wwPDB X-ray Structure Validation Summary Report (i)

Mar 17, 2026 – 07:52 PM UTC

PDB ID	:	7YQ2 / pdb_00007yq2
Title	:	Crystal structure of photosystem II expressing psbA2 gene only
Authors	:	Nakajima, Y.; Suga, M.; Shen, J.R.
Deposited on	:	2022-08-05
Resolution	:	1.90 Å(reported)

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

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

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

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

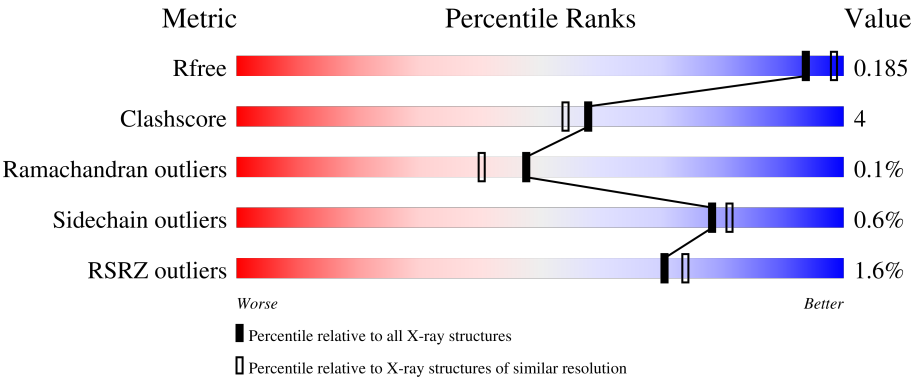
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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.



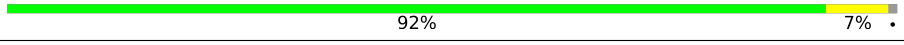
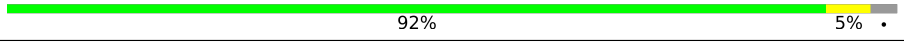
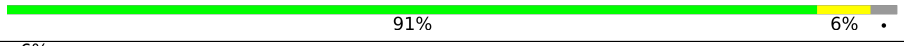
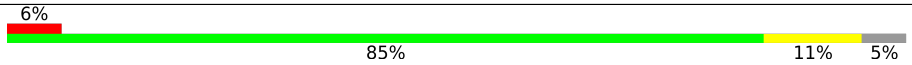
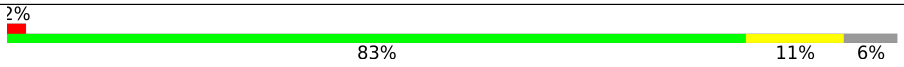
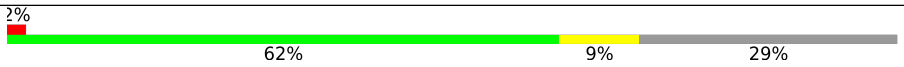
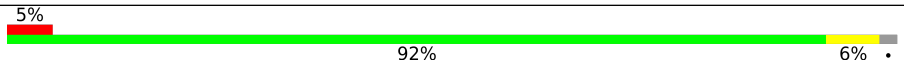
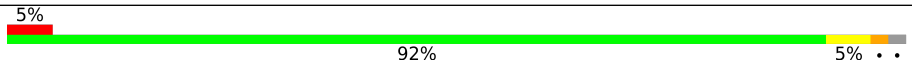
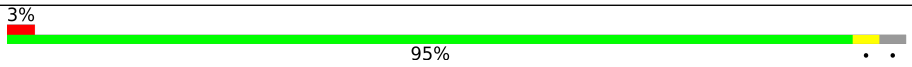
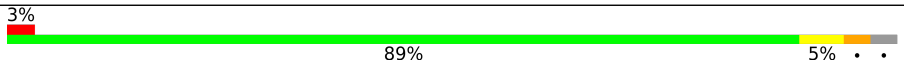
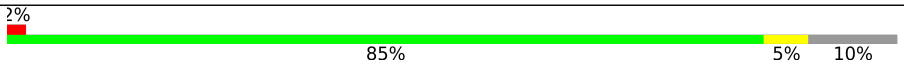
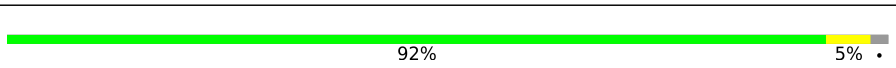
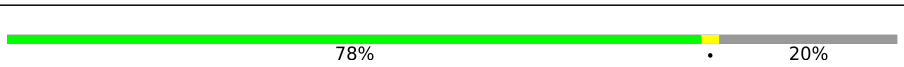
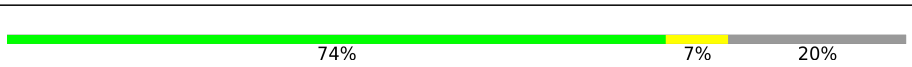
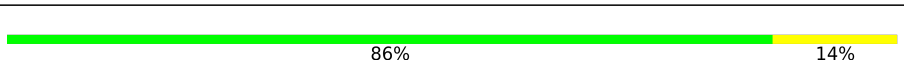
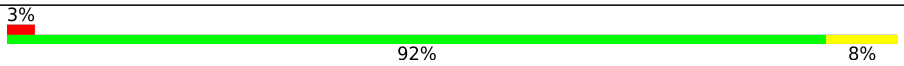
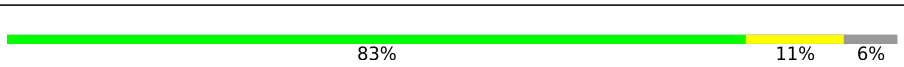
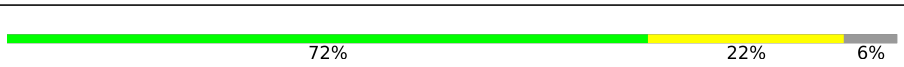
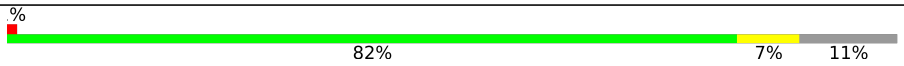
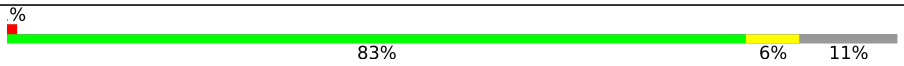
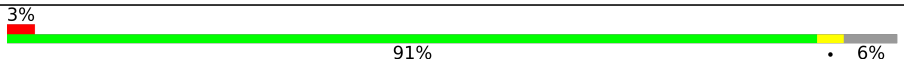
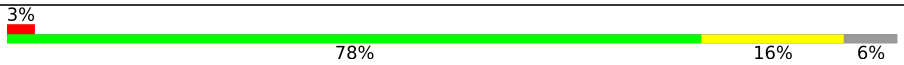
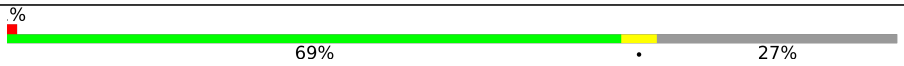
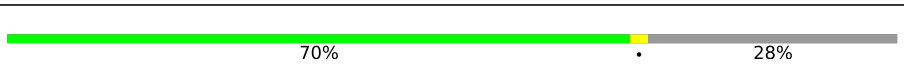
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	360	% 87% 6% 7%
1	a	360	% 85% 9% 7%
2	B	510	93% 6% •
2	b	510	3% 93% 6% •
3	C	461	92% 6% •

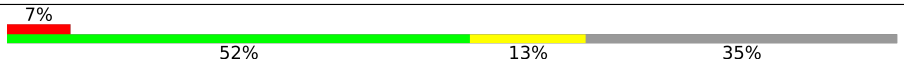
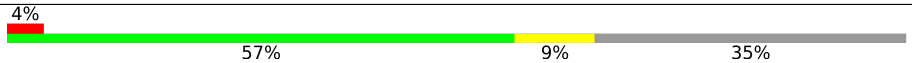
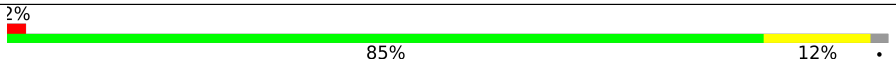
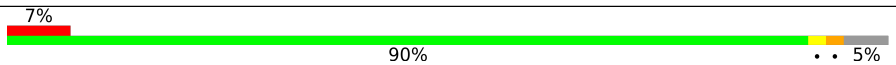
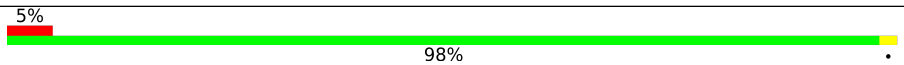
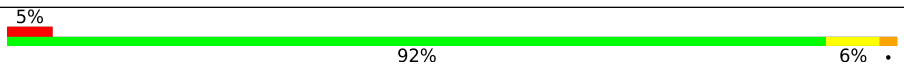
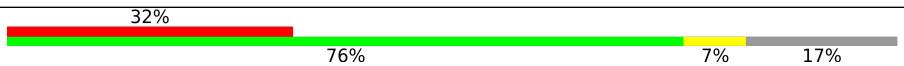
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Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	

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Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
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
24	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	413	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 55630 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2607	1712	427	455	13			
1	a	336	Total	C	N	O	S	0	3	0
			2632	1727	431	461	13			

- 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	8	0
			3995	2623	665	694	13			
2	b	504	Total	C	N	O	S	0	9	0
			3961	2600	656	692	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	6	0
			3507	2295	586	613	13			
3	c	456	Total	C	N	O	S	0	3	0
			3532	2314	589	616	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2713	1799	439	463	12			
4	d	342	Total	C	N	O	S	0	2	0
			2724	1806	442	463	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total 629	C 413	N 102	O 114	0	1	0
5	e	79	Total 644	C 423	N 102	O 119	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	32	Total 263	C 179	N 44	O 39	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 505	C 336	N 81	O 86	S 2	0	0	0
7	h	65	Total 516	C 343	N 85	O 86	S 2	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total 301	C 205	N 47	O 48	S 1	0	0	0
8	i	37	Total 297	C 203	N 47	O 46	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	39	Total 270	C 182	N 40	O 46	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 289	C 201	N 42	O 46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total 289	C 201	N 42	O 46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 311	C 209	N 49	O 52	S 1	0	2	0
11	l	37	Total 305	C 205	N 48	O 51	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 270	C 182	N 39	O 48	S 1	0	1	0
12	m	34	Total 274	C 184	N 40	O 49	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1895	C 1190	N 313	O 388	S 4	0	10	0
13	o	243	Total 1879	C 1177	N 311	O 387	S 4	0	5	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total 767	C 487	N 129	O 151	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

- 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	4	0
			1089	691	181	213	4			
16	v	137	Total	C	N	O	S	0	2	0
			1070	678	178	210	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
			218	144	35	36	3			
17	y	30	Total	C	N	O	S	0	1	0
			229	152	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			286	191	46	49			
18	x	39	Total	C	N	O	0	0	0
			286	191	46	49			

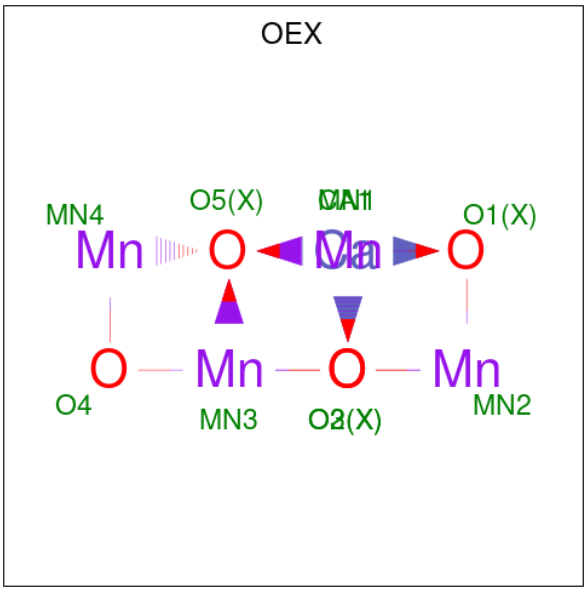
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			458	317	67	72	2			
19	z	62	Total	C	N	O	S	0	0	0
			455	312	67	74	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
			228	150	41	37			

- 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 10 1 4 5	0	0
21	a	1	Total Ca Mn O 10 1 4 5	0	0

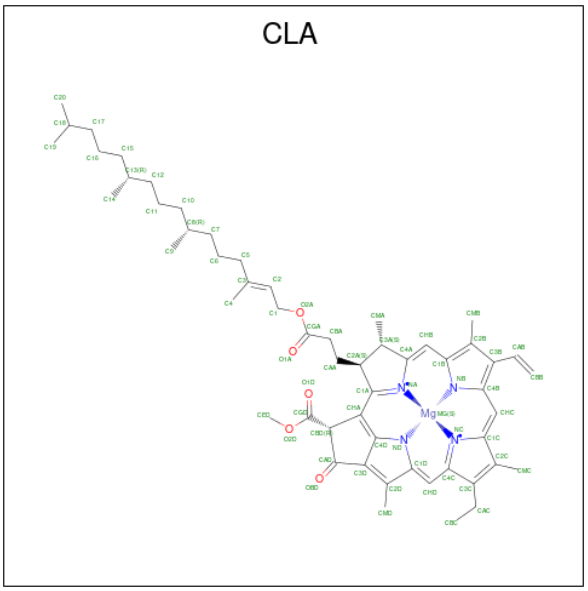
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

- 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	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		

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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	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	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		

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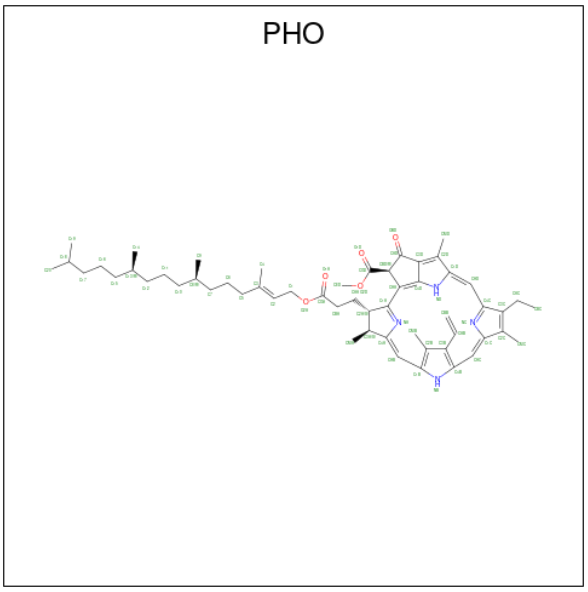
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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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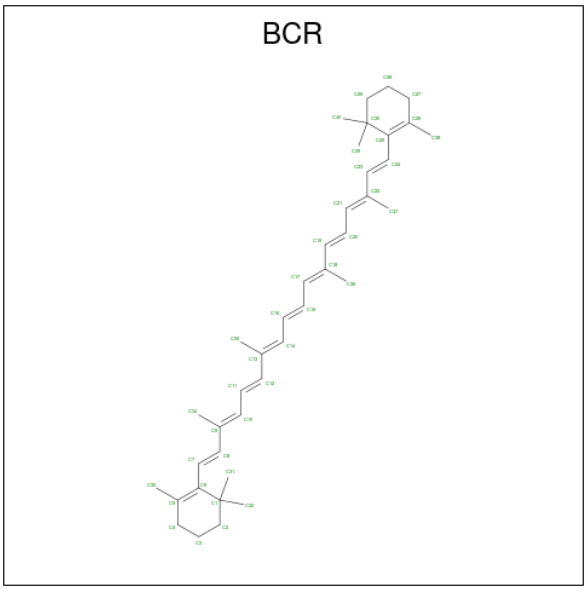
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



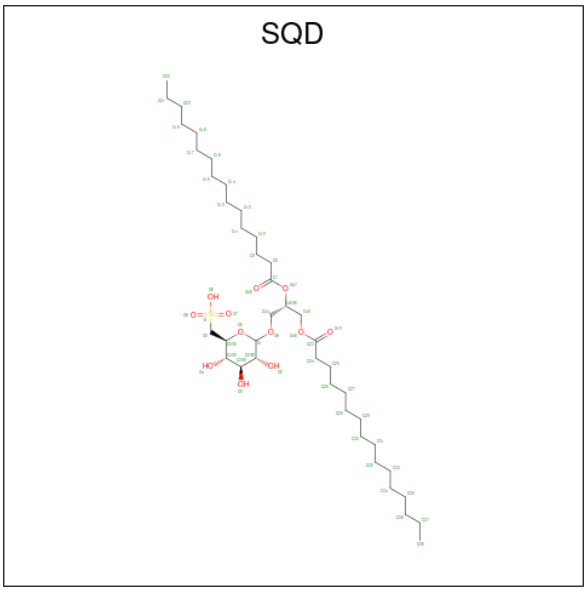
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



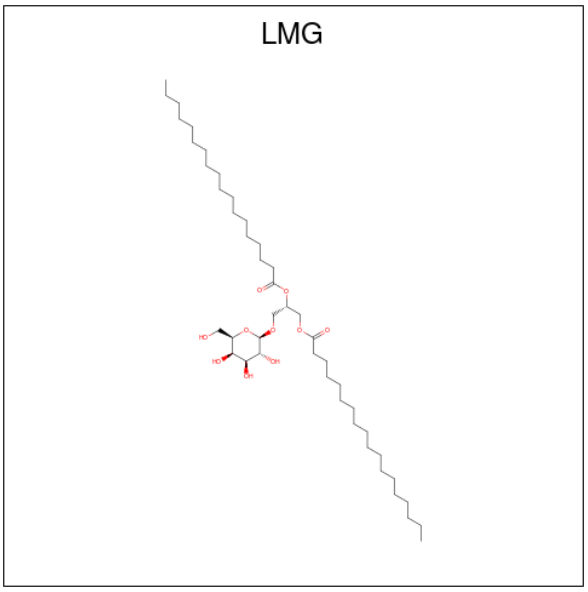
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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	d	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	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: $C_{41}H_{78}O_{12}S$).



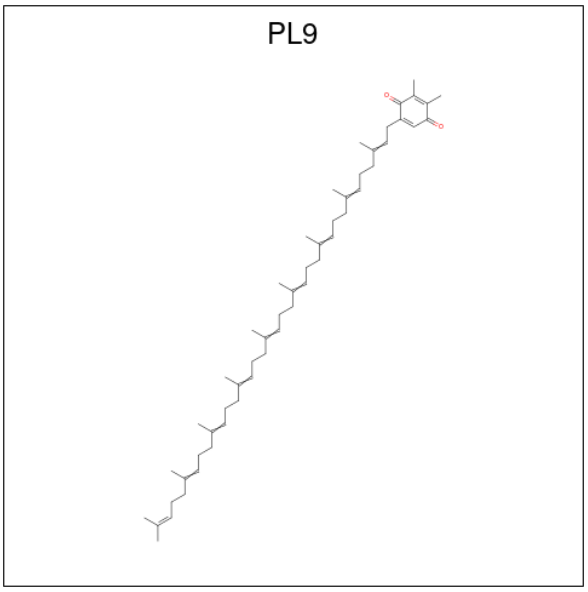
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			37	25	11	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		
27	l	1	Total	C	O	S	0	0
			54	41	12	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 51 41 10	0	0
28	D	1	Total C O 51 41 10	0	0
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 51 41 10	0	0
28	d	1	Total C O 51 41 10	0	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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

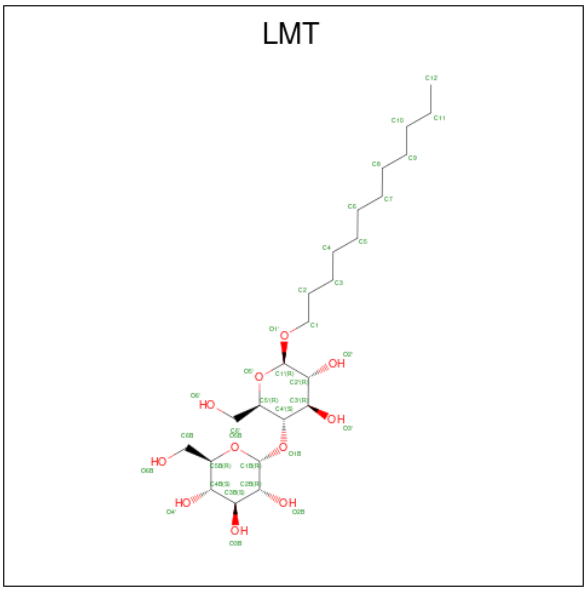
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	4	Total C O 57 52 5	0	0
30	B	4	Total C 24 24	0	0
30	C	3	Total C O 54 49 5	0	0
30	D	3	Total C O 60 55 5	0	0
30	E	4	Total C 22 22	0	0
30	H	2	Total C O 24 22 2	0	0
30	I	7	Total C 79 79	0	0
30	J	3	Total C 36 36	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	T	1	Total C 15 15	0	0
30	X	1	Total C 16 16	0	0
30	Z	3	Total C 20 20	0	0
30	a	2	Total C O 45 40 5	0	0
30	b	8	Total C O 87 85 2	0	0
30	c	6	Total C O 47 45 2	0	0
30	d	3	Total C O 65 58 7	0	0
30	e	2	Total C 15 15	0	0
30	h	3	Total C 29 29	0	0
30	i	5	Total C O 66 64 2	0	0
30	j	3	Total C 15 15	0	0
30	k	2	Total C O 39 34 5	0	0
30	l	1	Total C 13 13	0	0
30	m	1	Total C 11 11	0	0
30	t	1	Total C 12 12	0	0
30	y	1	Total C 4 4	0	0
30	x	4	Total C O 39 37 2	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



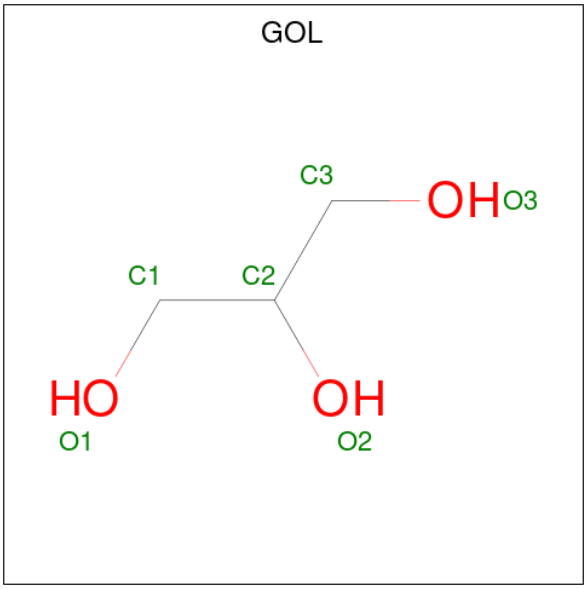
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0
31	A	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 24 18 6	0	0
31	F	1	Total C O 24 18 6	0	0
31	J	1	Total C O 24 18 6	0	0
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 25 19 6	0	0
31	Z	1	Total C O 35 24 11	0	0
31	a	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	c	1	Total C O 35 24 11	0	0
31	c	1	Total C O 35 24 11	0	0
31	e	1	Total C O 24 18 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	j	1	Total C O 24 18 6	0	0
31	m	1	Total C O 35 24 11	0	0
31	m	1	Total C O 35 24 11	0	0
31	t	1	Total C O 23 18 5	0	0
31	t	1	Total C O 35 24 11	0	0

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



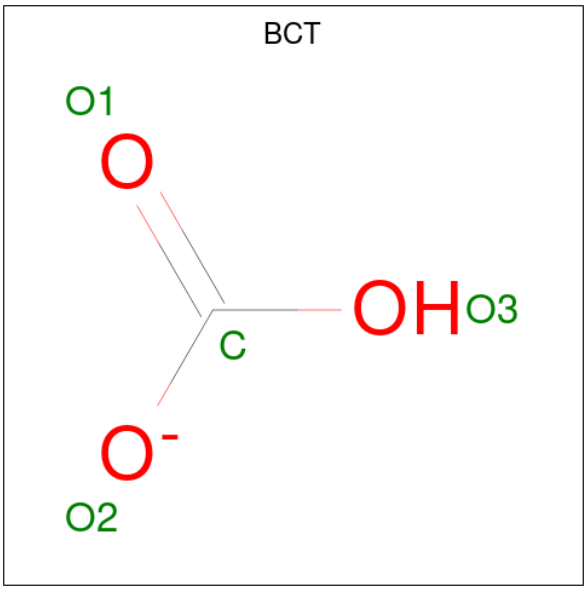
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 6 3 3	0	0
32	B	1	Total C O 6 3 3	0	0
32	B	1	Total C O 6 3 3	0	0
32	C	1	Total C O 6 3 3	0	0
32	O	1	Total C O 6 3 3	0	0
32	V	1	Total C O 6 3 3	0	0

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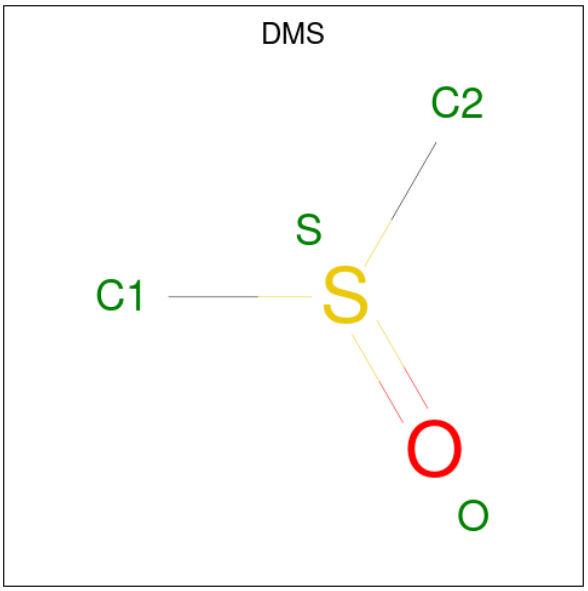
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	V	1	Total C O 6 3 3	0	0
32	a	1	Total C O 6 3 3	0	0
32	b	1	Total C O 6 3 3	0	0
32	c	1	Total C O 6 3 3	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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	1
33	d	1	Total C O 4 1 3	0	1

- 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	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		
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		

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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	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		
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	H	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	L	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	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	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	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	i	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	o	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	y	1	Total	C	O	S	0	0
			4	2	1	1		

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

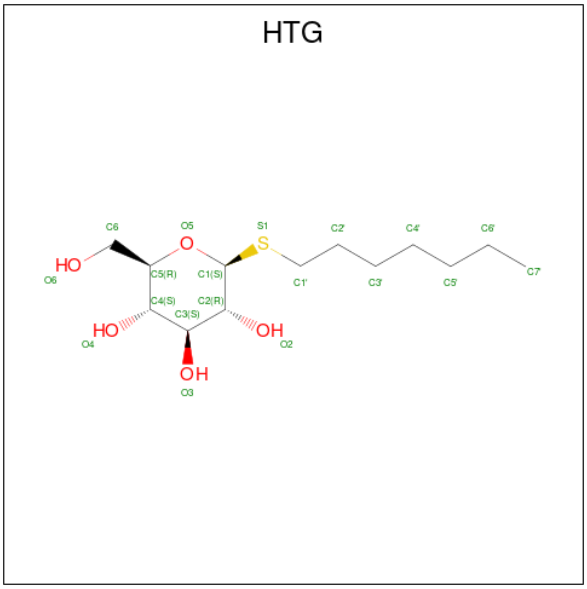
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	O	1	Total Ca 1 1	0	0
35	V	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
35	v	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 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	B	1	Total C O S 19 13 5 1	0	0

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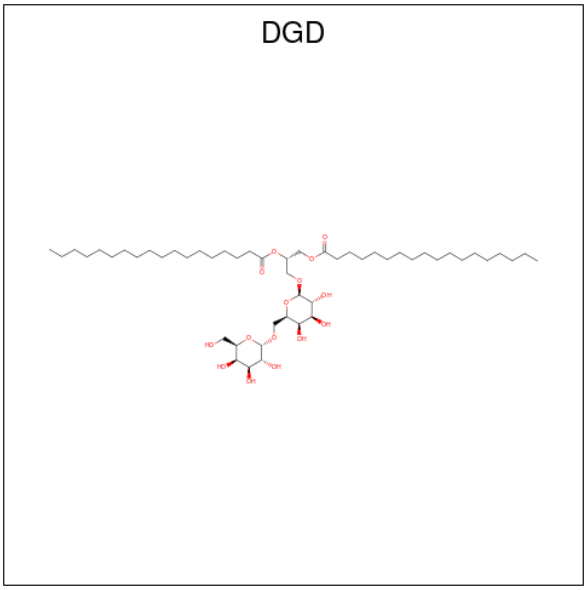
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	U	1	Total	C			0	0
			4	4				
36	V	1	Total	C	O	S	0	0
			13	7	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	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
			17	11	5	1		

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

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



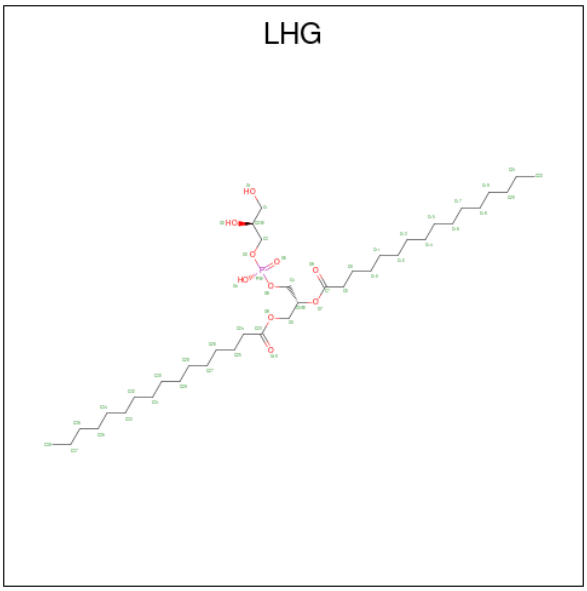
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total C O 62 47 15	0	0
37	C	1	Total C O 62 47 15	0	0
37	C	1	Total C O 62 47 15	0	0
37	D	1	Total C O 52 42 10	0	0
37	H	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	c	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	d	1	Total C O 50 41 9	0	0
37	h	1	Total C O 62 47 15	0	0

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



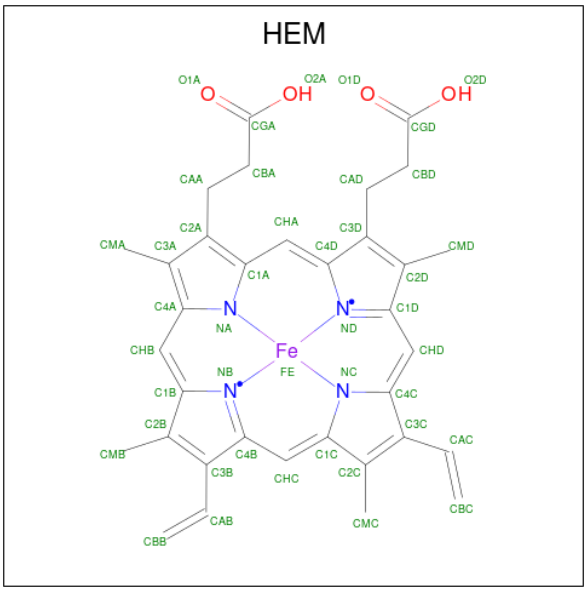
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 46 35 10 1	0	0
38	E	1	Total C O P 42 31 10 1	0	0
38	L	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0

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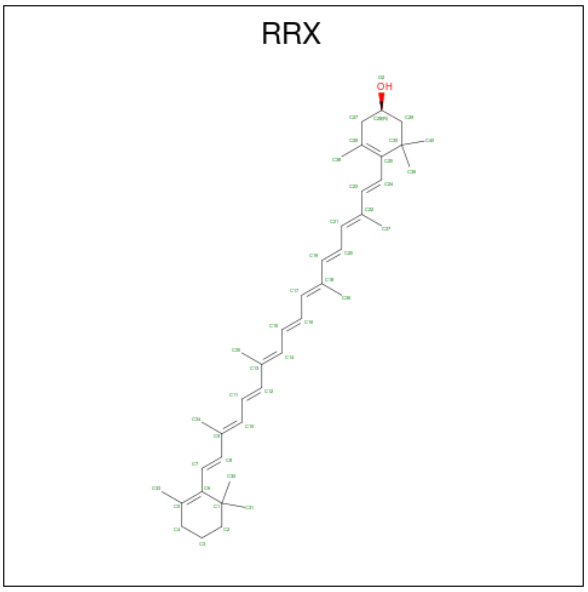
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	d	1	Total	C	O	P	0	0
			47	36	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



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

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

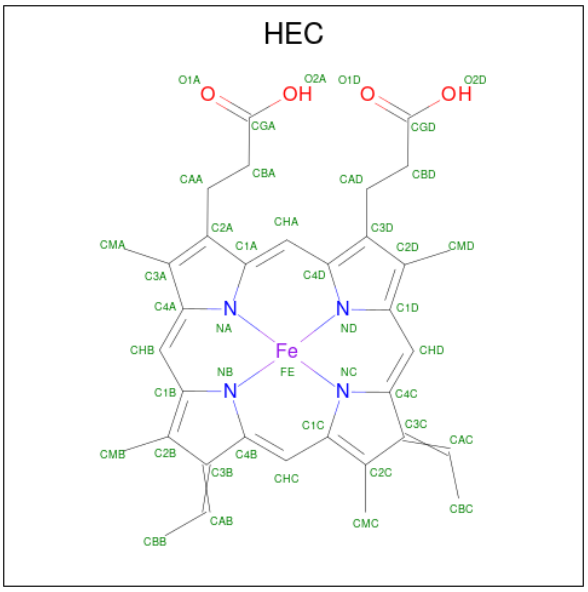


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	H	1	Total C O 41 40 1	0	0
40	h	1	Total C O 41 40 1	0	0

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 42 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	158	Total	O	0	1
			159	159		
43	B	406	Total	O	0	6
			411	411		
43	C	293	Total	O	0	2
			295	295		
43	D	173	Total	O	0	4
			177	177		
43	E	35	Total	O	0	0
			35	35		
43	F	15	Total	O	0	0
			15	15		
43	H	51	Total	O	0	0
			51	51		
43	I	11	Total	O	0	0
			11	11		
43	J	15	Total	O	0	0
			15	15		
43	K	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	16	Total O 16 16	0	0
43	M	20	Total O 20 20	0	0
43	O	217	Total O 224 224	0	7
43	T	14	Total O 14 14	0	0
43	U	116	Total O 117 117	0	1
43	V	153	Total O 157 157	0	4
43	Y	6	Total O 6 6	0	0
43	X	22	Total O 22 22	0	0
43	Z	4	Total O 4 4	0	0
43	a	157	Total O 159 159	0	2
43	b	394	Total O 399 399	0	5
43	c	316	Total O 320 320	0	5
43	d	170	Total O 172 172	0	2
43	e	38	Total O 39 39	0	1
43	f	12	Total O 12 12	0	0
43	h	51	Total O 52 52	0	1
43	i	12	Total O 12 12	0	0
43	j	12	Total O 12 12	0	0
43	k	6	Total O 6 6	0	0
43	l	20	Total O 20 20	0	0
43	m	20	Total O 20 20	0	0

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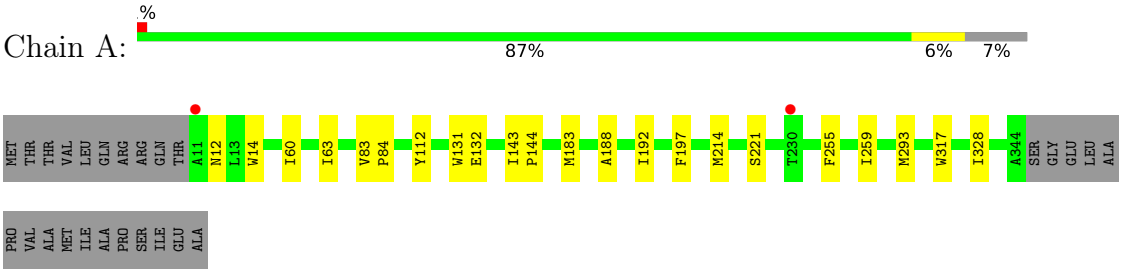
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	o	194	Total O 198 198	0	4
43	t	23	Total O 24 24	0	1
43	u	117	Total O 119 119	0	2
43	v	116	Total O 118 118	0	2
43	y	8	Total O 8 8	0	0
43	x	14	Total O 14 14	0	0
43	z	6	Total O 6 6	0	0

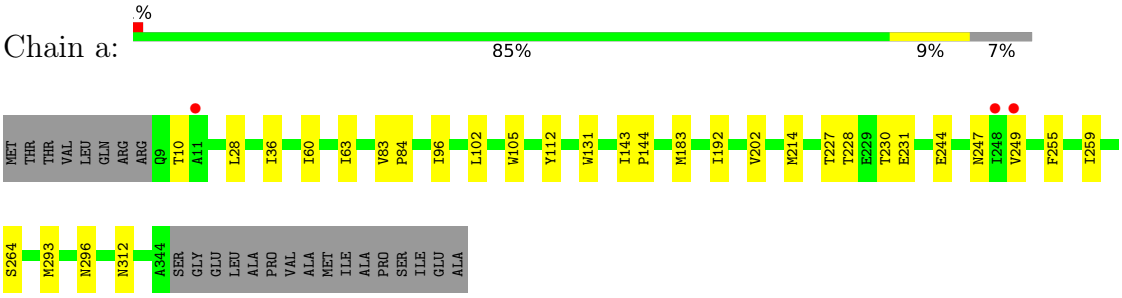
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

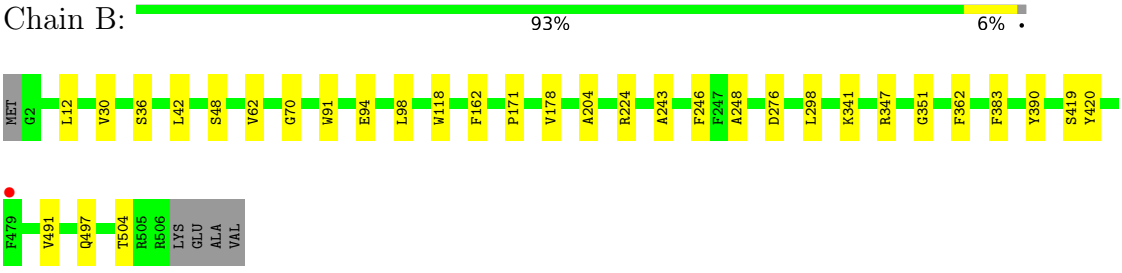
• Molecule 1: Photosystem II protein D1 2



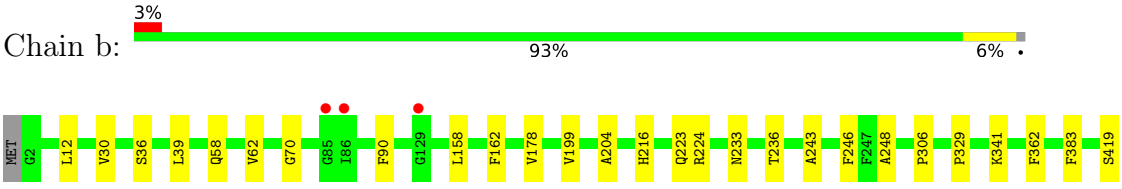
• Molecule 1: Photosystem II protein D1 2

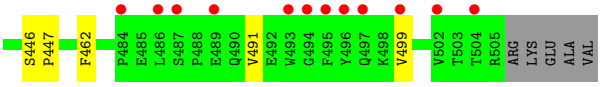


• Molecule 2: Photosystem II CP47 reaction center protein



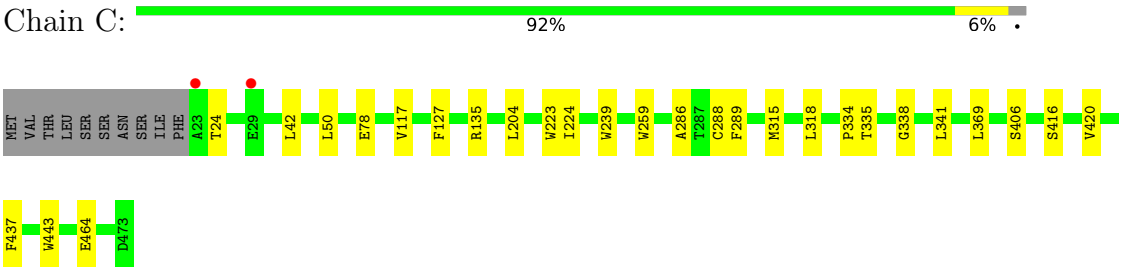
• Molecule 2: Photosystem II CP47 reaction center protein





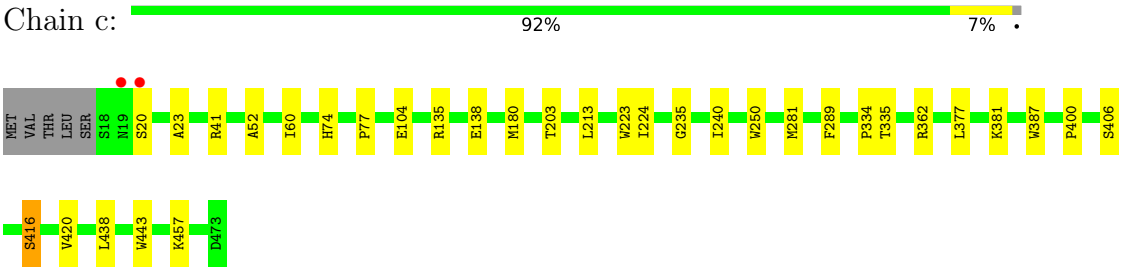
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



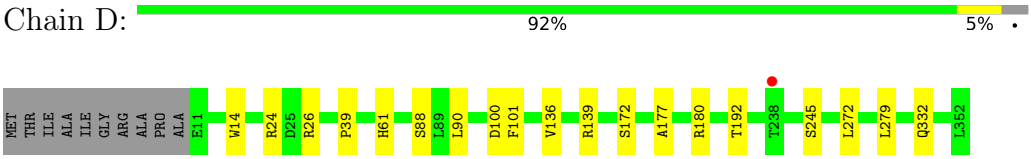
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



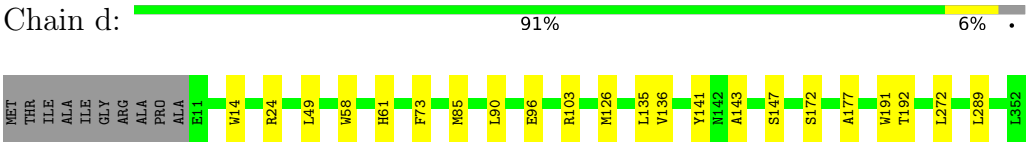
• Molecule 4: Photosystem II D2 protein

Chain D:



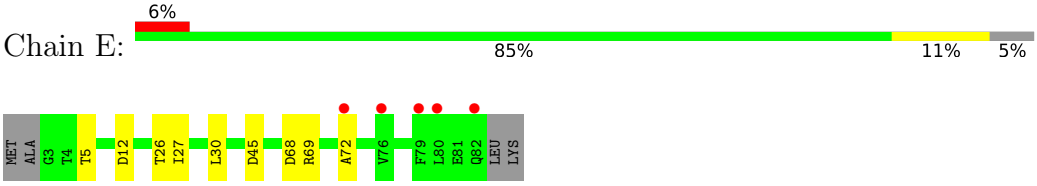
• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

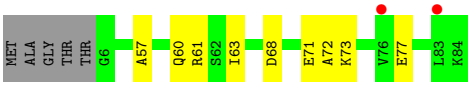
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

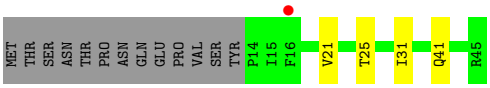




• Molecule 6: Cytochrome b559 subunit beta

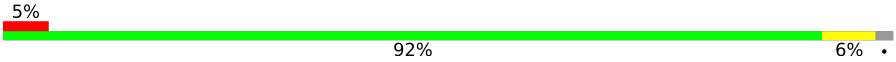
Chain f:





• Molecule 7: Photosystem II reaction center protein H

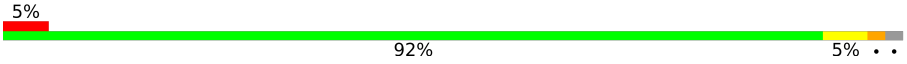
Chain H:

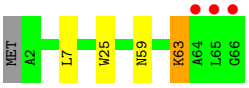




• Molecule 7: Photosystem II reaction center protein H

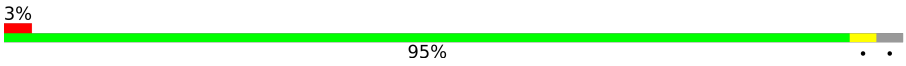
Chain h:





• Molecule 8: Photosystem II reaction center protein I

Chain I:

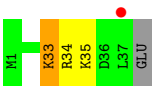




• Molecule 8: Photosystem II reaction center protein I

Chain i:

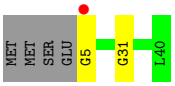




• Molecule 9: Photosystem II reaction center protein J

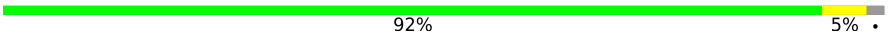
Chain J:

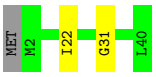




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

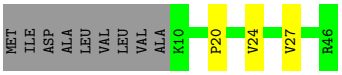




• Molecule 10: Photosystem II reaction center protein K

Chain k:

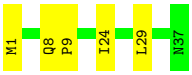




• Molecule 11: Photosystem II reaction center protein L

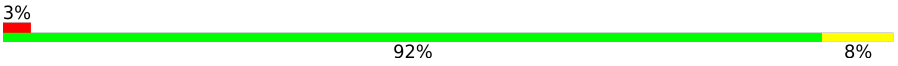
Chain L:

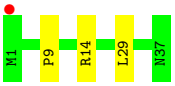




• Molecule 11: Photosystem II reaction center protein L

Chain l:

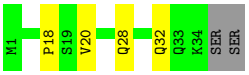




• Molecule 12: Photosystem II reaction center protein M

Chain M:

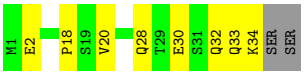




• Molecule 12: Photosystem II reaction center protein M

Chain m:

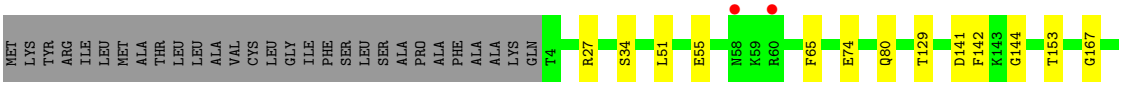




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



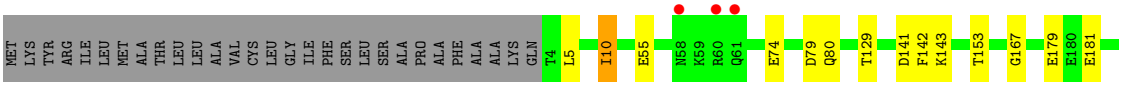


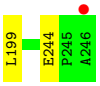


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

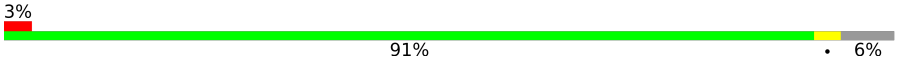


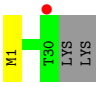




• Molecule 14: Photosystem II reaction center protein T

Chain T:

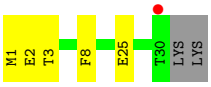




• Molecule 14: Photosystem II reaction center protein T

Chain t:

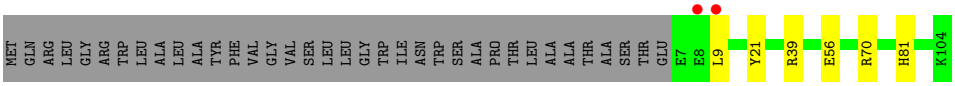




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

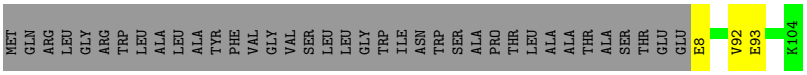




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:





• Molecule 16: Cytochrome c-550

Chain V:

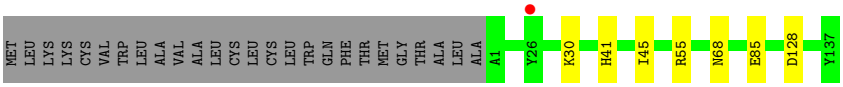




• Molecule 16: Cytochrome c-550

Chain v:

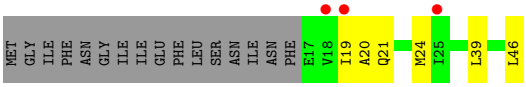




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

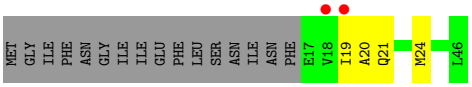




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

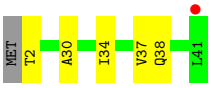




• Molecule 18: Photosystem II reaction center X protein

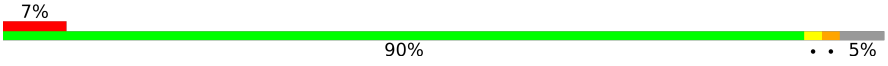
Chain X:





• Molecule 18: Photosystem II reaction center X protein

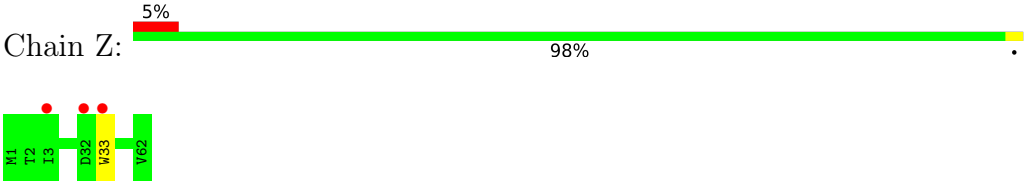
Chain x:





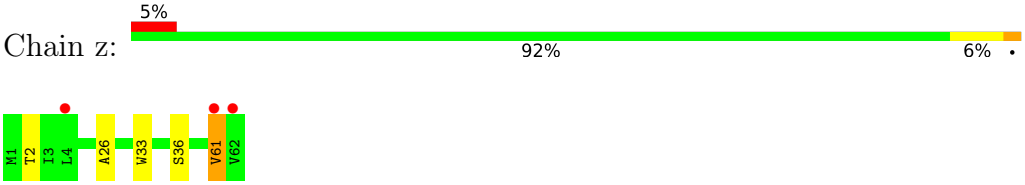
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



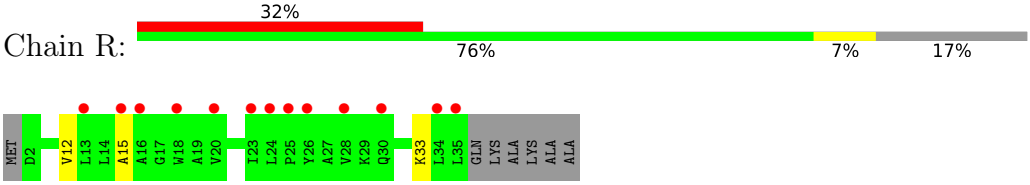
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• 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	122.14Å 228.17Å 286.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.6 (20.00-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0103	Depositor
R, R_{free}	0.151 , 0.184 0.151 , 0.185	Depositor DCC
R_{free} test set	31121 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	55630	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.38	0/2693	0.53	0/3680
1	a	0.37	0/2723	0.52	0/3719
2	B	0.34	0/4156	0.51	2/5665 (0.0%)
2	b	0.32	0/4122	0.48	0/5623
3	C	0.30	0/3638	0.46	0/4954
3	c	0.29	0/3655	0.46	0/4976
4	D	0.38	0/2811	0.51	0/3833
4	d	0.36	0/2825	0.49	0/3850
5	E	0.26	0/651	0.43	0/892
5	e	0.22	0/669	0.41	0/913
6	F	0.25	0/284	0.43	0/387
6	f	0.27	0/274	0.47	0/372
7	H	0.26	0/518	0.44	0/706
7	h	0.24	0/532	0.42	0/723
8	I	0.21	0/298	0.39	0/403
8	i	0.24	0/294	0.41	0/398
9	J	0.24	0/257	0.43	0/349
9	j	0.24	0/276	0.42	0/374
10	K	0.24	0/299	0.42	0/412
10	k	0.23	0/299	0.39	0/412
11	L	0.40	0/324	0.48	0/441
11	l	0.37	0/315	0.47	0/428
12	M	0.34	0/266	0.49	0/363
12	m	0.31	0/270	0.47	0/368
13	O	0.30	0/1956	0.50	0/2653
13	o	0.29	0/1925	0.50	0/2611
14	T	0.37	0/266	0.42	0/362
14	t	0.35	0/266	0.43	0/362
15	U	0.31	0/778	0.49	0/1057
15	u	0.32	0/785	0.47	0/1064
16	V	0.32	0/1122	0.46	0/1522

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.24	0/1097	0.42	0/1491
17	Y	0.20	0/219	0.34	0/294
17	y	0.19	0/233	0.36	0/312
18	X	0.19	0/289	0.31	0/391
18	x	0.18	0/289	0.33	0/391
19	Z	0.19	0/459	0.33	0/630
19	z	0.16	0/456	0.28	0/626
20	R	0.18	0/232	0.37	0/321
All	All	0.32	0/42821	0.48	2/58328 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	48	SER	CA-C-N	-7.62	115.57	122.28
2	B	48	SER	C-N-CA	-7.62	115.57	122.28

