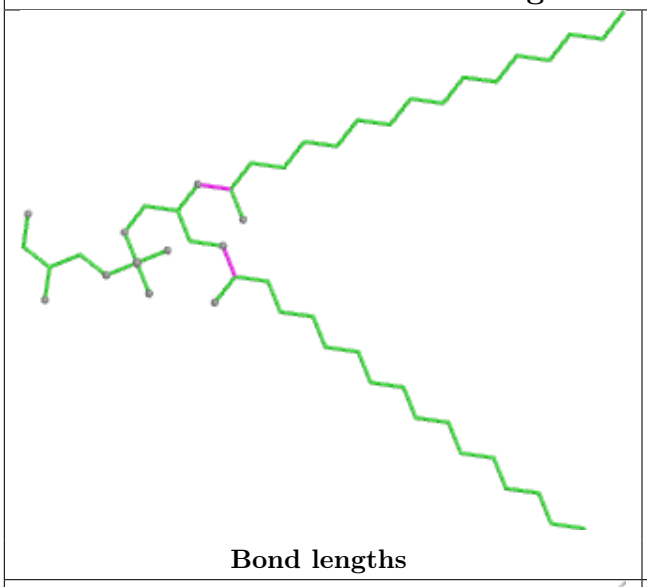


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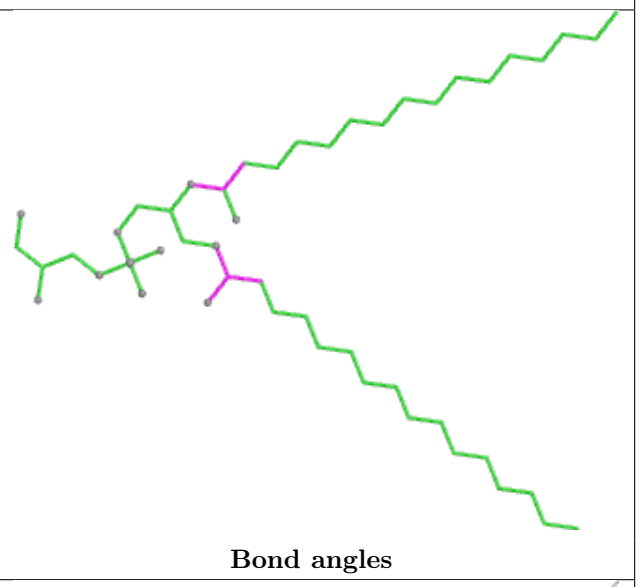


Rings

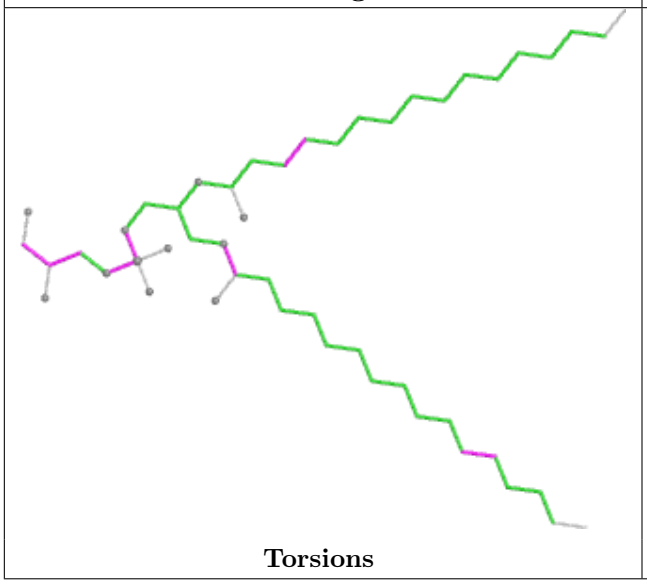
Ligand LHG d 409



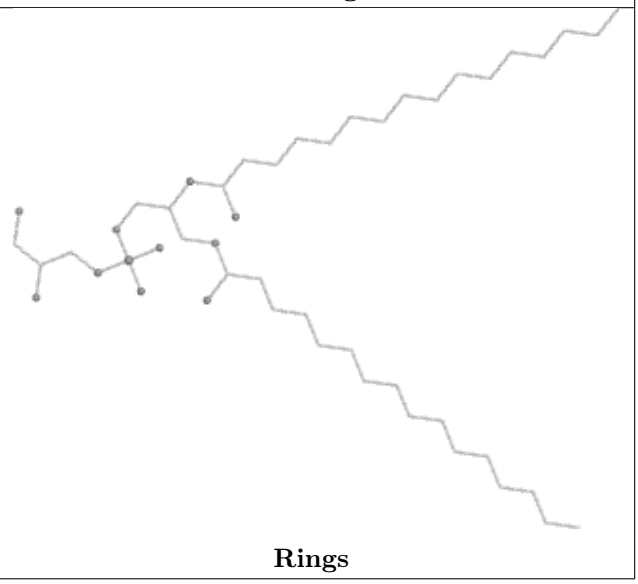
Bond lengths



Bond angles



Torsions



Rings

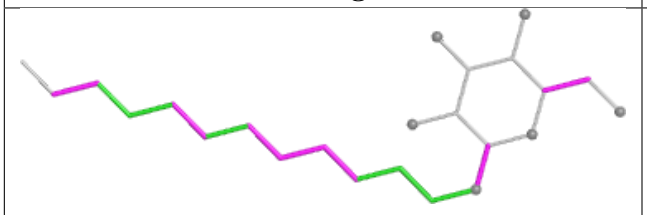
Ligand LMT B 637



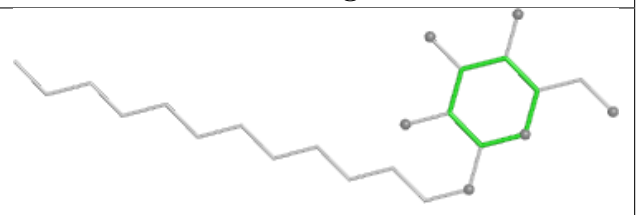
Bond lengths



Bond angles

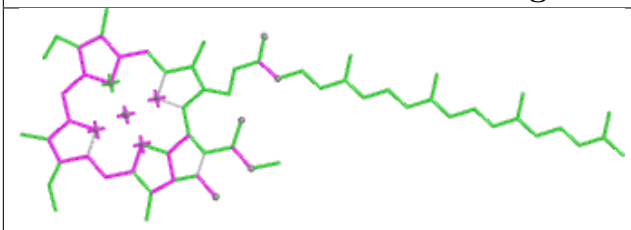


Torsions

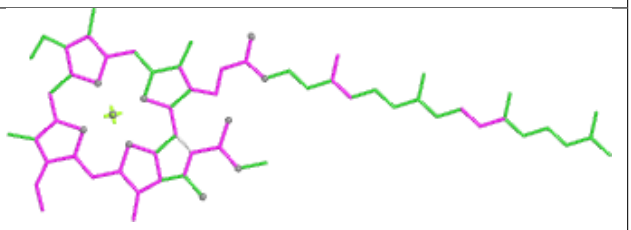


Rings

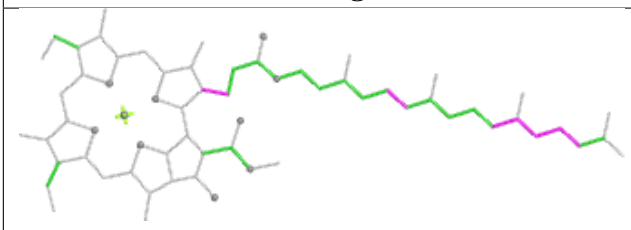
Ligand CLA c 508



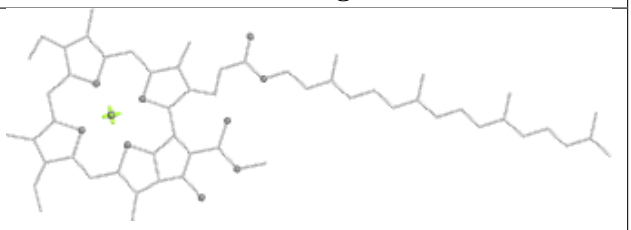
Bond lengths



Bond angles

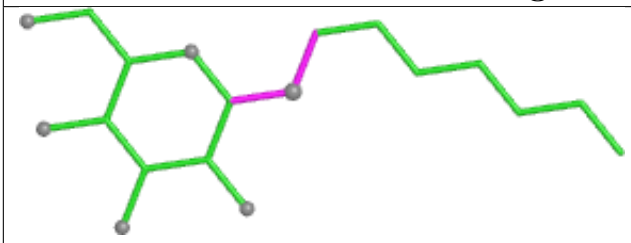


Torsions

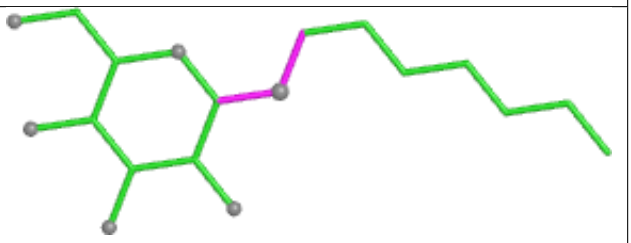


Rings

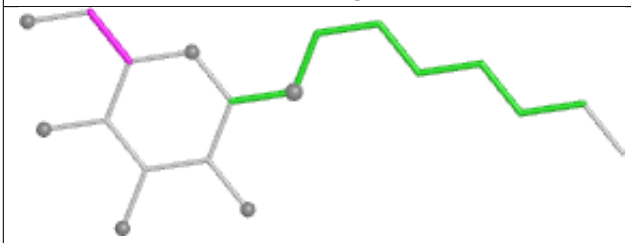
Ligand HTG i 103



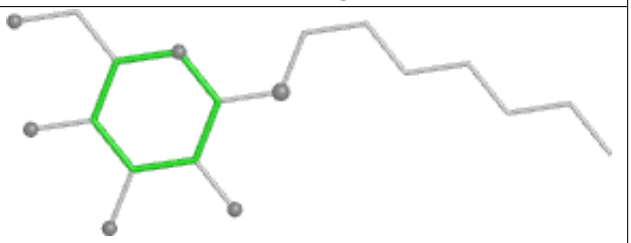
Bond lengths



Bond angles

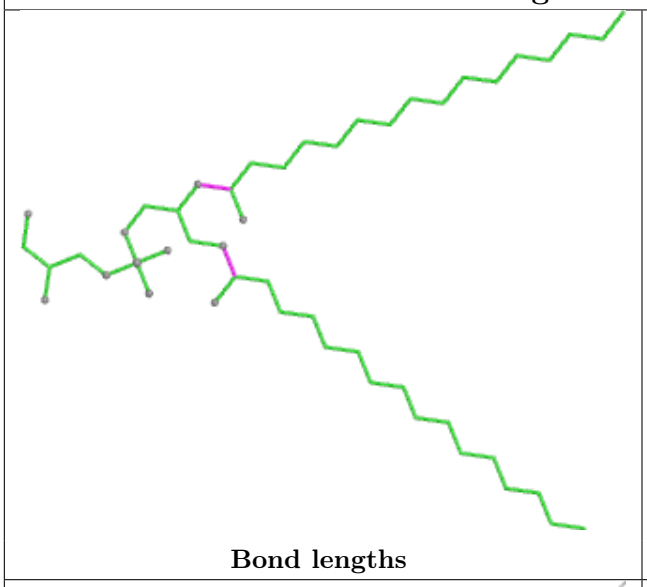


Torsions

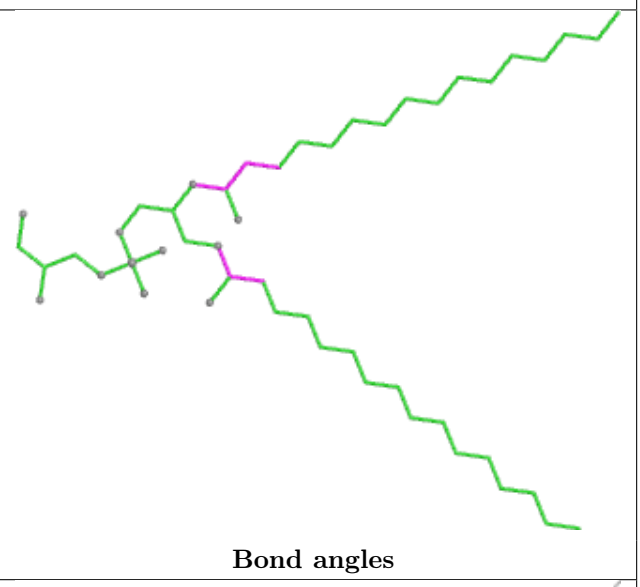


Rings

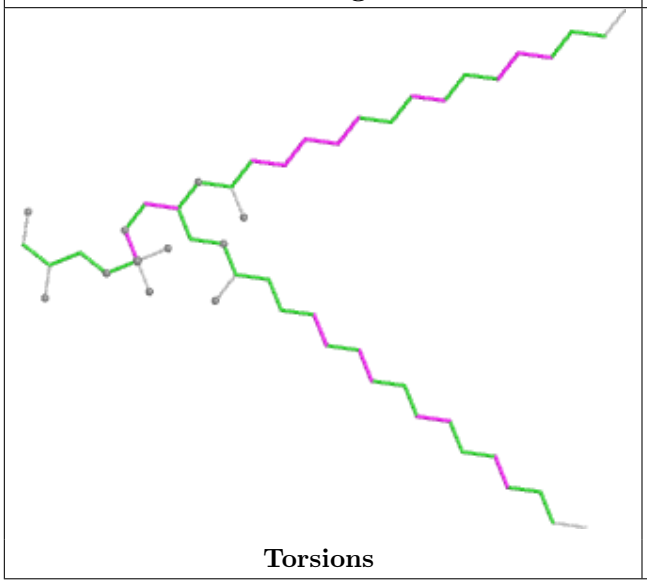
Ligand LHG l 101



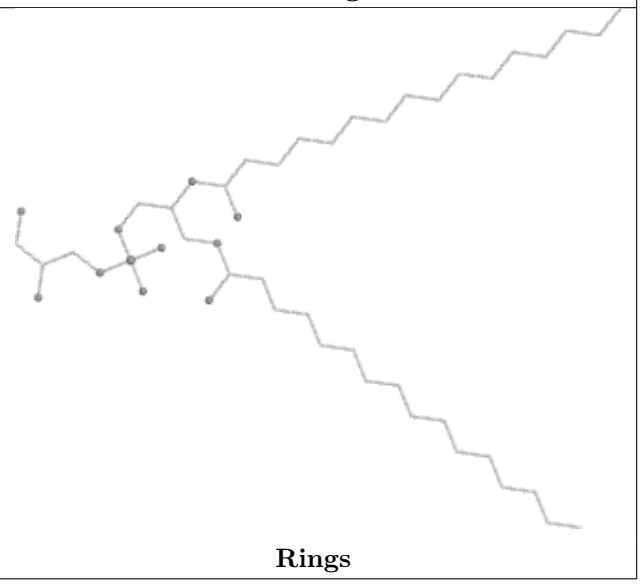
Bond lengths



Bond angles



Torsions

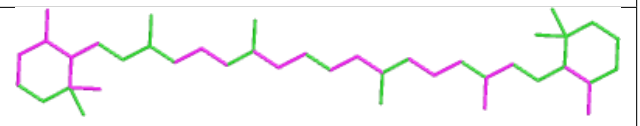


Rings

Ligand BCR Y 302



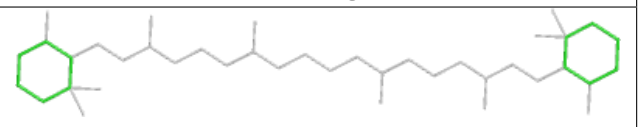
Bond lengths



Bond angles

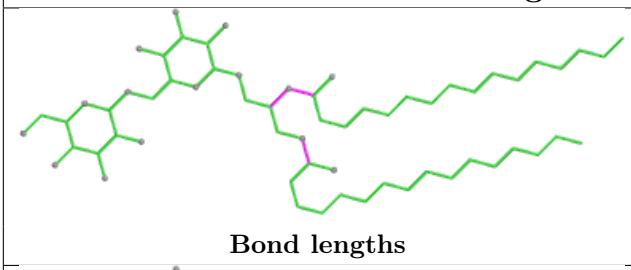


Torsions

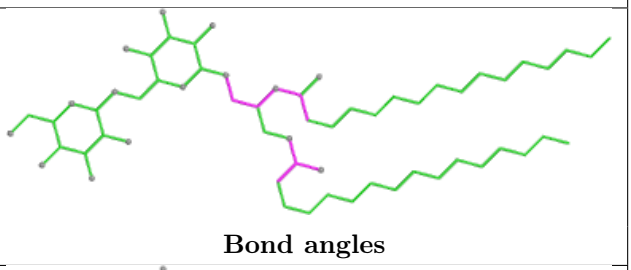


Rings

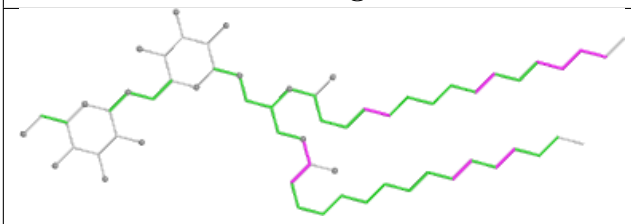
Ligand DGD c 520



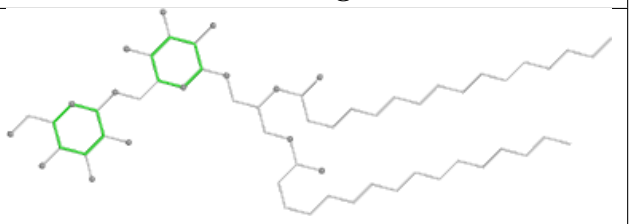
Bond lengths



Bond angles

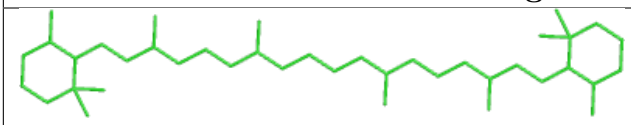


Torsions

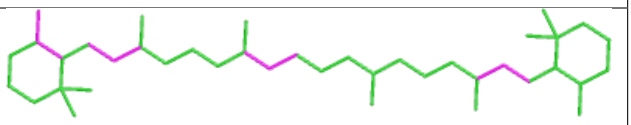


Rings

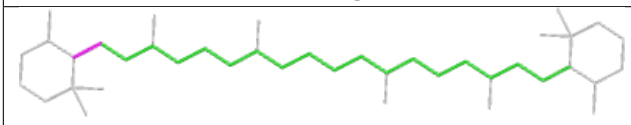
Ligand BCR b 620



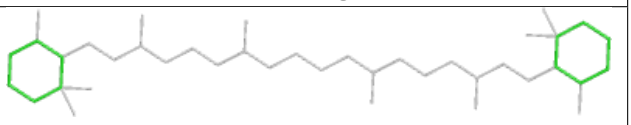
Bond lengths



Bond angles

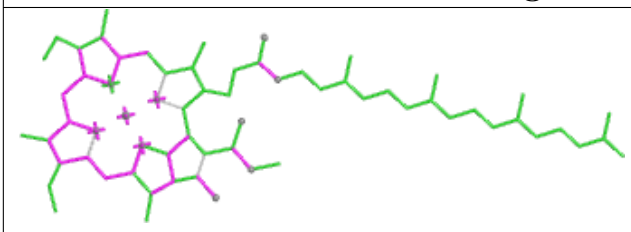


Torsions

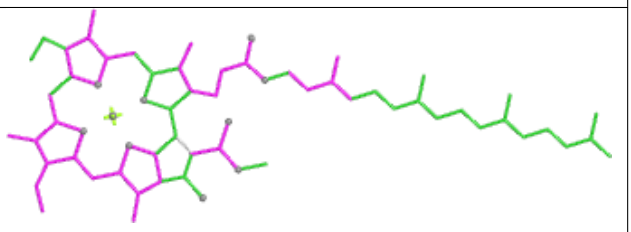


Rings

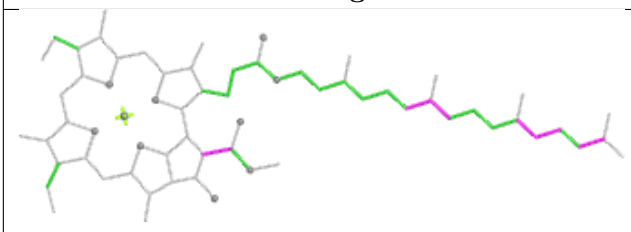
Ligand CLA A 406



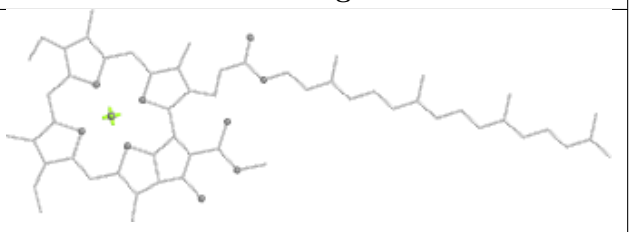
Bond lengths



Bond angles

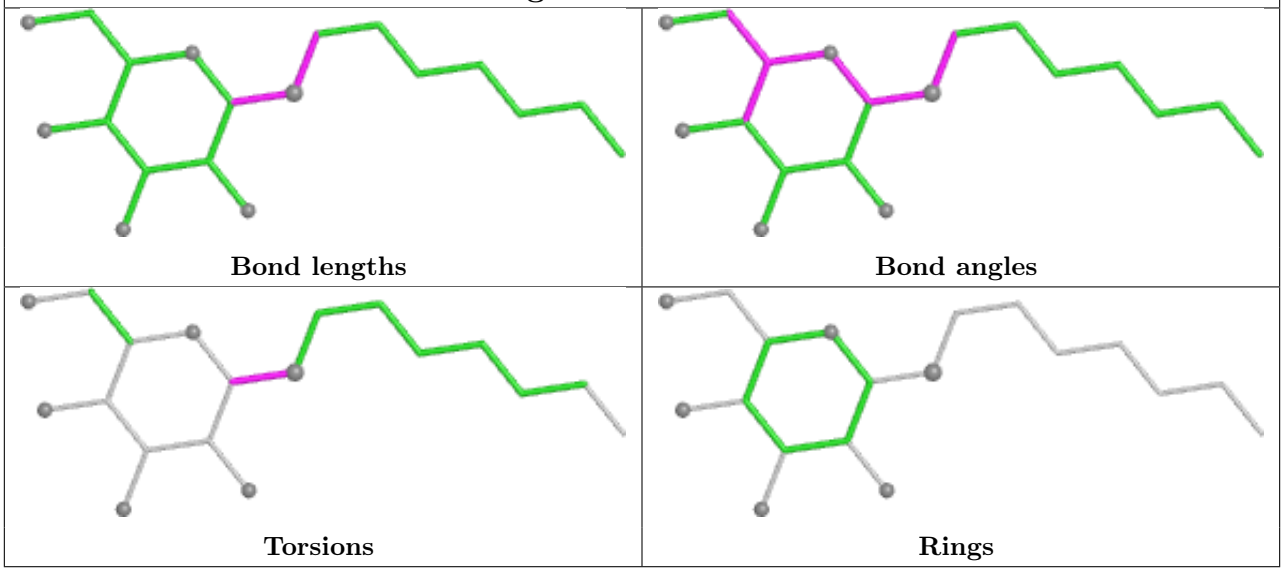


Torsions

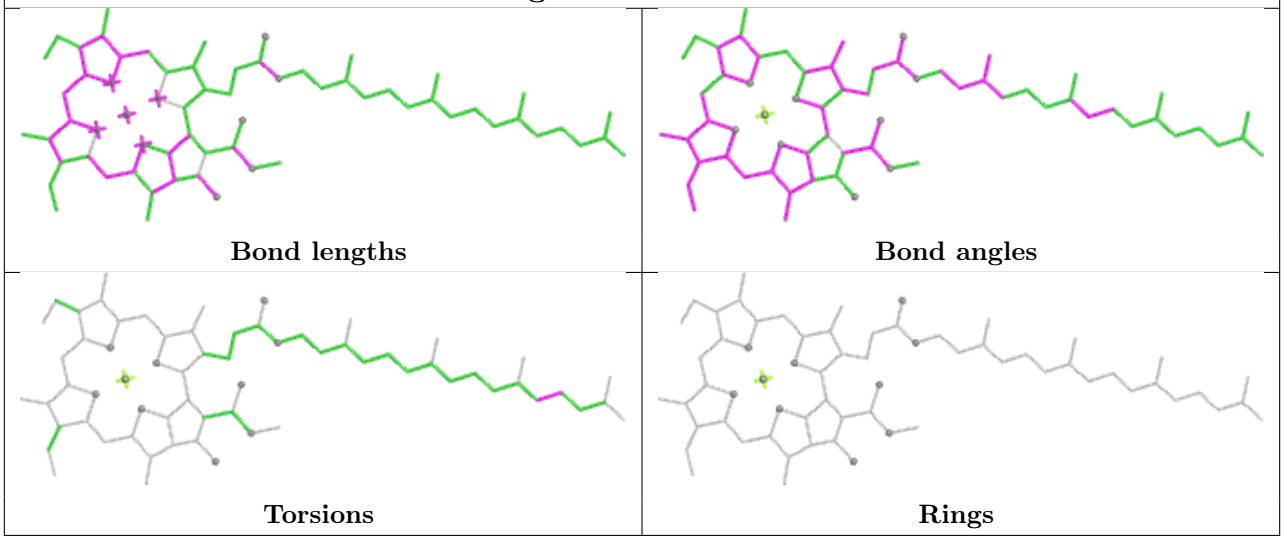


Rings

Ligand HTG c 523



Ligand CLA b 611



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.22	4 (1%) 76 78	27, 43, 72, 128	3 (0%)
1	a	334/344 (97%)	-0.07	7 (2%) 63 66	27, 45, 84, 116	3 (0%)
2	B	505/505 (100%)	-0.13	10 (1%) 65 67	27, 48, 79, 117	5 (0%)
2	b	503/505 (99%)	-0.05	17 (3%) 48 50	31, 50, 88, 168	8 (1%)
3	C	451/455 (99%)	-0.13	5 (1%) 78 80	35, 52, 71, 138	2 (0%)
3	c	455/455 (100%)	-0.00	4 (0%) 81 83	43, 57, 75, 119	0
4	D	340/342 (99%)	-0.25	1 (0%) 90 91	22, 44, 64, 107	1 (0%)
4	d	341/342 (99%)	-0.28	0 100 100	25, 46, 70, 114	3 (0%)
5	E	80/83 (96%)	0.28	4 (5%) 34 36	44, 66, 108, 118	1 (1%)
5	e	79/83 (95%)	0.29	3 (3%) 44 46	52, 67, 101, 124	0
6	F	34/44 (77%)	-0.20	1 (2%) 53 56	48, 56, 86, 104	0
6	f	32/44 (72%)	0.19	3 (9%) 14 14	49, 58, 104, 129	0
7	H	63/63 (100%)	0.15	1 (1%) 70 73	45, 57, 74, 103	0
7	h	63/63 (100%)	0.29	1 (1%) 70 73	46, 61, 80, 102	0
8	I	35/38 (92%)	0.61	1 (2%) 53 56	47, 63, 114, 124	0
8	i	35/38 (92%)	0.29	1 (2%) 53 56	47, 62, 109, 130	0
9	J	36/40 (90%)	-0.03	2 (5%) 30 32	45, 60, 95, 109	0
9	j	39/40 (97%)	-0.03	0 100 100	51, 62, 86, 108	0
10	K	37/37 (100%)	-0.07	0 100 100	38, 59, 73, 88	1 (2%)
10	k	37/37 (100%)	0.28	1 (2%) 56 59	54, 64, 85, 100	0
11	L	37/37 (100%)	-0.12	4 (10%) 11 11	22, 42, 94, 127	1 (2%)
11	l	36/37 (97%)	-0.24	1 (2%) 55 57	23, 43, 101, 128	2 (5%)
12	M	32/36 (88%)	-0.25	0 100 100	25, 44, 63, 86	1 (3%)
12	m	33/36 (91%)	-0.06	0 100 100	26, 45, 82, 105	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	0.02	3 (1%) 76 78	32, 55, 89, 169	2 (0%)
13	o	243/244 (99%)	0.00	4 (1%) 70 73	29, 57, 101, 138	3 (1%)
14	T	29/32 (90%)	-0.01	2 (6%) 23 24	36, 43, 72, 147	0
14	t	29/32 (90%)	-0.06	1 (3%) 48 50	37, 43, 76, 98	0
15	U	97/104 (93%)	-0.14	0 100 100	37, 52, 79, 92	1 (1%)
15	u	97/104 (93%)	-0.10	1 (1%) 79 81	46, 56, 75, 124	0
16	V	137/137 (100%)	-0.19	2 (1%) 72 74	32, 50, 68, 98	1 (0%)
16	v	137/137 (100%)	-0.13	0 100 100	48, 63, 87, 99	0
17	Y	30/30 (100%)	0.40	1 (3%) 49 51	59, 74, 114, 121	0
17	y	29/30 (96%)	0.51	1 (3%) 48 50	64, 78, 100, 113	0
18	X	38/40 (95%)	0.13	2 (5%) 32 34	53, 66, 85, 92	0
18	x	38/40 (95%)	0.34	2 (5%) 32 34	37, 66, 123, 143	1 (2%)
19	Z	61/62 (98%)	0.39	2 (3%) 49 51	58, 69, 110, 130	0
19	z	60/62 (96%)	0.64	8 (13%) 7 7	66, 79, 125, 142	0
20	R	34/41 (82%)	2.52	23 (67%) 0 0	99, 139, 163, 165	0
All	All	5274/5387 (97%)	-0.04	123 (2%) 61 64	22, 52, 89, 169	40 (0%)

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	28	VAL	5.7
14	T	30	THR	5.3
20	R	26	TYR	4.8
7	H	64	ALA	4.7
1	a	260	PHE	4.7

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
19	FME	Z	1	10/11	0.87	0.13	86,100,112,113	0
19	FME	z	1	10/11	0.87	0.11	108,131,143,145	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	0.94	0.09	45,52,78,79	0
14	FME	t	1	10/11	0.95	0.08	41,47,73,76	0
12	FME	M	1	10/11	0.95	0.09	42,48,82,86	0
4	HSK	d	336[A]	10/12	0.96	0.08	48,51,53,55	7
4	HSK	d	336[B]	11/12	0.96	0.08	48,51,55,59	8
12	FME	m	1	10/11	0.96	0.08	38,54,81,85	0
4	HSK	D	336[B]	11/12	0.96	0.08	45,48,49,50	8
4	HSK	D	336[A]	10/12	0.96	0.08	45,48,50,50	7
8	FME	I	1	10/11	0.97	0.06	45,54,63,64	0
8	FME	i	1	10/11	0.98	0.07	41,53,56,56	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	DMS	O	314	4/4	0.56	0.17	133,135,136,138	0
34	DMS	k	2004	4/4	0.57	0.23	147,149,149,150	0
29	LMT	A	420	35/35	0.62	0.17	91,129,142,147	0
30	UNL	D	415	9/-	0.62	0.25	89,92,97,98	0
37	GOL	Z	102	6/6	0.62	0.16	105,121,124,124	0
30	UNL	B	630	9/-	0.63	0.35	80,89,103,103	0
37	GOL	v	202	6/6	0.63	0.13	100,106,107,107	0
37	GOL	o	2603	6/6	0.66	0.27	76,86,87,90	0
34	DMS	C	536	4/4	0.66	0.22	109,110,113,114	0
34	DMS	o	2604	4/4	0.67	0.28	124,124,125,126	0
34	DMS	E	108	4/4	0.67	0.21	115,118,120,120	0
34	DMS	b	643	4/4	0.68	0.17	149,150,151,151	0
37	GOL	k	2001	6/6	0.68	0.15	86,107,121,126	0
30	UNL	i	105	10/-	0.69	0.21	85,95,98,99	0
34	DMS	B	647	4/4	0.69	0.20	106,110,112,116	0
34	DMS	c	539	4/4	0.69	0.20	120,122,123,123	0
34	DMS	T	106	4/4	0.70	0.31	121,124,125,126	0
34	DMS	O	306	4/4	0.70	0.21	114,121,122,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	b	627	11/-	0.70	0.24	91,97,103,103	0
34	DMS	C	527	4/4	0.71	0.26	111,114,115,117	0
34	DMS	o	2610	4/4	0.71	0.20	131,131,131,133	0
34	DMS	z	1802	4/4	0.72	0.17	139,141,144,144	0
34	DMS	B	650	4/4	0.72	0.26	130,131,132,134	0
34	DMS	B	646	4/4	0.72	0.21	111,111,113,115	0
29	LMT	a	2120	35/35	0.72	0.15	101,133,144,145	0
34	DMS	v	214	4/4	0.72	0.21	127,132,134,135	0
34	DMS	C	535	4/4	0.73	0.29	121,122,124,127	0
34	DMS	o	2612	4/4	0.73	0.23	94,95,103,105	0
30	UNL	B	634	10/-	0.74	0.18	81,96,108,108	0
34	DMS	a	2124	4/4	0.74	0.20	128,130,130,131	0
34	DMS	B	649	4/4	0.74	0.15	124,124,125,126	0
34	DMS	D	420	4/4	0.74	0.24	124,124,126,126	0
30	UNL	A	415	40/-	0.74	0.20	80,111,132,143	0
30	UNL	E	102	15/-	0.74	0.24	96,102,109,111	0
34	DMS	C	533	4/4	0.74	0.18	120,121,121,122	0
34	DMS	o	2607	4/4	0.75	0.21	140,140,141,142	0
34	DMS	o	2609	4/4	0.75	0.24	110,119,119,121	0
30	UNL	h	701	11/-	0.75	0.23	85,89,97,98	0
34	DMS	O	309	4/4	0.75	0.26	98,101,104,109	0
30	UNL	e	102	15/-	0.75	0.20	76,82,95,98	0
30	UNL	E	104	6/-	0.76	0.24	67,78,88,89	0
34	DMS	b	640	4/4	0.76	0.21	103,108,109,111	0
30	UNL	a	2116	17/-	0.76	0.17	85,96,115,118	0
34	DMS	c	536	4/4	0.76	0.25	83,86,90,95	0
34	DMS	c	537	4/4	0.76	0.25	109,111,112,114	0
34	DMS	D	417	4/4	0.76	0.21	74,86,91,95	0
30	UNL	I	1203	16/-	0.77	0.20	88,99,102,103	0
34	DMS	C	539	4/4	0.77	0.25	75,90,91,96	0
30	UNL	j	1602	16/-	0.77	0.21	80,88,100,101	0
34	DMS	d	419	4/4	0.77	0.20	100,101,102,104	0
36	HTG	B	625[A]	19/19	0.77	0.19	57,70,80,83	19
36	HTG	B	625[B]	19/19	0.77	0.19	57,70,80,83	19
34	DMS	B	644	4/4	0.77	0.31	116,119,120,121	0
37	GOL	d	415	6/6	0.77	0.15	94,106,109,110	0
30	UNL	I	1204	13/-	0.77	0.18	80,87,94,95	0
37	GOL	o	2601	6/6	0.77	0.15	89,94,98,103	0
34	DMS	b	642	4/4	0.77	0.20	135,136,137,138	0
29	LMT	B	636	35/35	0.77	0.18	66,146,168,168	0
38	DGD	D	408	46/66	0.77	0.19	77,106,140,148	0
29	LMT	m	103	35/35	0.78	0.17	75,143,152,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	B	631	15/-	0.78	0.29	87,100,112,114	0
34	DMS	B	640	4/4	0.78	0.22	119,120,122,123	0
34	DMS	O	311	4/4	0.78	0.23	103,108,112,113	0
34	DMS	o	2605	4/4	0.78	0.28	111,114,114,122	0
34	DMS	b	639	4/4	0.79	0.19	93,94,94,99	0
30	UNL	B	629	18/-	0.79	0.17	78,85,103,105	0
34	DMS	d	422	4/4	0.79	0.19	113,118,118,121	0
34	DMS	O	312	4/4	0.79	0.23	112,116,117,118	0
30	UNL	E	106	16/-	0.79	0.27	93,104,113,114	0
29	LMT	f	101	24/35	0.79	0.15	93,112,125,126	0
30	UNL	b	628	15/-	0.79	0.22	85,97,105,106	0
34	DMS	x	802	4/4	0.80	0.21	110,115,116,118	0
34	DMS	O	304	4/4	0.80	0.28	129,133,136,141	0
34	DMS	b	635	4/4	0.80	0.19	102,104,106,108	0
30	UNL	c	525	12/-	0.80	0.24	88,97,118,118	0
36	HTG	B	626	19/19	0.80	0.15	53,114,123,126	19
36	HTG	B	628	19/19	0.80	0.14	56,128,134,137	0
36	HTG	I	1202	19/19	0.80	0.13	72,116,134,134	0
37	GOL	B	635	6/6	0.80	0.12	70,80,94,97	0
37	GOL	D	403	6/6	0.80	0.16	74,79,84,85	0
34	DMS	C	538	4/4	0.80	0.18	121,122,124,126	0
30	UNL	d	413	10/-	0.80	0.17	85,88,96,100	0
29	LMT	E	105	24/35	0.80	0.16	89,104,131,136	0
29	LMT	a	2103	35/35	0.80	0.18	60,100,116,118	0
34	DMS	T	104	4/4	0.80	0.24	118,127,127,129	0
34	DMS	c	538	4/4	0.80	0.18	111,113,114,116	0
30	UNL	J	103	15/-	0.80	0.24	86,93,99,99	0
29	LMT	j	1601	23/35	0.81	0.16	77,104,149,151	0
34	DMS	d	420	4/4	0.81	0.27	117,117,120,122	0
34	DMS	b	637	4/4	0.81	0.24	131,135,135,137	0
34	DMS	d	423	4/4	0.81	0.19	143,144,144,145	0
34	DMS	e	104	4/4	0.81	0.20	117,119,120,120	0
30	UNL	Y	301	10/-	0.81	0.21	93,101,108,109	0
36	HTG	d	414	19/19	0.81	0.17	76,99,110,110	19
30	UNL	k	2002	12/-	0.81	0.24	84,93,114,115	0
34	DMS	O	313	4/4	0.81	0.16	99,102,104,111	0
37	GOL	U	501	6/6	0.81	0.24	86,95,97,103	0
30	UNL	A	416	15/-	0.81	0.20	70,89,101,102	0
34	DMS	c	533	4/4	0.81	0.21	110,116,116,117	0
34	DMS	O	305	4/4	0.81	0.21	101,101,103,112	0
30	UNL	h	704	12/-	0.81	0.23	83,89,104,106	0
34	DMS	v	208	4/4	0.81	0.20	115,115,120,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	a	2122	4/4	0.81	0.16	128,128,129,129	0
37	GOL	v	204	6/6	0.81	0.15	85,89,93,97	0
34	DMS	O	307	4/4	0.81	0.20	119,120,120,120	0
39	LHG	e	101	32/49	0.81	0.17	77,130,154,158	0
30	UNL	i	102	19/-	0.82	0.16	86,96,114,114	0
30	UNL	C	501	40/-	0.82	0.19	75,102,126,129	0
34	DMS	c	534	4/4	0.82	0.15	120,120,122,123	0
37	GOL	b	631	6/6	0.82	0.15	94,99,103,109	0
36	HTG	C	522	19/19	0.82	0.13	66,115,134,137	0
36	HTG	D	413	19/19	0.82	0.15	74,106,124,127	0
34	DMS	V	206	4/4	0.82	0.16	88,96,102,105	0
36	HTG	b	626	19/19	0.82	0.14	96,137,142,142	0
36	HTG	d	403	19/19	0.82	0.14	83,114,127,128	0
30	UNL	C	523	10/-	0.82	0.21	81,88,98,100	0
37	GOL	B	632	6/6	0.82	0.18	95,101,103,106	0
39	LHG	E	101	49/49	0.82	0.17	77,108,122,123	0
29	LMT	A	414	34/35	0.82	0.17	68,107,122,131	0
30	UNL	b	629	9/-	0.83	0.20	76,90,96,96	0
37	GOL	H	103	6/6	0.83	0.17	85,97,100,102	0
30	UNL	E	103	6/-	0.83	0.16	82,82,84,85	0
37	GOL	V	203	6/6	0.83	0.15	84,103,106,107	0
34	DMS	j	1604	4/4	0.83	0.23	126,129,130,133	0
34	DMS	t	103	4/4	0.83	0.19	109,112,116,117	0
34	DMS	u	204	4/4	0.83	0.21	106,108,109,110	0
30	UNL	d	402	40/-	0.83	0.23	61,88,130,131	0
34	DMS	v	210	4/4	0.83	0.17	122,123,124,125	0
34	DMS	v	211	4/4	0.83	0.18	95,111,113,114	0
34	DMS	v	213	4/4	0.83	0.18	108,108,109,109	0
34	DMS	A	424	4/4	0.83	0.16	78,84,87,89	0
36	HTG	i	103	19/19	0.83	0.14	74,133,147,148	0
34	DMS	T	105	4/4	0.83	0.24	134,134,135,135	0
29	LMT	I	1201	24/35	0.83	0.17	56,96,144,148	0
34	DMS	c	540	4/4	0.84	0.15	118,124,125,128	0
34	DMS	A	423	4/4	0.84	0.22	113,115,117,121	0
34	DMS	C	537	4/4	0.84	0.17	112,114,116,118	0
36	HTG	b	602	19/19	0.84	0.14	68,120,134,138	0
34	DMS	o	2611	4/4	0.84	0.18	96,99,99,99	0
36	HTG	c	523	19/19	0.84	0.14	95,110,115,116	0
36	HTG	c	524	19/19	0.84	0.15	73,97,108,110	19
34	DMS	B	642	4/4	0.84	0.23	109,111,113,115	0
34	DMS	E	107	4/4	0.84	0.19	124,128,129,133	0
37	GOL	c	527	6/6	0.85	0.18	81,86,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	Z	101	35/35	0.85	0.15	60,125,151,156	0
27	SQD	L	102	54/54	0.85	0.17	55,78,119,123	0
34	DMS	B	638	4/4	0.85	0.20	124,124,126,126	0
29	LMT	J	102	24/35	0.85	0.16	76,101,135,137	0
37	GOL	O	303	6/6	0.85	0.12	91,94,95,96	0
37	GOL	v	203	6/6	0.85	0.14	78,80,83,87	0
30	UNL	b	630	21/-	0.85	0.14	61,79,105,107	0
34	DMS	C	534	4/4	0.85	0.22	119,119,120,121	0
30	UNL	c	501	36/-	0.85	0.19	80,98,127,130	0
30	UNL	m	101	13/-	0.85	0.21	70,75,95,99	0
34	DMS	v	212	4/4	0.86	0.17	119,121,122,124	0
29	LMT	z	1801	33/35	0.86	0.14	74,116,131,136	0
27	SQD	F	101	45/54	0.86	0.14	69,97,121,132	0
37	GOL	C	525	6/6	0.86	0.15	83,98,100,101	0
34	DMS	A	425	4/4	0.86	0.19	93,96,96,98	0
34	DMS	u	201	4/4	0.86	0.26	104,109,110,111	0
34	DMS	b	636	4/4	0.86	0.15	69,96,97,100	0
29	LMT	m	102	35/35	0.86	0.13	49,82,99,101	0
36	HTG	c	526	19/19	0.86	0.12	97,131,146,149	0
30	UNL	a	2117	9/-	0.86	0.17	72,79,83,84	0
28	LMG	C	526	48/55	0.86	0.16	63,111,128,134	0
36	HTG	V	204	19/19	0.87	0.13	67,84,115,118	0
34	DMS	B	645	4/4	0.87	0.13	86,91,92,93	0
29	LMT	b	624	25/35	0.87	0.17	80,110,138,139	0
29	LMT	B	623	35/35	0.87	0.13	74,104,121,122	0
34	DMS	C	529	4/4	0.87	0.24	123,124,124,127	0
30	UNL	D	402	40/-	0.88	0.18	60,82,118,122	0
29	LMT	M	101	35/35	0.88	0.12	57,89,104,107	0
27	SQD	B	621	54/54	0.88	0.14	48,87,130,133	0
34	DMS	c	535	4/4	0.88	0.17	95,103,106,106	0
36	HTG	b	625	19/19	0.88	0.16	46,69,88,89	19
27	SQD	f	102	37/54	0.88	0.15	73,101,129,134	0
30	UNL	M	102	15/-	0.88	0.17	58,68,108,113	0
30	UNL	T	103	9/-	0.88	0.21	78,85,93,95	0
29	LMT	i	104	24/35	0.88	0.15	64,103,141,147	0
34	DMS	V	208	4/4	0.88	0.14	81,91,94,96	0
34	DMS	c	541	4/4	0.88	0.14	104,106,106,106	0
31	PL9	A	417	39/55	0.89	0.18	73,85,102,105	0
34	DMS	b	641	4/4	0.89	0.14	67,70,72,74	0
34	DMS	V	207	4/4	0.89	0.14	92,93,99,100	0
34	DMS	C	530	4/4	0.89	0.15	88,93,97,99	0
34	DMS	c	530	4/4	0.89	0.20	121,122,122,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	PL9	x	801	39/55	0.89	0.19	71,91,119,122	0
28	LMG	i	101	51/55	0.89	0.15	65,82,94,101	0
34	DMS	b	634	4/4	0.89	0.17	96,98,98,104	0
37	GOL	C	524	6/6	0.89	0.12	91,98,103,105	0
27	SQD	A	413	54/54	0.89	0.13	62,81,122,128	0
30	UNL	B	633	22/-	0.89	0.13	61,84,112,113	0
34	DMS	O	310	4/4	0.89	0.15	102,103,103,107	0
34	DMS	o	2606	4/4	0.89	0.18	109,111,111,111	0
34	DMS	V	202	4/4	0.89	0.17	96,97,99,101	0
28	LMG	c	522	48/55	0.90	0.14	55,110,127,139	0
34	DMS	v	209	4/4	0.90	0.14	82,93,93,101	0
34	DMS	d	421	4/4	0.90	0.20	85,92,95,96	0
34	DMS	o	2608	4/4	0.90	0.12	102,107,110,114	0
34	DMS	V	209	4/4	0.90	0.16	87,103,104,110	0
24	CLA	B	602	65/65	0.90	0.10	45,68,113,120	0
29	LMT	B	637	24/35	0.90	0.13	50,77,118,128	0
34	DMS	U	503	4/4	0.90	0.20	95,109,110,112	0
34	DMS	B	648	4/4	0.90	0.14	63,65,67,80	0
28	LMG	C	520	51/55	0.90	0.15	48,81,101,108	0
34	DMS	u	203	4/4	0.90	0.14	76,85,86,89	0
27	SQD	a	2102	53/54	0.90	0.13	52,80,111,115	0
26	BCR	t	102	40/40	0.91	0.10	42,55,75,77	0
24	CLA	C	507	65/65	0.91	0.13	50,69,110,117	0
36	HTG	B	627	19/19	0.91	0.13	59,90,110,116	0
29	LMT	T	102	24/35	0.91	0.15	48,79,108,114	0
36	HTG	C	521	19/19	0.91	0.13	90,106,113,116	0
34	DMS	v	207	4/4	0.91	0.15	96,97,99,100	0
34	DMS	A	426	4/4	0.91	0.18	79,80,80,84	0
34	DMS	a	2123	4/4	0.91	0.19	113,115,118,123	0
36	HTG	B	624	19/19	0.91	0.13	60,69,74,76	0
34	DMS	d	417	4/4	0.91	0.22	84,87,87,90	0
30	UNL	D	414	16/-	0.92	0.16	55,70,85,89	0
28	LMG	B	622	51/55	0.92	0.13	51,70,83,92	0
34	DMS	b	633	4/4	0.92	0.16	79,80,81,92	0
32	K2I	A	418[A]	10/10	0.92	0.14	94,96,102,105	10
32	K2I	A	418[B]	10/10	0.92	0.14	74,95,100,112	10
26	BCR	C	516	40/40	0.92	0.11	48,56,69,72	0
34	DMS	u	202	4/4	0.92	0.14	79,80,89,90	0
26	BCR	T	101	40/40	0.92	0.09	39,52,71,75	0
34	DMS	D	419	4/4	0.92	0.15	88,95,95,104	0
28	LMG	b	623	51/55	0.92	0.13	56,70,83,100	0
36	HTG	b	601	19/19	0.92	0.11	63,84,94,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	X	801	18/-	0.92	0.12	65,71,96,98	0
34	DMS	C	528	4/4	0.92	0.17	88,96,97,98	0
34	DMS	i	106	4/4	0.92	0.15	95,96,97,98	0
34	DMS	F	103	4/4	0.92	0.13	77,78,79,88	0
24	CLA	b	604	65/65	0.92	0.11	52,73,118,121	0
28	LMG	A	412	51/55	0.92	0.13	57,79,100,104	0
30	UNL	t	101	8/-	0.92	0.16	75,81,88,89	0
34	DMS	B	643	4/4	0.92	0.17	81,85,90,91	0
34	DMS	V	210	4/4	0.92	0.15	87,96,98,100	0
34	DMS	O	308	4/4	0.92	0.18	102,105,106,108	0
32	K2I	a	2118[A]	10/10	0.93	0.10	103,106,111,114	10
37	GOL	a	2101	6/6	0.93	0.13	66,76,77,80	0
32	K2I	a	2118[B]	10/10	0.93	0.10	82,105,107,112	10
30	UNL	d	412	14/-	0.93	0.17	56,73,79,82	0
34	DMS	b	638	4/4	0.93	0.14	81,85,89,94	0
26	BCR	c	516	40/40	0.93	0.12	63,76,81,85	0
36	HTG	O	302	19/19	0.93	0.11	51,68,78,81	0
30	UNL	d	416	18/-	0.93	0.11	59,74,105,105	0
24	CLA	c	508	65/65	0.93	0.11	51,67,102,107	0
24	CLA	a	2113	65/65	0.93	0.11	40,46,116,121	0
34	DMS	c	542	4/4	0.93	0.11	113,114,117,118	0
27	SQD	a	2115	47/54	0.93	0.13	59,80,97,104	0
38	DGD	c	518	62/66	0.93	0.12	42,54,95,100	0
24	CLA	B	617	65/65	0.93	0.11	40,52,119,123	0
28	LMG	c	521	49/55	0.93	0.14	53,88,105,108	0
27	SQD	A	411	49/54	0.94	0.12	66,82,98,99	0
24	CLA	b	619	65/65	0.94	0.11	43,56,119,121	0
34	DMS	D	416	4/4	0.94	0.12	61,76,81,82	0
33	BCT	A	421	4/4	0.94	0.09	51,56,61,64	0
33	BCT	a	2108	4/4	0.94	0.10	55,57,63,68	0
24	CLA	C	514	65/65	0.94	0.09	54,65,95,98	0
24	CLA	c	514	65/65	0.94	0.10	56,64,100,102	0
24	CLA	c	515	65/65	0.94	0.10	55,68,98,106	0
34	DMS	d	418	4/4	0.94	0.14	69,73,81,88	0
24	CLA	d	405	65/65	0.94	0.09	46,55,105,115	0
24	CLA	B	615	65/65	0.94	0.10	35,45,99,107	0
34	DMS	C	531	4/4	0.94	0.14	63,70,77,78	0
24	CLA	C	513	65/65	0.94	0.10	51,65,107,110	0
26	BCR	a	2114	40/40	0.94	0.08	35,45,51,53	0
24	CLA	b	609	65/65	0.94	0.09	39,50,86,88	0
34	DMS	v	206	4/4	0.94	0.14	78,93,93,98	0
39	LHG	D	409	49/49	0.94	0.11	48,59,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	c	517	40/40	0.94	0.10	47,59,75,78	0
24	CLA	b	617	65/65	0.94	0.11	36,45,100,113	0
41	RRX	H	101	41/41	0.94	0.09	45,59,68,78	0
41	RRX	h	702	41/41	0.94	0.10	46,59,81,93	0
24	CLA	B	607	65/65	0.95	0.09	37,46,74,84	0
26	BCR	D	406	40/40	0.95	0.09	42,52,85,86	0
26	BCR	K	101	40/40	0.95	0.09	50,57,63,67	0
24	CLA	D	405	65/65	0.95	0.09	42,52,106,112	0
26	BCR	Y	302	40/40	0.95	0.07	48,56,62,63	0
24	CLA	c	505	65/65	0.95	0.09	43,57,63,70	0
26	BCR	b	622	40/40	0.95	0.09	45,57,71,76	0
24	CLA	c	506	65/65	0.95	0.10	44,52,86,90	0
24	CLA	B	611	65/65	0.95	0.08	41,49,57,68	0
28	LMG	d	411	48/55	0.95	0.10	47,56,86,95	0
26	BCR	c	528	40/40	0.95	0.09	48,58,68,69	0
26	BCR	d	406	40/40	0.95	0.09	47,55,75,82	0
24	CLA	c	510	65/65	0.95	0.09	41,51,114,126	0
24	CLA	C	511	65/65	0.95	0.09	37,51,59,70	0
34	DMS	c	531	4/4	0.95	0.14	97,99,101,106	0
38	DGD	C	517	62/66	0.95	0.10	40,51,93,96	0
38	DGD	C	518	62/66	0.95	0.10	41,54,109,119	0
38	DGD	C	519	62/66	0.95	0.10	39,51,92,103	0
24	CLA	A	409	65/65	0.95	0.11	35,45,117,121	0
38	DGD	H	102	62/66	0.95	0.10	45,54,66,70	0
24	CLA	b	610	65/65	0.95	0.08	31,43,58,62	0
38	DGD	c	519	62/66	0.95	0.10	47,59,107,117	0
38	DGD	h	703	62/66	0.95	0.10	46,57,74,79	0
26	BCR	B	618	40/40	0.95	0.08	38,47,54,55	0
26	BCR	B	620	40/40	0.95	0.08	42,52,63,67	0
39	LHG	d	408	49/49	0.95	0.10	45,58,73,78	0
26	BCR	C	515	40/40	0.95	0.08	47,65,74,79	0
39	LHG	l	101	49/49	0.95	0.10	43,52,71,79	0
31	PL9	D	407	55/55	0.95	0.08	34,43,50,55	0
31	PL9	d	407	55/55	0.95	0.09	33,44,55,60	0
24	CLA	A	406	65/65	0.96	0.09	34,42,100,104	0
24	CLA	c	507	65/65	0.96	0.08	42,52,66,74	0
24	CLA	C	508	65/65	0.96	0.09	47,56,73,77	0
24	CLA	c	509	65/65	0.96	0.09	45,56,77,79	0
24	CLA	C	509	65/65	0.96	0.08	38,50,106,117	0
24	CLA	c	511	65/65	0.96	0.09	43,55,79,90	0
24	CLA	c	513	65/65	0.96	0.08	45,59,70,79	0
24	CLA	C	510	65/65	0.96	0.09	46,54,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	LMG	D	412	44/55	0.96	0.09	44,53,80,83	0
24	CLA	B	608	65/65	0.96	0.08	33,42,57,67	0
24	CLA	C	512	65/65	0.96	0.07	41,56,65,69	0
34	DMS	v	205	4/4	0.96	0.13	75,76,84,85	0
25	PHO	A	407	64/64	0.96	0.07	33,39,48,49	0
37	GOL	U	502	6/6	0.96	0.09	69,78,90,95	0
25	PHO	A	408	64/64	0.96	0.07	34,45,52,55	0
24	CLA	B	610	65/65	0.96	0.07	42,49,58,60	0
34	DMS	c	532	4/4	0.96	0.11	72,72,73,75	0
26	BCR	B	619	40/40	0.96	0.07	40,50,62,67	0
24	CLA	B	603	65/65	0.96	0.08	41,48,57,58	0
24	CLA	B	614	65/65	0.96	0.07	34,41,79,93	0
24	CLA	a	2110	65/65	0.96	0.10	35,44,106,111	0
24	CLA	B	604	65/65	0.96	0.07	36,45,57,63	0
24	CLA	B	606	65/65	0.96	0.07	34,43,59,64	0
24	CLA	b	608	65/65	0.96	0.07	37,45,58,61	0
24	CLA	C	502	65/65	0.96	0.08	43,52,68,88	0
34	DMS	B	641	4/4	0.96	0.12	63,65,69,71	0
24	CLA	C	503	65/65	0.96	0.07	39,48,62,66	0
26	BCR	b	620	40/40	0.96	0.08	40,49,58,59	0
26	BCR	b	621	40/40	0.96	0.08	39,51,63,71	0
24	CLA	b	612	65/65	0.96	0.08	43,52,62,70	0
24	CLA	b	613	65/65	0.96	0.08	42,50,57,64	0
24	CLA	b	615	65/65	0.96	0.07	37,45,52,56	0
24	CLA	b	616	65/65	0.96	0.08	37,41,80,84	0
38	DGD	c	520	62/66	0.96	0.10	44,57,80,88	0
34	DMS	V	205	4/4	0.96	0.11	66,69,70,75	0
24	CLA	C	504	65/65	0.96	0.07	42,52,59,67	0
39	LHG	D	410	49/49	0.96	0.09	41,47,65,81	0
39	LHG	D	411	44/49	0.96	0.10	44,53,90,98	0
26	BCR	k	2003	40/40	0.96	0.09	50,60,69,71	0
24	CLA	b	618	65/65	0.96	0.09	41,51,70,78	0
39	LHG	d	409	49/49	0.96	0.09	40,46,72,84	0
39	LHG	d	410	36/49	0.96	0.08	46,54,79,85	0
24	CLA	C	505	65/65	0.96	0.09	41,49,81,86	0
24	CLA	c	503	65/65	0.96	0.09	44,55,68,73	0
24	CLA	c	504	65/65	0.96	0.08	40,50,64,81	0
24	CLA	C	506	65/65	0.96	0.09	45,52,70,76	0
25	PHO	a	2112	64/64	0.97	0.06	36,46,54,56	0
26	BCR	A	410	40/40	0.97	0.06	37,45,50,52	0
24	CLA	D	401	65/65	0.97	0.06	33,39,49,59	0
24	CLA	D	404	65/65	0.97	0.06	31,38,59,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	b	611	65/65	0.97	0.07	42,49,57,63	0
24	CLA	B	616	65/65	0.97	0.08	39,50,70,78	0
24	CLA	a	2109	65/65	0.97	0.07	33,40,51,74	0
24	CLA	b	614	65/65	0.97	0.07	34,44,61,64	0
24	CLA	B	612	65/65	0.97	0.07	35,44,57,68	0
24	CLA	c	512	65/65	0.97	0.08	42,52,62,74	0
34	DMS	D	418	4/4	0.97	0.11	77,82,88,90	0
24	CLA	B	613	65/65	0.97	0.06	34,43,50,53	0
34	DMS	c	529	4/4	0.97	0.15	57,60,62,63	0
24	CLA	B	605	65/65	0.97	0.08	31,42,75,81	0
39	LHG	L	101	49/49	0.97	0.08	44,51,68,70	0
24	CLA	b	605	65/65	0.97	0.07	40,51,62,65	0
24	CLA	d	401	65/65	0.97	0.06	34,39,47,55	0
24	CLA	d	404	65/65	0.97	0.07	31,41,59,71	0
24	CLA	b	606	65/65	0.97	0.07	38,48,60,64	0
24	CLA	b	607	65/65	0.97	0.08	34,44,84,89	0
40	HEM	e	103	43/43	0.97	0.09	52,63,90,105	0
24	CLA	B	609	65/65	0.97	0.06	40,48,58,61	0
25	PHO	a	2111	64/64	0.97	0.06	33,41,47,55	0
35	CA	o	2602	1/1	0.98	0.04	71,71,71,71	0
34	DMS	b	632	4/4	0.98	0.07	47,48,54,58	0
24	CLA	A	405	65/65	0.98	0.06	30,38,50,72	0
34	DMS	C	532	4/4	0.98	0.07	62,63,63,67	0
32	K2I	A	419	10/10	0.98	0.09	43,52,58,64	10
34	DMS	A	422	4/4	0.98	0.08	45,48,53,55	0
32	K2I	a	2119	10/10	0.98	0.08	48,57,64,73	10
34	DMS	B	639	4/4	0.98	0.08	42,46,47,58	0
40	HEM	F	102	43/43	0.98	0.07	52,62,73,90	0
35	CA	B	601	1/1	0.98	0.05	64,64,64,64	0
35	CA	O	301	1/1	0.98	0.04	72,72,72,72	0
35	CA	b	603	1/1	0.98	0.04	72,72,72,72	0
42	MG	J	101	1/1	0.98	0.09	53,53,53,53	0
43	HEC	V	201	43/43	0.98	0.06	37,45,50,53	0
43	HEC	v	201	43/43	0.98	0.07	45,55,61,64	0
23	CL	A	404	1/1	0.99	0.03	41,41,41,41	0
23	CL	a	2106	1/1	0.99	0.07	47,47,47,47	0
34	DMS	a	2121	4/4	0.99	0.06	42,48,52,52	0
23	CL	a	2107	1/1	0.99	0.04	46,46,46,46	0
21	OEX	A	401	10/10	0.99	0.03	39,42,46,48	0
42	MG	j	1603	1/1	0.99	0.08	57,57,57,57	0
23	CL	A	403	1/1	0.99	0.08	42,42,42,42	0
35	CA	c	502	1/1	0.99	0.05	66,66,66,66	0