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	2607	0	2508	15	0
1	a	2632	0	2551	21	0
2	B	3995	0	3853	28	0
2	b	3961	0	3794	25	0
3	C	3507	0	3436	23	0
3	c	3532	0	3456	30	0
4	D	2713	0	2606	16	0
4	d	2724	0	2626	19	0
5	E	629	0	601	8	0
5	e	644	0	619	8	0
6	F	275	0	282	1	0
6	f	263	0	277	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	505	0	514	6	0
7	h	516	0	536	4	0
8	I	301	0	320	0	0
8	i	297	0	316	2	0
9	J	251	0	257	2	0
9	j	270	0	273	2	0
10	K	289	0	294	1	0
10	k	289	0	294	2	0
11	L	311	0	331	5	0
11	l	305	0	323	4	0
12	M	270	0	293	5	0
12	m	274	0	299	7	0
13	O	1895	0	1877	16	0
13	o	1879	0	1848	11	0
14	T	264	0	267	0	0
14	t	264	0	267	4	0
15	U	767	0	756	6	0
15	u	774	0	773	2	0
16	V	1089	0	1104	9	0
16	v	1070	0	1070	5	0
17	Y	218	0	241	4	0
17	y	229	0	263	2	0
18	X	286	0	309	4	0
18	x	286	0	314	2	0
19	Z	458	0	479	1	0
19	z	455	0	463	3	0
20	R	228	0	201	3	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	260	0	288	11	0
24	B	1040	0	1152	35	0
24	C	845	0	936	36	0
24	D	130	0	144	1	0
24	a	195	0	216	10	0
24	b	1040	0	1152	33	0
24	c	845	0	936	22	0
24	d	195	0	216	4	0
25	A	128	0	148	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	a	128	0	148	2	0
26	A	40	0	56	0	0
26	B	160	0	224	10	0
26	C	80	0	112	4	0
26	D	40	0	56	0	0
26	K	40	0	56	1	0
26	T	40	0	56	4	0
26	Y	40	0	56	2	0
26	a	40	0	56	2	0
26	b	120	0	168	7	0
26	c	80	0	112	4	0
26	d	40	0	56	2	0
26	k	80	0	112	2	0
27	A	108	0	156	2	0
27	F	37	0	46	2	0
27	a	108	0	156	9	0
27	b	54	0	78	1	0
27	f	43	0	53	0	0
27	l	54	0	78	1	0
28	A	51	0	72	3	0
28	B	51	0	72	1	0
28	C	102	0	144	6	0
28	D	51	0	72	1	0
28	a	51	0	72	1	0
28	b	51	0	72	1	0
28	c	102	0	144	3	0
28	d	51	0	72	3	0
29	A	55	0	80	4	0
29	D	55	0	80	1	0
29	a	55	0	80	3	0
29	d	55	0	80	3	0
30	A	57	0	0	0	0
30	B	24	0	0	0	0
30	C	54	0	0	0	0
30	D	60	0	0	0	0
30	E	22	0	0	0	0
30	H	24	0	0	0	0
30	I	79	0	0	0	0
30	J	36	0	0	0	0
30	T	15	0	0	0	0
30	X	16	0	0	0	0
30	Z	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	45	0	0	0	0
30	b	87	0	0	0	0
30	c	47	0	0	0	0
30	d	65	0	0	1	0
30	e	15	0	0	0	0
30	h	29	0	0	0	0
30	i	66	0	0	0	0
30	j	15	0	0	0	0
30	k	39	0	0	0	0
30	l	13	0	0	0	0
30	m	11	0	0	0	0
30	t	12	0	0	0	0
30	x	39	0	0	0	0
30	y	4	0	0	0	0
31	A	70	0	92	7	0
31	B	59	0	81	2	0
31	F	24	0	35	0	0
31	J	24	0	35	0	0
31	M	60	0	81	3	0
31	Z	35	0	46	1	0
31	a	35	0	46	2	0
31	b	35	0	46	2	0
31	c	70	0	92	1	0
31	e	24	0	35	0	0
31	j	24	0	35	2	0
31	m	70	0	92	2	0
31	t	58	0	80	0	0
32	A	6	0	8	0	0
32	B	12	0	16	4	0
32	C	6	0	8	0	0
32	O	6	0	8	0	0
32	V	12	0	16	2	0
32	a	6	0	8	0	0
32	b	6	0	8	0	0
32	c	6	0	8	2	0
33	A	4	0	0	0	0
33	a	4	0	0	0	0
33	d	4	0	0	0	0
34	A	20	0	30	1	0
34	B	48	0	72	4	0
34	C	44	0	66	1	0
34	D	16	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	4	0	6	0	0
34	K	4	0	6	0	0
34	L	4	0	6	1	0
34	O	48	0	72	5	0
34	T	4	0	6	0	0
34	U	12	0	18	3	0
34	V	36	0	54	1	0
34	a	24	0	36	1	0
34	b	48	0	72	2	0
34	c	48	0	72	8	0
34	d	16	0	24	1	0
34	e	12	0	18	0	0
34	h	4	0	6	2	0
34	i	4	0	6	0	0
34	o	24	0	36	2	0
34	u	8	0	12	0	0
34	v	32	0	48	0	0
34	y	4	0	6	2	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	V	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
35	v	1	0	0	0	0
36	B	114	0	156	7	0
36	C	76	0	104	4	0
36	D	19	0	26	2	0
36	O	38	0	52	1	0
36	U	4	0	4	1	0
36	V	32	0	37	1	0
36	b	76	0	104	4	0
36	c	112	0	149	4	0
36	d	57	0	78	5	0
36	v	19	0	26	2	0
36	y	19	0	26	0	0
37	C	186	0	246	4	0
37	D	52	0	71	7	0
37	H	62	0	82	1	0
37	c	186	0	246	3	0
37	d	50	0	69	4	0
37	h	62	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	D	144	0	213	9	0
38	E	42	0	57	1	0
38	L	49	0	74	3	0
38	d	145	0	215	10	0
38	l	49	0	74	2	0
39	F	43	0	30	2	0
39	f	43	0	30	3	0
40	H	41	0	56	3	0
40	h	41	0	56	2	0
41	J	1	0	0	0	0
41	j	1	0	0	0	0
42	V	43	0	30	0	0
42	v	43	0	30	0	0
43	A	159	0	0	1	0
43	B	411	0	0	1	0
43	C	295	0	0	0	0
43	D	177	0	0	1	0
43	E	35	0	0	0	0
43	F	15	0	0	0	0
43	H	51	0	0	1	0
43	I	11	0	0	0	0
43	J	15	0	0	0	0
43	K	9	0	0	0	0
43	L	16	0	0	0	0
43	M	20	0	0	0	0
43	O	224	0	0	3	0
43	T	14	0	0	0	0
43	U	117	0	0	2	0
43	V	157	0	0	4	0
43	X	22	0	0	0	0
43	Y	6	0	0	0	0
43	Z	4	0	0	0	0
43	a	159	0	0	1	0
43	b	399	0	0	0	0
43	c	320	0	0	2	0
43	d	172	0	0	1	0
43	e	39	0	0	0	0
43	f	12	0	0	0	0
43	h	52	0	0	2	0
43	i	12	0	0	0	0
43	j	12	0	0	0	0
43	k	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	l	20	0	0	0	0
43	m	20	0	0	0	0
43	o	198	0	0	3	0
43	t	24	0	0	0	0
43	u	119	0	0	0	0
43	v	118	0	0	3	0
43	x	14	0	0	0	0
43	y	8	0	0	1	0
43	z	6	0	0	0	0
All	All	55630	0	52949	469	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 469 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)
24:a:413:CLA:H152	24:c:907:CLA:H142	1.62	0.80
4:D:101:PHE:H	37:D:405:DGD:HB31	1.48	0.78
2:B:347[B]:ARG:NH1	32:B:637:GOL:O2	2.19	0.76
37:D:405:DGD:HD5	5:E:45:ASP:HB3	1.70	0.72
38:D:408:LHG:H141	38:D:408:LHG:H342	1.72	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/360 (93%)	329 (98%)	4 (1%)	1 (0%)	36	29
1	a	337/360 (94%)	332 (98%)	4 (1%)	1 (0%)	36	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	511/510 (100%)	503 (98%)	8 (2%)	0	100	100
2	b	511/510 (100%)	503 (98%)	8 (2%)	0	100	100
3	C	455/461 (99%)	445 (98%)	8 (2%)	2 (0%)	30	22
3	c	457/461 (99%)	446 (98%)	10 (2%)	1 (0%)	43	36
4	D	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
4	d	342/352 (97%)	335 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	79 (100%)	0	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	251/272 (92%)	246 (98%)	5 (2%)	0	100	100
13	o	246/272 (90%)	241 (98%)	5 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	96/134 (72%)	93 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	139/163 (85%)	136 (98%)	3 (2%)	0	100	100
16	v	137/163 (84%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/46 (61%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	y	29/46 (63%)	29 (100%)	0	0	100	100
18	X	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5292/5691 (93%)	5194 (98%)	93 (2%)	5 (0%)	48	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
1	A	259	ILE
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	266/290 (92%)	266 (100%)	0	100	100
1	a	271/290 (93%)	269 (99%)	2 (1%)	76	78
2	B	405/407 (100%)	404 (100%)	1 (0%)	87	90
2	b	397/407 (98%)	395 (100%)	2 (0%)	81	84
3	C	357/362 (99%)	355 (99%)	2 (1%)	78	81
3	c	358/362 (99%)	356 (99%)	2 (1%)	78	81
4	D	275/283 (97%)	273 (99%)	2 (1%)	76	78
4	d	277/283 (98%)	275 (99%)	2 (1%)	76	78
5	E	65/73 (89%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	68/73 (93%)	68 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	52/55 (94%)	52 (100%)	0	100	100
7	h	54/55 (98%)	53 (98%)	1 (2%)	50	47
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	29
8	i	31/34 (91%)	30 (97%)	1 (3%)	34	27
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	31/32 (97%)	30 (97%)	1 (3%)	34	27
13	O	211/228 (92%)	211 (100%)	0	100	100
13	o	208/228 (91%)	203 (98%)	5 (2%)	43	38
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	81/112 (72%)	81 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	63
16	V	121/138 (88%)	119 (98%)	2 (2%)	53	52
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	22/37 (60%)	21 (96%)	1 (4%)	24	17
17	y	24/37 (65%)	23 (96%)	1 (4%)	26	19
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	27
19	Z	45/51 (88%)	45 (100%)	0	100	100
19	z	44/51 (86%)	43 (98%)	1 (2%)	44	40
20	R	16/33 (48%)	16 (100%)	0	100	100
All	All	4289/4639 (92%)	4260 (99%)	29 (1%)	78	78

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	416	SER
18	x	37	VAL
7	h	63	LYS
13	o	181	GLU
4	d	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	415	ASN
13	o	155	ASN
16	v	86	GLN
15	u	78	ASN
4	d	301	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.95	0	8,9,11	0.86	0
19	FME	z	1	19	8,9,10	0.93	0	8,9,11	1.04	0
8	FME	I	1	8	8,9,10	0.95	0	8,9,11	0.90	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.78	0
14	FME	t	1	14	8,9,10	1.01	0	8,9,11	1.36	1 (12%)
19	FME	Z	1	19	8,9,10	0.95	0	8,9,11	1.02	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	FME	T	1	14	8,9,10	1.02	0	8,9,11	1.28	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
19	FME	z	1	19	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
19	FME	Z	1	19	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	C-CA-N	2.54	114.41	109.50
14	t	1	FME	C-CA-N	2.10	113.55	109.50

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	t	1	FME	O-C-CA-CB
19	Z	1	FME	CA-CB-CG-SD
19	z	1	FME	CA-CB-CG-SD

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 414 ligands modelled in this entry, 15 are monoatomic and 77 are unknown - leaving 322 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	$\#\|Z\| > 2$
27	SQD	a	401	-	52,54,54	0.98	2 (3%)	62,65,65	1.08	3 (4%)
34	DMS	T	103	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
32	GOL	V	207	-	5,5,5	1.05	0	5,5,5	0.93	0
28	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.13	4 (6%)
36	HTG	O	316	-	19,19,19	0.82	1 (5%)	23,24,24	1.21	2 (8%)
24	CLA	C	504	43	69,73,73	2.29	22 (31%)	82,113,113	2.44	29 (35%)
34	DMS	u	201	-	3,3,3	2.73	1 (33%)	3,3,3	0.84	0
26	BCR	K	101	-	41,41,41	0.76	0	56,56,56	1.35	7 (12%)
26	BCR	b	623	-	41,41,41	0.78	1 (2%)	56,56,56	1.48	12 (21%)
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.08	3 (6%)
31	LMT	c	927	-	36,36,36	0.43	0	47,47,47	0.91	3 (6%)
25	PHO	A	408	-	58,69,69	2.57	12 (20%)	55,99,99	3.00	16 (29%)
34	DMS	c	940	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
34	DMS	C	527	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
24	CLA	c	914	-	69,73,73	2.48	23 (33%)	82,113,113	2.29	26 (31%)
34	DMS	o	305	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
24	CLA	D	402	-	69,73,73	2.31	22 (31%)	82,113,113	2.41	28 (34%)
34	DMS	C	530	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
24	CLA	B	602	43	69,73,73	2.34	26 (37%)	82,113,113	2.36	29 (35%)
24	CLA	c	910	-	69,73,73	2.40	23 (33%)	82,113,113	2.41	32 (39%)
36	HTG	V	204	-	12,13,19	0.60	0	17,18,24	2.08	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	V	212	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
34	DMS	a	423	-	3,3,3	2.75	1 (33%)	3,3,3	0.68	0
34	DMS	c	932	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	C	509	-	69,73,73	2.43	24 (34%)	82,113,113	2.43	29 (35%)
34	DMS	c	938	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
34	DMS	B	633	-	3,3,3	2.66	1 (33%)	3,3,3	0.38	0
37	DGD	c	917	-	63,63,67	0.85	2 (3%)	77,77,81	1.13	6 (7%)
36	HTG	C	536	-	19,19,19	0.99	2 (10%)	23,24,24	1.14	1 (4%)
32	GOL	A	419	-	5,5,5	1.01	0	5,5,5	1.08	1 (20%)
24	CLA	d	401	43	69,73,73	2.34	21 (30%)	82,113,113	2.56	33 (40%)
34	DMS	c	936	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	B	608	43	69,73,73	2.24	22 (31%)	82,113,113	2.40	28 (34%)
37	DGD	d	408	-	50,50,67	0.96	2 (4%)	58,58,81	1.39	8 (13%)
24	CLA	A	405	-	69,73,73	2.50	22 (31%)	82,113,113	2.38	29 (35%)
24	CLA	b	618	-	69,73,73	2.36	23 (33%)	82,113,113	2.55	29 (35%)
28	LMG	D	409	41	51,51,55	0.83	2 (3%)	59,59,63	0.90	3 (5%)
31	LMT	M	102	-	25,25,36	0.48	0	30,30,47	0.93	1 (3%)
34	DMS	b	632	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
34	DMS	V	201	-	3,3,3	2.70	1 (33%)	3,3,3	0.47	0
36	HTG	b	626	-	19,19,19	0.79	1 (5%)	23,24,24	1.22	3 (13%)
24	CLA	a	410	43	69,73,73	2.28	24 (34%)	82,113,113	2.56	29 (35%)
31	LMT	t	102	-	36,36,36	0.43	0	47,47,47	0.87	1 (2%)
34	DMS	B	641	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
26	BCR	C	515	-	41,41,41	0.73	0	56,56,56	1.47	7 (12%)
34	DMS	a	425	-	3,3,3	2.75	1 (33%)	3,3,3	0.54	0
36	HTG	c	928	-	19,19,19	0.98	2 (10%)	23,24,24	1.38	3 (13%)
34	DMS	O	307	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
34	DMS	e	102	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
36	HTG	v	211	-	19,19,19	0.96	2 (10%)	23,24,24	1.55	4 (17%)
29	PL9	d	407	-	55,55,55	0.77	1 (1%)	68,69,69	1.49	12 (17%)
24	CLA	B	617	-	69,73,73	2.34	22 (31%)	82,113,113	2.51	32 (39%)
34	DMS	o	307	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
36	HTG	U	201	-	3,3,19	0.32	0	2,2,24	0.73	0
34	DMS	c	939	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
24	CLA	C	508	-	69,73,73	2.56	23 (33%)	82,113,113	2.37	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HTG	b	603	-	19,19,19	0.94	2 (10%)	23,24,24	1.27	3 (13%)
26	BCR	d	406	-	41,41,41	0.85	0	56,56,56	1.73	11 (19%)
32	GOL	V	206	-	5,5,5	0.88	0	5,5,5	1.04	0
24	CLA	C	513	-	69,73,73	2.37	25 (36%)	82,113,113	2.37	28 (34%)
34	DMS	D	414	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
34	DMS	v	210	-	3,3,3	2.76	1 (33%)	3,3,3	0.55	0
34	DMS	U	204	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
27	SQD	A	412	-	52,54,54	0.89	2 (3%)	62,65,65	1.68	12 (19%)
36	HTG	C	537	-	19,19,19	0.91	1 (5%)	23,24,24	1.38	3 (13%)
34	DMS	C	529	-	3,3,3	2.72	1 (33%)	3,3,3	0.46	0
34	DMS	O	313	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
29	PL9	D	404	-	55,55,55	0.74	2 (3%)	68,69,69	1.53	13 (19%)
38	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	1.05	4 (7%)
34	DMS	a	421	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
36	HTG	O	303	-	19,19,19	1.01	1 (5%)	23,24,24	1.08	2 (8%)
26	BCR	B	619	-	41,41,41	0.90	0	56,56,56	1.16	6 (10%)
38	LHG	d	409	-	48,48,48	0.89	3 (6%)	51,54,54	1.17	5 (9%)
32	GOL	a	419	-	5,5,5	1.15	0	5,5,5	0.71	0
34	DMS	L	102	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
36	HTG	c	943	-	17,17,19	0.96	1 (5%)	21,22,24	1.27	1 (4%)
34	DMS	B	632	-	3,3,3	2.51	1 (33%)	3,3,3	0.39	0
31	LMT	m	102	-	36,36,36	0.44	0	47,47,47	0.89	0
34	DMS	c	934	-	3,3,3	2.76	1 (33%)	3,3,3	0.56	0
34	DMS	a	422	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
24	CLA	C	511	3	69,73,73	2.52	23 (33%)	82,113,113	2.31	28 (34%)
26	BCR	c	915	-	41,41,41	0.76	0	56,56,56	1.38	7 (12%)
24	CLA	C	506	-	69,73,73	2.51	24 (34%)	82,113,113	2.38	29 (35%)
34	DMS	c	933	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
34	DMS	O	315	-	3,3,3	2.77	1 (33%)	3,3,3	0.62	0
24	CLA	C	502	-	69,73,73	2.50	24 (34%)	82,113,113	2.44	28 (34%)
34	DMS	A	423	-	3,3,3	2.47	1 (33%)	3,3,3	0.75	0
32	GOL	c	929	-	5,5,5	1.03	0	5,5,5	1.00	0
26	BCR	b	622	-	41,41,41	0.87	0	56,56,56	1.09	3 (5%)
34	DMS	i	106	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
29	PL9	a	417	-	55,55,55	0.64	2 (3%)	68,69,69	1.82	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	DGD	C	518	-	63,63,67	0.83	3 (4%)	77,77,81	0.99	4 (5%)
34	DMS	V	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
36	HTG	B	629	-	19,19,19	0.92	2 (10%)	23,24,24	1.33	3 (13%)
26	BCR	A	411	-	41,41,41	0.79	0	56,56,56	1.35	5 (8%)
34	DMS	v	203	-	3,3,3	2.69	1 (33%)	3,3,3	0.42	0
28	LMG	C	523	-	51,51,55	0.95	2 (3%)	59,59,63	1.28	8 (13%)
24	CLA	b	607	-	69,73,73	2.37	24 (34%)	82,113,113	2.42	28 (34%)
24	CLA	B	605	-	69,73,73	2.28	20 (28%)	82,113,113	2.49	28 (34%)
34	DMS	B	646	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
24	CLA	b	616	-	69,73,73	2.23	21 (30%)	82,113,113	2.55	29 (35%)
24	CLA	C	501	-	69,73,73	2.28	22 (31%)	82,113,113	2.42	27 (32%)
34	DMS	u	202	-	3,3,3	2.67	1 (33%)	3,3,3	0.74	0
36	HTG	C	520	-	19,19,19	0.92	2 (10%)	23,24,24	1.15	1 (4%)
36	HTG	d	419	-	19,19,19	0.96	2 (10%)	23,24,24	1.12	1 (4%)
24	CLA	b	613	-	69,73,73	2.54	23 (33%)	82,113,113	2.28	27 (32%)
25	PHO	a	411	-	58,69,69	2.54	12 (20%)	55,99,99	2.89	17 (30%)
24	CLA	C	503	-	69,73,73	2.63	20 (28%)	82,113,113	2.33	24 (29%)
34	DMS	e	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.58	0
32	GOL	b	637	-	5,5,5	0.94	0	5,5,5	1.04	0
21	OEX	A	401	3,1,43	0,15,15	-	-	-		
32	GOL	B	637	-	5,5,5	0.99	0	5,5,5	0.97	0
36	HTG	B	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.15	1 (4%)
34	DMS	v	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
24	CLA	b	609	-	69,73,73	2.27	24 (34%)	82,113,113	2.52	30 (36%)
36	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.36	2 (8%)
34	DMS	b	647	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
24	CLA	B	613	-	69,73,73	2.29	21 (30%)	82,113,113	2.32	24 (29%)
36	HTG	c	924	-	19,19,19	0.95	2 (10%)	23,24,24	1.17	2 (8%)
34	DMS	B	647	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
31	LMT	F	103	-	24,24,36	0.46	0	29,29,47	0.58	0
38	LHG	D	407	-	48,48,48	0.88	3 (6%)	51,54,54	0.92	3 (5%)
34	DMS	b	640	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
34	DMS	V	210	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
26	BCR	c	916	-	41,41,41	0.79	0	56,56,56	1.38	7 (12%)
28	LMG	C	519	-	51,51,55	0.91	3 (5%)	59,59,63	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	y	101	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	b	611	43	69,73,73	2.30	21 (30%)	82,113,113	2.33	29 (35%)
24	CLA	B	612	-	69,73,73	2.41	20 (28%)	82,113,113	2.54	32 (39%)
34	DMS	v	207	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
24	CLA	B	611	43	69,73,73	2.49	24 (34%)	82,113,113	2.43	31 (37%)
25	PHO	a	412	-	58,69,69	2.72	12 (20%)	55,99,99	3.00	15 (27%)
24	CLA	b	610	-	69,73,73	2.42	21 (30%)	82,113,113	2.39	29 (35%)
33	BCT	A	422	22	3,3,3	0.52	0	2,3,3	0.61	0
36	HTG	c	941	-	19,19,19	0.92	1 (5%)	23,24,24	1.76	5 (21%)
31	LMT	j	102	-	24,24,36	0.55	1 (4%)	29,29,47	0.89	0
34	DMS	O	309	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
34	DMS	b	641	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
24	CLA	B	615	-	69,73,73	2.19	20 (28%)	82,113,113	2.56	30 (36%)
27	SQD	f	102	-	41,43,54	1.12	2 (4%)	51,54,65	1.47	6 (11%)
27	SQD	A	416	-	52,54,54	0.98	2 (3%)	62,65,65	1.09	4 (6%)
28	LMG	c	921	-	51,51,55	0.97	2 (3%)	59,59,63	1.20	6 (10%)
36	HTG	y	102	-	19,19,19	0.98	2 (10%)	23,24,24	1.08	1 (4%)
34	DMS	C	532	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
34	DMS	C	534	-	3,3,3	2.71	1 (33%)	3,3,3	0.44	0
26	BCR	D	403	-	41,41,41	0.86	0	56,56,56	1.71	9 (16%)
36	HTG	B	625	-	19,19,19	0.93	1 (5%)	23,24,24	1.74	3 (13%)
24	CLA	B	607	-	69,73,73	2.46	22 (31%)	82,113,113	2.42	30 (36%)
29	PL9	A	414	-	55,55,55	0.62	1 (1%)	68,69,69	1.92	20 (29%)
24	CLA	B	616	-	69,73,73	2.42	23 (33%)	82,113,113	2.43	29 (35%)
24	CLA	b	620	-	69,73,73	2.43	22 (31%)	82,113,113	2.48	27 (32%)
34	DMS	c	935	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
34	DMS	O	314	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0
34	DMS	V	211	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
34	DMS	o	306	-	3,3,3	2.76	1 (33%)	3,3,3	0.68	0
34	DMS	d	416	-	3,3,3	2.72	1 (33%)	3,3,3	0.44	0
34	DMS	C	524	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
24	CLA	c	909	-	69,73,73	2.36	24 (34%)	82,113,113	2.58	30 (36%)
26	BCR	B	618	-	41,41,41	0.78	0	56,56,56	1.34	6 (10%)
34	DMS	O	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
37	DGD	c	918	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	b	642	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
38	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.93	3 (5%)
34	DMS	D	415	-	3,3,3	2.77	1 (33%)	3,3,3	0.56	0
38	LHG	d	411	-	46,46,48	0.88	2 (4%)	49,52,54	1.03	4 (8%)
36	HTG	b	627	-	19,19,19	1.02	2 (10%)	23,24,24	1.56	4 (17%)
26	BCR	T	101	-	41,41,41	0.73	0	56,56,56	1.71	12 (21%)
34	DMS	V	209	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
34	DMS	b	645	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
34	DMS	v	208	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
33	BCT	a	408[A]	22	3,3,3	0.52	0	2,3,3	0.72	0
27	SQD	b	601	-	52,54,54	1.00	3 (5%)	62,65,65	1.58	12 (19%)
24	CLA	c	906	-	69,73,73	2.36	22 (31%)	82,113,113	2.31	30 (36%)
37	DGD	C	516	-	63,63,67	0.83	3 (4%)	77,77,81	1.11	5 (6%)
31	LMT	A	417	-	36,36,36	0.47	0	47,47,47	1.21	3 (6%)
26	BCR	Y	101	-	41,41,41	0.81	0	56,56,56	1.55	10 (17%)
42	HEC	v	202	16	46,50,50	2.03	8 (17%)	58,82,82	1.31	6 (10%)
26	BCR	k	103	-	41,41,41	0.74	0	56,56,56	1.30	6 (10%)
34	DMS	B	634	-	3,3,3	2.76	1 (33%)	3,3,3	0.75	0
36	HTG	d	414	-	19,19,19	0.95	1 (5%)	23,24,24	1.52	3 (13%)
31	LMT	e	101	-	24,24,36	0.47	0	29,29,47	0.64	0
34	DMS	A	425	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
24	CLA	c	908	43	69,73,73	2.41	21 (30%)	82,113,113	2.53	31 (37%)
34	DMS	D	416	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
40	RRX	H	101	-	42,42,42	0.72	0	56,58,58	1.33	6 (10%)
34	DMS	b	646	-	3,3,3	2.79	1 (33%)	3,3,3	0.62	0
36	HTG	V	215	-	19,19,19	0.95	1 (5%)	23,24,24	1.92	3 (13%)
26	BCR	B	636	-	41,41,41	0.74	0	56,56,56	1.61	12 (21%)
34	DMS	b	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.61	0
39	HEM	F	102	5,6	50,50,50	1.88	9 (18%)	67,82,82	1.31	5 (7%)
24	CLA	c	903	-	69,73,73	2.40	22 (31%)	82,113,113	2.35	26 (31%)
34	DMS	b	631	-	3,3,3	2.43	1 (33%)	3,3,3	0.43	0
24	CLA	b	619	-	69,73,73	2.37	23 (33%)	82,113,113	2.33	29 (35%)
34	DMS	C	528	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
31	LMT	Z	101	-	36,36,36	0.42	0	47,47,47	0.92	1 (2%)
36	HTG	B	631	-	19,19,19	0.90	1 (5%)	23,24,24	1.57	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HTG	d	420	-	19,19,19	0.92	1 (5%)	23,24,24	1.29	2 (8%)
24	CLA	C	510	-	69,73,73	2.48	25 (36%)	82,113,113	2.46	34 (41%)
34	DMS	V	213	-	3,3,3	2.73	1 (33%)	3,3,3	0.64	0
24	CLA	B	610	-	69,73,73	2.50	21 (30%)	82,113,113	2.31	29 (35%)
24	CLA	C	512	-	69,73,73	2.56	24 (34%)	82,113,113	2.35	30 (36%)
34	DMS	e	103	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
39	HEM	f	101	5,6	50,50,50	1.89	8 (16%)	67,82,82	1.34	7 (10%)
31	LMT	c	922	-	36,36,36	0.50	1 (2%)	47,47,47	1.26	4 (8%)
34	DMS	v	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
24	CLA	b	605	43	69,73,73	2.46	23 (33%)	82,113,113	2.33	27 (32%)
24	CLA	c	911	-	69,73,73	2.43	24 (34%)	82,113,113	2.38	26 (31%)
42	HEC	V	203	16	46,50,50	1.96	7 (15%)	58,82,82	1.45	5 (8%)
34	DMS	A	427	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
34	DMS	O	310	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
34	DMS	C	526	-	3,3,3	2.69	1 (33%)	3,3,3	0.41	0
31	LMT	t	101	-	23,23,36	0.47	0	26,27,47	0.97	1 (3%)
34	DMS	U	203	-	3,3,3	2.75	1 (33%)	3,3,3	0.88	0
34	DMS	O	302	-	3,3,3	2.74	1 (33%)	3,3,3	0.64	0
28	LMG	A	413	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	6 (10%)
24	CLA	c	902	-	69,73,73	2.40	22 (31%)	82,113,113	2.57	30 (36%)
34	DMS	B	643	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
34	DMS	K	102	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
32	GOL	O	304	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)
36	HTG	b	602	-	19,19,19	0.93	2 (10%)	23,24,24	1.29	3 (13%)
24	CLA	b	617	-	69,73,73	2.44	22 (31%)	82,113,113	2.45	30 (36%)
36	HTG	D	412	-	19,19,19	0.96	1 (5%)	23,24,24	1.33	3 (13%)
24	CLA	b	612	-	69,73,73	2.71	23 (33%)	82,113,113	2.33	26 (31%)
38	LHG	D	408	-	45,45,48	0.91	2 (4%)	48,51,54	0.97	4 (8%)
34	DMS	V	208	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
34	DMS	a	424	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
34	DMS	o	304	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
25	PHO	A	409	-	58,69,69	2.81	13 (22%)	55,99,99	3.10	15 (27%)
24	CLA	b	608	-	69,73,73	2.66	22 (31%)	82,113,113	2.47	28 (34%)
34	DMS	A	424	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
31	LMT	B	626	-	24,24,36	0.47	0	29,29,47	1.13	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	C	535	-	3,3,3	2.77	1 (33%)	3,3,3	0.58	0
31	LMT	a	402	-	36,36,36	0.43	0	47,47,47	1.14	4 (8%)
24	CLA	b	615	-	69,73,73	2.40	22 (31%)	82,113,113	2.37	32 (39%)
28	LMG	B	621	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
21	OEX	a	404	3,1,43	0,15,15	-	-	-		
37	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.90	3 (3%)
34	DMS	C	531	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
32	GOL	B	638	-	5,5,5	1.09	0	5,5,5	1.29	1 (20%)
36	HTG	B	624	-	19,19,19	0.73	1 (5%)	23,24,24	1.34	2 (8%)
24	CLA	A	410	-	69,73,73	2.18	22 (31%)	82,113,113	2.52	31 (37%)
34	DMS	h	105	-	3,3,3	2.71	1 (33%)	3,3,3	0.38	0
31	LMT	m	103	-	36,36,36	0.41	0	47,47,47	0.81	1 (2%)
34	DMS	O	308	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
26	BCR	b	621	-	41,41,41	0.76	0	56,56,56	1.49	9 (16%)
24	CLA	d	404	-	69,73,73	2.48	23 (33%)	82,113,113	2.47	31 (37%)
28	LMG	a	416	-	51,51,55	0.96	3 (5%)	59,59,63	1.29	9 (15%)
34	DMS	c	926	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
34	DMS	H	104	-	3,3,3	2.71	1 (33%)	3,3,3	0.58	0
26	BCR	B	620	-	41,41,41	0.69	0	56,56,56	1.27	8 (14%)
24	CLA	B	603	-	69,73,73	2.34	24 (34%)	82,113,113	2.55	31 (37%)
24	CLA	c	904	-	69,73,73	2.65	24 (34%)	82,113,113	2.21	29 (35%)
26	BCR	C	514	-	41,41,41	0.77	0	56,56,56	1.36	7 (12%)
24	CLA	C	507	43	69,73,73	2.55	22 (31%)	82,113,113	2.47	30 (36%)
24	CLA	B	614	-	69,73,73	2.25	21 (30%)	82,113,113	2.47	31 (37%)
38	LHG	D	406	-	48,48,48	0.83	2 (4%)	51,54,54	1.21	7 (13%)
24	CLA	d	405	-	69,73,73	2.27	22 (31%)	82,113,113	2.53	32 (39%)
34	DMS	B	640	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
26	BCR	a	414	-	41,41,41	0.80	0	56,56,56	1.28	5 (8%)
32	GOL	C	525	-	5,5,5	0.95	0	5,5,5	1.04	0
34	DMS	o	302	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
34	DMS	d	417	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
24	CLA	B	609	-	69,73,73	2.37	23 (33%)	82,113,113	2.28	27 (32%)
24	CLA	C	505	-	69,73,73	2.66	22 (31%)	82,113,113	2.22	25 (30%)
24	CLA	b	614	43	69,73,73	2.26	22 (31%)	82,113,113	2.38	29 (35%)
24	CLA	c	907	-	69,73,73	2.43	24 (34%)	82,113,113	2.39	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	A	426	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
24	CLA	c	905	43	69,73,73	2.19	24 (34%)	82,113,113	2.56	32 (39%)
34	DMS	a	420	-	3,3,3	2.57	1 (33%)	3,3,3	0.43	0
27	SQD	a	415	-	52,54,54	0.89	2 (3%)	62,65,65	1.66	11 (17%)
24	CLA	c	912	3	69,73,73	2.36	22 (31%)	82,113,113	2.37	30 (36%)
33	BCT	d	402[B]	22	3,3,3	0.55	0	2,3,3	0.43	0
34	DMS	d	415	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
28	LMG	d	412	41	51,51,55	0.90	2 (3%)	59,59,63	0.89	3 (5%)
34	DMS	O	311	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
36	HTG	c	923	-	19,19,19	0.94	2 (10%)	23,24,24	1.39	3 (13%)
34	DMS	U	202	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
28	LMG	b	624	-	51,51,55	0.95	2 (3%)	59,59,63	1.08	4 (6%)
34	DMS	v	206	-	3,3,3	2.78	1 (33%)	3,3,3	0.57	0
24	CLA	D	401	-	69,73,73	2.16	24 (34%)	82,113,113	2.61	29 (35%)
27	SQD	l	101	-	52,54,54	0.97	3 (5%)	62,65,65	1.32	5 (8%)
24	CLA	a	413	-	69,73,73	2.15	23 (33%)	82,113,113	2.47	32 (39%)
34	DMS	B	645	-	3,3,3	2.74	1 (33%)	3,3,3	0.64	0
34	DMS	b	643	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
34	DMS	D	413	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
31	LMT	b	625	-	36,36,36	0.39	0	47,47,47	1.28	7 (14%)
38	LHG	L	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.13	4 (7%)
34	DMS	d	418	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
26	BCR	k	102	-	41,41,41	0.78	0	56,56,56	1.55	8 (14%)
34	DMS	c	931	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
34	DMS	C	533	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
31	LMT	J	102	-	24,24,36	0.51	0	29,29,47	0.76	0
24	CLA	c	913	-	69,73,73	2.57	23 (33%)	82,113,113	2.46	29 (35%)
37	DGD	D	405	-	52,52,67	0.93	2 (3%)	60,60,81	1.18	6 (10%)
36	HTG	B	630	-	19,19,19	0.92	2 (10%)	23,24,24	1.25	2 (8%)
31	LMT	M	101	-	36,36,36	0.39	0	47,47,47	0.83	1 (2%)
34	DMS	O	312	-	3,3,3	2.74	1 (33%)	3,3,3	0.50	0
24	CLA	A	406	43	69,73,73	2.29	24 (34%)	82,113,113	2.60	27 (32%)
37	DGD	c	919	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	4 (5%)
24	CLA	A	407	43	69,73,73	2.15	20 (28%)	82,113,113	2.60	32 (39%)
40	RRX	h	101	-	42,42,42	0.74	0	56,58,58	1.32	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	SQD	F	101	-	35,37,54	0.90	1 (2%)	44,47,65	1.89	9 (20%)
34	DMS	b	638	-	3,3,3	2.80	1 (33%)	3,3,3	0.69	0
34	DMS	V	214	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
31	LMT	A	421	-	36,36,36	0.43	0	47,47,47	1.01	1 (2%)
24	CLA	a	409	-	69,73,73	2.39	23 (33%)	82,113,113	2.45	28 (34%)
34	DMS	B	639	-	3,3,3	2.70	1 (33%)	3,3,3	0.49	0
24	CLA	b	606	-	69,73,73	2.43	24 (34%)	82,113,113	2.44	30 (36%)
34	DMS	c	930	-	3,3,3	2.59	1 (33%)	3,3,3	0.37	0
24	CLA	B	606	-	69,73,73	2.28	23 (33%)	82,113,113	2.43	30 (36%)
34	DMS	o	303	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
34	DMS	v	204	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
34	DMS	B	642	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
31	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.60	12 (25%)
37	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.99	7 (9%)
34	DMS	b	644	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
34	DMS	O	306	-	3,3,3	2.73	1 (33%)	3,3,3	0.48	0
37	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.06	6 (7%)
34	DMS	B	644	-	3,3,3	2.65	1 (33%)	3,3,3	0.33	0
24	CLA	B	604	-	69,73,73	2.26	24 (34%)	82,113,113	2.55	28 (34%)
36	HTG	c	942	-	19,19,19	0.93	2 (10%)	23,24,24	1.21	3 (13%)
34	DMS	c	937	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	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
29	PL9	a	417	-	-	11/53/73/73	0/1/1/1
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	CLA	C	507	43	1/1/15/20	8/39/115/115	-
27	SQD	a	401	-	-	20/49/69/69	0/1/1/1
36	HTG	B	629	-	-	2/10/30/30	0/1/1/1
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
32	GOL	V	207	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	c	920	-	-	8/46/66/70	0/1/1/1
36	HTG	O	316	-	-	1/10/30/30	0/1/1/1
24	CLA	B	614	-	1/1/15/20	5/39/115/115	-
24	CLA	C	504	43	1/1/15/20	4/39/115/115	-
38	LHG	D	406	-	-	8/53/53/53	-
24	CLA	d	405	-	1/1/15/20	4/39/115/115	-
40	RRX	H	101	-	-	2/29/65/65	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	LMG	C	523	-	-	9/46/66/70	0/1/1/1
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
24	CLA	b	607	-	1/1/15/20	1/39/115/115	-
24	CLA	B	605	-	1/1/15/20	0/39/115/115	-
26	BCR	B	636	-	-	1/29/63/63	0/2/2/2
26	BCR	a	414	-	-	0/29/63/63	0/2/2/2
36	HTG	V	215	-	-	1/10/30/30	0/1/1/1
38	LHG	E	101	-	-	10/46/46/53	-
24	CLA	b	616	-	1/1/15/20	3/39/115/115	-
32	GOL	C	525	-	-	0/4/4/4	-
39	HEM	F	102	5,6	-	2/14/54/54	-
31	LMT	c	927	-	-	11/21/61/61	0/2/2/2
24	CLA	c	903	-	1/1/15/20	5/39/115/115	-
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	C	501	-	1/1/15/20	3/39/115/115	-
24	CLA	b	619	-	1/1/15/20	7/39/115/115	-
31	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
36	HTG	C	520	-	-	3/10/30/30	0/1/1/1
36	HTG	d	419	-	-	1/10/30/30	0/1/1/1
36	HTG	B	631	-	-	1/10/30/30	0/1/1/1
24	CLA	b	613	-	1/1/15/20	2/39/115/115	-
24	CLA	B	609	-	-	2/39/115/115	-
24	CLA	C	505	-	1/1/15/20	1/39/115/115	-
36	HTG	d	420	-	-	3/10/30/30	0/1/1/1
25	PHO	a	411	-	-	2/37/103/103	0/5/6/6
24	CLA	C	510	-	1/1/15/20	3/39/115/115	-
24	CLA	b	614	43	1/1/15/20	2/39/115/115	-
24	CLA	c	914	-	1/1/15/20	2/39/115/115	-
24	CLA	C	503	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	402	-	1/1/15/20	5/39/115/115	-
32	GOL	b	637	-	-	0/4/4/4	-
24	CLA	B	602	43	1/1/15/20	12/39/115/115	-
24	CLA	c	907	-	1/1/15/20	8/39/115/115	-
32	GOL	B	637	-	-	4/4/4/4	-
36	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	c	910	-	1/1/15/20	6/39/115/115	-
24	CLA	b	609	-	1/1/15/20	3/39/115/115	-
36	HTG	C	521	-	-	1/10/30/30	0/1/1/1
36	HTG	V	204	-	-	3/4/24/30	0/1/1/1
24	CLA	c	905	43	1/1/15/20	4/39/115/115	-
24	CLA	B	610	-	1/1/15/20	5/39/115/115	-
24	CLA	C	512	-	1/1/15/20	3/39/115/115	-
27	SQD	a	415	-	-	6/49/69/69	0/1/1/1
24	CLA	B	613	-	1/1/15/20	1/39/115/115	-
36	HTG	c	924	-	-	0/10/30/30	0/1/1/1
31	LMT	F	103	-	-	4/15/35/61	0/1/1/2
24	CLA	c	912	3	-	0/39/115/115	-
39	HEM	f	101	5,6	-	0/14/54/54	-
38	LHG	D	407	-	-	4/53/53/53	-
31	LMT	c	922	-	-	5/21/61/61	0/2/2/2
24	CLA	C	509	-	1/1/15/20	8/39/115/115	-
26	BCR	c	916	-	-	3/29/63/63	0/2/2/2
28	LMG	C	519	-	-	14/46/66/70	0/1/1/1
24	CLA	b	611	43	1/1/15/20	1/39/115/115	-
24	CLA	B	612	-	1/1/15/20	1/39/115/115	-
24	CLA	b	605	43	1/1/15/20	3/39/115/115	-
24	CLA	B	611	43	1/1/15/20	2/39/115/115	-
25	PHO	a	412	-	-	1/37/103/103	0/5/6/6
28	LMG	d	412	41	-	8/46/66/70	0/1/1/1
24	CLA	c	911	-	1/1/15/20	2/39/115/115	-
36	HTG	c	923	-	-	0/10/30/30	0/1/1/1
24	CLA	b	610	-	1/1/15/20	2/39/115/115	-
42	HEC	V	203	16	-	6/14/54/54	-
37	DGD	c	917	-	-	13/51/91/95	0/2/2/2
36	HTG	C	536	-	-	1/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	b	624	-	-	11/46/66/70	0/1/1/1
24	CLA	D	401	-	1/1/15/20	4/39/115/115	-
27	SQD	l	101	-	-	21/49/69/69	0/1/1/1
32	GOL	A	419	-	-	2/4/4/4	-
36	HTG	c	941	-	-	1/10/30/30	0/1/1/1
31	LMT	t	101	-	-	3/15/31/61	0/1/1/2
24	CLA	a	413	-	1/1/15/20	6/39/115/115	-
24	CLA	d	401	43	1/1/15/20	3/39/115/115	-
24	CLA	B	608	43	1/1/15/20	1/39/115/115	-
37	DGD	d	408	-	-	20/44/64/95	0/1/1/2
24	CLA	A	405	-	1/1/15/20	2/39/115/115	-
24	CLA	b	618	-	1/1/15/20	11/39/115/115	-
28	LMG	D	409	41	-	3/46/66/70	0/1/1/1
28	LMG	A	413	-	-	16/46/66/70	0/1/1/1
31	LMT	j	102	-	-	3/15/35/61	0/1/1/2
24	CLA	c	902	-	1/1/15/20	3/39/115/115	-
31	LMT	b	625	-	-	8/21/61/61	0/2/2/2
31	LMT	M	102	-	-	7/17/37/61	0/1/1/2
32	GOL	O	304	-	-	2/4/4/4	-
38	LHG	L	101	-	-	13/53/53/53	-
24	CLA	B	615	-	1/1/15/20	2/39/115/115	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
36	HTG	b	602	-	-	2/10/30/30	0/1/1/1
24	CLA	a	410	43	-	2/39/115/115	-
31	LMT	t	102	-	-	9/21/61/61	0/2/2/2
24	CLA	b	617	-	1/1/15/20	2/39/115/115	-
27	SQD	A	416	-	-	11/49/69/69	0/1/1/1
28	LMG	c	921	-	-	1/46/66/70	0/1/1/1
36	HTG	b	626	-	-	2/10/30/30	0/1/1/1
36	HTG	y	102	-	-	3/10/30/30	0/1/1/1
26	BCR	C	515	-	-	1/29/63/63	0/2/2/2
36	HTG	D	412	-	-	3/10/30/30	0/1/1/1
36	HTG	c	928	-	-	0/10/30/30	0/1/1/1
24	CLA	b	612	-	-	2/39/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	D	408	-	-	8/50/50/53	-
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2
36	HTG	v	211	-	-	1/10/30/30	0/1/1/1
31	LMT	J	102	-	-	3/15/35/61	0/1/1/2
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	B	607	-	1/1/15/20	5/39/115/115	-
24	CLA	c	913	-	1/1/15/20	4/39/115/115	-
37	DGD	D	405	-	-	20/47/67/95	0/1/1/2
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1
24	CLA	B	616	-	1/1/15/20	10/39/115/115	-
24	CLA	b	620	-	1/1/15/20	9/39/115/115	-
29	PL9	d	407	-	-	6/53/73/73	0/1/1/1
24	CLA	B	617	-	1/1/15/20	10/39/115/115	-
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6
24	CLA	b	608	-	1/1/15/20	4/39/115/115	-
36	HTG	U	201	-	-	0/1/1/30	-
24	CLA	C	508	-	1/1/15/20	4/39/115/115	-
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
32	GOL	V	206	-	-	4/4/4/4	-
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
31	LMT	B	626	-	-	9/15/35/61	0/1/1/2
31	LMT	M	101	-	-	3/21/61/61	0/2/2/2
24	CLA	C	513	-	-	9/39/115/115	-
24	CLA	c	909	-	1/1/15/20	7/39/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
31	LMT	a	402	-	-	7/21/61/61	0/2/2/2
24	CLA	A	406	43	-	3/39/115/115	-
37	DGD	c	919	-	-	9/51/91/95	0/2/2/2
37	DGD	c	918	-	-	15/51/91/95	0/2/2/2
24	CLA	b	615	-	1/1/15/20	2/39/115/115	-
28	LMG	B	621	-	-	13/46/66/70	0/1/1/1
27	SQD	A	412	-	-	9/49/69/69	0/1/1/1
36	HTG	C	537	-	-	2/10/30/30	0/1/1/1
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	407	43	-	2/39/115/115	-
38	LHG	d	410	-	-	9/53/53/53	-
38	LHG	d	411	-	-	9/51/51/53	-
36	HTG	b	627	-	-	3/10/30/30	0/1/1/1
40	RRX	h	101	-	-	1/29/65/65	0/2/2/2
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
32	GOL	B	638	-	-	4/4/4/4	-
27	SQD	F	101	-	-	8/31/51/69	0/1/1/1
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
29	PL9	D	404	-	-	1/53/73/73	0/1/1/1
38	LHG	l	103	-	-	13/53/53/53	-
27	SQD	b	601	-	-	17/49/69/69	0/1/1/1
24	CLA	A	410	-	-	8/39/115/115	-
36	HTG	O	303	-	-	2/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	c	906	-	1/1/15/20	6/39/115/115	-
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
38	LHG	d	409	-	-	6/53/53/53	-
31	LMT	m	103	-	-	2/21/61/61	0/2/2/2
31	LMT	A	417	-	-	6/21/61/61	0/2/2/2
32	GOL	a	419	-	-	2/4/4/4	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
31	LMT	A	421	-	-	8/21/61/61	0/2/2/2
36	HTG	c	943	-	-	2/8/28/30	0/1/1/1
42	HEC	v	202	16	-	6/14/54/54	-
24	CLA	a	409	-	1/1/15/20	3/39/115/115	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/15/20	5/39/115/115	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
24	CLA	B	606	-	1/1/15/20	4/39/115/115	-
24	CLA	C	511	3	1/1/15/20	3/39/115/115	-
26	BCR	c	915	-	-	0/29/63/63	0/2/2/2
26	BCR	k	103	-	-	0/29/63/63	0/2/2/2
24	CLA	C	506	-	1/1/15/20	5/39/115/115	-
24	CLA	d	404	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	a	416	-	-	18/46/66/70	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
24	CLA	C	502	-	-	4/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
36	HTG	d	414	-	-	4/10/30/30	0/1/1/1
24	CLA	B	603	-	1/1/15/20	4/39/115/115	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
32	GOL	c	929	-	-	2/4/4/4	-
31	LMT	e	101	-	-	3/15/35/61	0/1/1/2
37	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	B	604	-	1/1/15/20	3/39/115/115	-
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
36	HTG	c	942	-	-	2/10/30/30	0/1/1/1
24	CLA	c	908	43	1/1/15/20	5/39/115/115	-
24	CLA	c	904	-	1/1/15/20	3/39/115/115	-

The worst 5 of 1918 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	MG-NA	10.97	2.32	2.06
24	C	507	CLA	MG-NA	10.43	2.31	2.06
24	C	511	CLA	MG-NA	10.27	2.30	2.06
24	C	503	CLA	MG-NA	10.00	2.30	2.06
24	b	612	CLA	MG-ND	-9.99	1.86	2.05

The worst 5 of 2680 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	PHO	C2D-C1D-ND	12.48	118.45	109.43
25	A	408	PHO	C2D-C1D-ND	12.25	118.28	109.43
24	c	909	CLA	C1D-ND-C4D	-11.41	98.31	106.31
24	D	401	CLA	C1D-ND-C4D	-11.32	98.37	106.31
25	a	411	PHO	C2D-C1D-ND	11.18	117.51	109.43

5 of 61 chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND

5 of 967 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

185 monomers are involved in 327 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	401	SQD	6	0
32	V	207	GOL	1	0
28	c	920	LMG	3	0
24	C	504	CLA	3	0
26	K	101	BCR	1	0
26	b	623	BCR	2	0
38	E	101	LHG	1	0
31	c	927	LMT	1	0
34	c	940	DMS	2	0
24	B	602	CLA	1	0
24	c	910	CLA	2	0
34	c	932	DMS	2	0
24	C	509	CLA	1	0
34	B	633	DMS	1	0
37	c	917	DGD	1	0
36	C	536	HTG	2	0
24	d	401	CLA	3	0
24	B	608	CLA	1	0
37	d	408	DGD	4	0
24	A	405	CLA	3	0
28	D	409	LMG	1	0
31	M	102	LMT	1	0
36	b	626	HTG	3	0
24	a	410	CLA	3	0
26	C	515	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	928	HTG	1	0
36	v	211	HTG	2	0
29	d	407	PL9	3	0
24	B	617	CLA	3	0
34	o	307	DMS	1	0
36	U	201	HTG	1	0
24	C	508	CLA	7	0
26	d	406	BCR	2	0
32	V	206	GOL	1	0
24	C	513	CLA	4	0
34	U	204	DMS	2	0
36	C	537	HTG	2	0
29	D	404	PL9	1	0
38	l	103	LHG	2	0
36	O	303	HTG	1	0
26	B	619	BCR	3	0
38	d	409	LHG	3	0
34	L	102	DMS	1	0
34	B	632	DMS	1	0
31	m	102	LMT	2	0
34	c	934	DMS	1	0
24	C	511	CLA	3	0
26	c	915	BCR	2	0
24	C	506	CLA	5	0
34	c	933	DMS	1	0
34	O	315	DMS	2	0
24	C	502	CLA	2	0
32	c	929	GOL	2	0
26	b	622	BCR	2	0
29	a	417	PL9	3	0
37	C	518	DGD	1	0
28	C	523	LMG	3	0
24	b	607	CLA	2	0
24	B	605	CLA	1	0
24	b	616	CLA	3	0
24	C	501	CLA	4	0
36	d	419	HTG	3	0
24	b	613	CLA	3	0
25	a	411	PHO	1	0
24	C	503	CLA	3	0
32	B	637	GOL	2	0
36	B	623	HTG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	609	CLA	5	0
34	b	647	DMS	1	0
24	B	613	CLA	1	0
34	V	210	DMS	1	0
26	c	916	BCR	2	0
28	C	519	LMG	3	0
34	y	101	DMS	2	0
24	B	612	CLA	1	0
24	B	611	CLA	5	0
25	a	412	PHO	1	0
24	b	610	CLA	6	0
36	c	941	HTG	1	0
31	j	102	LMT	2	0
24	B	615	CLA	5	0
27	A	416	SQD	2	0
34	C	534	DMS	1	0
24	B	607	CLA	4	0
29	A	414	PL9	4	0
24	B	616	CLA	3	0
24	b	620	CLA	4	0
34	O	314	DMS	1	0
34	V	211	DMS	1	0
24	c	909	CLA	4	0
26	B	618	BCR	3	0
37	c	918	DGD	2	0
38	d	410	LHG	2	0
38	d	411	LHG	5	0
36	b	627	HTG	1	0
26	T	101	BCR	4	0
27	b	601	SQD	1	0
24	c	906	CLA	6	0
37	C	516	DGD	2	0
31	A	417	LMT	3	0
26	Y	101	BCR	2	0
26	k	103	BCR	1	0
34	B	634	DMS	1	0
36	d	414	HTG	2	0
24	c	908	CLA	1	0
34	D	416	DMS	1	0
40	H	101	RRX	3	0
36	V	215	HTG	1	0
26	B	636	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	b	639	DMS	1	0
39	F	102	HEM	2	0
24	c	903	CLA	2	0
24	b	619	CLA	4	0
31	Z	101	LMT	1	0
24	C	510	CLA	4	0
24	B	610	CLA	1	0
24	C	512	CLA	1	0
39	f	101	HEM	3	0
24	b	605	CLA	1	0
24	c	911	CLA	1	0
28	A	413	LMG	3	0
24	c	902	CLA	2	0
24	b	617	CLA	2	0
36	D	412	HTG	2	0
38	D	408	LHG	6	0
34	a	424	DMS	1	0
25	A	409	PHO	2	0
24	b	608	CLA	1	0
31	B	626	LMT	2	0
31	a	402	LMT	2	0
24	b	615	CLA	3	0
28	B	621	LMG	1	0
32	B	638	GOL	2	0
36	B	624	HTG	3	0
24	A	410	CLA	4	0
34	h	105	DMS	2	0
26	b	621	BCR	3	0
24	d	404	CLA	1	0
28	a	416	LMG	1	0
26	B	620	BCR	1	0
24	B	603	CLA	5	0
24	c	904	CLA	2	0
26	C	514	BCR	2	0
24	C	507	CLA	2	0
24	B	614	CLA	2	0
38	D	406	LHG	3	0
26	a	414	BCR	2	0
24	C	505	CLA	5	0
24	b	614	CLA	3	0
24	c	907	CLA	2	0
34	A	426	DMS	1	0

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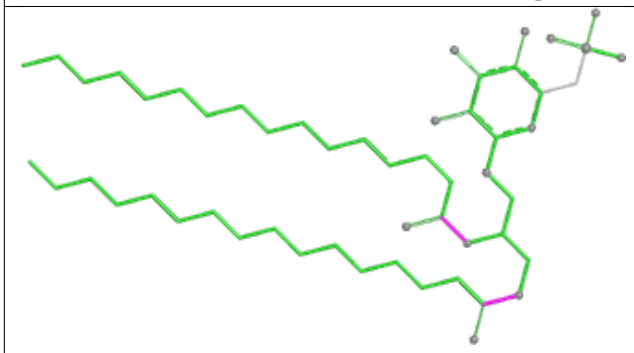
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	905	CLA	2	0
27	a	415	SQD	3	0
24	c	912	CLA	2	0
34	d	415	DMS	1	0
28	d	412	LMG	3	0
34	O	311	DMS	1	0
34	U	202	DMS	1	0
28	b	624	LMG	1	0
24	D	401	CLA	1	0
27	l	101	SQD	1	0
24	a	413	CLA	3	0
31	b	625	LMT	2	0
38	L	101	LHG	3	0
26	k	102	BCR	1	0
37	D	405	DGD	7	0
36	B	630	HTG	1	0
31	M	101	LMT	2	0
24	A	406	CLA	4	0
24	A	407	CLA	1	0
40	h	101	RRX	2	0
27	F	101	SQD	2	0
31	A	421	LMT	4	0
24	a	409	CLA	4	0
34	B	639	DMS	1	0
24	b	606	CLA	1	0
34	c	930	DMS	1	0
24	B	606	CLA	6	0
34	o	303	DMS	1	0
37	H	102	DGD	1	0
34	O	306	DMS	1	0
37	C	517	DGD	1	0
24	B	604	CLA	3	0
36	c	942	HTG	2	0
34	c	937	DMS	1	0

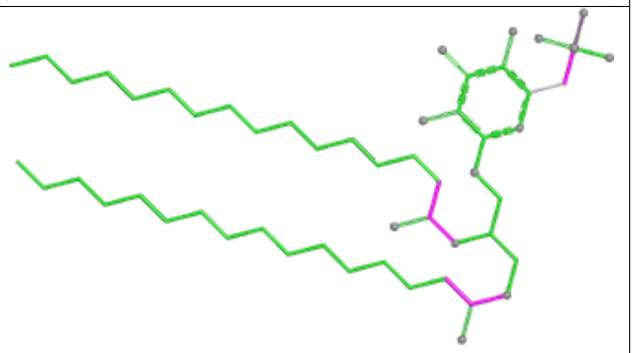
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

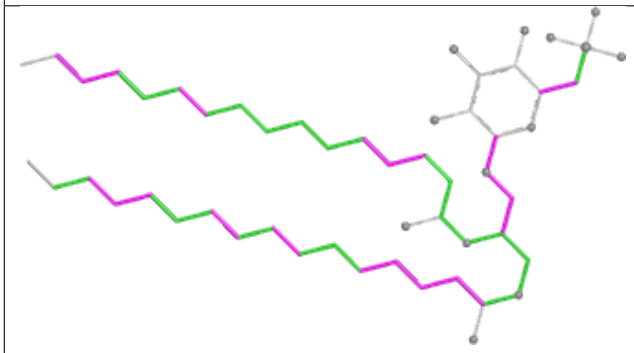
Ligand SQD a 401



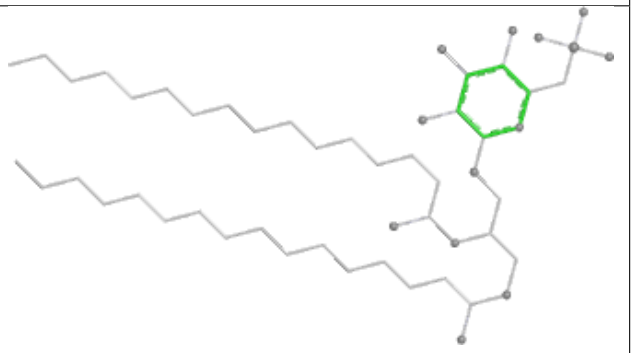
Bond lengths



Bond angles

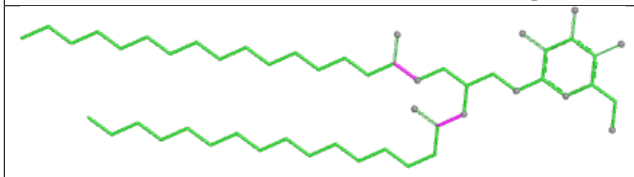


Torsions

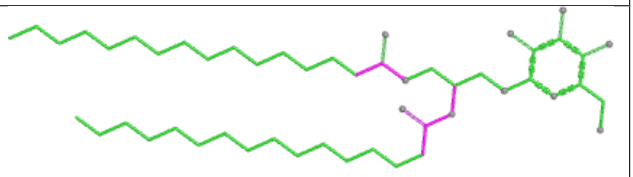


Rings

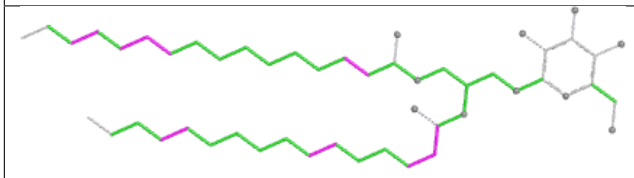
Ligand LMG c 920



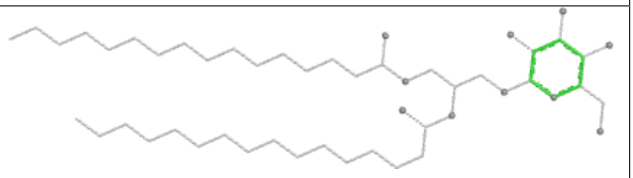
Bond lengths



Bond angles

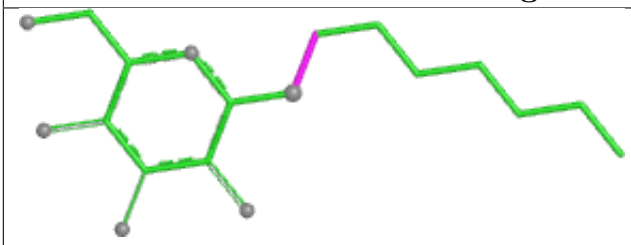


Torsions

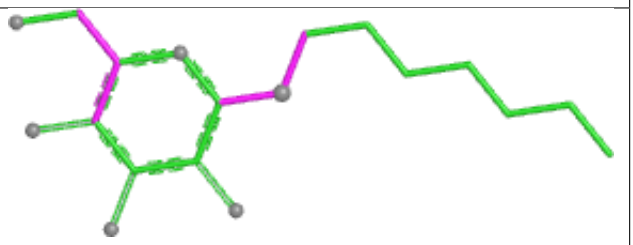


Rings

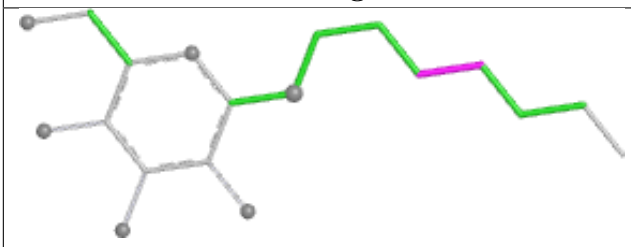
Ligand HTG O 316



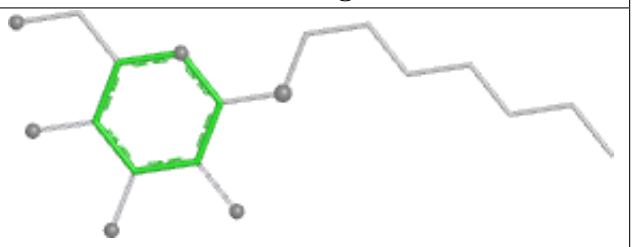
Bond lengths



Bond angles

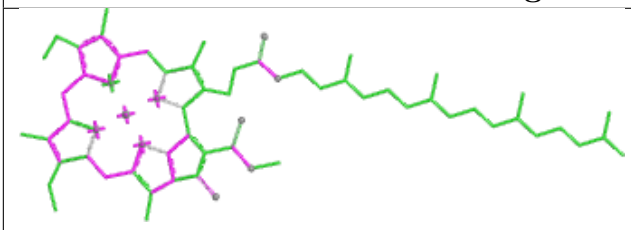


Torsions

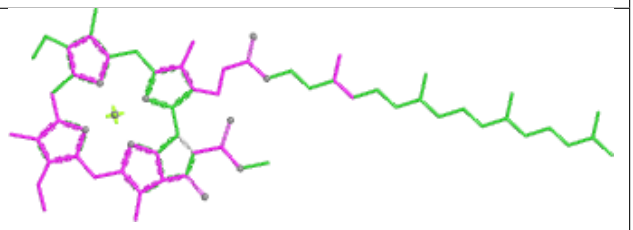


Rings

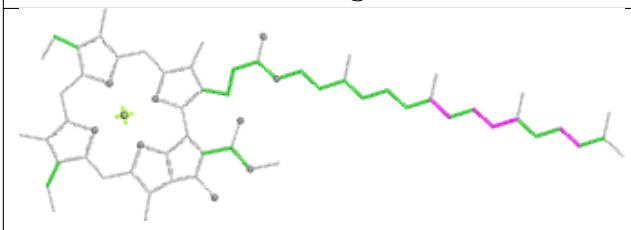
Ligand CLA C 504



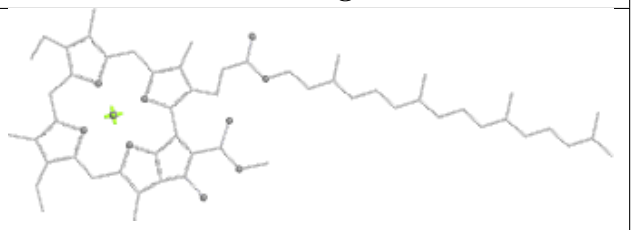
Bond lengths



Bond angles

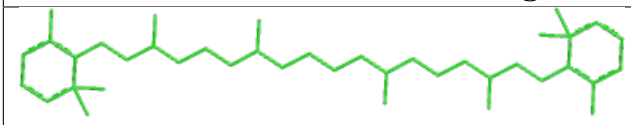


Torsions

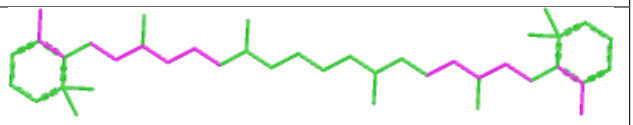


Rings

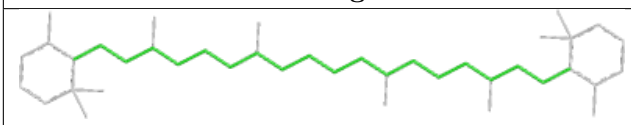
Ligand BCR K 101



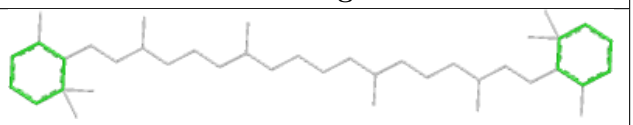
Bond lengths



Bond angles

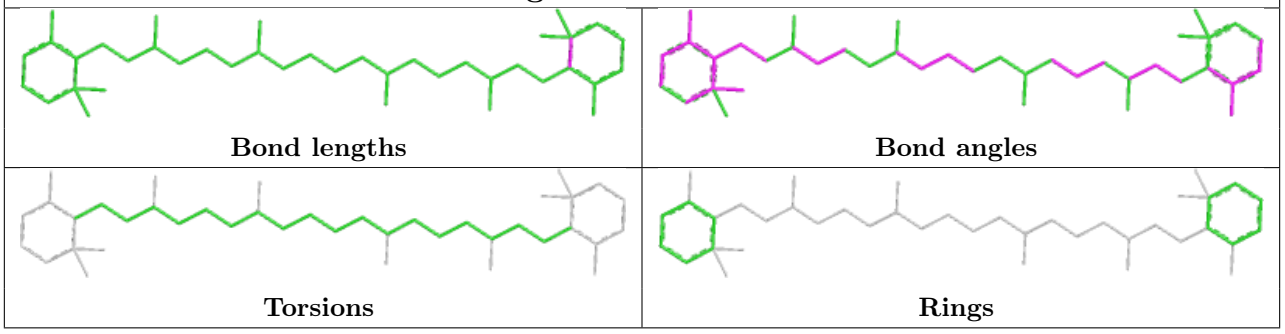


Torsions

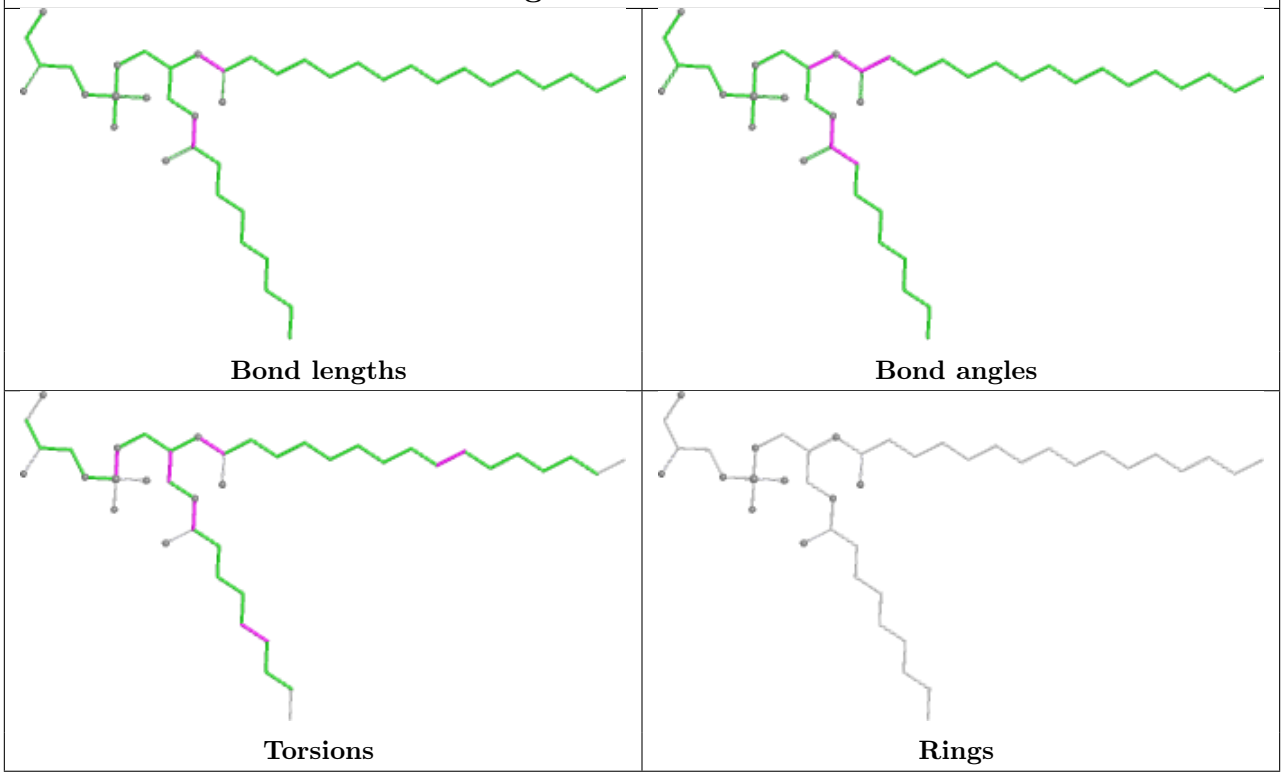


Rings

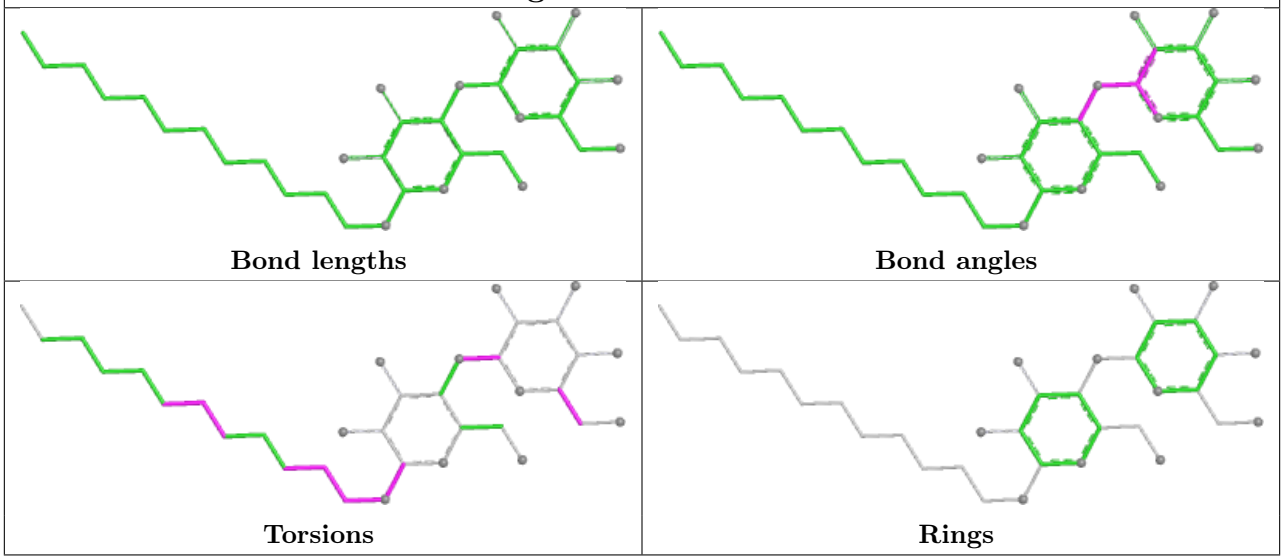
Ligand BCR b 623



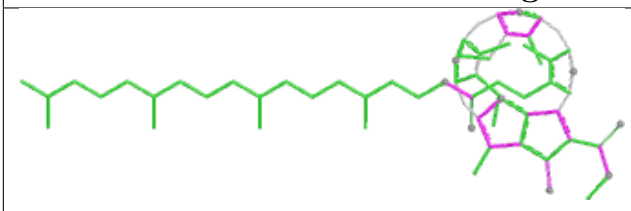
Ligand LHG E 101



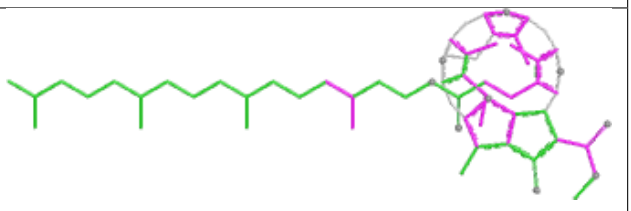
Ligand LMT c 927



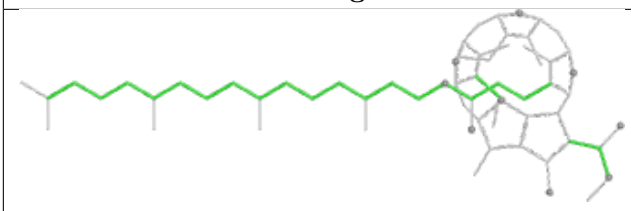
Ligand PHO A 408



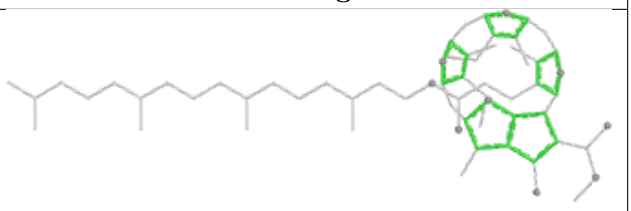
Bond lengths



Bond angles

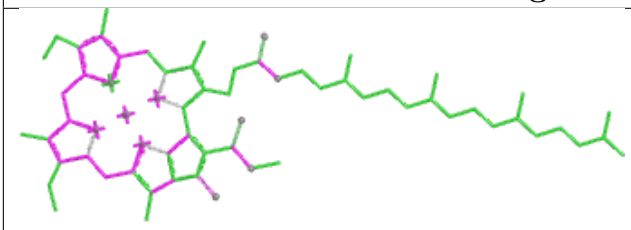


Torsions

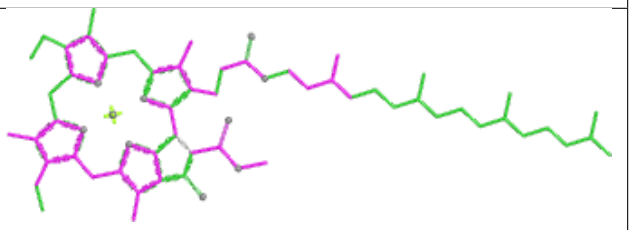


Rings

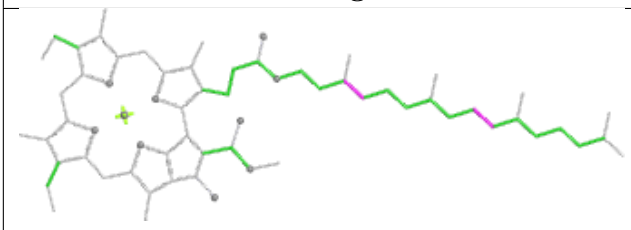
Ligand CLA c 914



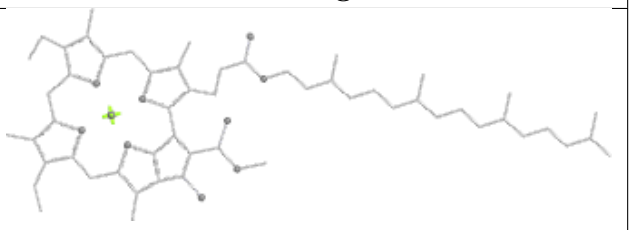
Bond lengths



Bond angles

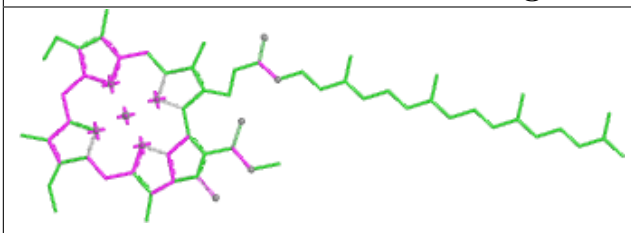


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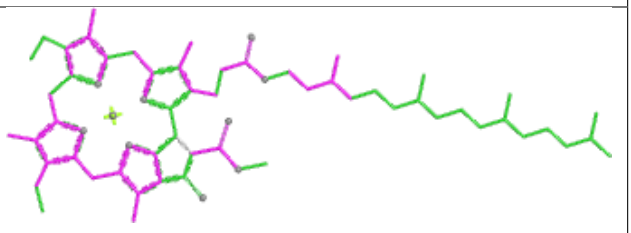


Rings

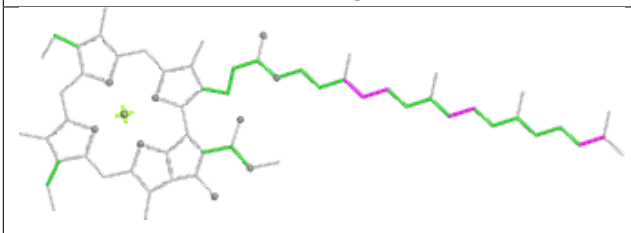
Ligand CLA D 402



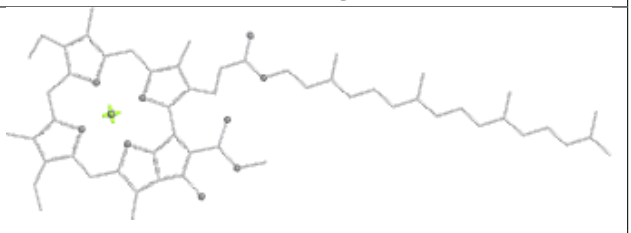
Bond lengths



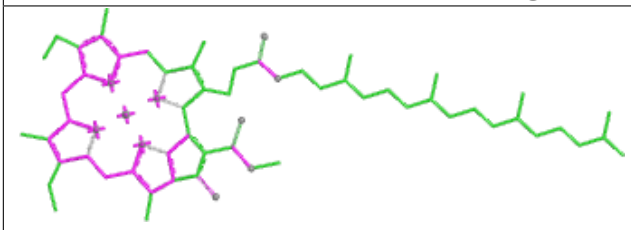
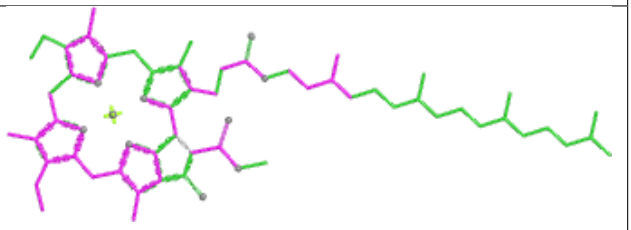
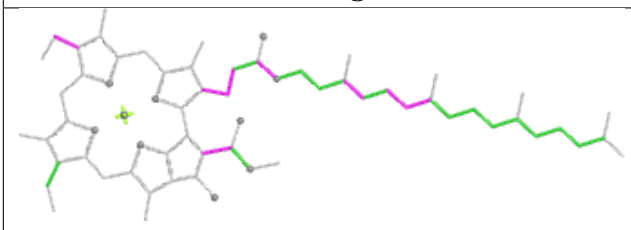
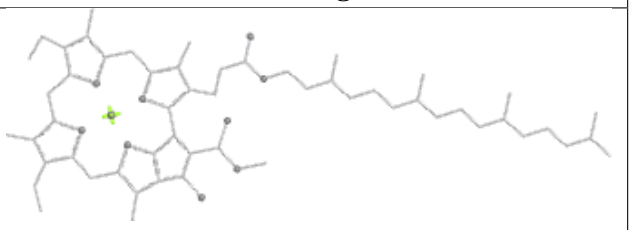
Bond angles

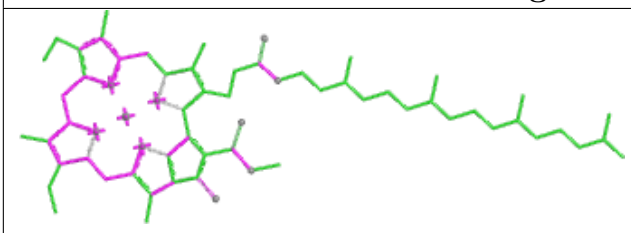
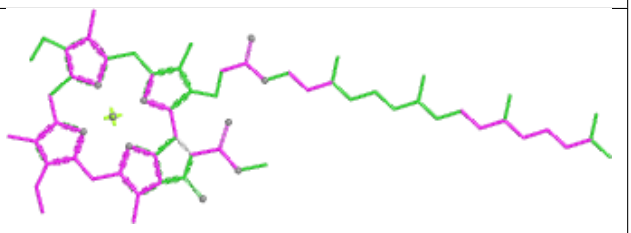
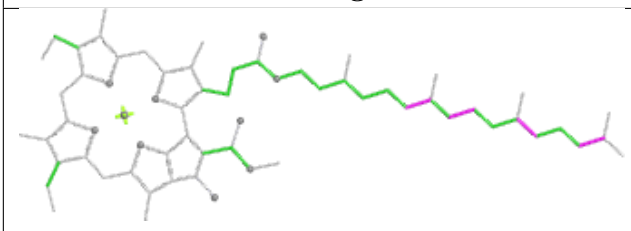
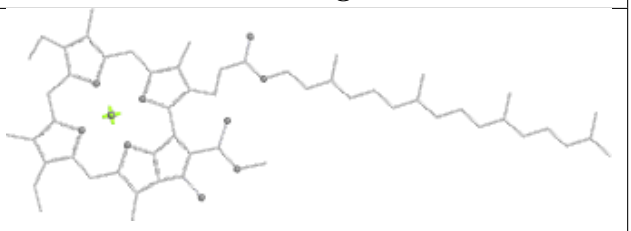


Torsions

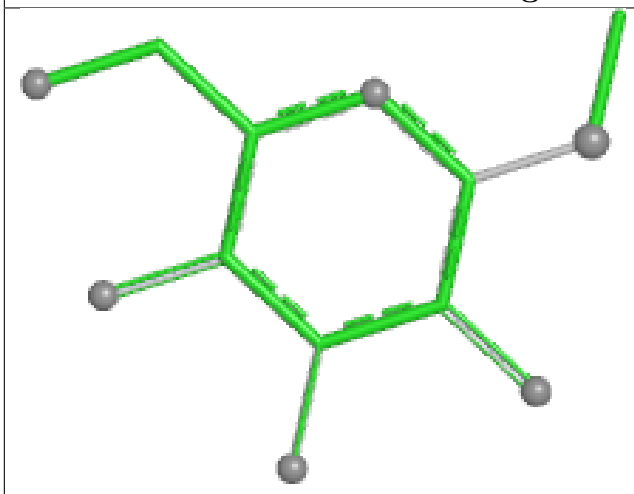


Rings

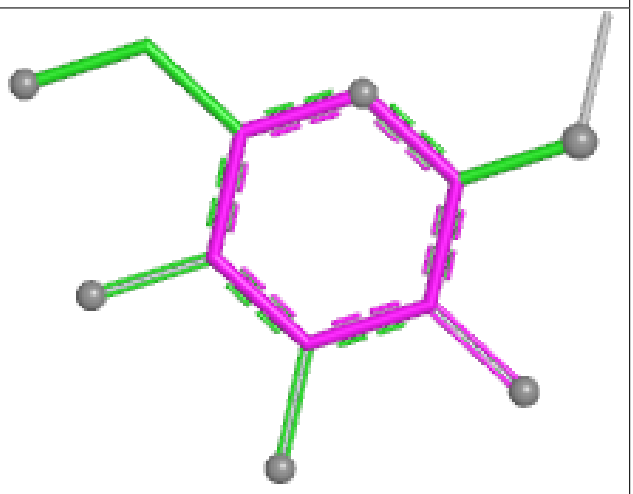
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 910	
 Bond lengths	 Bond angles
 Torsions	 Rings

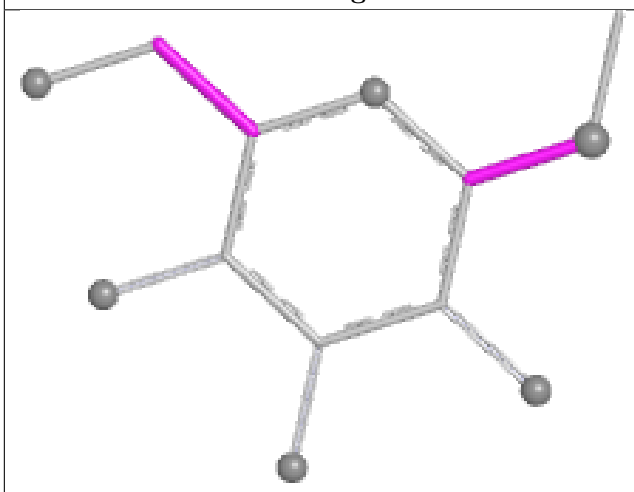
Ligand HTG V 204



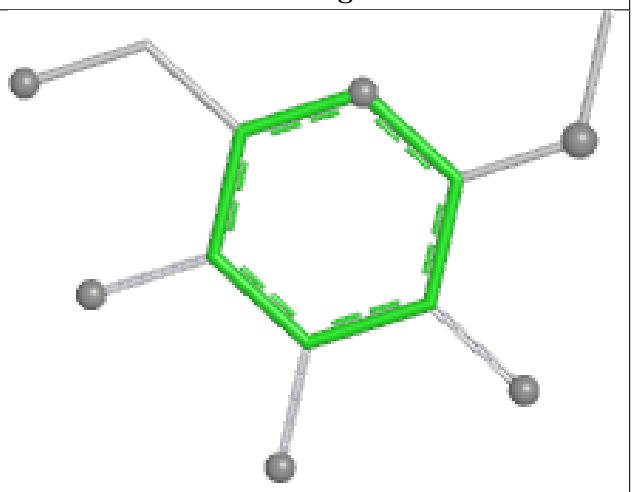
Bond lengths



Bond angles

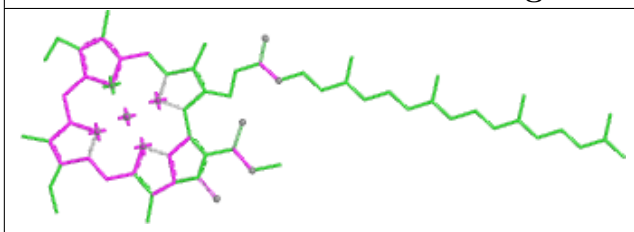


Torsions

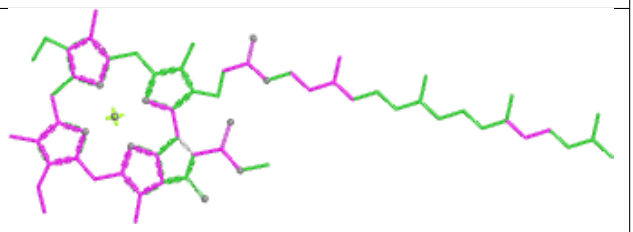


Rings

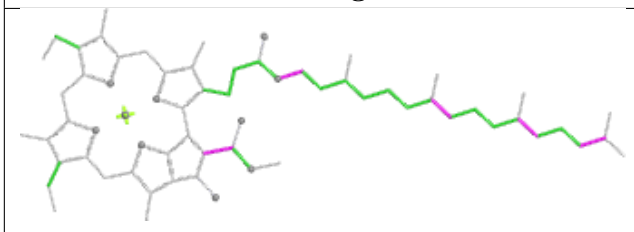
Ligand CLA C 509



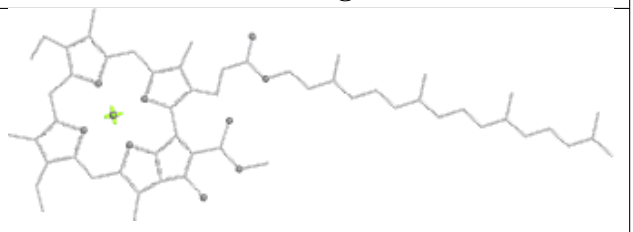
Bond lengths



Bond angles

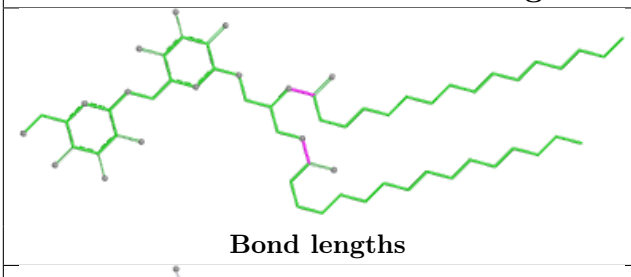


Torsions

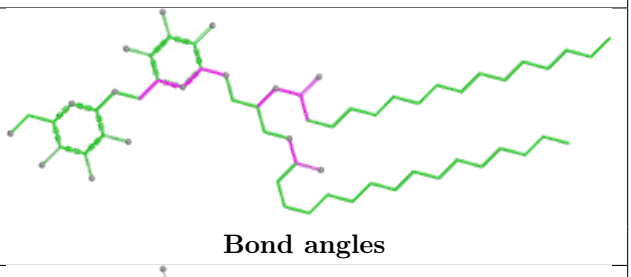


Rings

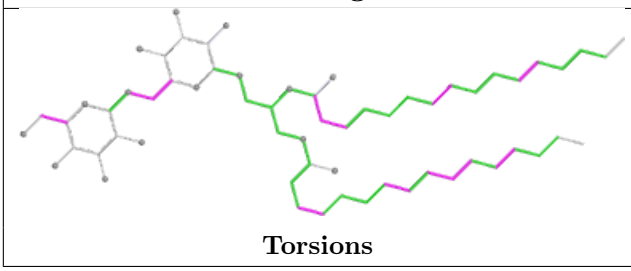
Ligand DGD c 917



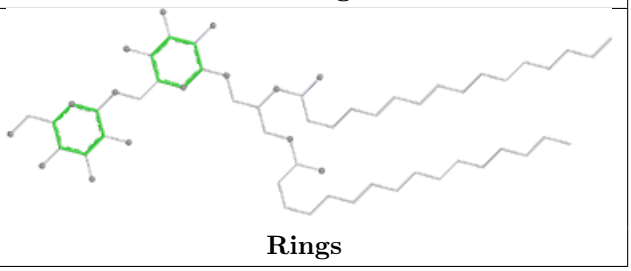
Bond lengths



Bond angles

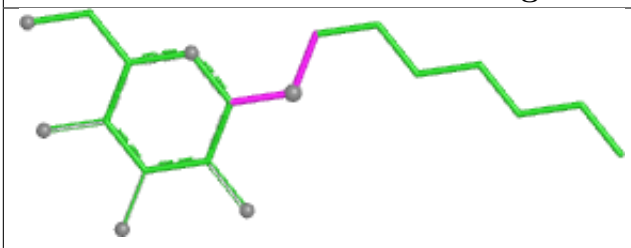


Torsions

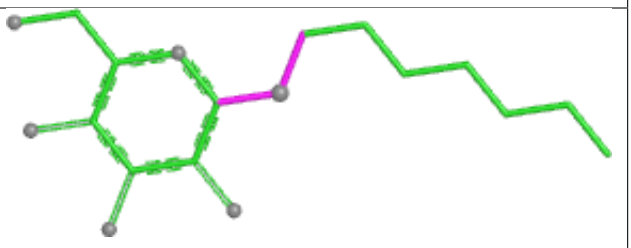


Rings

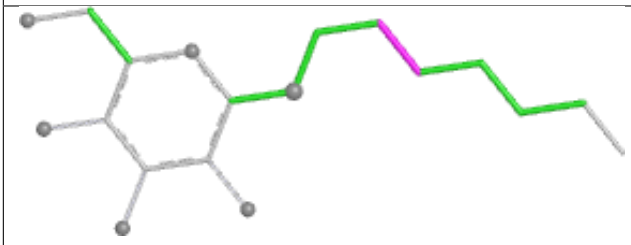
Ligand HTG C 536



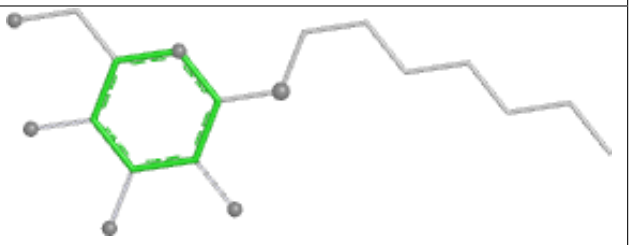
Bond lengths



Bond angles

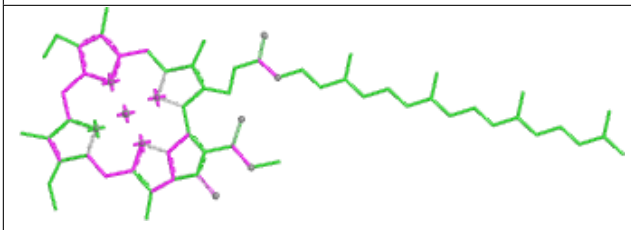


Torsions

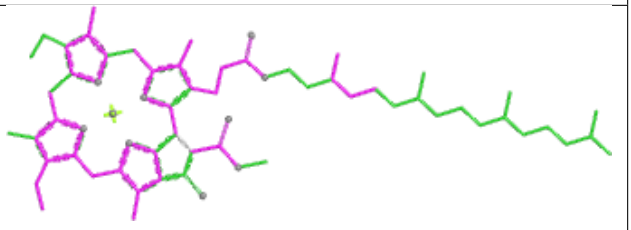


Rings

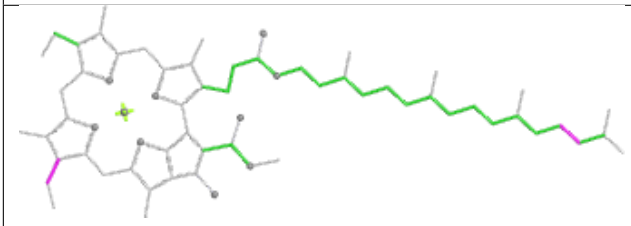
Ligand CLA d 401



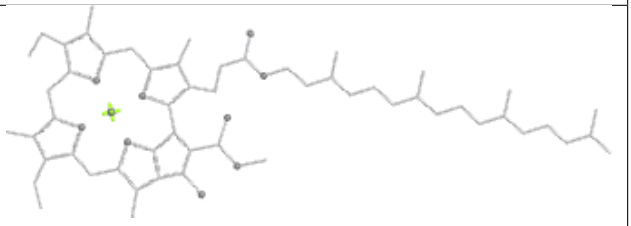
Bond lengths



Bond angles

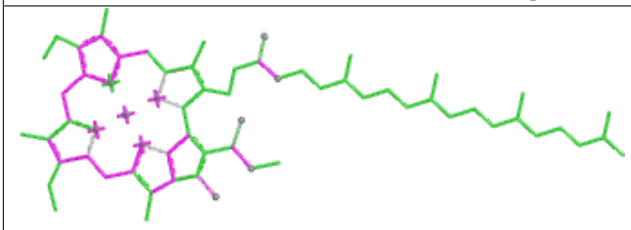


Torsions

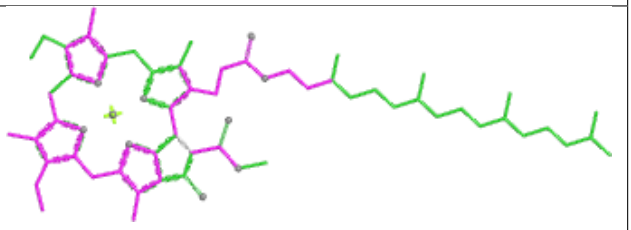


Rings

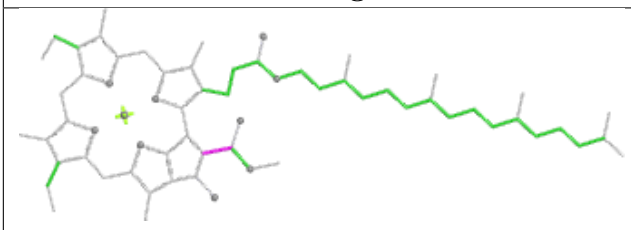
Ligand CLA B 608



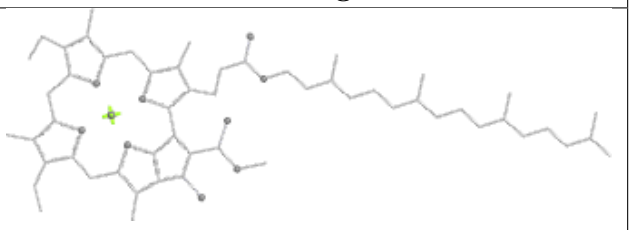
Bond lengths



Bond angles

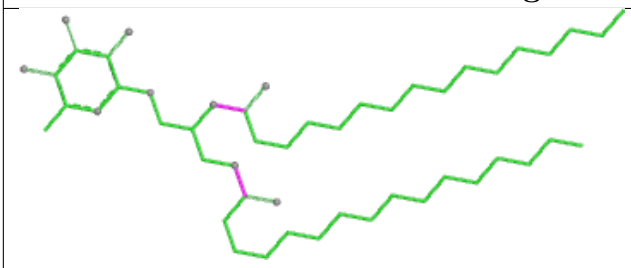


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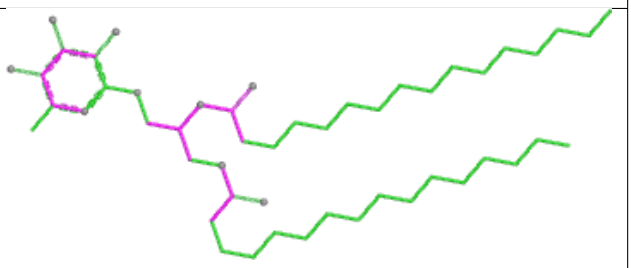


Rings

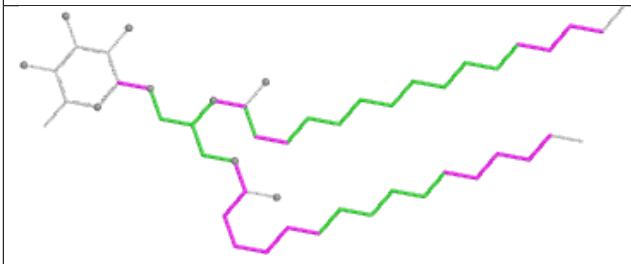
Ligand DGD d 408



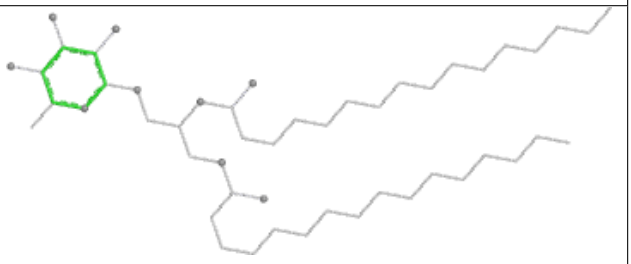
Bond lengths



Bond angles

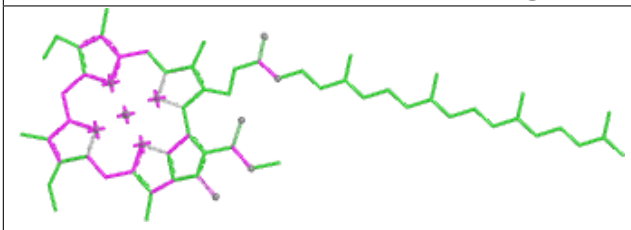


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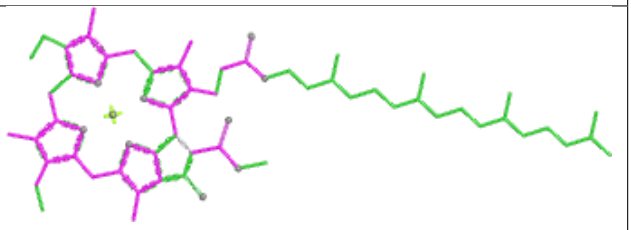


Rings

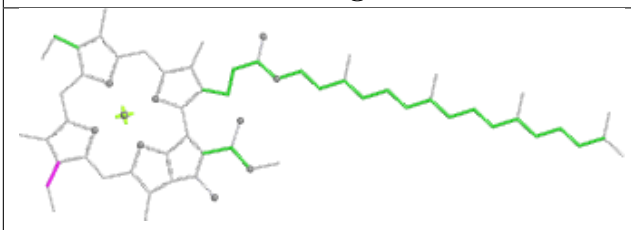
Ligand CLA A 405



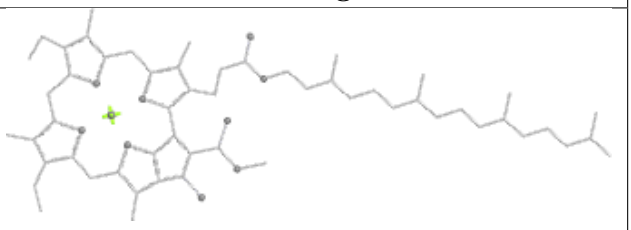
Bond lengths



Bond angles

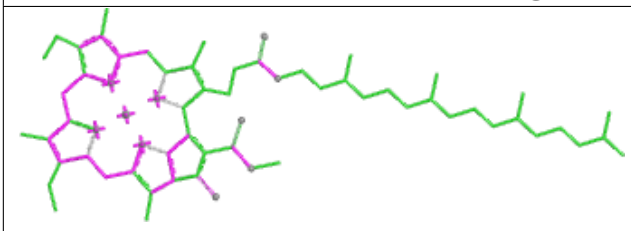


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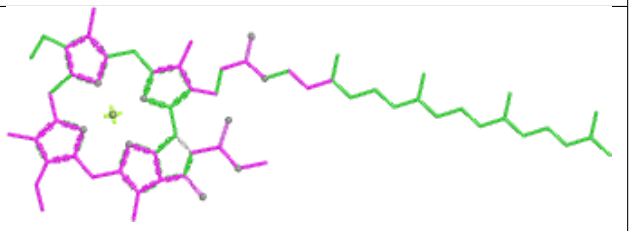


Rings

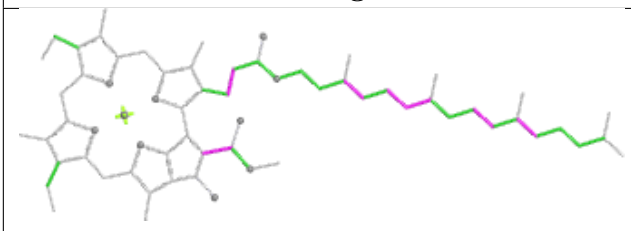
Ligand CLA b 618



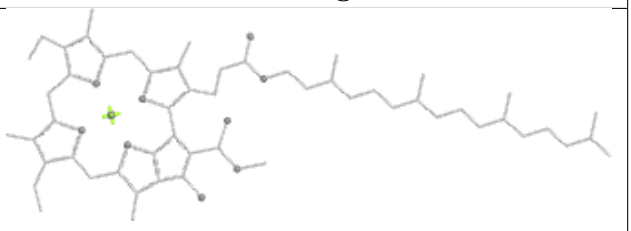
Bond lengths



Bond angles

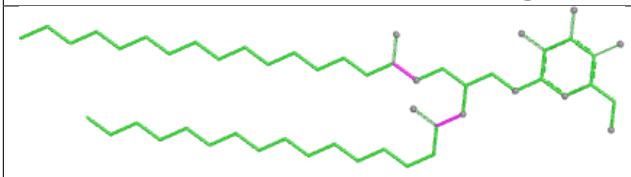


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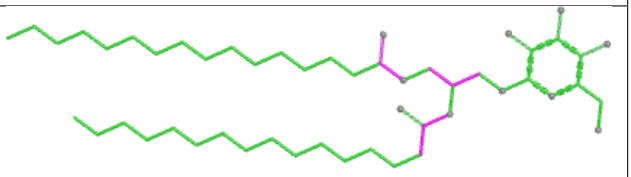


Rings

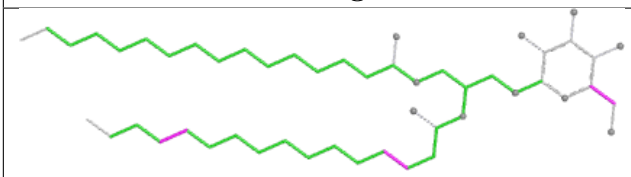
Ligand LMG D 409



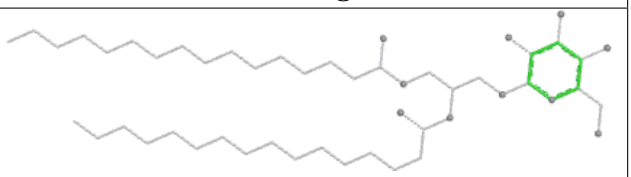
Bond lengths



Bond angles

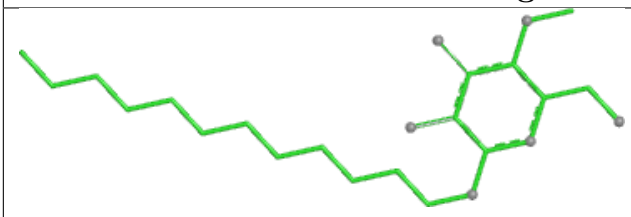


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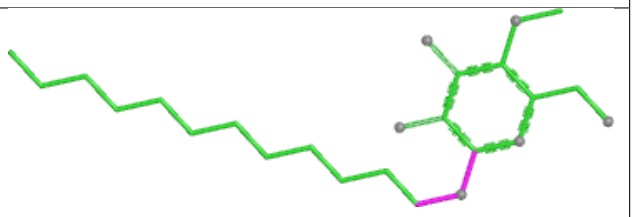


Rings

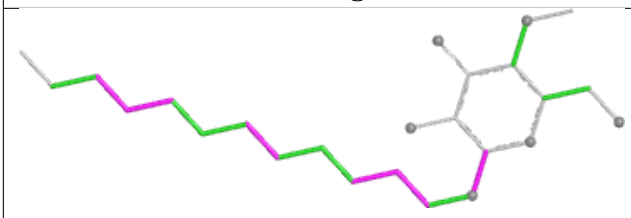
Ligand LMT M 102



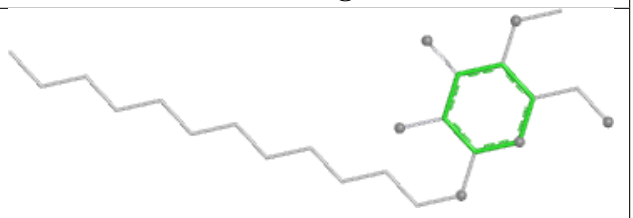
Bond lengths



Bond angles

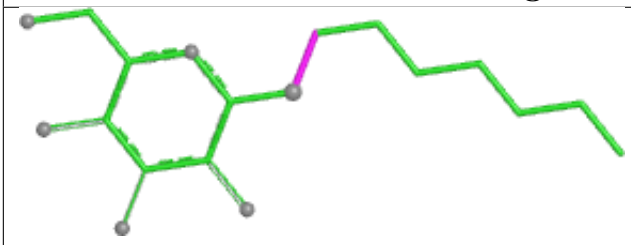


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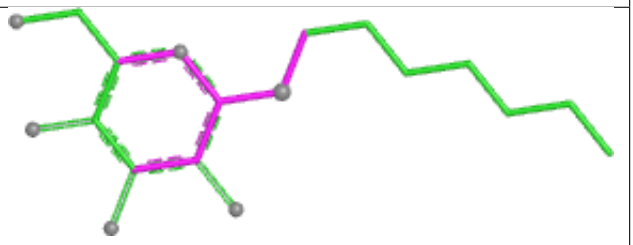


Rings

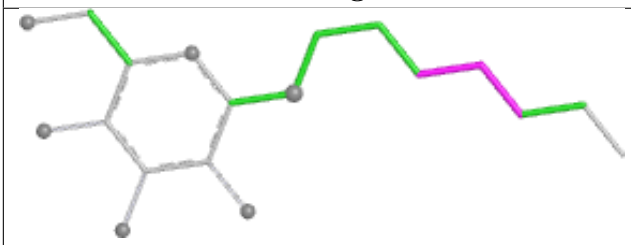
Ligand HTG b 626



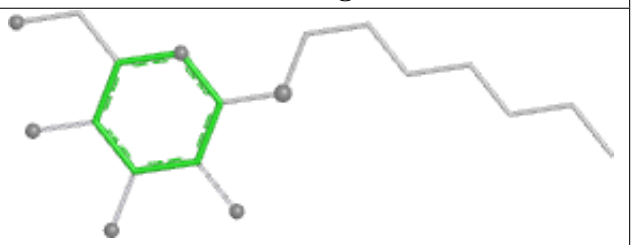
Bond lengths



Bond angles

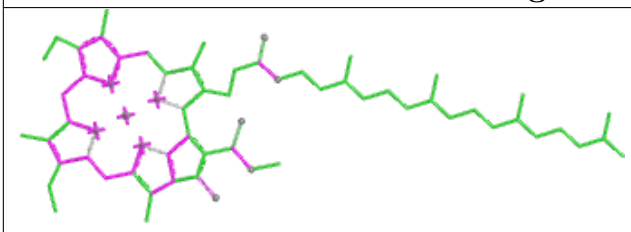


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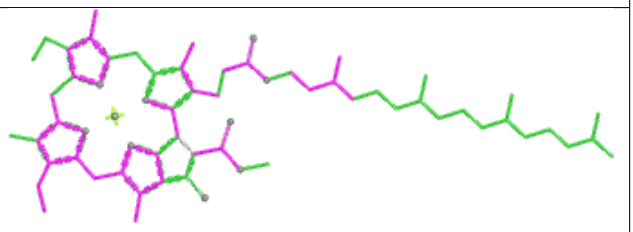