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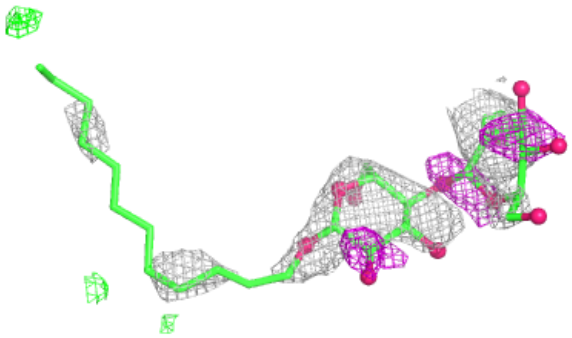
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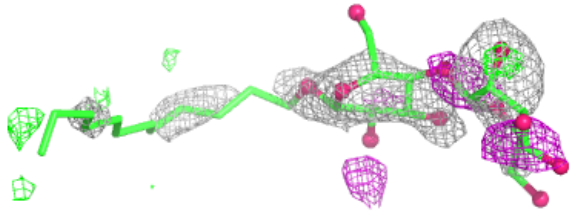
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	FE2	a	2105	1/1	1.00	0.02	47,47,47,47	0
21	OEX	a	2104	10/10	1.00	0.02	38,43,49,52	0
22	FE2	A	402	1/1	1.00	0.01	48,48,48,48	0

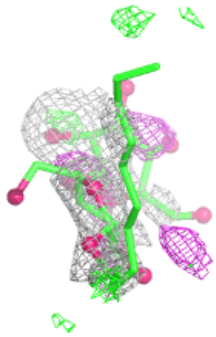
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 420:

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

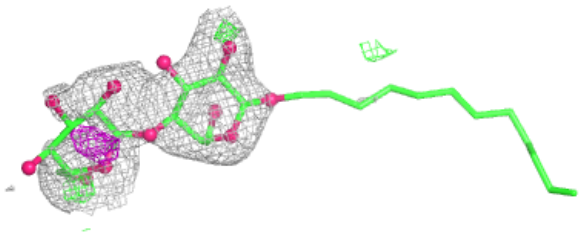


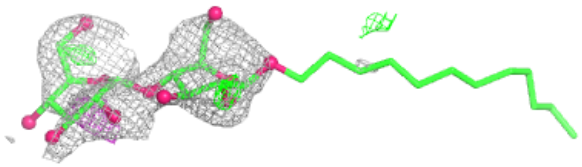


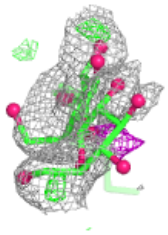


Electron density around LMT a 2120:

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

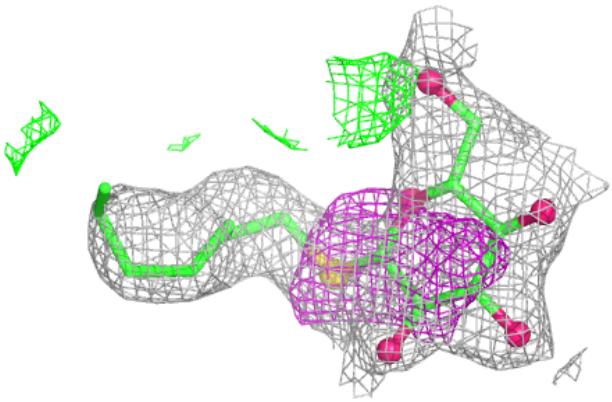


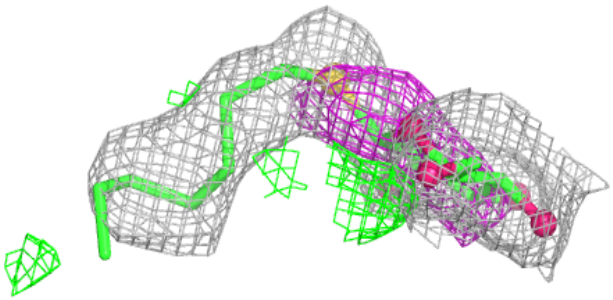


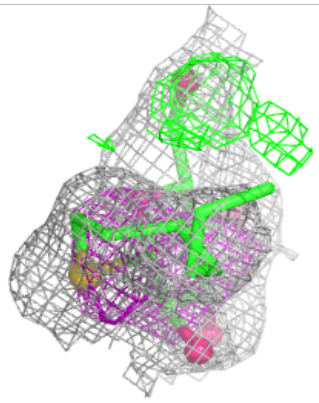


Electron density around HTG B 625 (A):

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

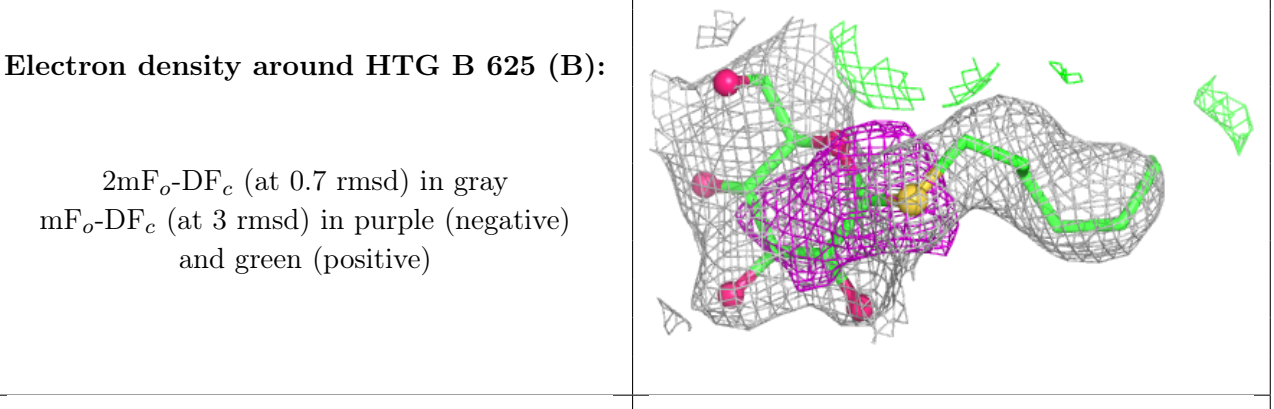






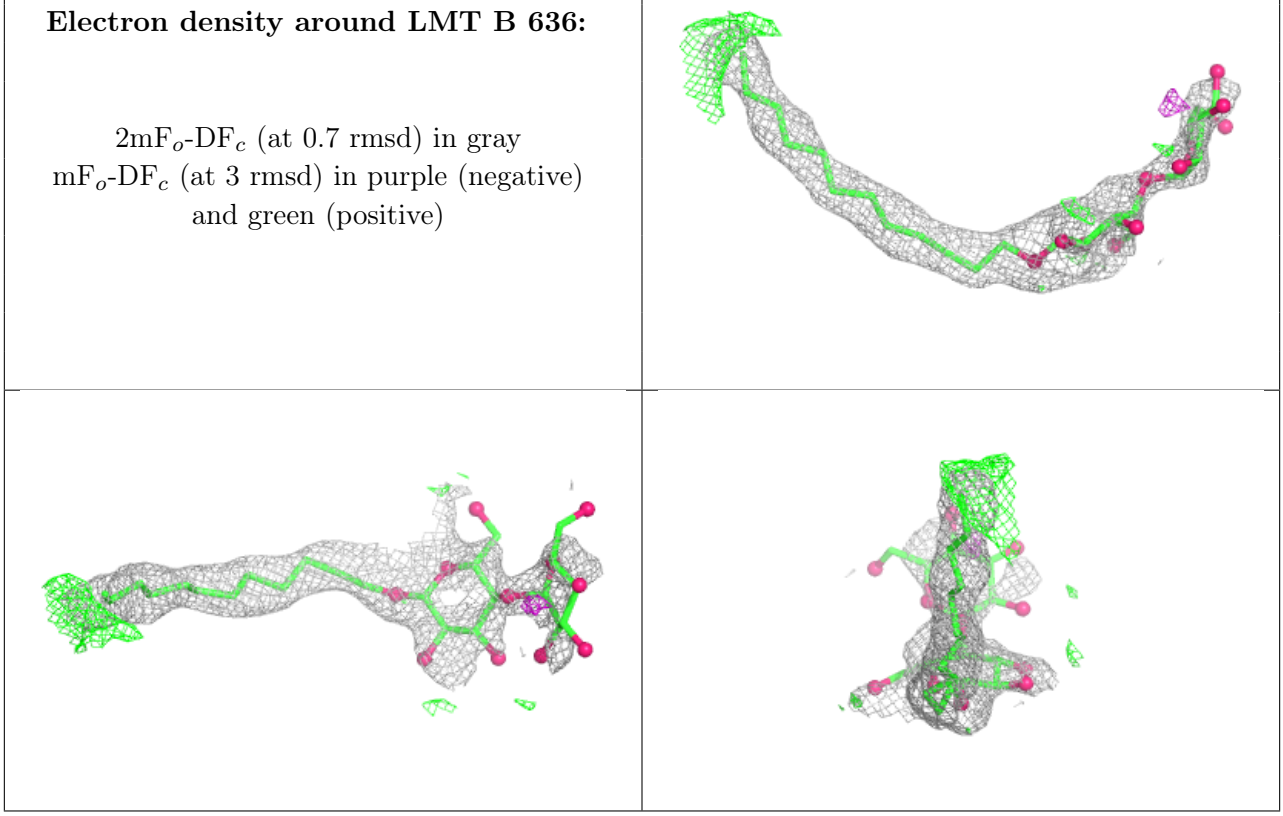
Electron density around HTG B 625 (B):

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



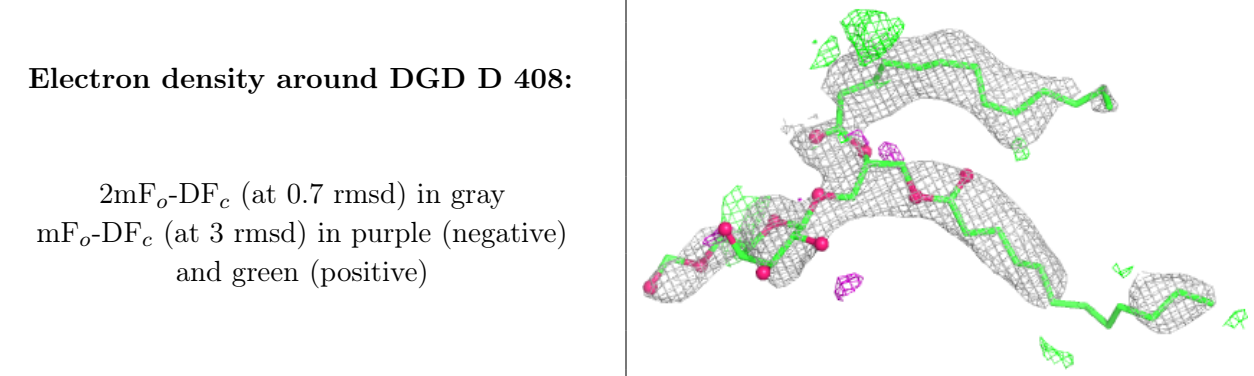
Electron density around LMT B 636:

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



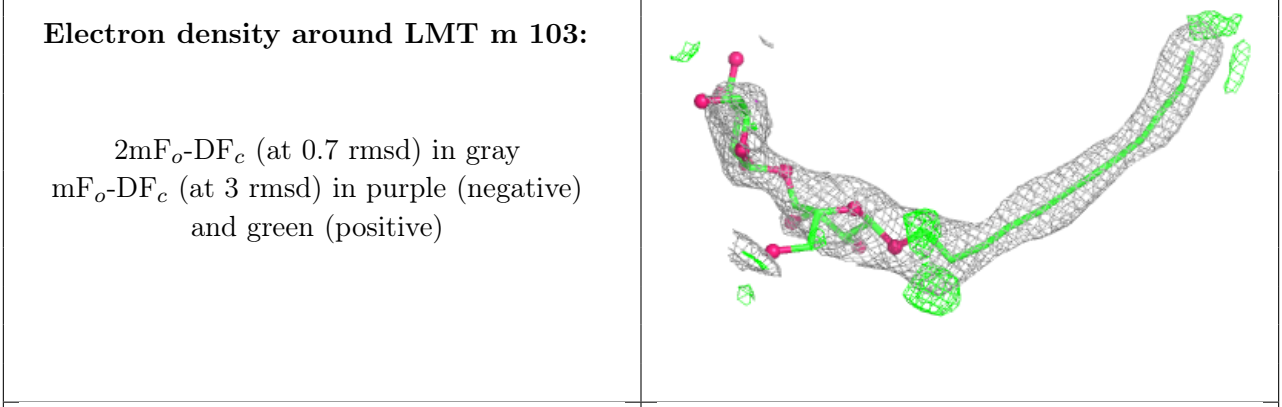
Electron density around DGD D 408:

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



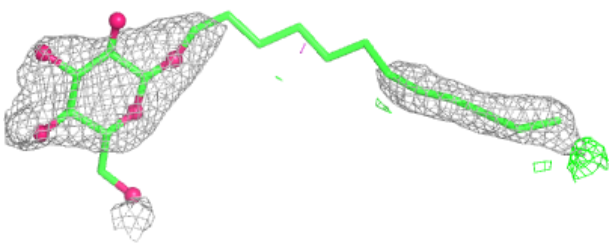
Electron density around LMT m 103:

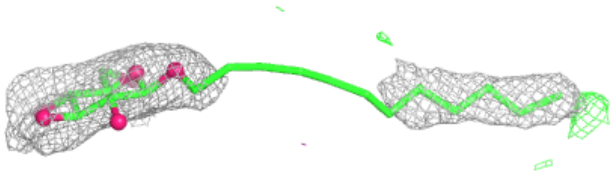
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

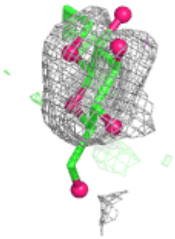


Electron density around LMT f 101:

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

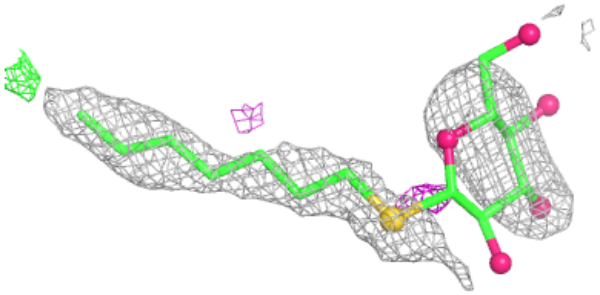


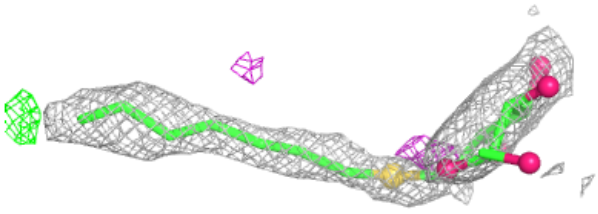


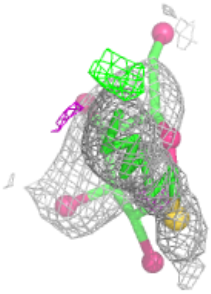


Electron density around HTG B 626:

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

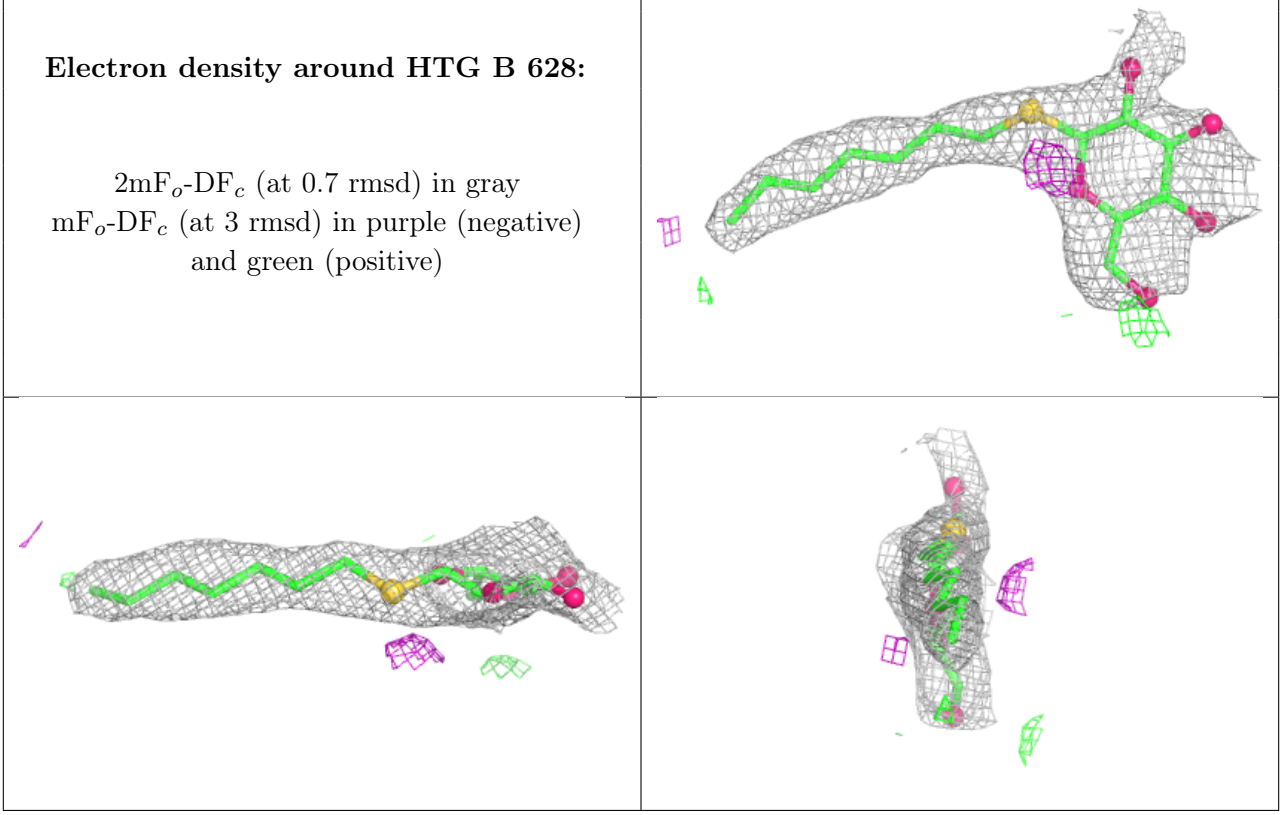






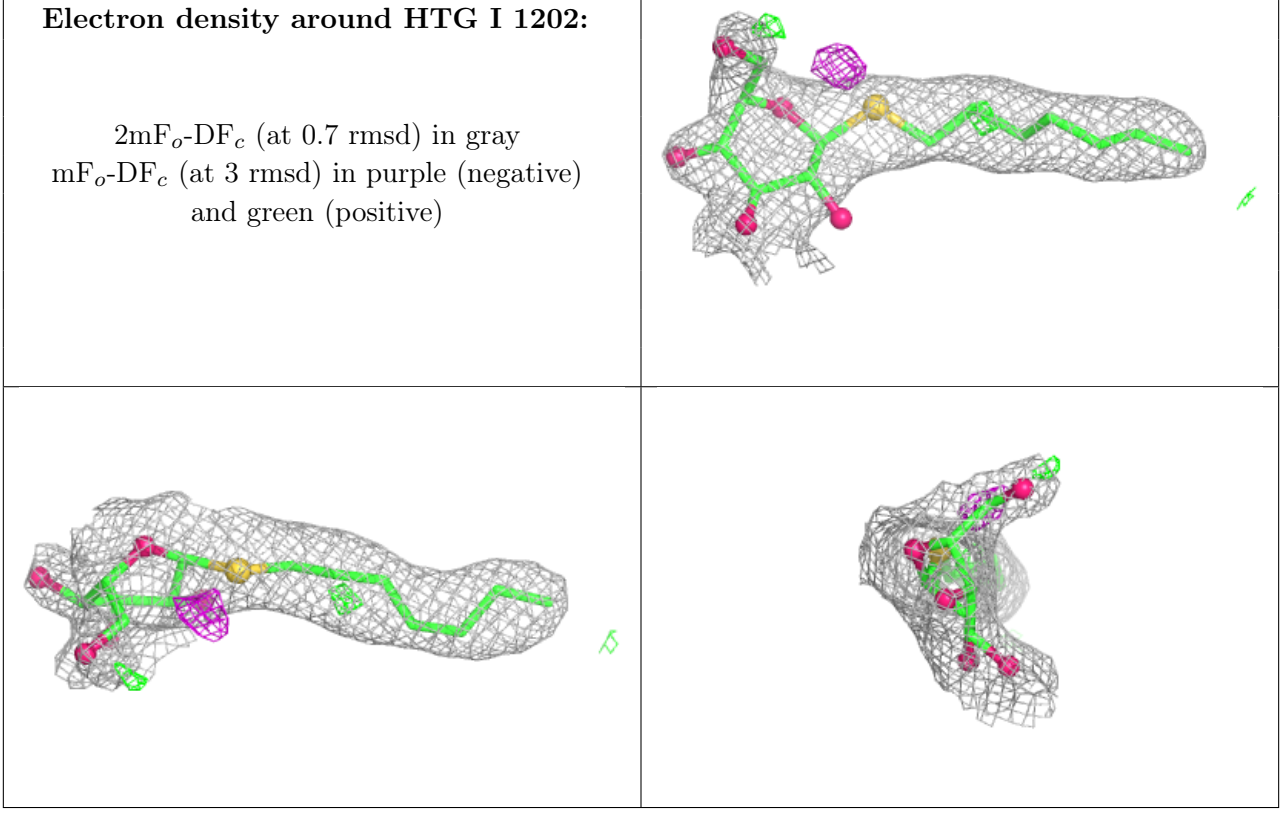
Electron density around HTG B 628:

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



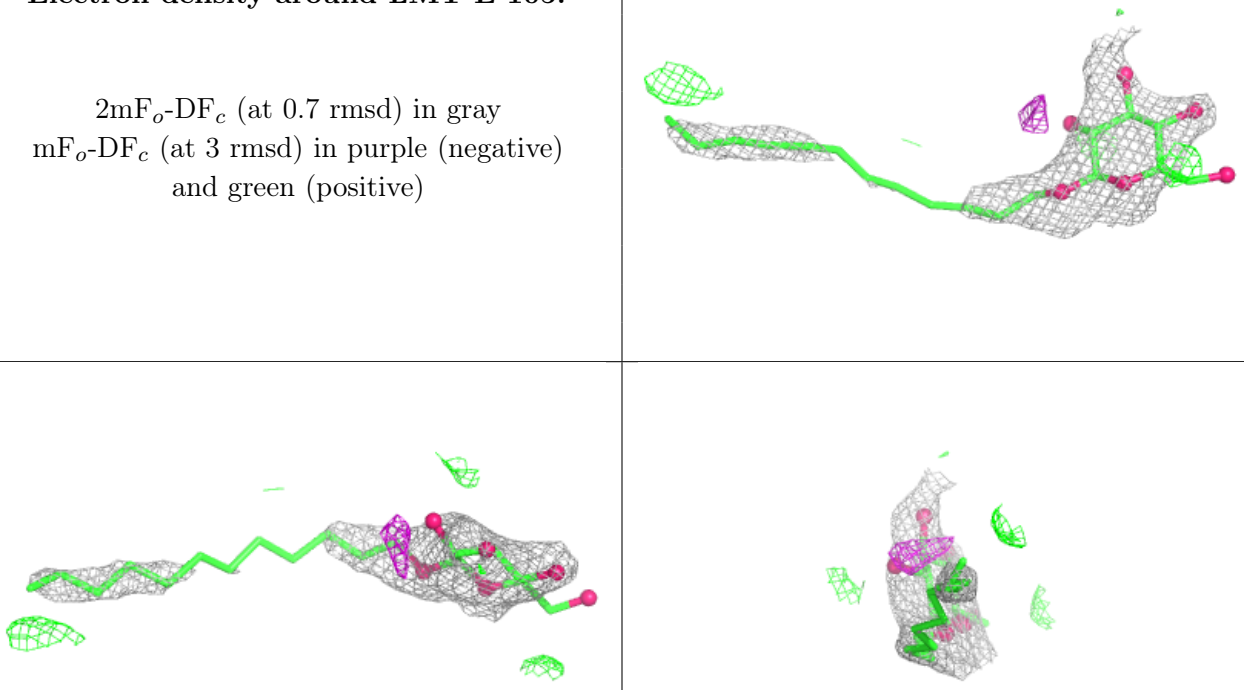
Electron density around HTG I 1202:

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



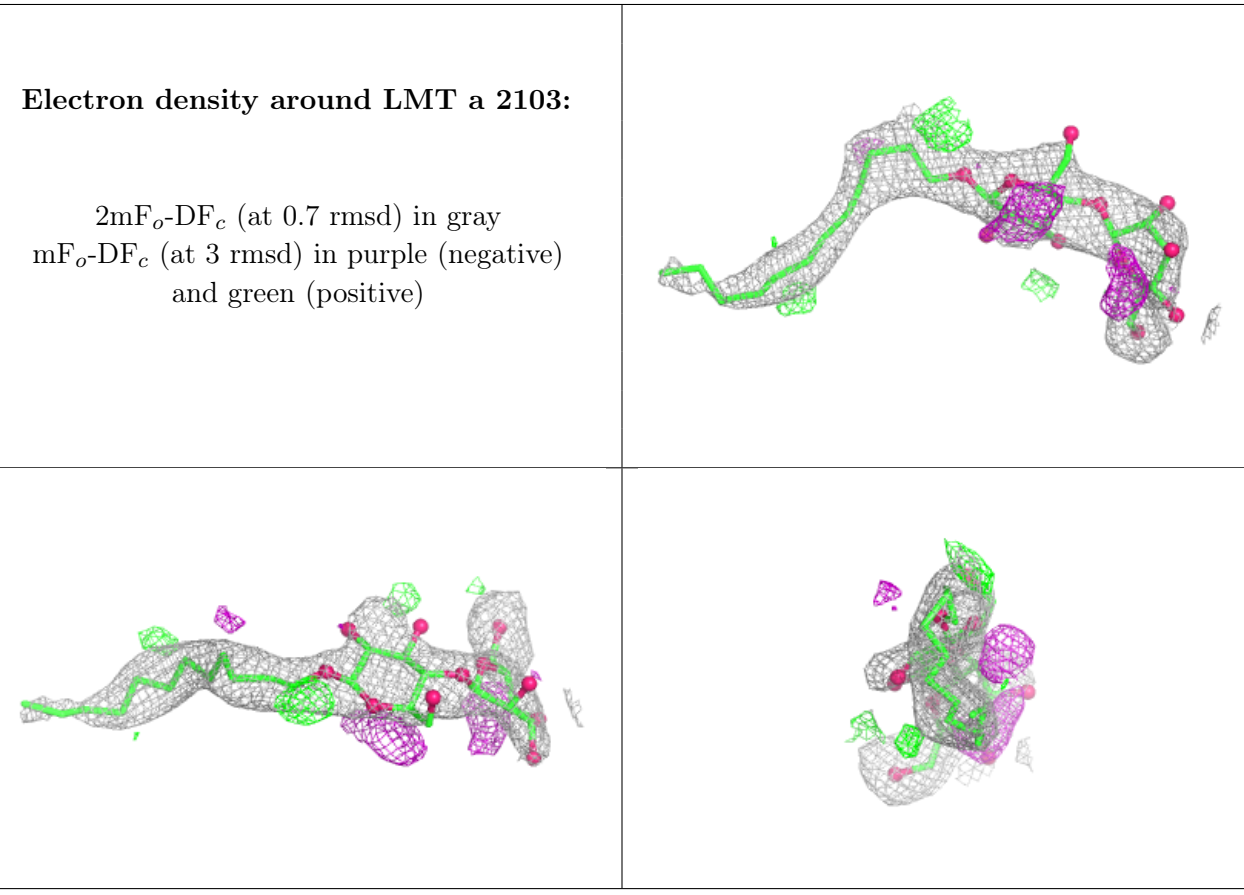
Electron density around LMT E 105:

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



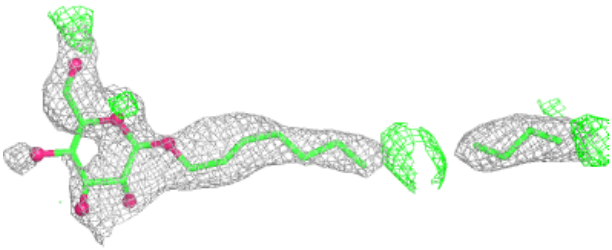
Electron density around LMT a 2103:

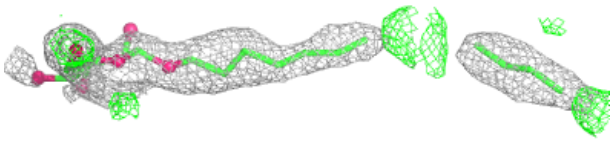
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

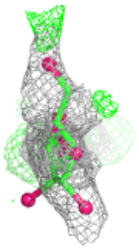


Electron density around LMT j 1601:

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

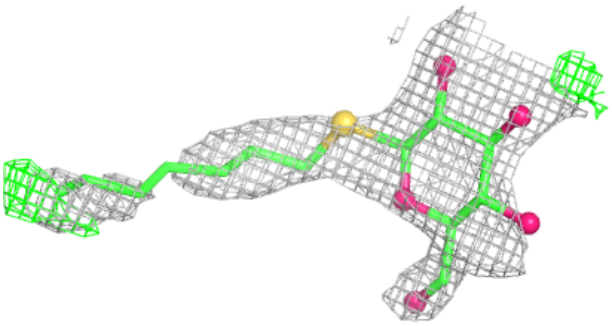


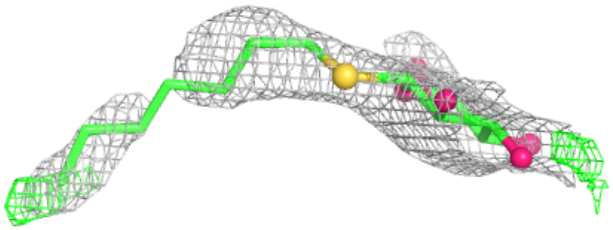


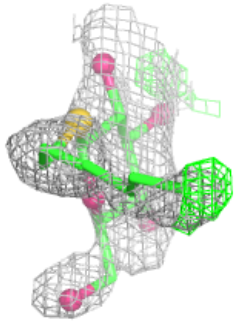


Electron density around HTG d 414:

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

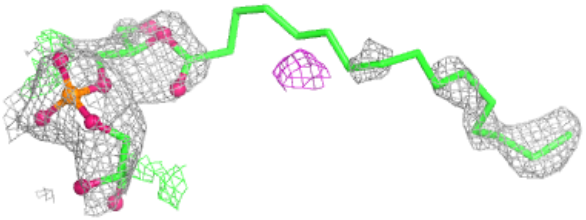


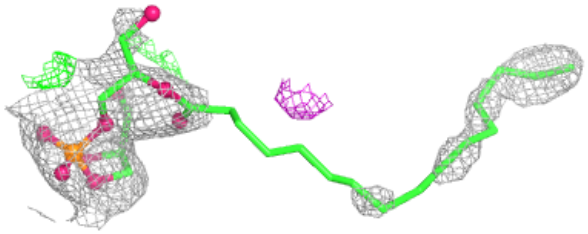


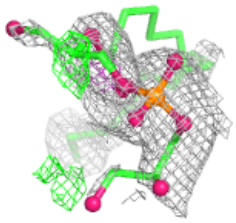


Electron density around LHG e 101:

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

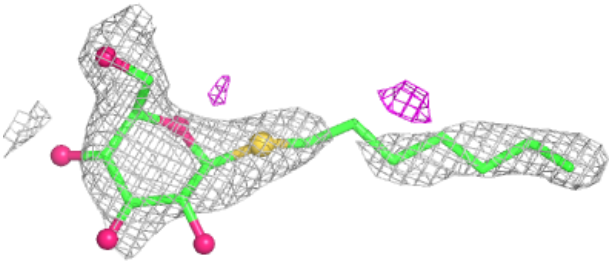


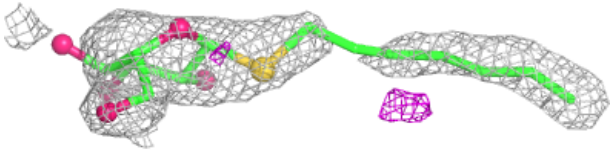


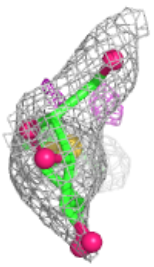


Electron density around HTG C 522:

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

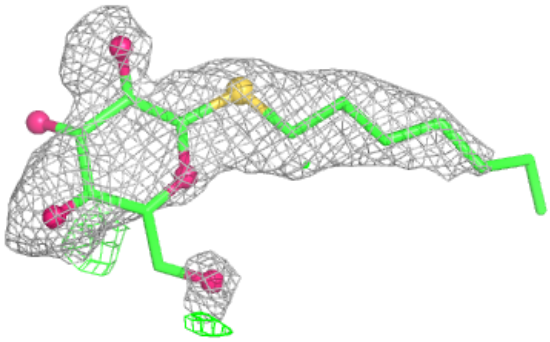


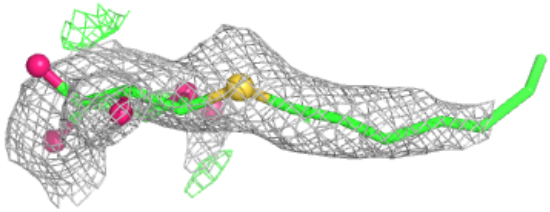


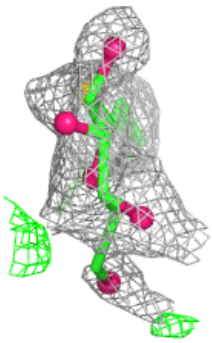


Electron density around HTG D 413:

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

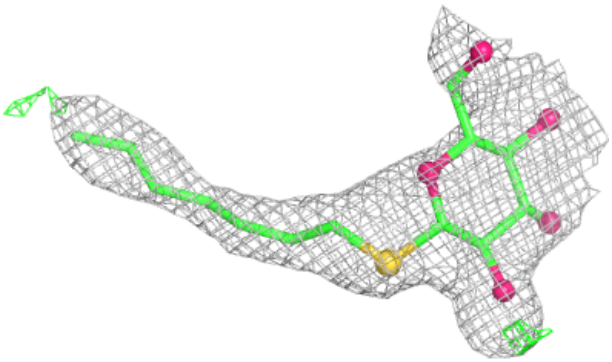


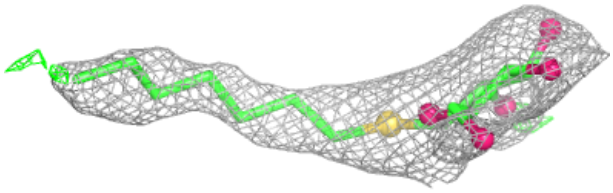


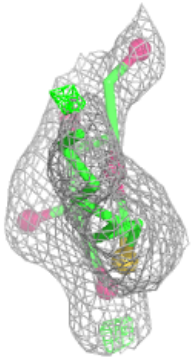


Electron density around HTG b 626:

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

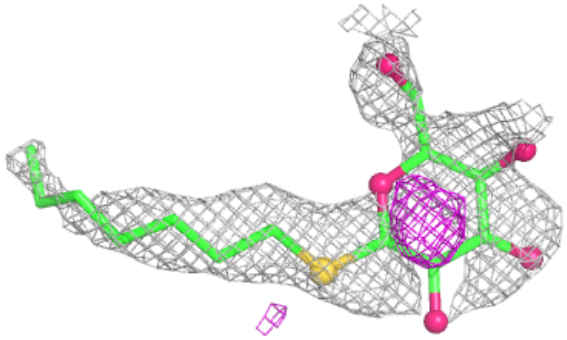


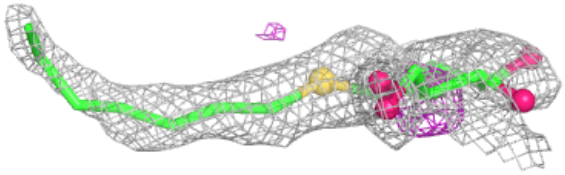


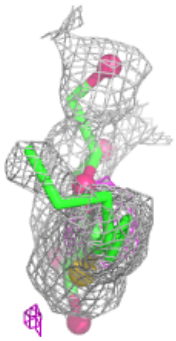


Electron density around HTG d 403:

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

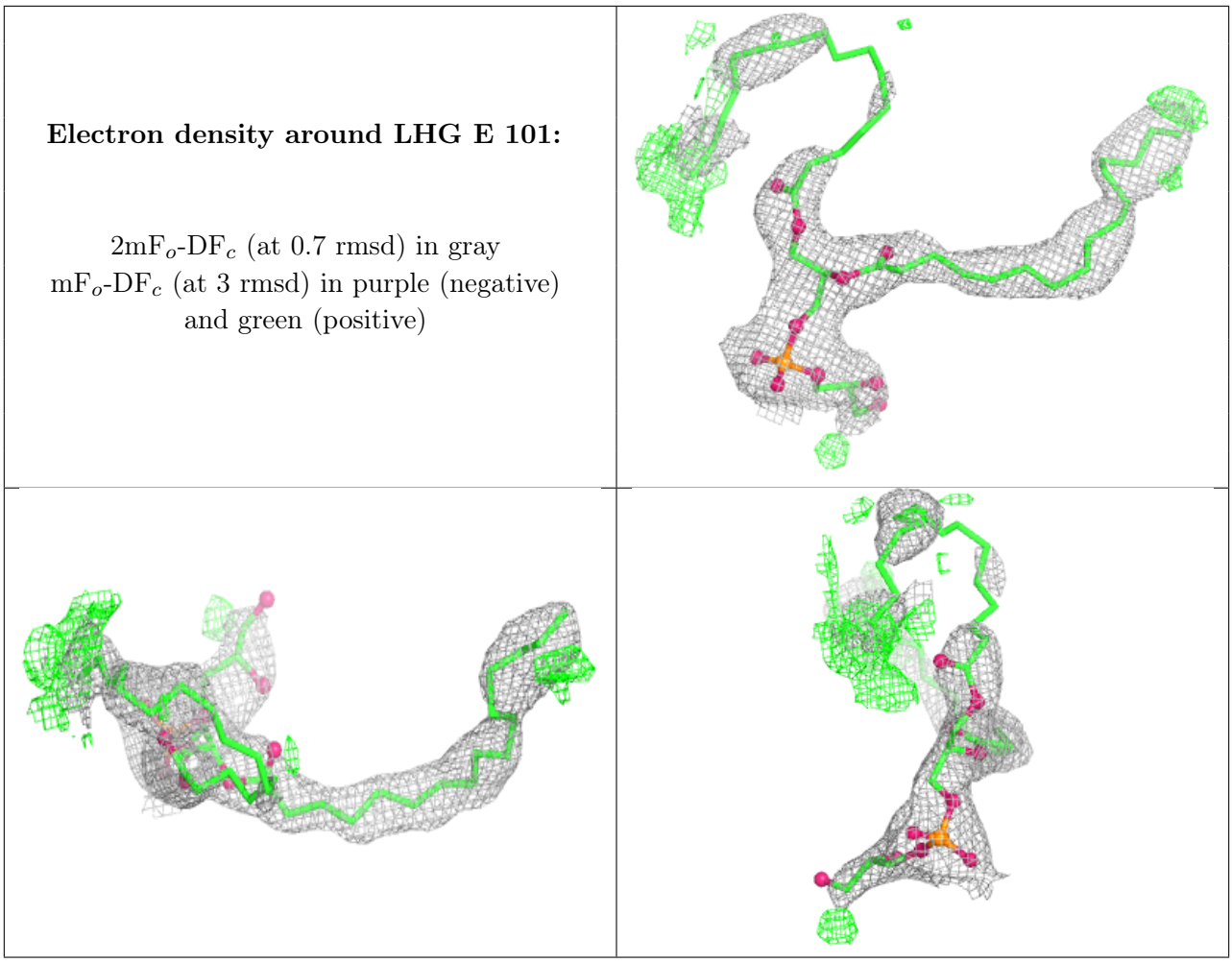






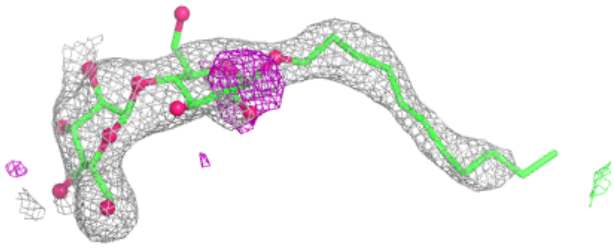
Electron density around LHG E 101:

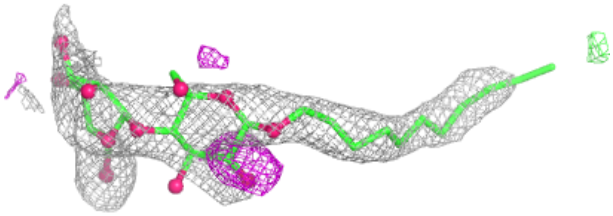
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

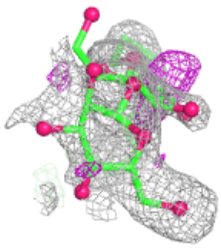


Electron density around LMT A 414:

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

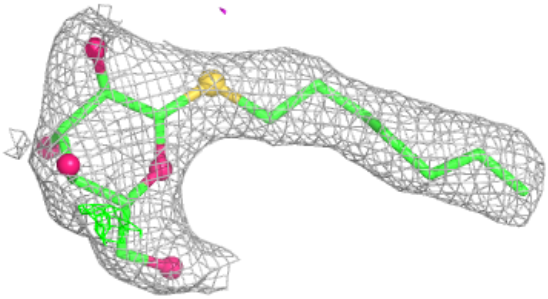


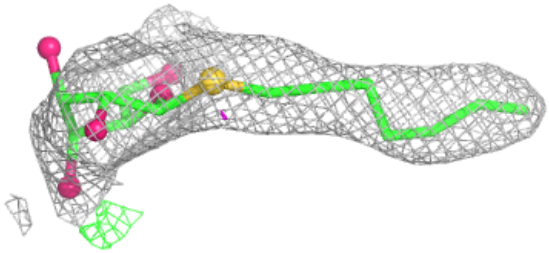


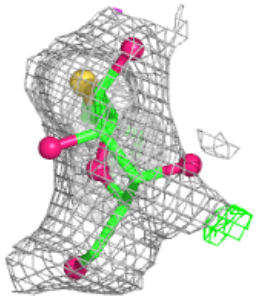


Electron density around HTG i 103:

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

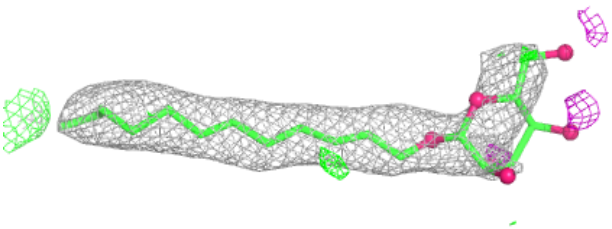


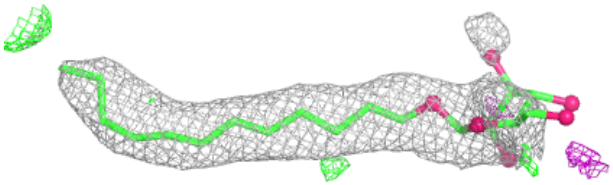


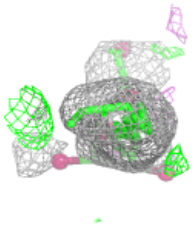


Electron density around LMT I 1201:

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

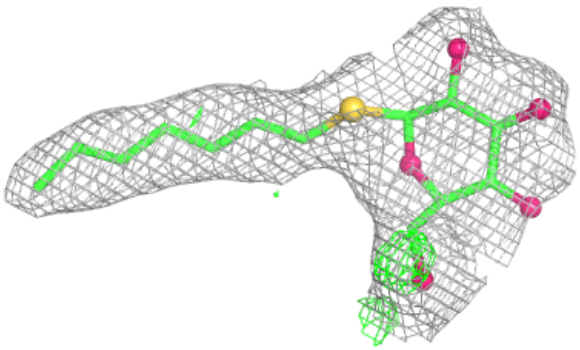


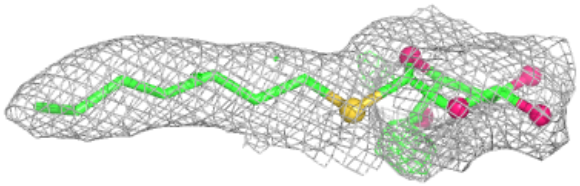


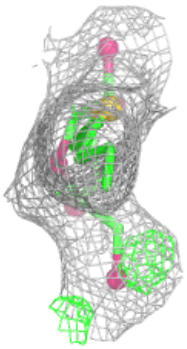


Electron density around HTG b 602:

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

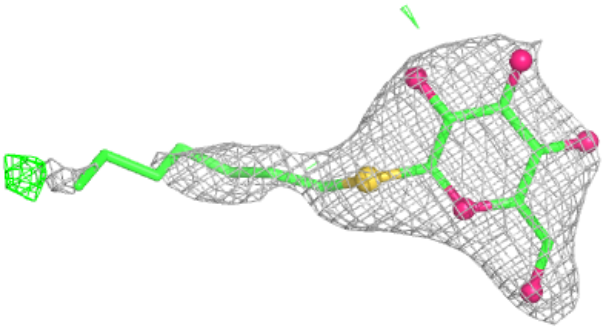


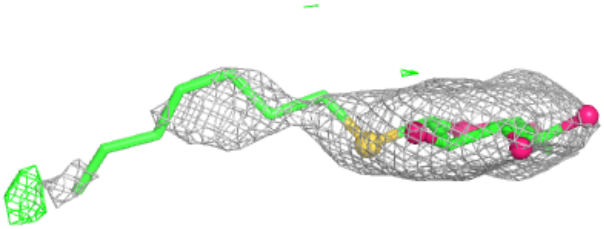


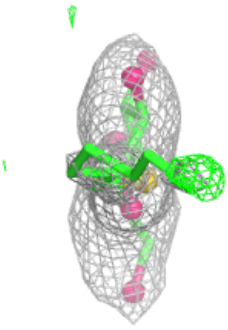


Electron density around HTG c 523:

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

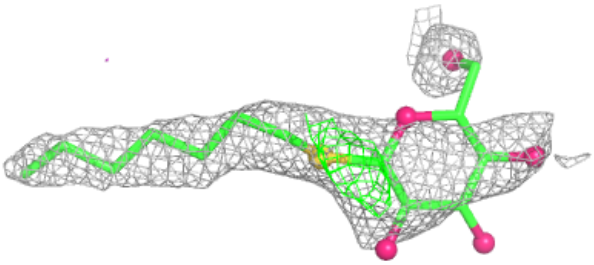


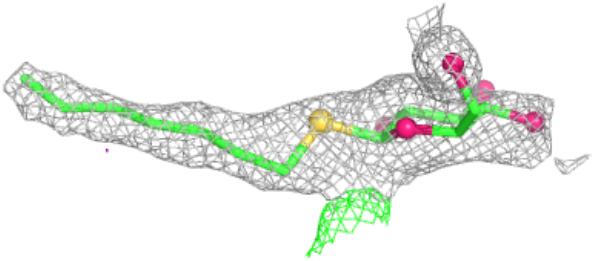


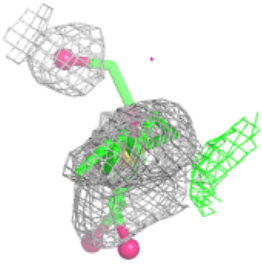


Electron density around HTG c 524:

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

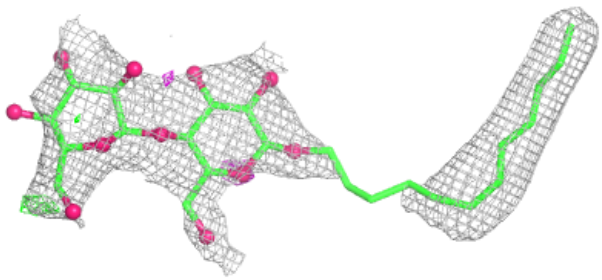


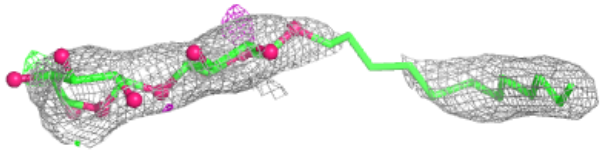


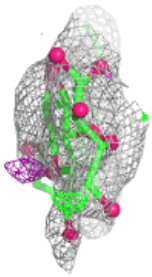


Electron density around LMT Z 101:

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

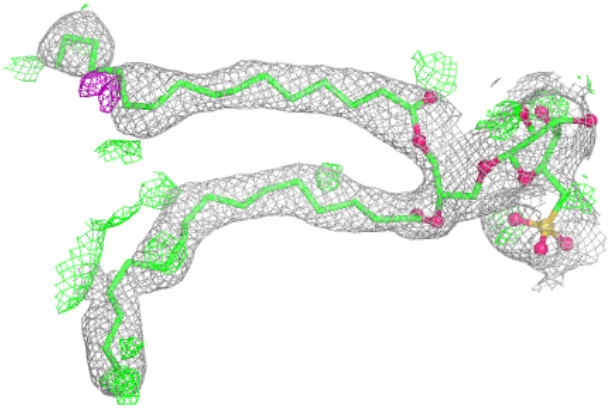


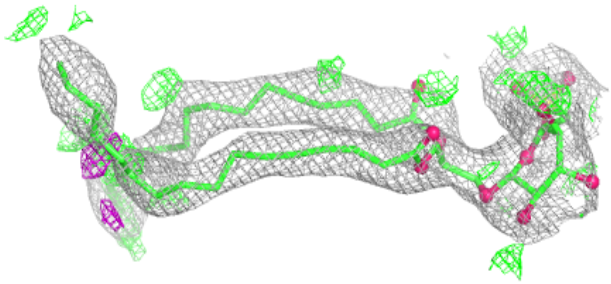


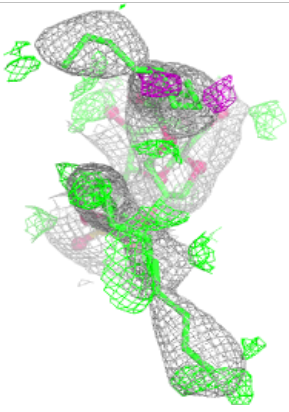


Electron density around SQD L 102:

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

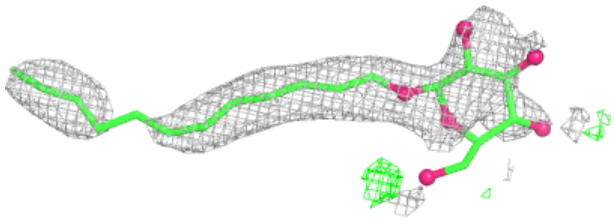


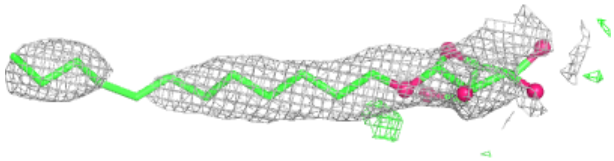


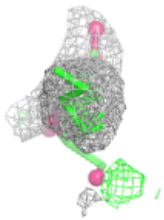


Electron density around LMT J 102:

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

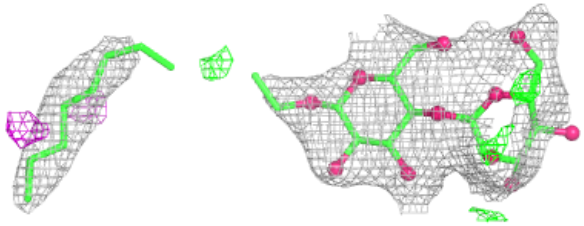


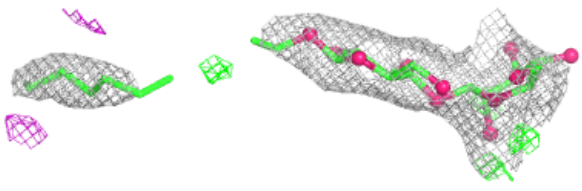


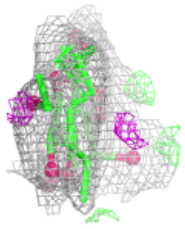


Electron density around LMT z 1801:

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

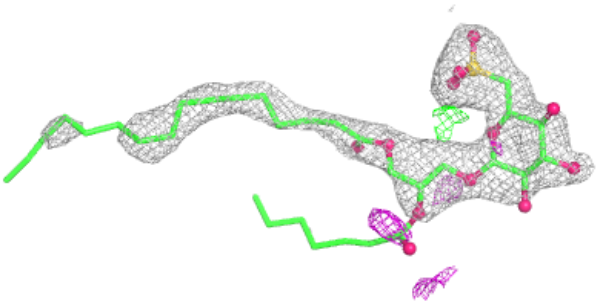


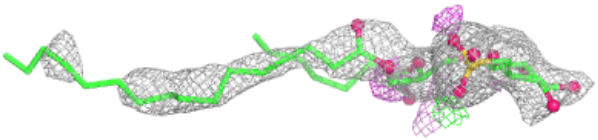


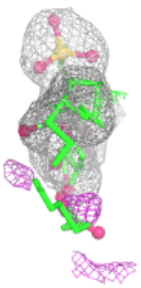


Electron density around SQD F 101:

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

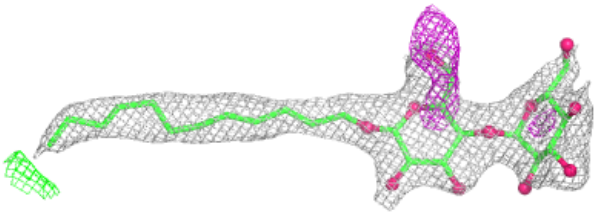


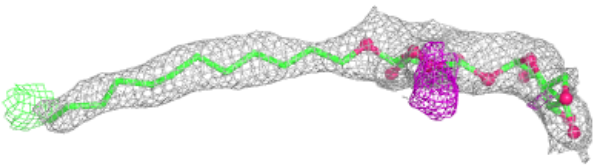


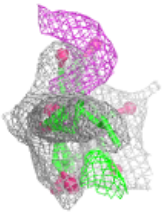


Electron density around LMT m 102:

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

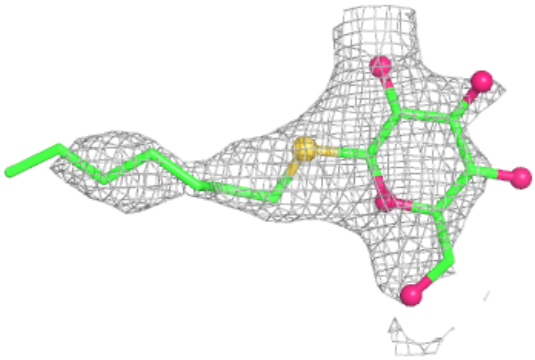


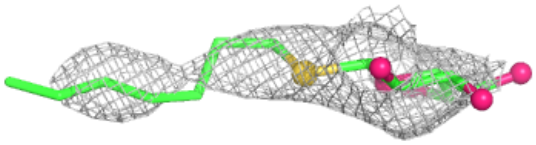


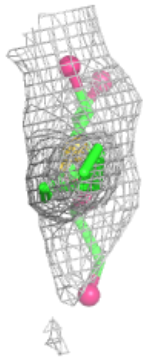


Electron density around HTG c 526:

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

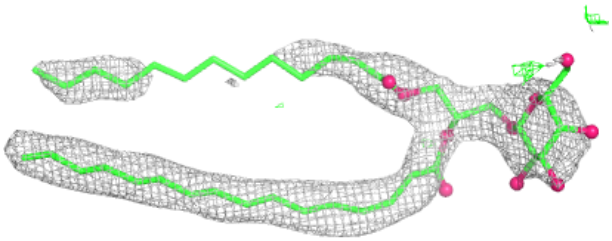


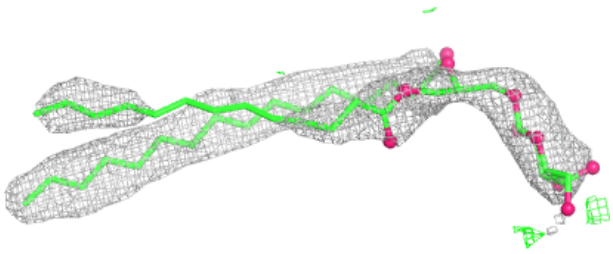


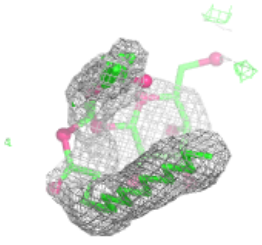


Electron density around LMG C 526:

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

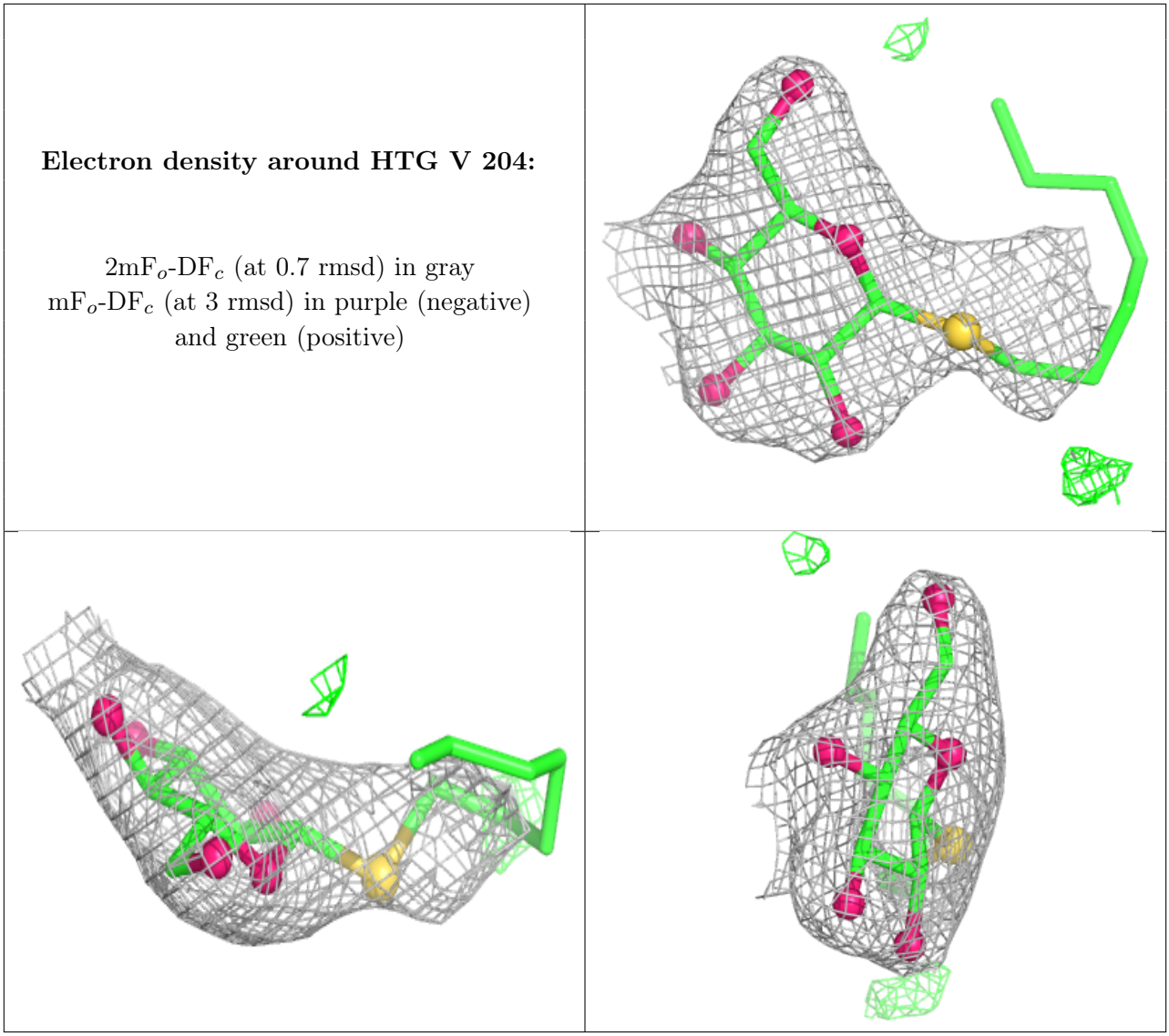






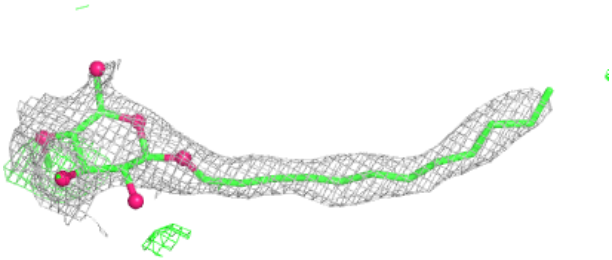
Electron density around HTG V 204:

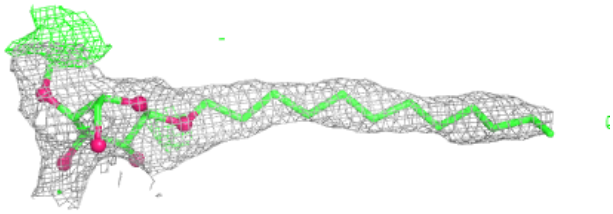
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

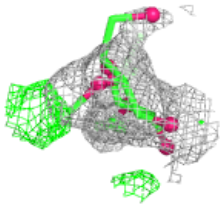


Electron density around LMT b 624:

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

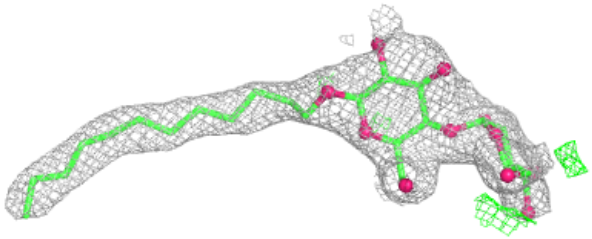


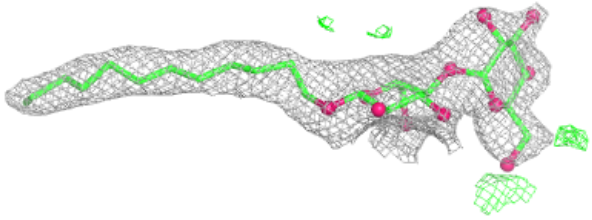


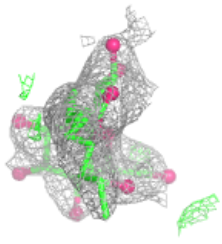


Electron density around LMT B 623:

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

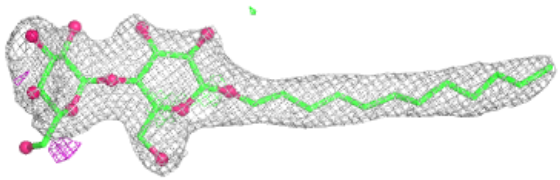


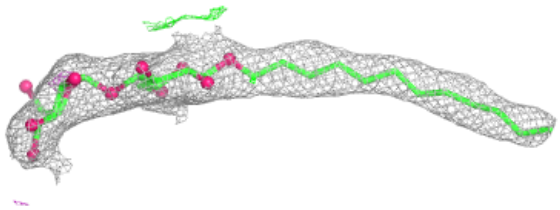


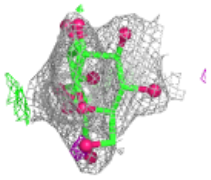


Electron density around LMT M 101:

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

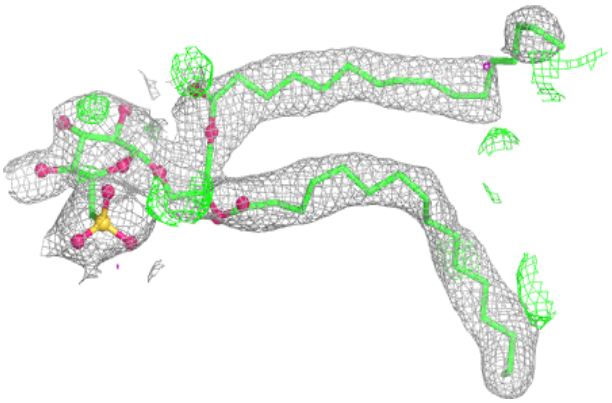


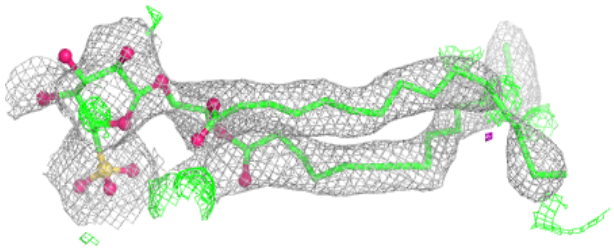


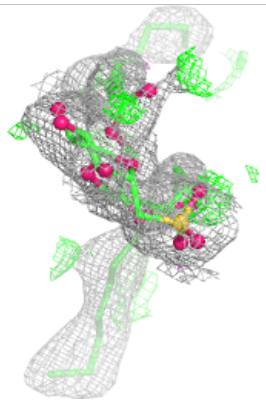


Electron density around SQD B 621:

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

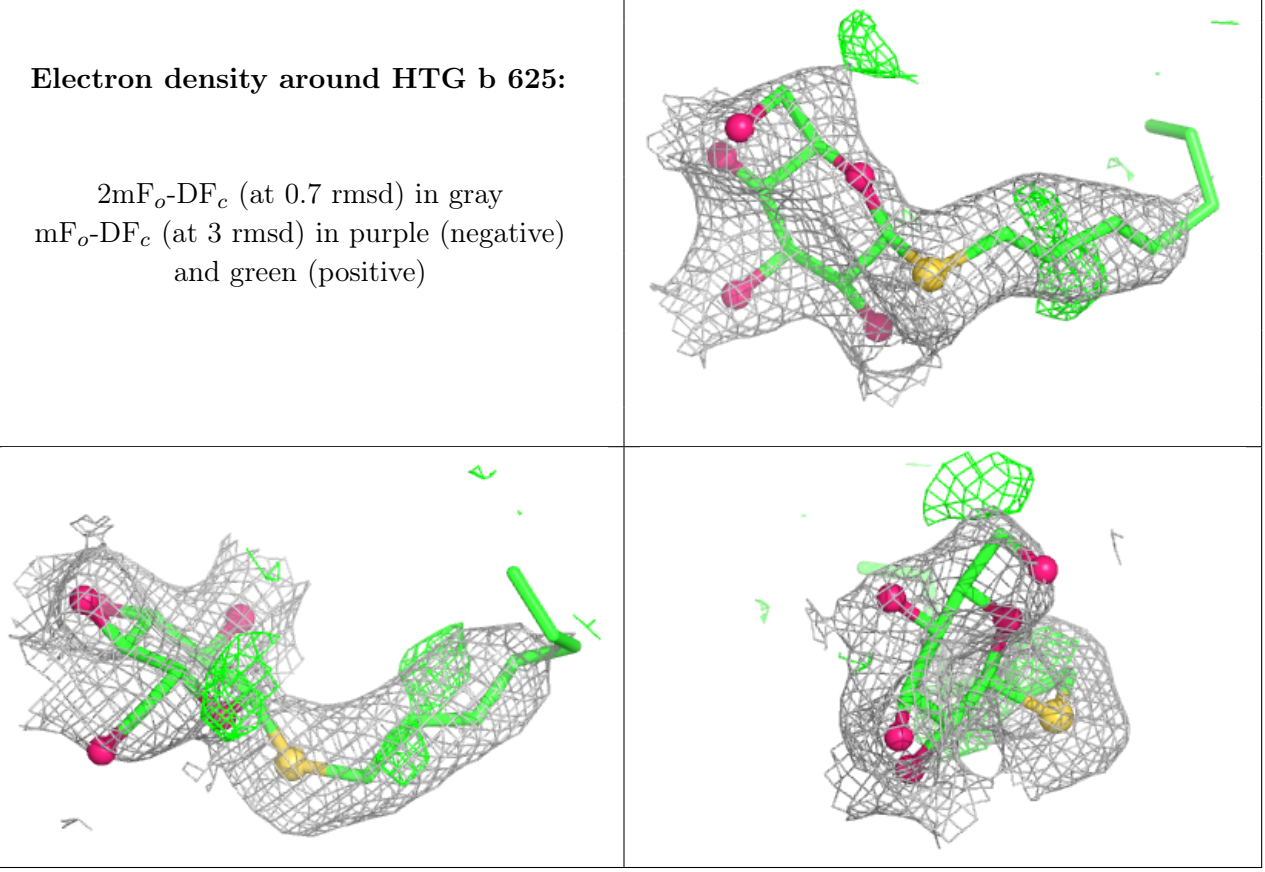






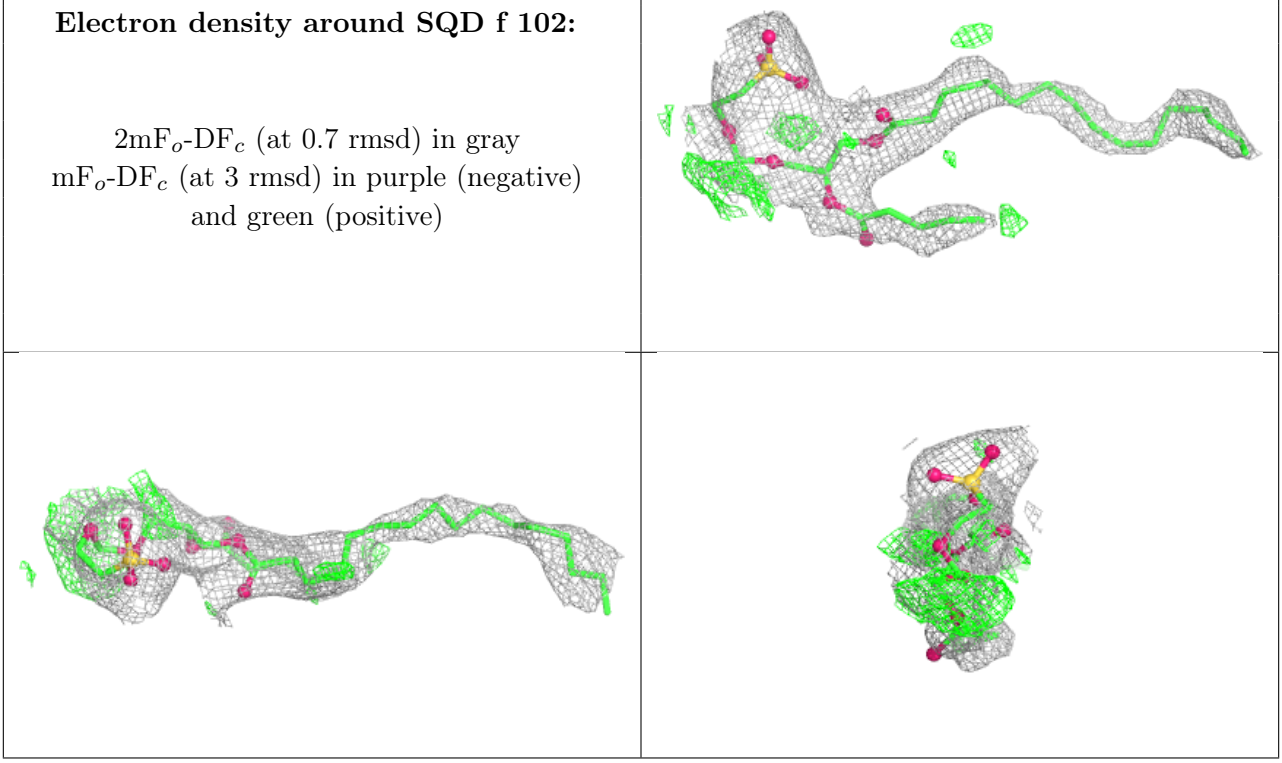
Electron density around HTG b 625:

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



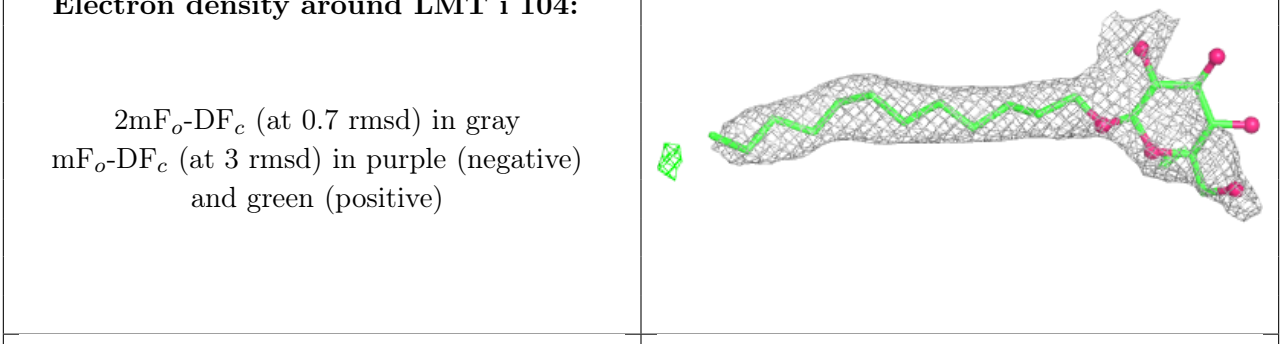
Electron density around SQD f 102:

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



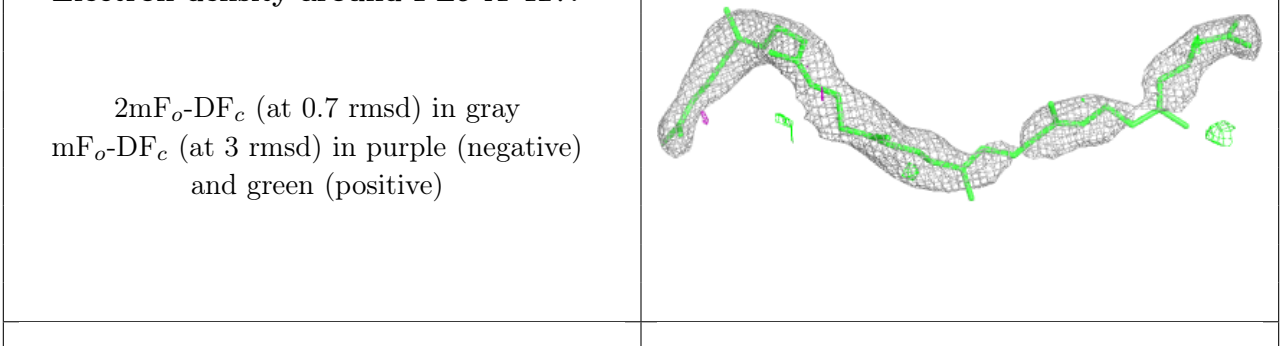
Electron density around LMT i 104:

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



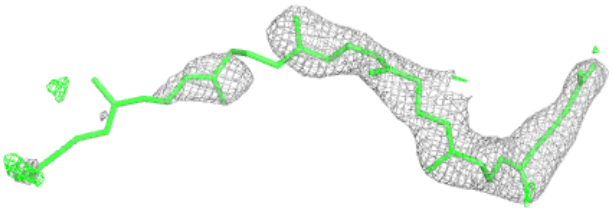
Electron density around PL9 A 417:

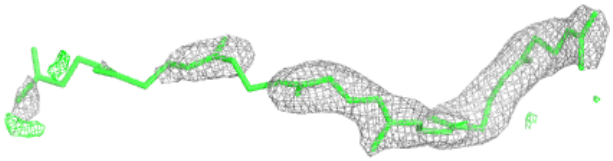
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

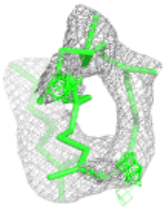


Electron density around PL9 x 801:

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

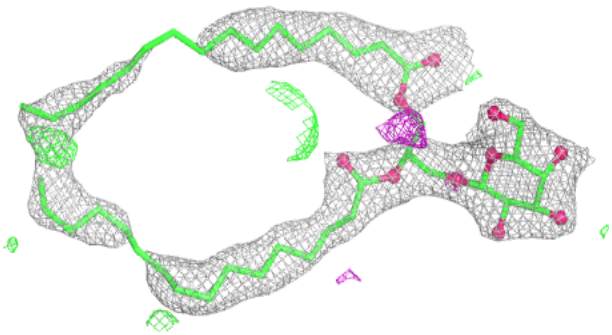


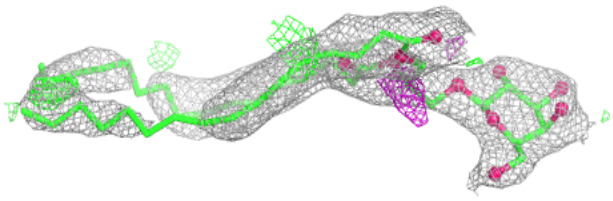


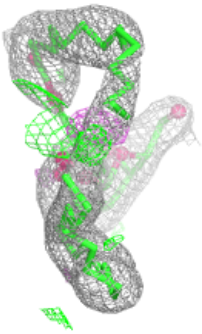


Electron density around LMG i 101:

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

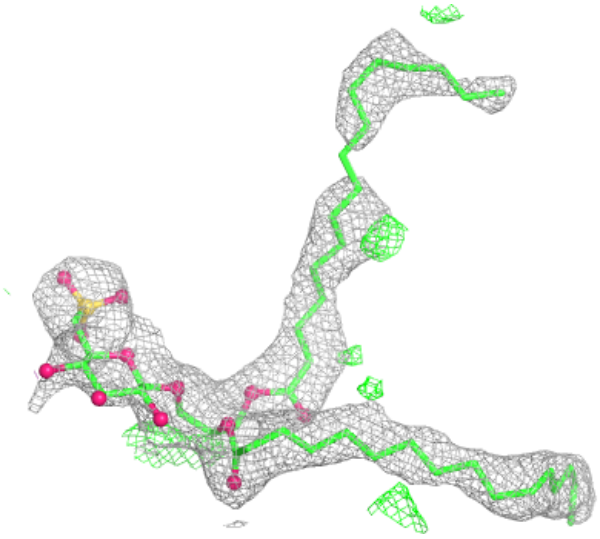


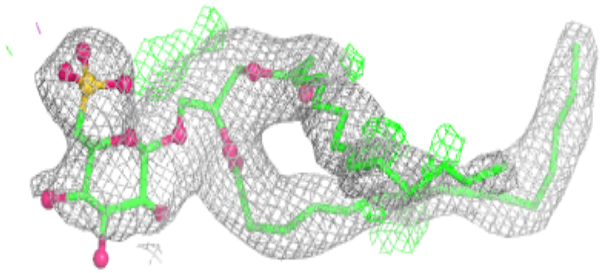


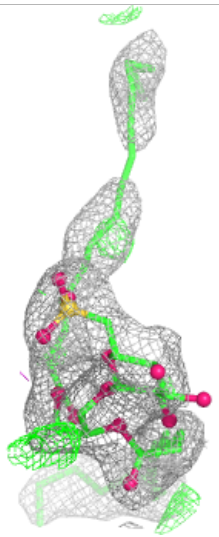


Electron density around SQD A 413:

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

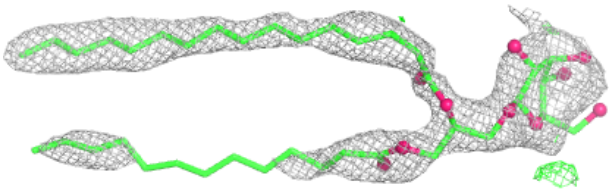


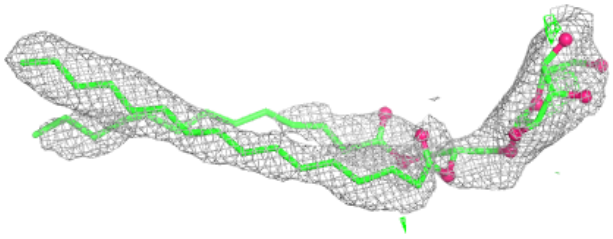


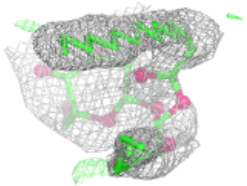


Electron density around LMG c 522:

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

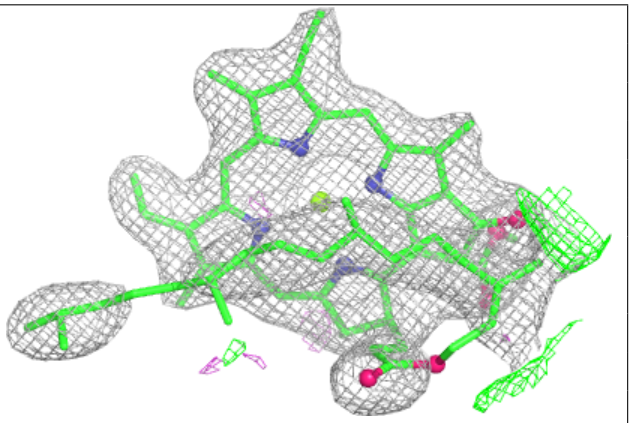


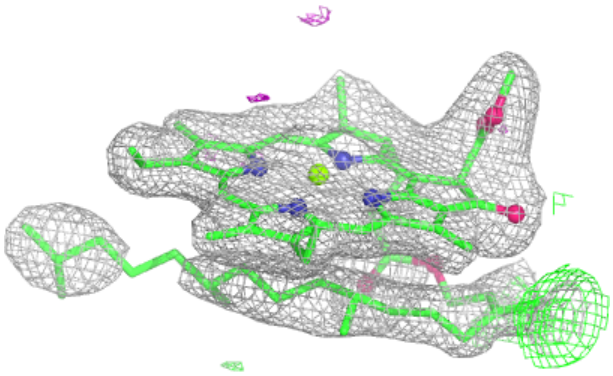


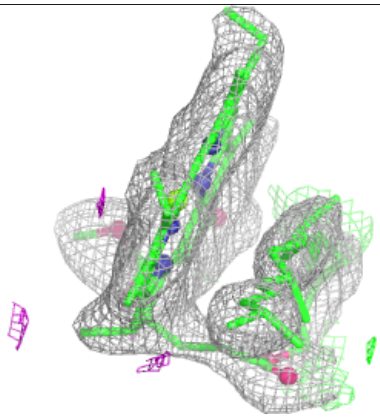


Electron density around CLA B 602:

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

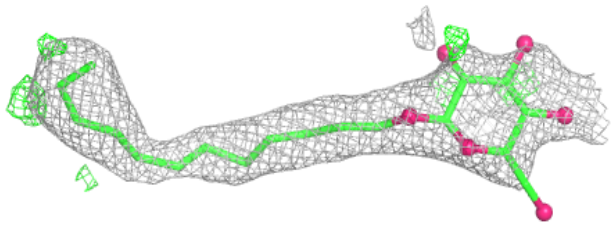


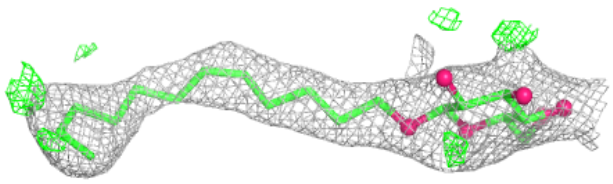


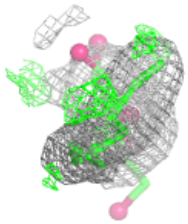


Electron density around LMT B 637:

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

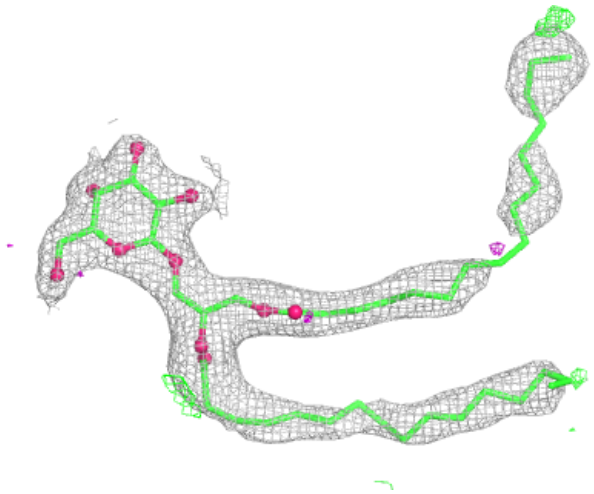


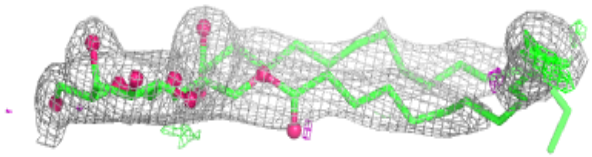


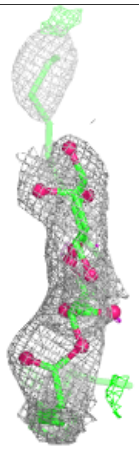


Electron density around LMG C 520:

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

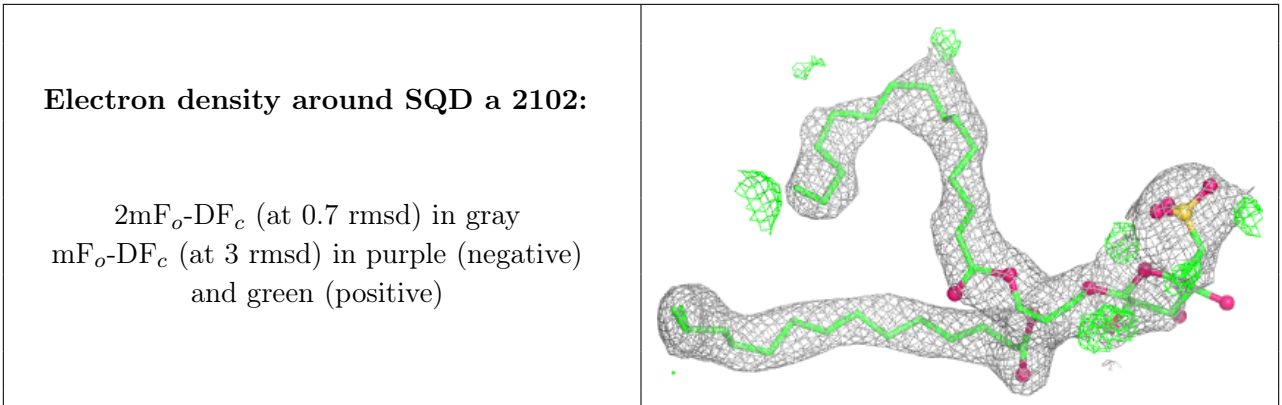


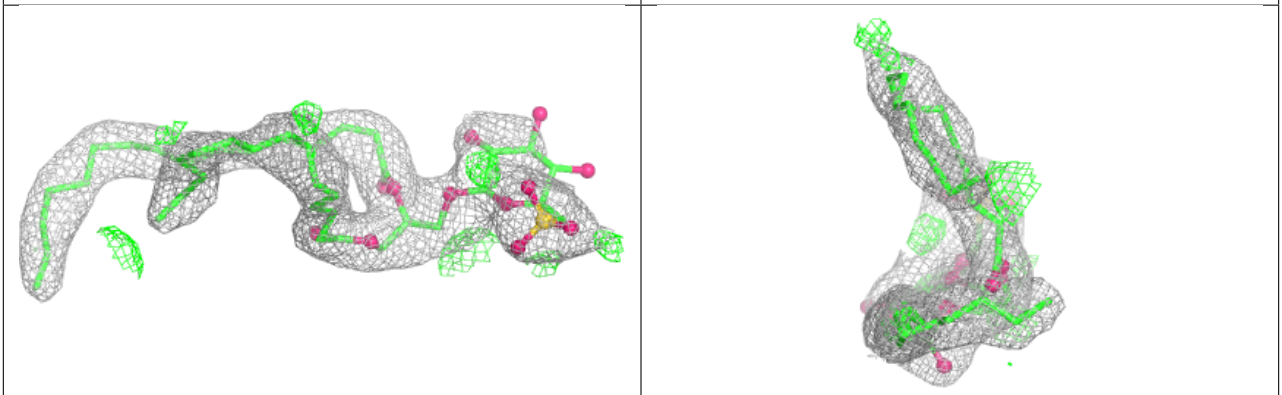




Electron density around SQD a 2102:

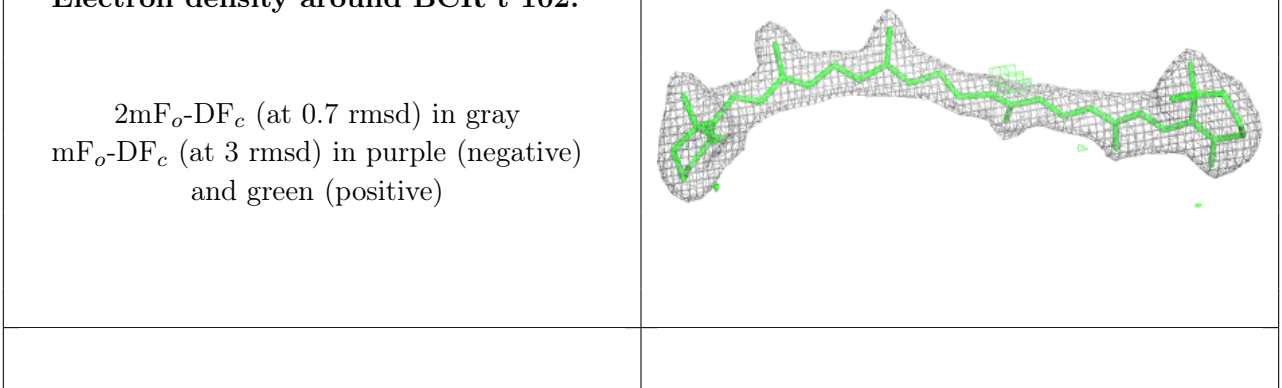
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

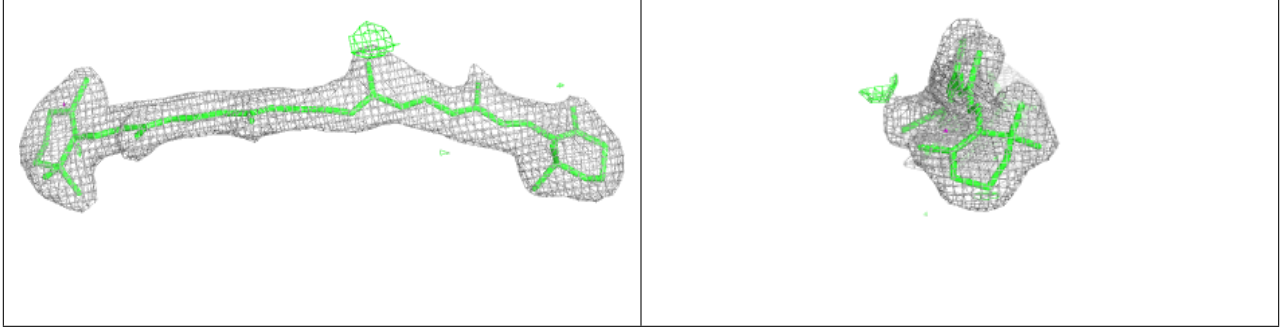




Electron density around BCR t 102:

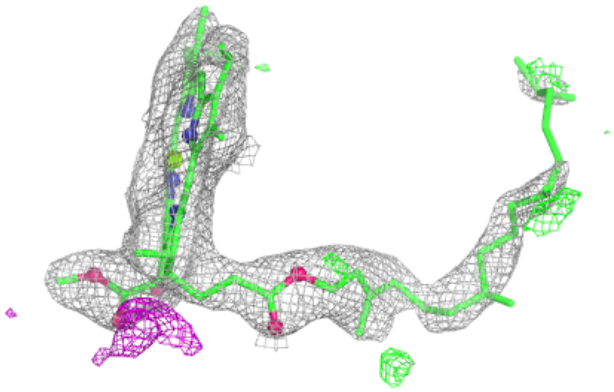
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

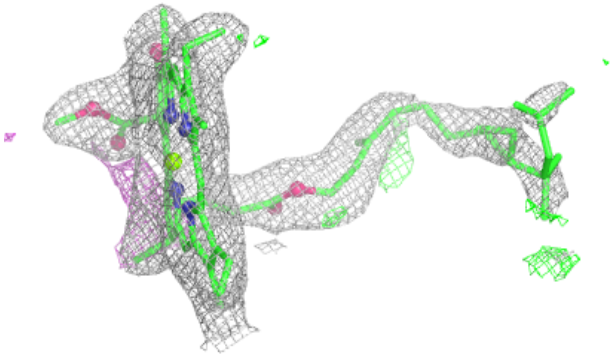


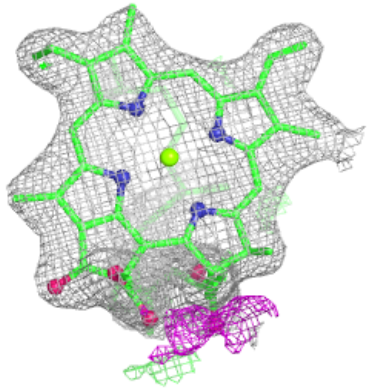


Electron density around CLA C 507:

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

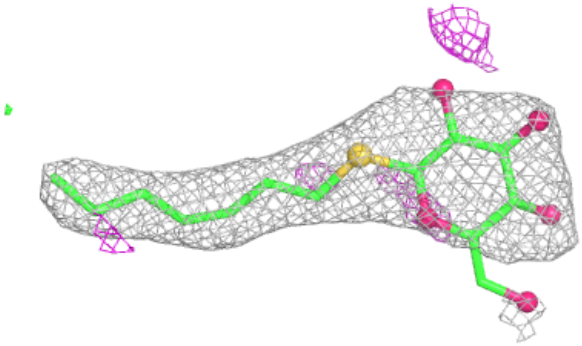


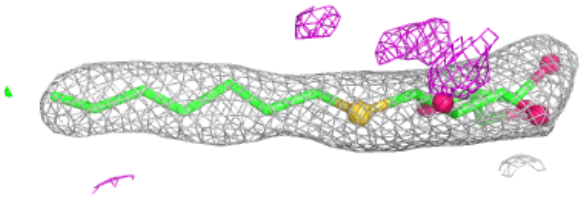


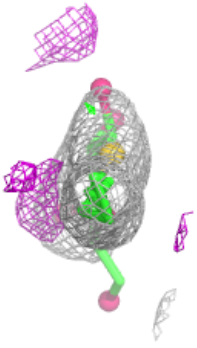


Electron density around HTG B 627:

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

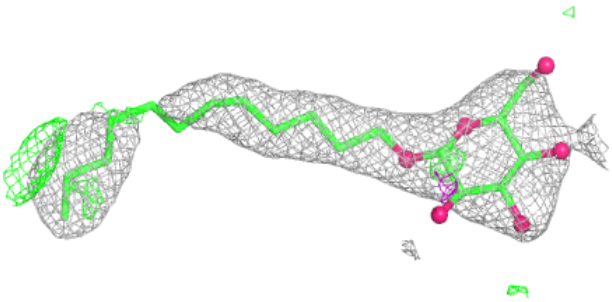


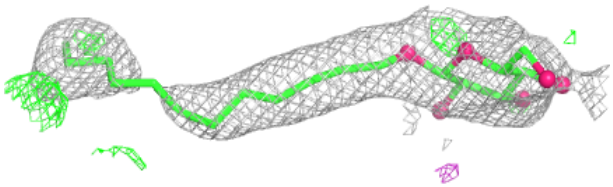


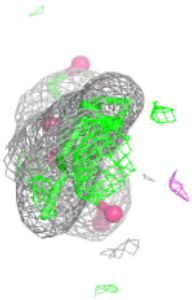


Electron density around LMT T 102:

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

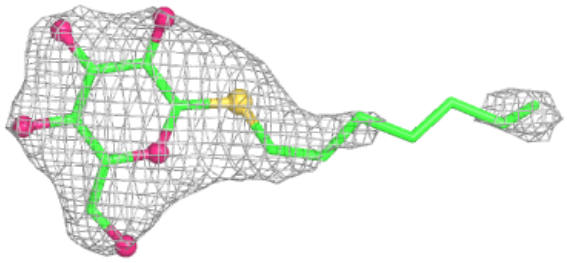


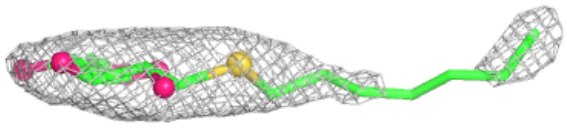


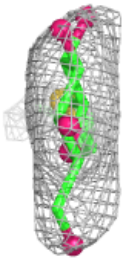


Electron density around HTG C 521:

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

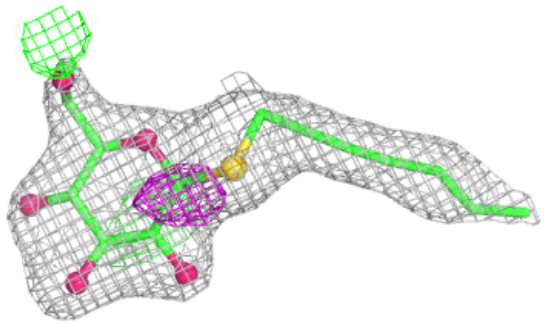


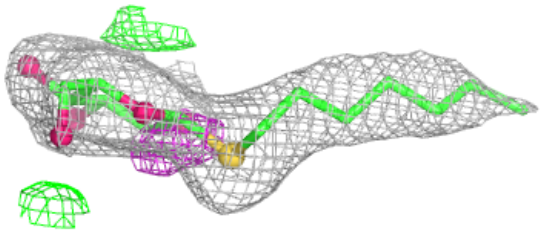


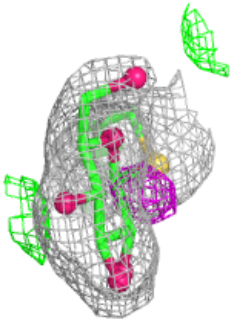


Electron density around HTG B 624:

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

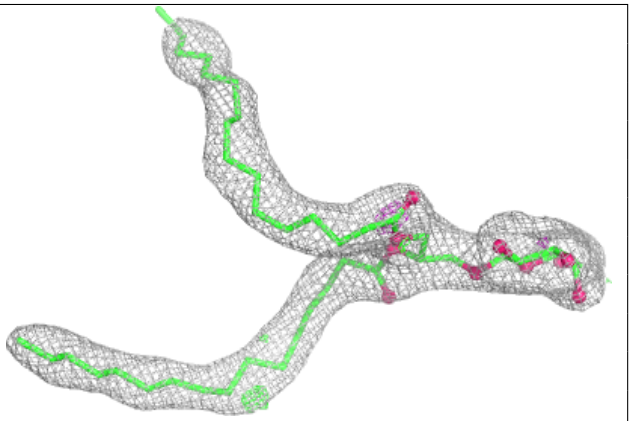


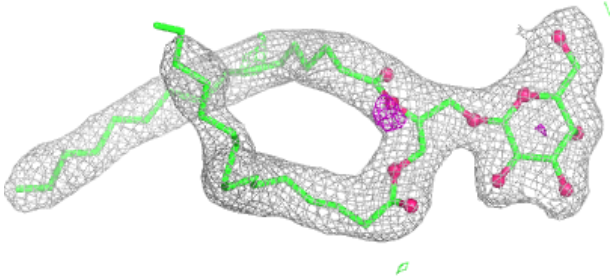


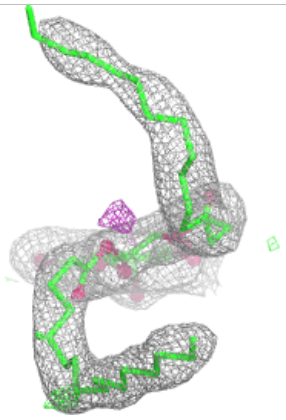


Electron density around LMG B 622:

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

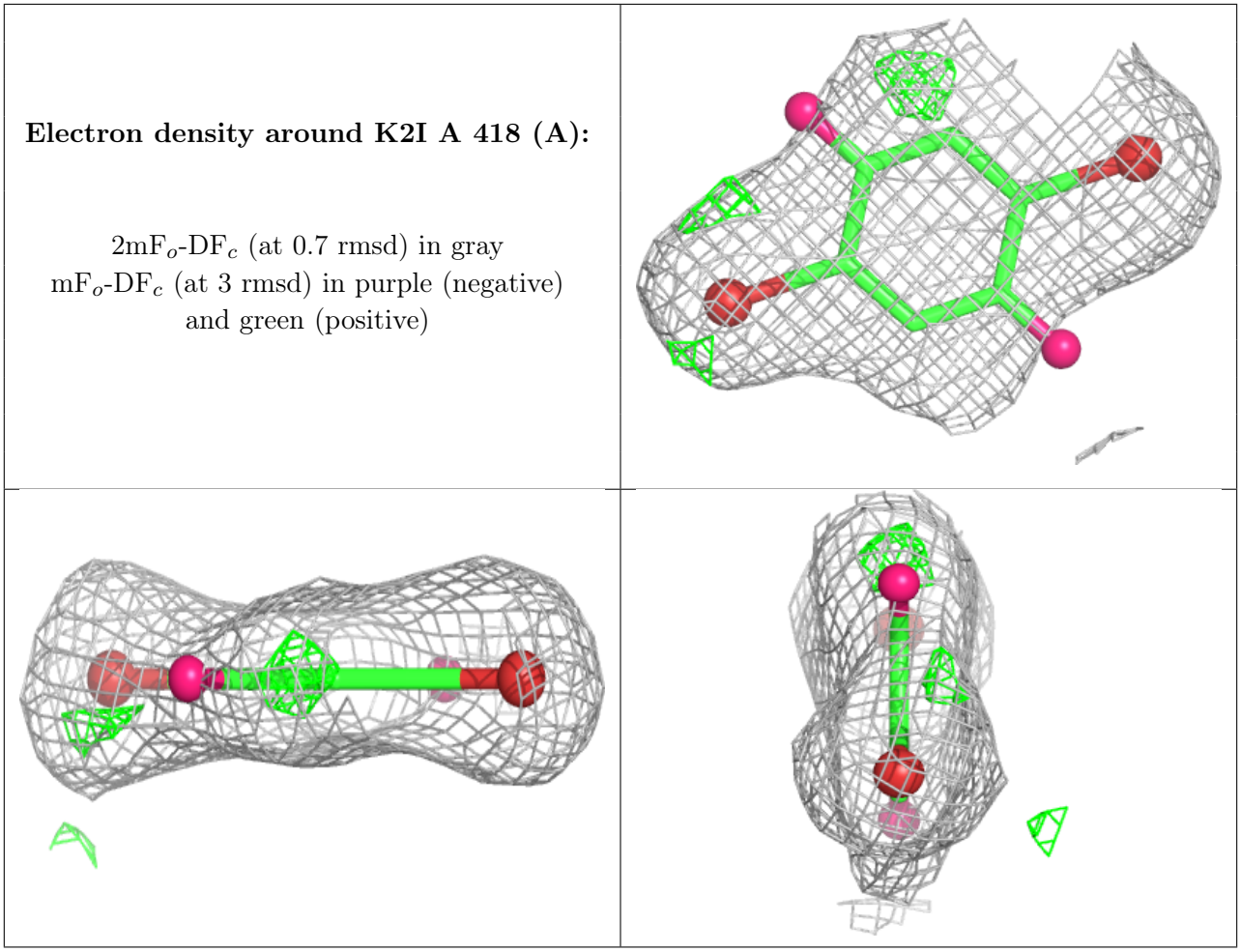






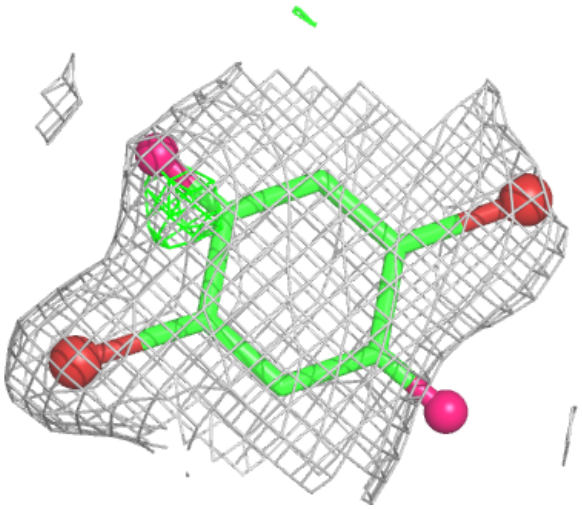
Electron density around K2I A 418 (A):

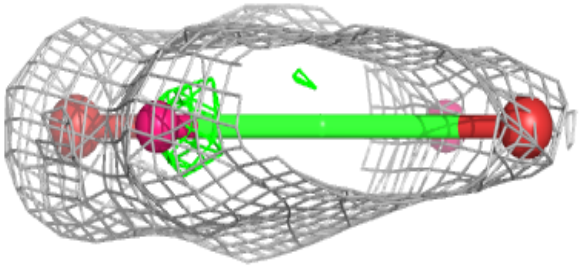
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

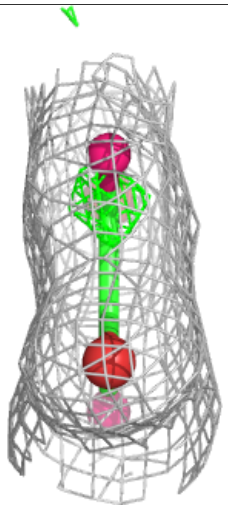


Electron density around K2I A 418 (B):

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



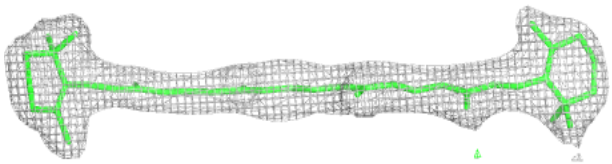




Electron density around BCR C 516:

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

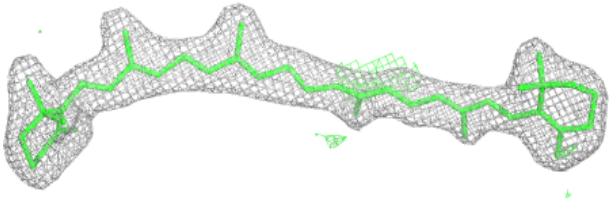


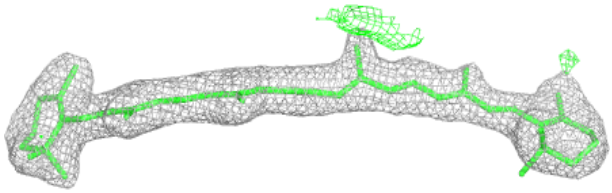


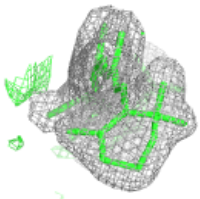


Electron density around BCR T 101:

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

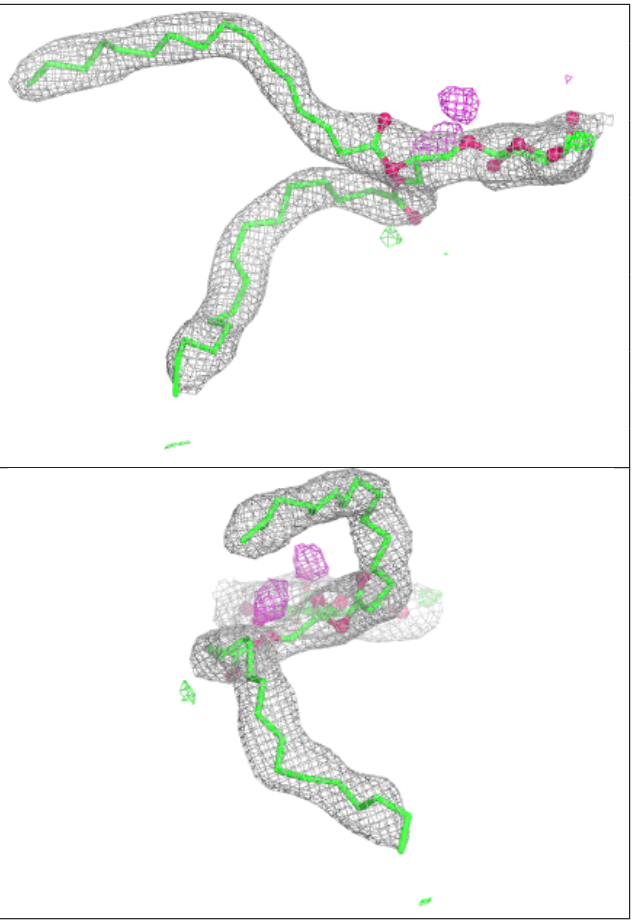


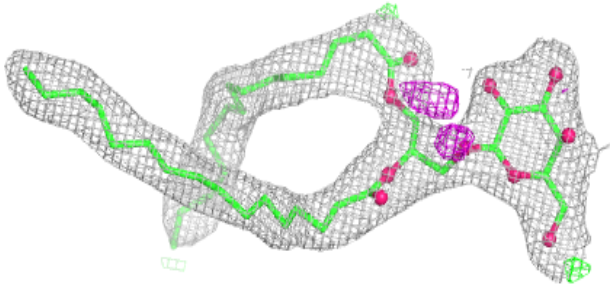




Electron density around LMG b 623:

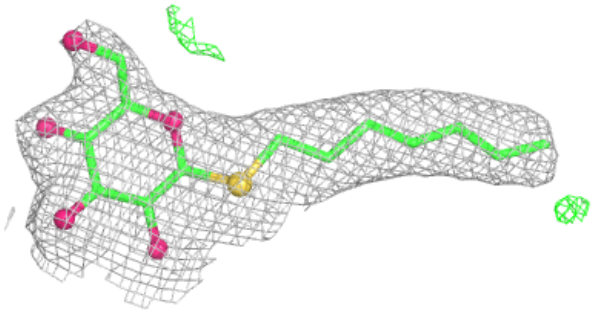
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

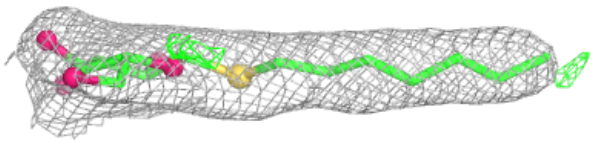


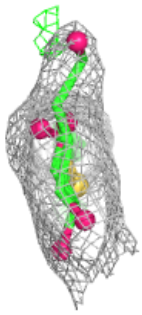


Electron density around HTG b 601:

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

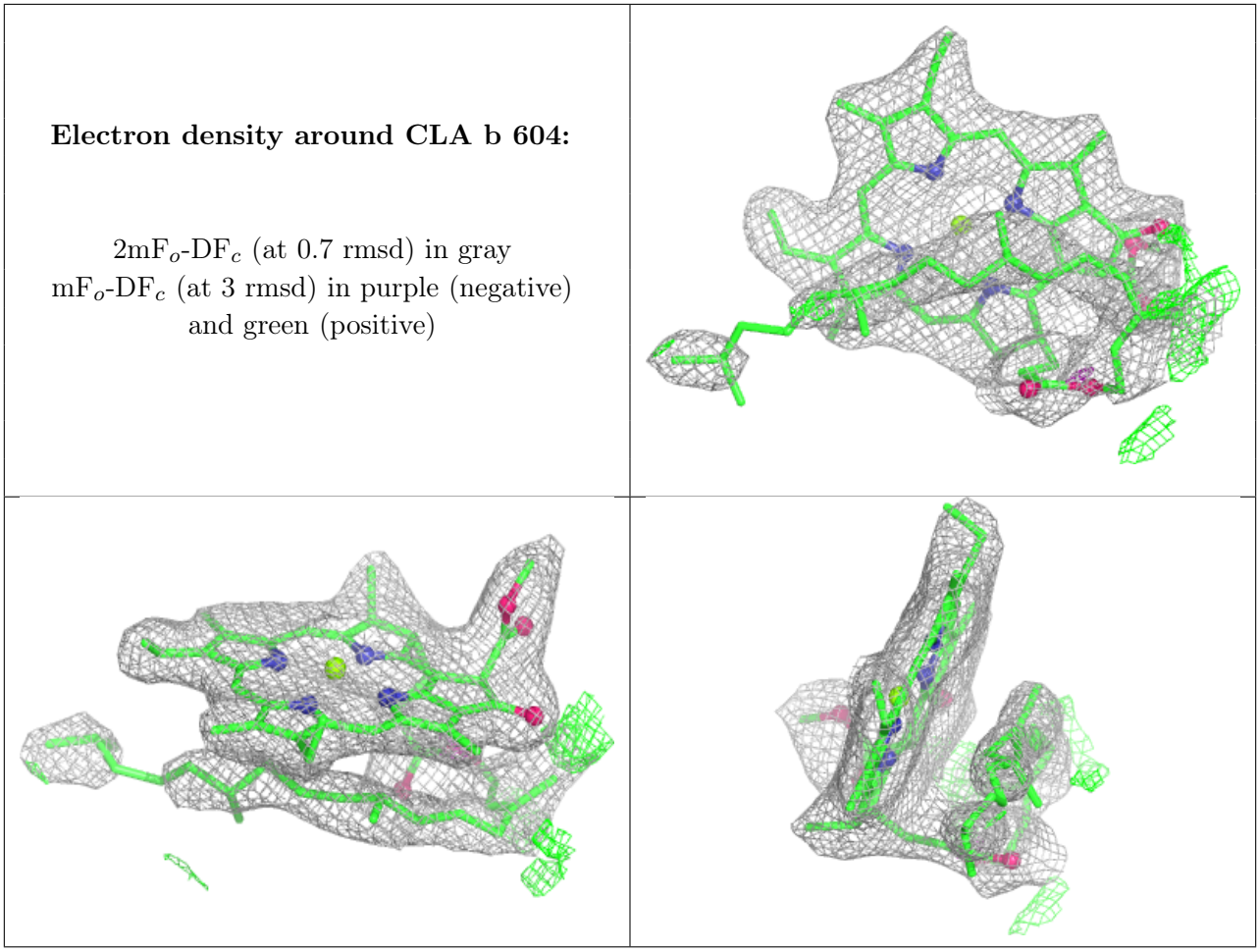






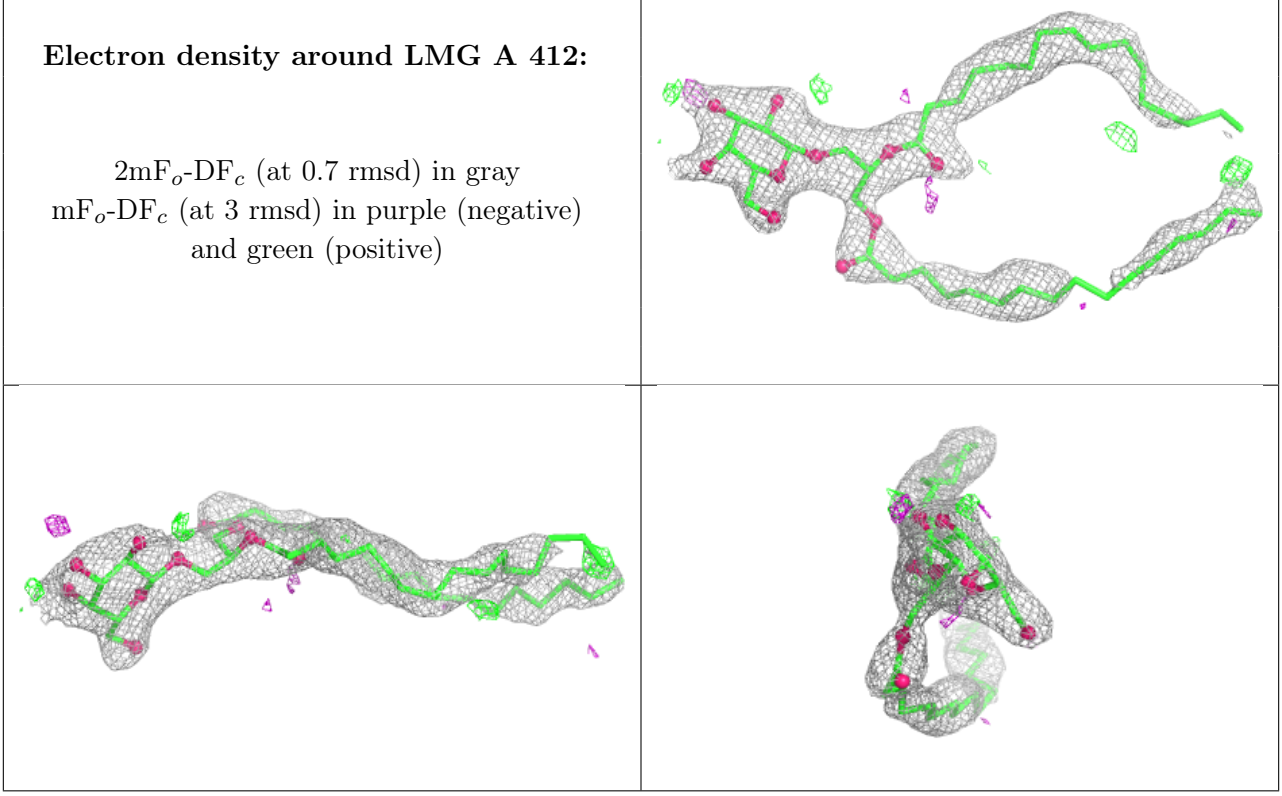
Electron density around CLA b 604:

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



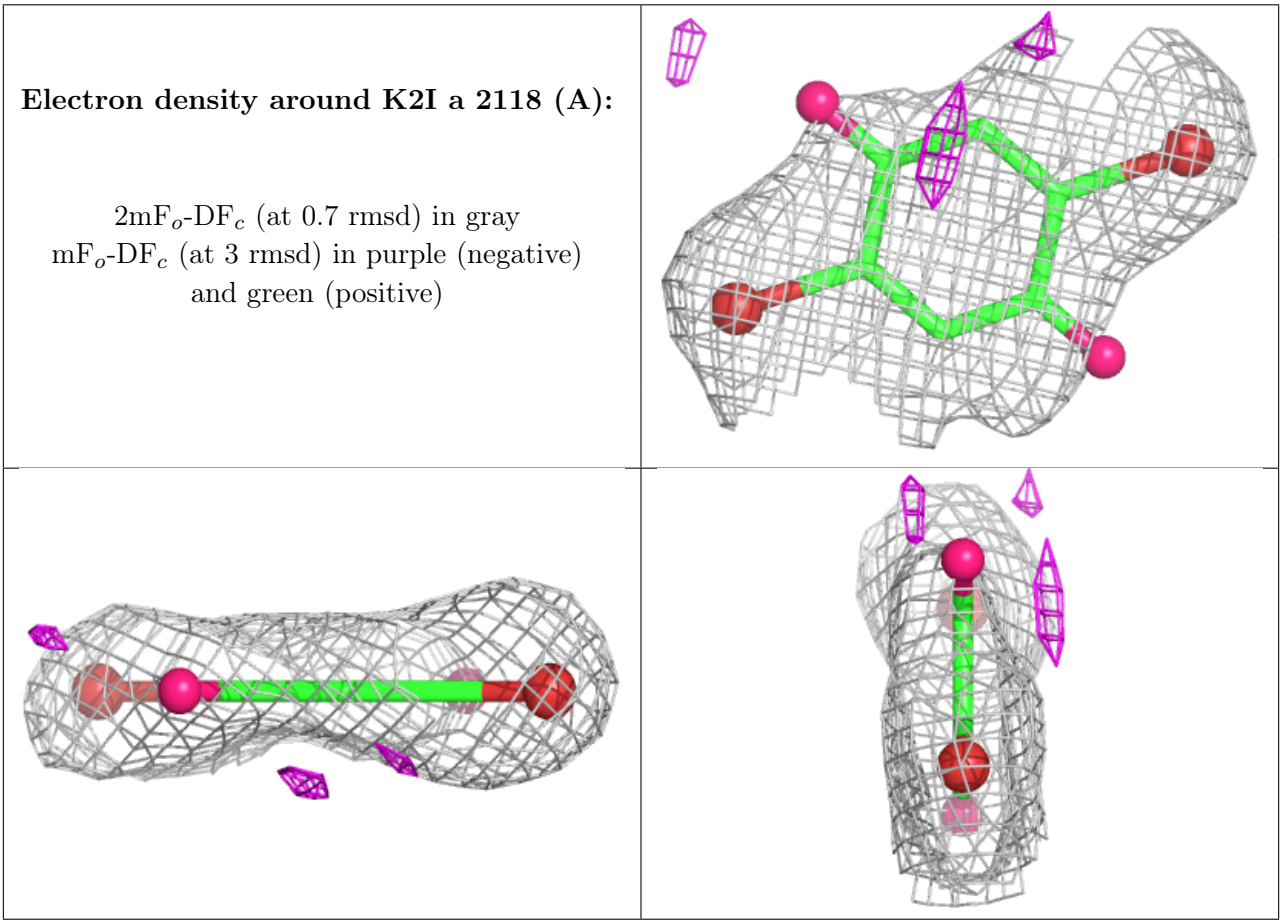
Electron density around LMG A 412:

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



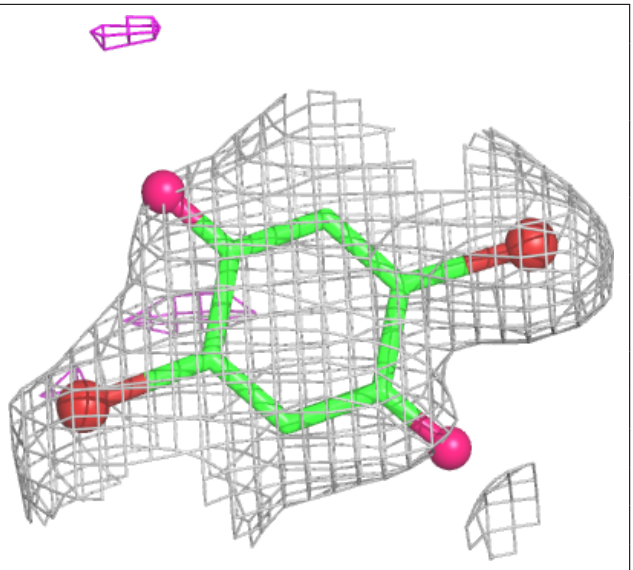
Electron density around K2I a 2118 (A):

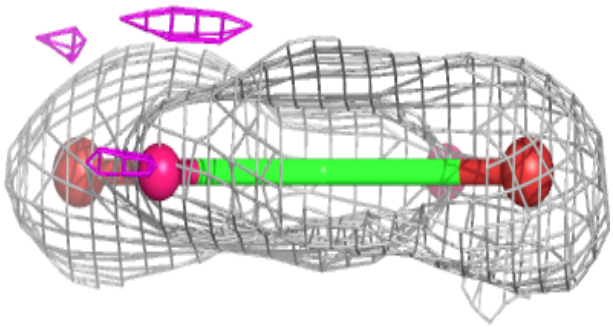
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

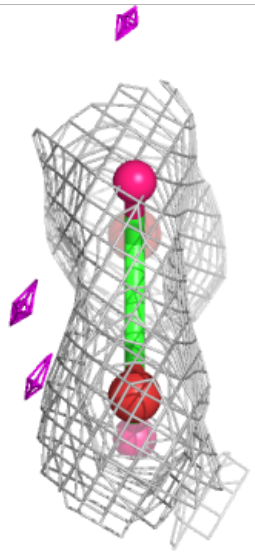


Electron density around K2I a 2118 (B):

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

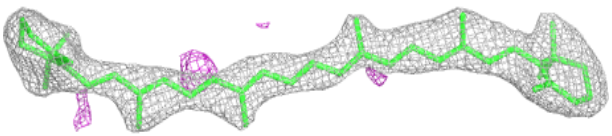


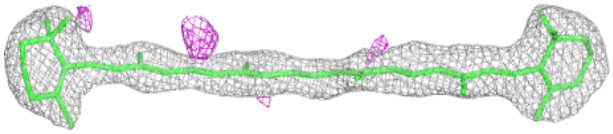


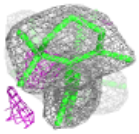


Electron density around BCR c 516:

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

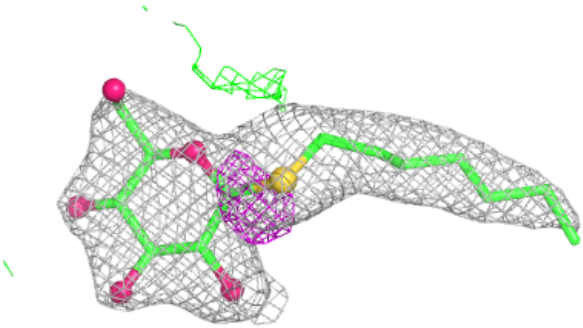


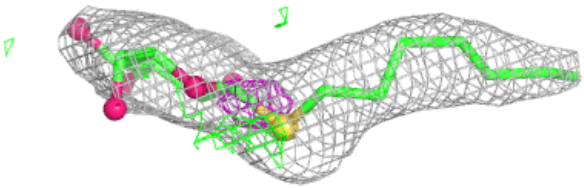


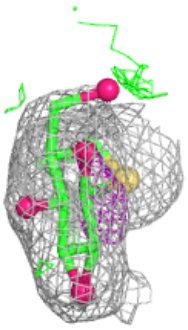


Electron density around HTG O 302:

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

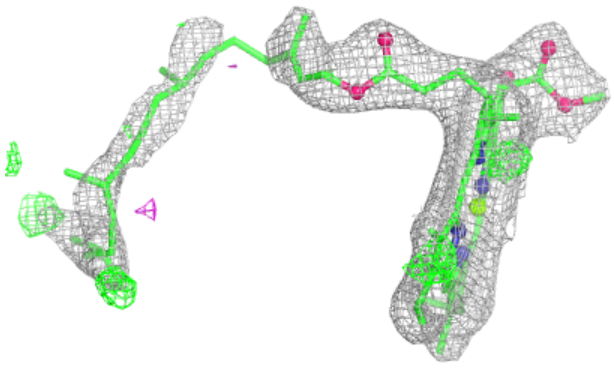


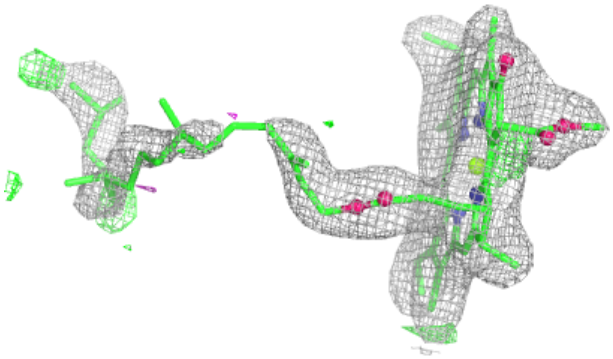


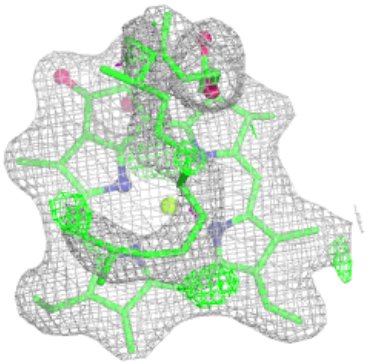


Electron density around CLA c 508:

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

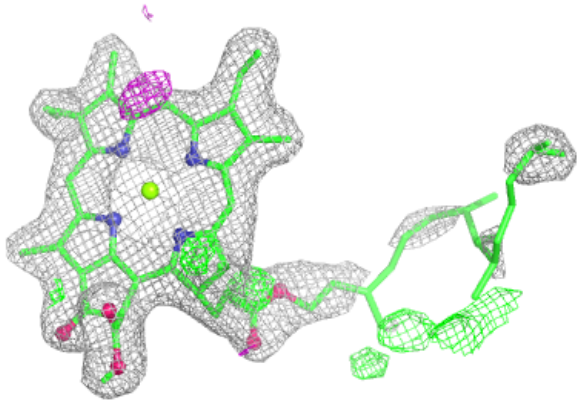


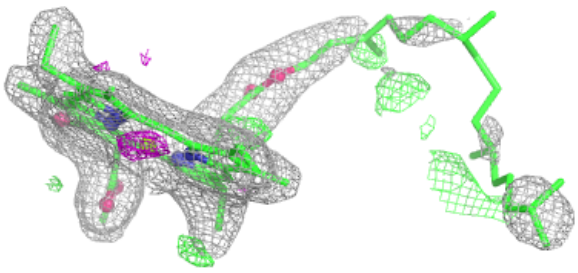




Electron density around CLA a 2113:

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

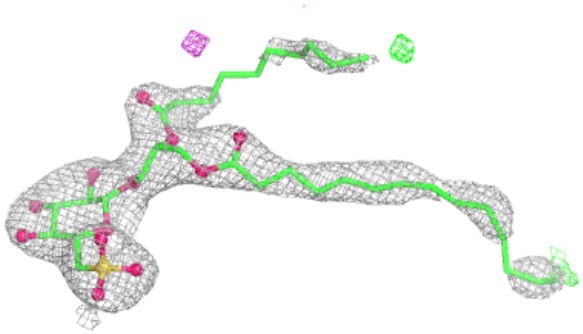


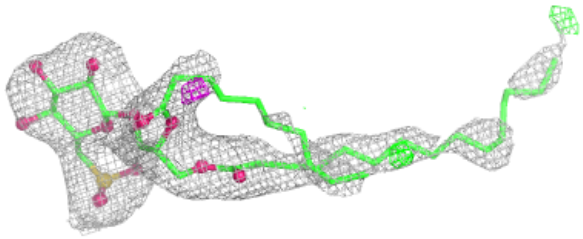


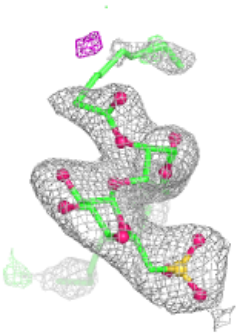


Electron density around SQD a 2115:

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

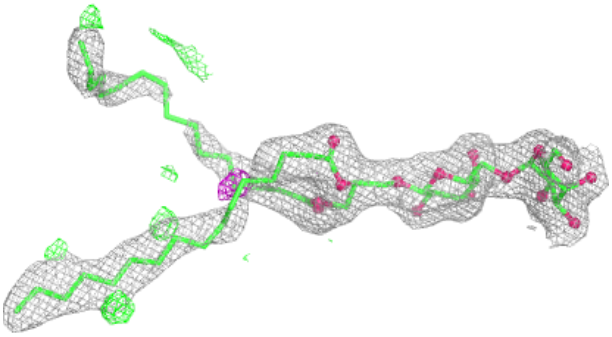


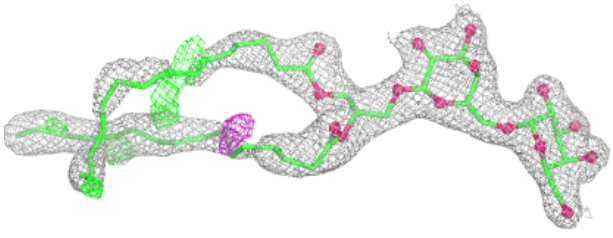


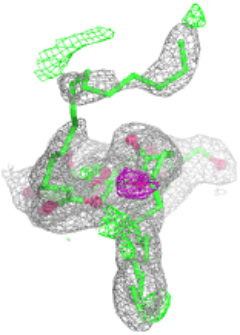


Electron density around DGD c 518:

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

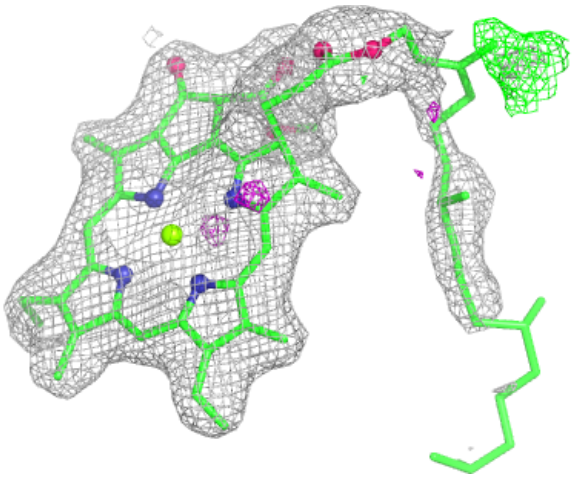


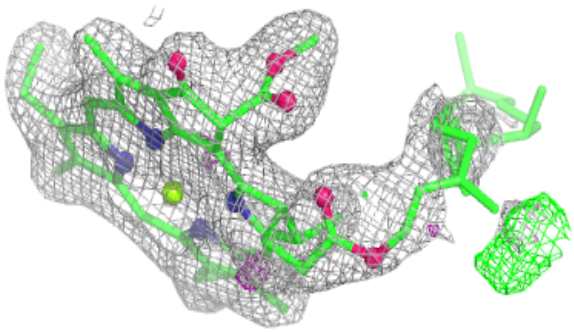


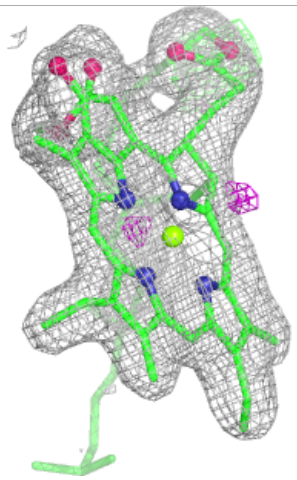


Electron density around CLA B 617:

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

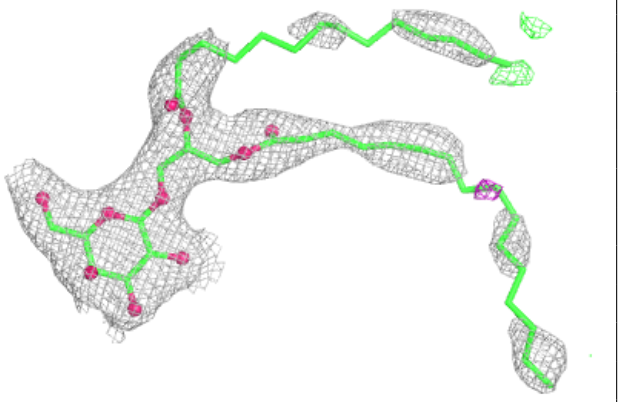


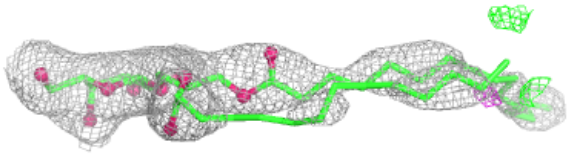


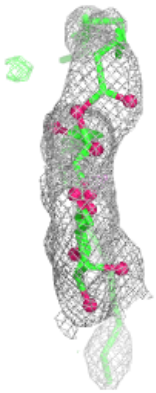


Electron density around LMG c 521:

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

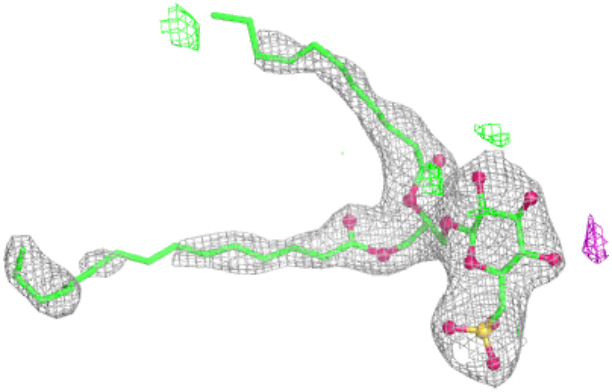


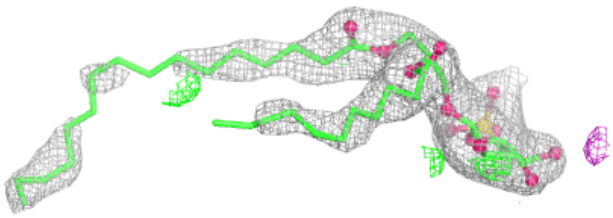


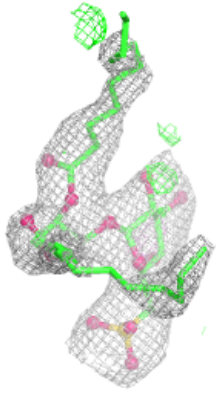


Electron density around SQD A 411:

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

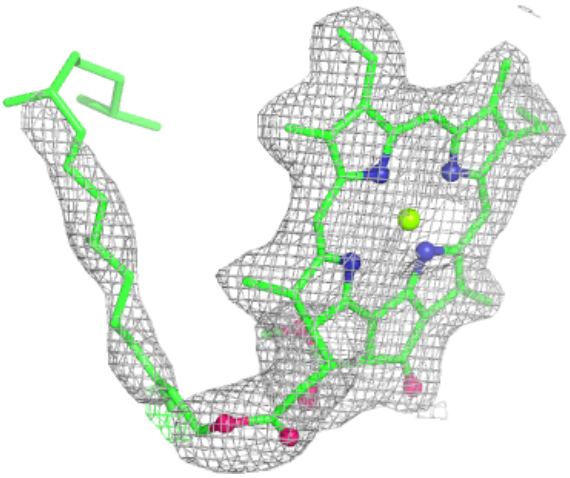


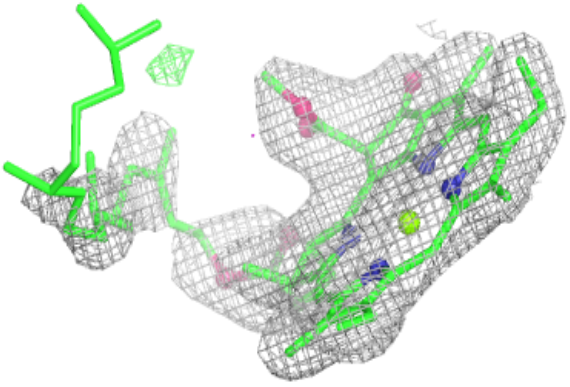


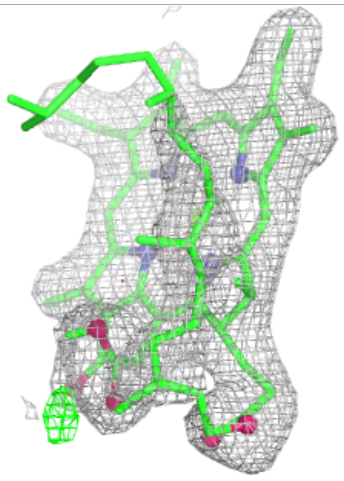


Electron density around CLA b 619:

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

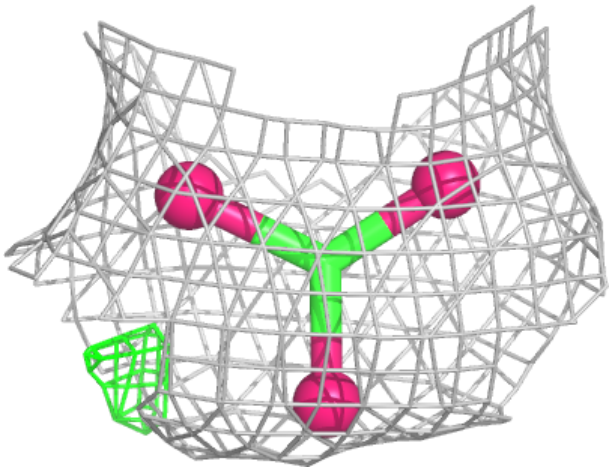


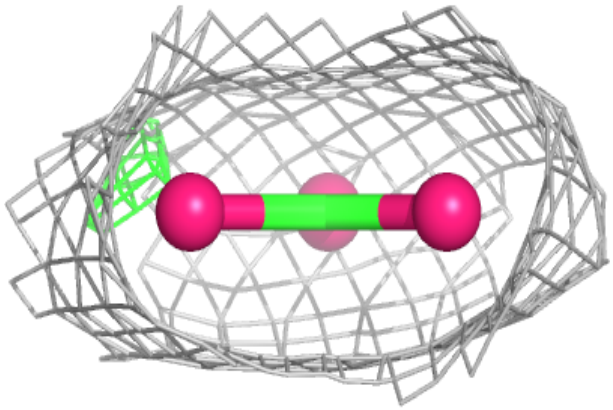


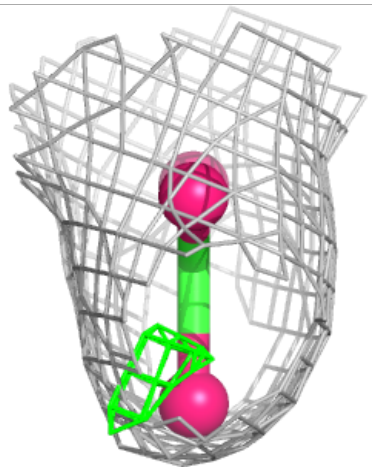


Electron density around BCT A 421:

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

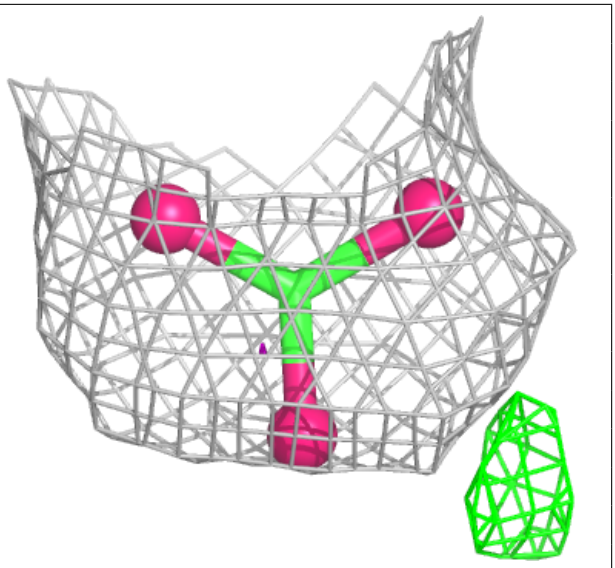


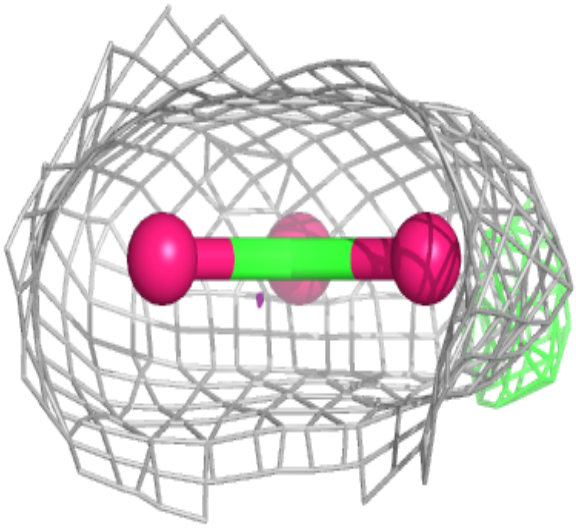


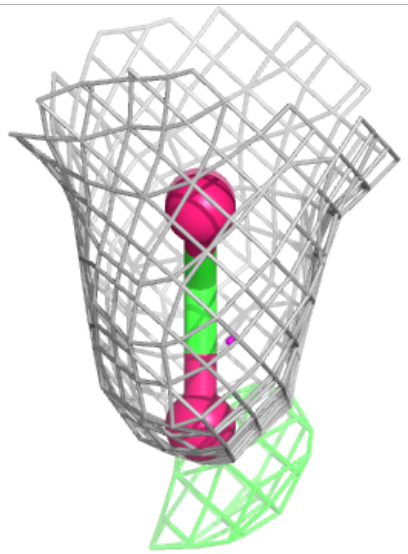


Electron density around BCT a 2108:

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

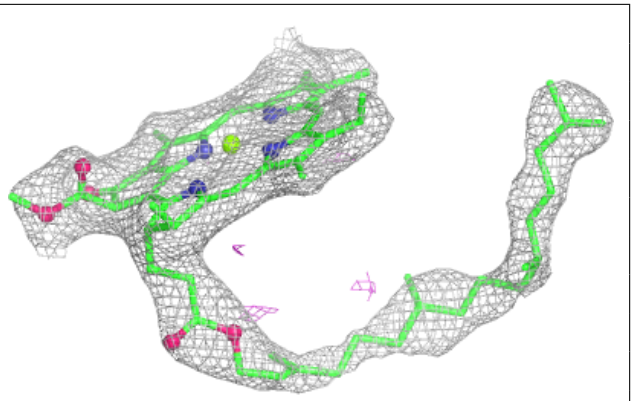


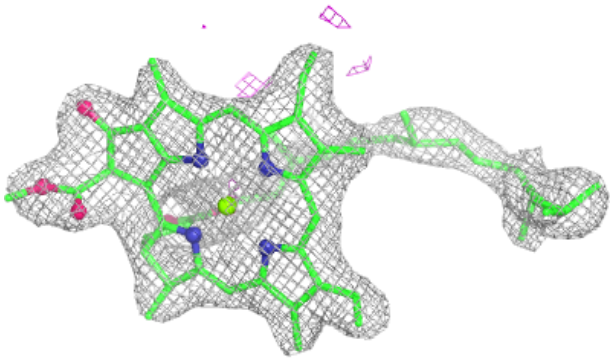


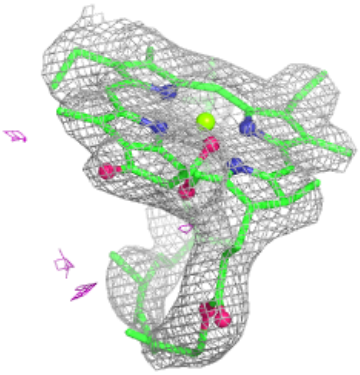


Electron density around CLA C 514:

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

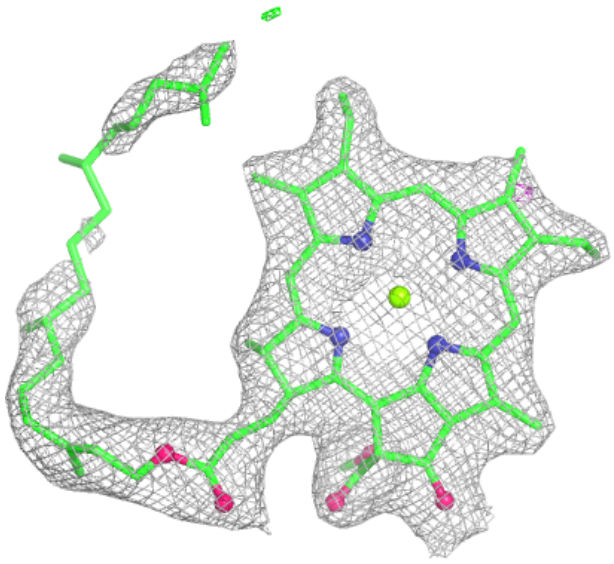


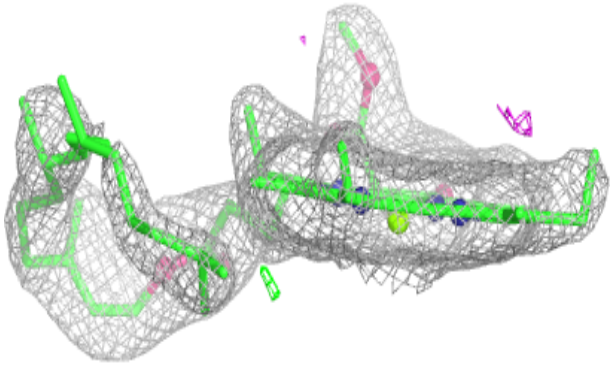


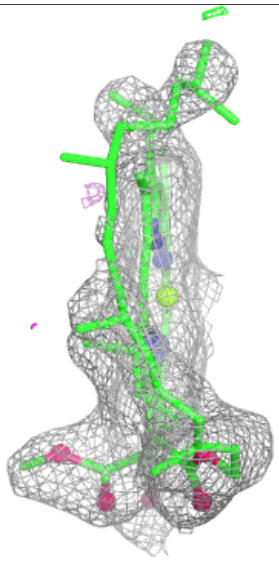


Electron density around CLA c 514:

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

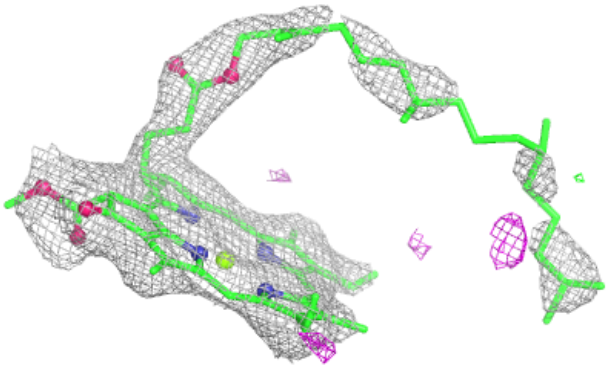


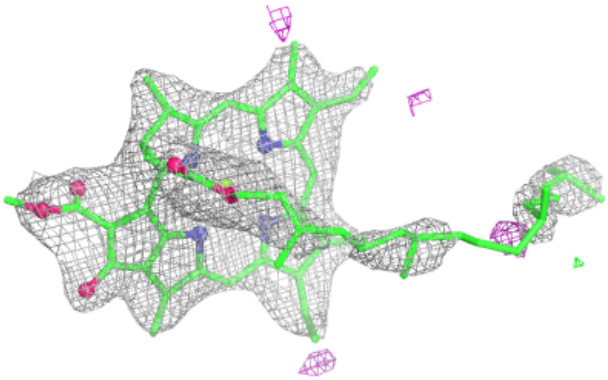


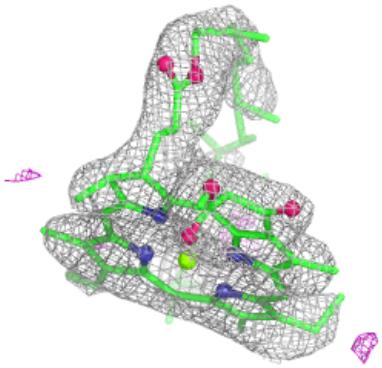


Electron density around CLA c 515:

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

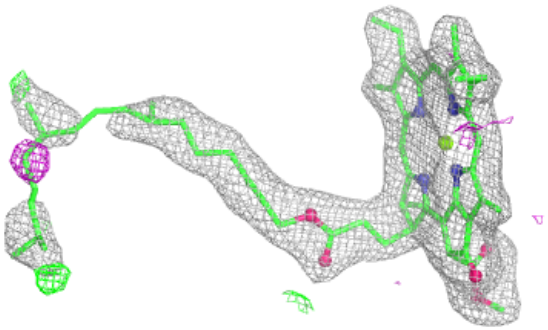


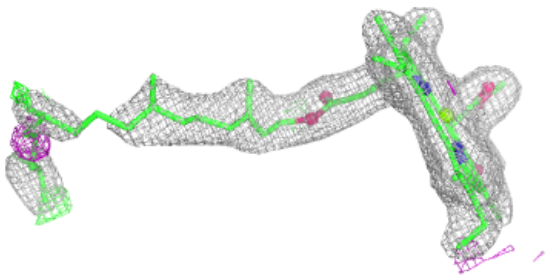


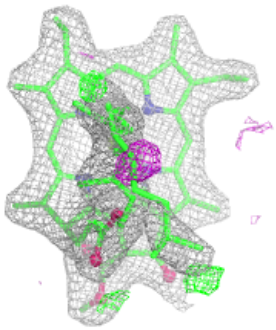


Electron density around CLA d 405:

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

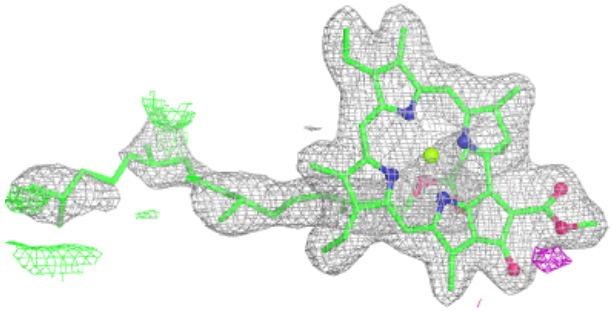


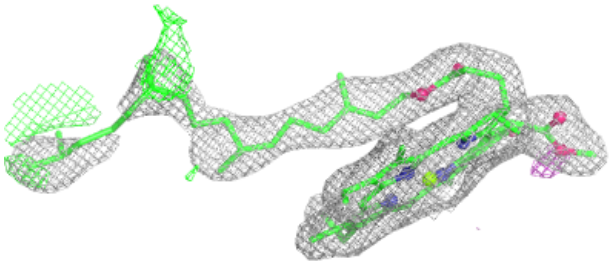


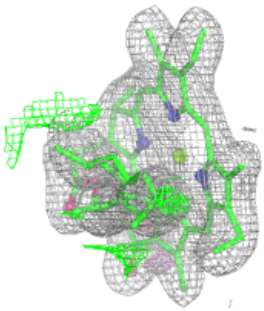


Electron density around CLA B 615:

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

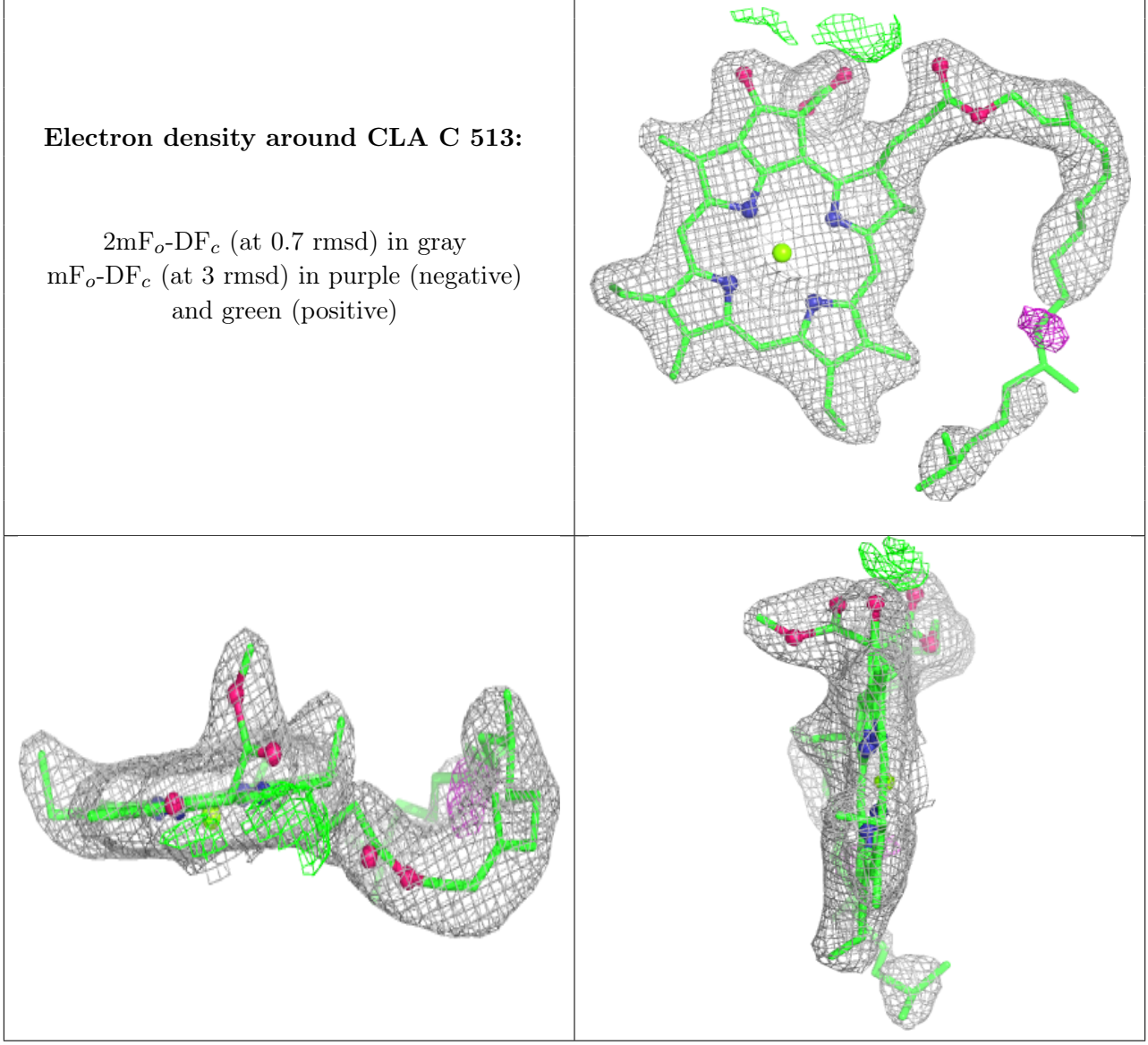






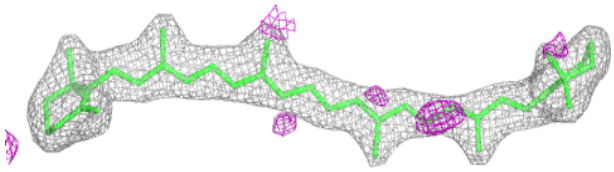
Electron density around CLA C 513:

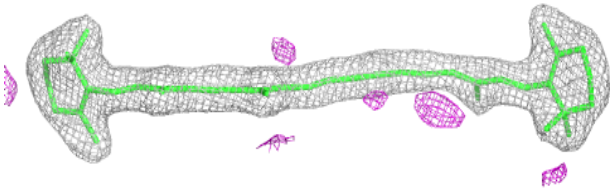
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

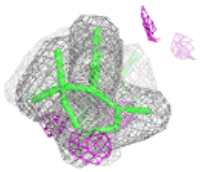


Electron density around BCR a 2114:

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

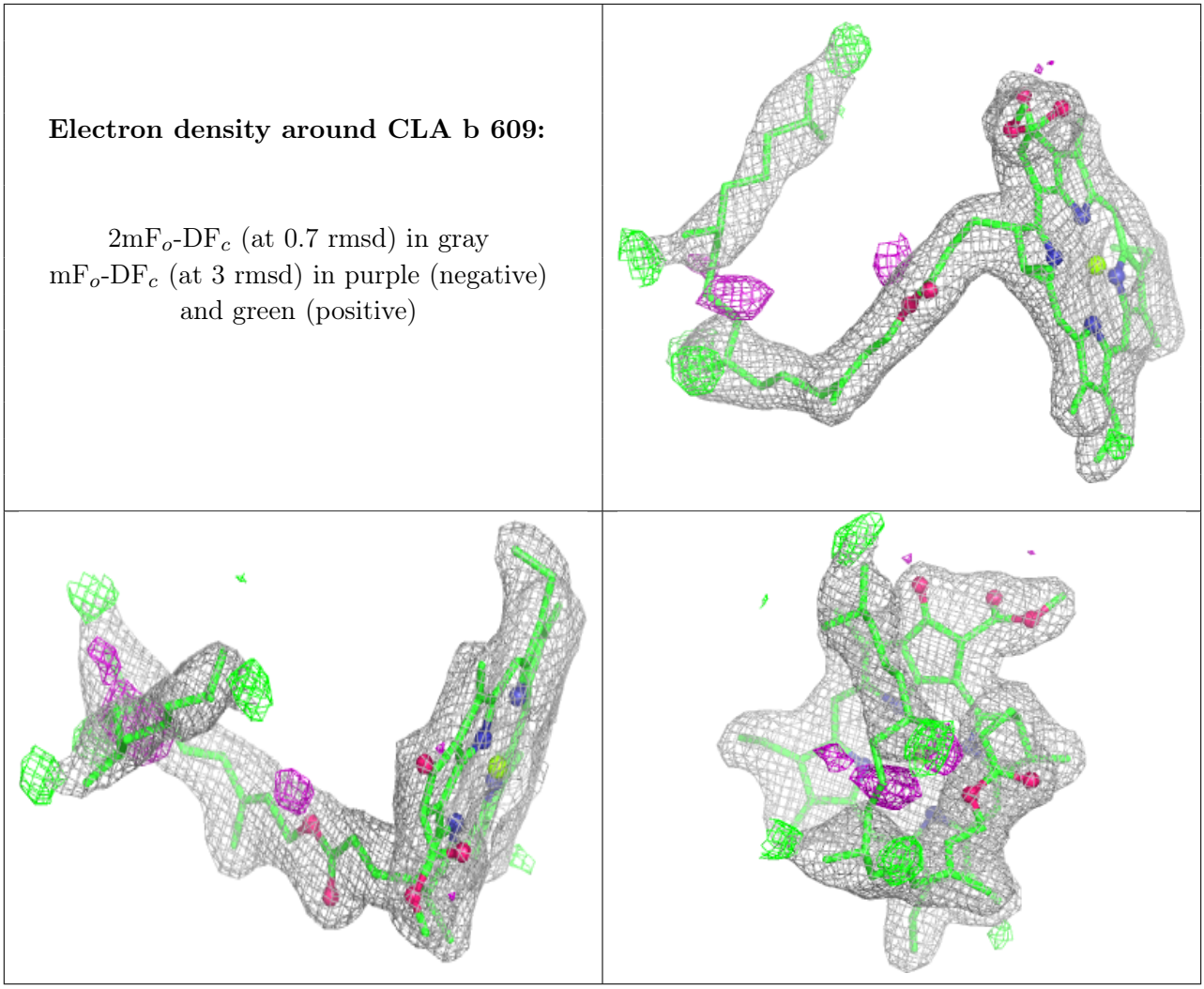






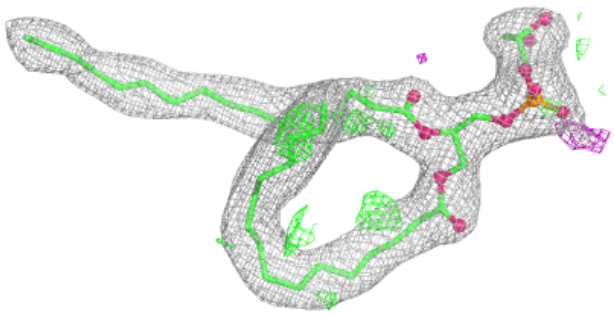
Electron density around CLA b 609:

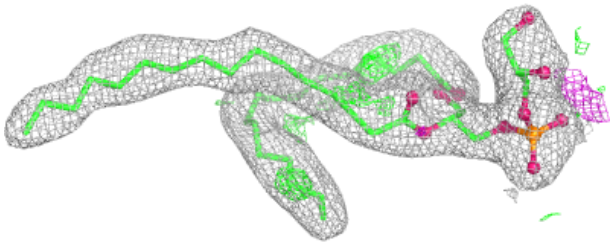
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

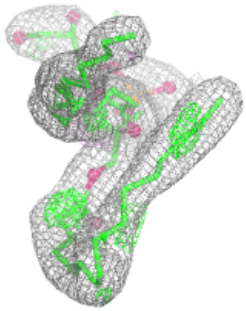


Electron density around LHG D 409:

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

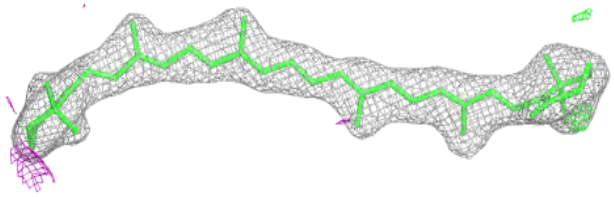


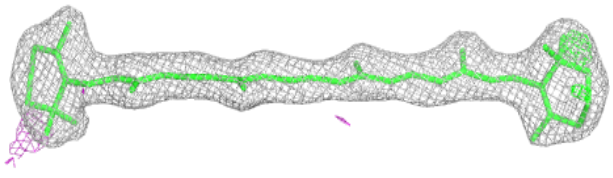


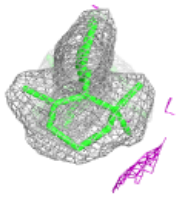


Electron density around BCR c 517:

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

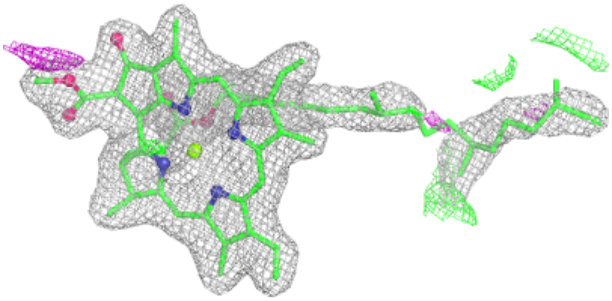


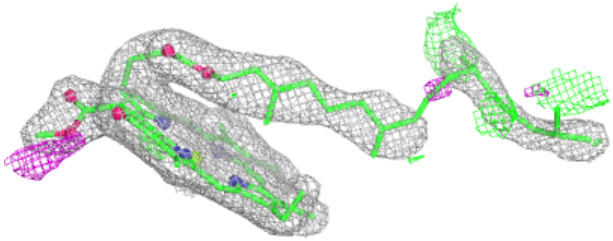


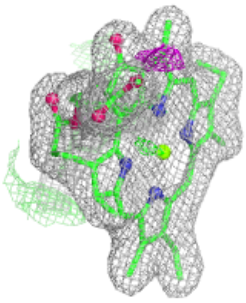


Electron density around CLA b 617:

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

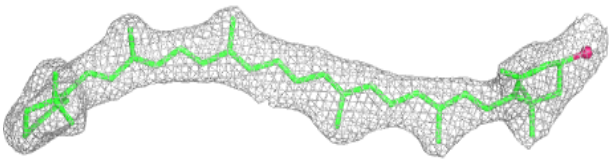


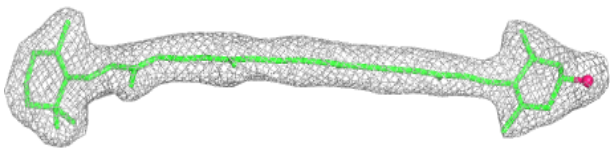


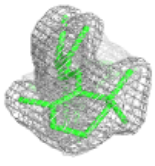


Electron density around RRX H 101:

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

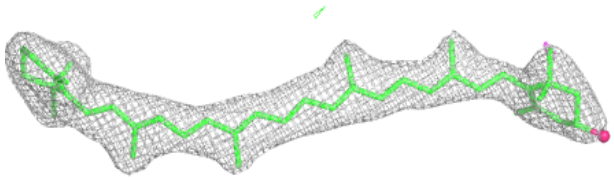


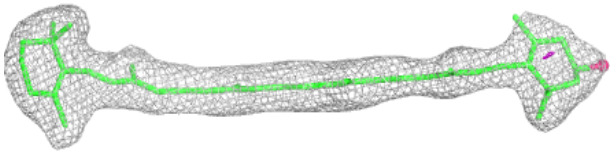


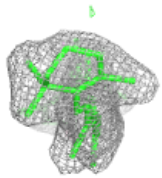


Electron density around RRX h 702:

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

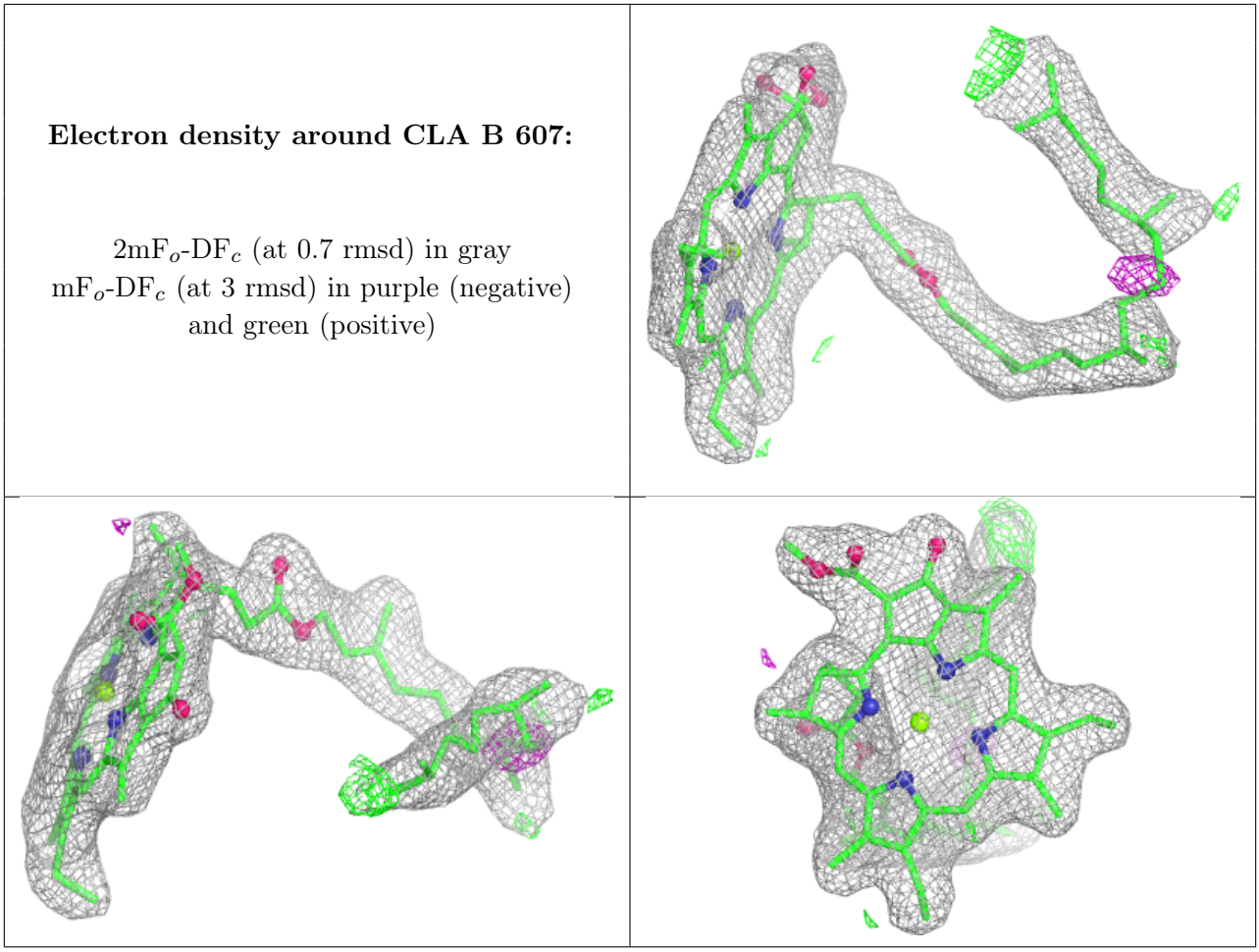






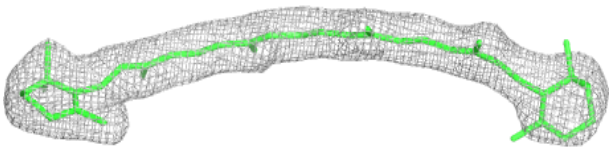
Electron density around CLA B 607:

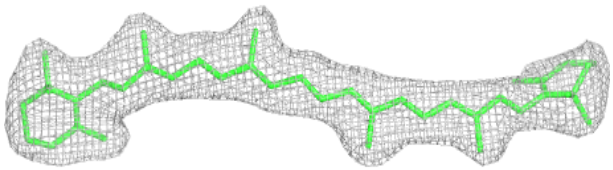
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

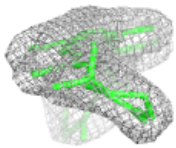


Electron density around BCR D 406:

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

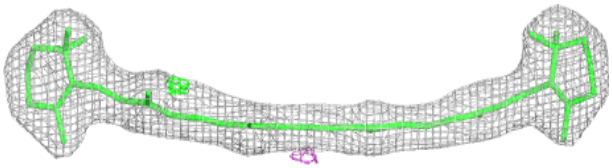


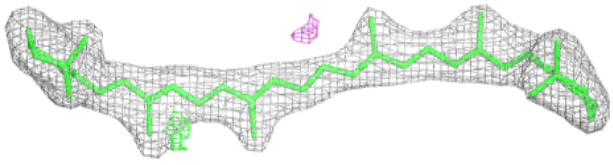


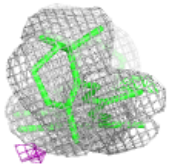


Electron density around BCR K 101:

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

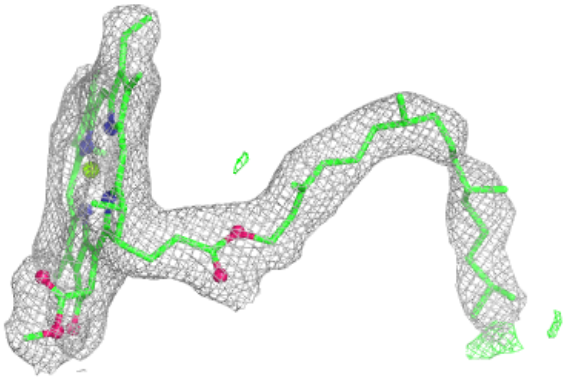


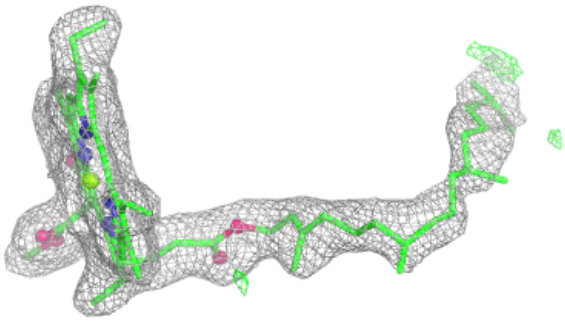


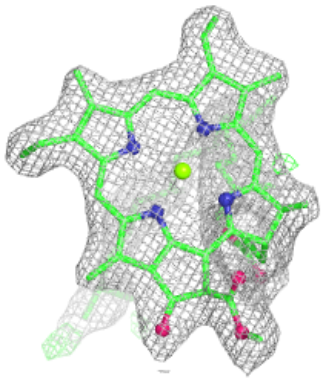


Electron density around CLA D 405:

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

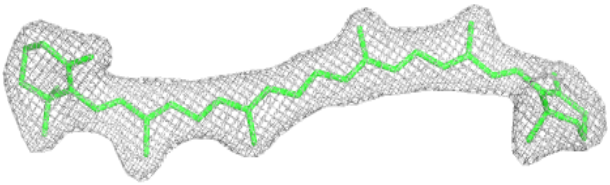


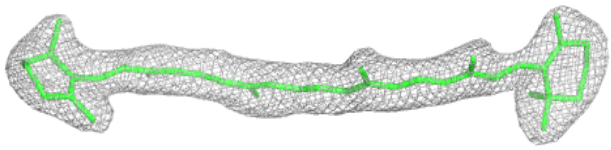


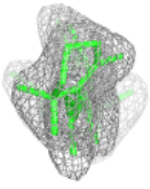


Electron density around BCR Y 302:

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

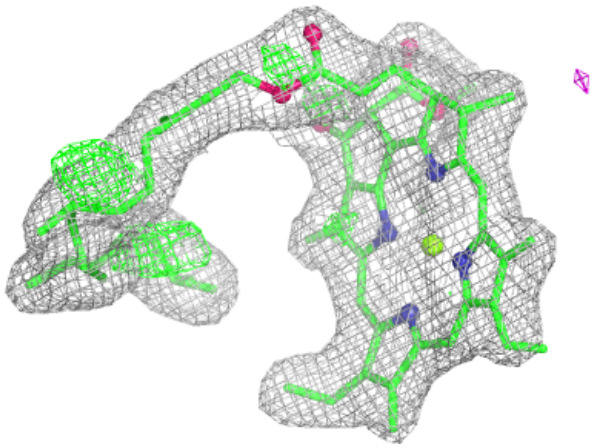


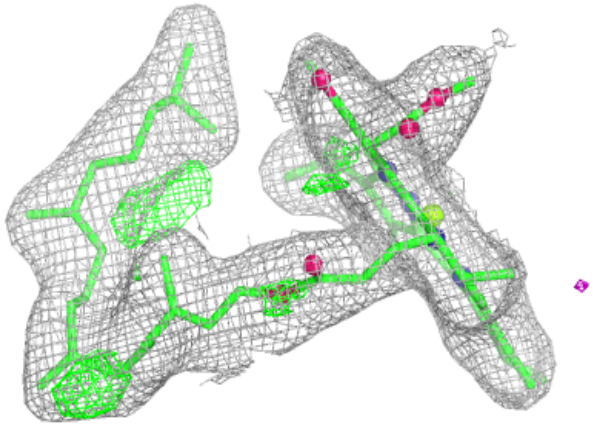


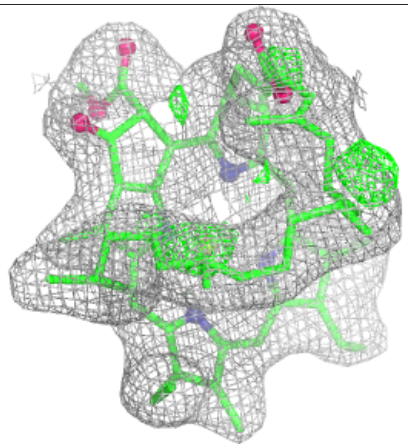


Electron density around CLA c 505:

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

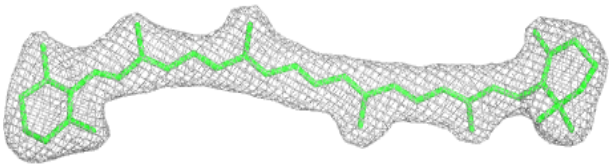


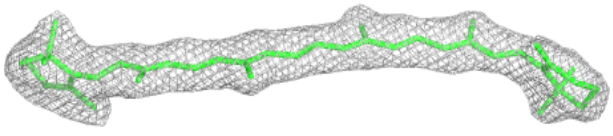


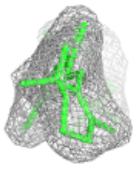


Electron density around BCR b 622:

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

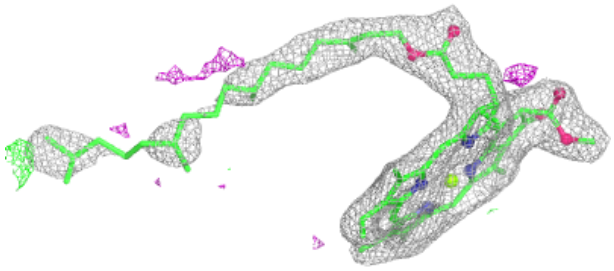


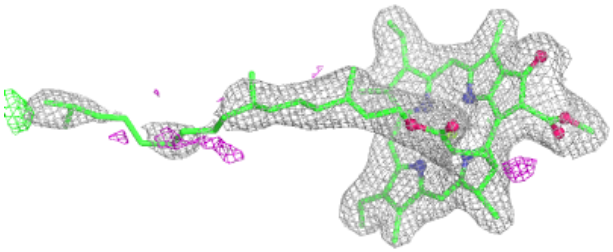


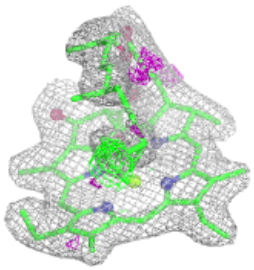


Electron density around CLA c 506:

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

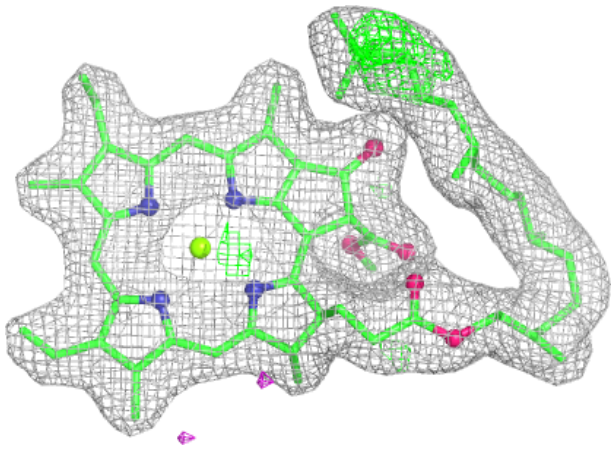


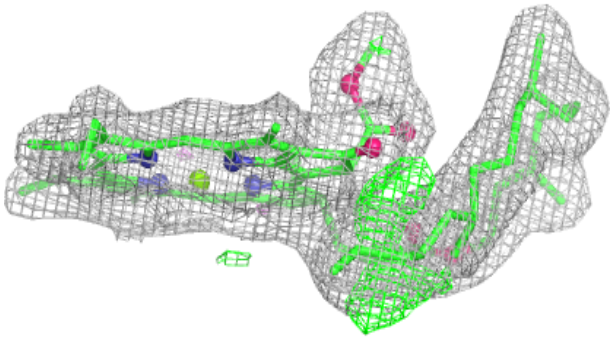


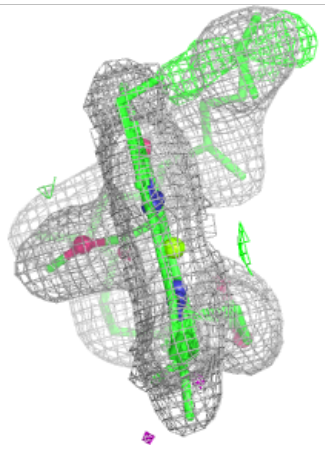


Electron density around CLA B 611:

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

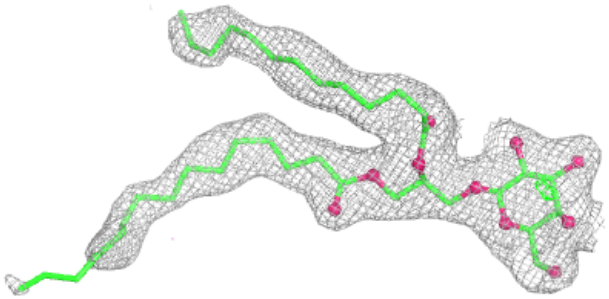


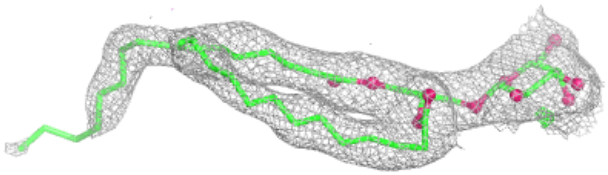


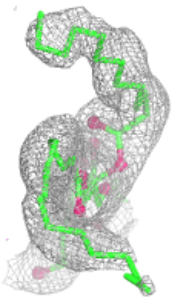


Electron density around LMG d 411:

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

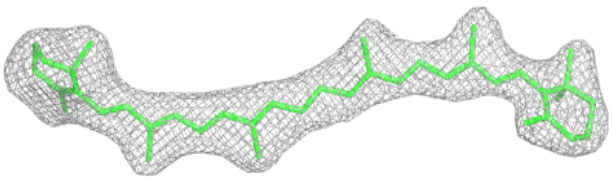


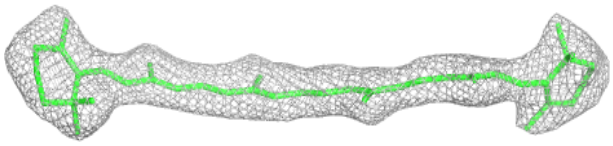


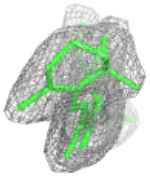


Electron density around BCR c 528:

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

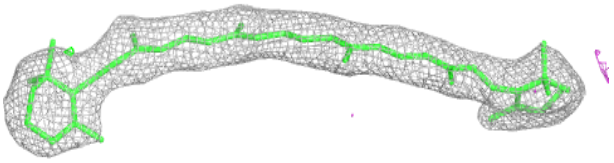


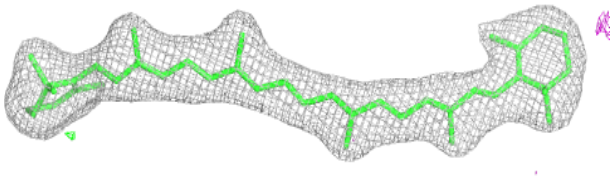


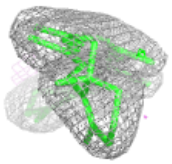


Electron density around BCR d 406:

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

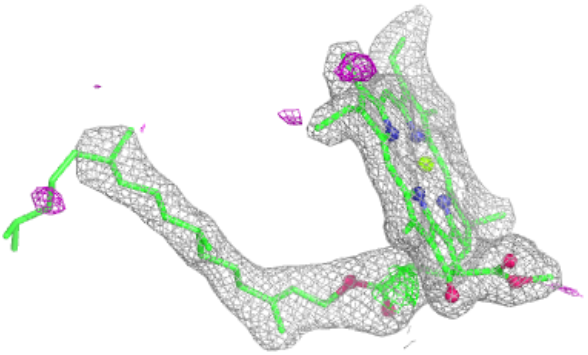


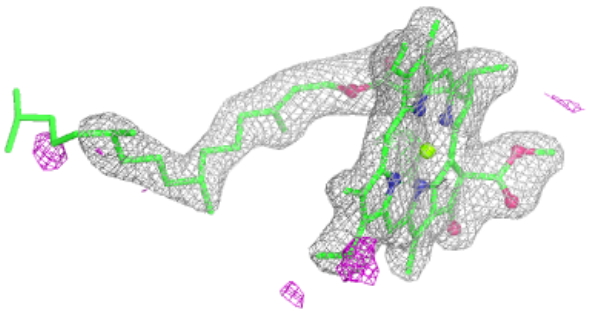


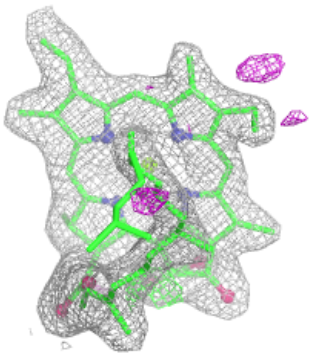


Electron density around CLA c 510:

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

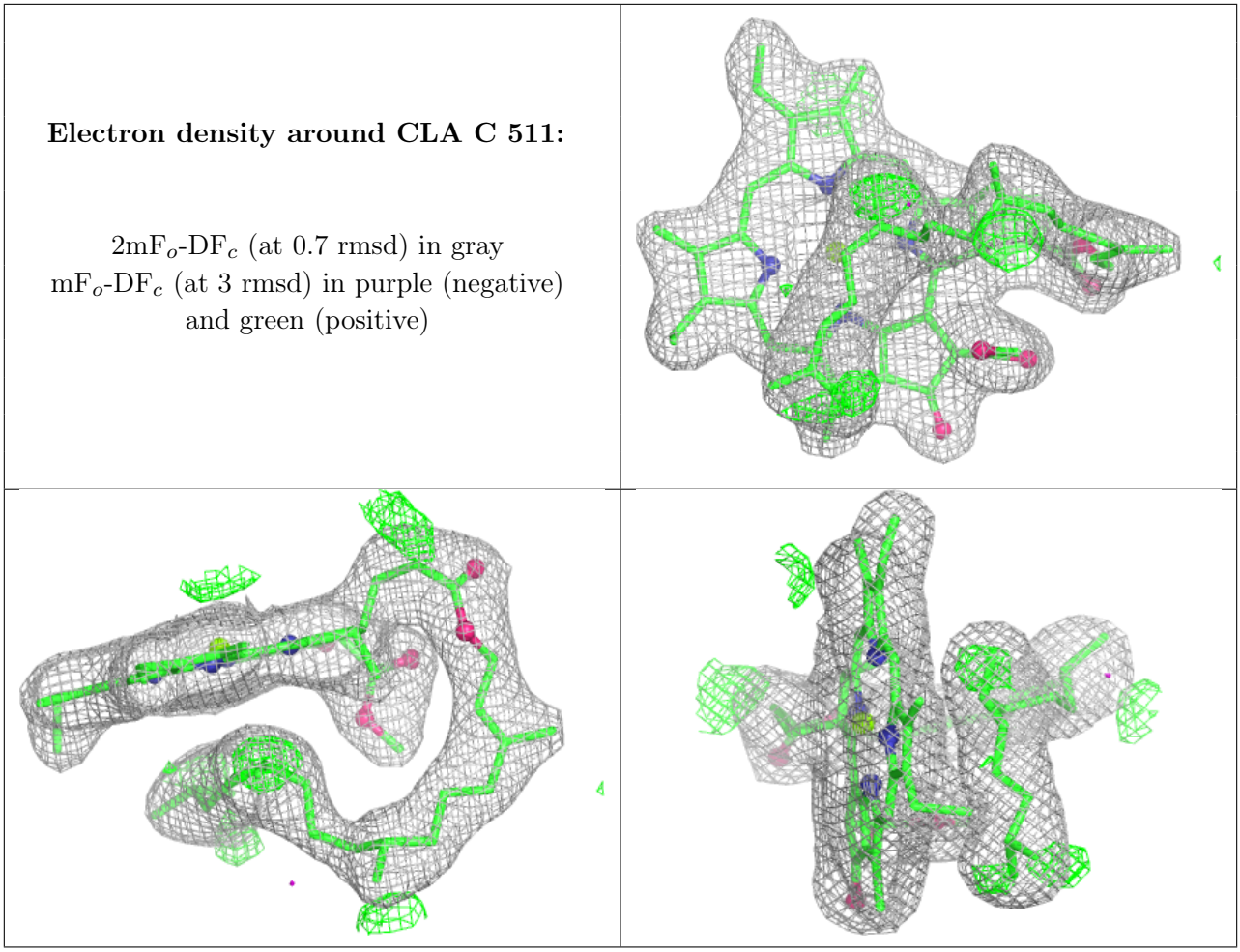






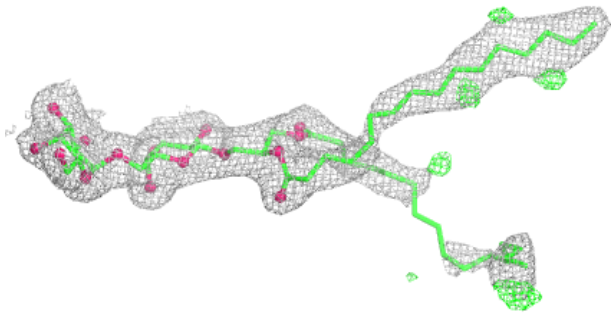
Electron density around CLA C 511:

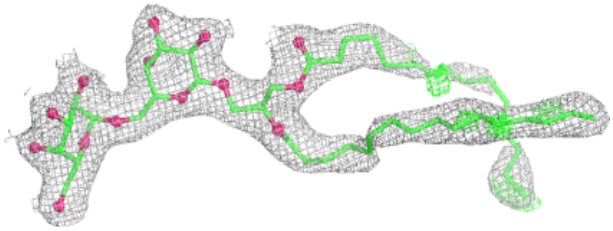
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

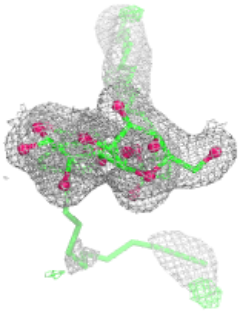


Electron density around DGD C 517:

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

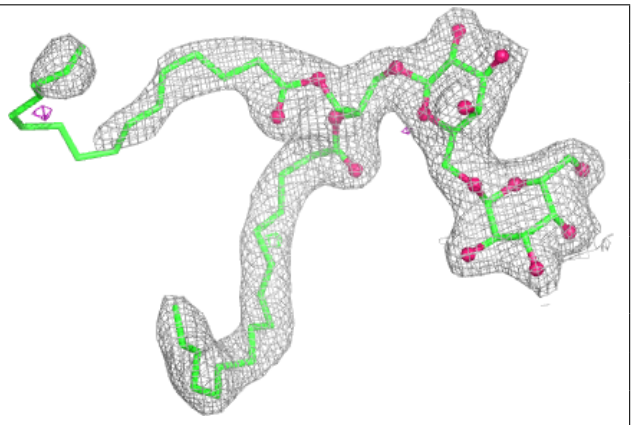


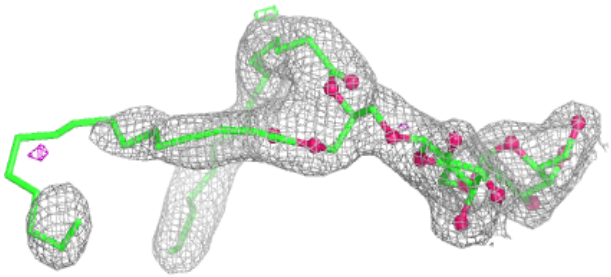


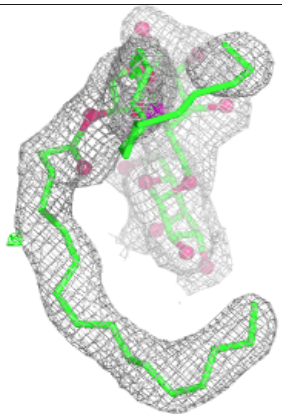


Electron density around DGD C 518:

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

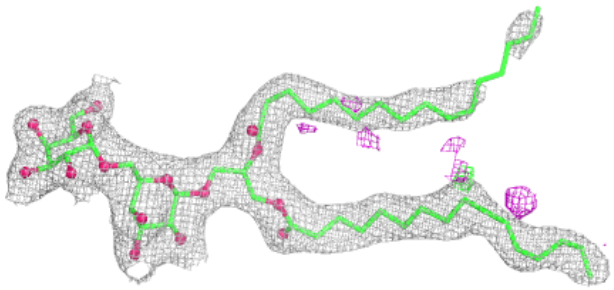


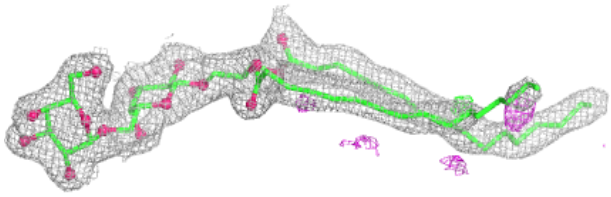


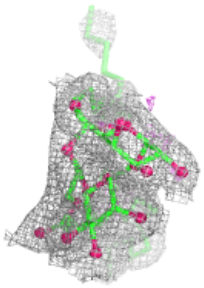


Electron density around DGD C 519:

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

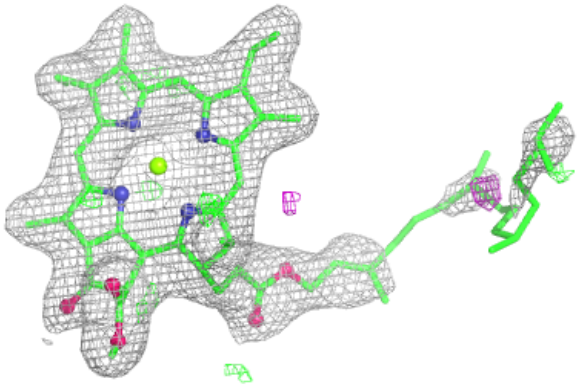


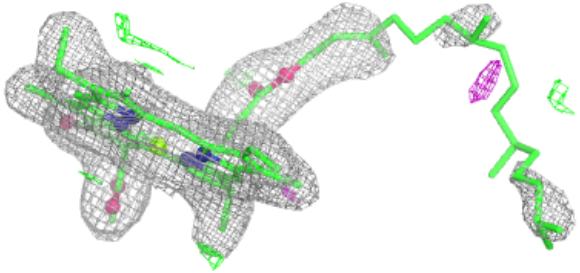




Electron density around CLA A 409:

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

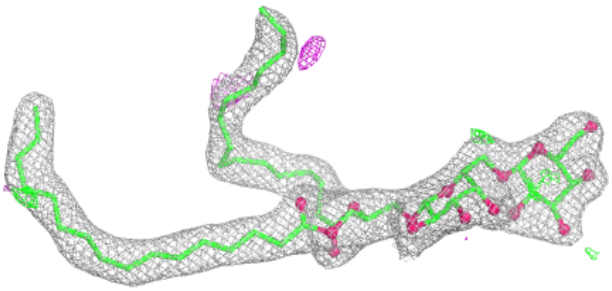


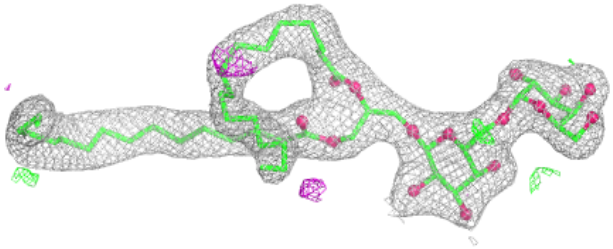


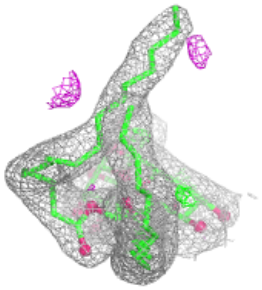


Electron density around DGD H 102:

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

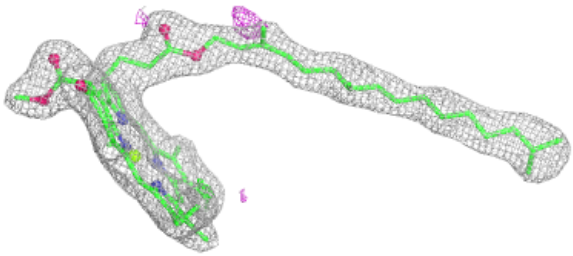


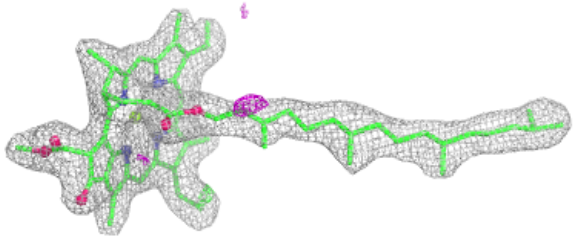


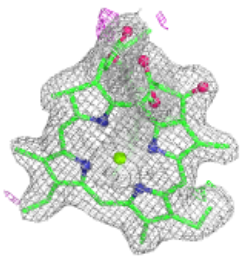


Electron density around CLA b 610:

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

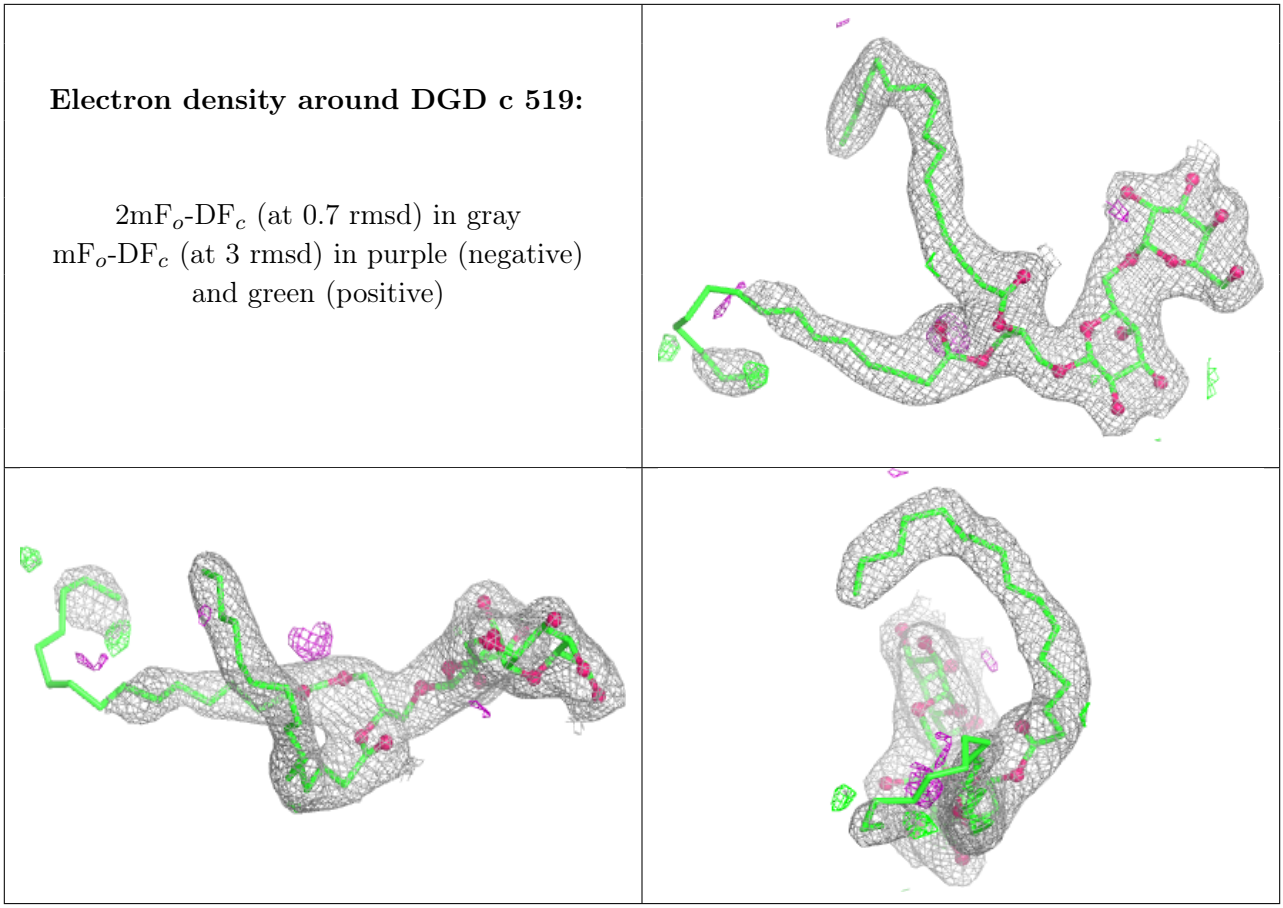






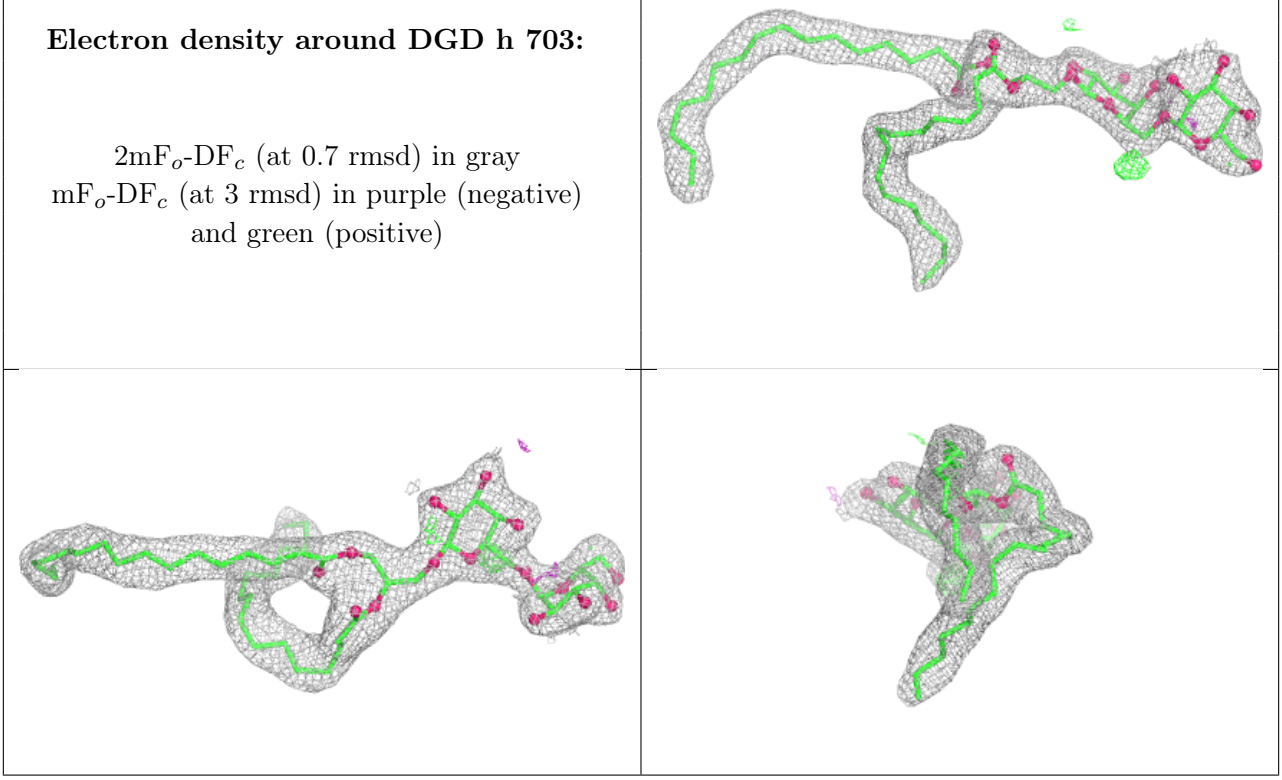
Electron density around DGD c 519:

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



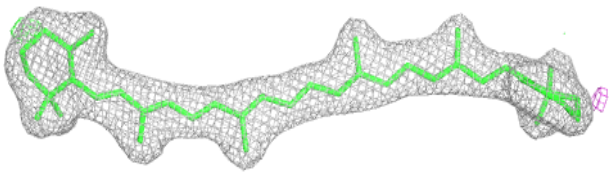
Electron density around DGD h 703:

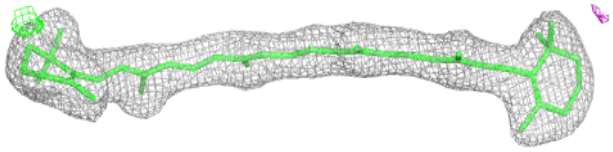
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

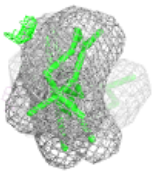


Electron density around BCR B 618:

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

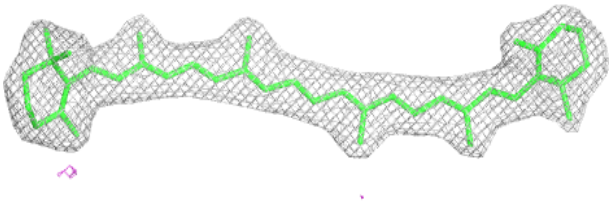


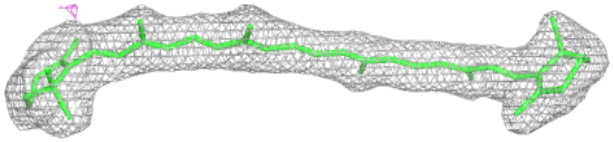


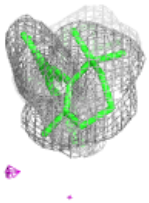


Electron density around BCR B 620:

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

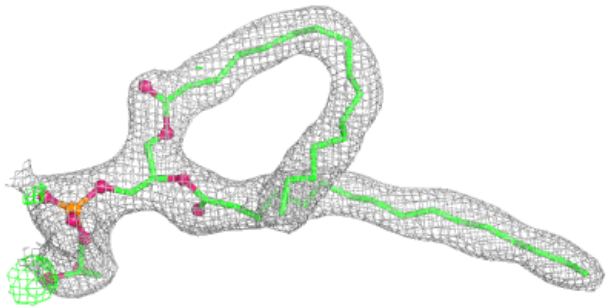


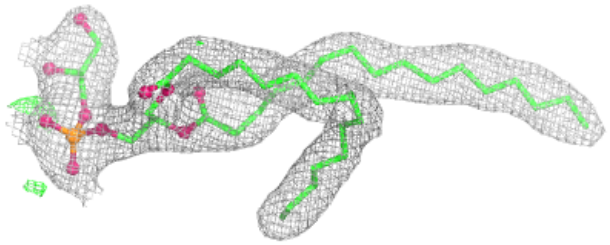


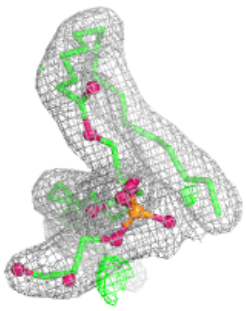


Electron density around LHG d 408:

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

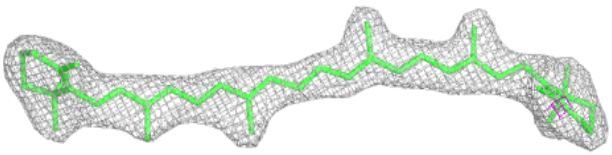


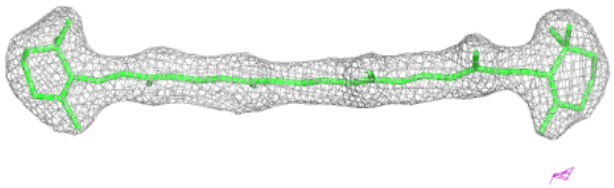


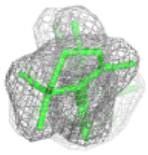


Electron density around BCR C 515:

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

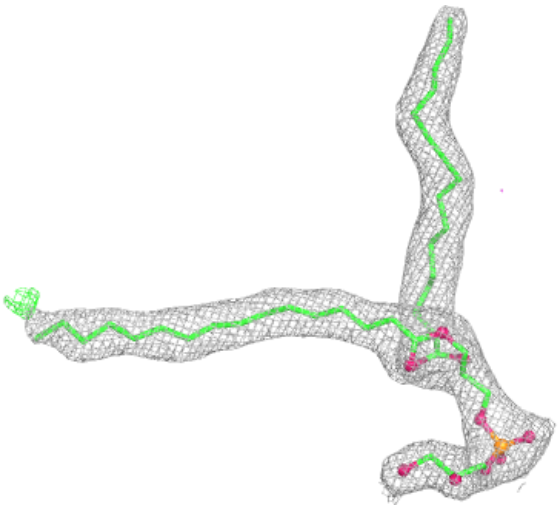


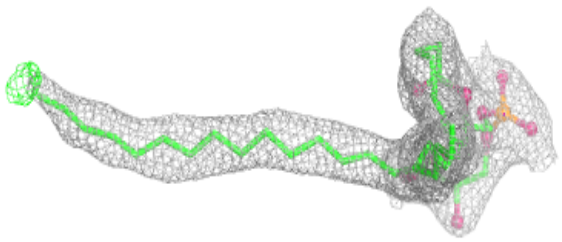


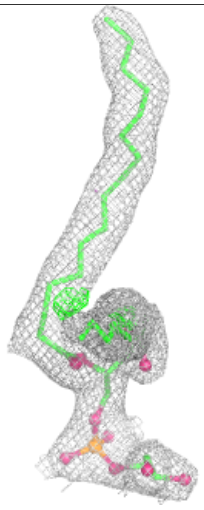


Electron density around LHG l 101:

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

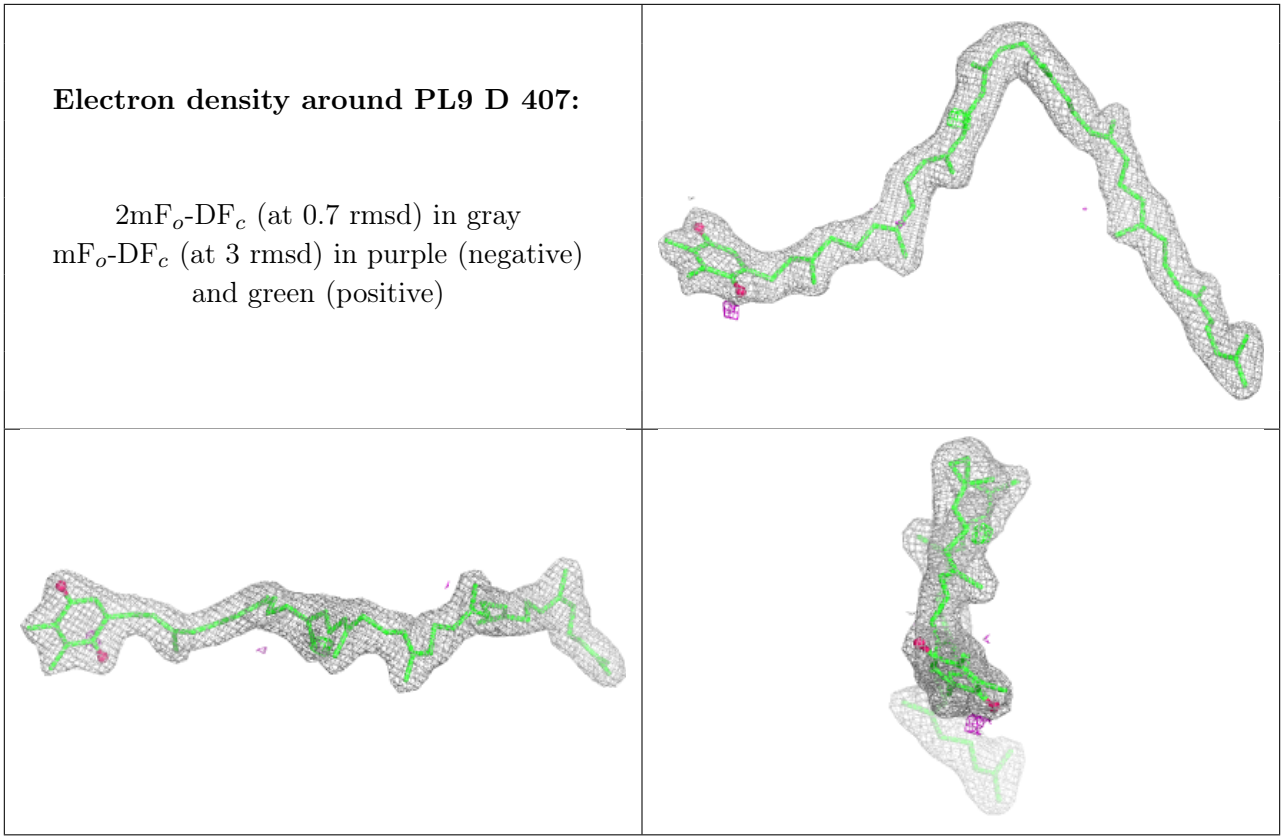






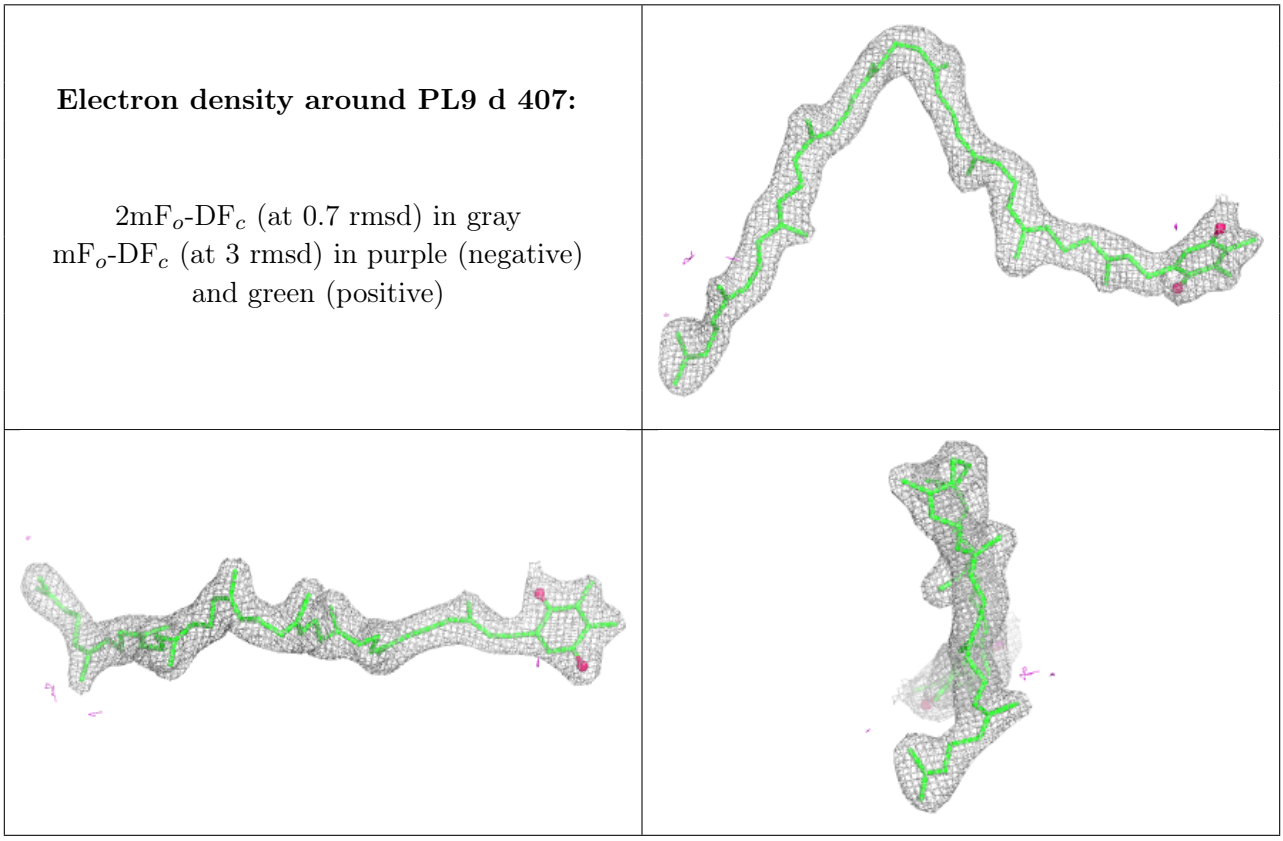
Electron density around PL9 D 407:

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



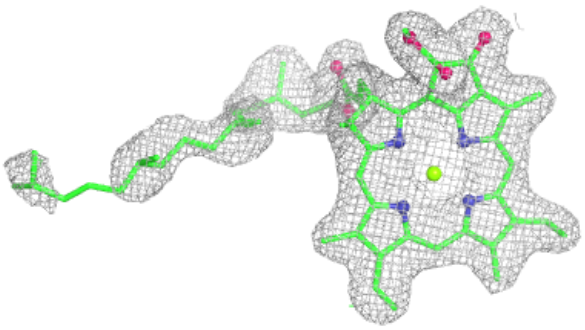
Electron density around PL9 d 407:

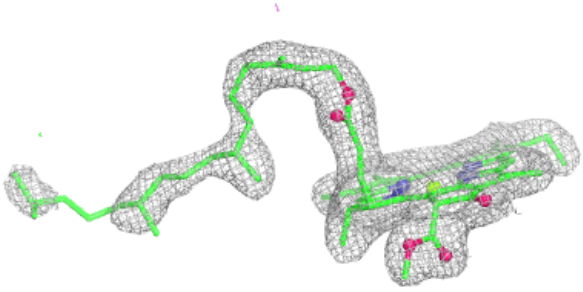
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

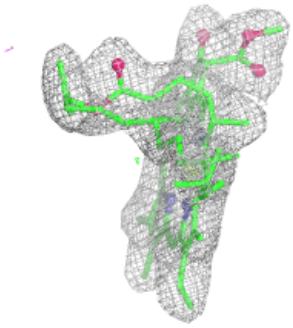


Electron density around CLA A 406:

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

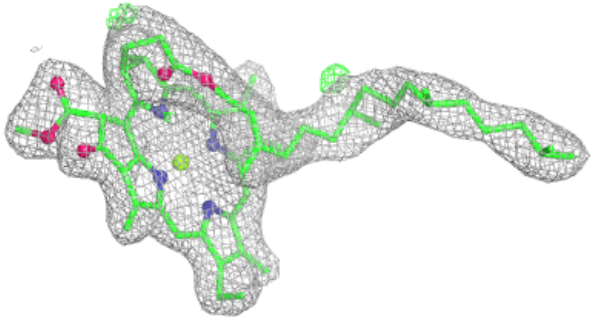


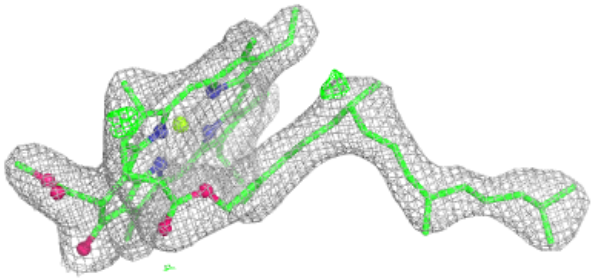


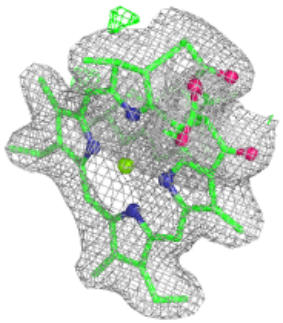


Electron density around CLA c 507:

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

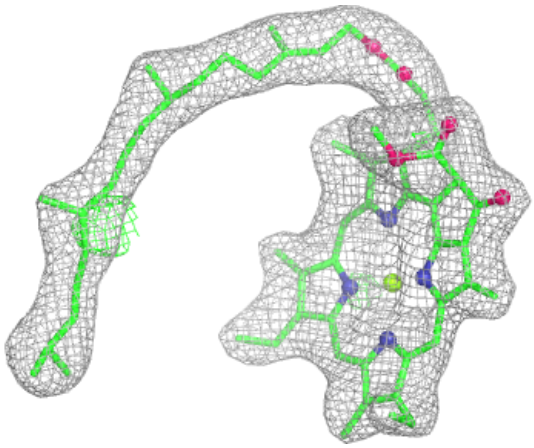


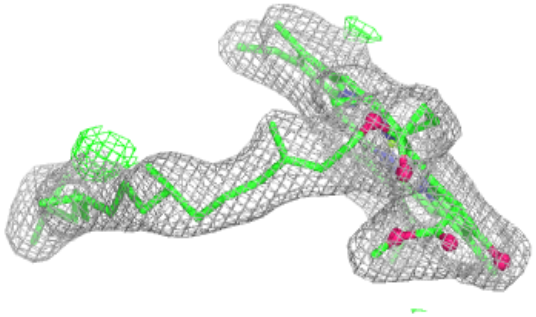


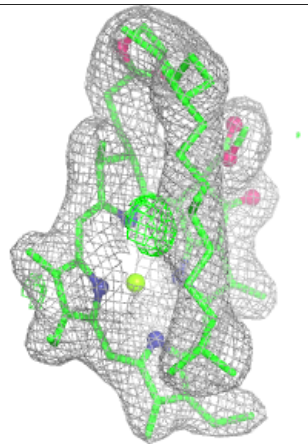


Electron density around CLA C 508:

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

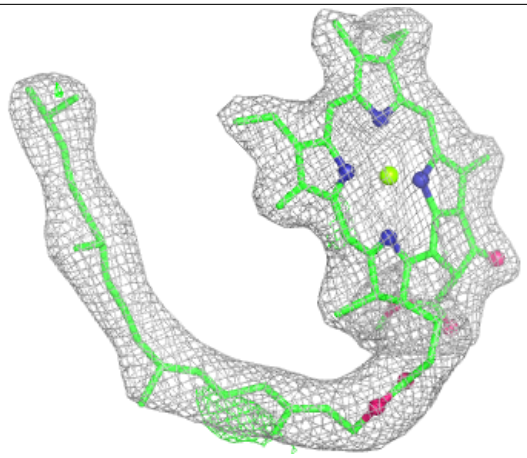


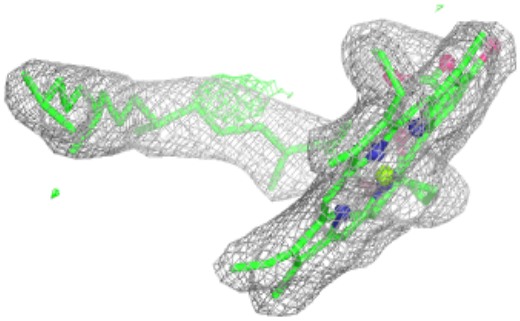




Electron density around CLA c 509:

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

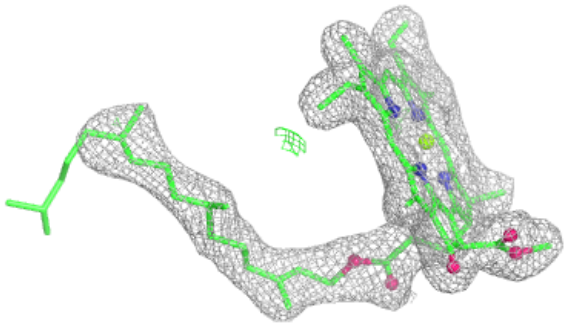


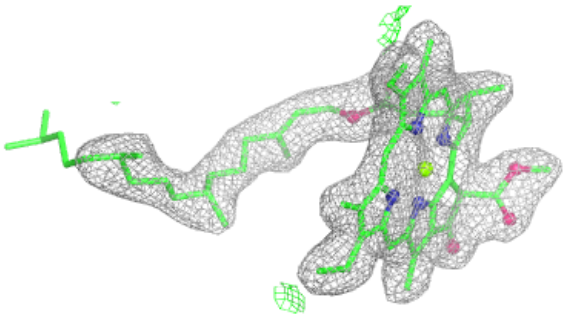


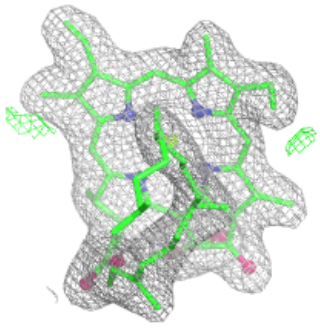


Electron density around CLA C 509:

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

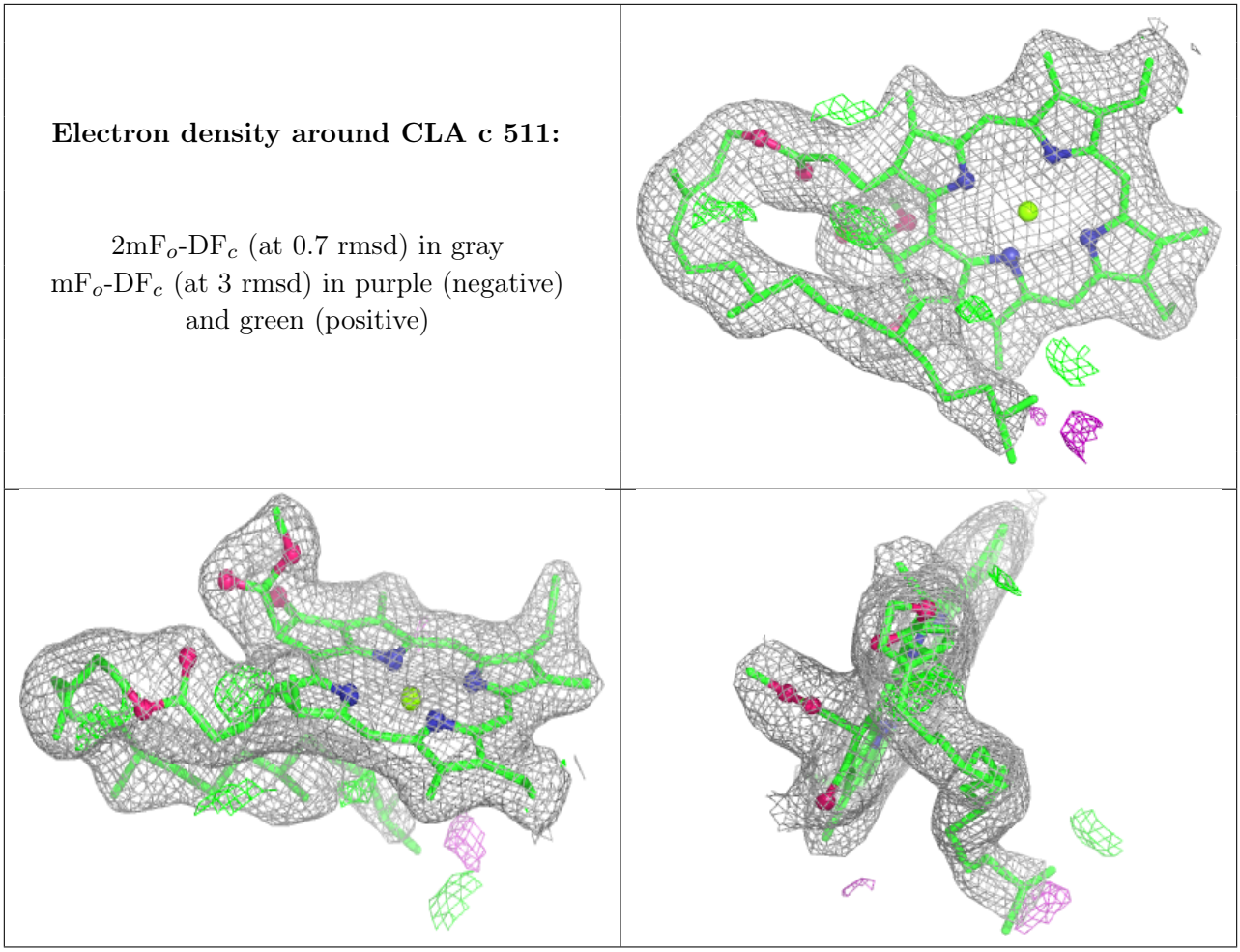






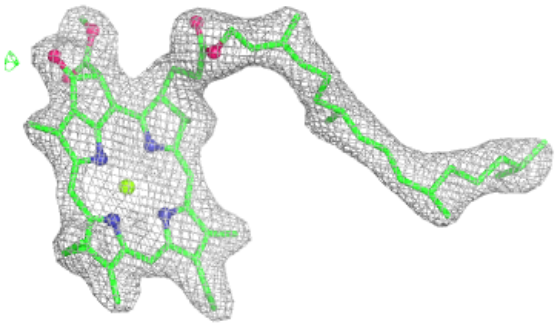
Electron density around CLA c 511:

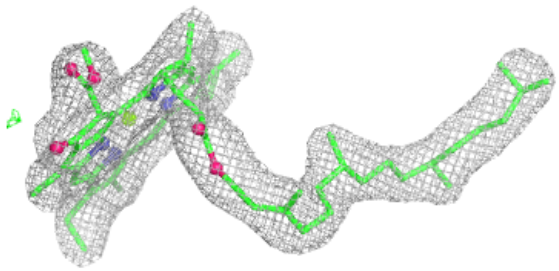
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

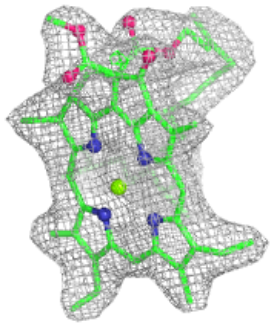


Electron density around CLA c 513:

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

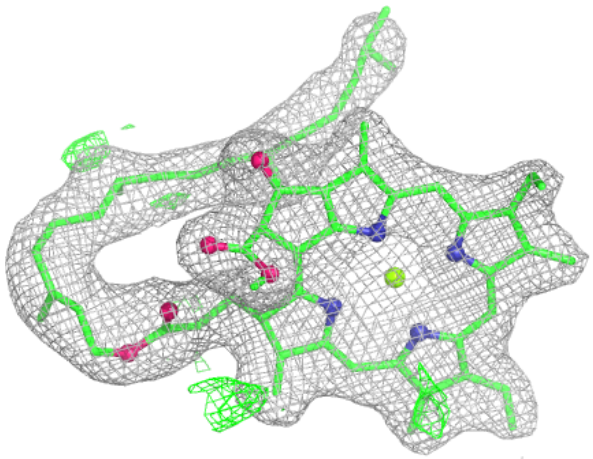


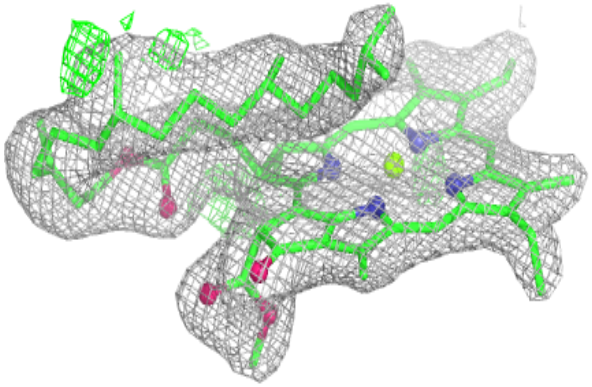


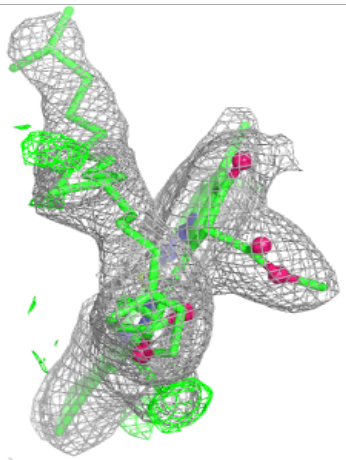


Electron density around CLA C 510:

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

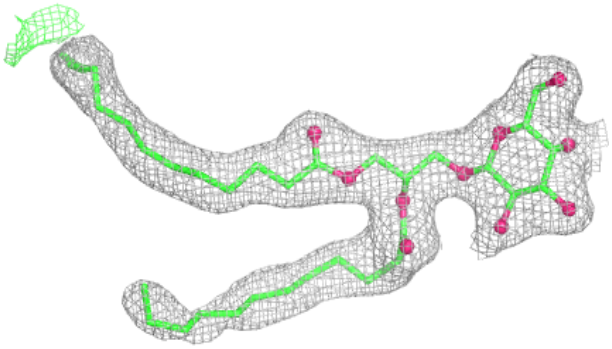


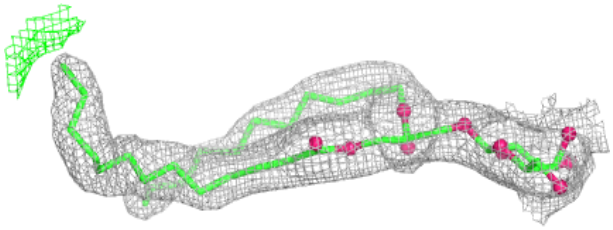


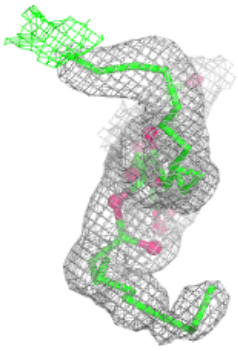


Electron density around LMG D 412:

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

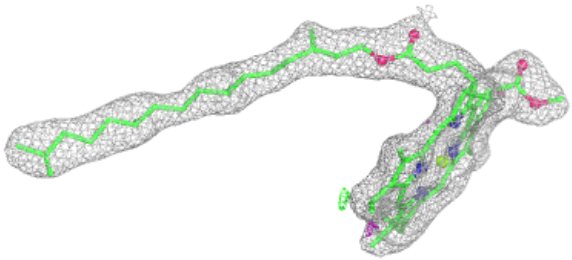


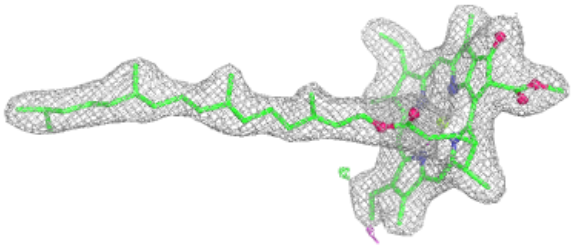


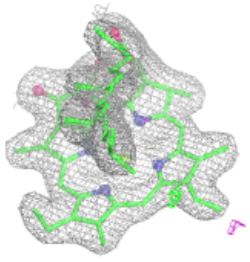


Electron density around CLA B 608:

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

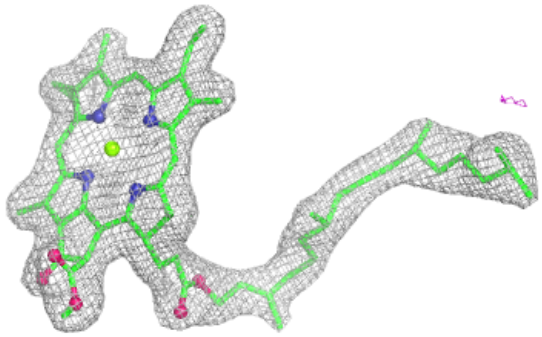


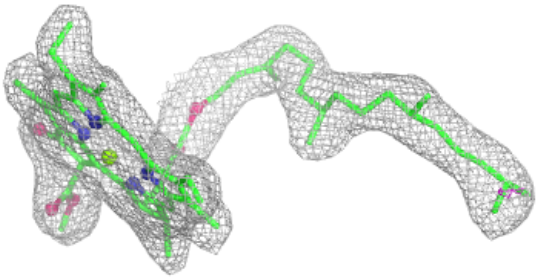


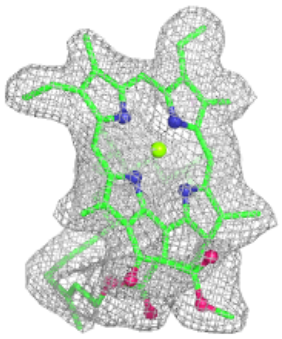


Electron density around CLA C 512:

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

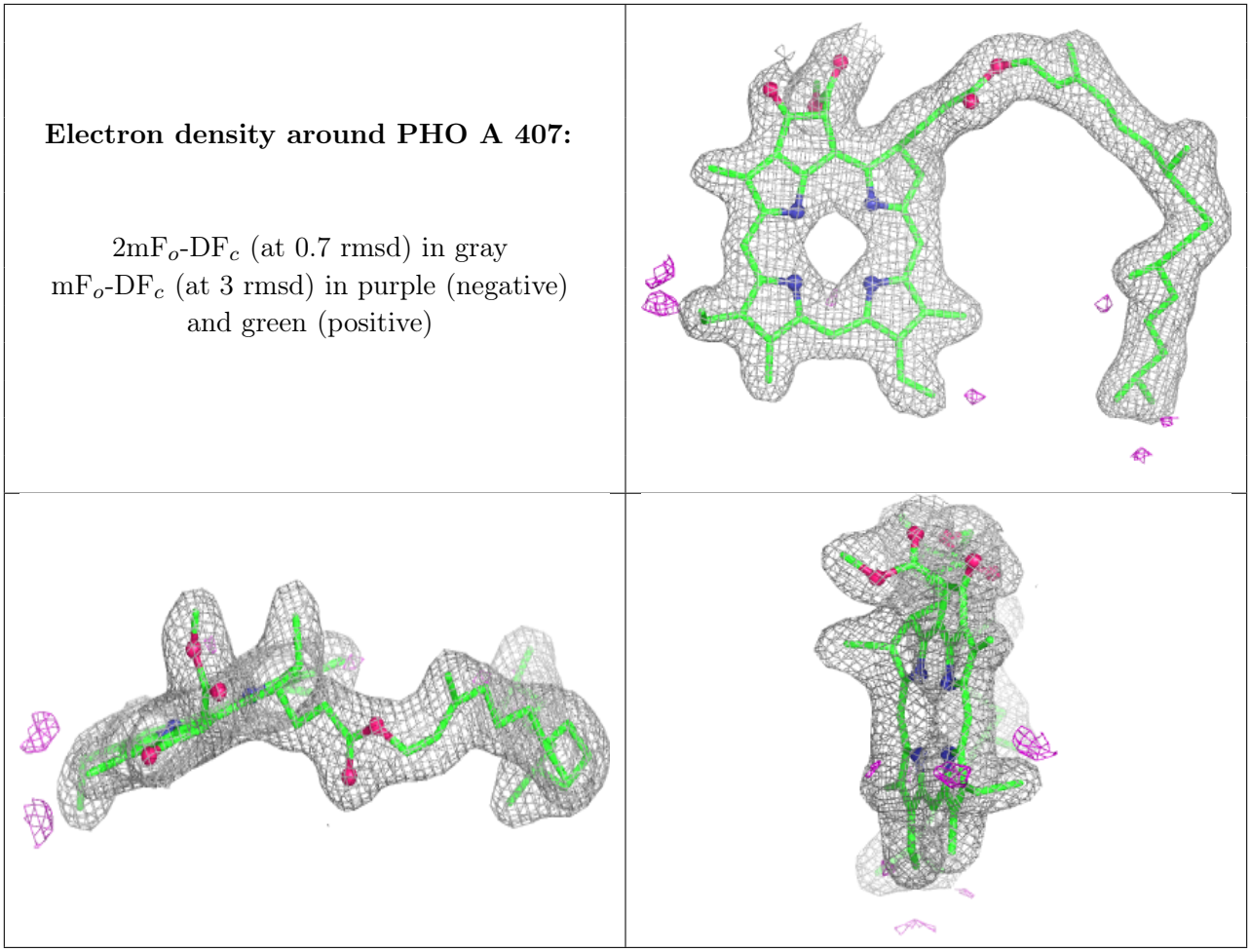






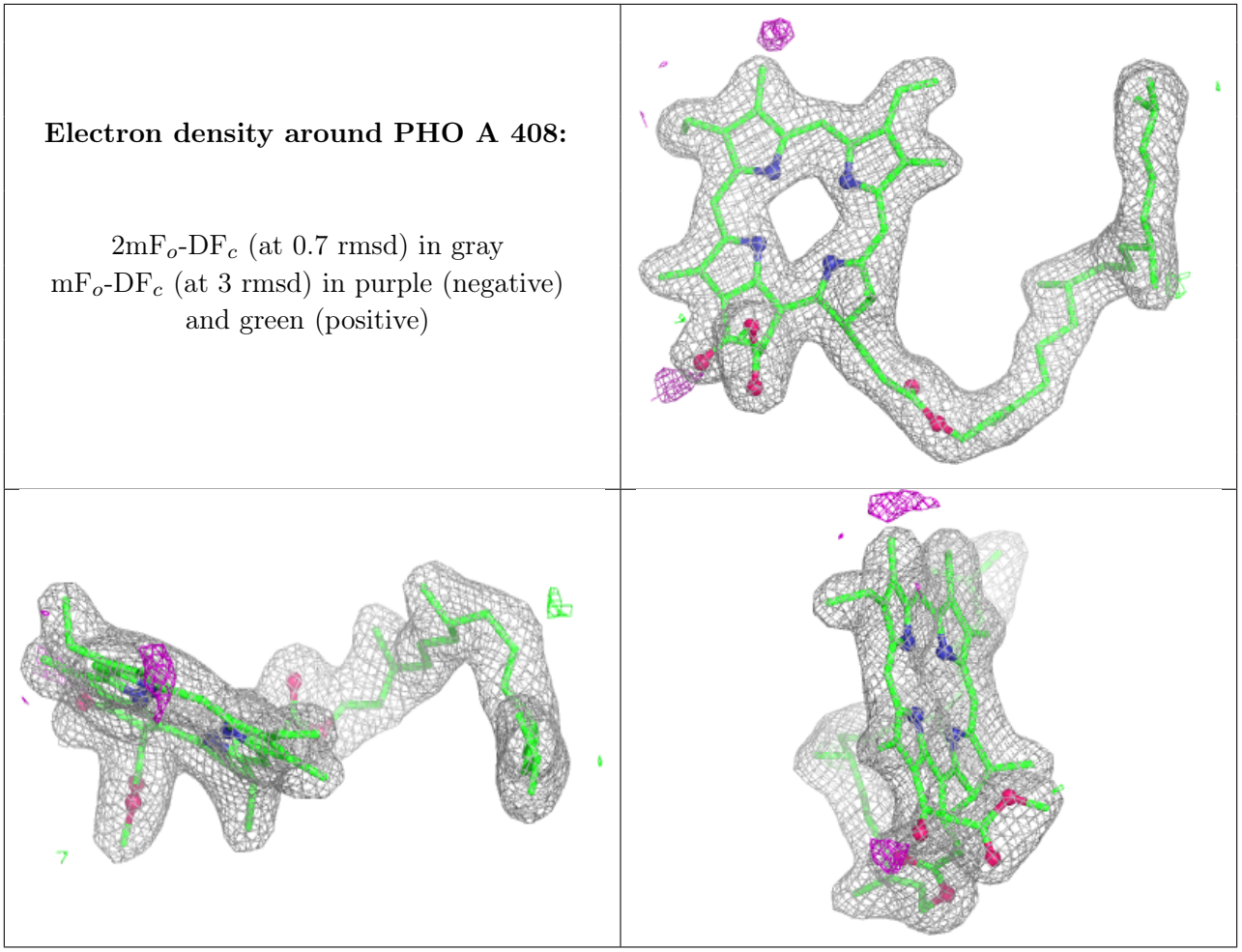
Electron density around PHO A 407:

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



Electron density around PHO A 408:

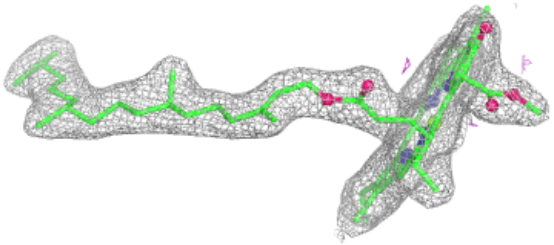
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

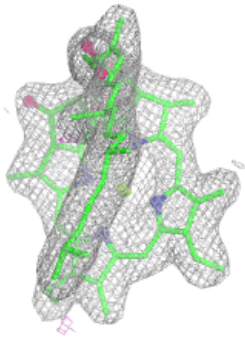


Electron density around CLA B 610:

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

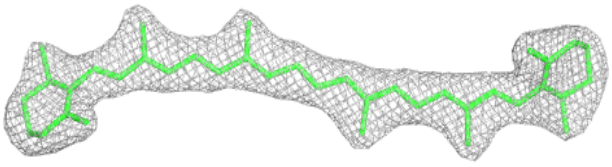


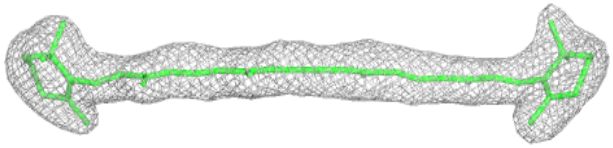


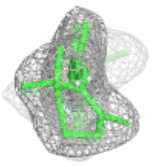


Electron density around BCR B 619:

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

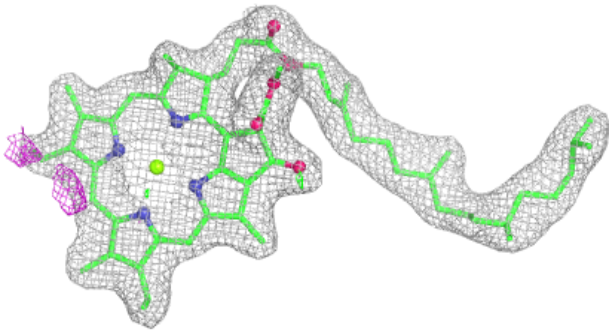


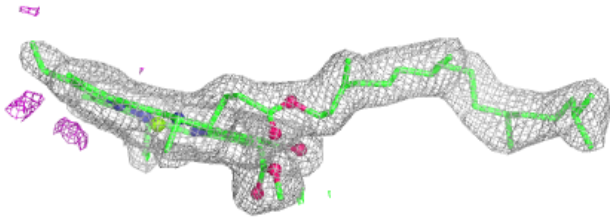


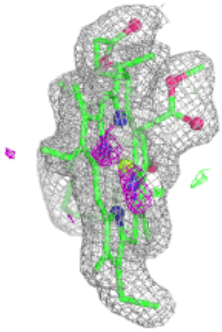


Electron density around CLA B 603:

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

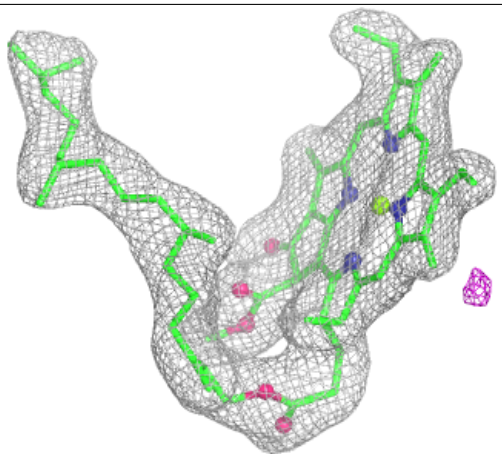


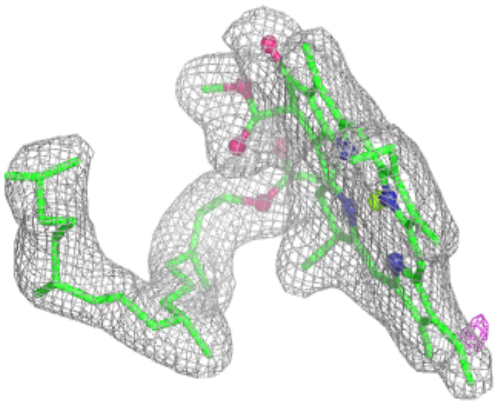


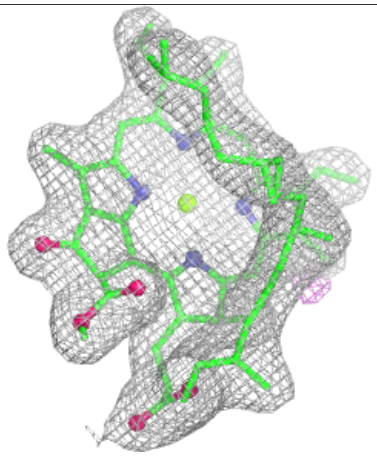


Electron density around CLA B 614:

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

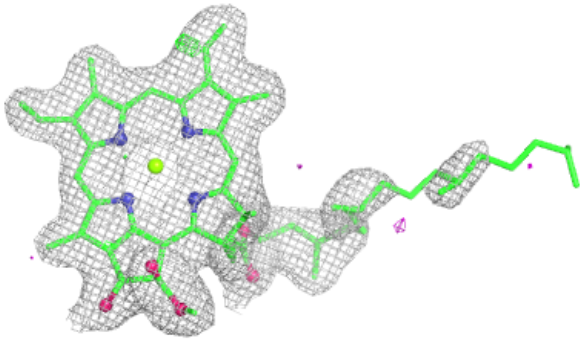


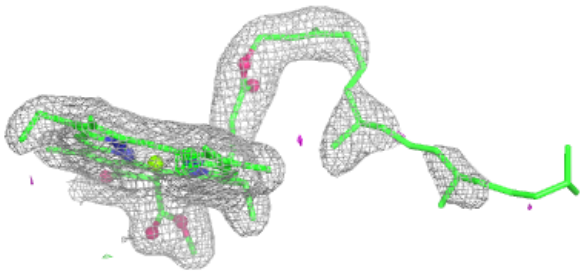


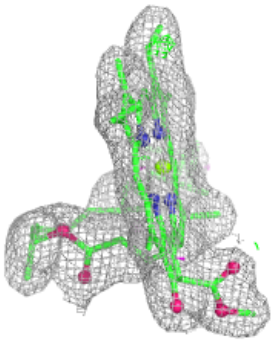


Electron density around CLA a 2110:

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

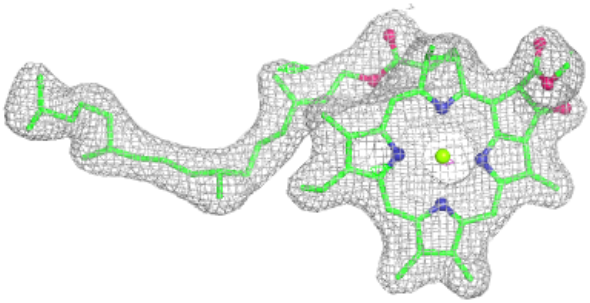


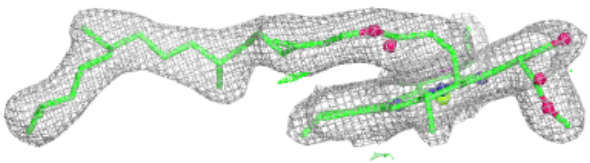


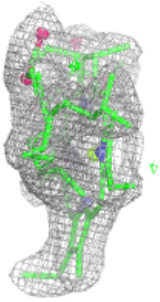


Electron density around CLA B 604:

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

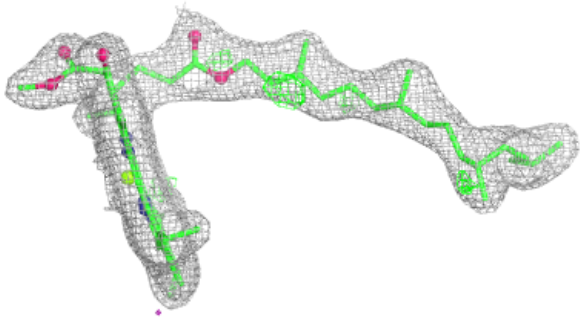


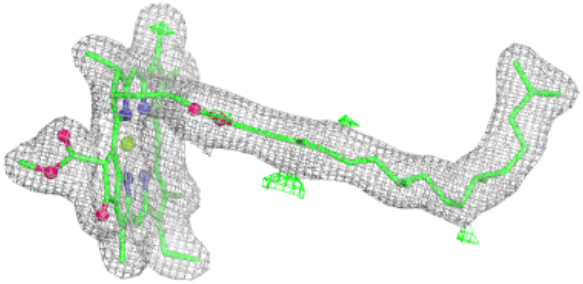


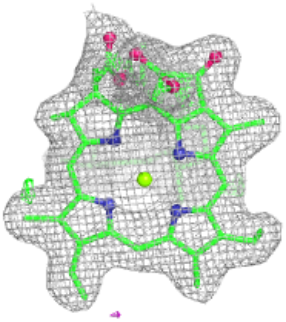


Electron density around CLA B 606:

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

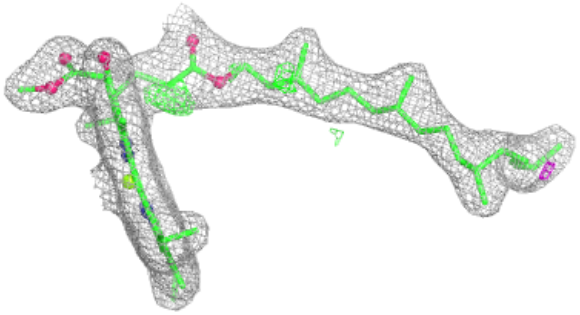


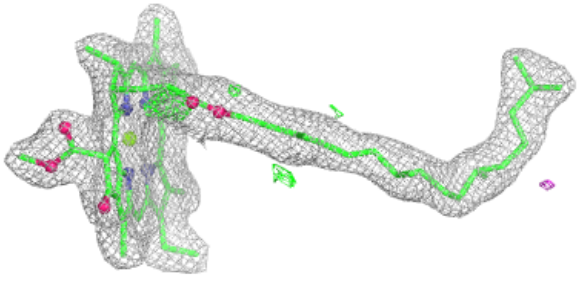


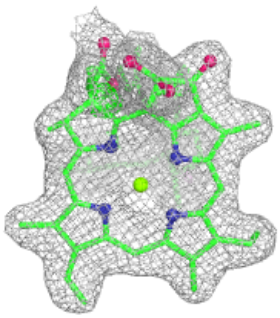


Electron density around CLA b 608:

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

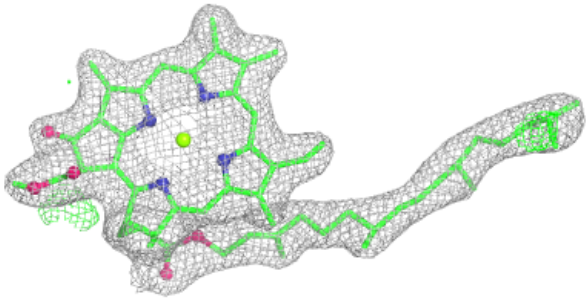


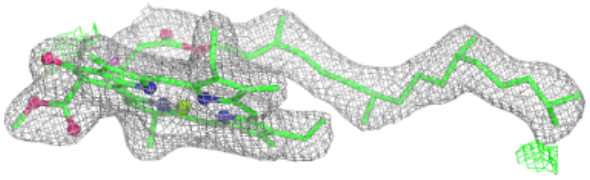


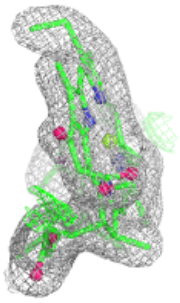


Electron density around CLA C 502:

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

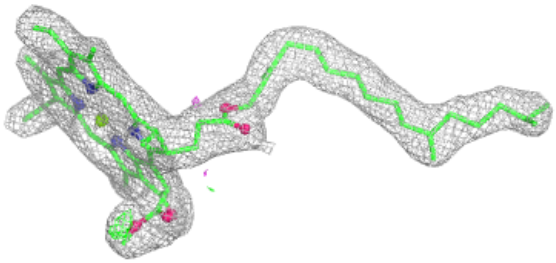


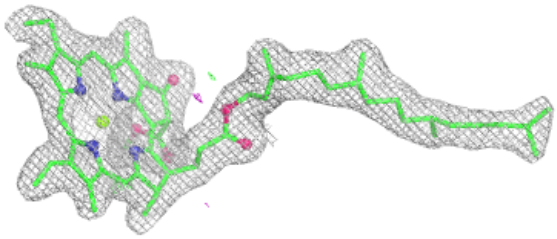


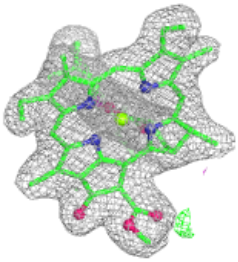


Electron density around CLA C 503:

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

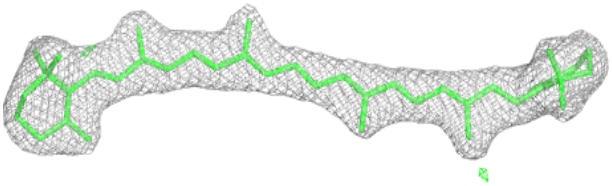


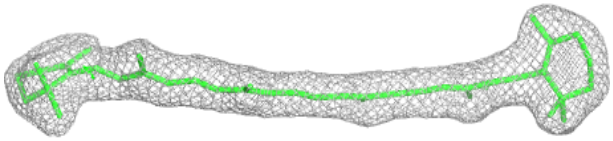


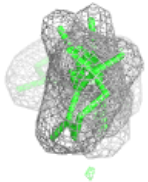


Electron density around BCR b 620:

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

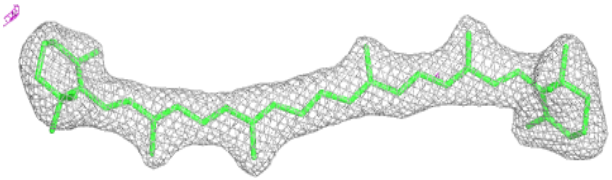


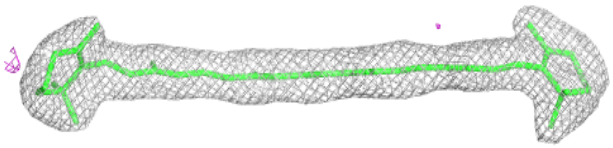


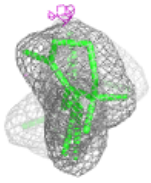


Electron density around BCR b 621:

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

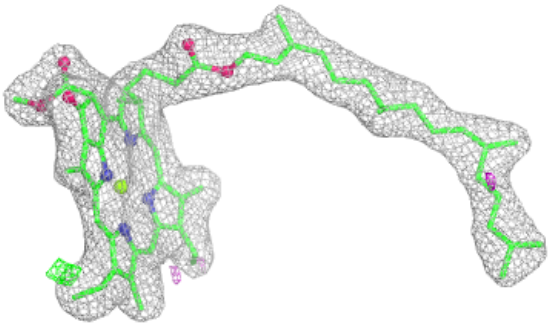


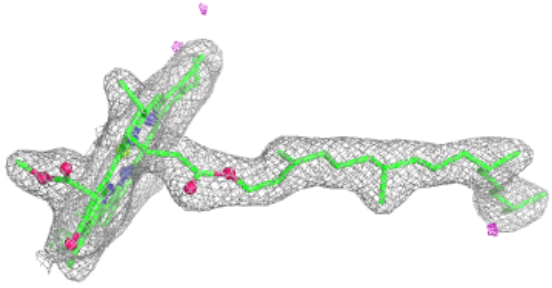


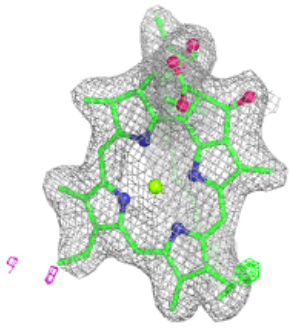


Electron density around CLA b 612:

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

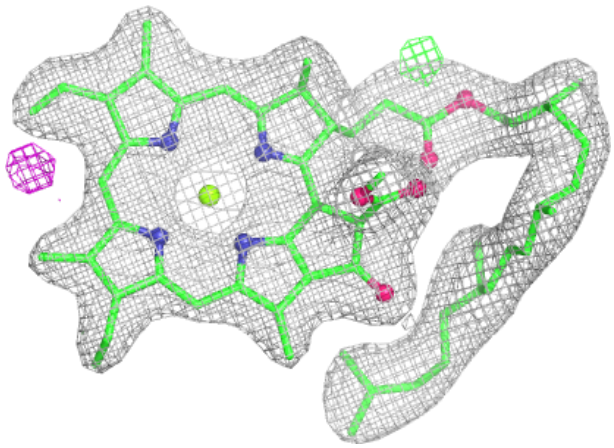


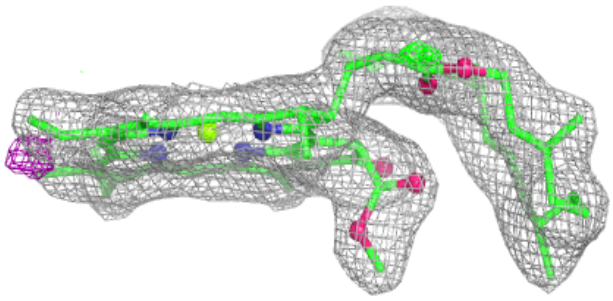


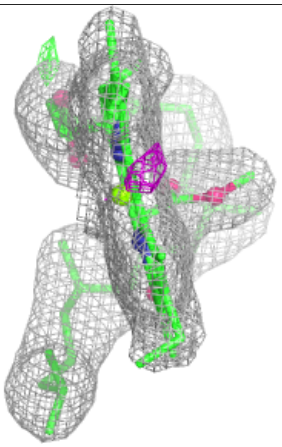


Electron density around CLA b 613:

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

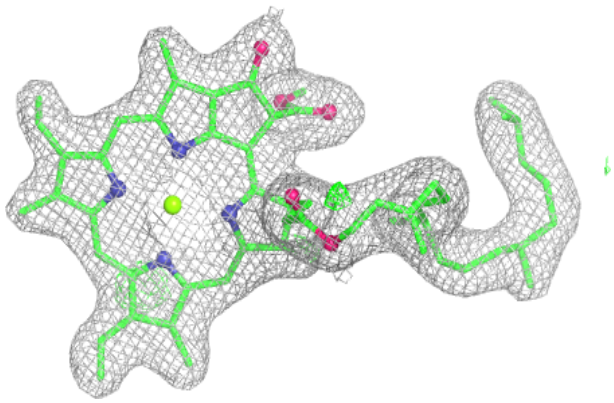


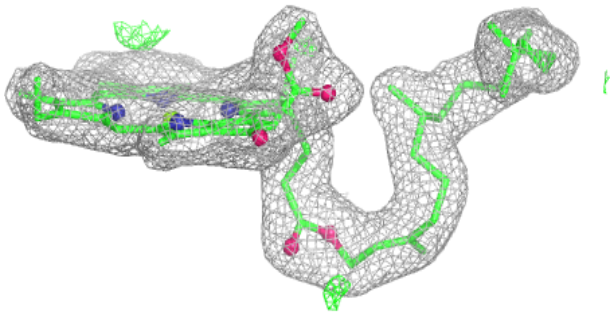


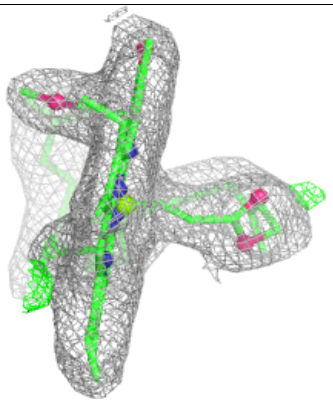


Electron density around CLA b 615:

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

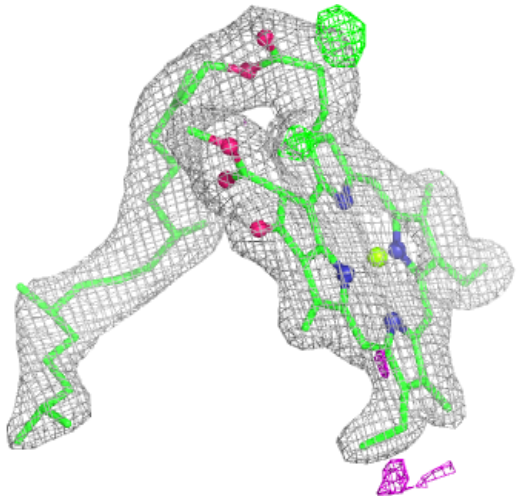


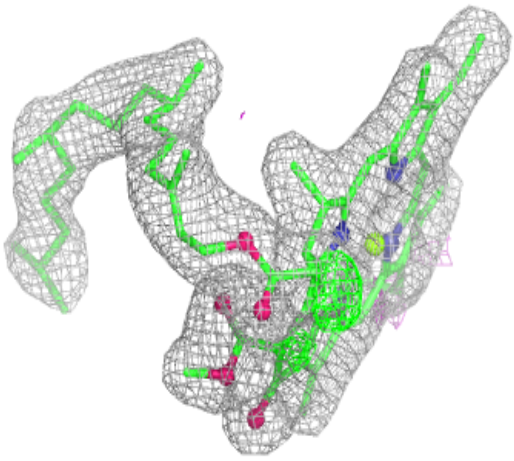


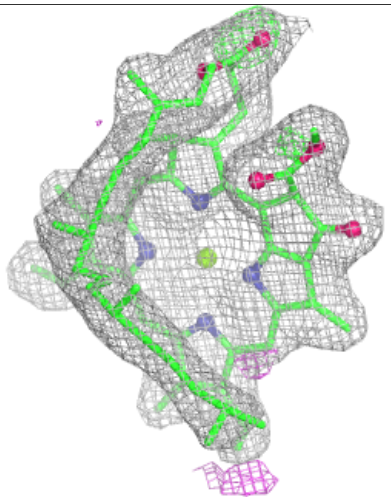


Electron density around CLA b 616:

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

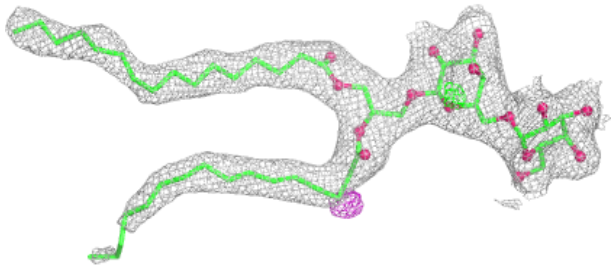


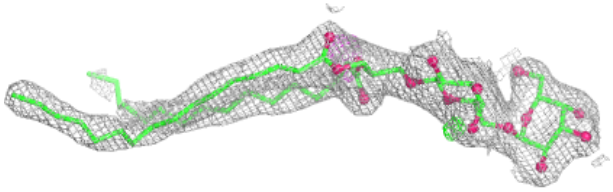


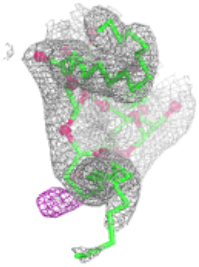


Electron density around DGD c 520:

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

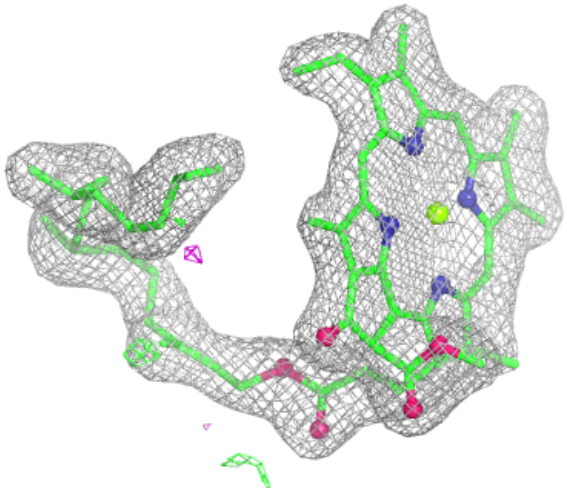


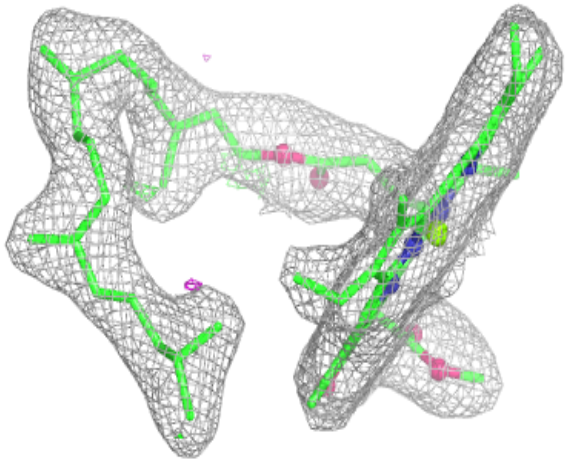


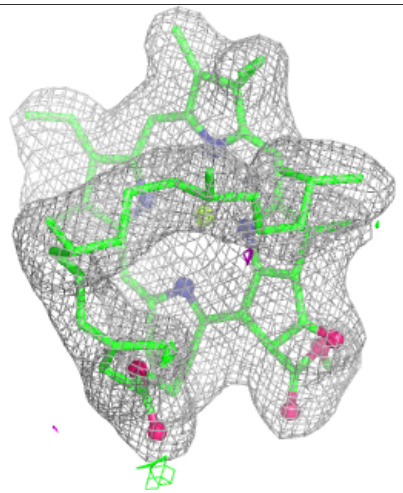


Electron density around CLA C 504:

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

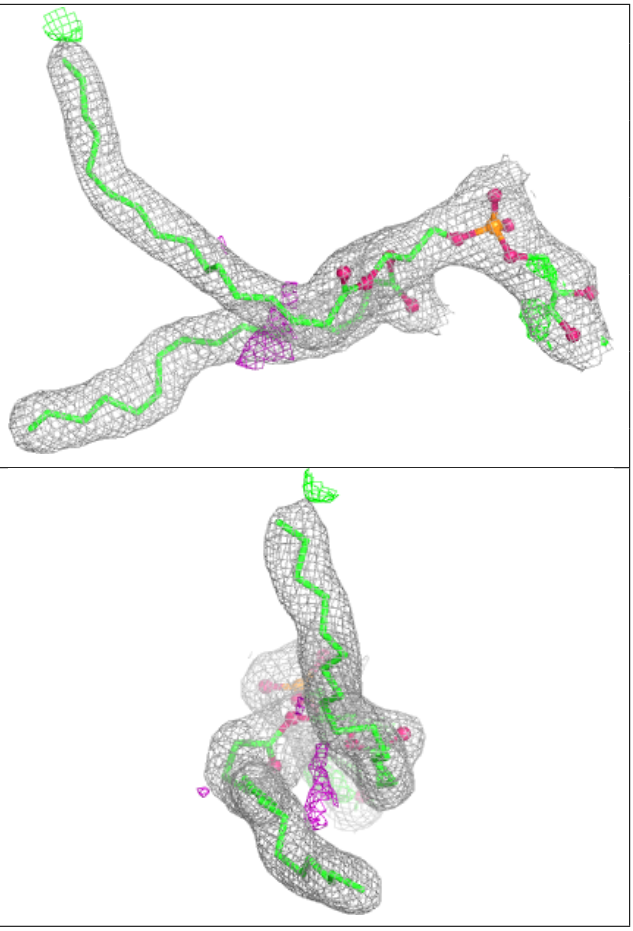


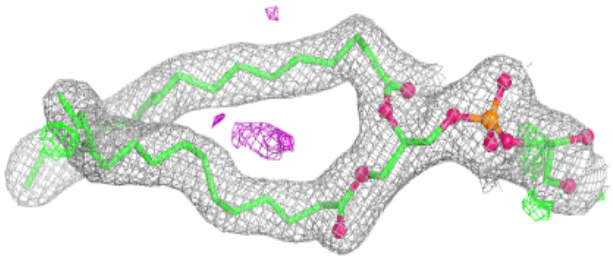




Electron density around LHG D 410:

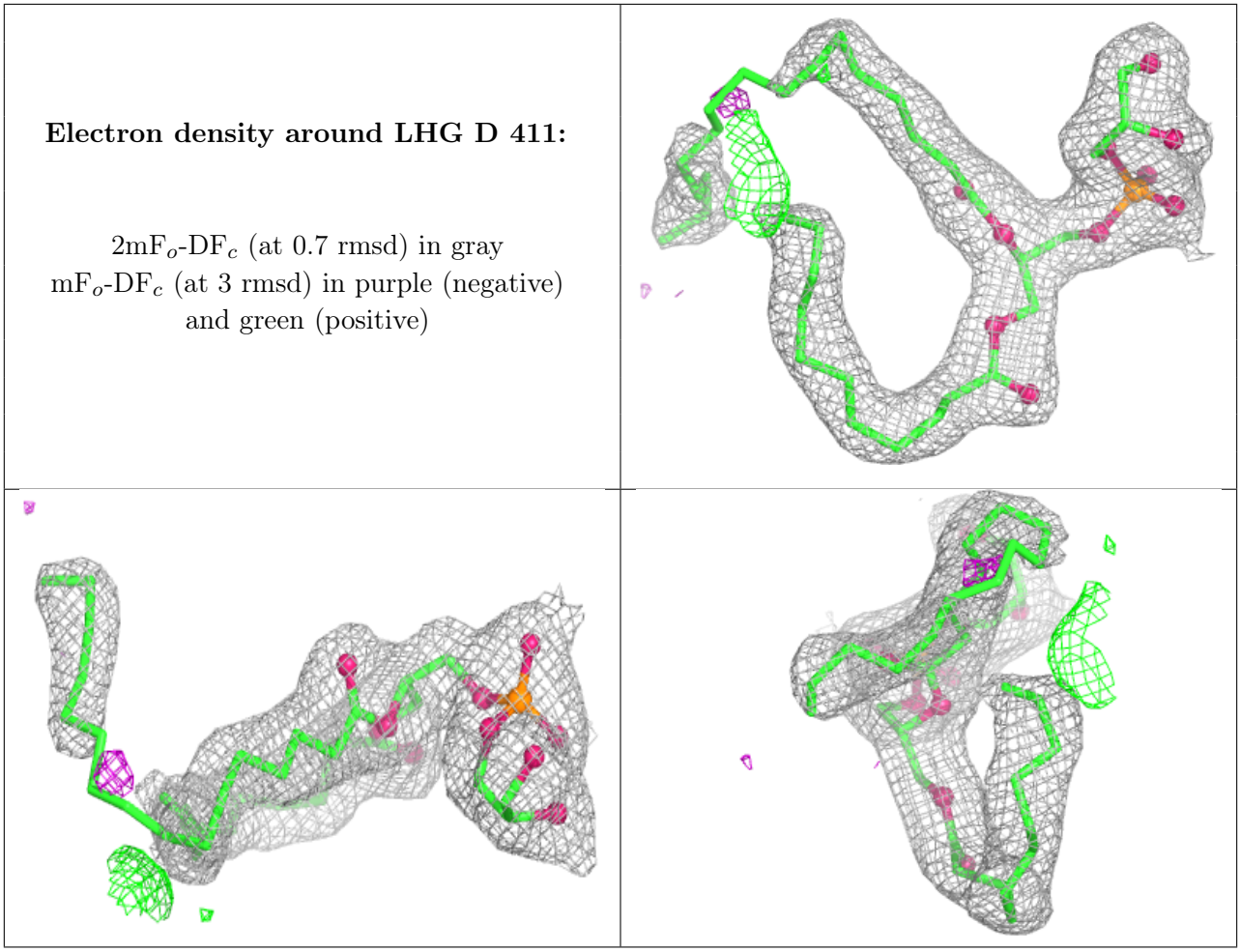
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





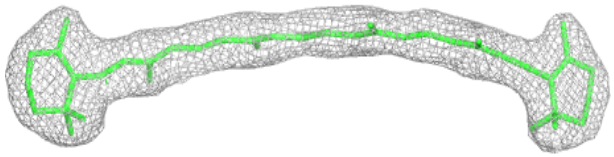
Electron density around LHG D 411:

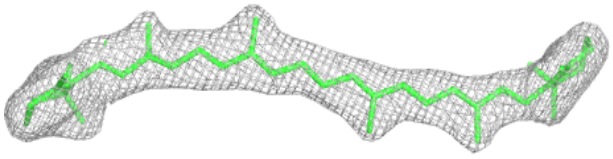
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

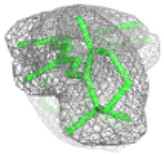


Electron density around BCR k 2003:

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

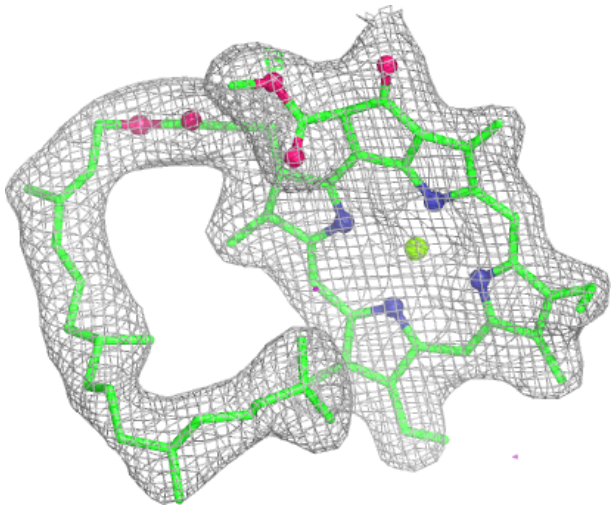


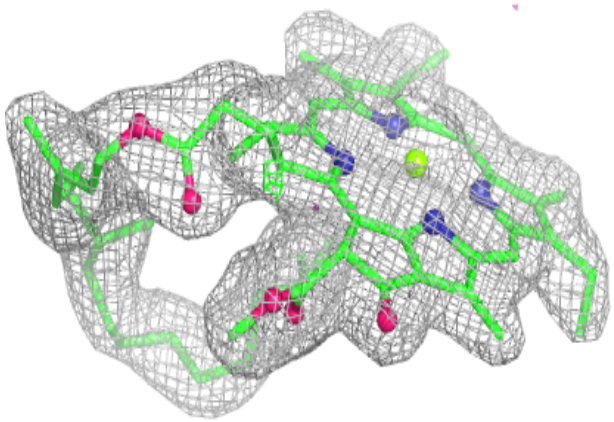




Electron density around CLA b 618:

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

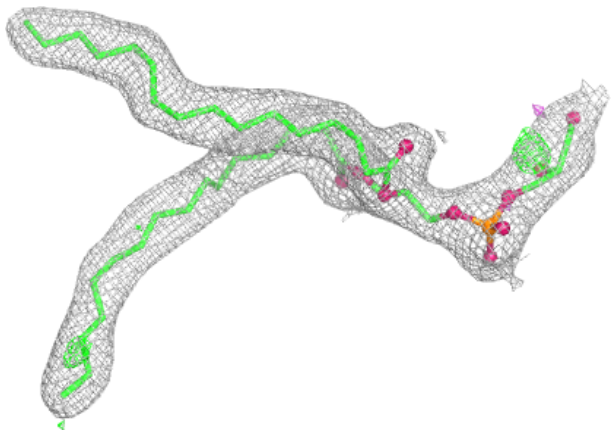


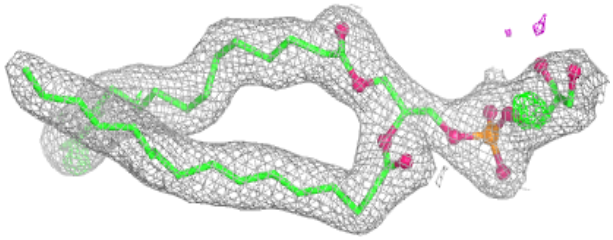


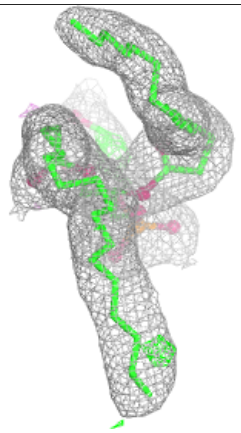


Electron density around LHG d 409:

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

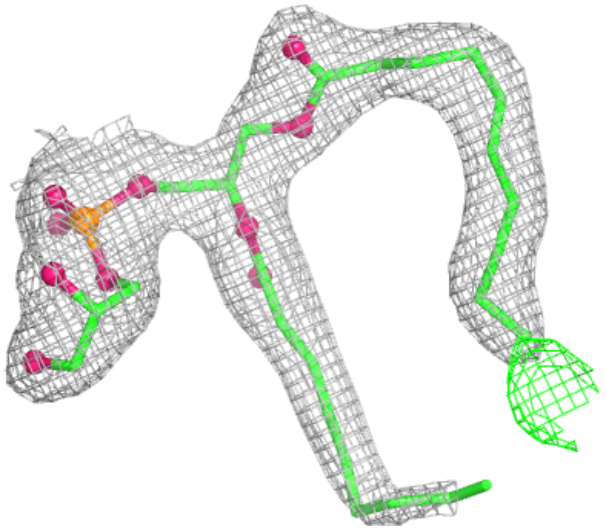


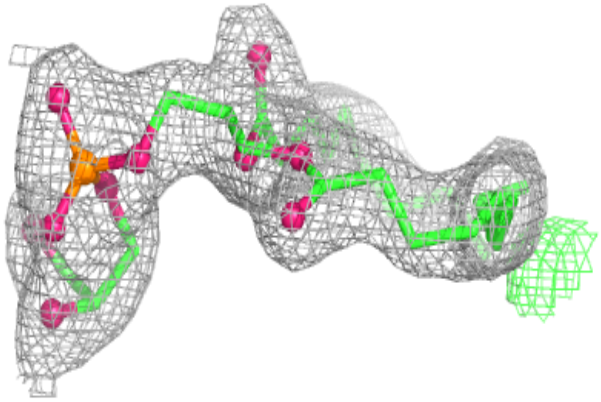




Electron density around LHG d 410:

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

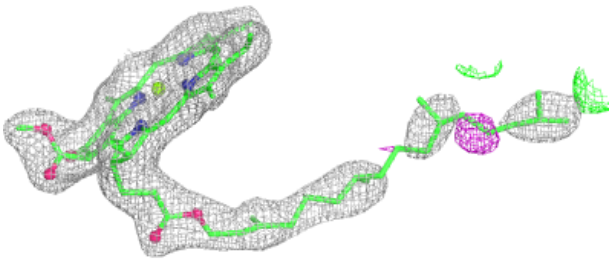


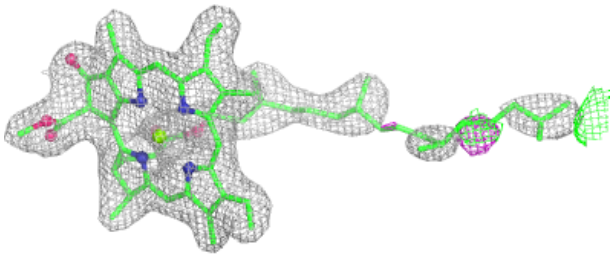


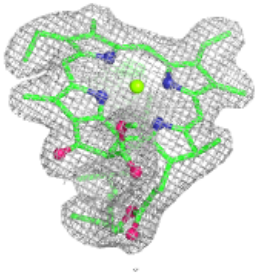


Electron density around CLA C 505:

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

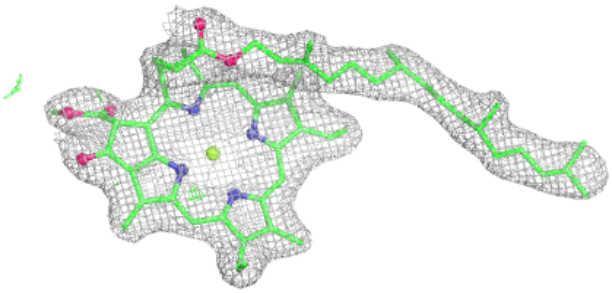


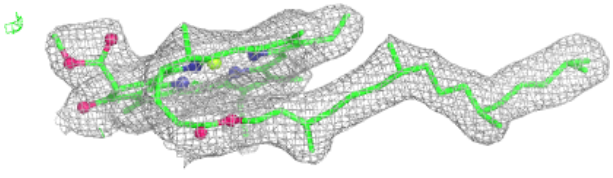




Electron density around CLA c 503:

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

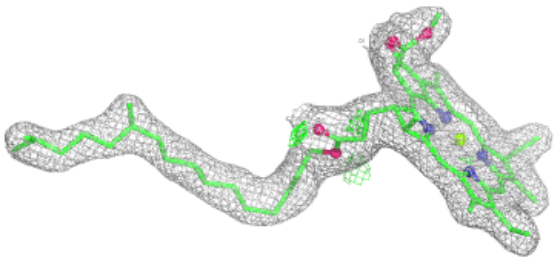


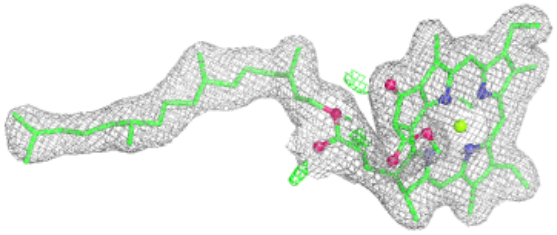


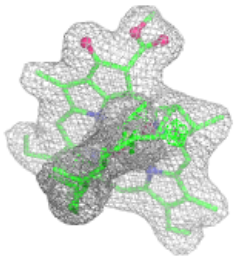


Electron density around CLA c 504:

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

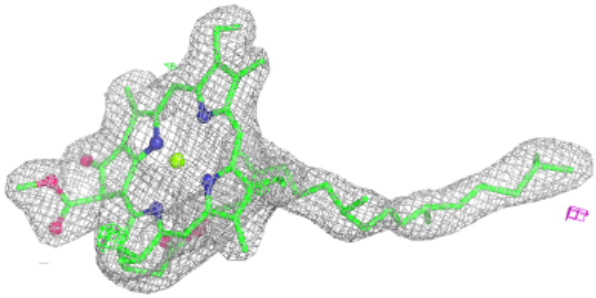


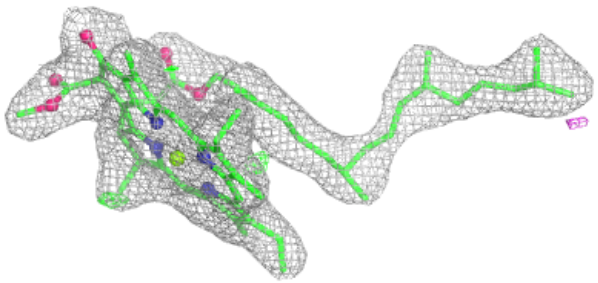


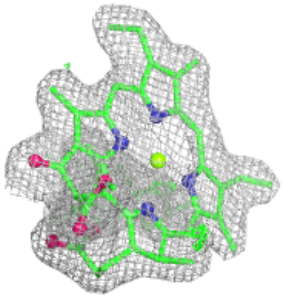


Electron density around CLA C 506:

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

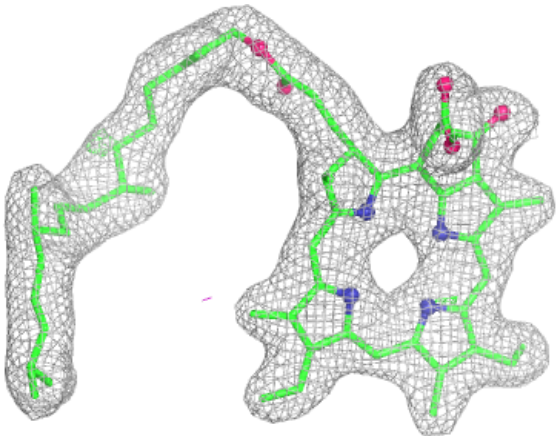


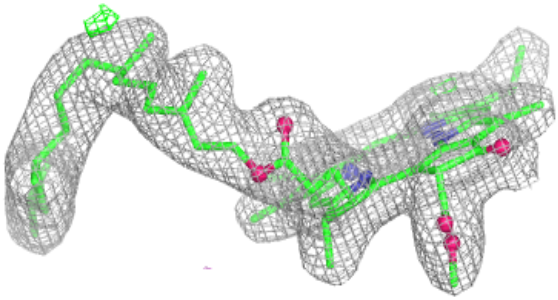


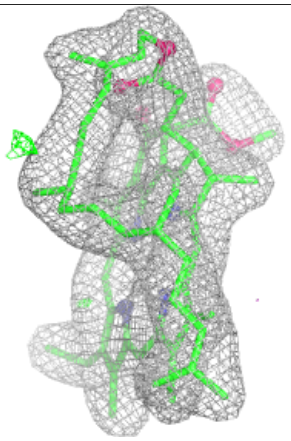


Electron density around PHO a 2112:

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

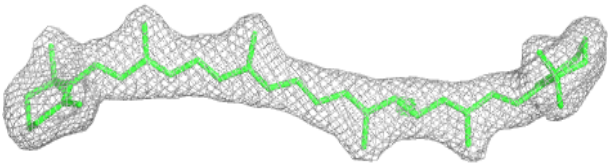


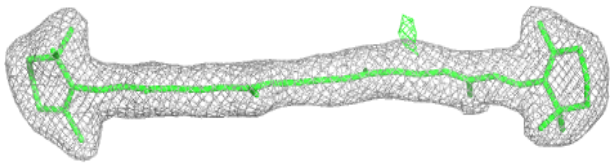


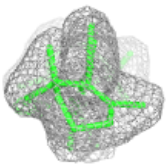


Electron density around BCR A 410:

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

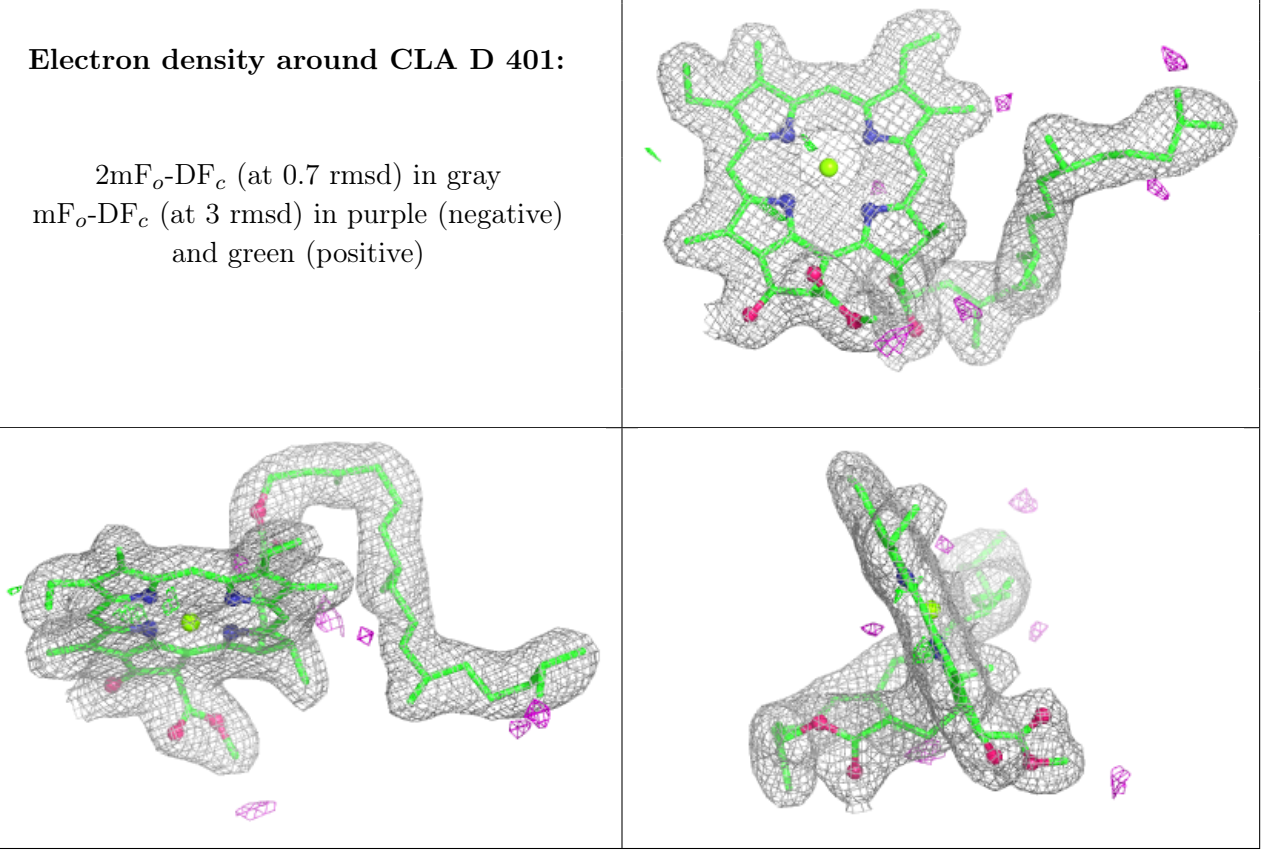






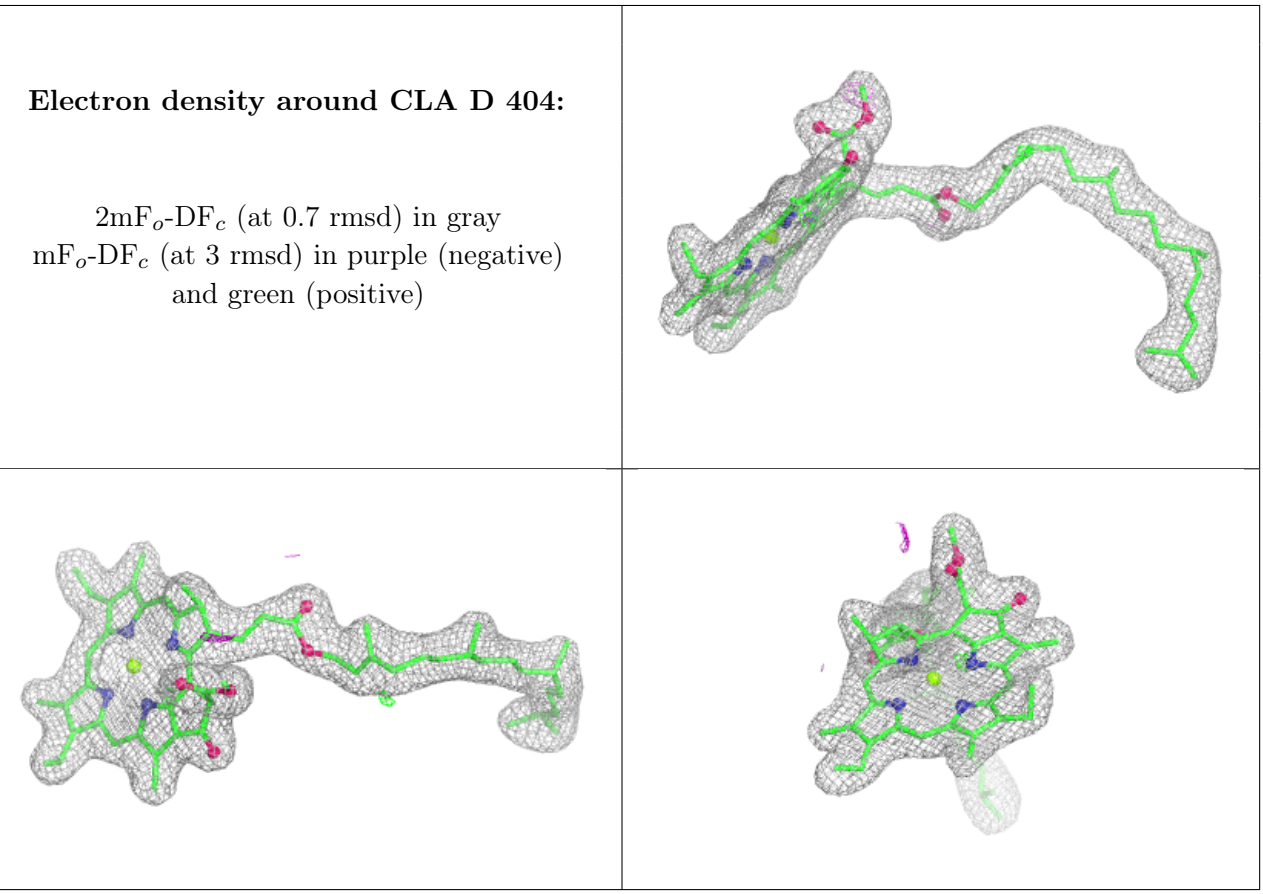
Electron density around CLA D 401:

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



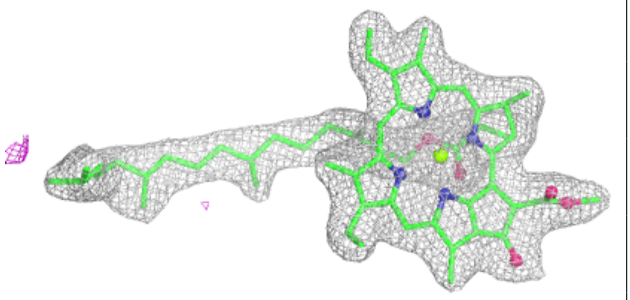
Electron density around CLA D 404:

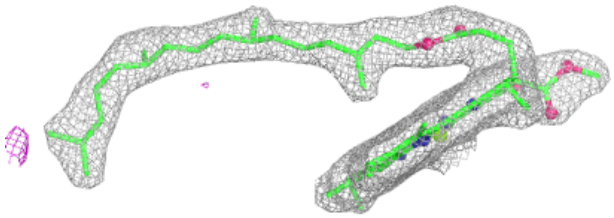
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

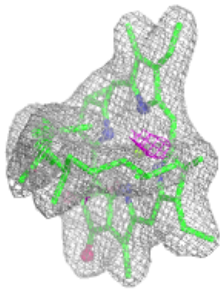


Electron density around CLA b 611:

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

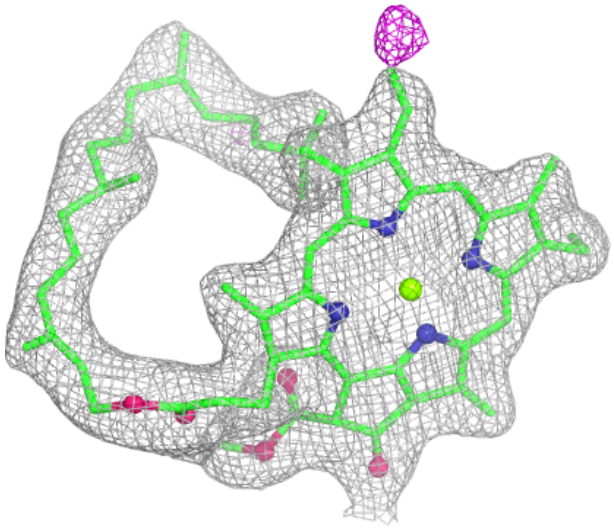


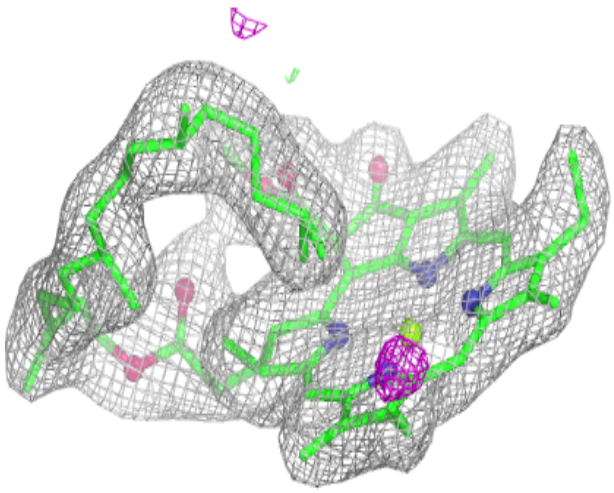


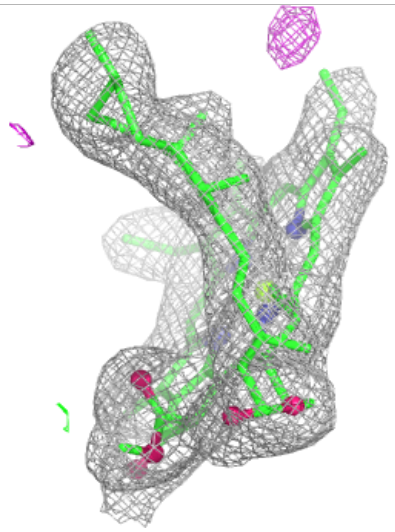


Electron density around CLA B 616:

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

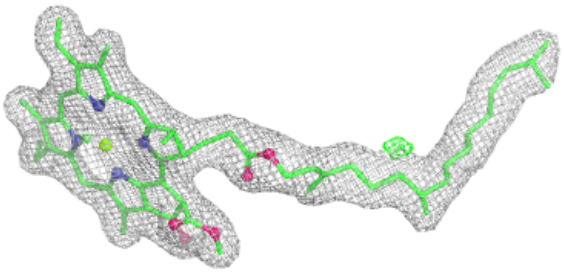


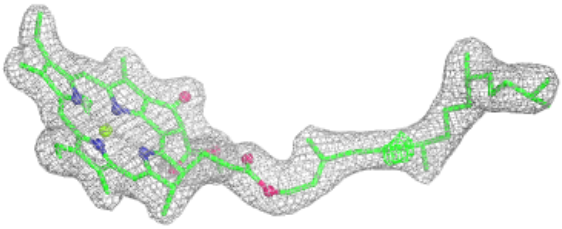


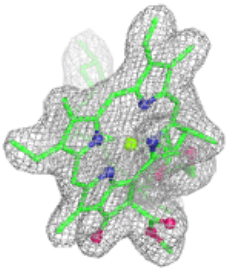


Electron density around CLA a 2109:

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

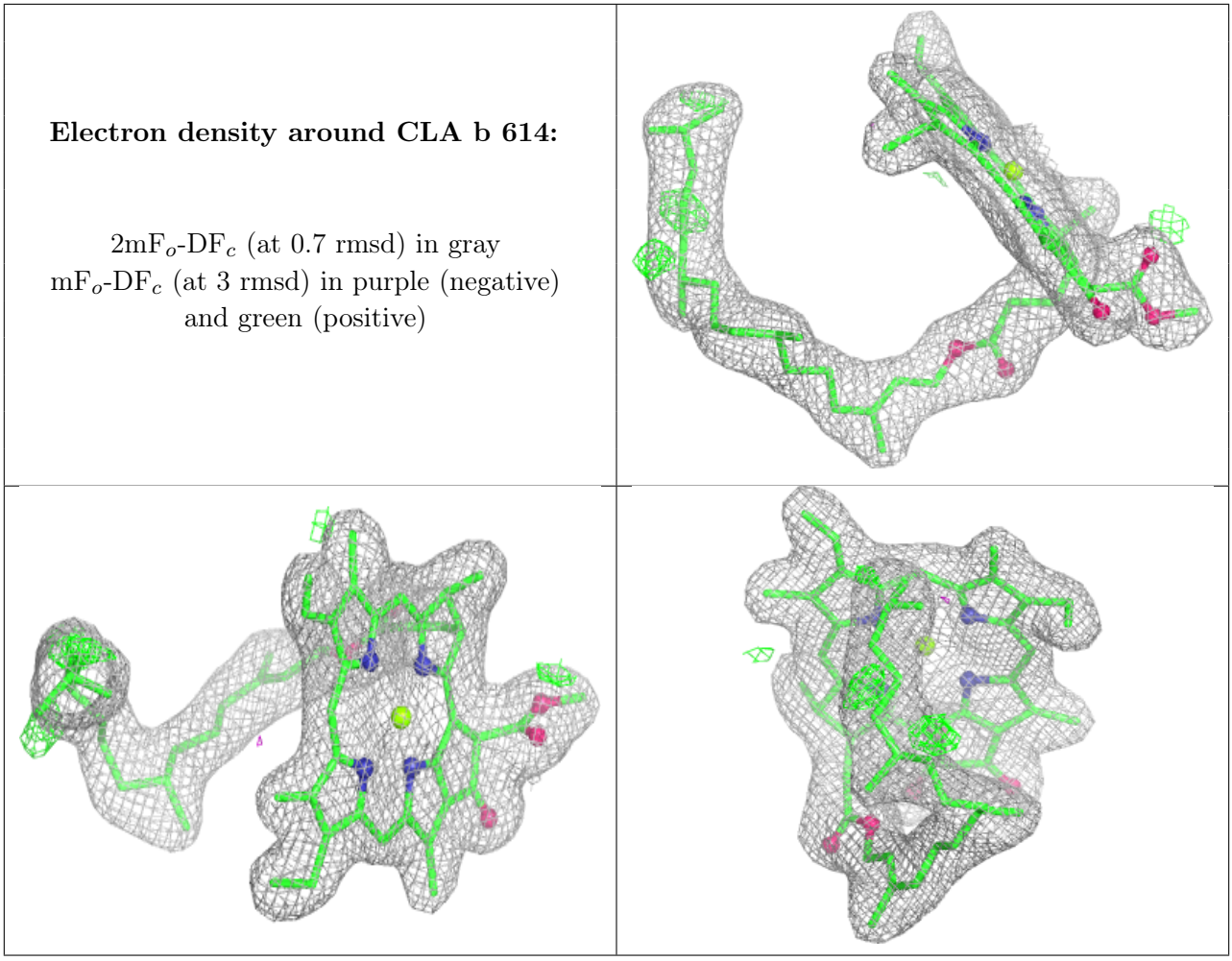






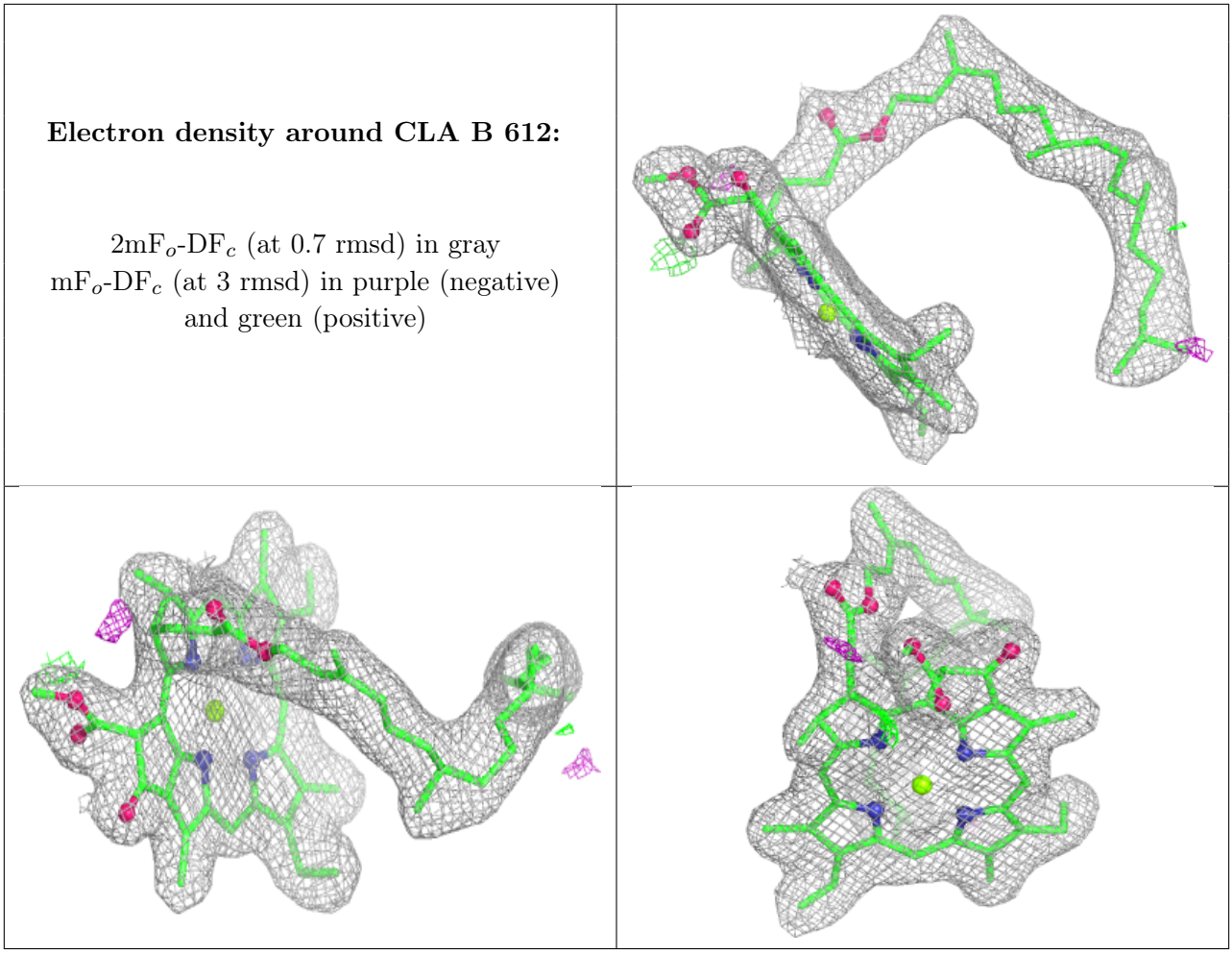
Electron density around CLA b 614:

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



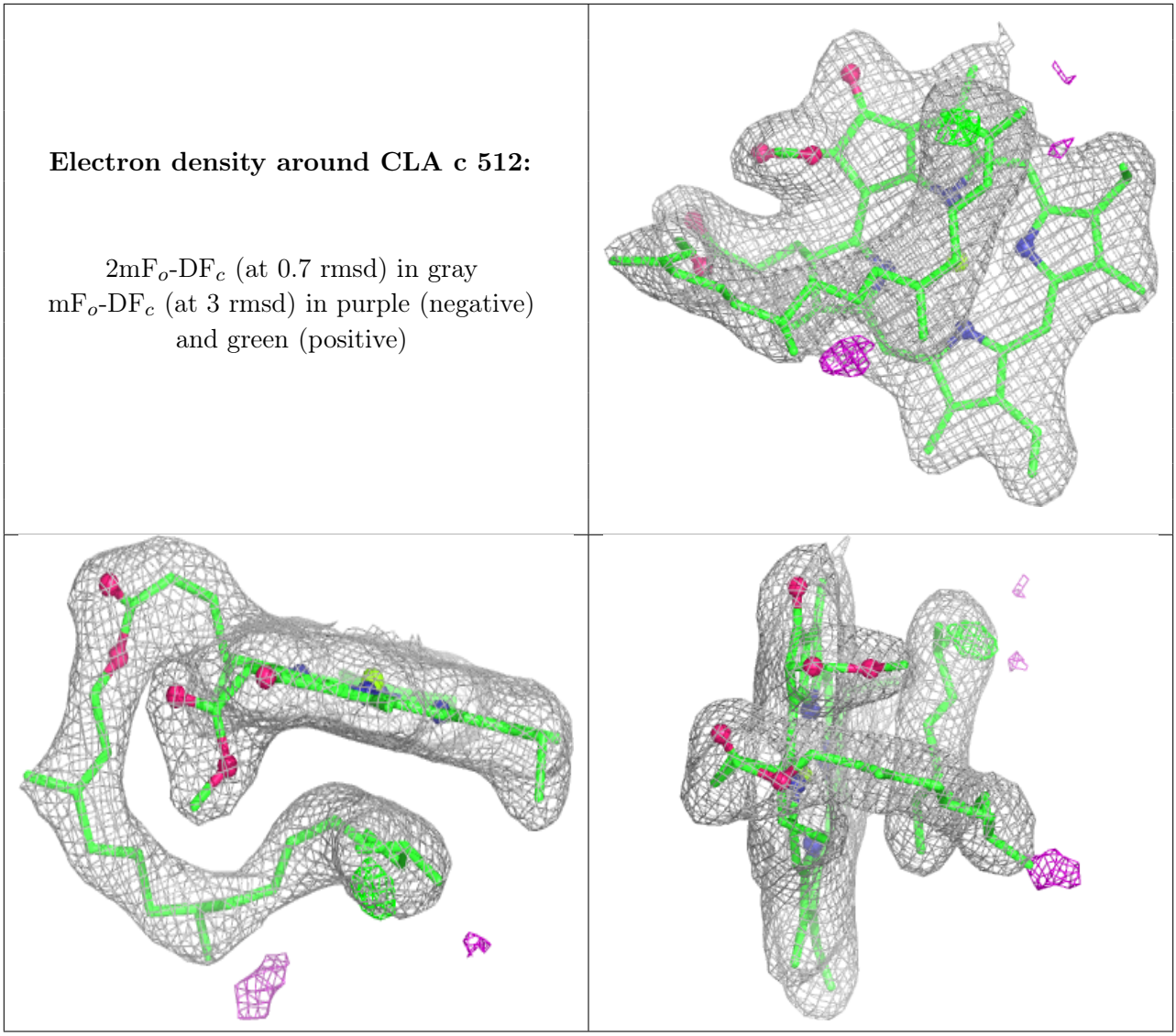
Electron density around CLA B 612:

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



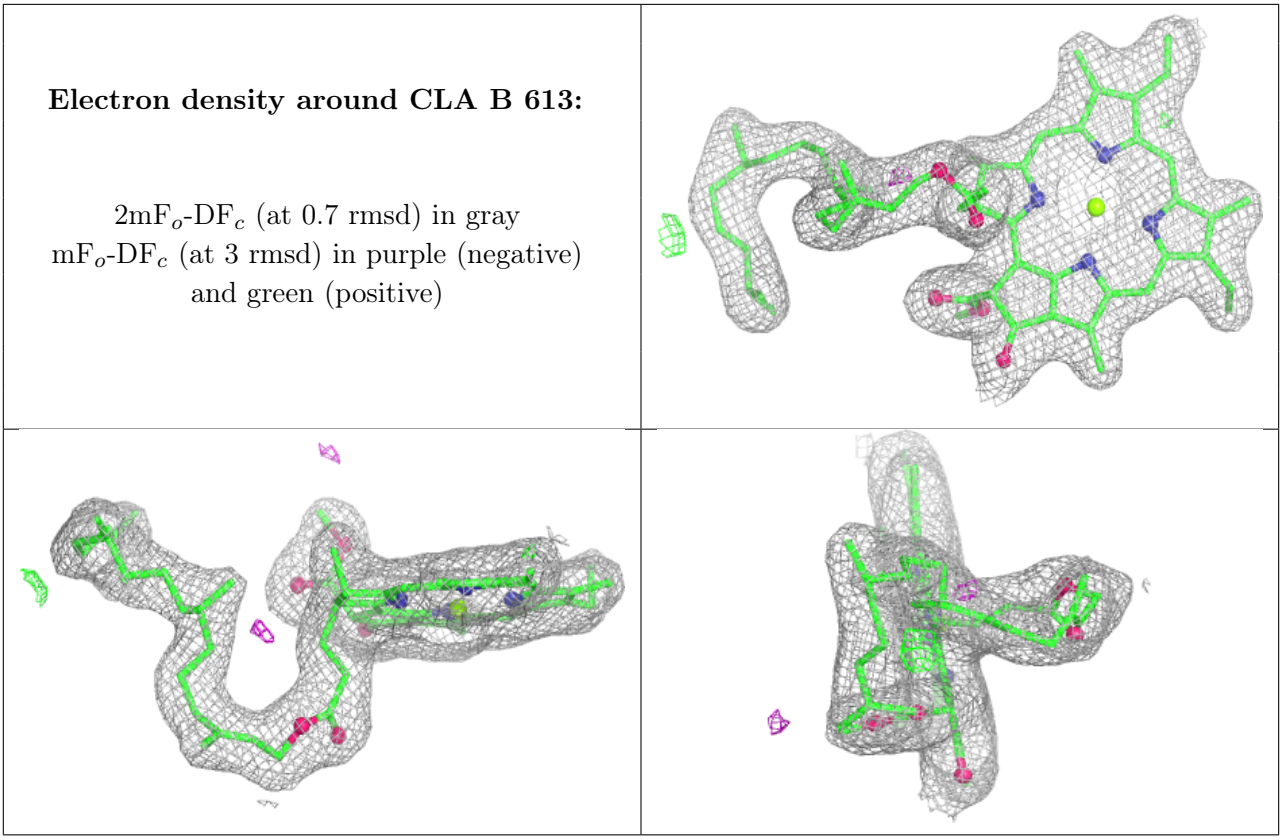
Electron density around CLA c 512:

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



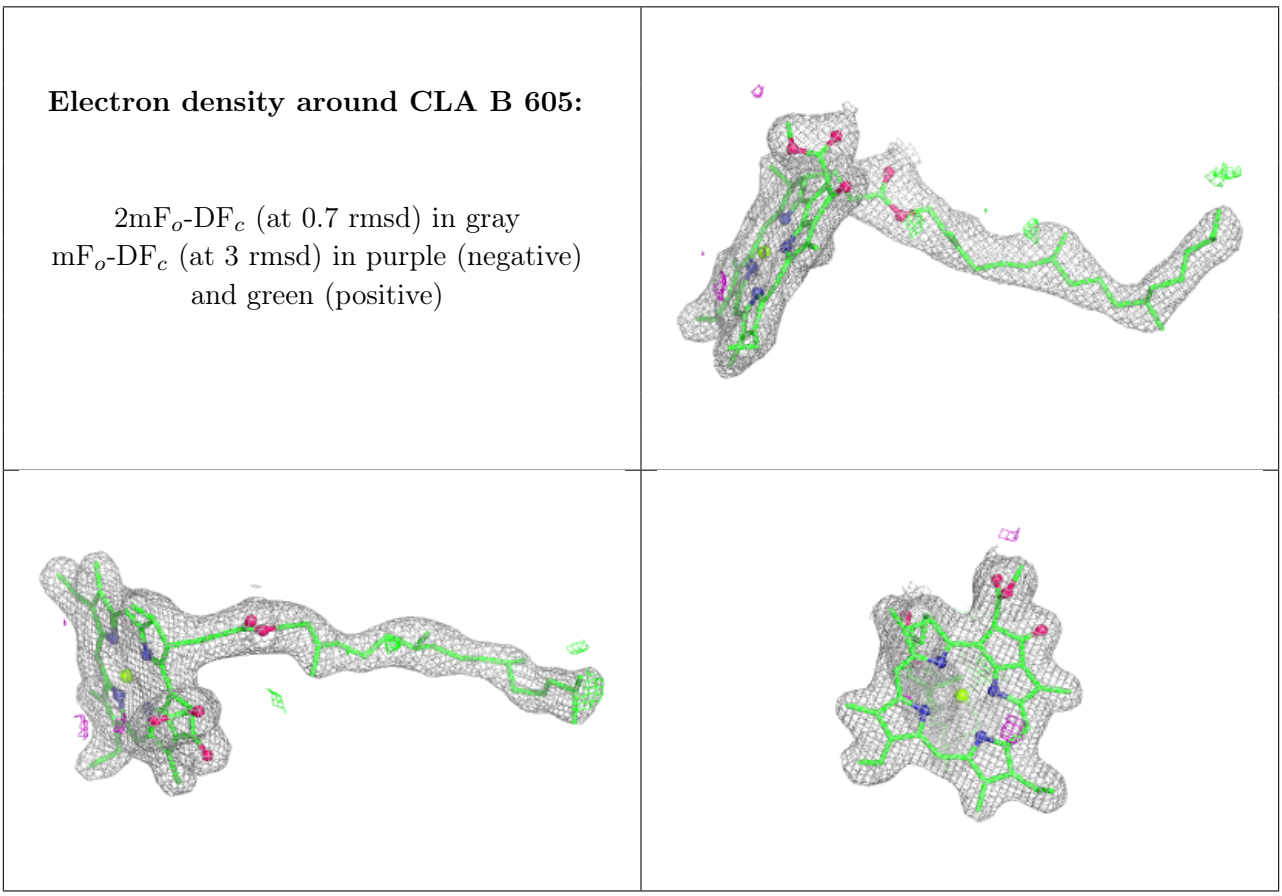
Electron density around CLA B 613:

$2mF_o$-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 605:

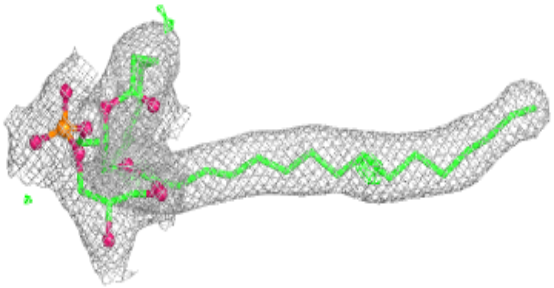
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

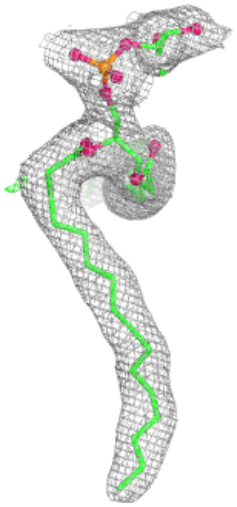


Electron density around LHG L 101:

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

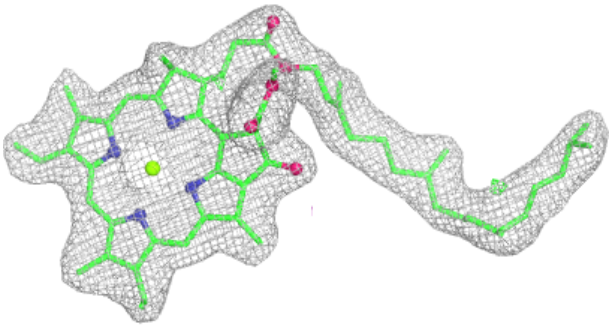


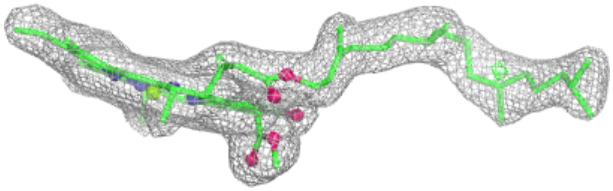




Electron density around CLA b 605:

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

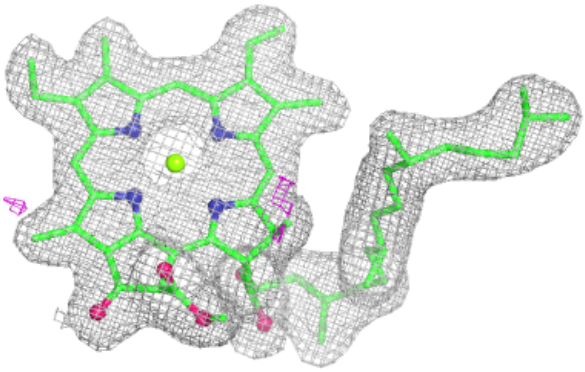


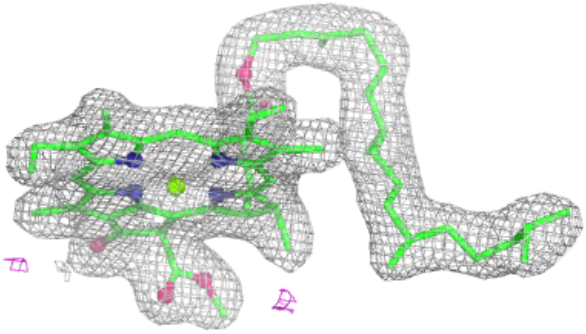


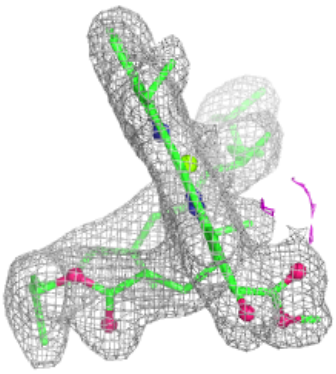


Electron density around CLA d 401:

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

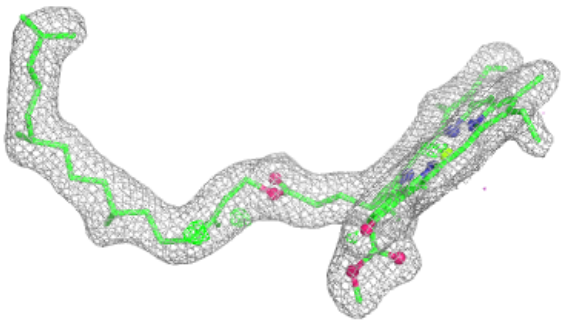


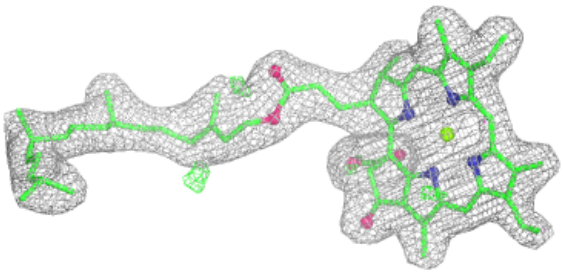


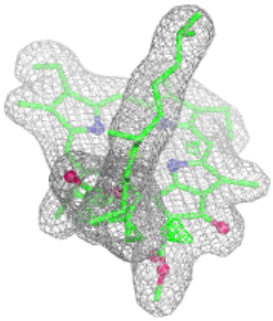


Electron density around CLA d 404:

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

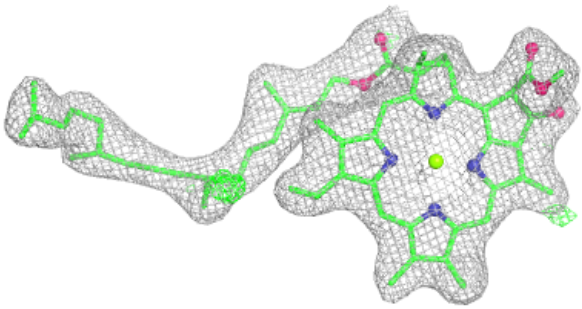


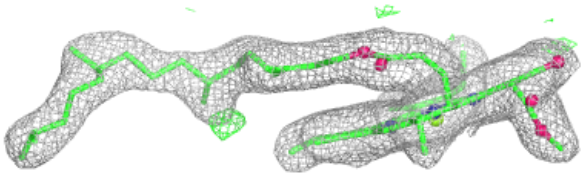


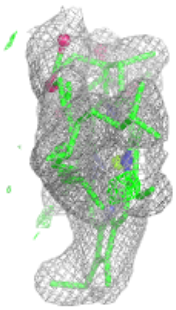


Electron density around CLA b 606:

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

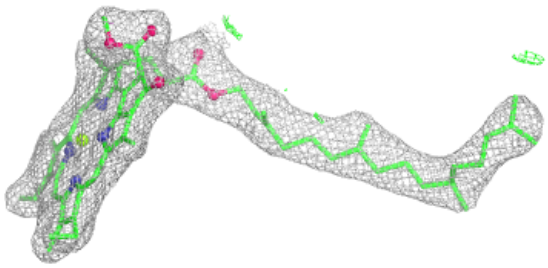


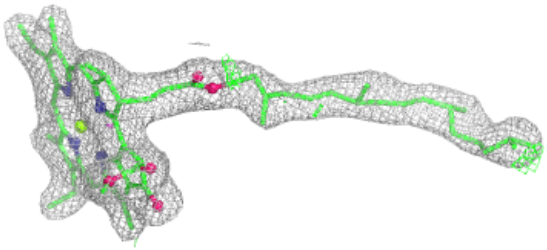


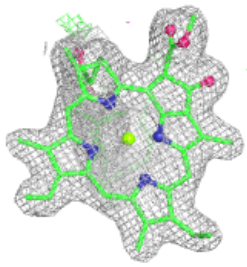


Electron density around CLA b 607:

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

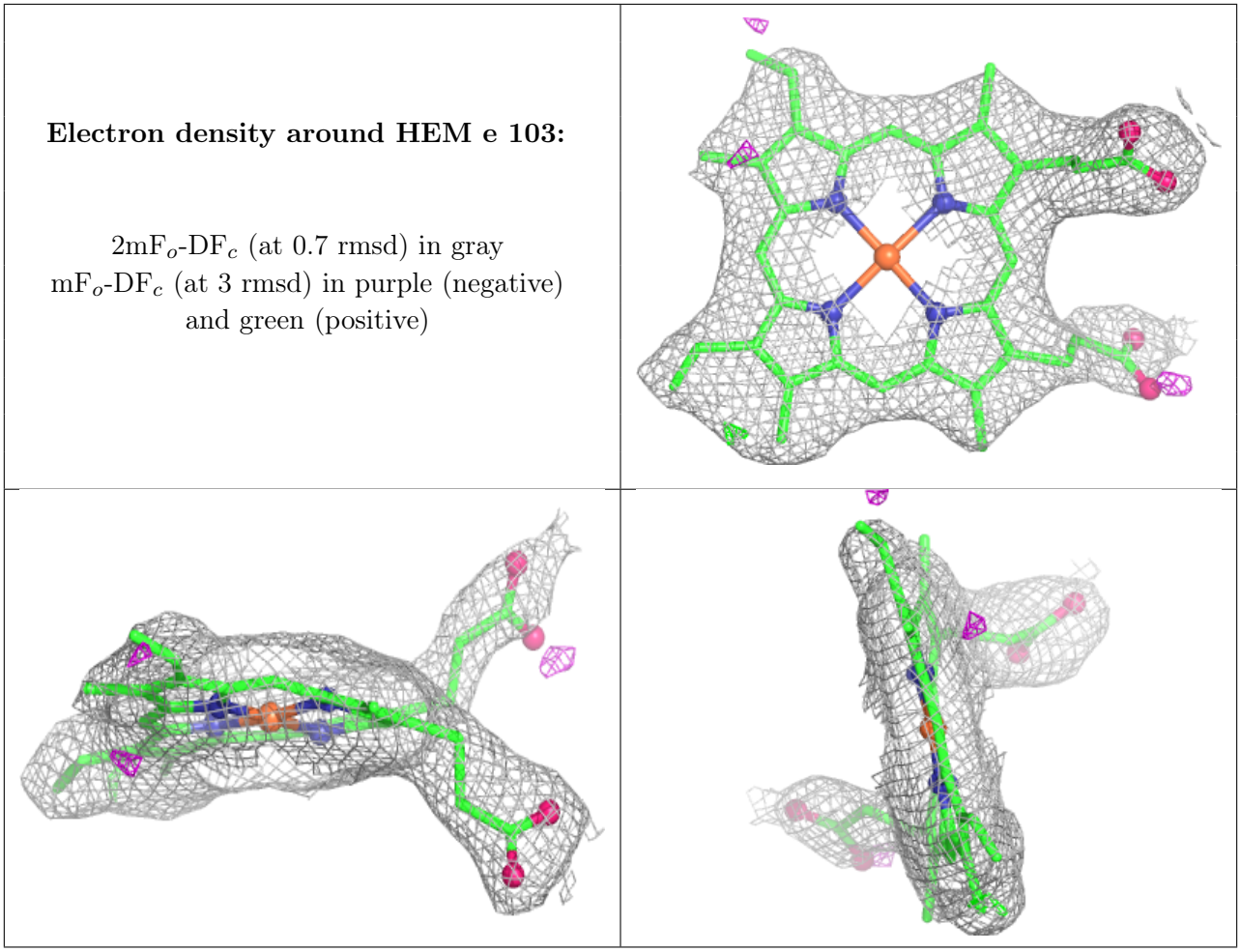






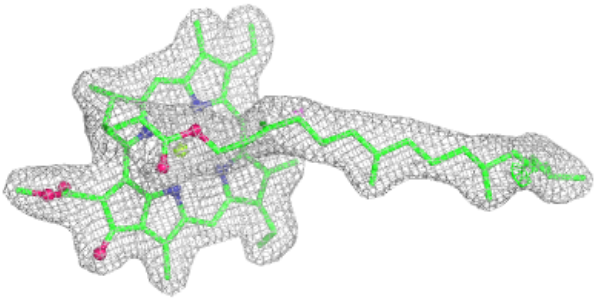
Electron density around HEM e 103:

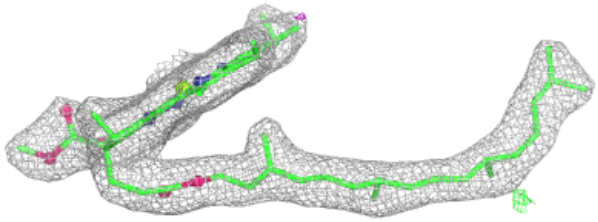
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

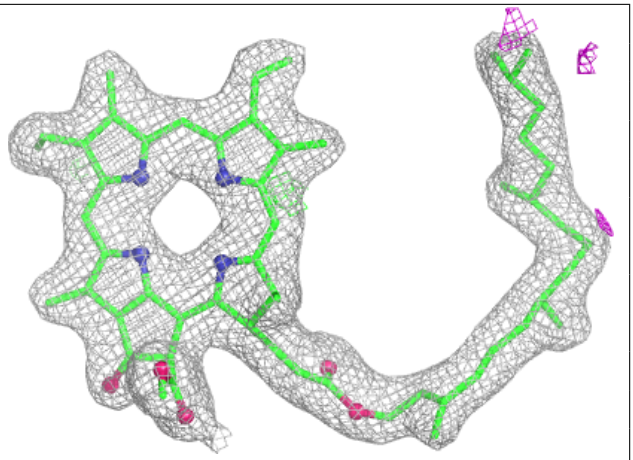


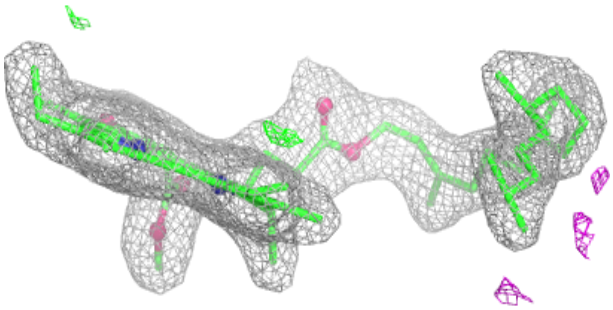


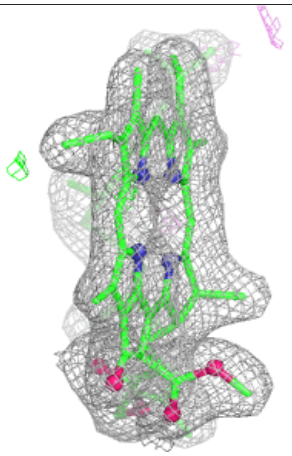


Electron density around PHO a 2111:

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

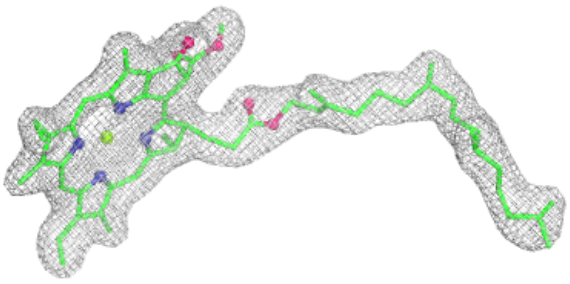


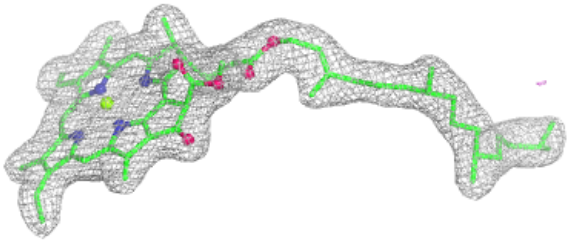


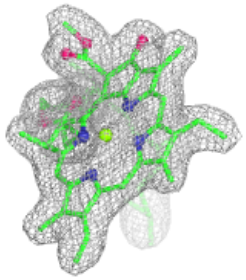


Electron density around CLA A 405:

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

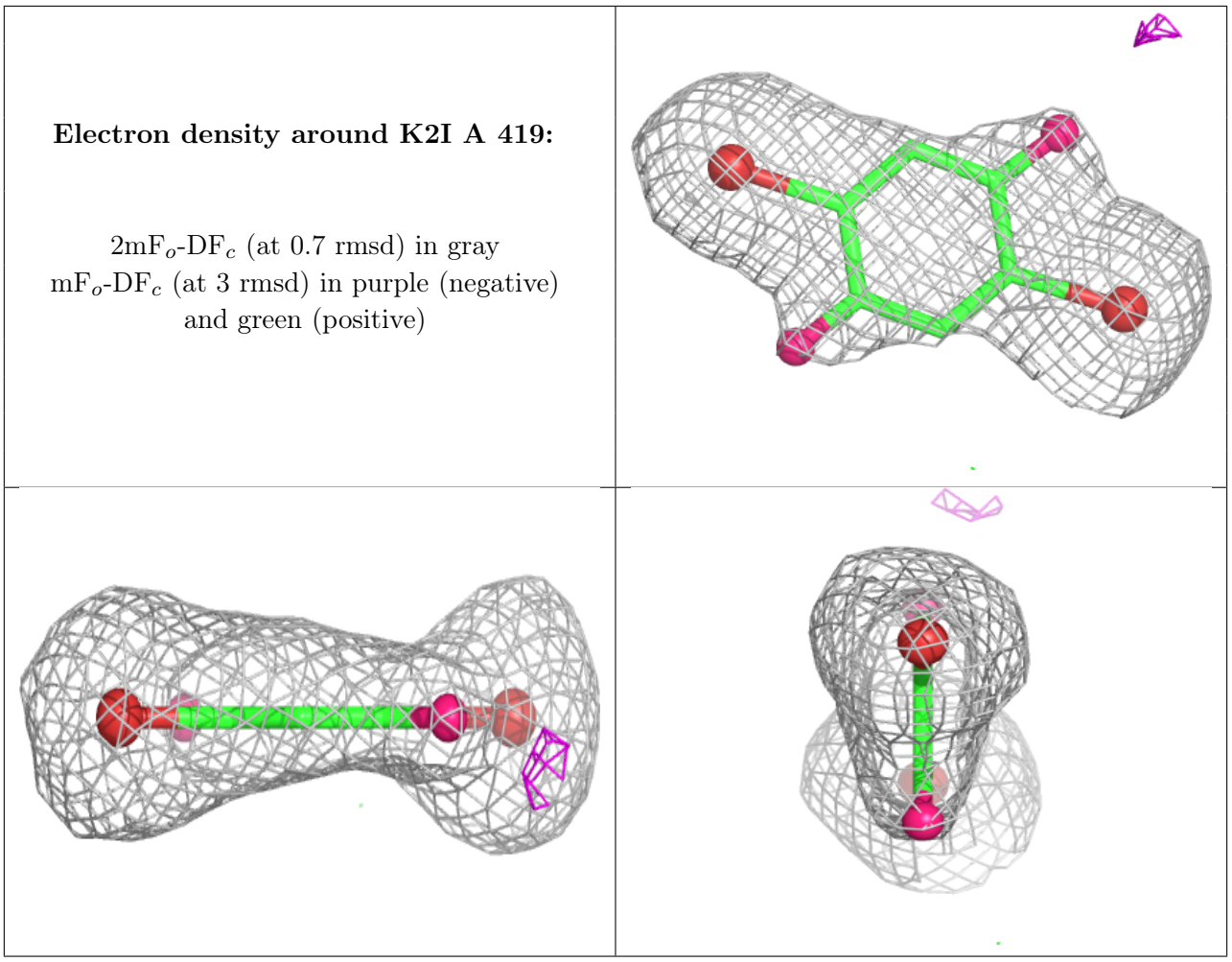






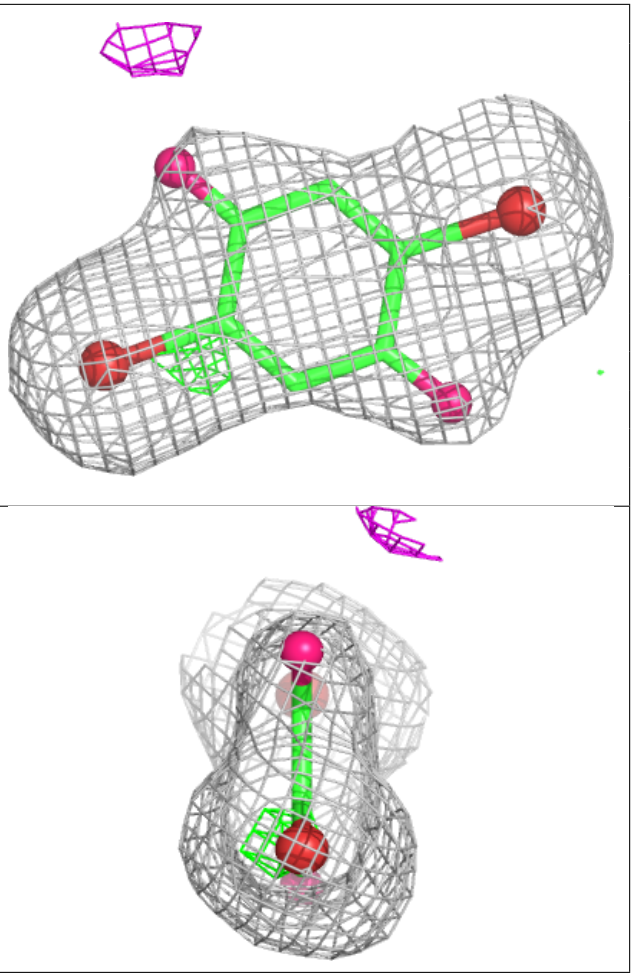
Electron density around K2I A 419:

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



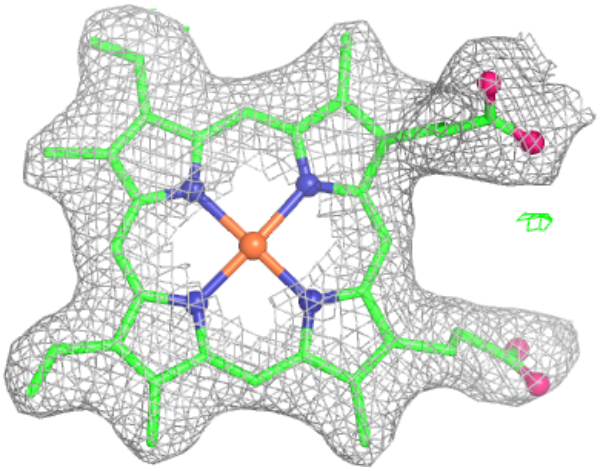
Electron density around K2I a 2119:

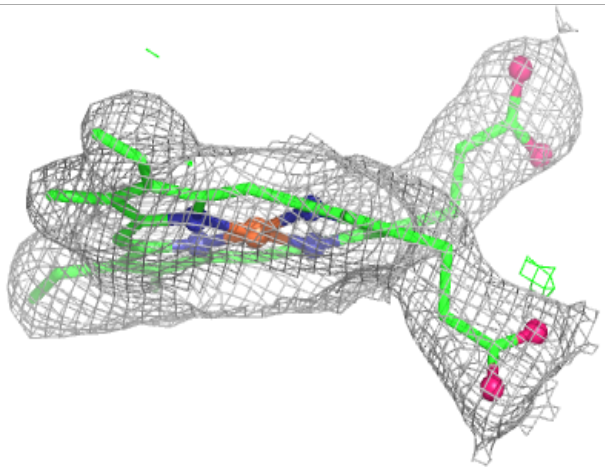
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

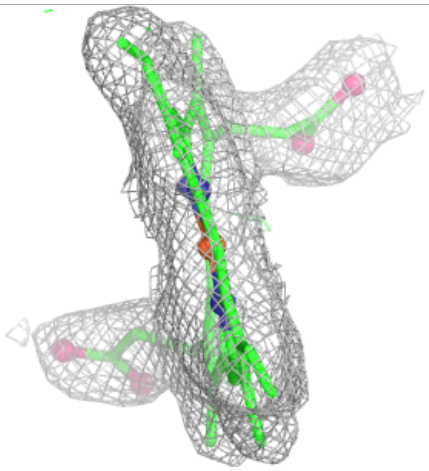


Electron density around HEM F 102:

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

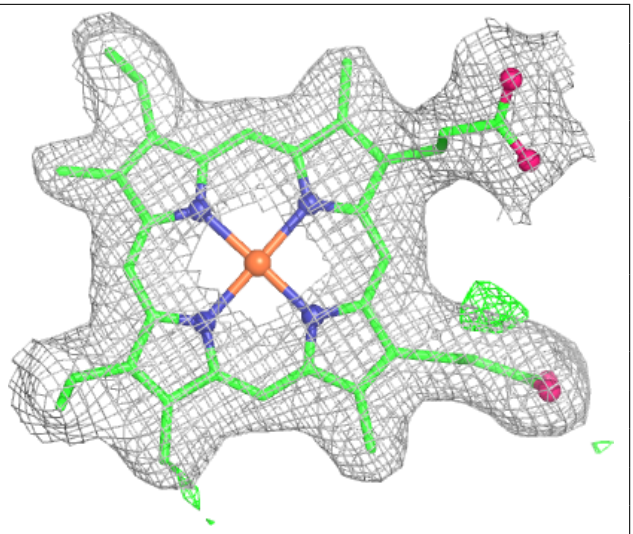


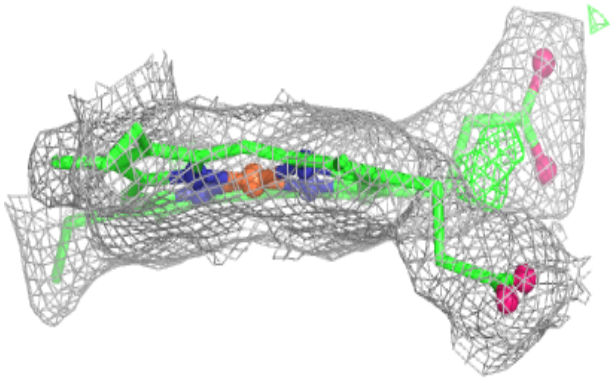


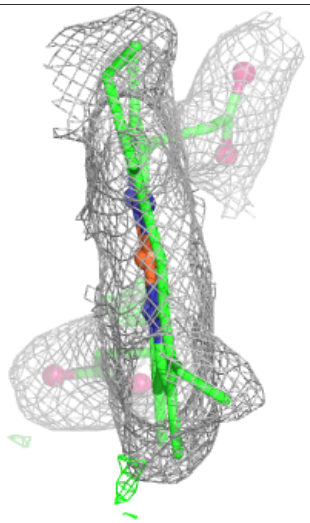


Electron density around HEC V 201:

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

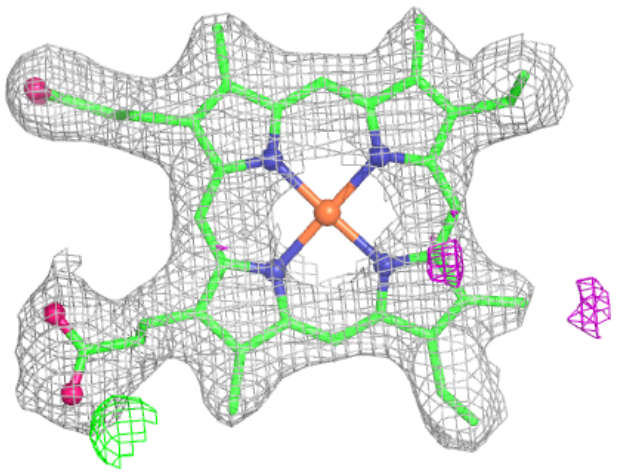


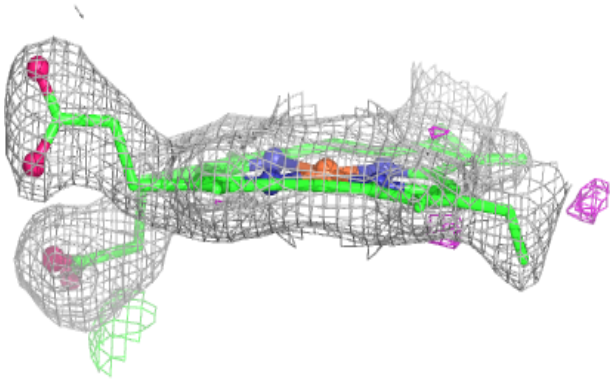




Electron density around HEC v 201:

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

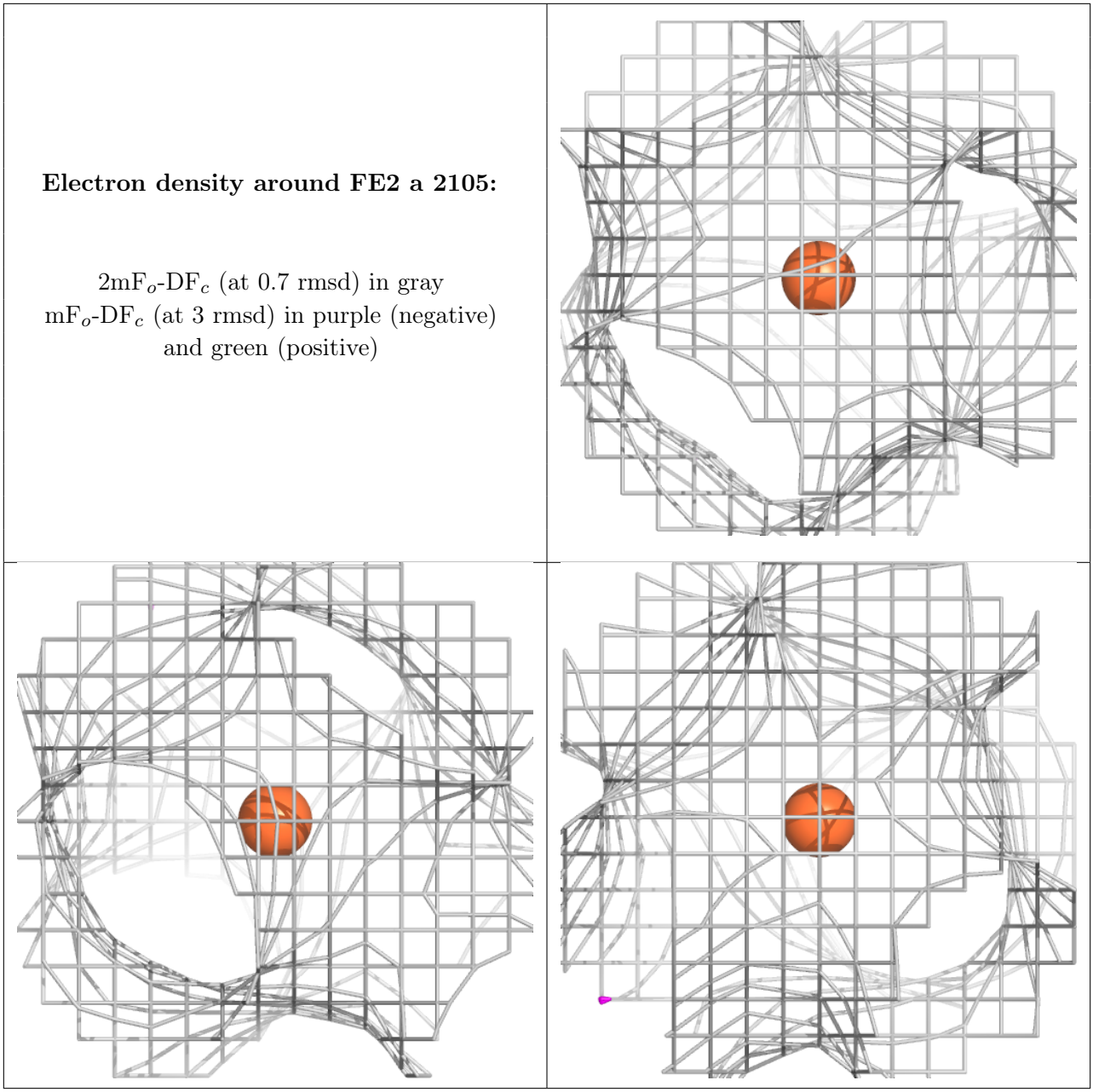






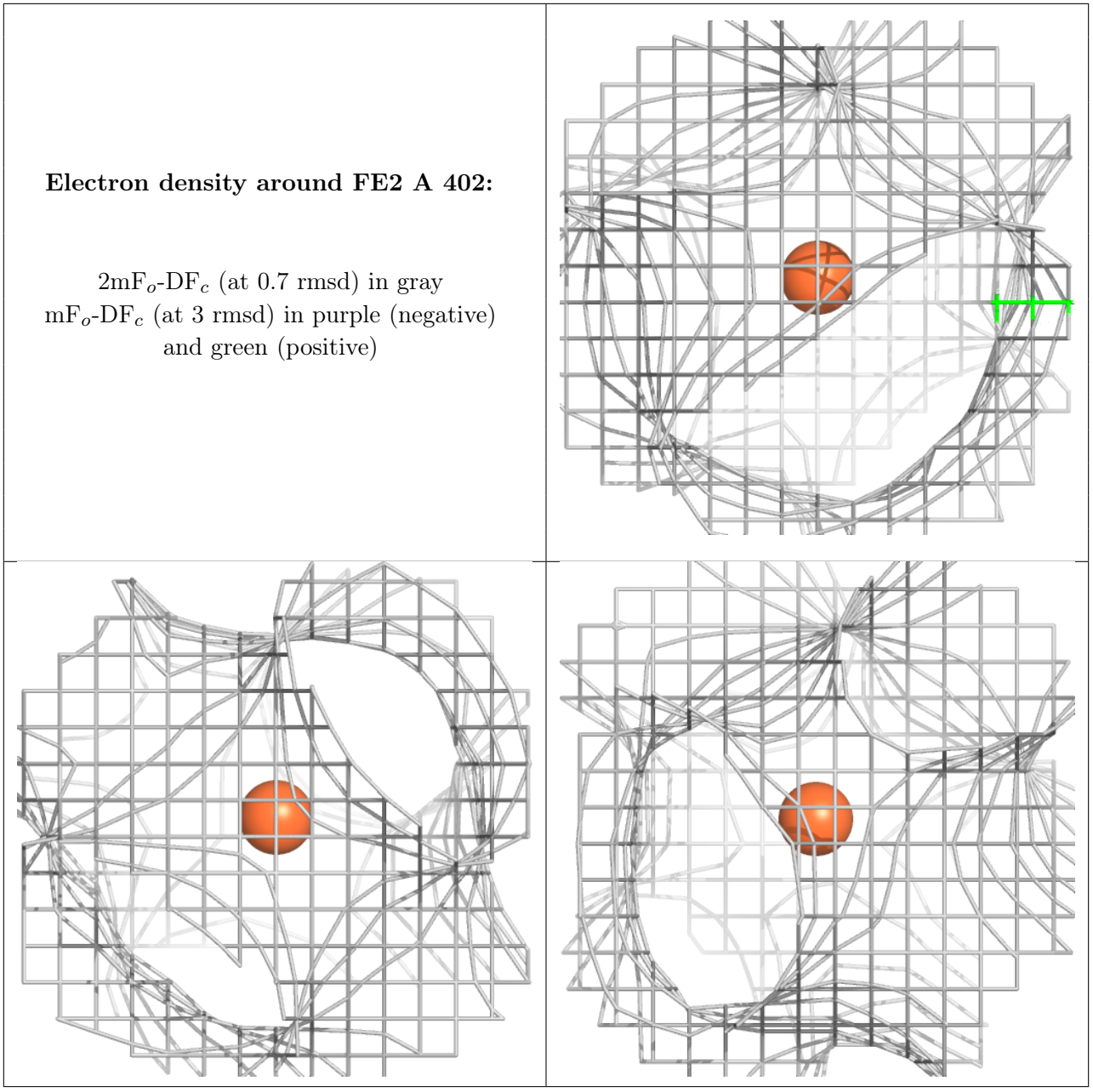
Electron density around FE2 a 2105:

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



Electron density around FE2 A 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.