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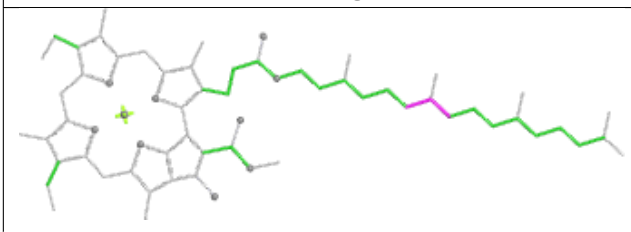
Ligand CLA a 410



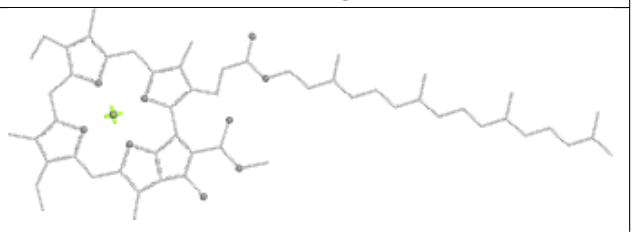
Bond lengths



Bond angles

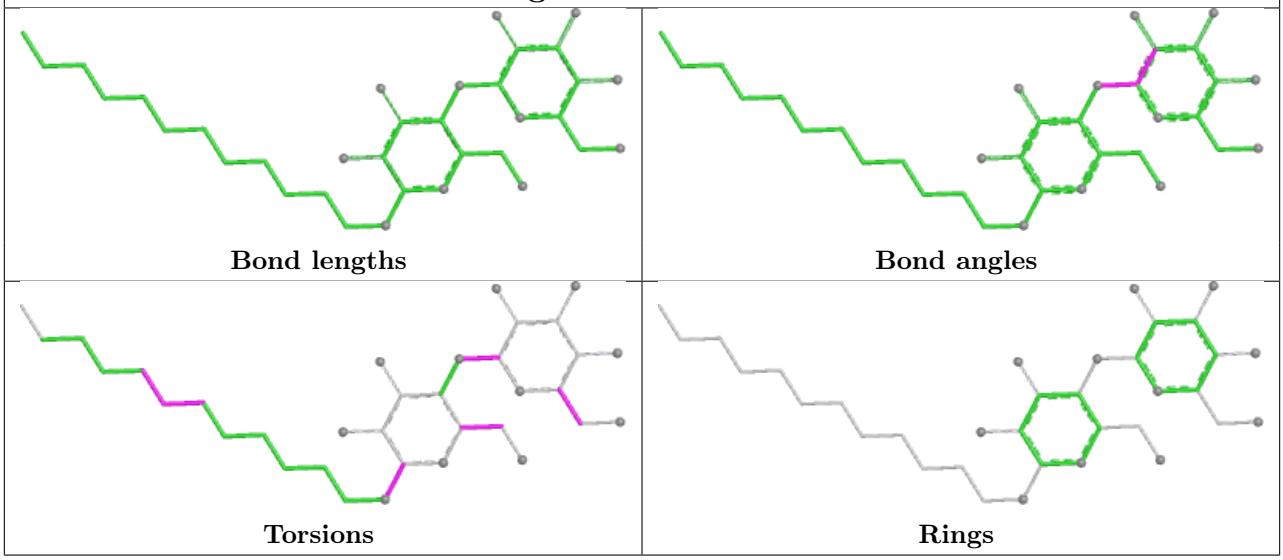


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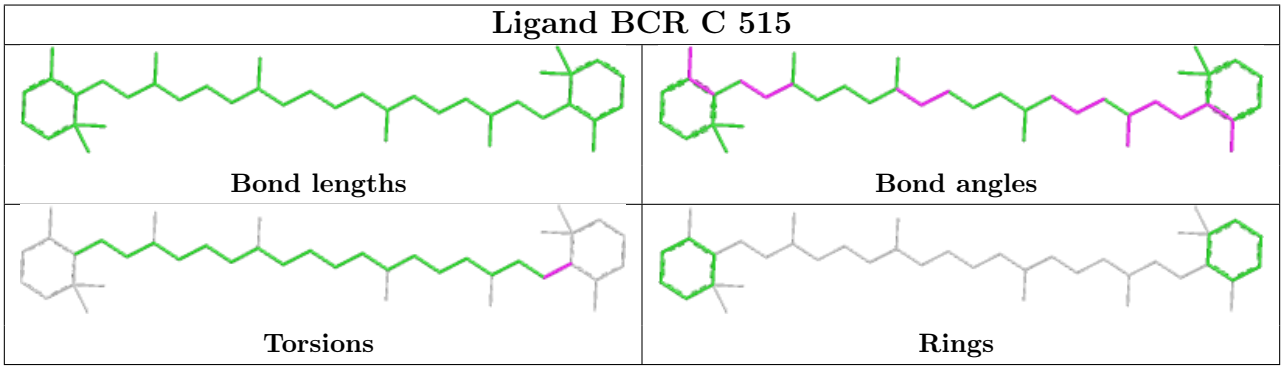


Rings

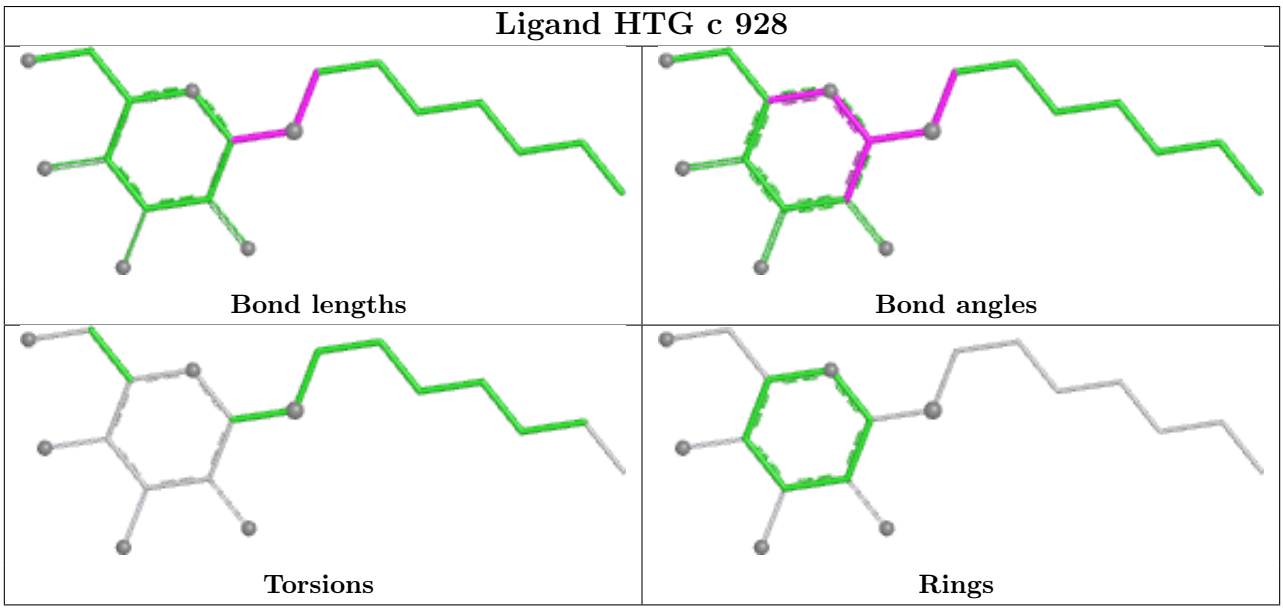
Ligand LMT t 102



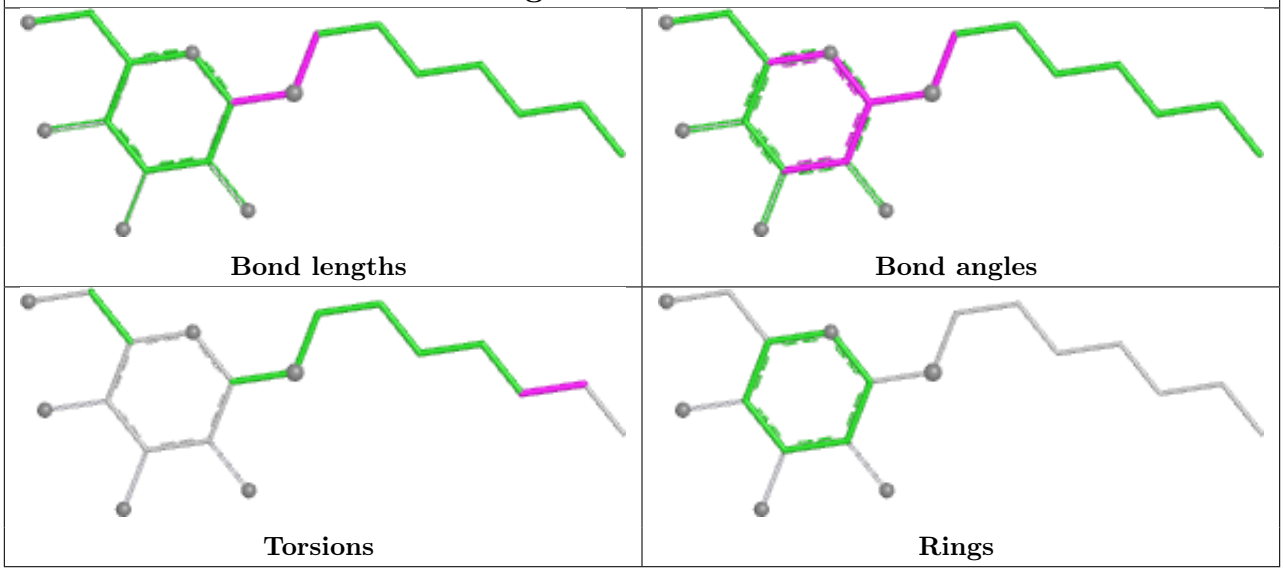
Ligand BCR C 515



Ligand HTG c 928



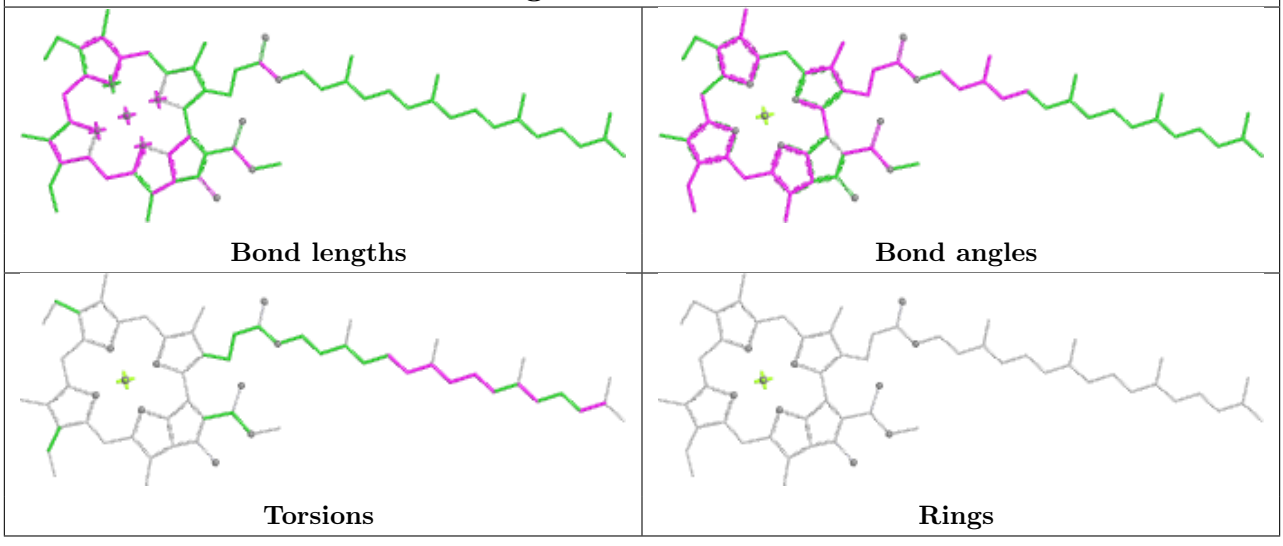
Ligand HTG v 211



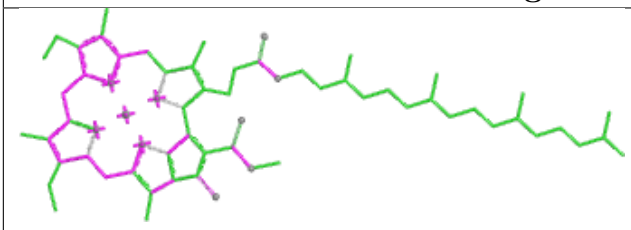
Ligand PL9 d 407



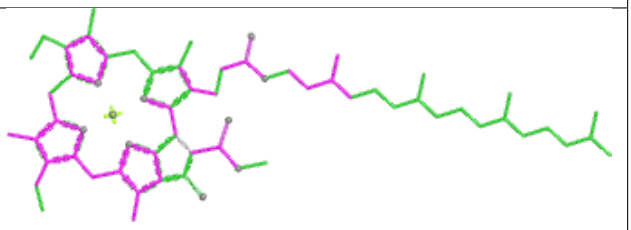
Ligand CLA B 617



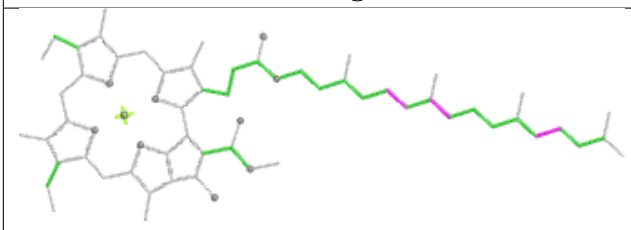
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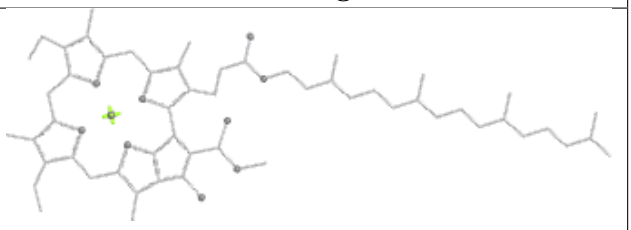
Bond lengths



Bond angles

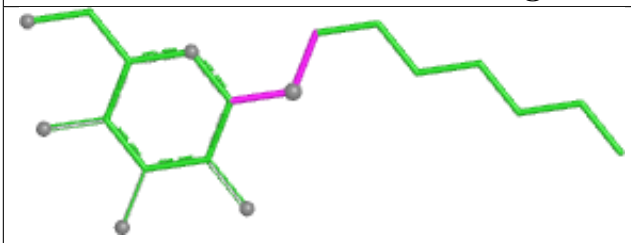


Torsions

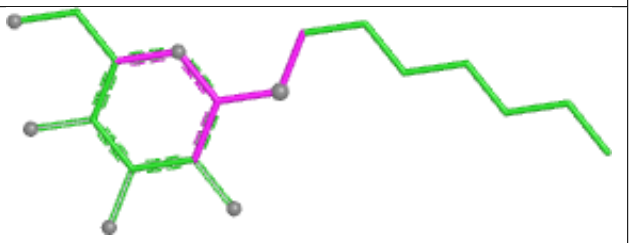


Rings

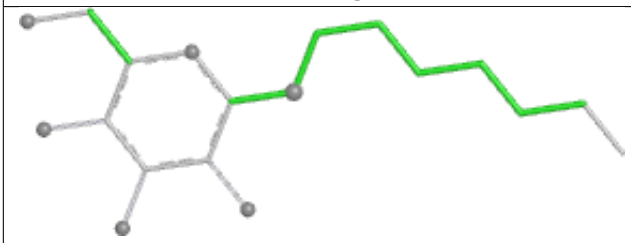
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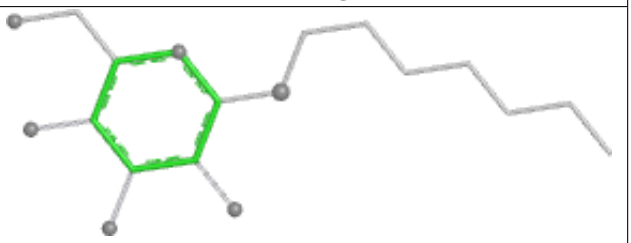
Bond lengths



Bond angles

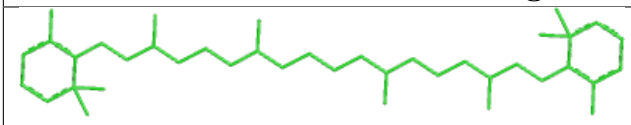


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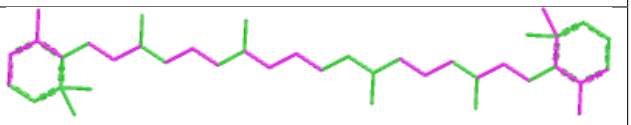


Rings

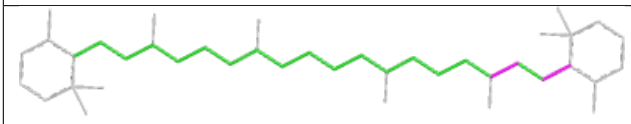
Ligand BCR d 406



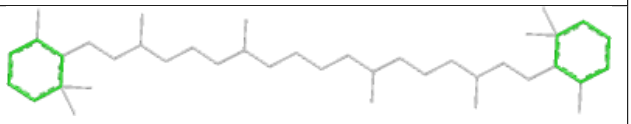
Bond lengths



Bond angles

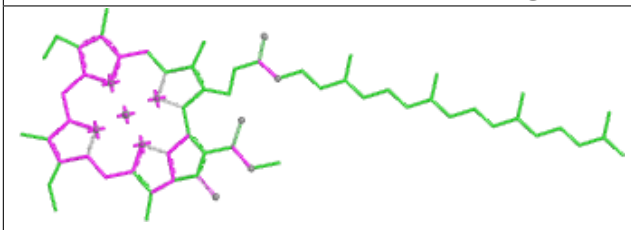


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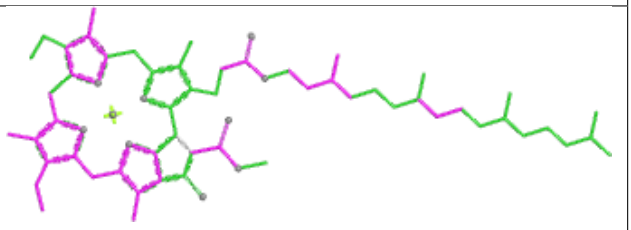


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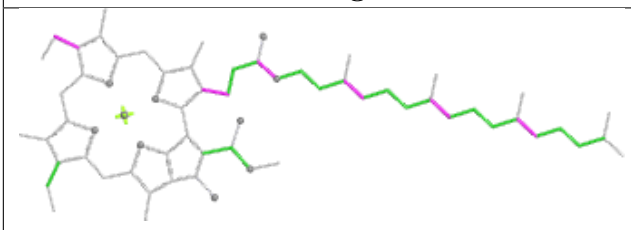
Ligand CLA C 513



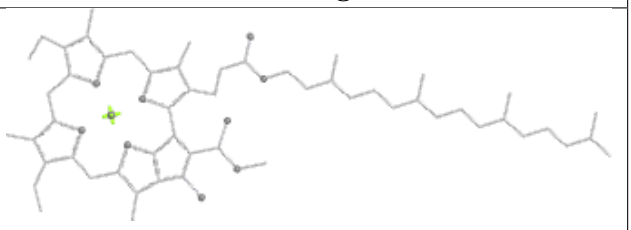
Bond lengths



Bond angles

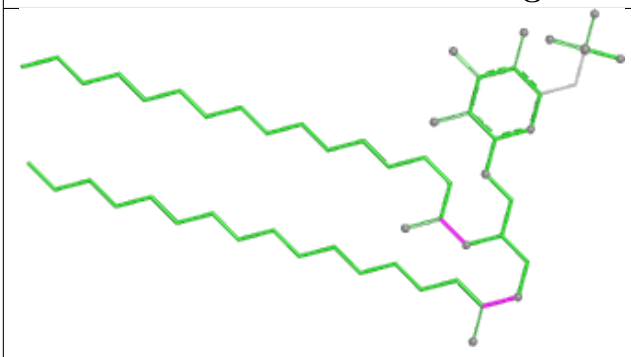


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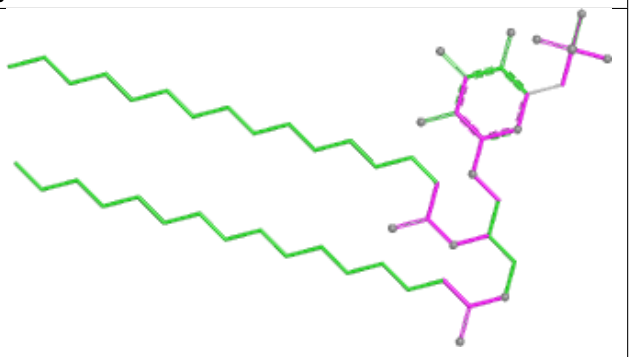


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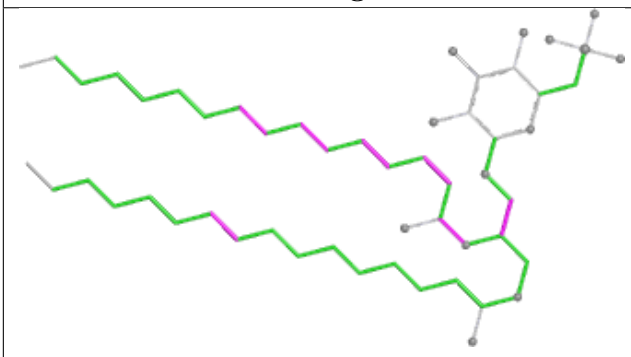
Ligand SQD A 412



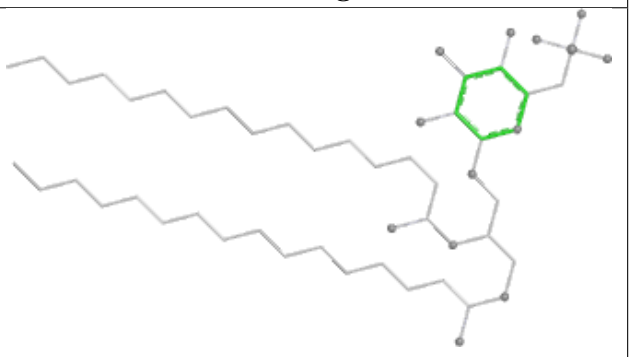
Bond lengths



Bond angles

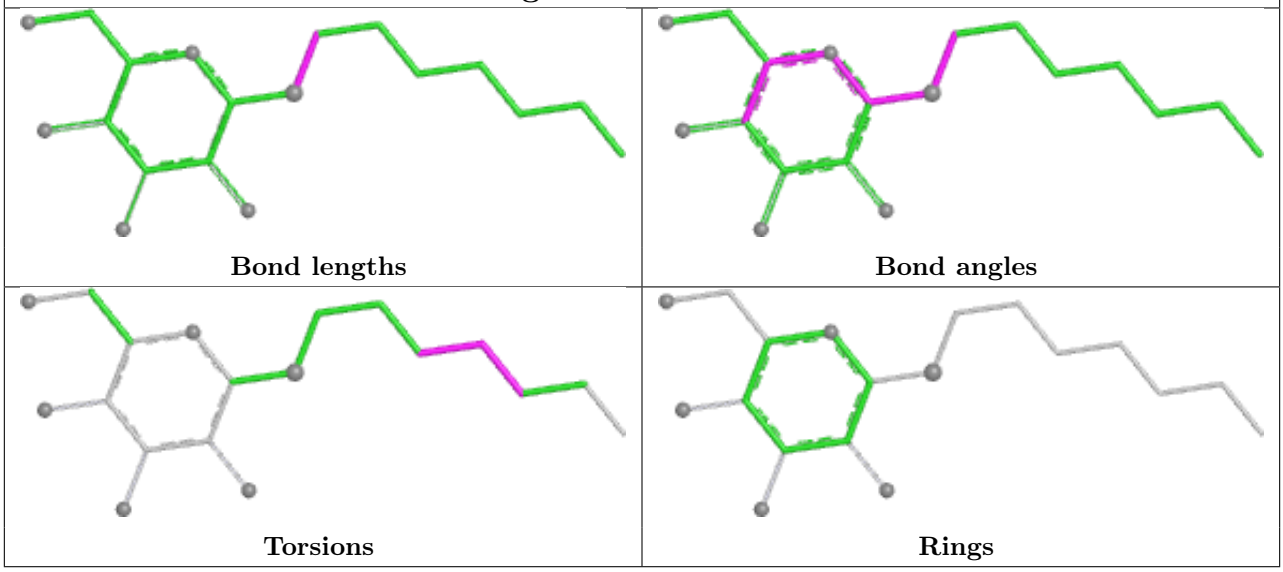


Torsions



Rings

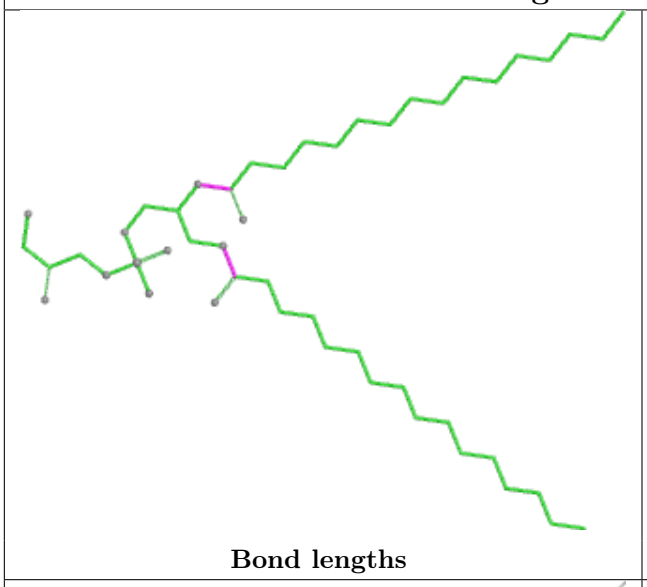
Ligand HTG C 537



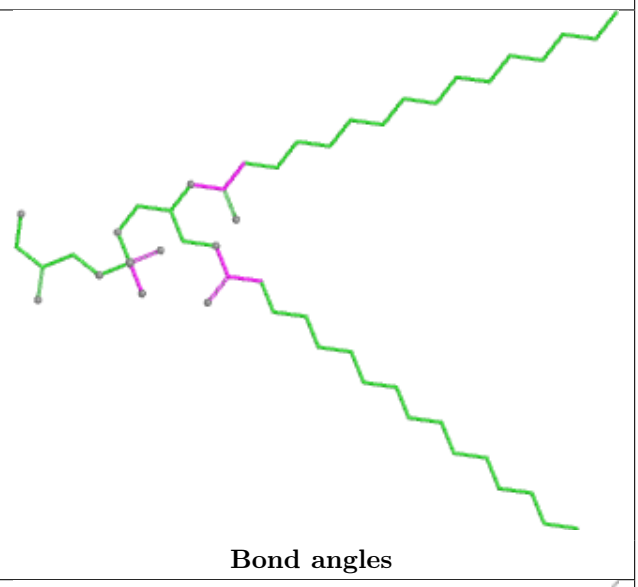
Ligand PL9 D 404



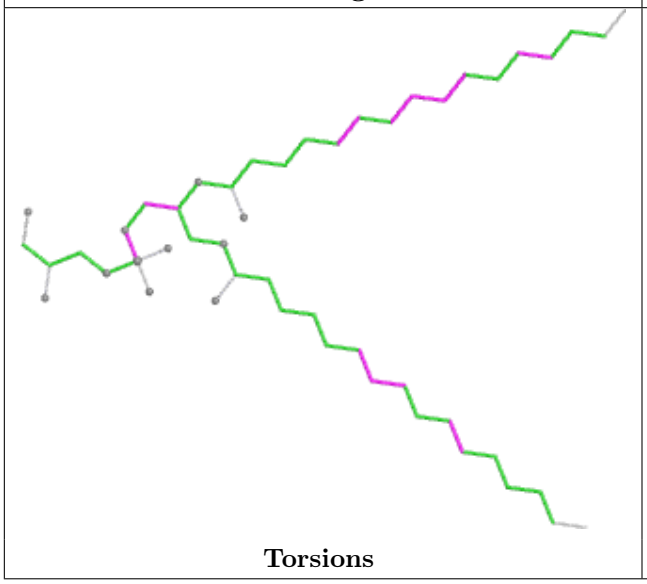
Ligand LHG l 103



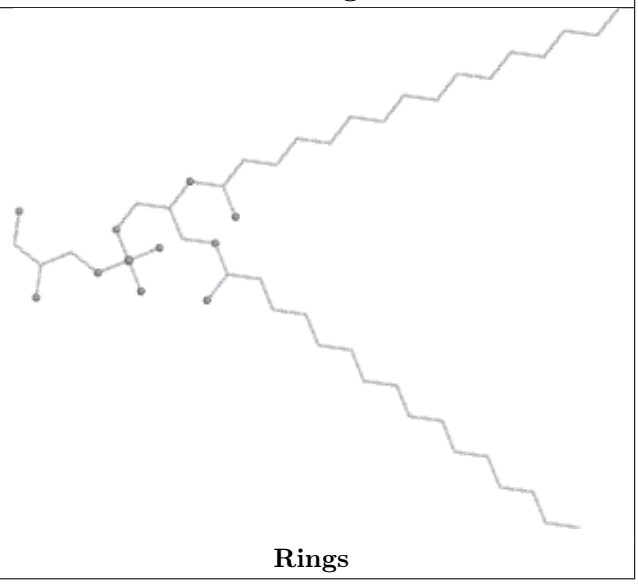
Bond lengths



Bond angles

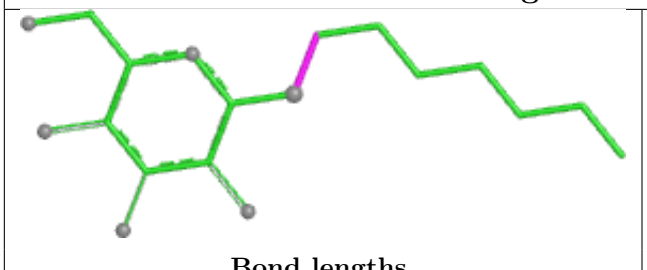


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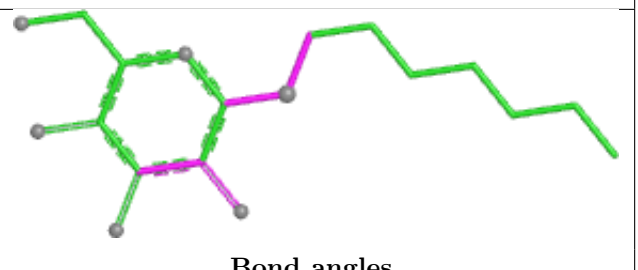


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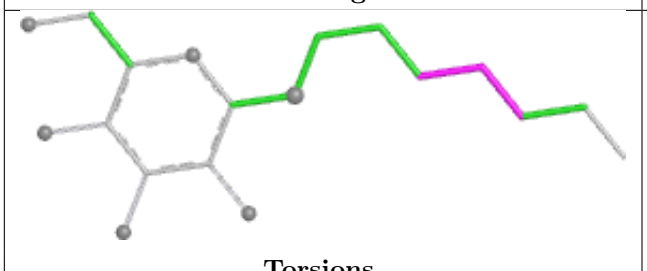
Ligand HTG O 303



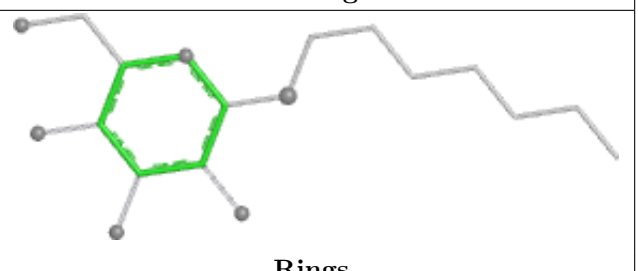
Bond lengths



Bond angles

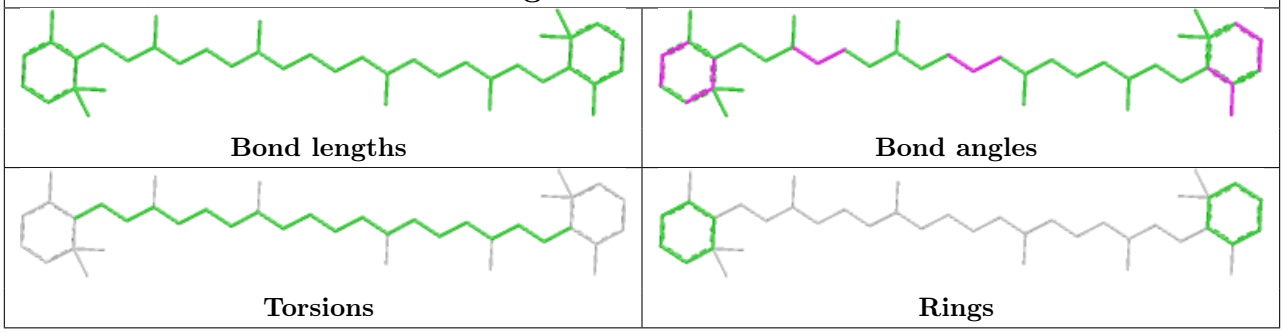


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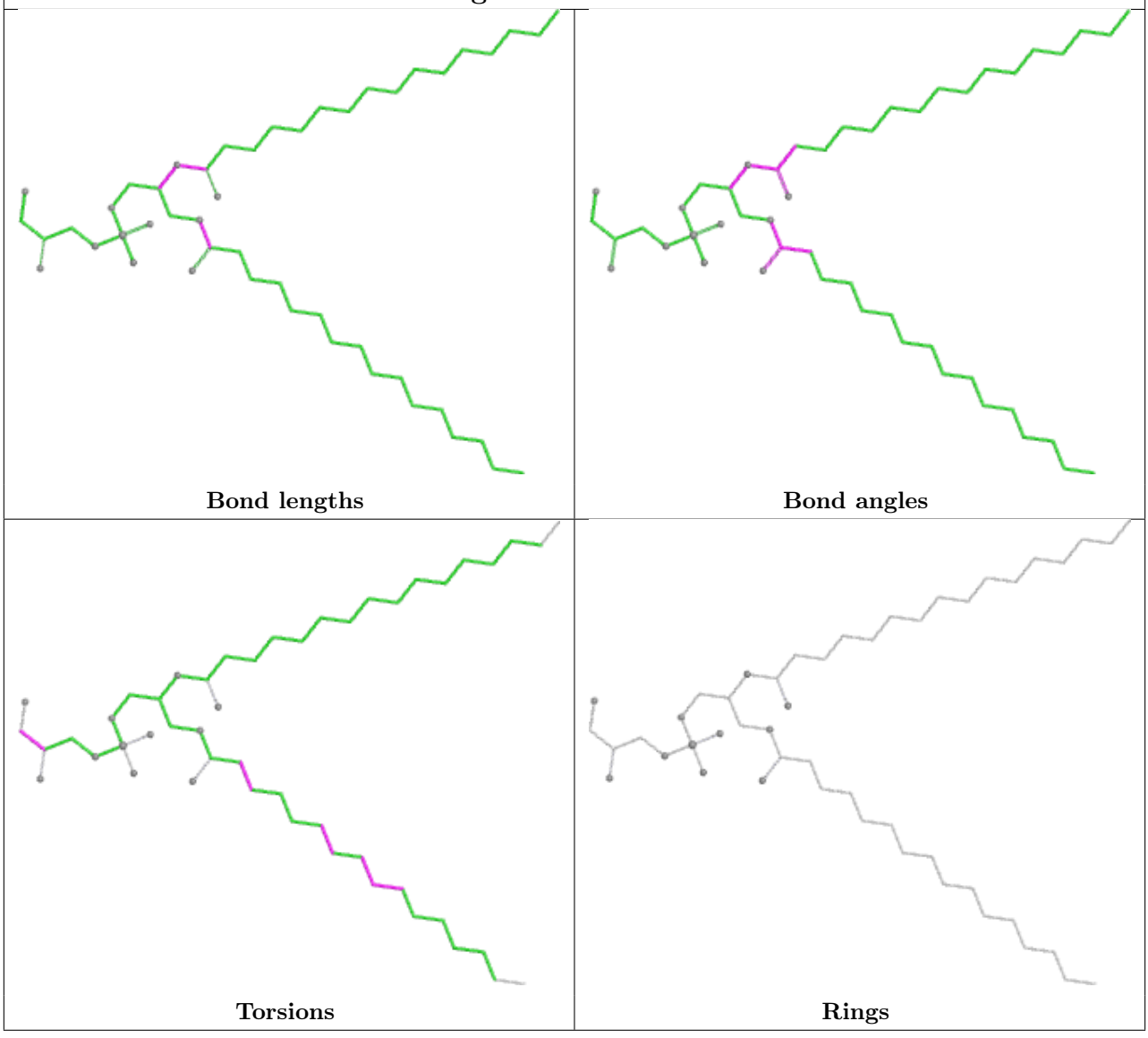


Rings

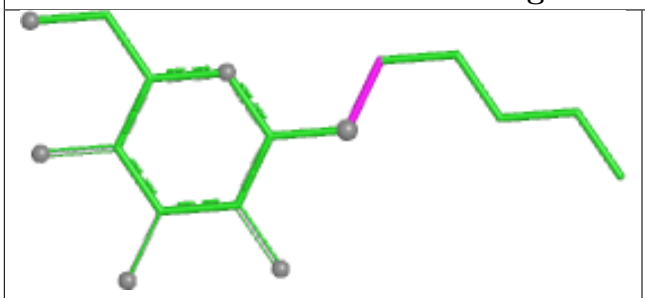
Ligand BCR B 619



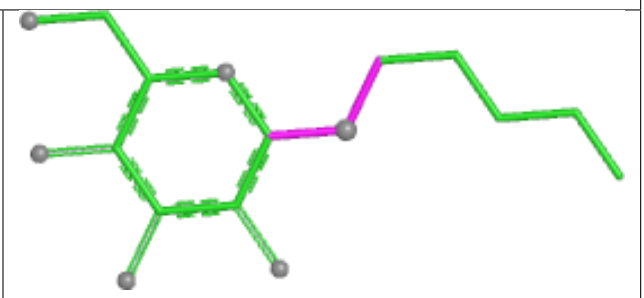
Ligand LHG d 409



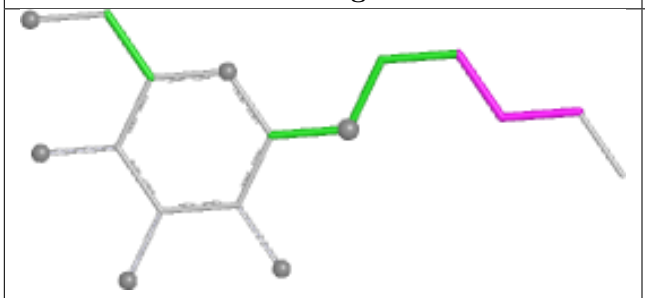
Ligand HTG c 943



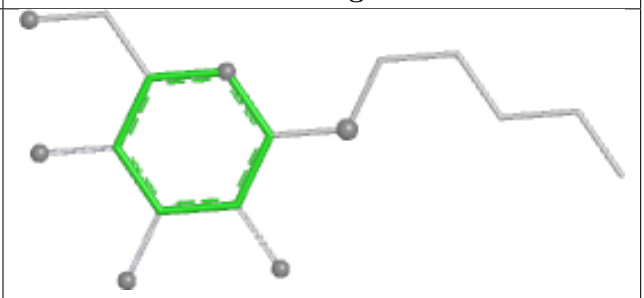
Bond lengths



Bond angles

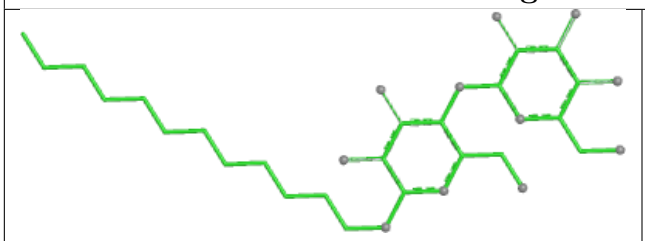


Torsions

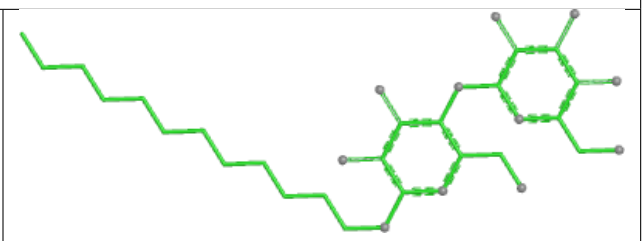


Rings

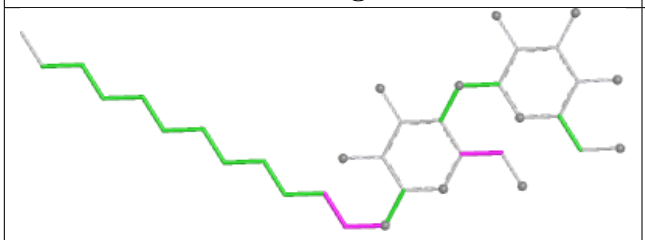
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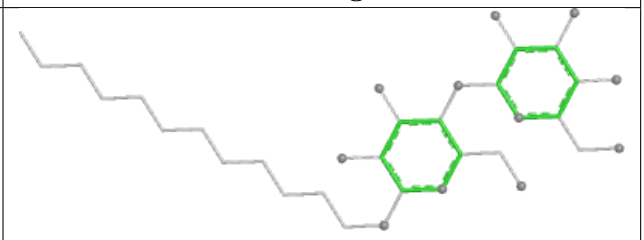
Bond lengths



Bond angles

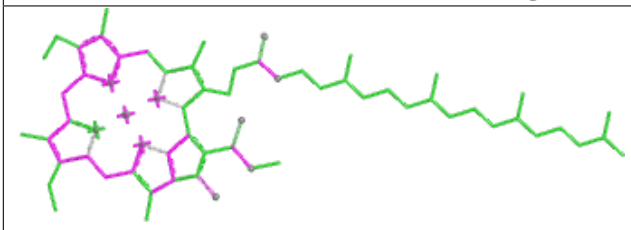


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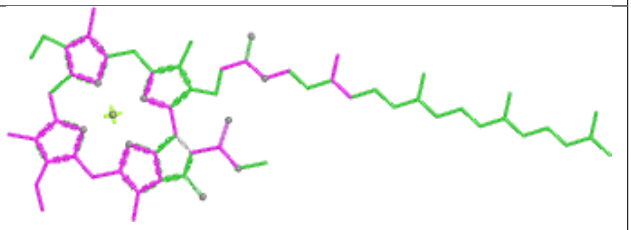


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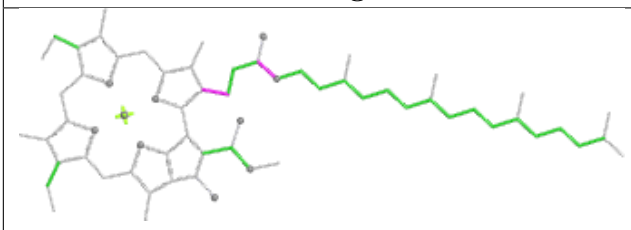
Ligand CLA C 511



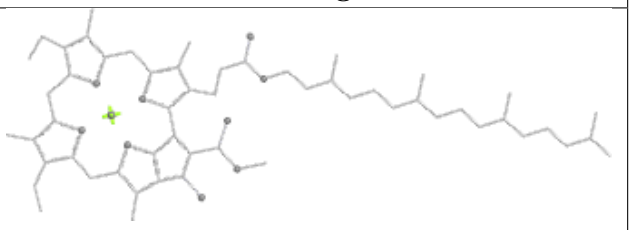
Bond lengths



Bond angles



Torsions

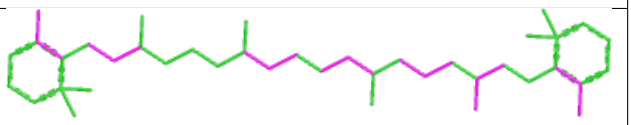


Rings

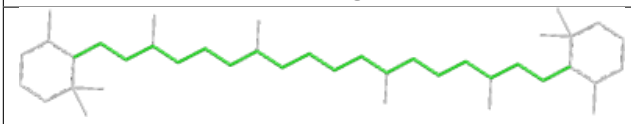
Ligand BCR c 915



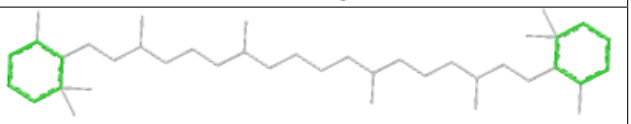
Bond lengths



Bond angles

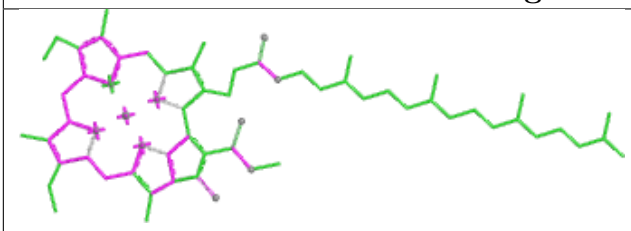


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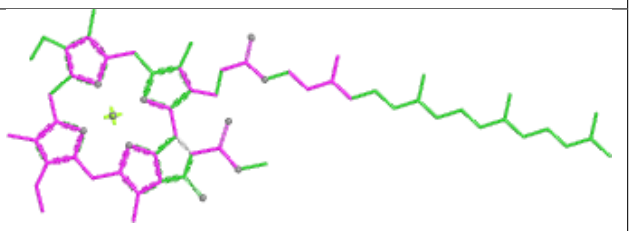


Rings

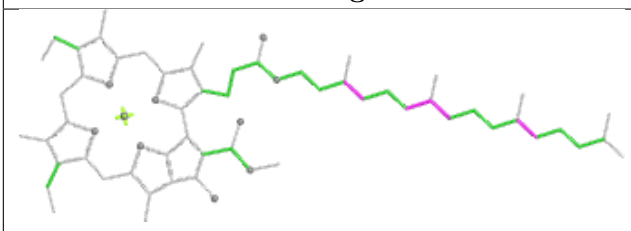
Ligand CLA C 506



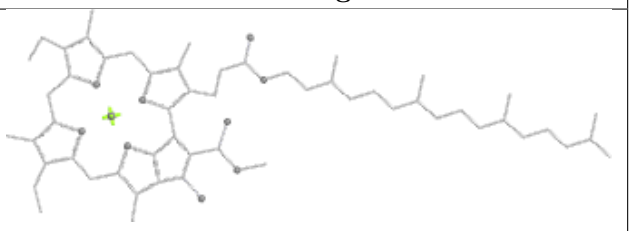
Bond lengths



Bond angles

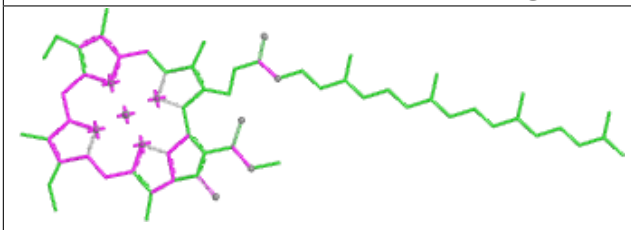


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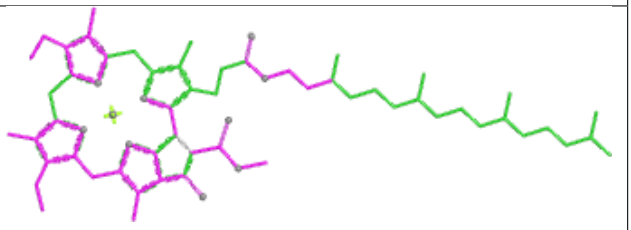


Rings

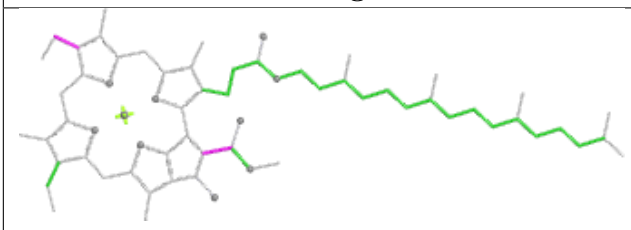
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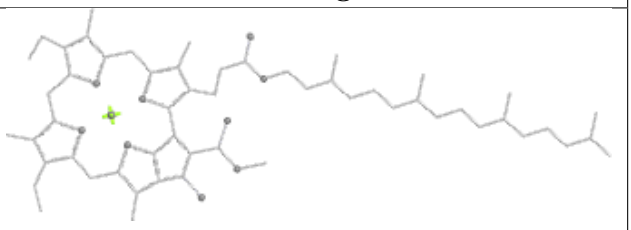
Bond lengths



Bond angles



Torsions

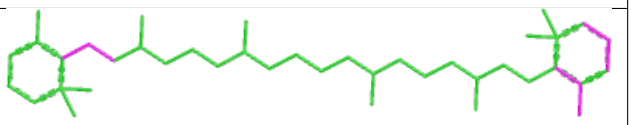


Rings

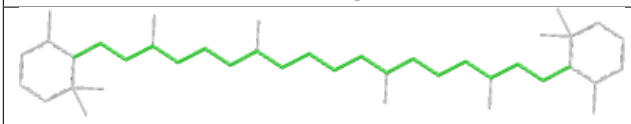
Ligand BCR b 622



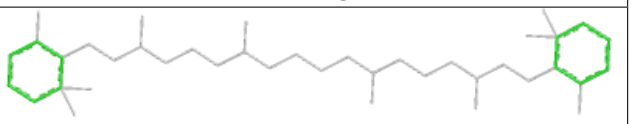
Bond lengths



Bond angles

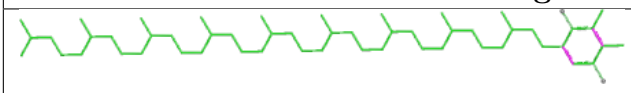


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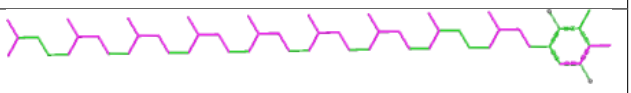


Rings

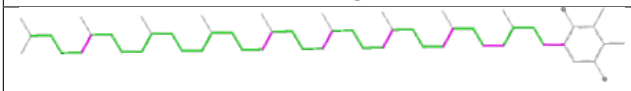
Ligand PL9 a 417



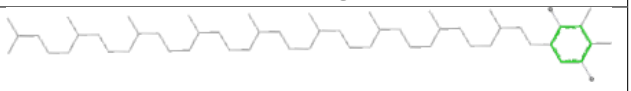
Bond lengths



Bond angles

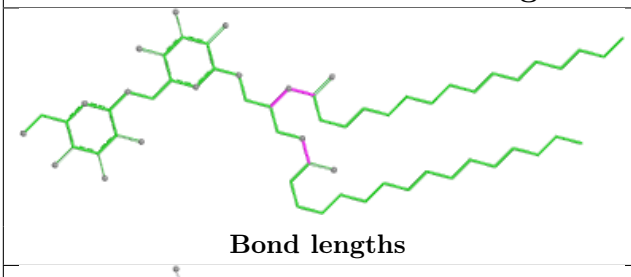


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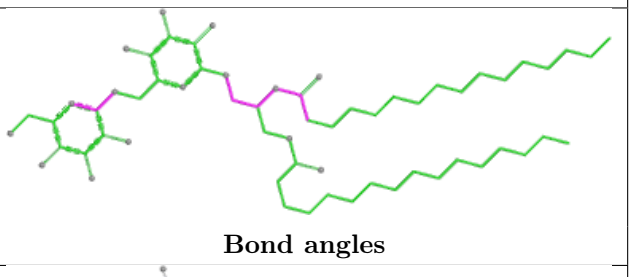


Rings

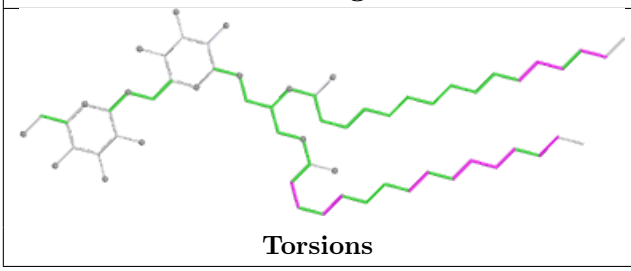
Ligand DGD C 518



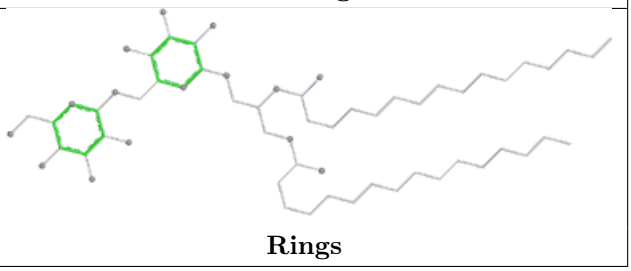
Bond lengths



Bond angles

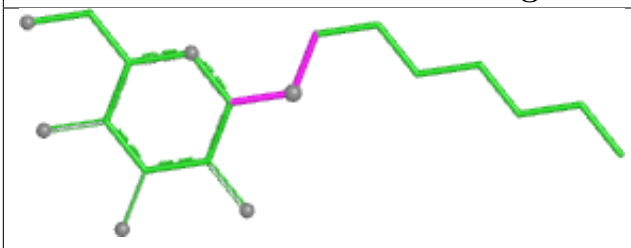


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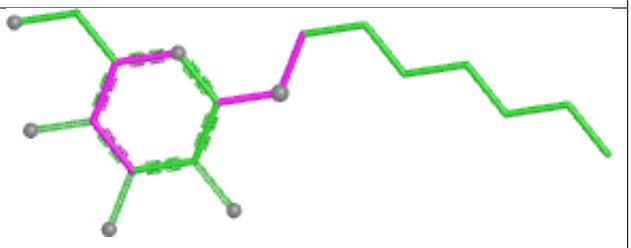


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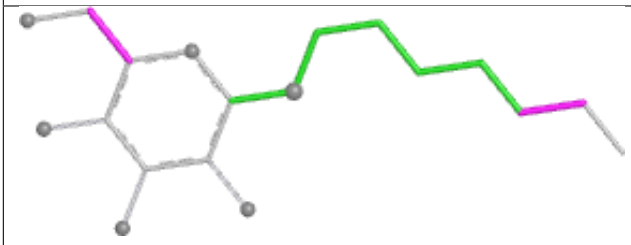
Ligand HTG B 629



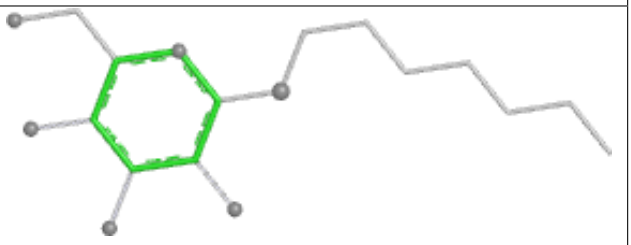
Bond lengths



Bond angles



Torsions

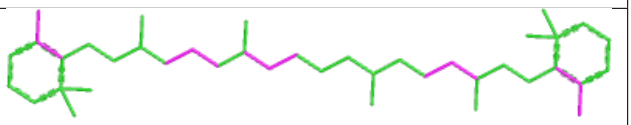


Rings

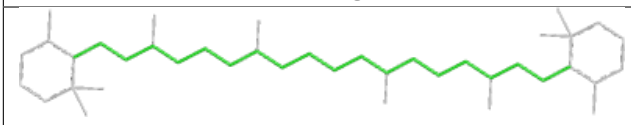
Ligand BCR A 411



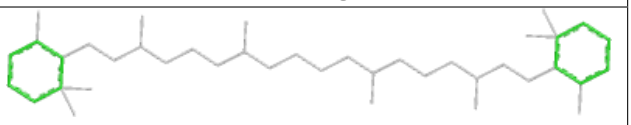
Bond lengths



Bond angles

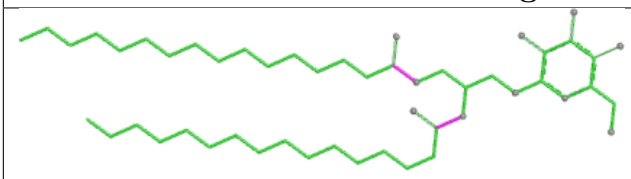


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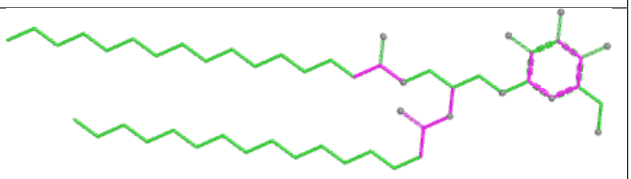


Rings

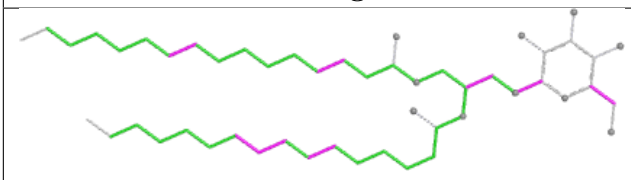
Ligand LMG C 523



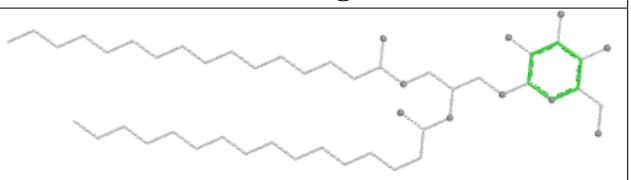
Bond lengths



Bond angles

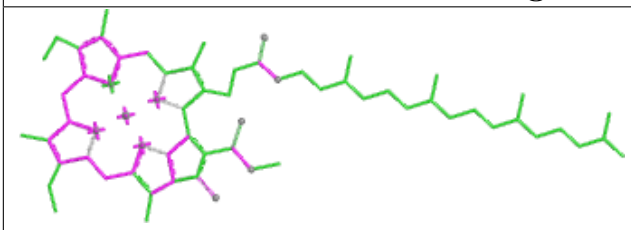


Torsions

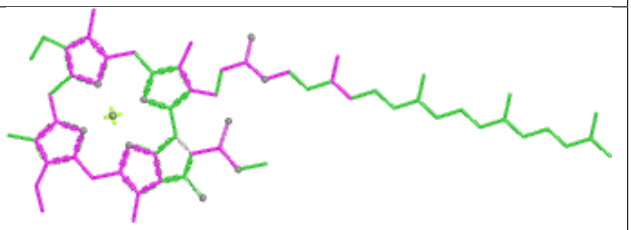


Rings

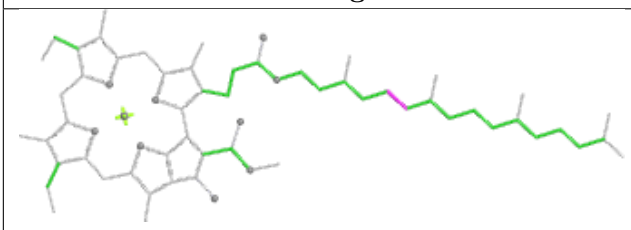
Ligand CLA b 607



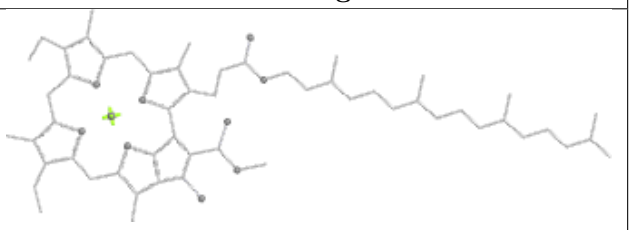
Bond lengths



Bond angles

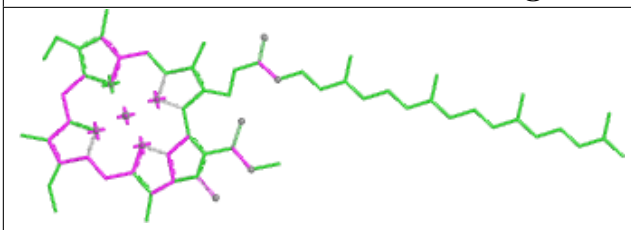


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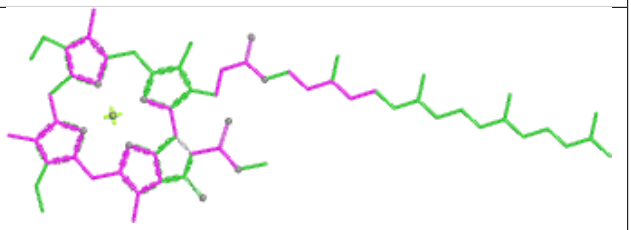


Rings

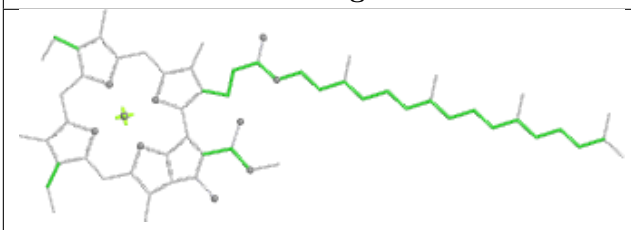
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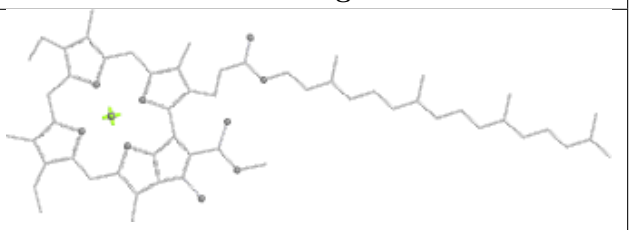
Bond lengths



Bond angles

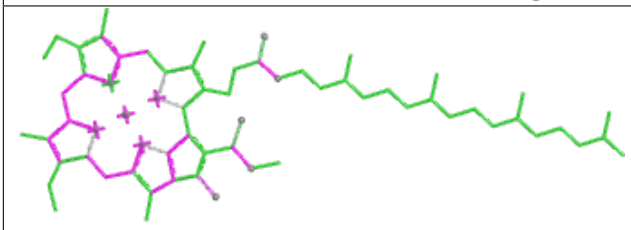


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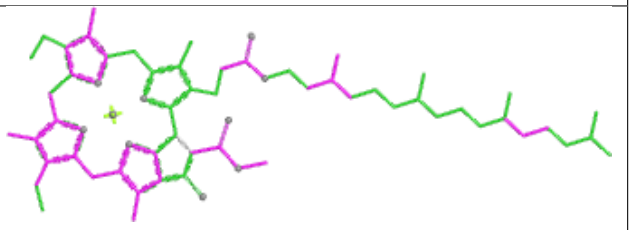


Rings

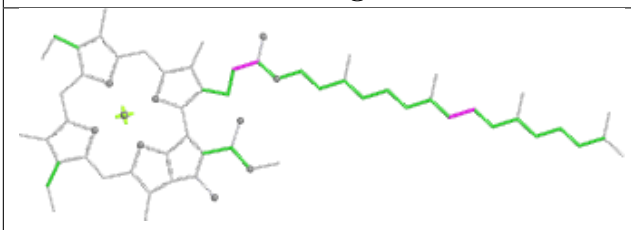
Ligand CLA b 616



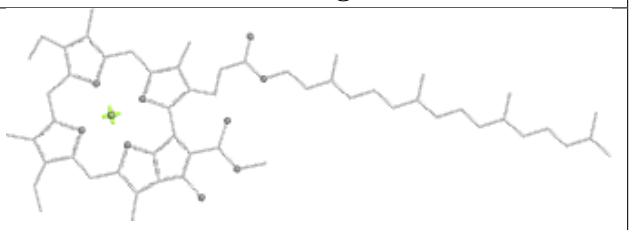
Bond lengths



Bond angles

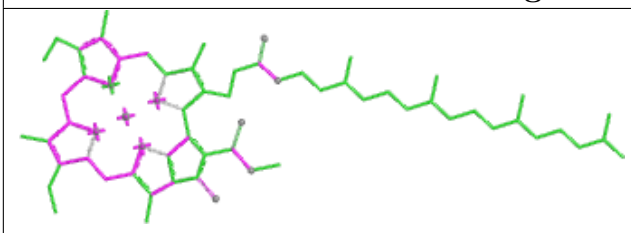


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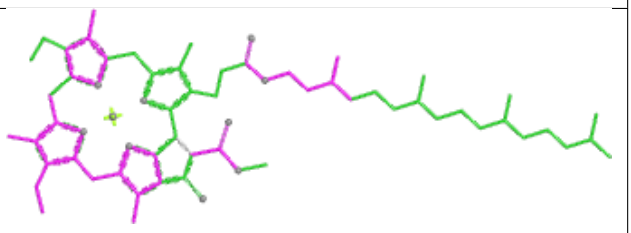


Rings

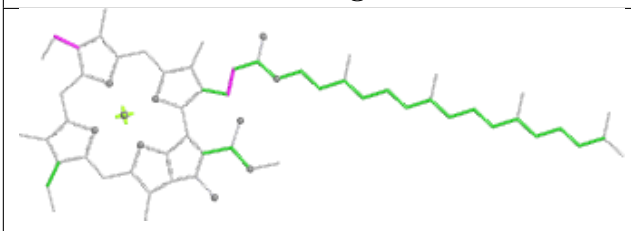
Ligand CLA C 501



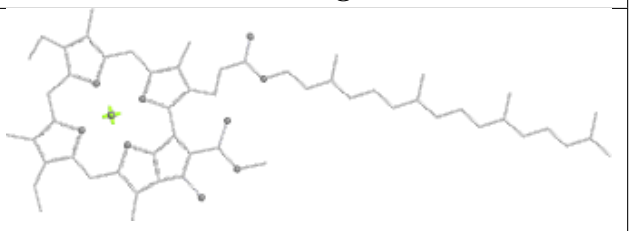
Bond lengths



Bond angles

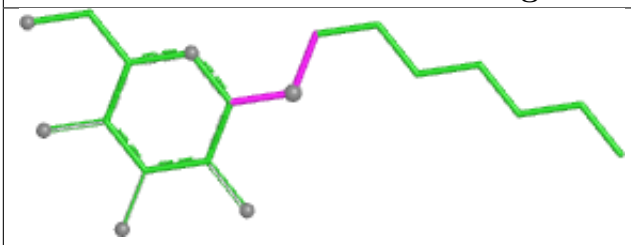


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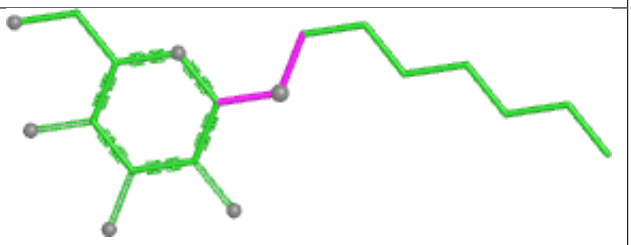


Rings

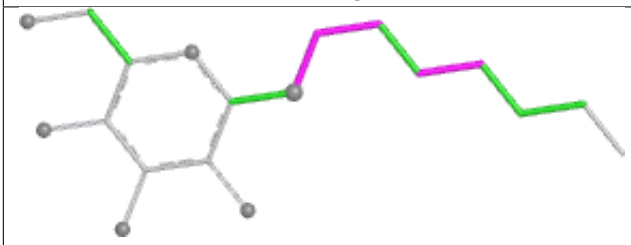
Ligand HTG C 520



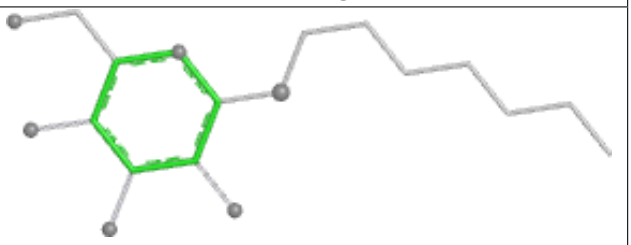
Bond lengths



Bond angles

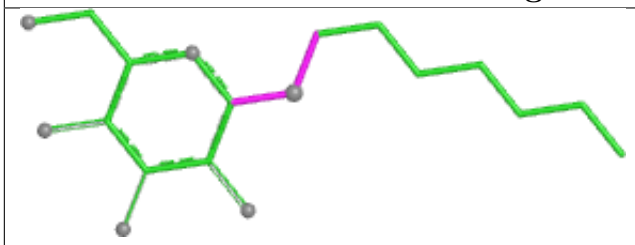


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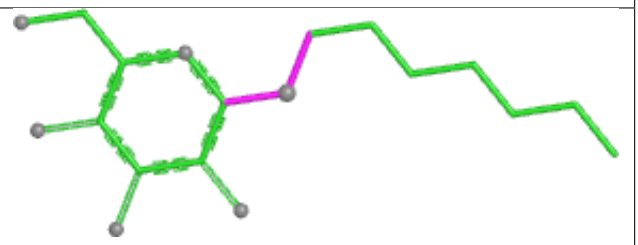


Rings

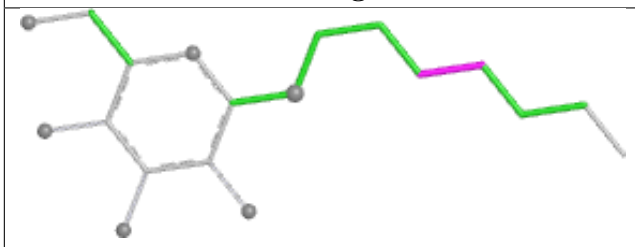
Ligand HTG d 419



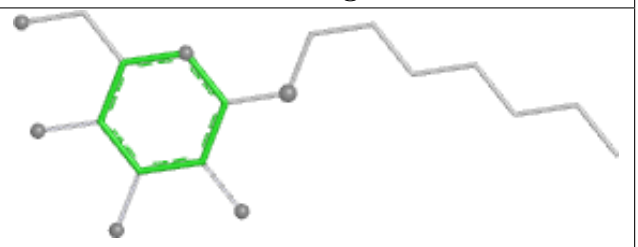
Bond lengths



Bond angles

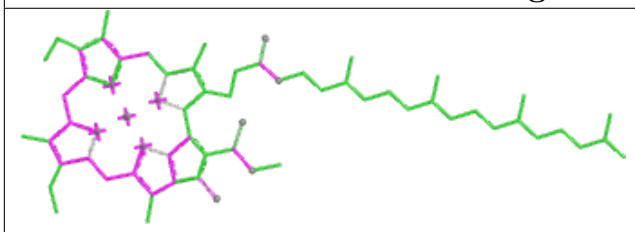


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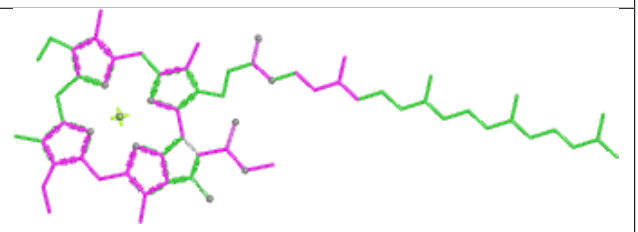


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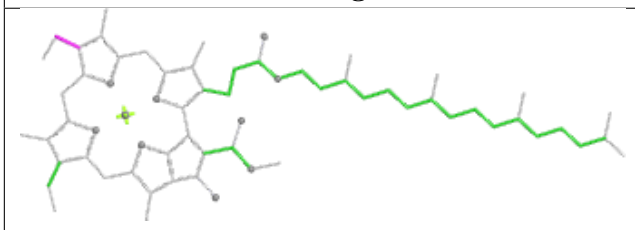
Ligand CLA b 613



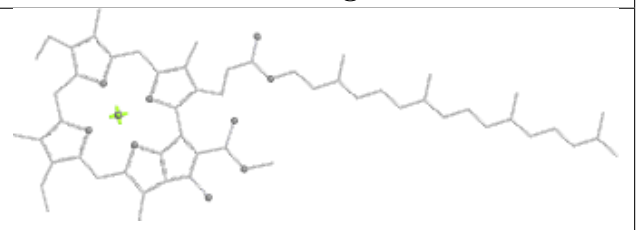
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Bond angles

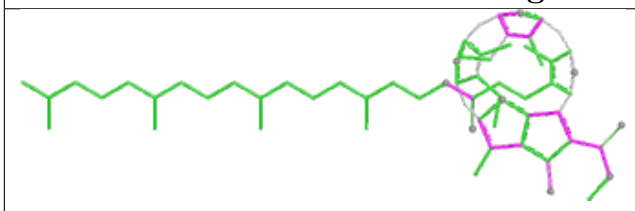


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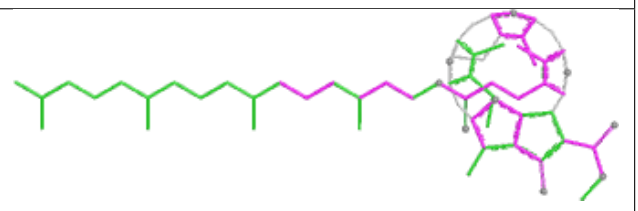


Rings

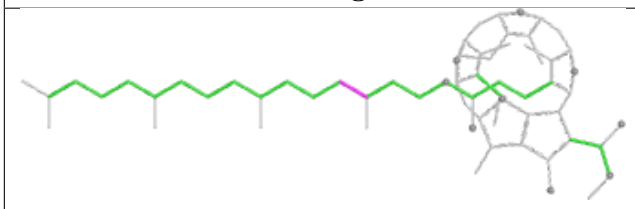
Ligand PHO a 411



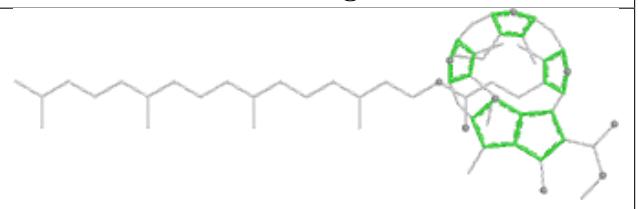
Bond lengths



Bond angles

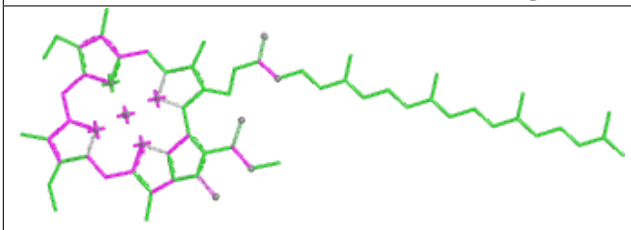


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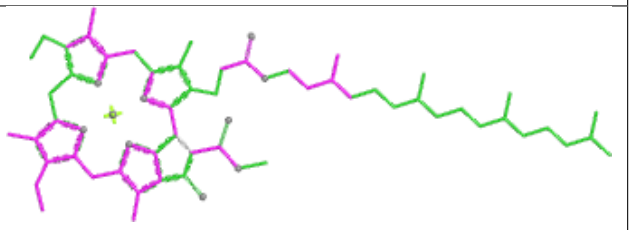


Rings

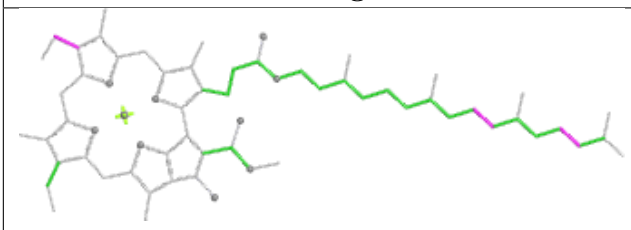
Ligand CLA C 503



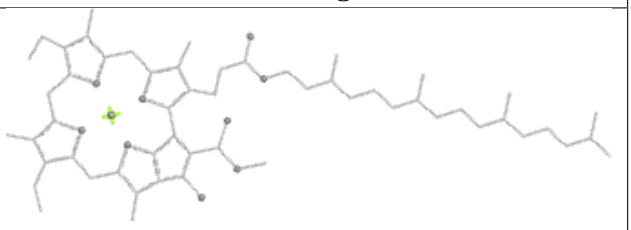
Bond lengths



Bond angles

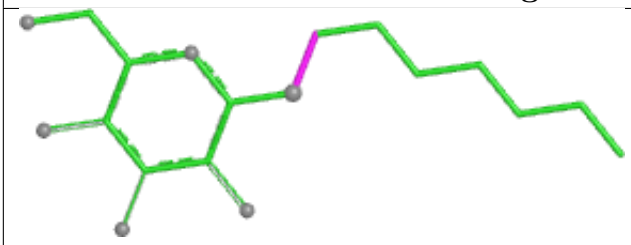


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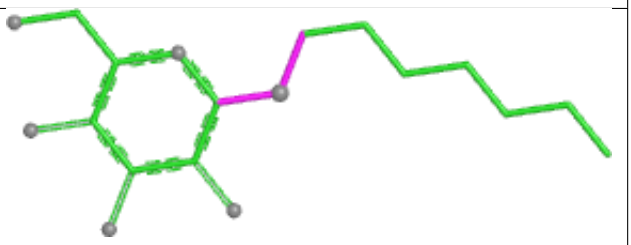


Rings

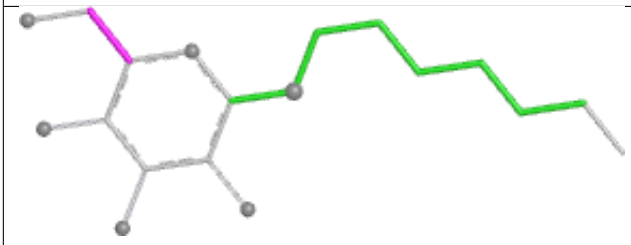
Ligand HTG B 623



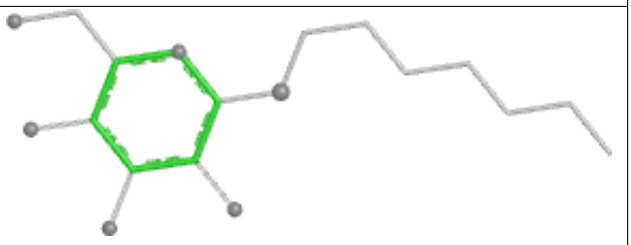
Bond lengths



Bond angles

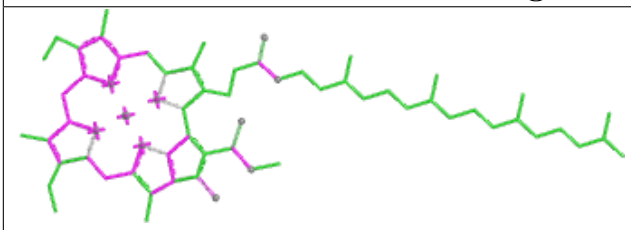


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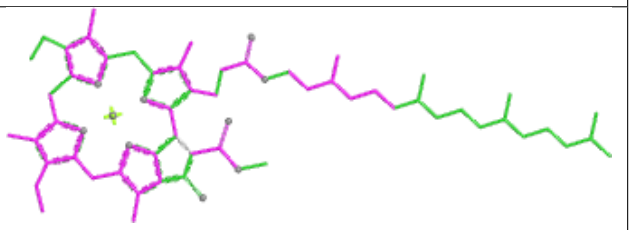


Rings

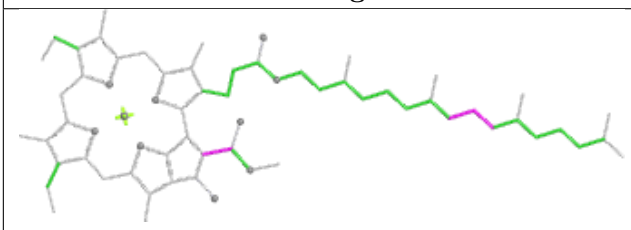
Ligand CLA b 609



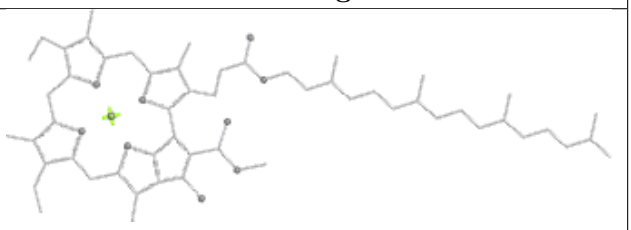
Bond lengths



Bond angles

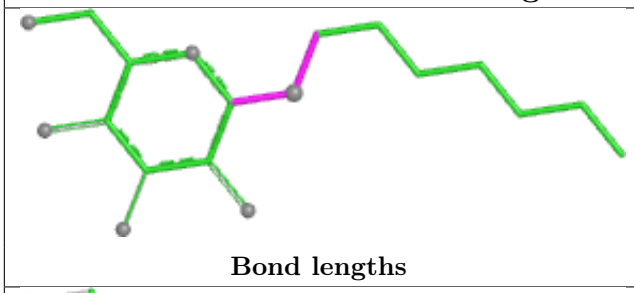


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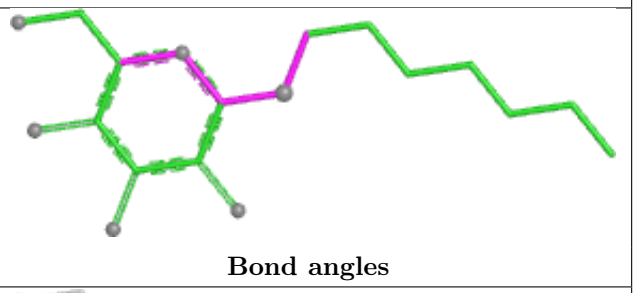


Rings

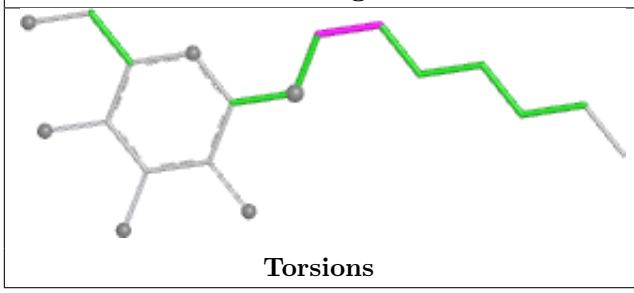
Ligand HTG C 521



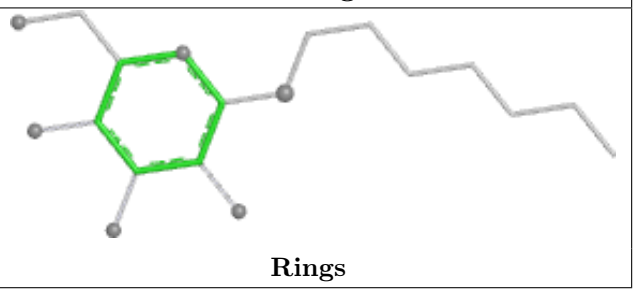
Bond lengths



Bond angles

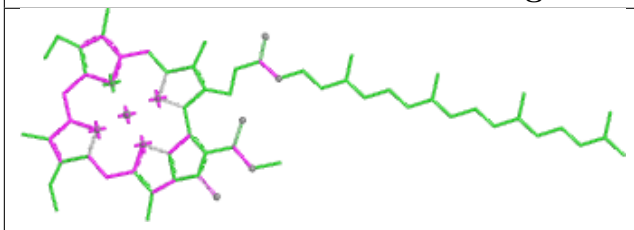


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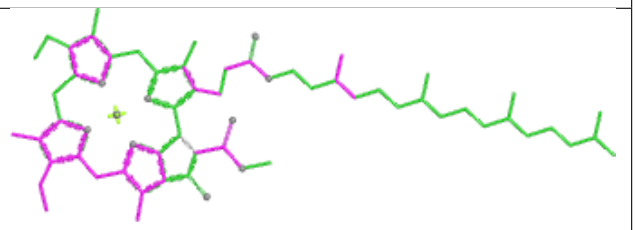


Rings

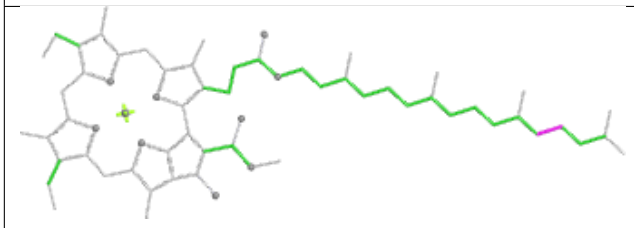
Ligand CLA B 613



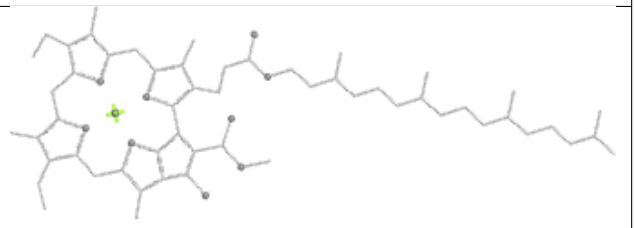
Bond lengths



Bond angles

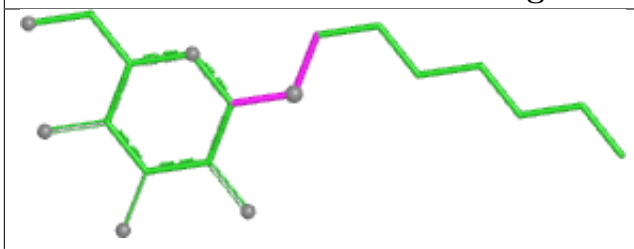


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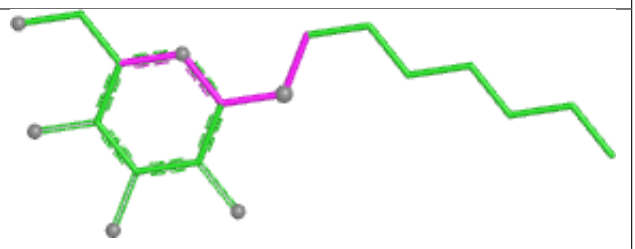


Rings

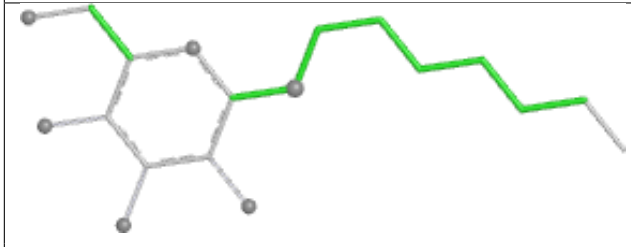
Ligand HTG c 924



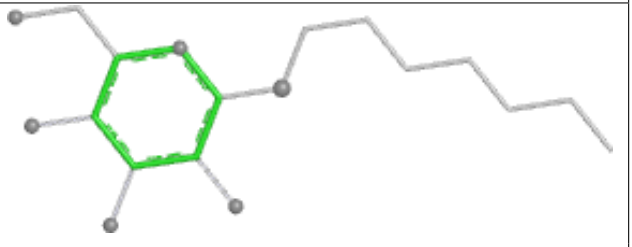
Bond lengths



Bond angles

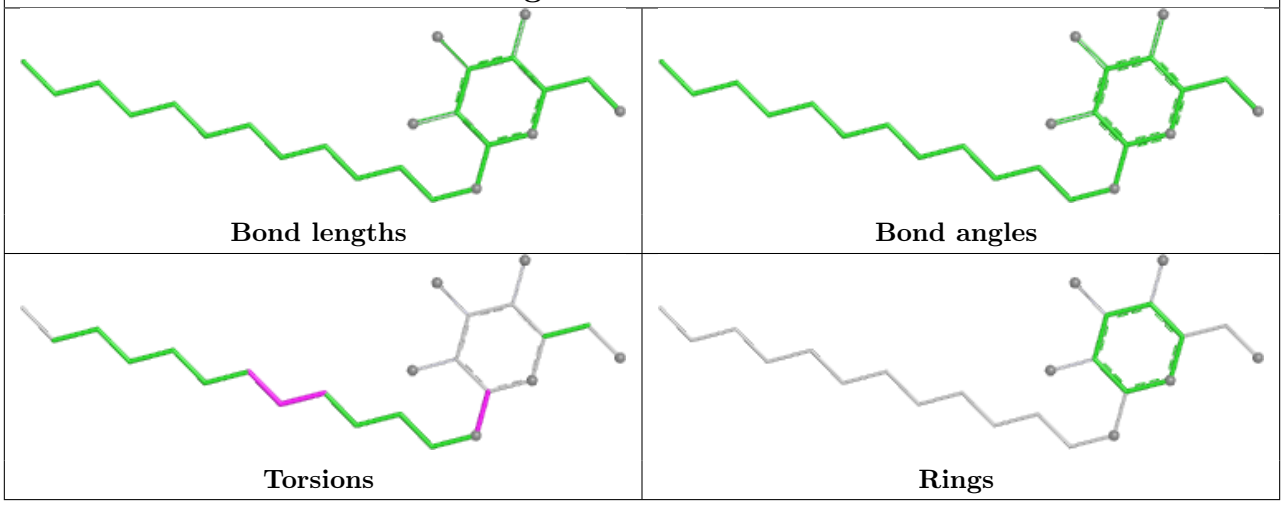


Torsions

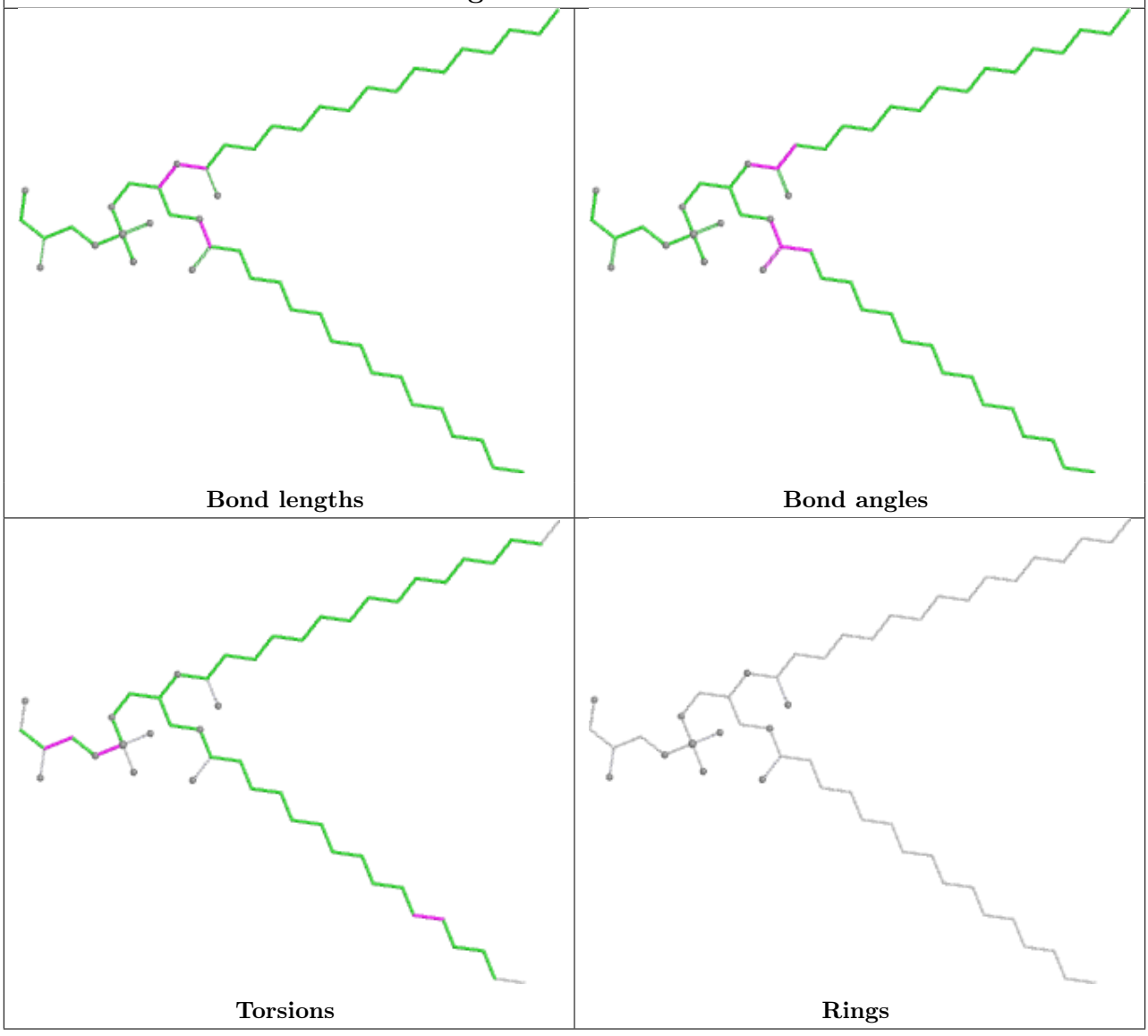


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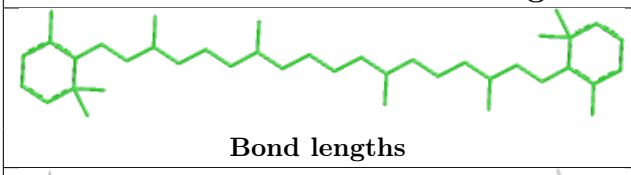
Ligand LMT F 103



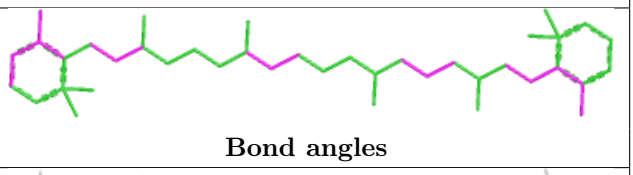
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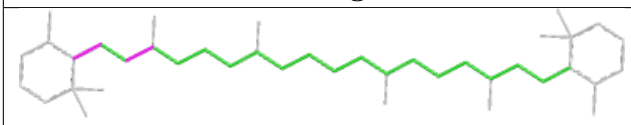
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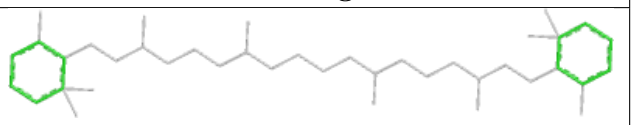
Bond lengths



Bond angles

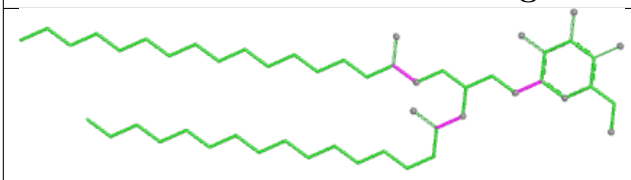


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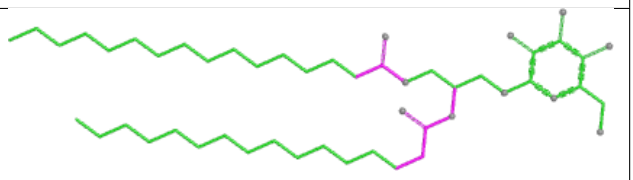


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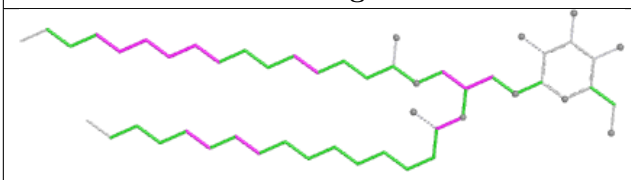
Ligand LMG C 519



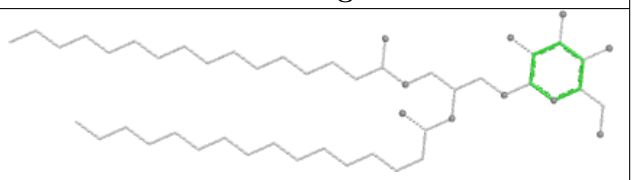
Bond lengths



Bond angles

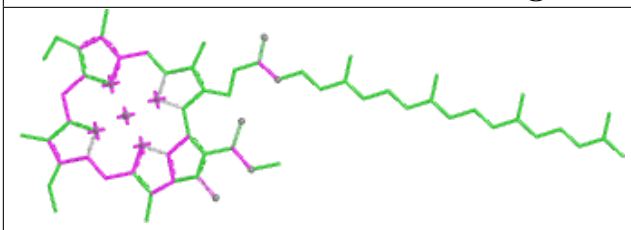


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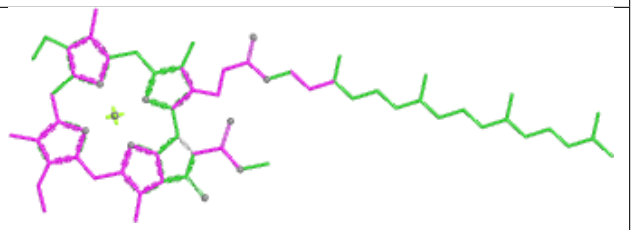


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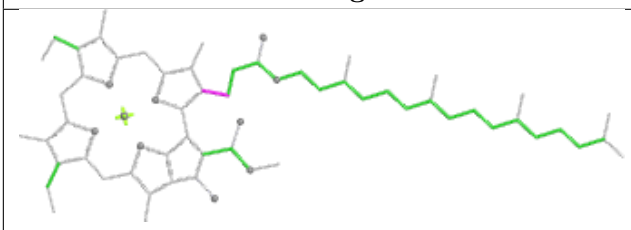
Ligand CLA b 611



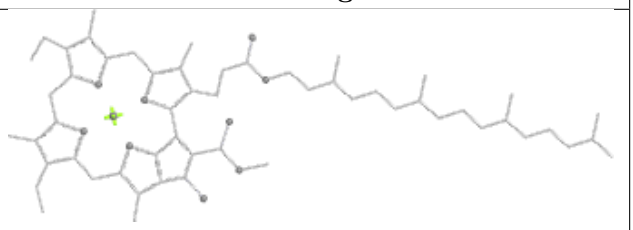
Bond lengths



Bond angles

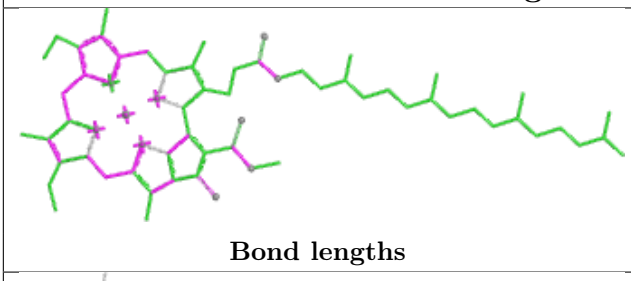


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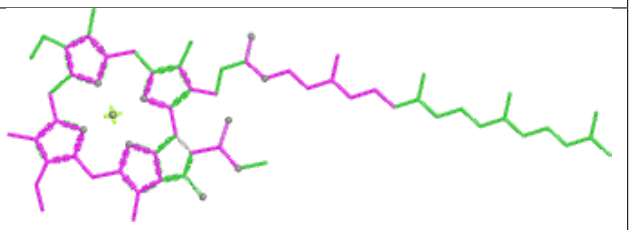


Rings

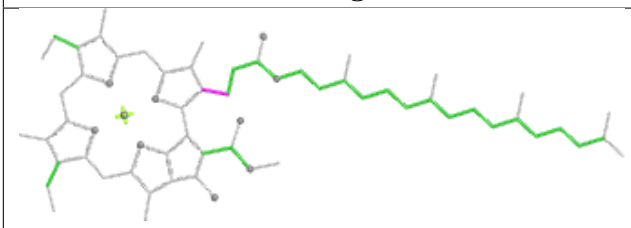
Ligand CLA B 612



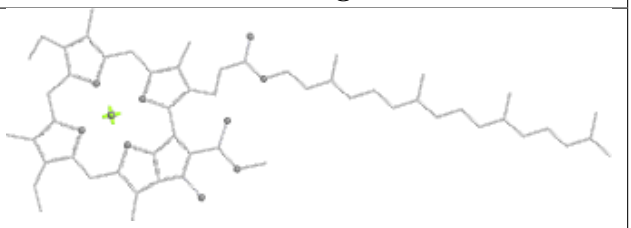
Bond lengths



Bond angles

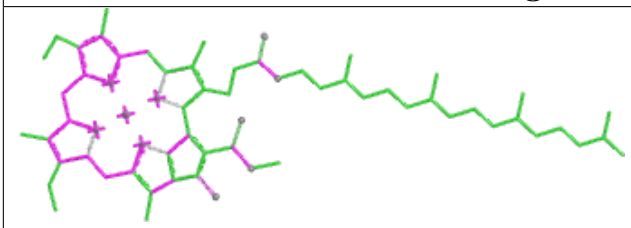


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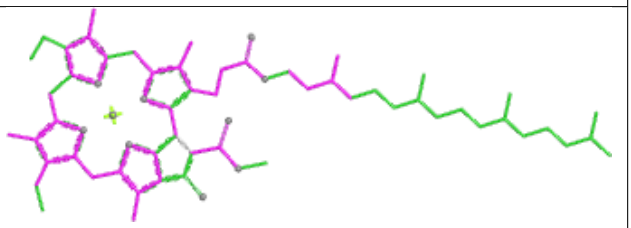


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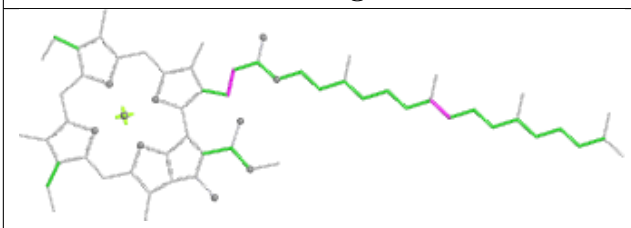
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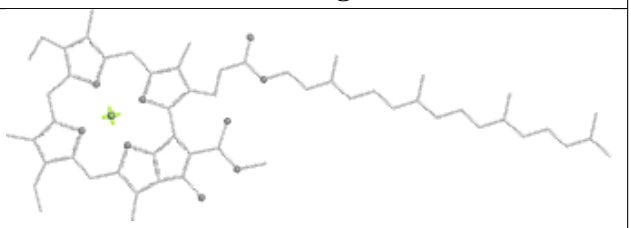
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Bond angles

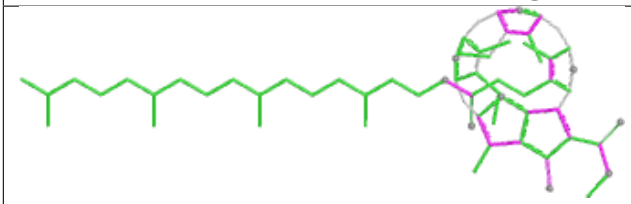


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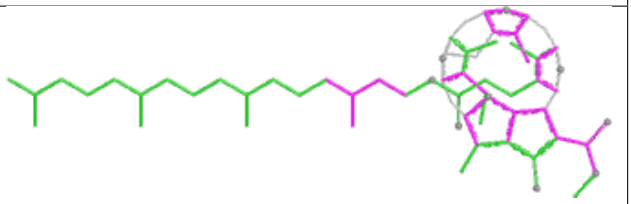


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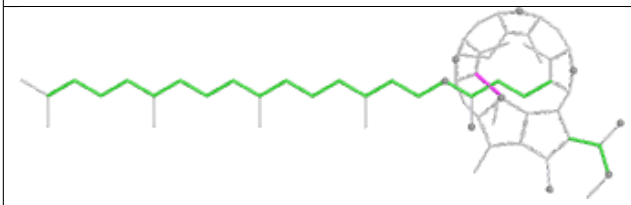
Ligand PHO a 412



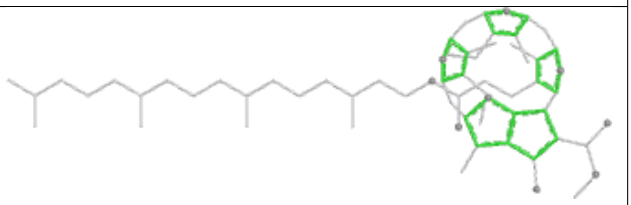
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Bond angles

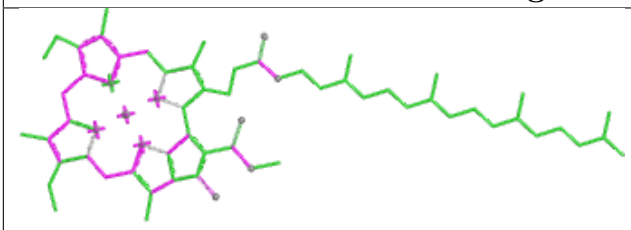


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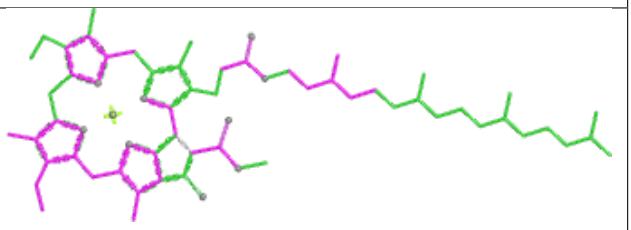


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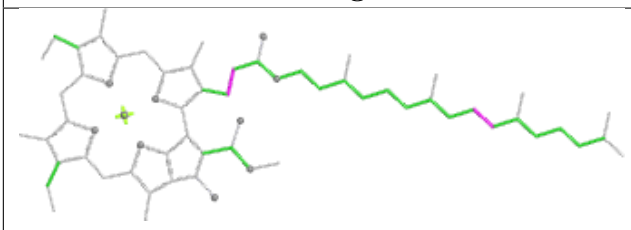
Ligand CLA b 610



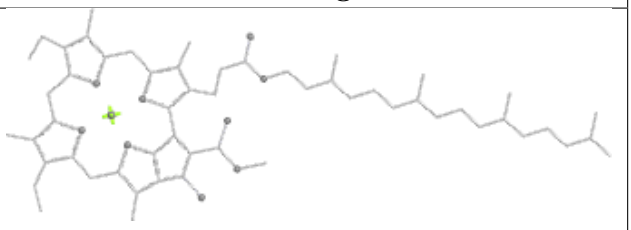
Bond lengths



Bond angles

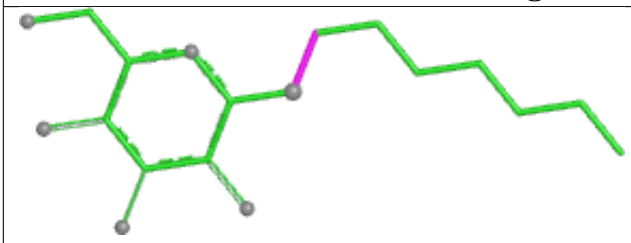


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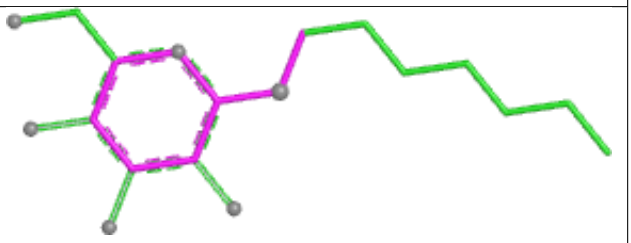


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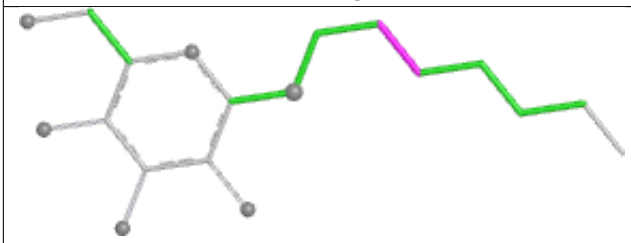
Ligand HTG c 941



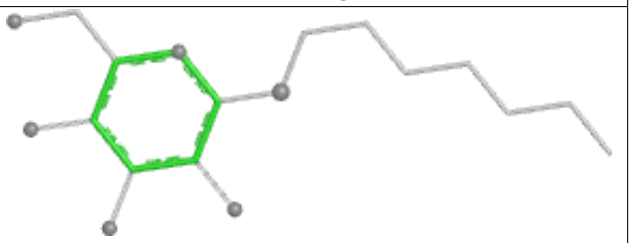
Bond lengths



Bond angles

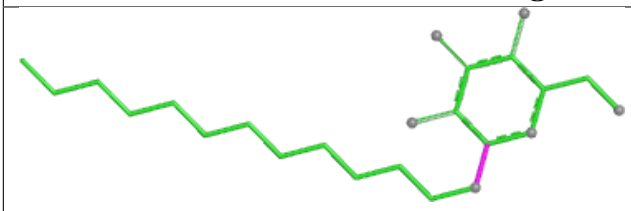


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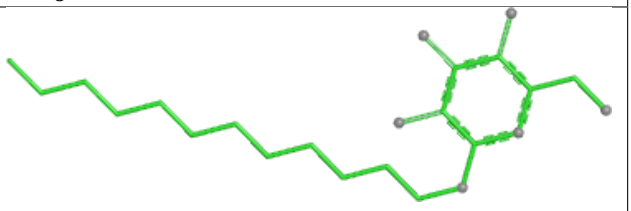


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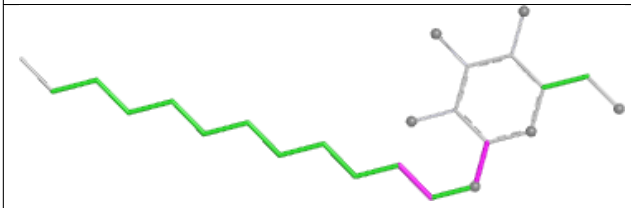
Ligand LMT j 102



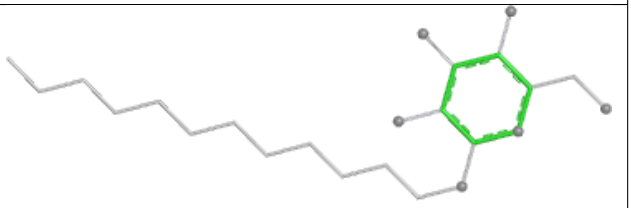
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Bond angles

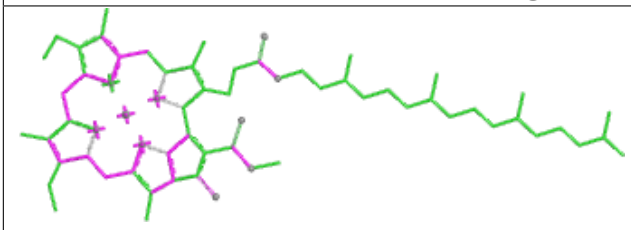


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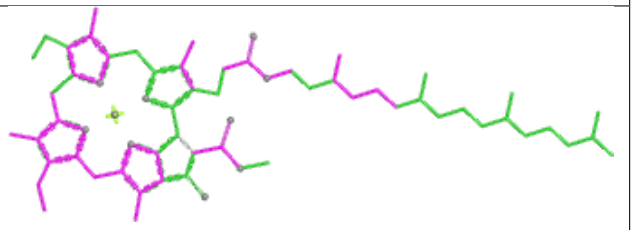


Rings

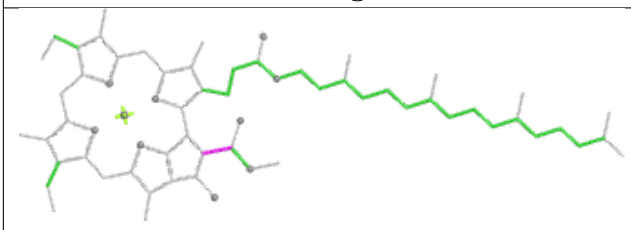
Ligand CLA B 615



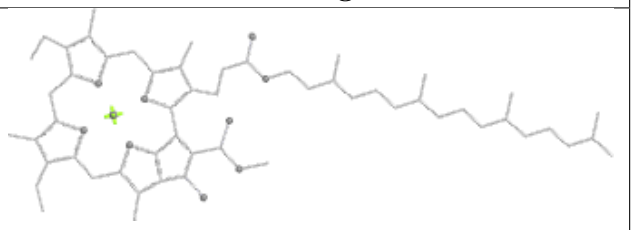
Bond lengths



Bond angles

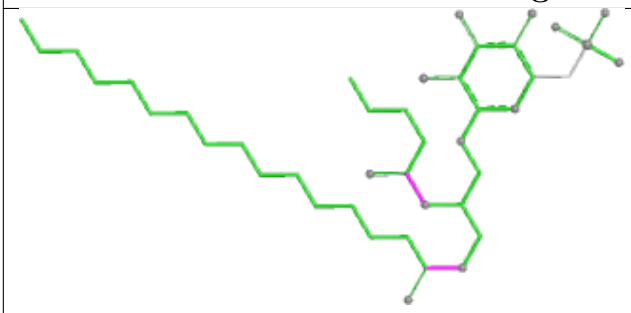


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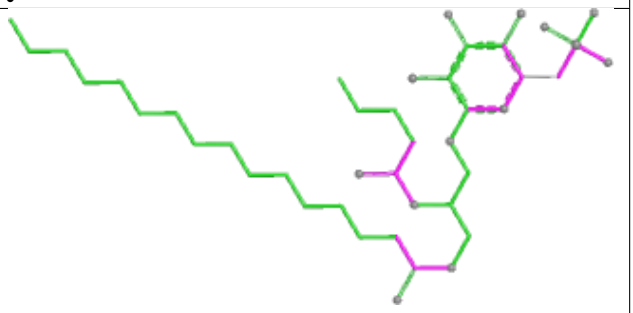


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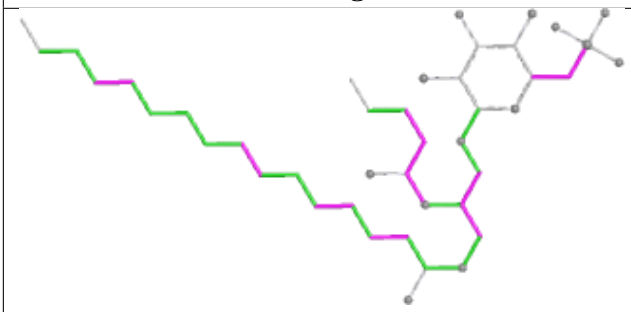
Ligand SQD f 102



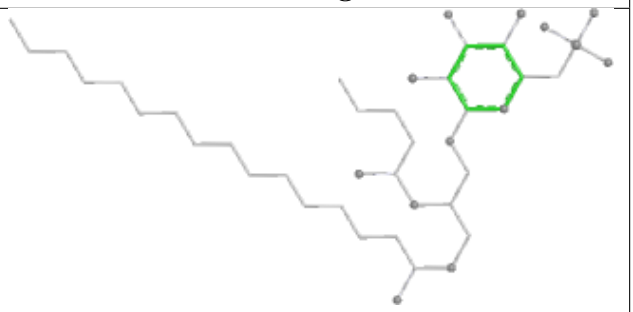
Bond lengths



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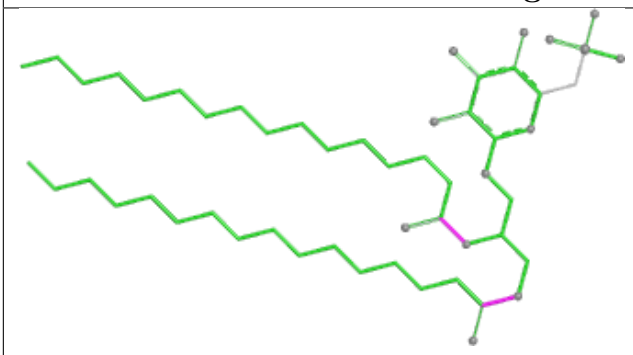


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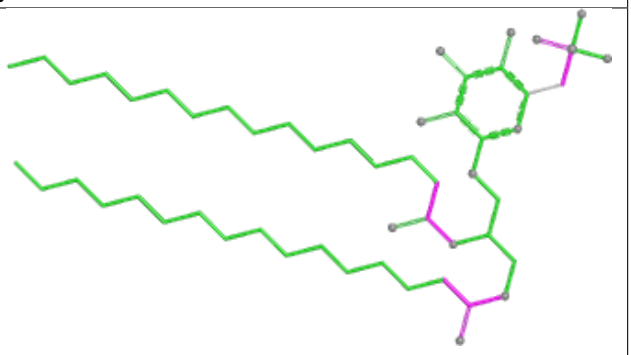


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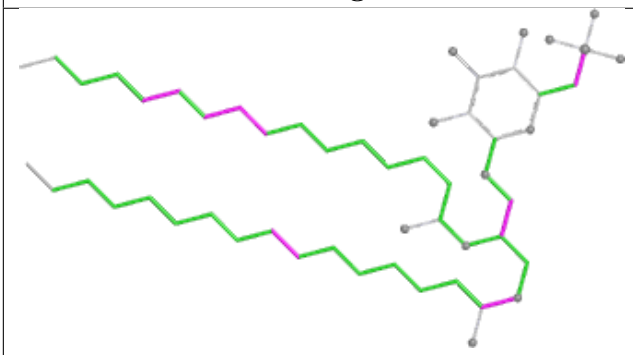
Ligand SQD A 416



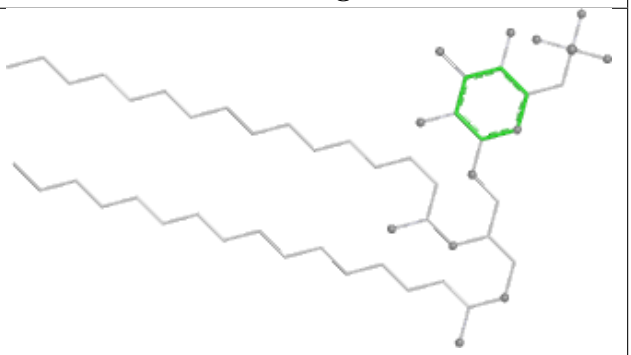
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Bond angles

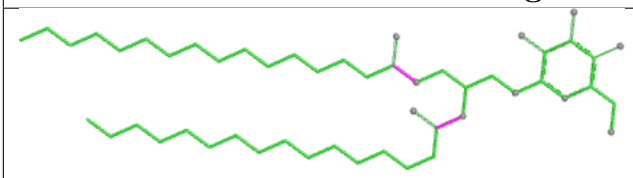


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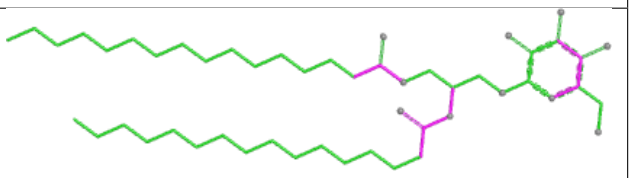


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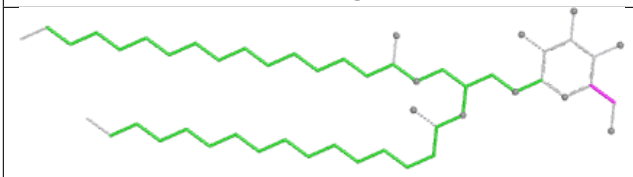
Ligand LMG c 921



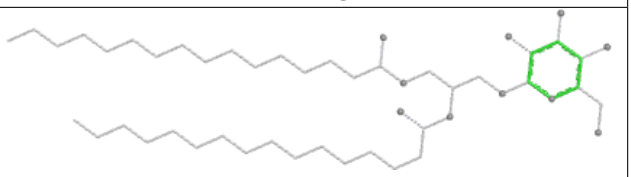
Bond lengths



Bond angles

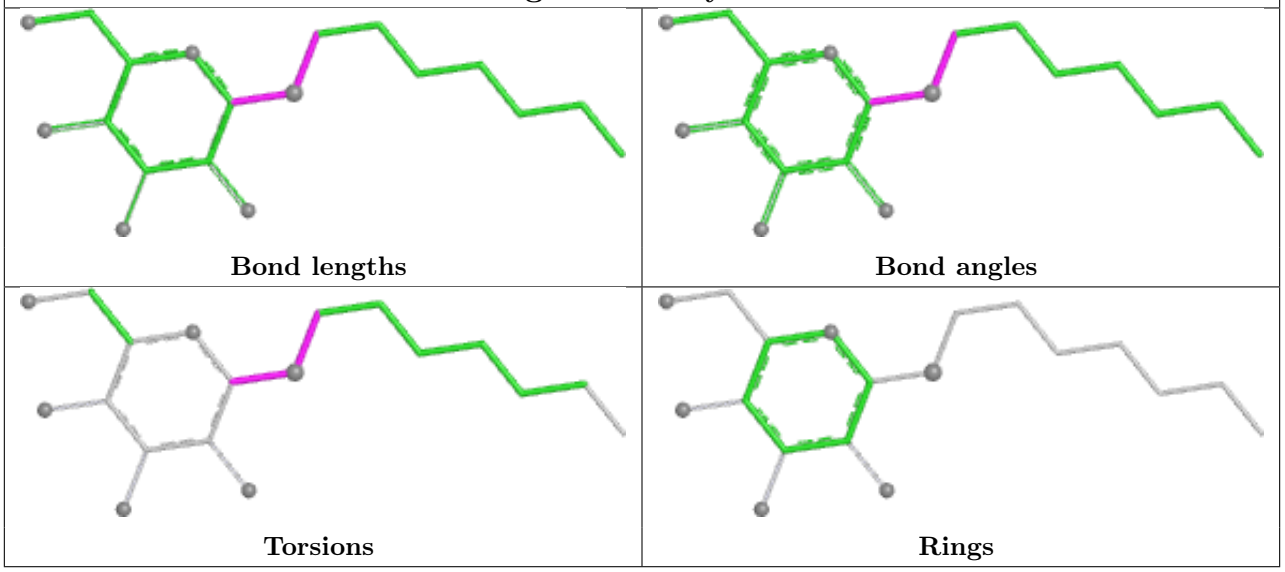


Torsions

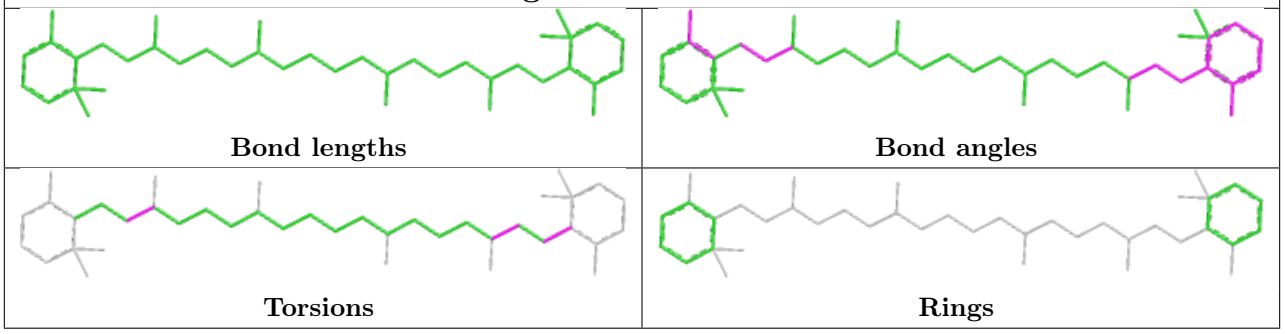


Rings

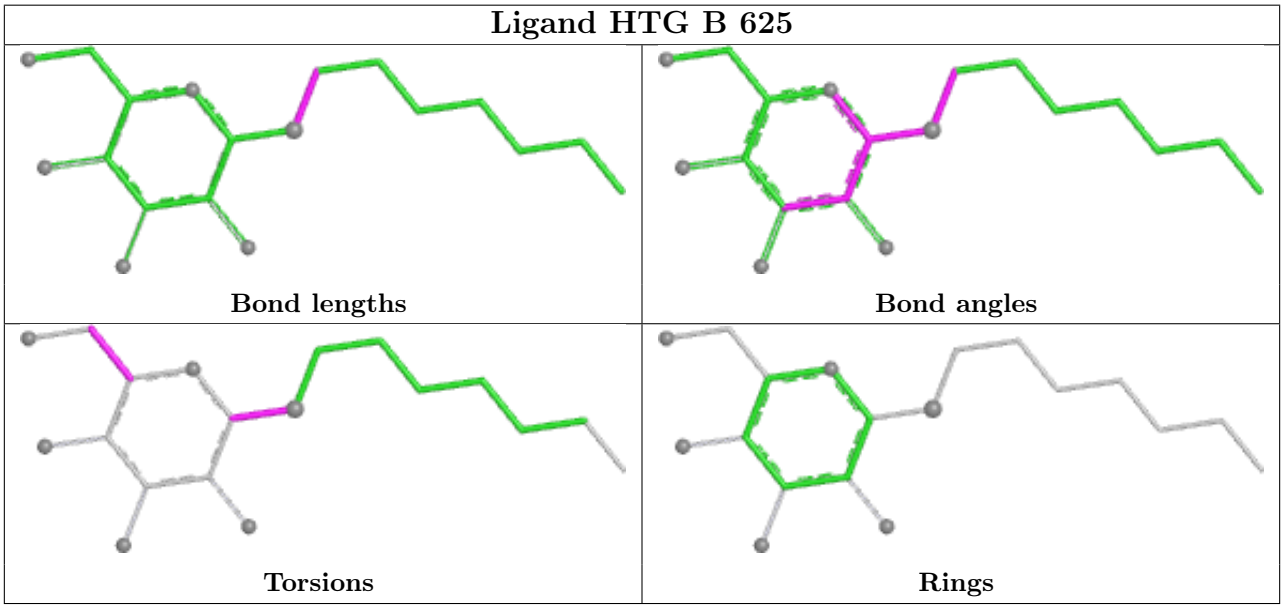
Ligand HTG y 102



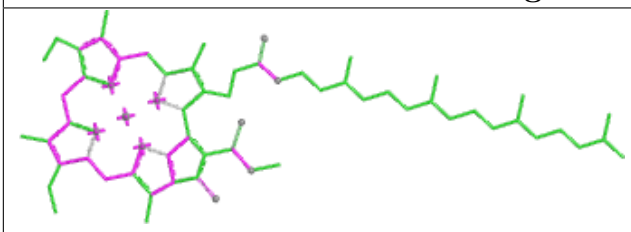
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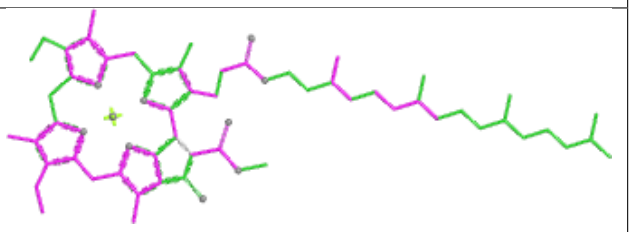
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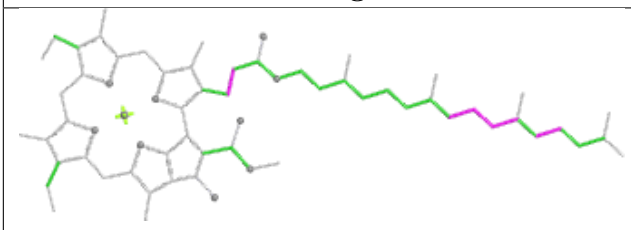
Ligand CLA B 607



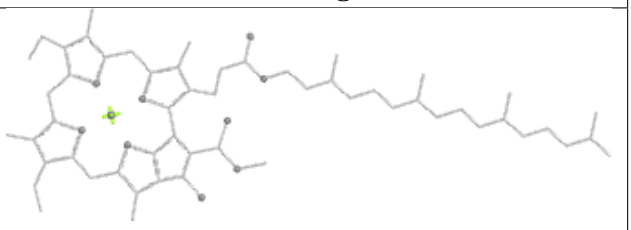
Bond lengths



Bond angles



Torsions

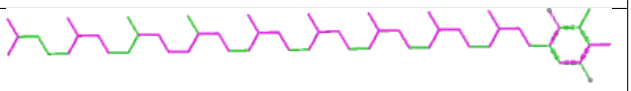


Rings

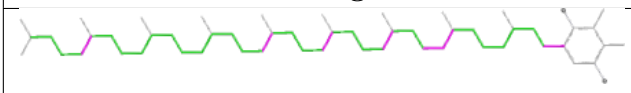
Ligand PL9 A 414



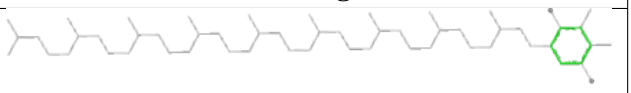
Bond lengths



Bond angles

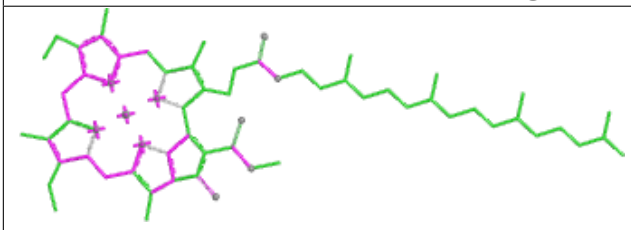


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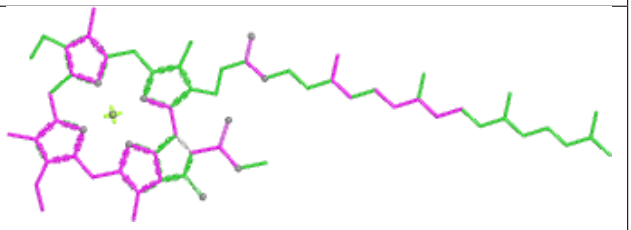


Rings

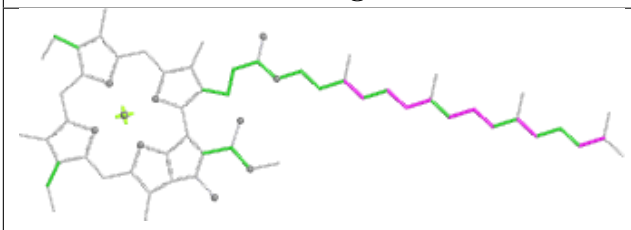
Ligand CLA B 616



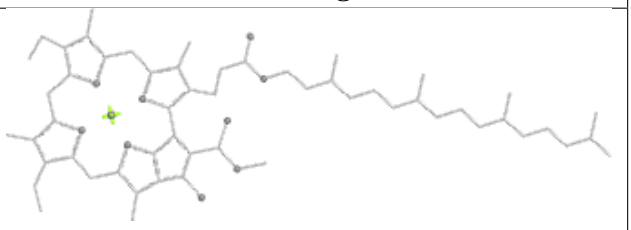
Bond lengths



Bond angles

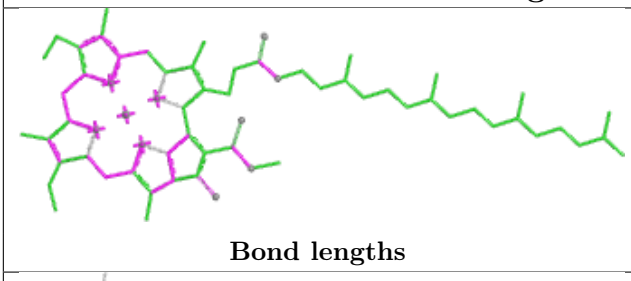


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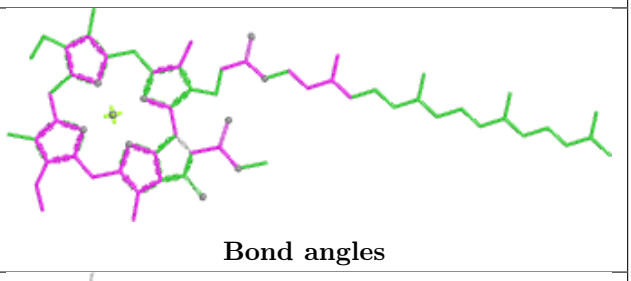


Rings

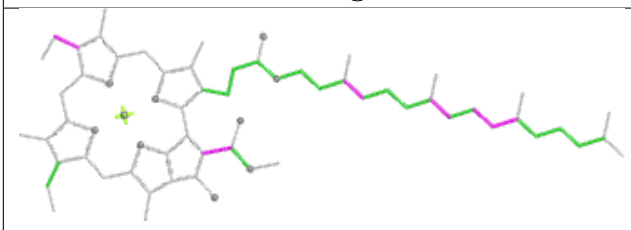
Ligand CLA b 620



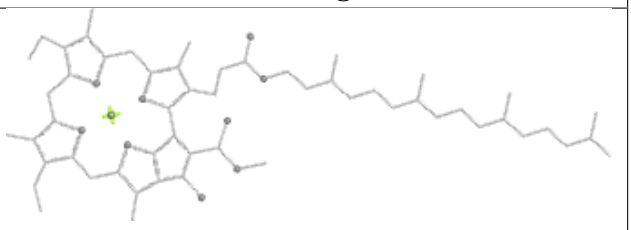
Bond lengths



Bond angles

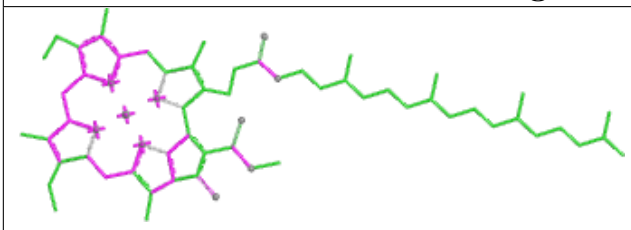


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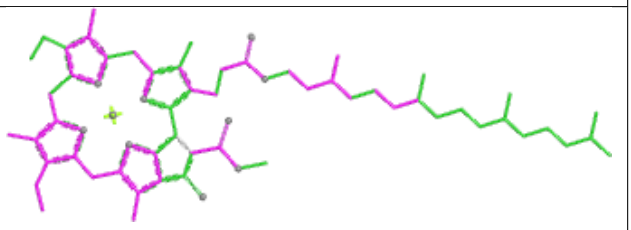


Rings

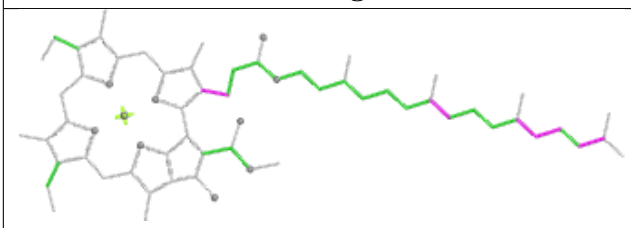
Ligand CLA c 909



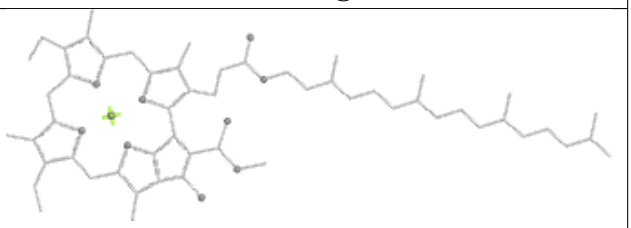
Bond lengths



Bond angles

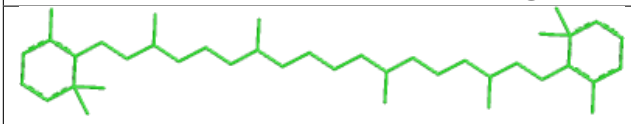


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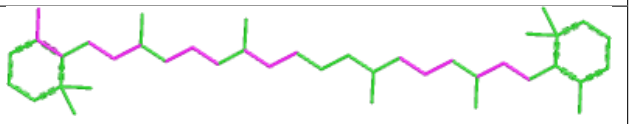


Rings

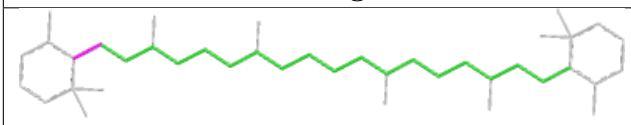
Ligand BCR B 618



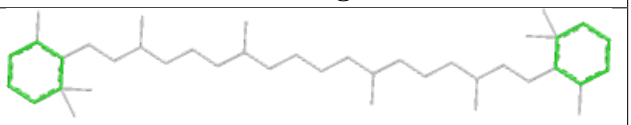
Bond lengths



Bond angles

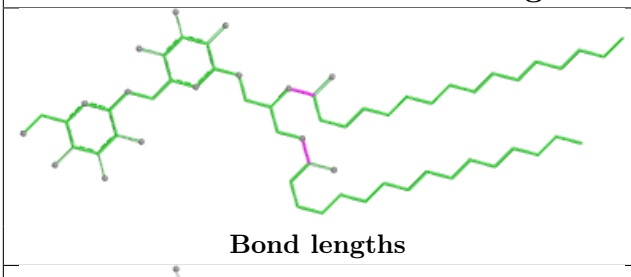


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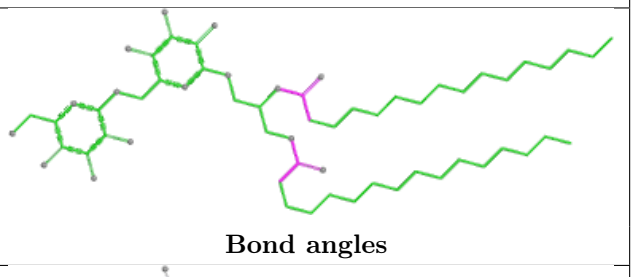


Rings

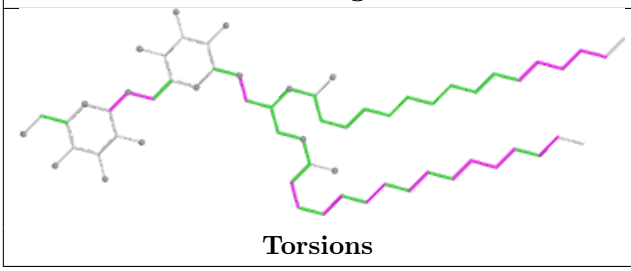
Ligand DGD c 918



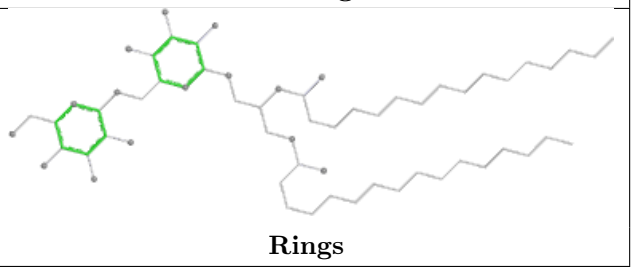
Bond lengths



Bond angles

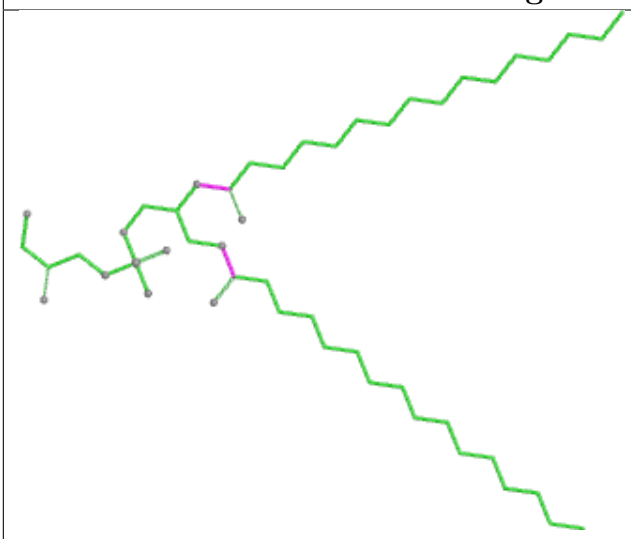


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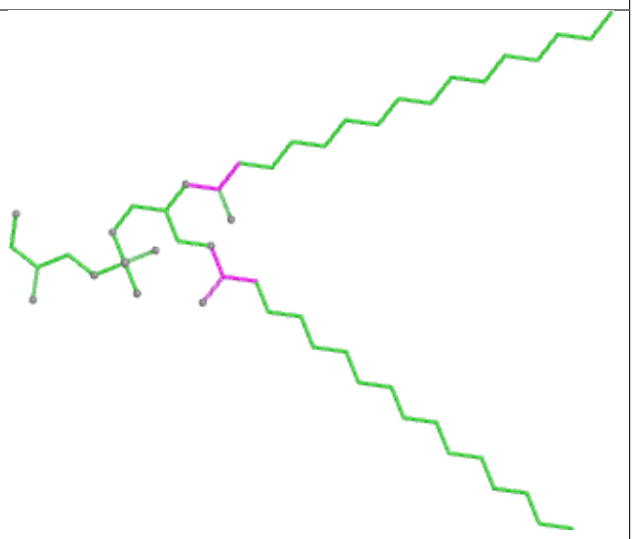


Rings

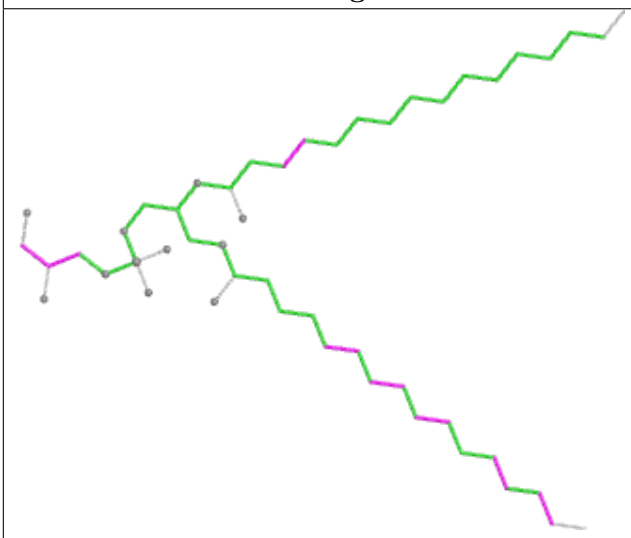
Ligand LHG d 410



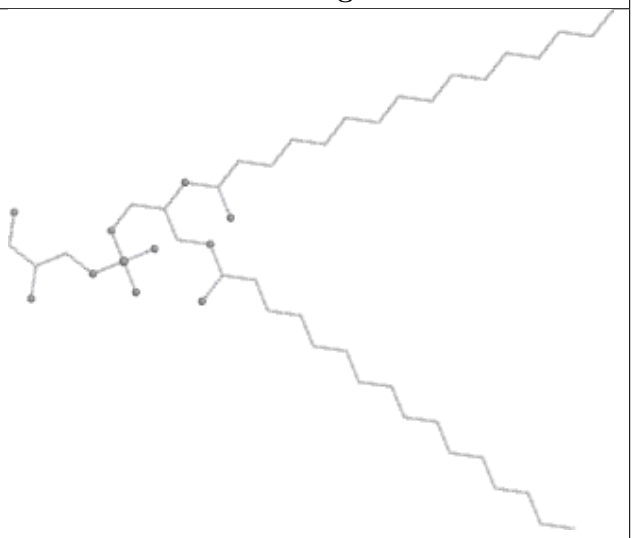
Bond lengths



Bond angles

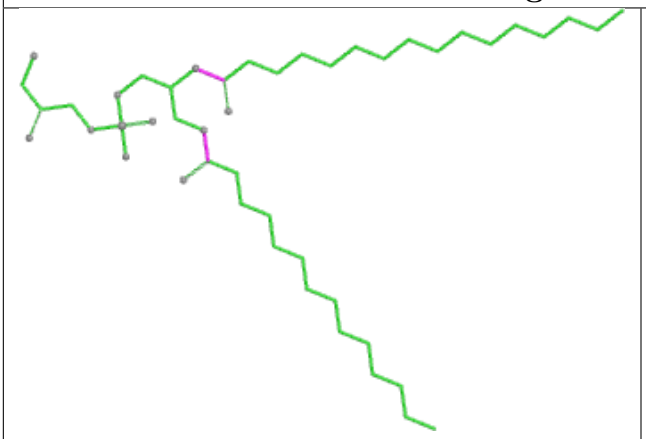


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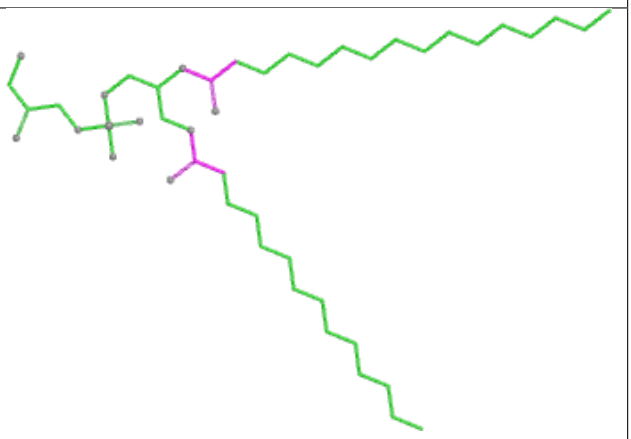


Rings

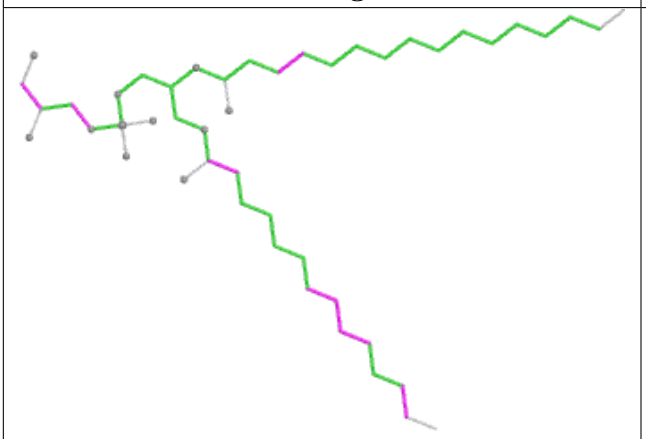
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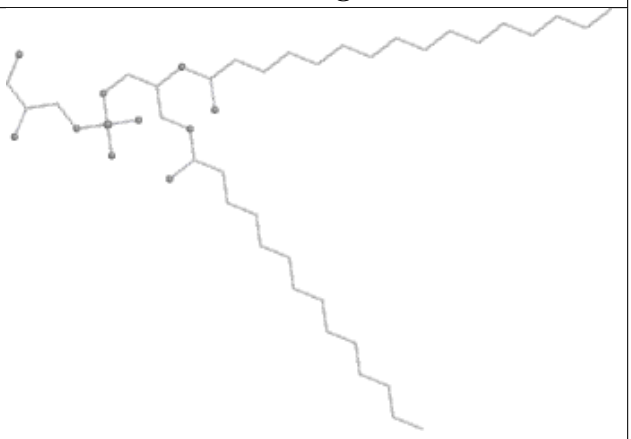
Bond lengths



Bond angles

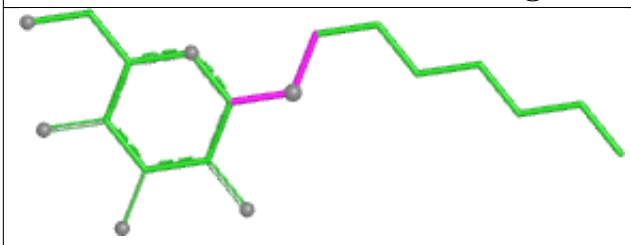


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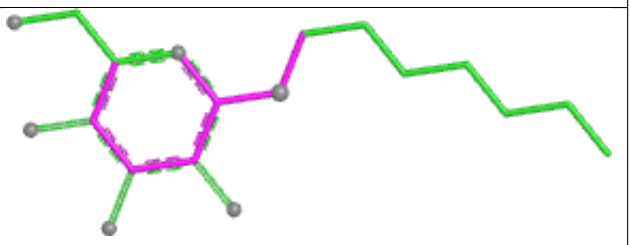


Rings

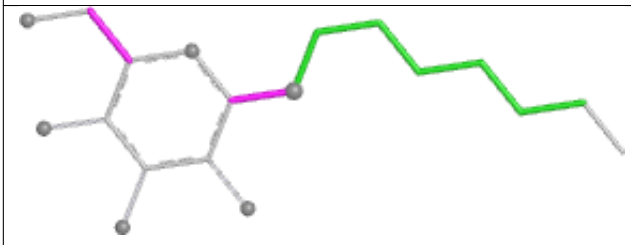
Ligand HTG b 627



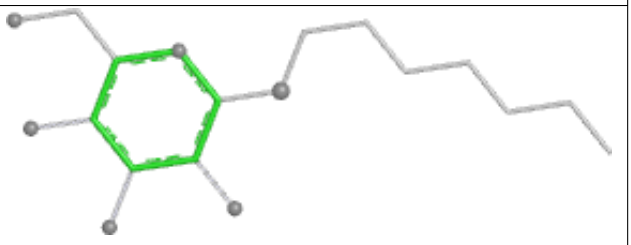
Bond lengths



Bond angles

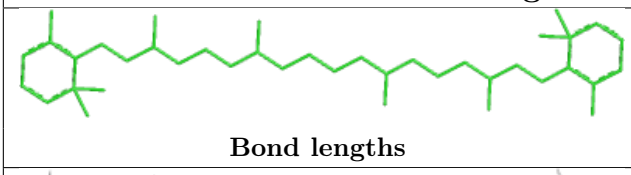


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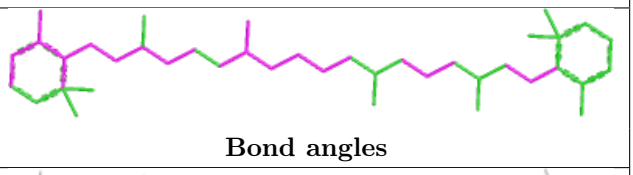


Rings

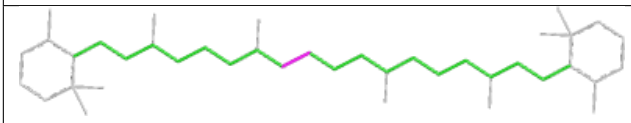
Ligand BCR T 101



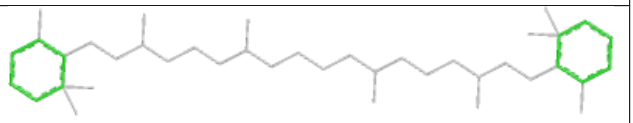
Bond lengths



Bond angles

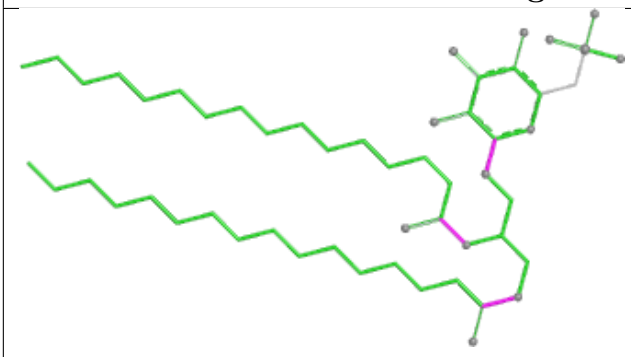


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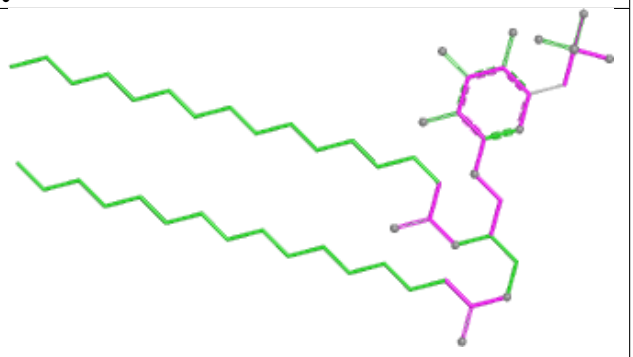


Rings

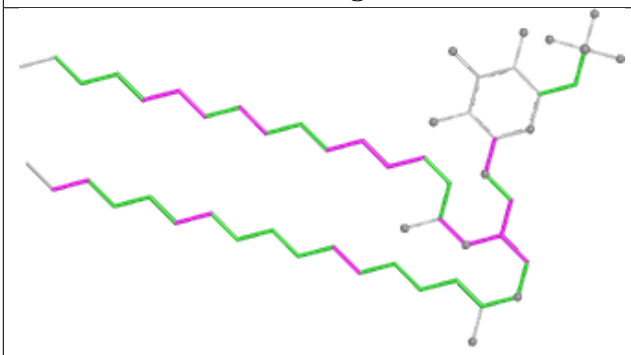
Ligand SQD b 601



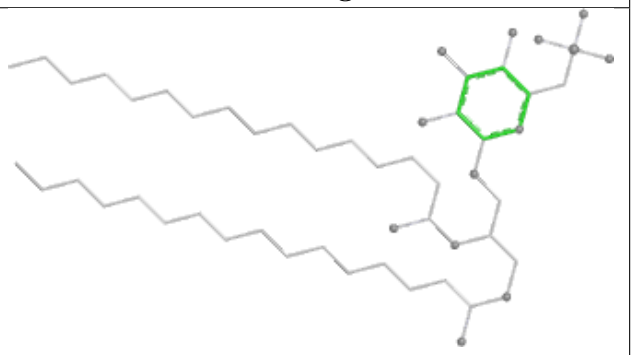
Bond lengths



Bond angles

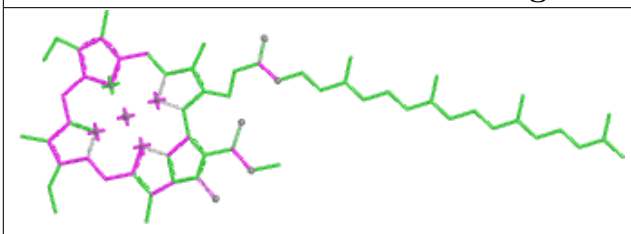


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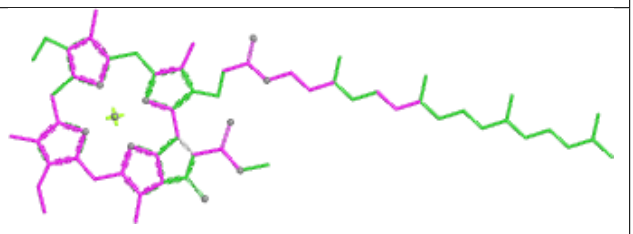


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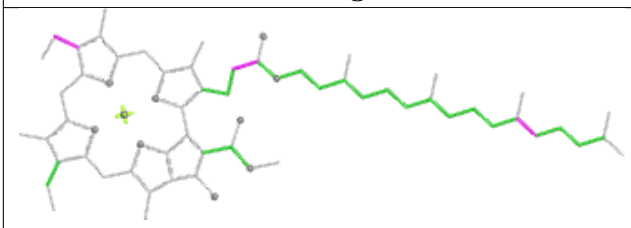
Ligand CLA c 906



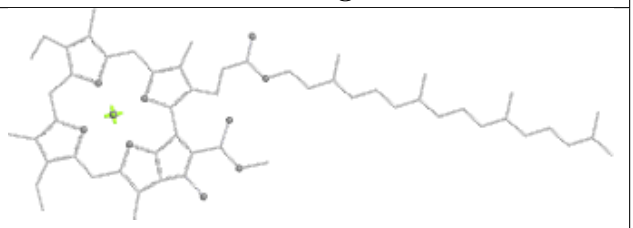
Bond lengths



Bond angles

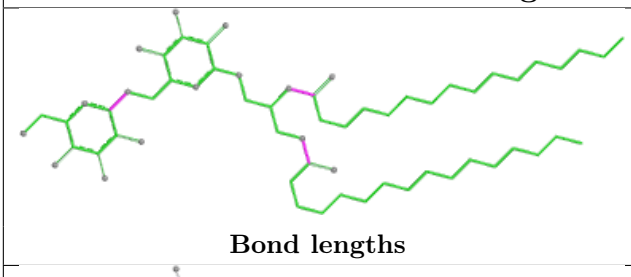


Torsions

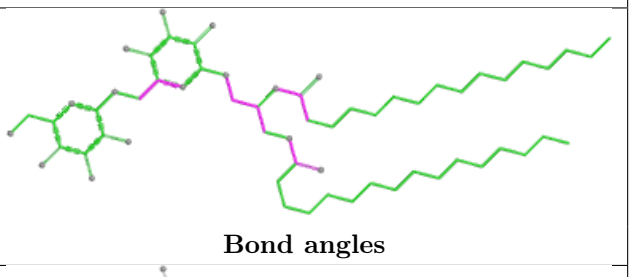


Rings

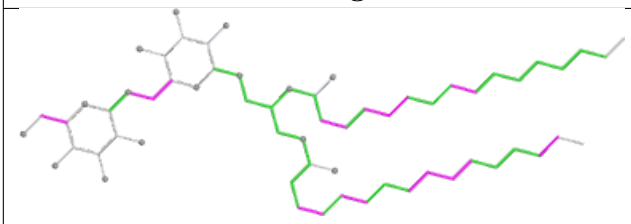
Ligand DGD C 516



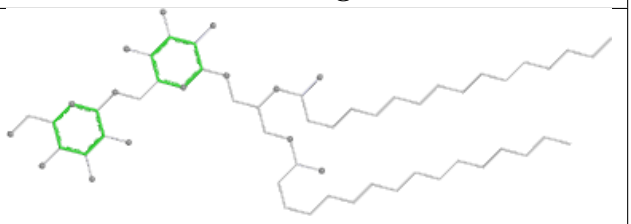
Bond lengths



Bond angles

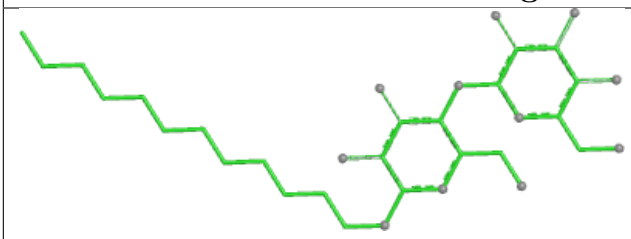


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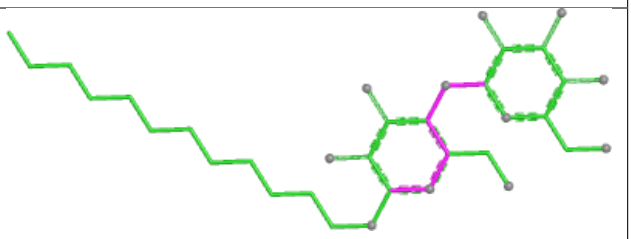


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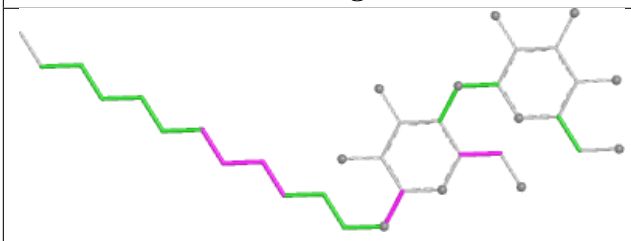
Ligand LMT A 417



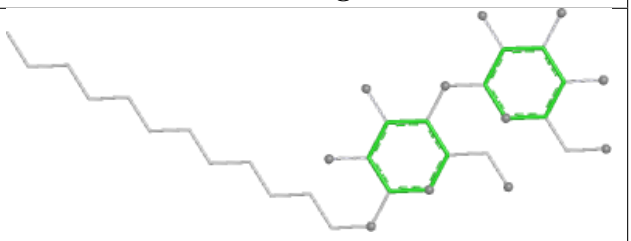
Bond lengths



Bond angles

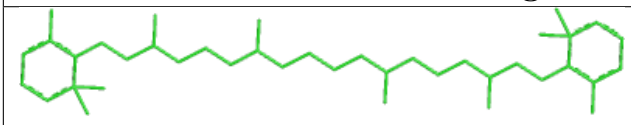


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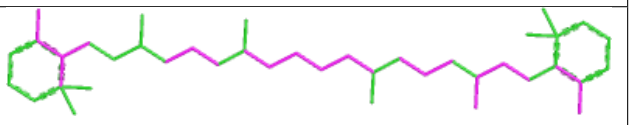


Rings

Ligand BCR Y 101



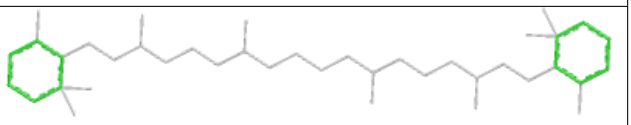
Bond lengths



Bond angles

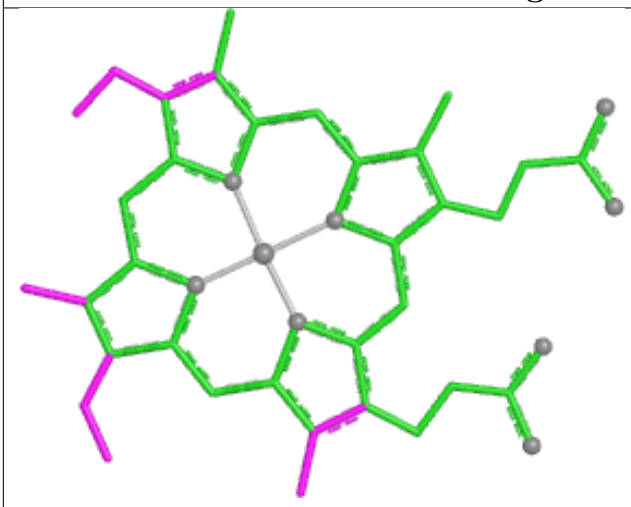


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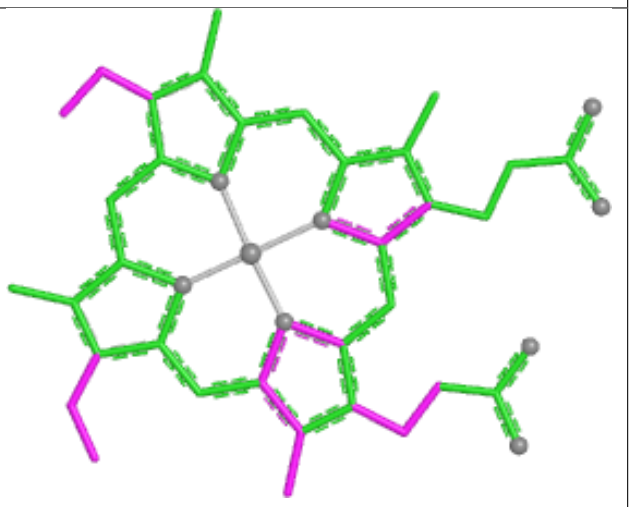


Rings

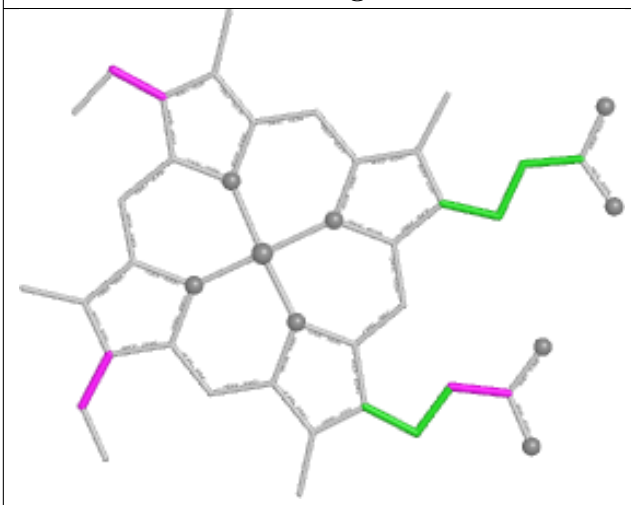
Ligand HEC v 202



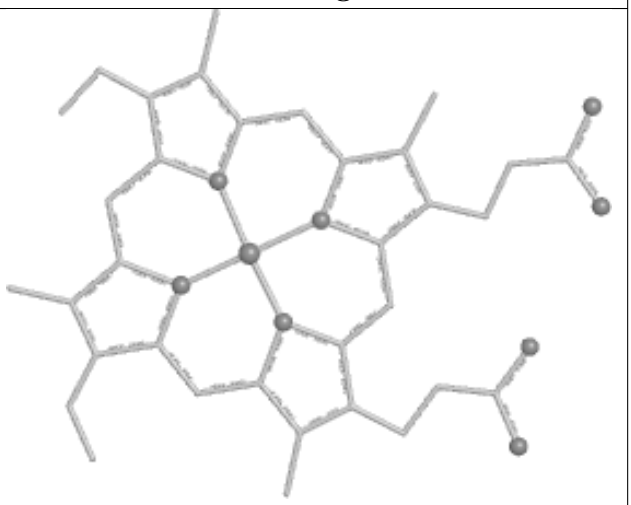
Bond lengths



Bond angles



Torsions

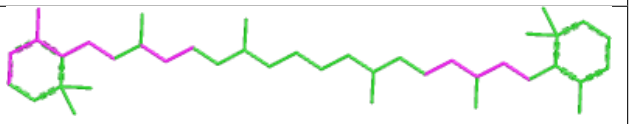


Rings

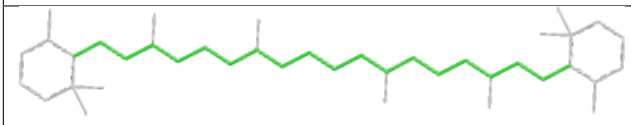
Ligand BCR k 103



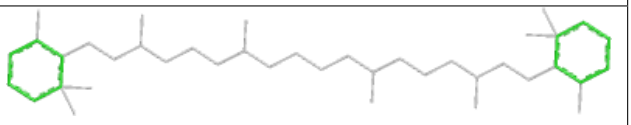
Bond lengths



Bond angles

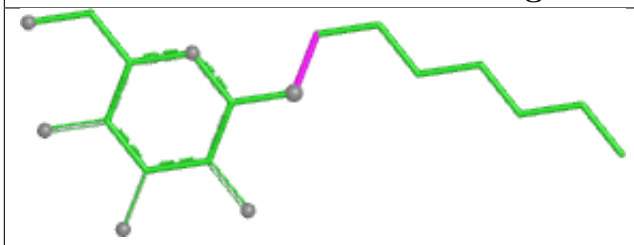


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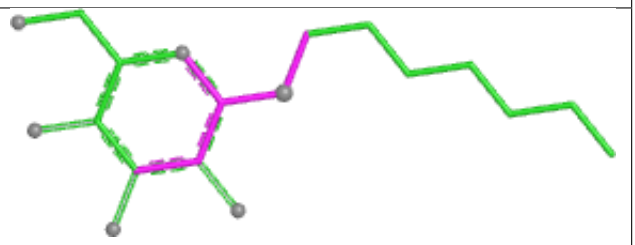


Rings

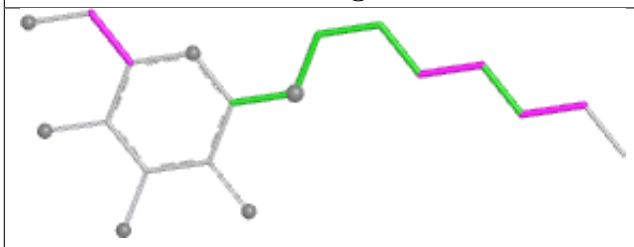
Ligand HTG d 414



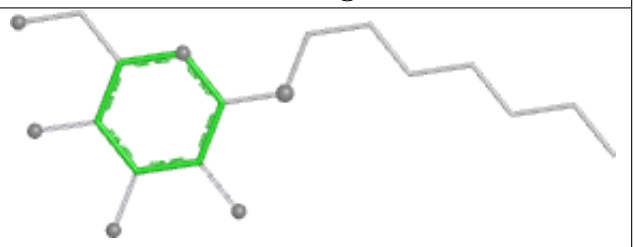
Bond lengths



Bond angles

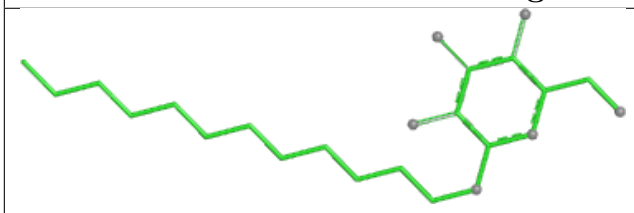


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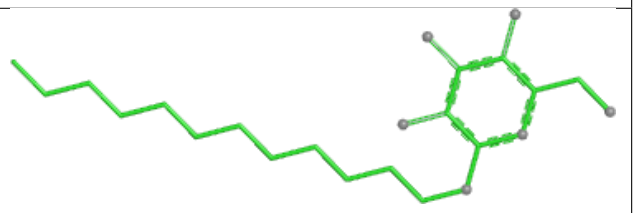


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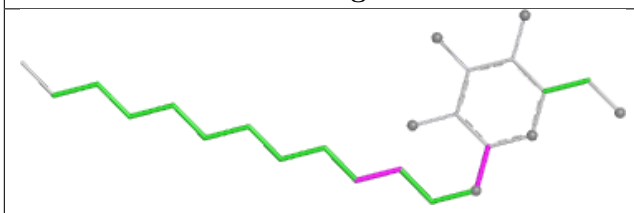
Ligand LMT e 101



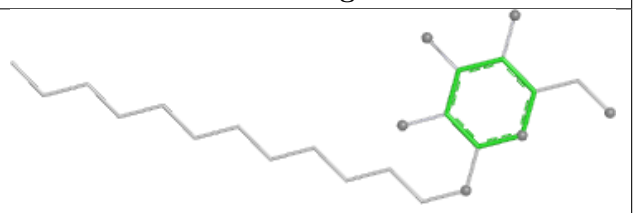
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Bond angles

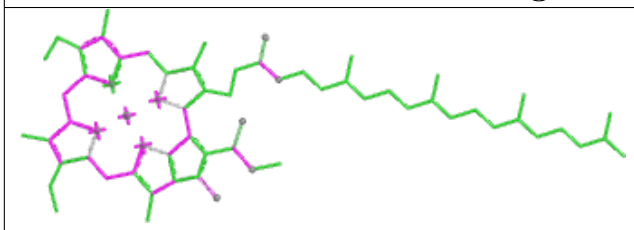


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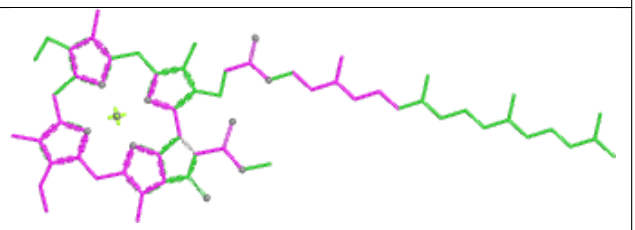


Rings

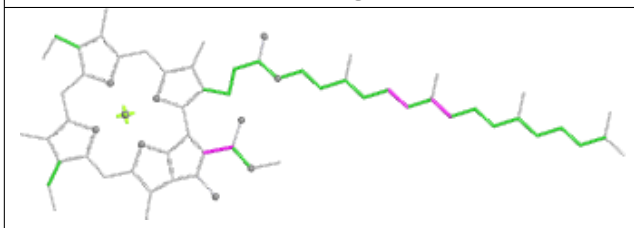
Ligand CLA c 908



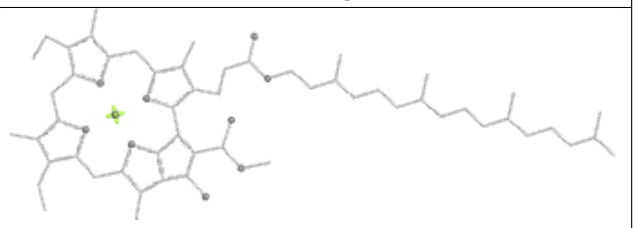
Bond lengths



Bond angles

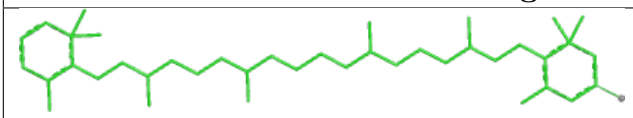


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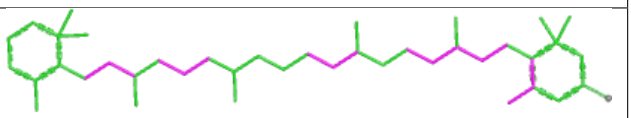


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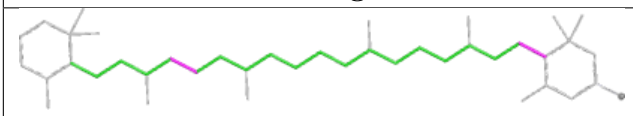
Ligand RRX H 101



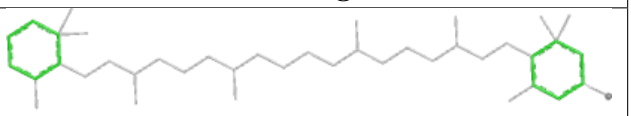
Bond lengths



Bond angles

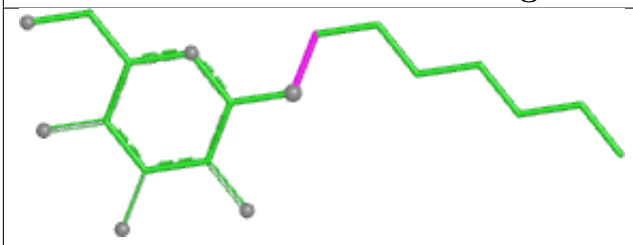


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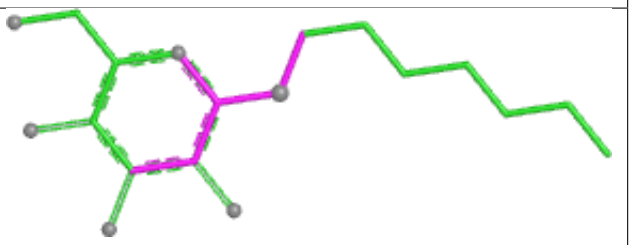


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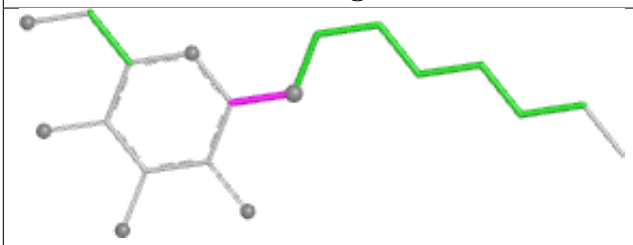
Ligand HTG V 215



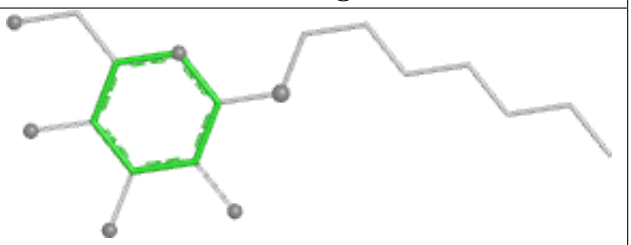
Bond lengths



Bond angles



Torsions

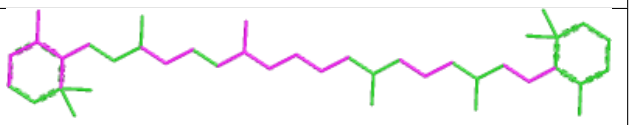


Rings

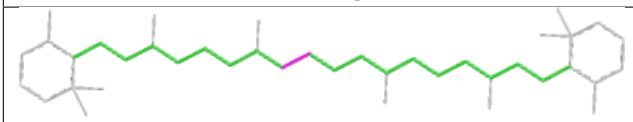
Ligand BCR B 636



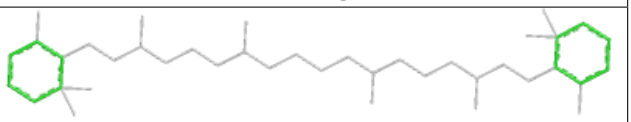
Bond lengths



Bond angles

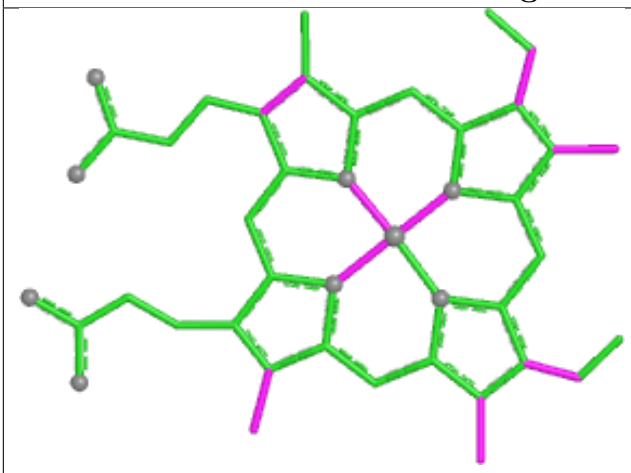


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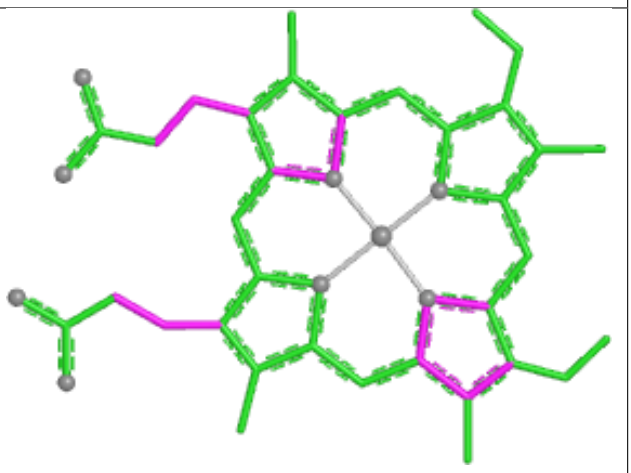


Rings

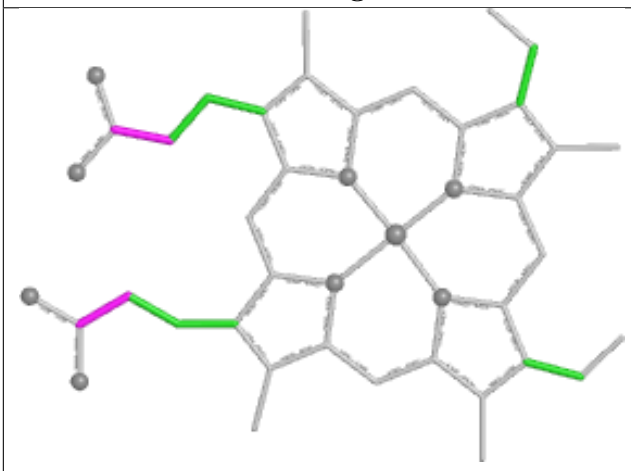
Ligand HEM F 102



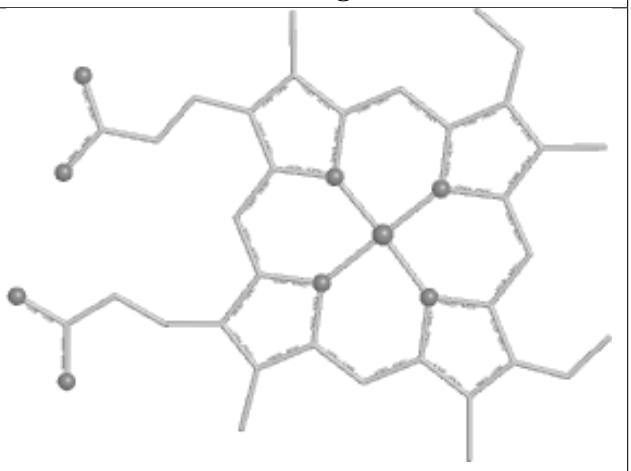
Bond lengths



Bond angles

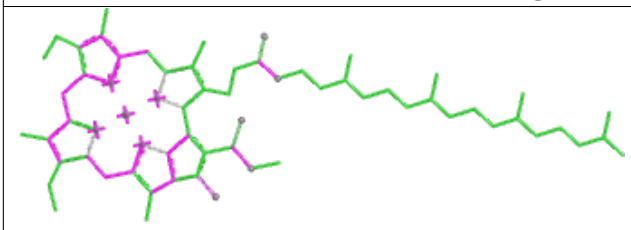


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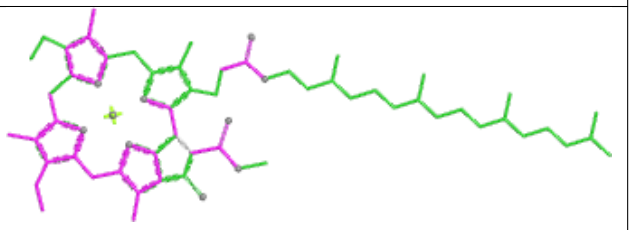


Rings

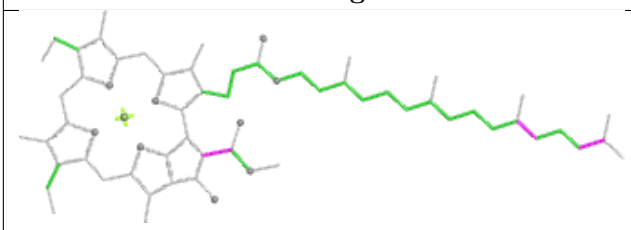
Ligand CLA c 903



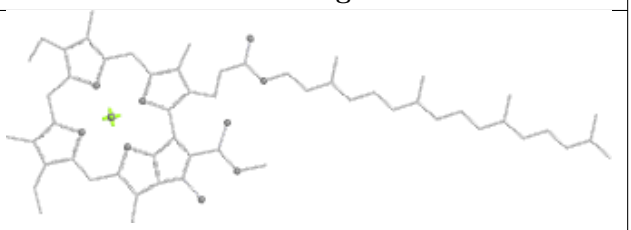
Bond lengths



Bond angles

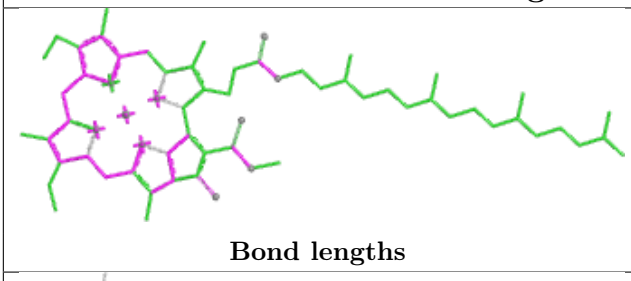


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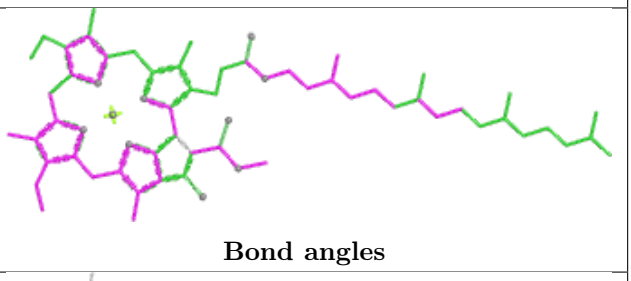


Rings

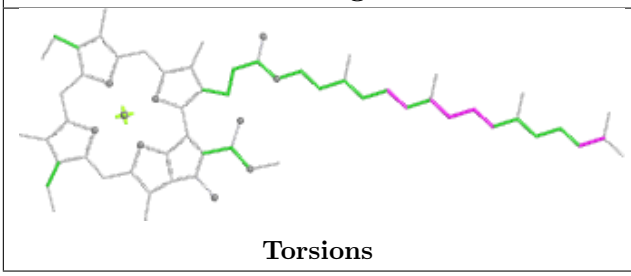
Ligand CLA b 619



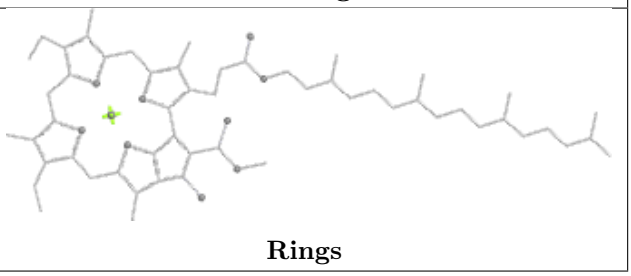
Bond lengths



Bond angles

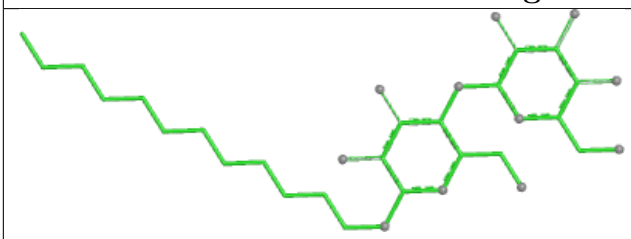


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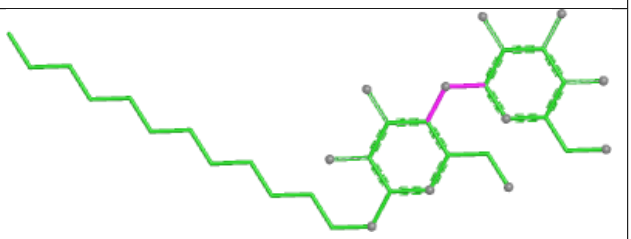


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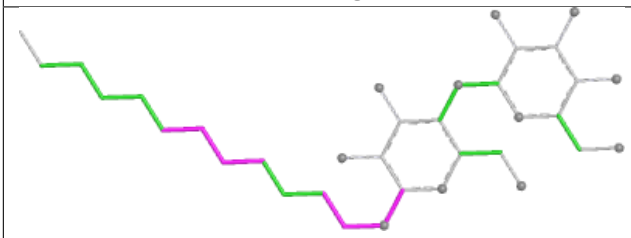
Ligand LMT Z 101



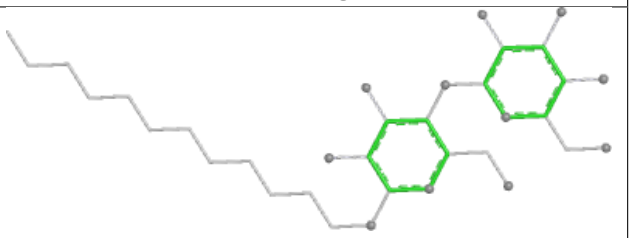
Bond lengths



Bond angles

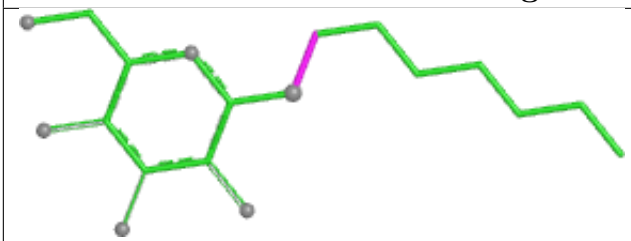


Torsions

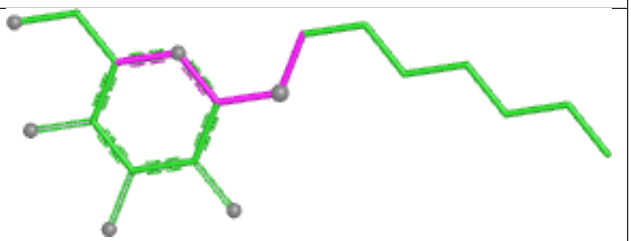


Rings

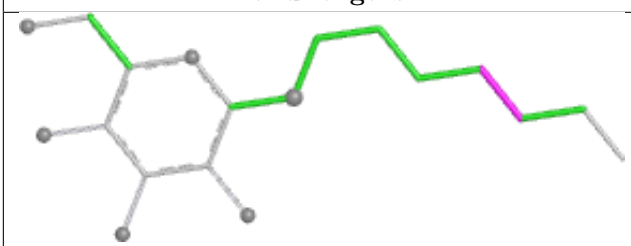
Ligand HTG B 631



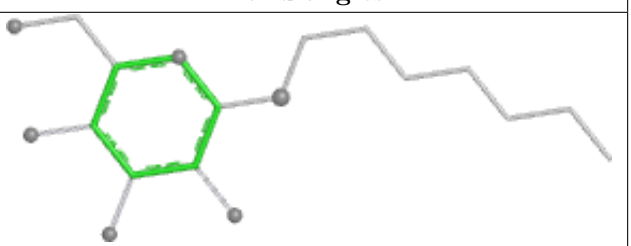
Bond lengths



Bond angles

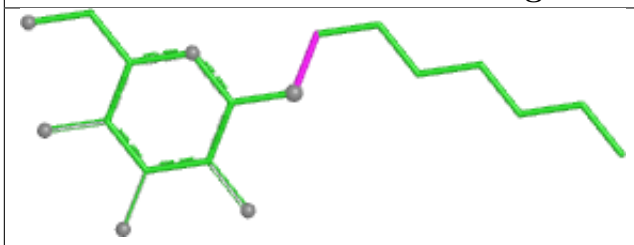


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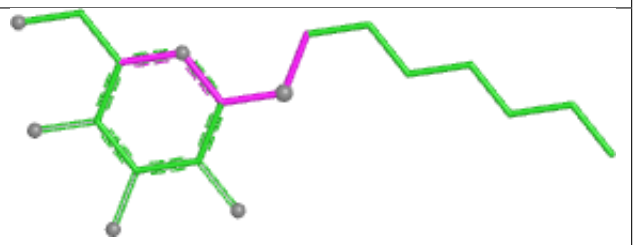


Rings

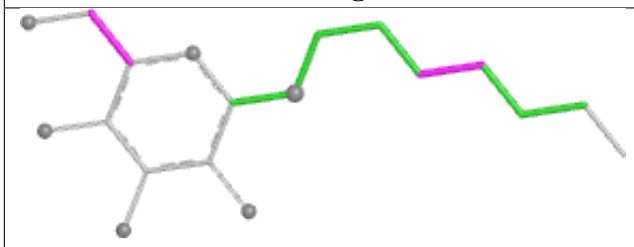
Ligand HTG d 420



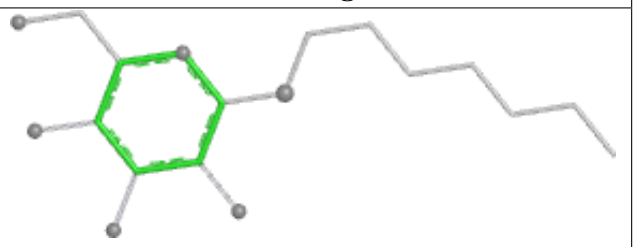
Bond lengths



Bond angles

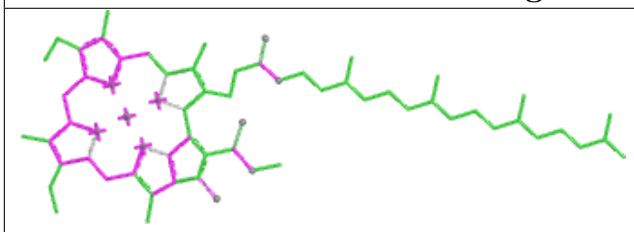


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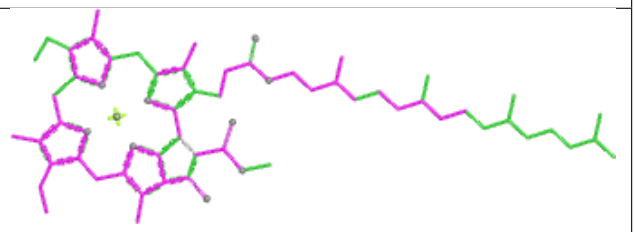


Rings

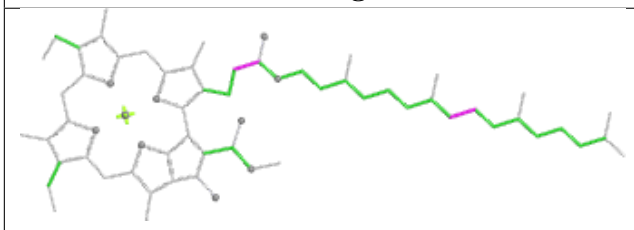
Ligand CLA C 510



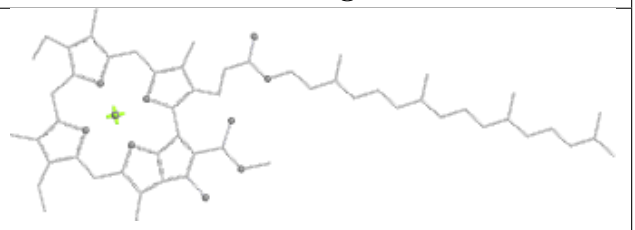
Bond lengths



Bond angles

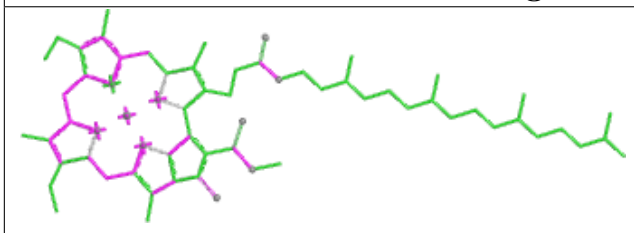


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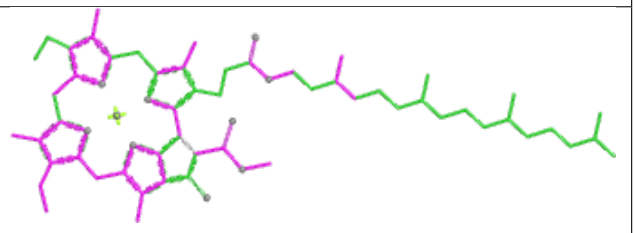


Rings

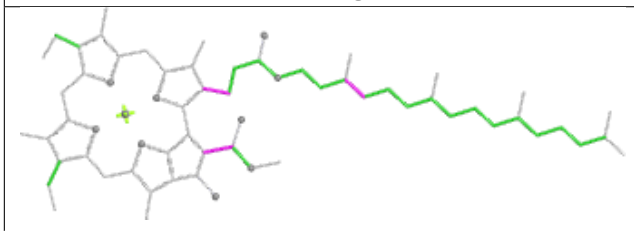
Ligand CLA B 610



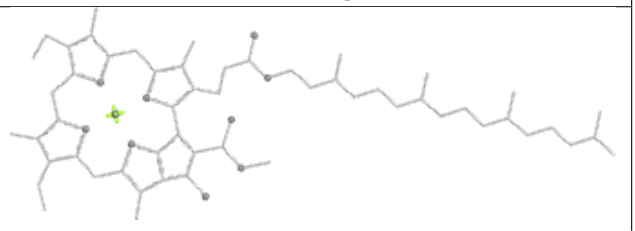
Bond lengths



Bond angles

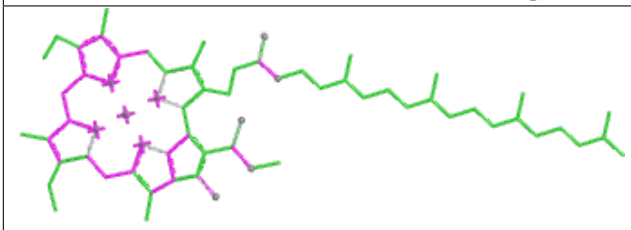


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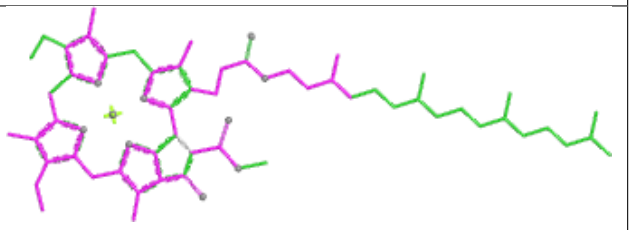


Rings

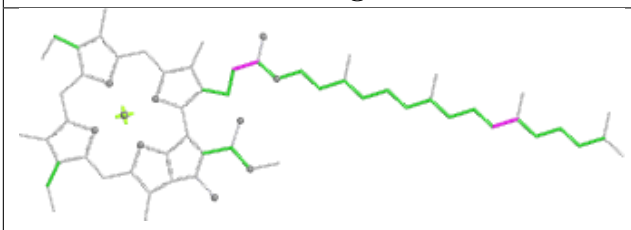
Ligand CLA C 512



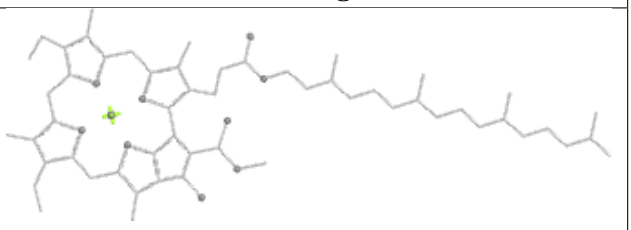
Bond lengths



Bond angles

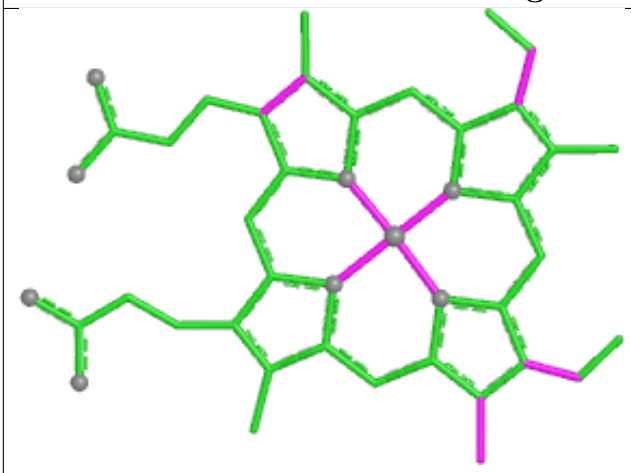


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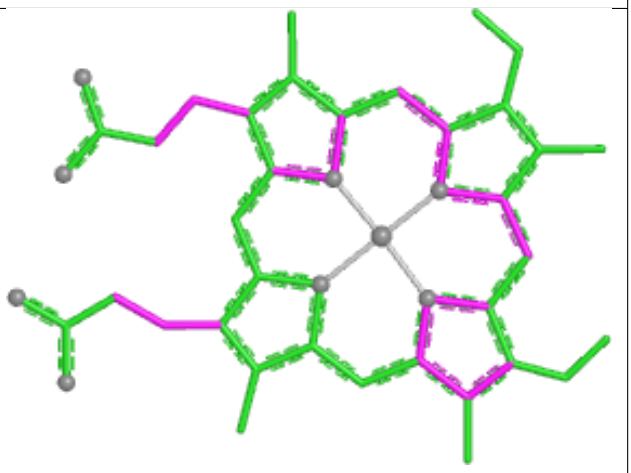


Rings

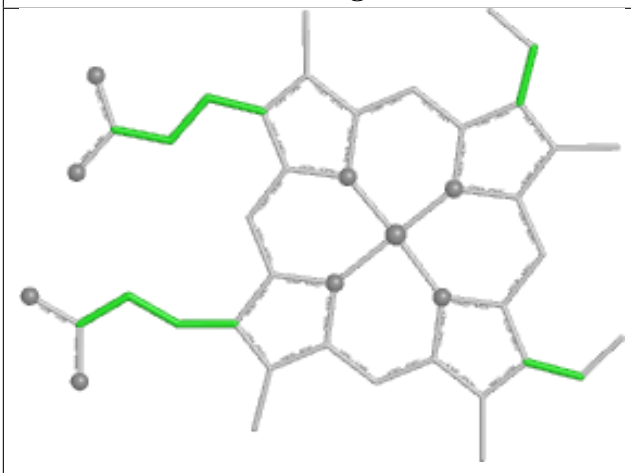
Ligand HEM f 101



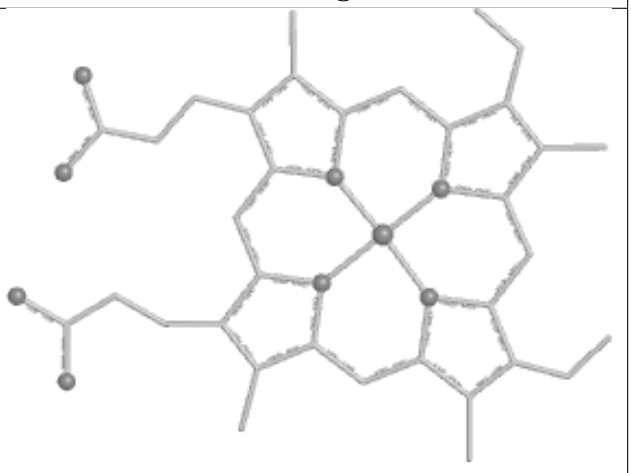
Bond lengths



Bond angles

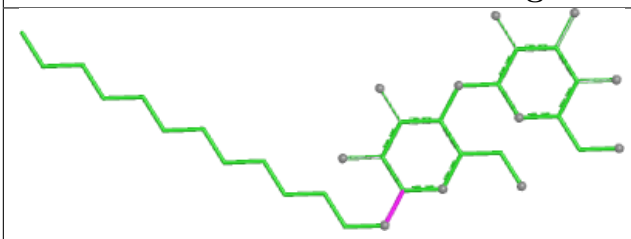


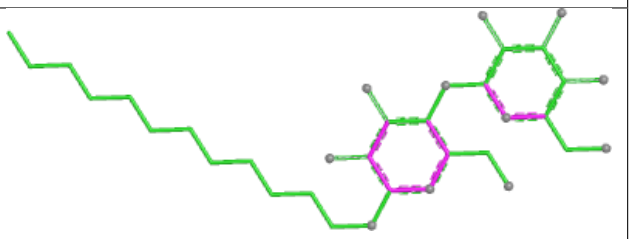
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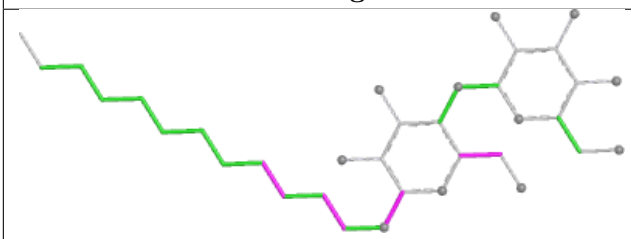


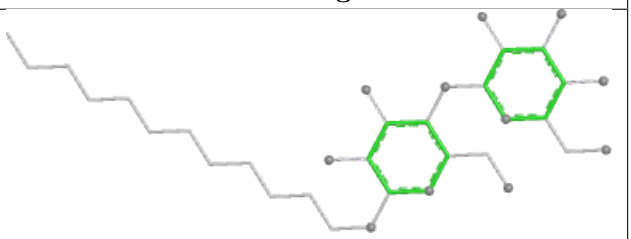
Rings

Ligand LMT c 922

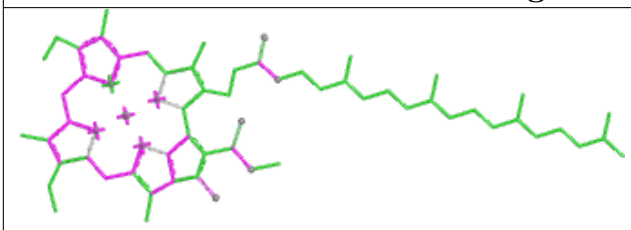

Bond lengths

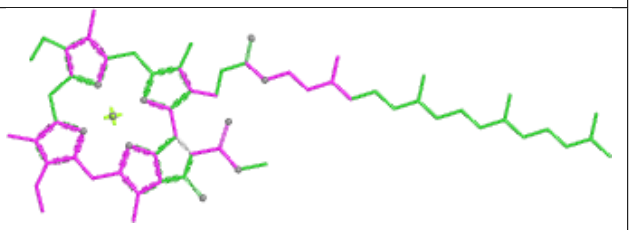

Bond angles

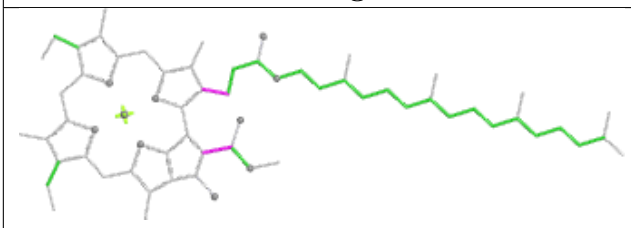

Torsions

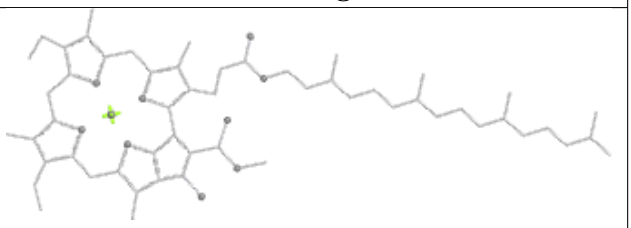

Rings

Ligand CLA b 605

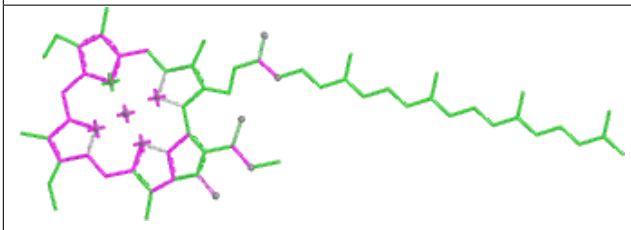

Bond lengths

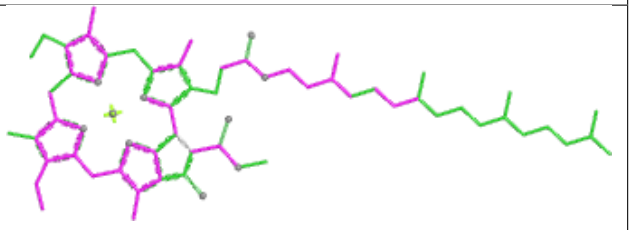

Bond angles

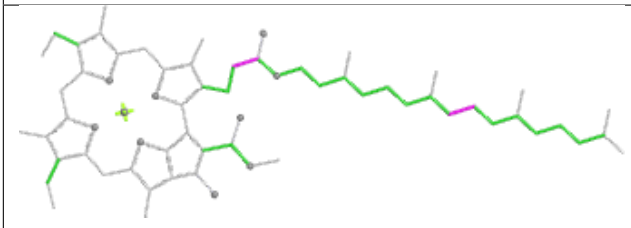

Torsions

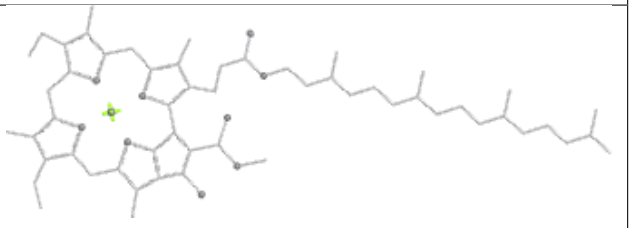

Rings

Ligand CLA c 911

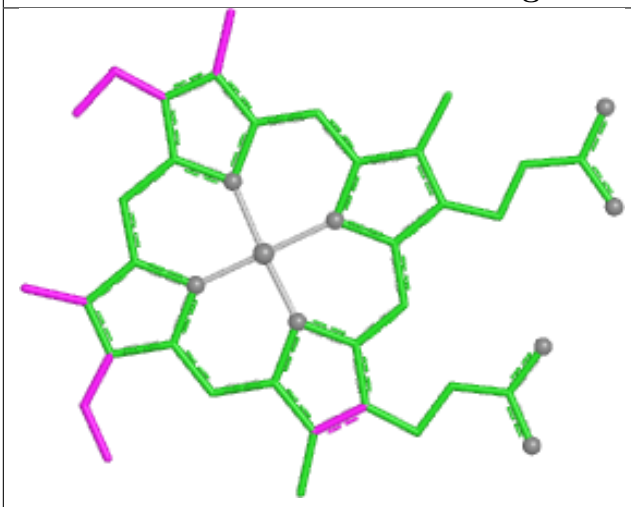

Bond lengths


Bond angles

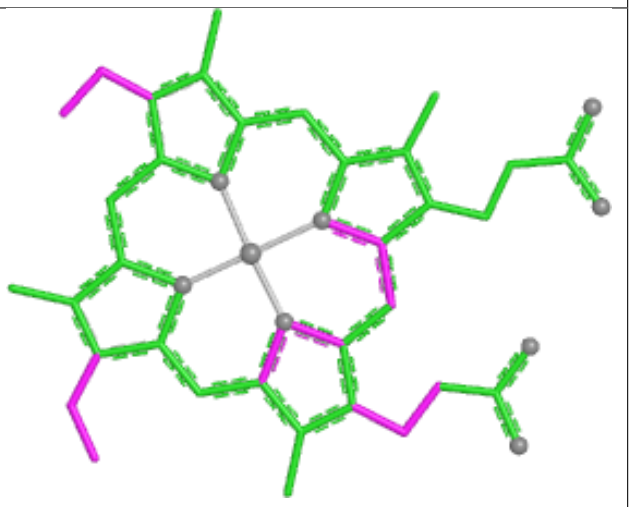

Torsions


Rings

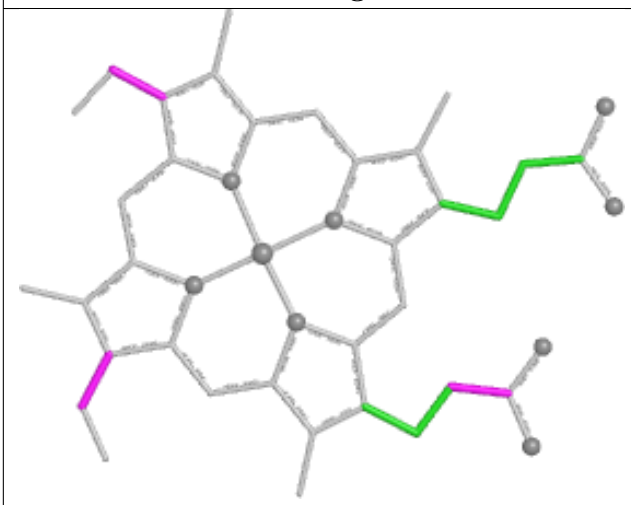
Ligand HEC V 203



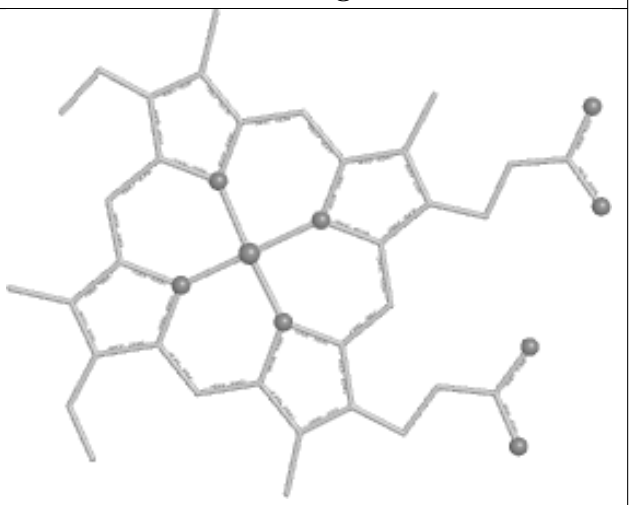
Bond lengths



Bond angles



Torsions

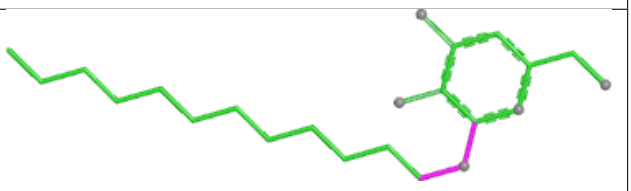


Rings

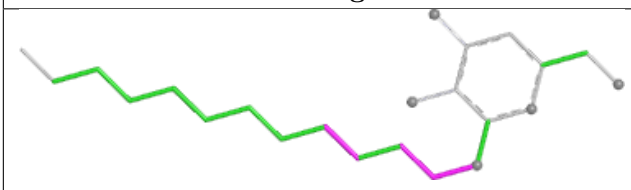
Ligand LMT t 101



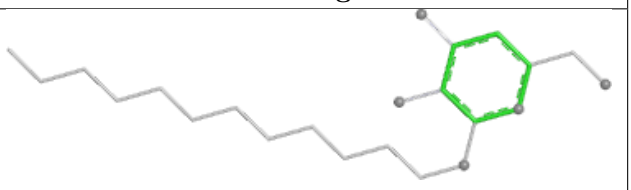
Bond lengths



Bond angles

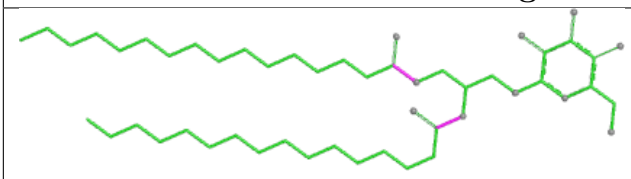


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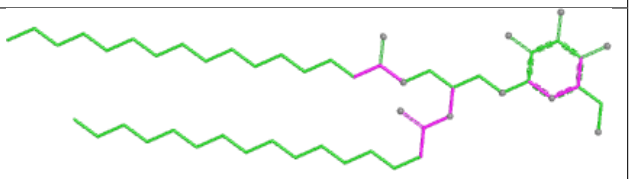


Rings

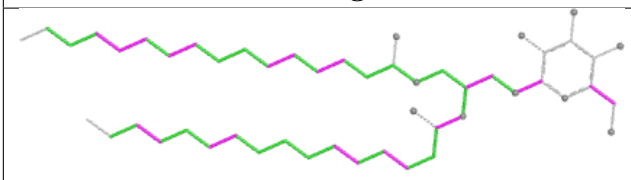
Ligand LMG A 413



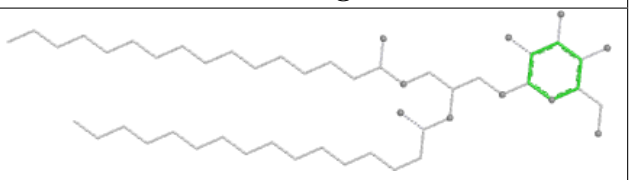
Bond lengths



Bond angles

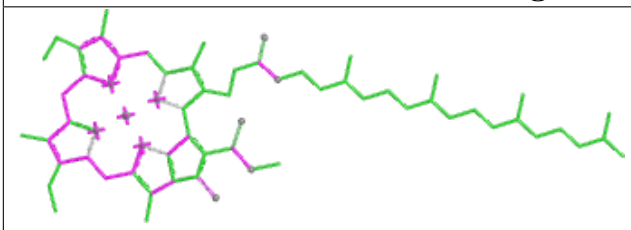


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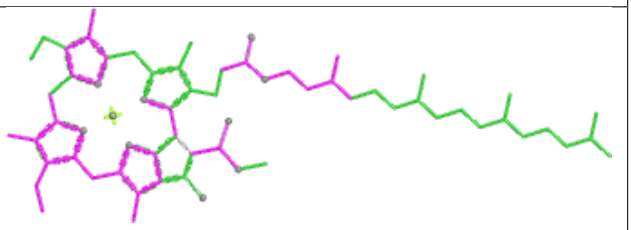


Rings

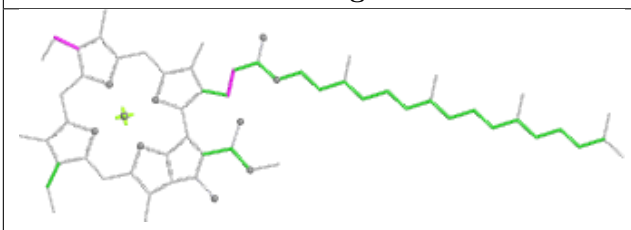
Ligand CLA c 902



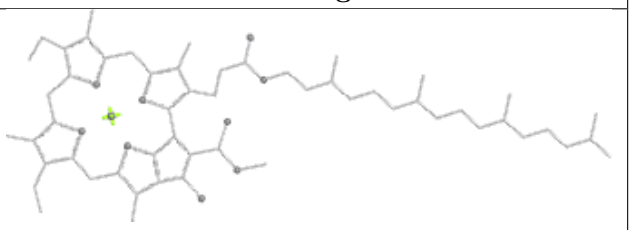
Bond lengths



Bond angles

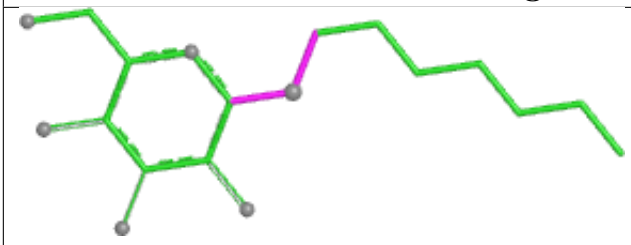


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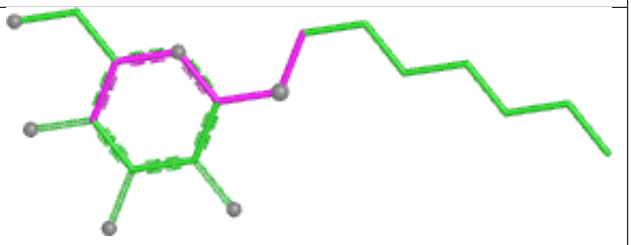


Rings

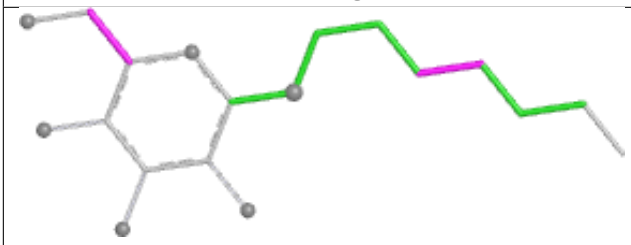
Ligand HTG b 602



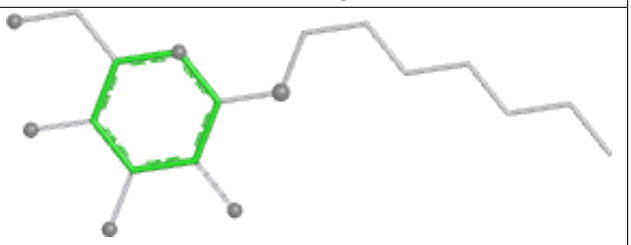
Bond lengths



Bond angles

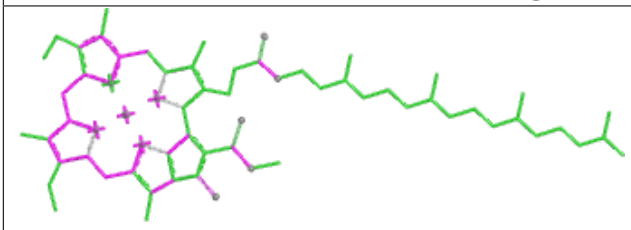


Torsions

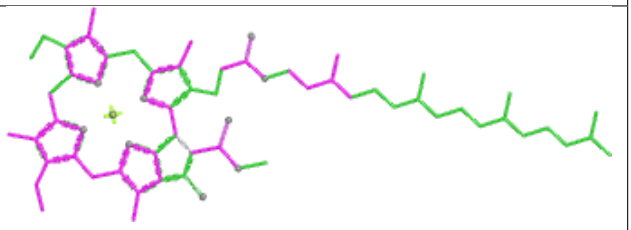


Rings

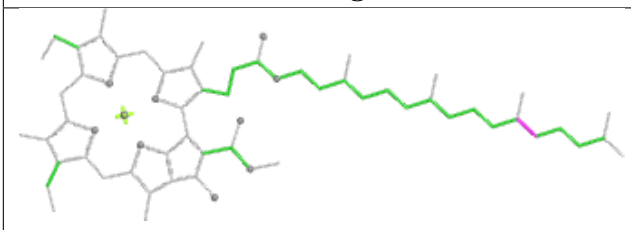
Ligand CLA b 617



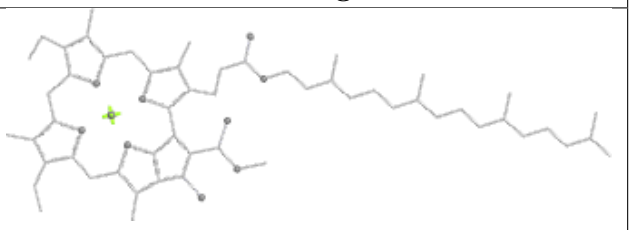
Bond lengths



Bond angles

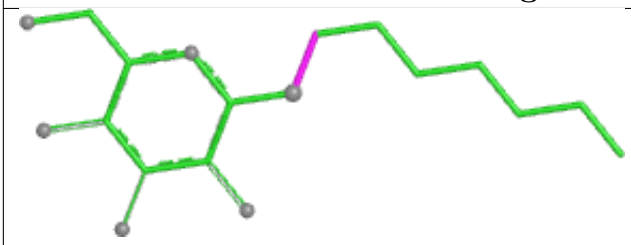


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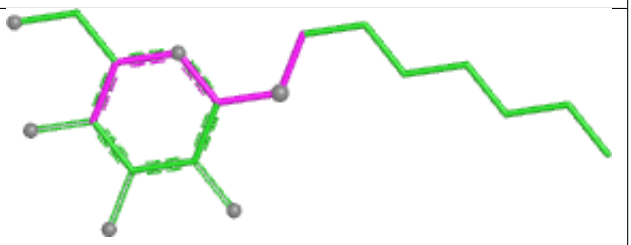


Rings

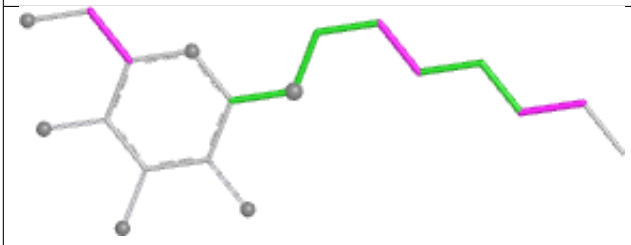
Ligand HTG D 412



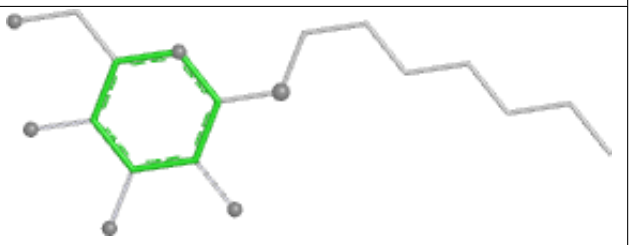
Bond lengths



Bond angles

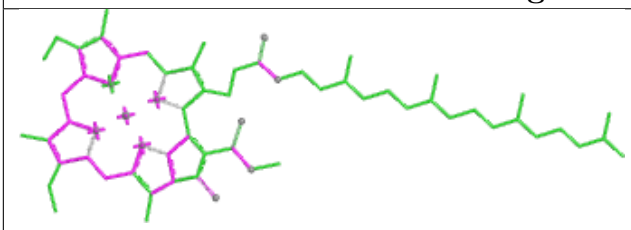


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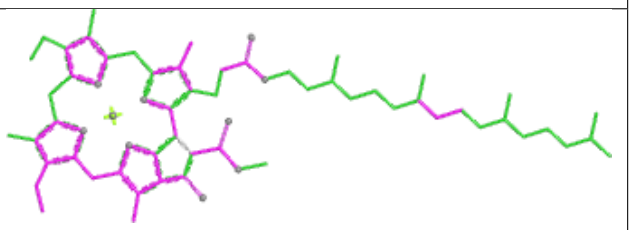


Rings

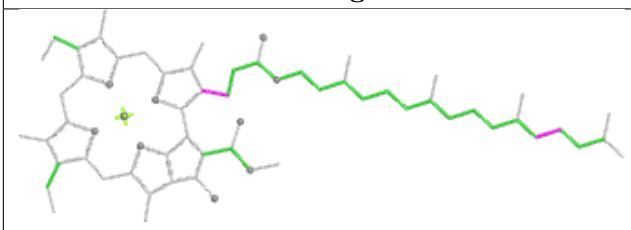
Ligand CLA b 612



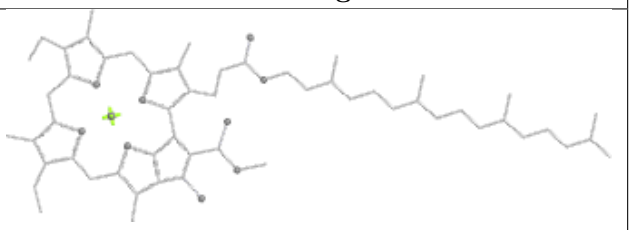
Bond lengths



Bond angles

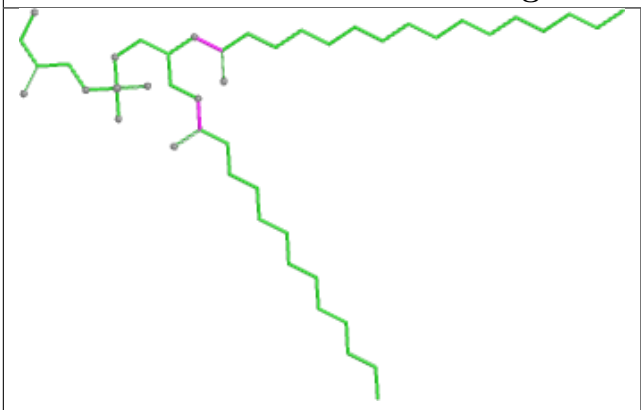


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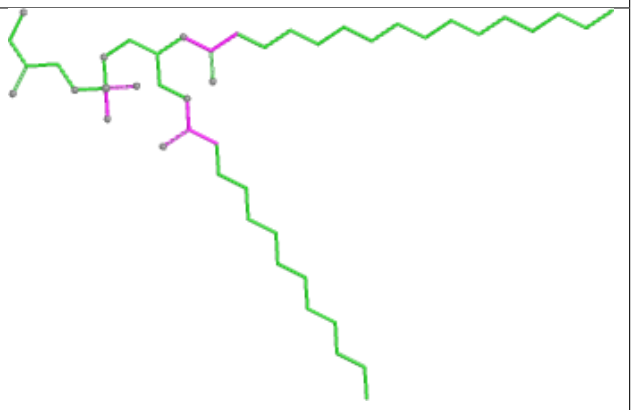


Rings

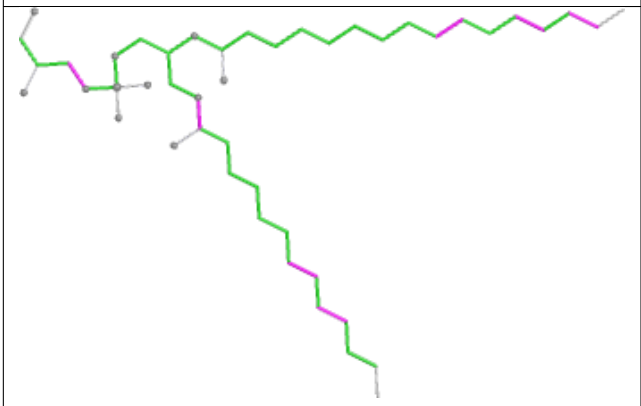
Ligand LHG D 408



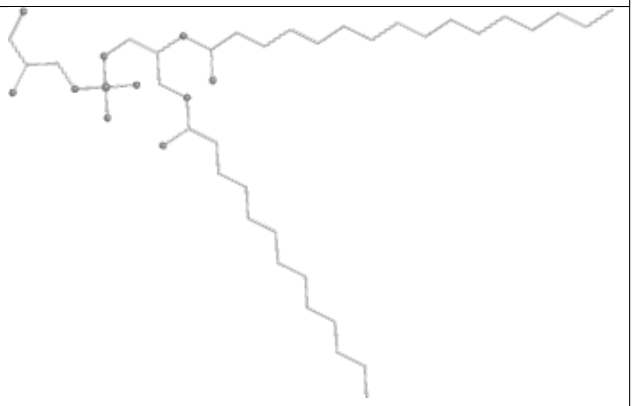
Bond lengths



Bond angles

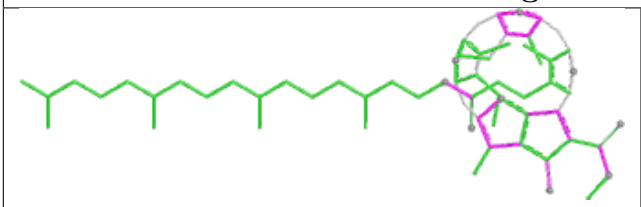


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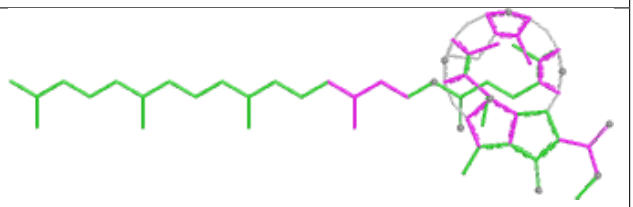


Rings

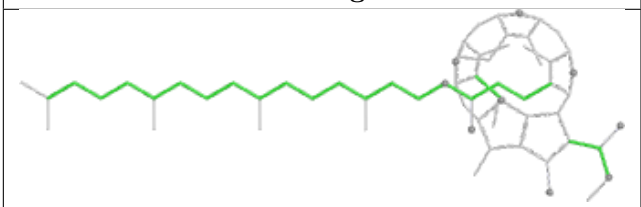
Ligand PHO A 409



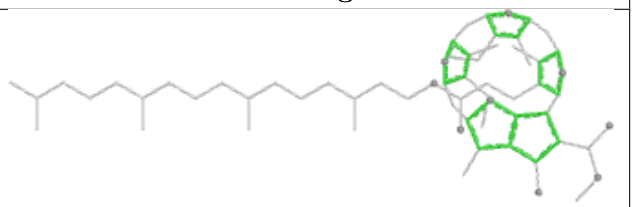
Bond lengths



Bond angles

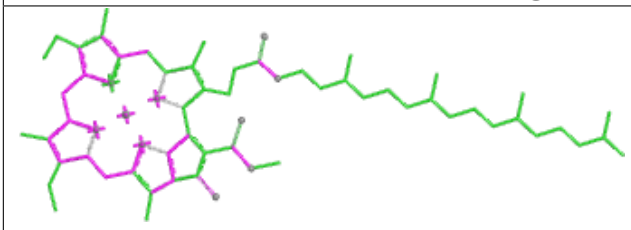


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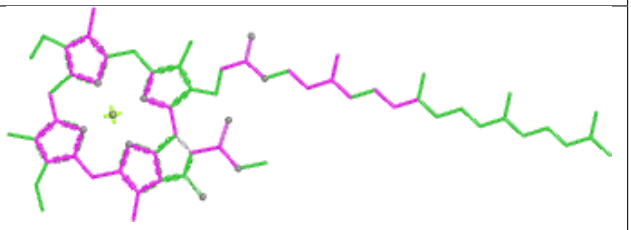


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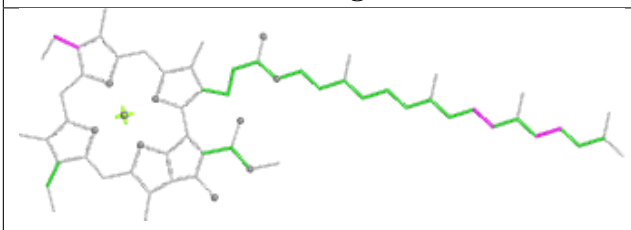
Ligand CLA b 608



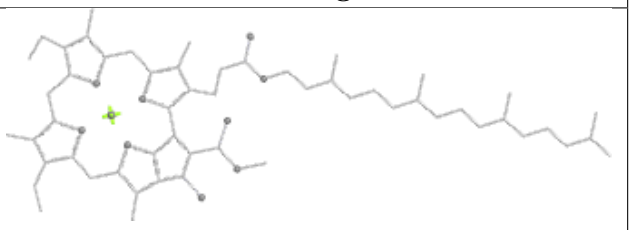
Bond lengths



Bond angles



Torsions



Rings

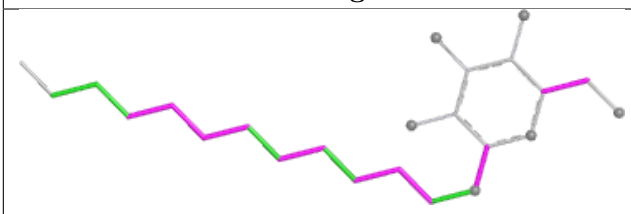
Ligand LMT B 626



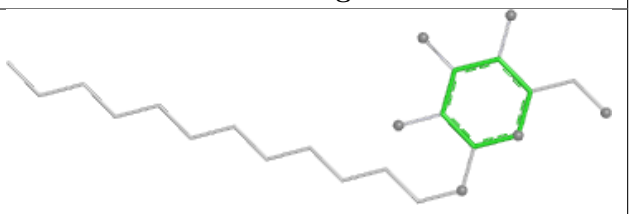
Bond lengths



Bond angles

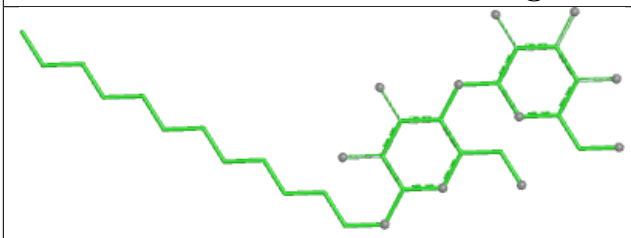


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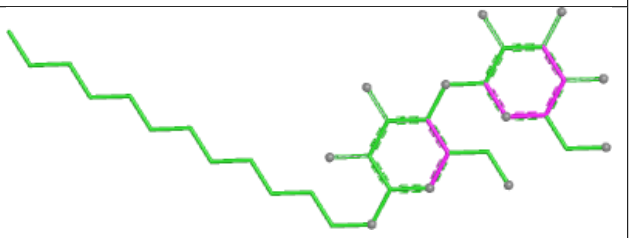


Rings

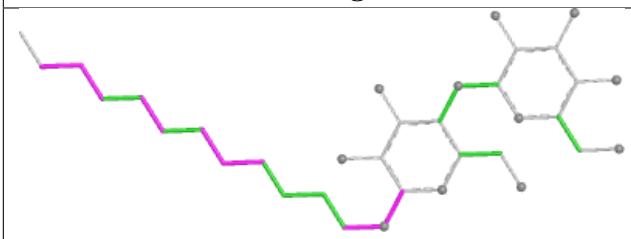
Ligand LMT a 402



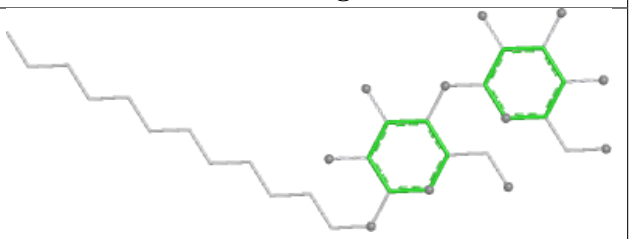
Bond lengths



Bond angles

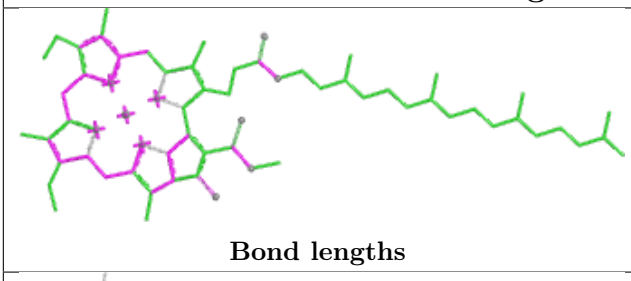


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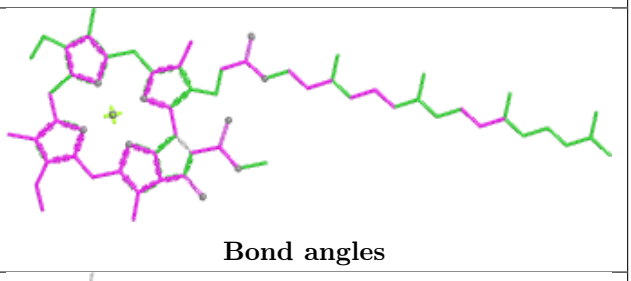


Rings

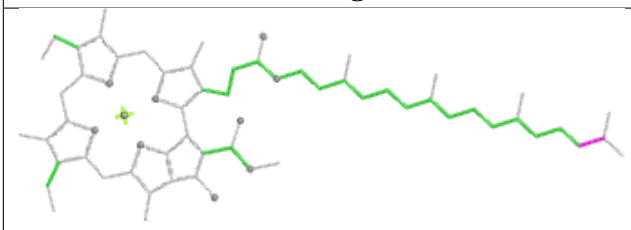
Ligand CLA b 615



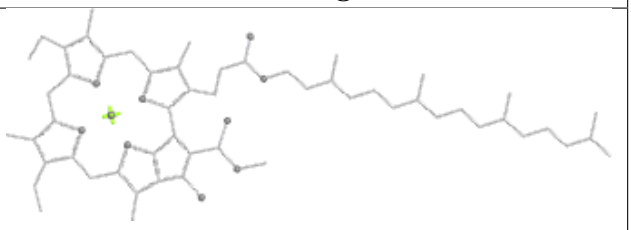
Bond lengths



Bond angles

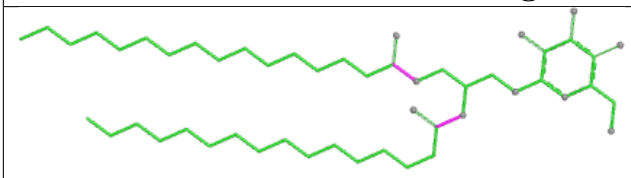


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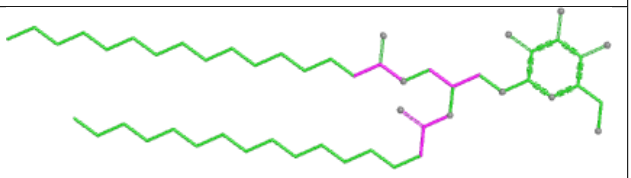


Rings

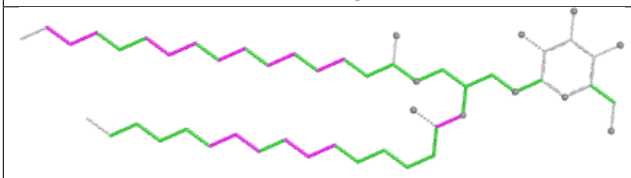
Ligand LMG B 621



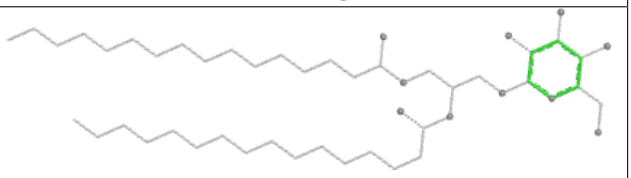
Bond lengths



Bond angles

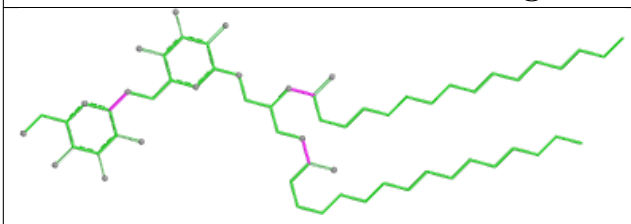


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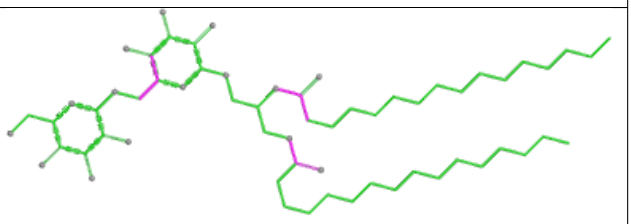


Rings

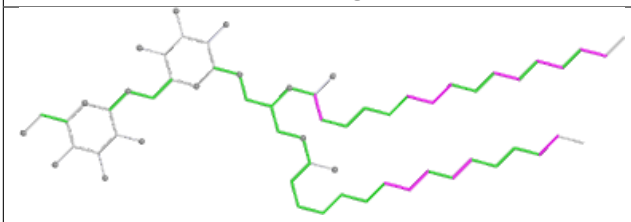
Ligand DGD h 102



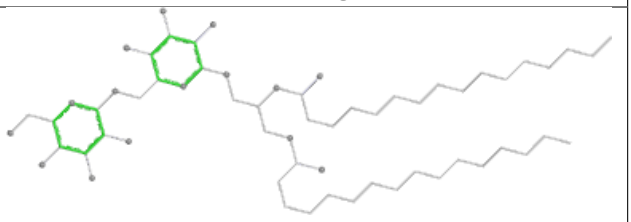
Bond lengths



Bond angles

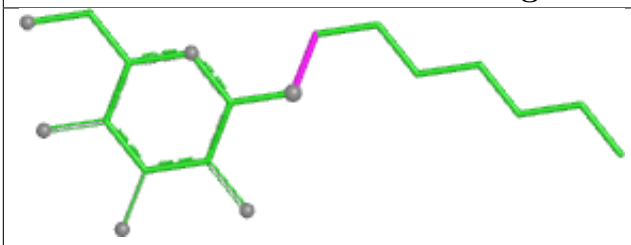


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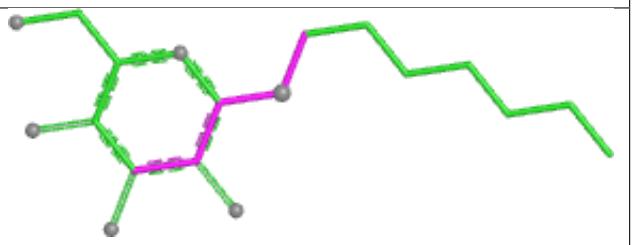


Rings

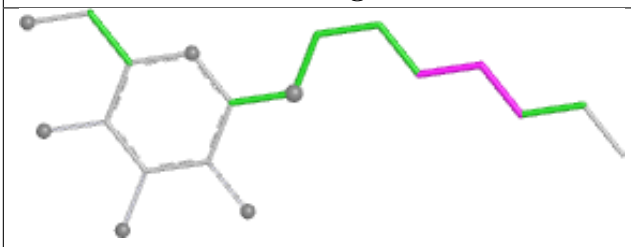
Ligand HTG B 624



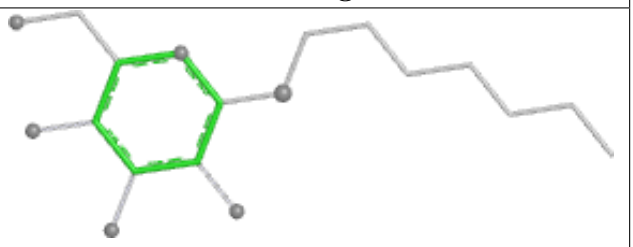
Bond lengths



Bond angles

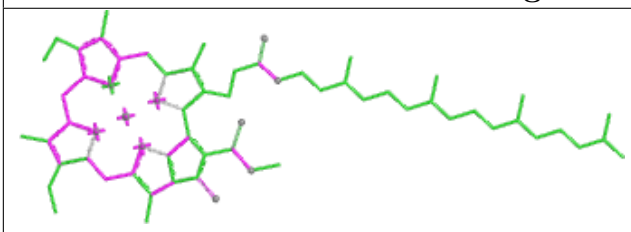


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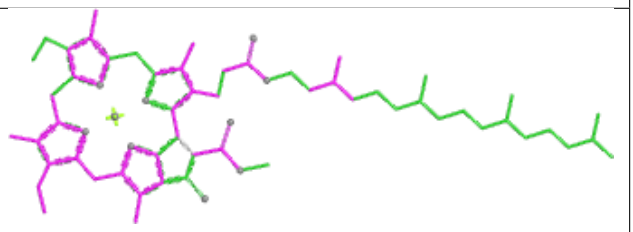


Rings

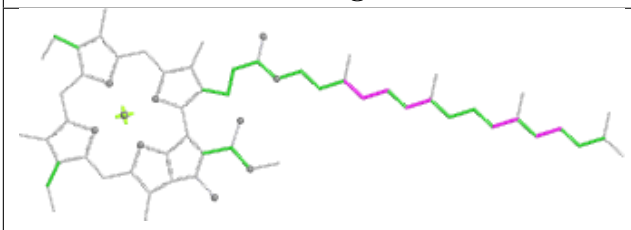
Ligand CLA A 410



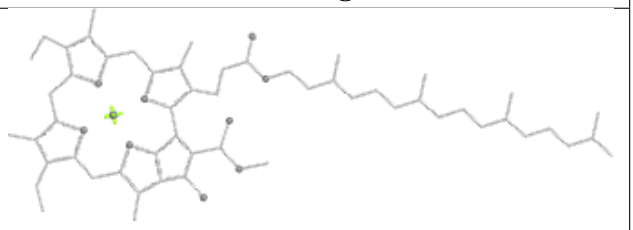
Bond lengths



Bond angles

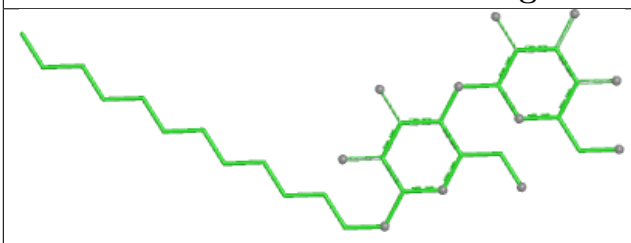


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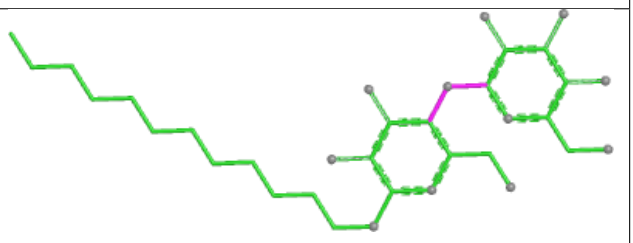


Rings

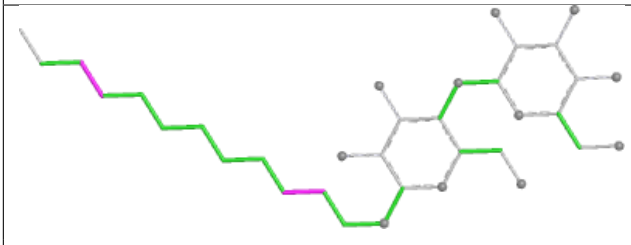
Ligand LMT m 103



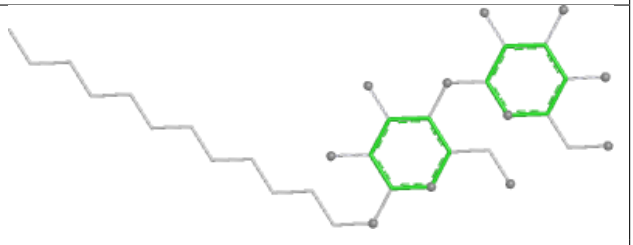
Bond lengths



Bond angles

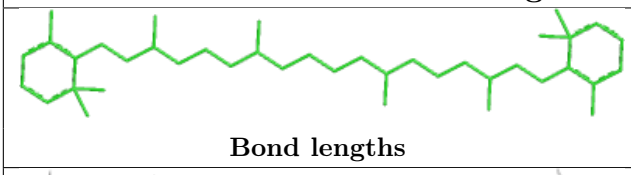


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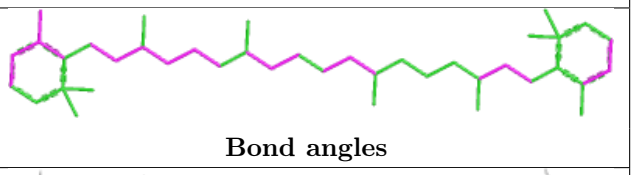


Rings

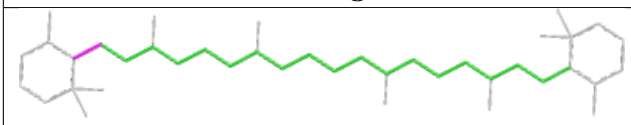
Ligand BCR b 621



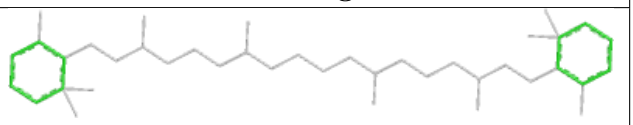
Bond lengths



Bond angles

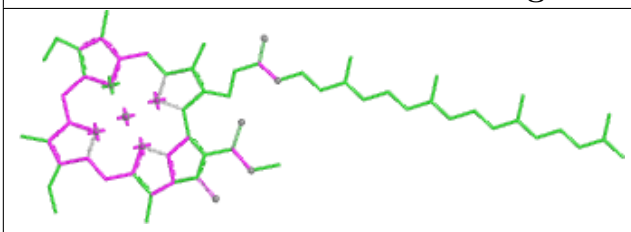


Torsions

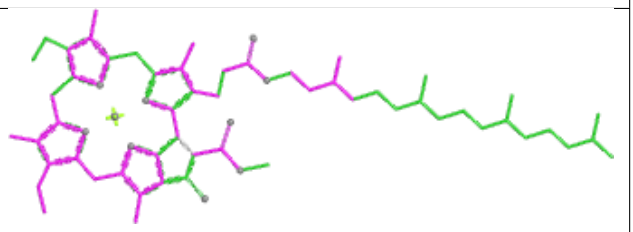


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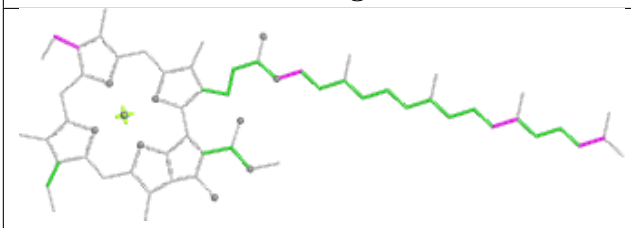
Ligand CLA d 404



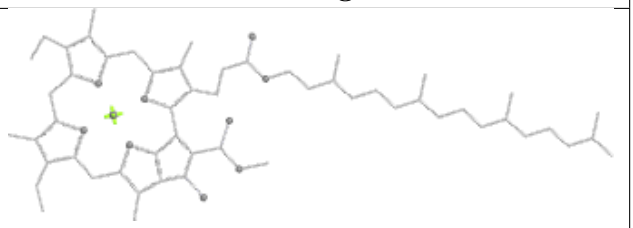
Bond lengths



Bond angles

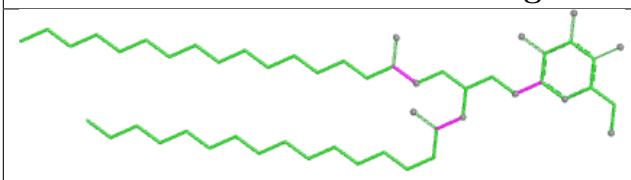


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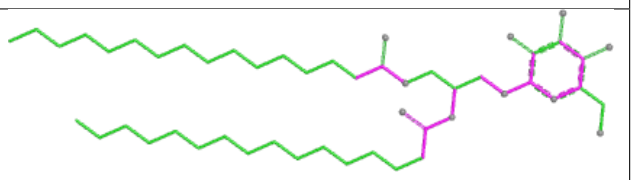


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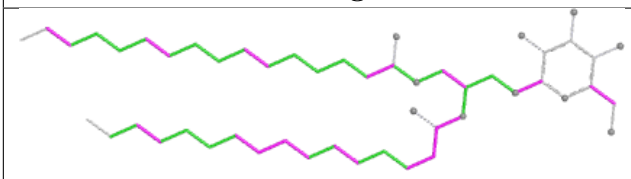
Ligand LMG a 416



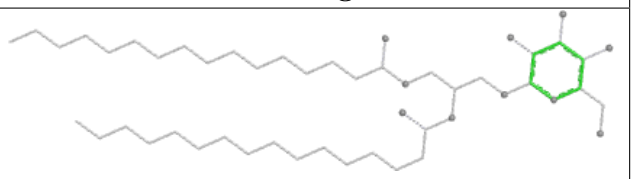
Bond lengths



Bond angles

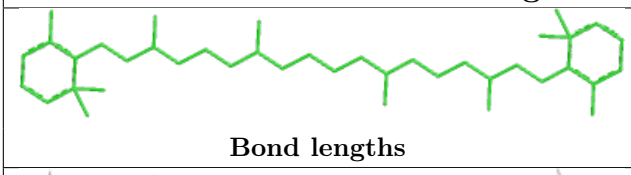


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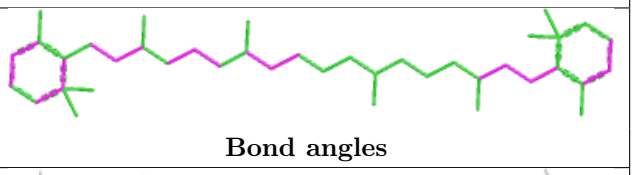


Rings

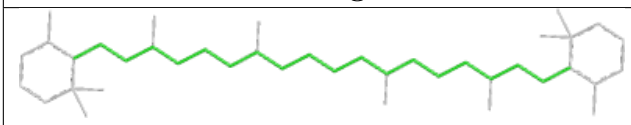
Ligand BCR B 620



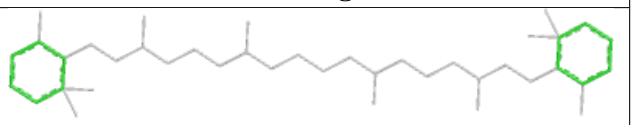
Bond lengths



Bond angles

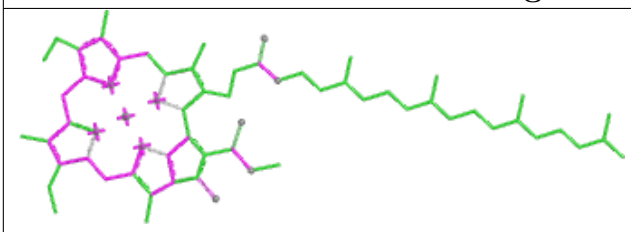


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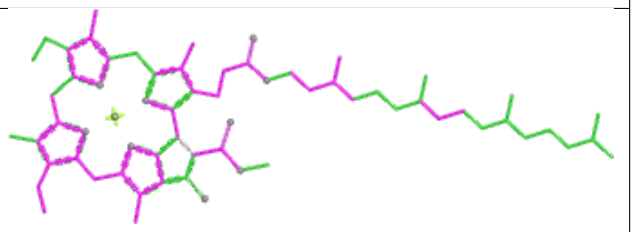


Rings

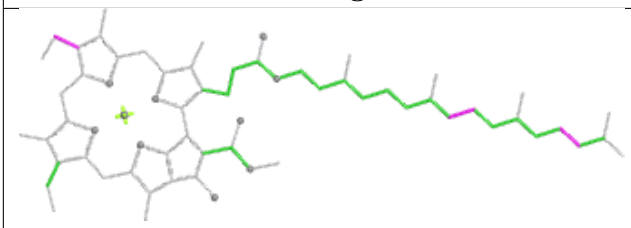
Ligand CLA B 603



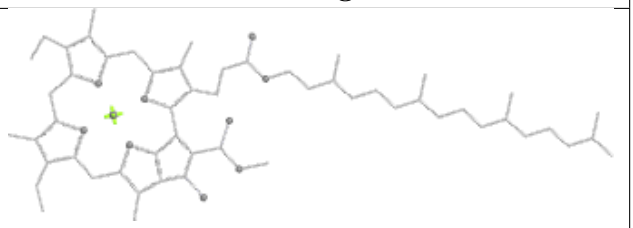
Bond lengths



Bond angles

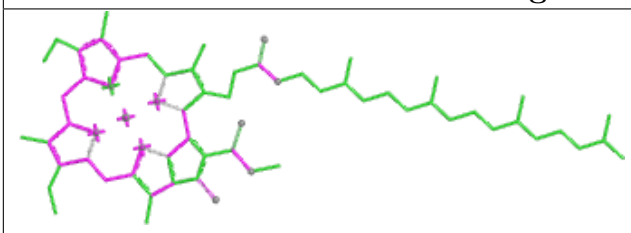


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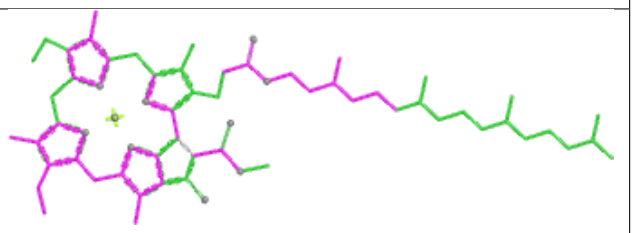


Rings

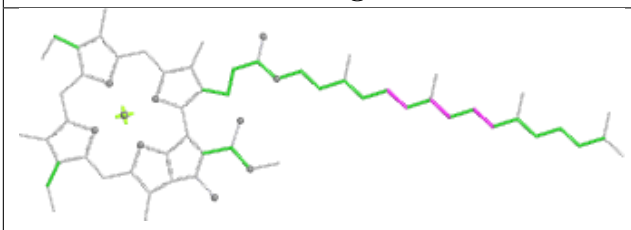
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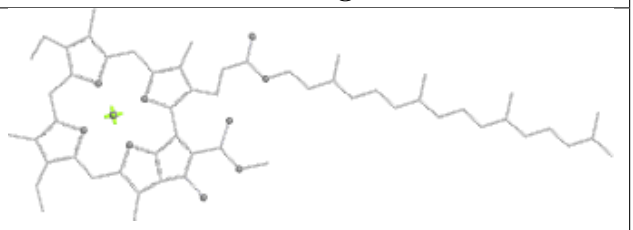
Bond lengths



Bond angles

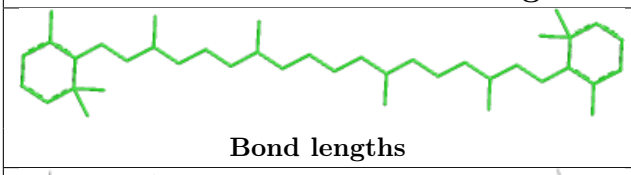


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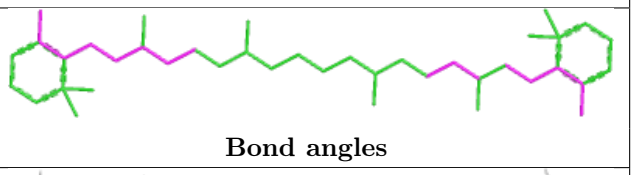


Rings

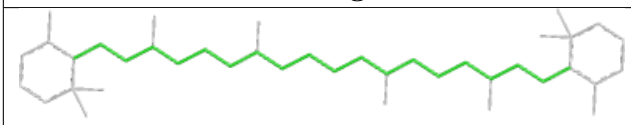
Ligand BCR C 514



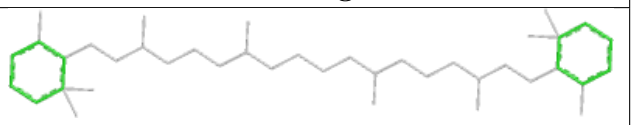
Bond lengths



Bond angles

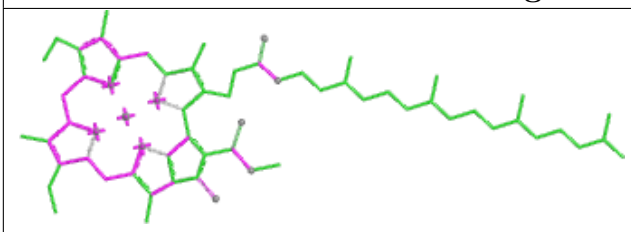


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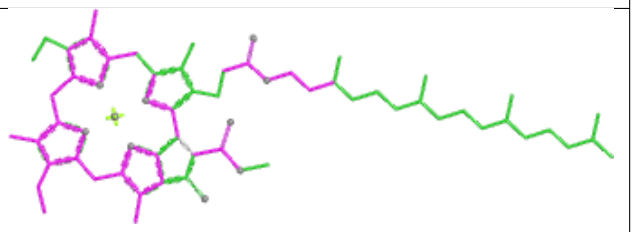


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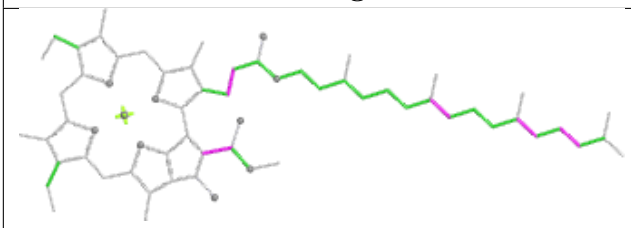
Ligand CLA C 507



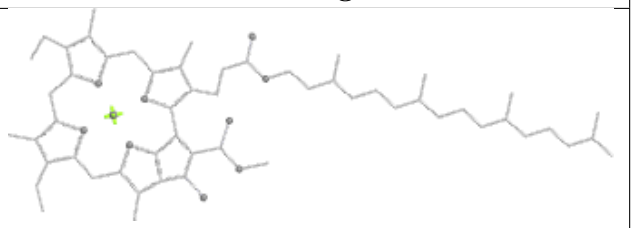
Bond lengths



Bond angles

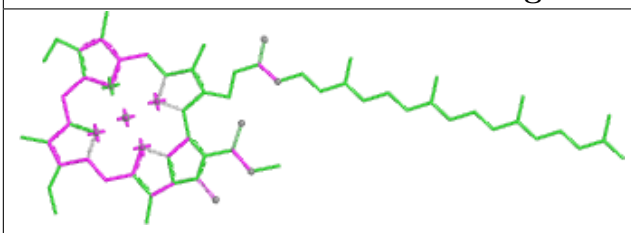


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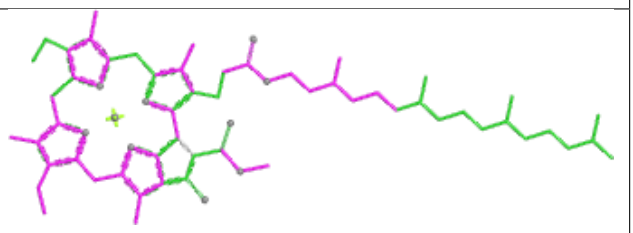


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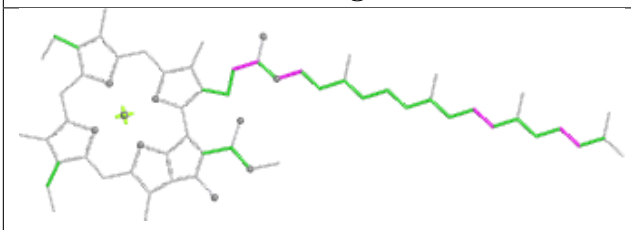
Ligand CLA B 614



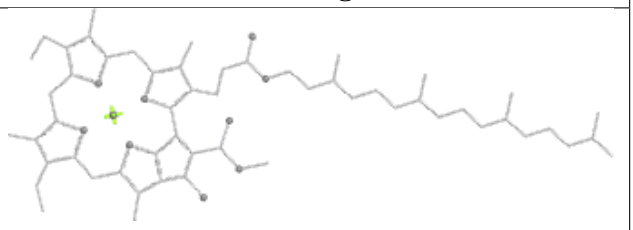
Bond lengths



Bond angles

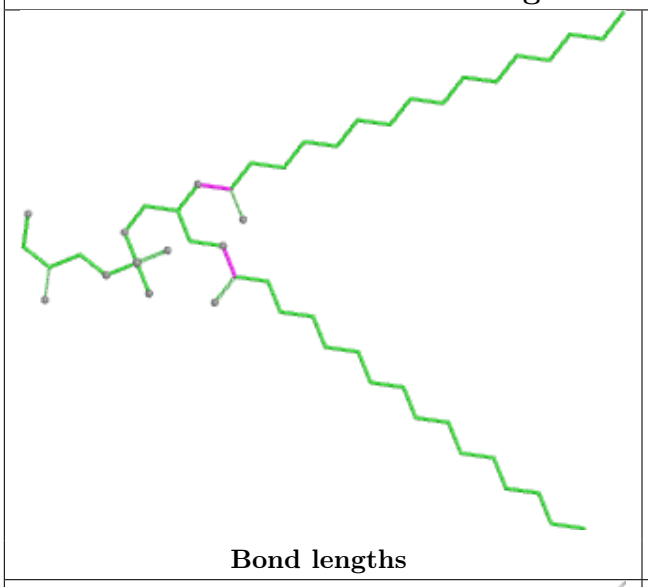


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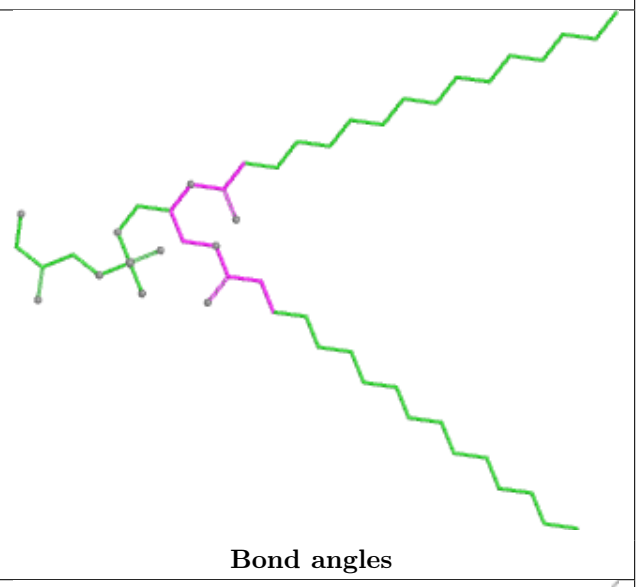


Rings

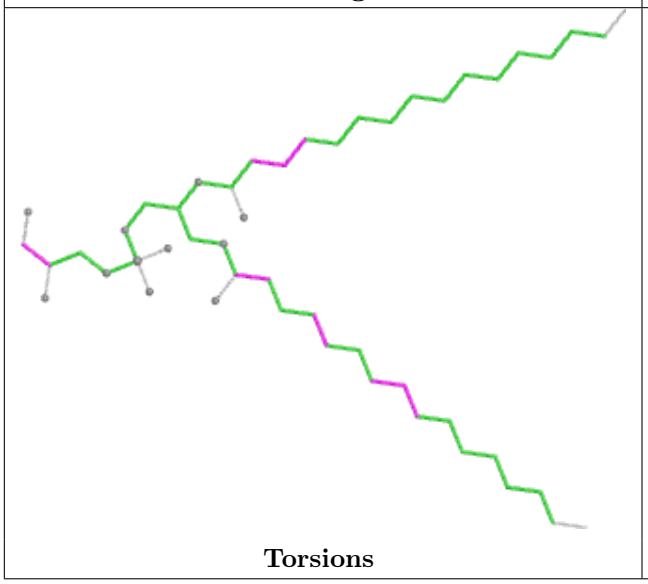
Ligand LHG D 406



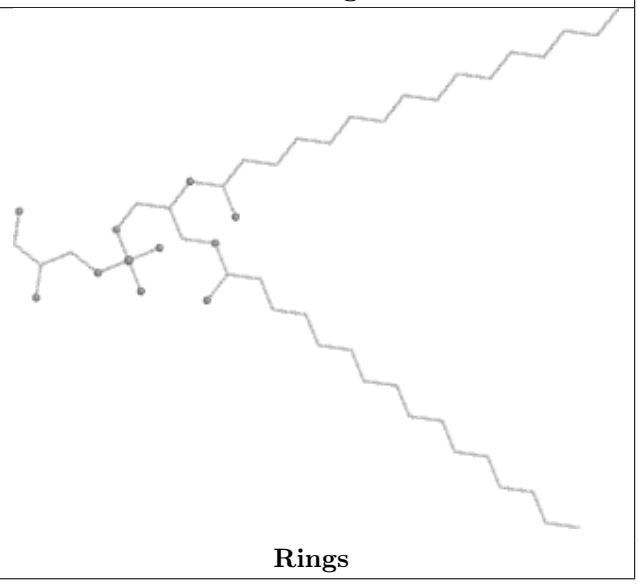
Bond lengths



Bond angles

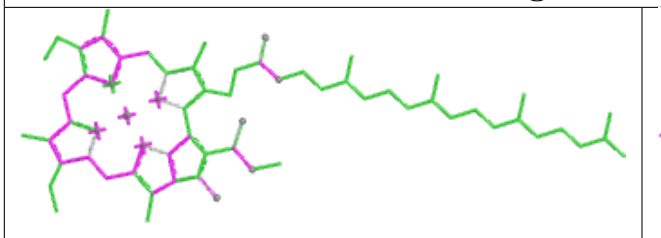


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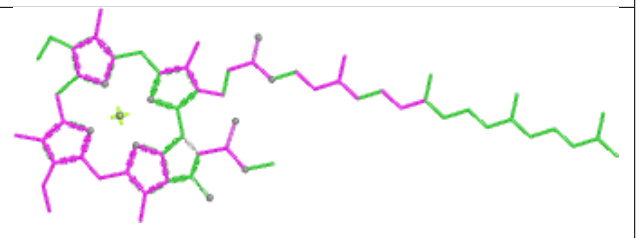


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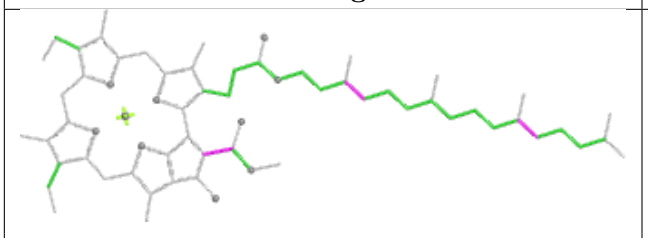
Ligand CLA d 405



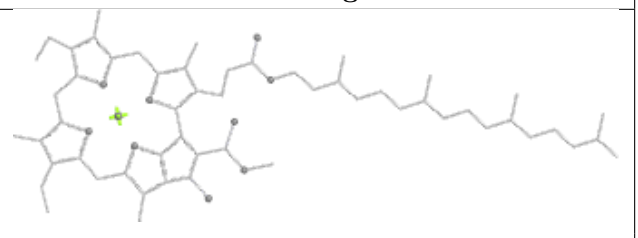
Bond lengths



Bond angles

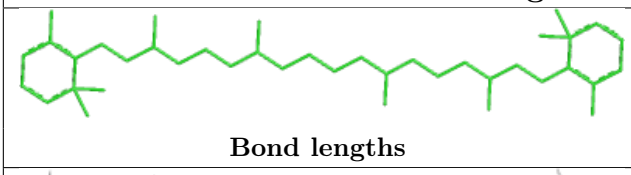


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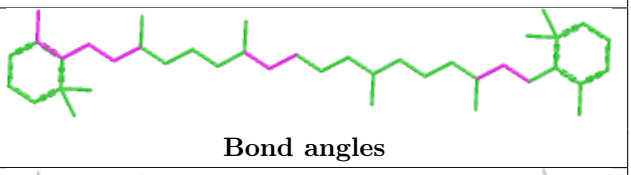


Rings

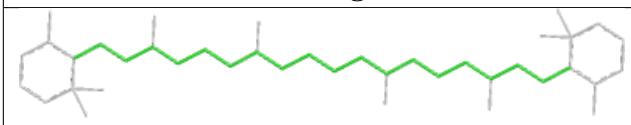
Ligand BCR a 414



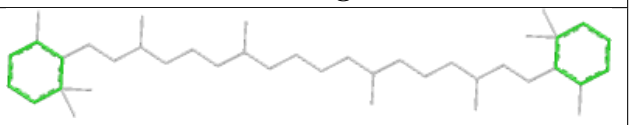
Bond lengths



Bond angles

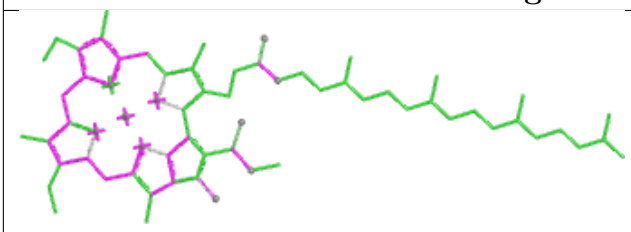


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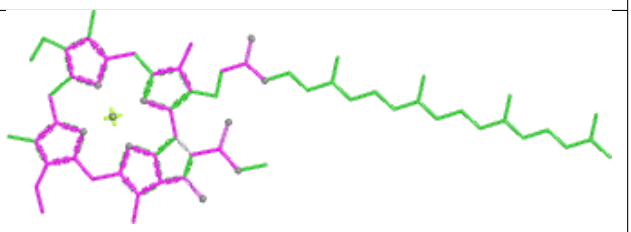


Rings

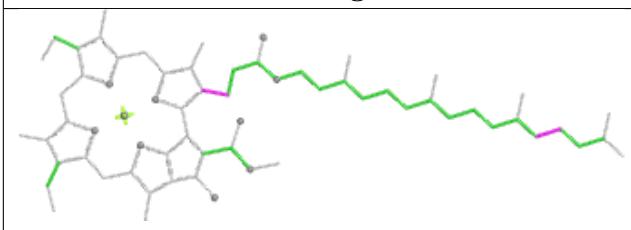
Ligand CLA B 609



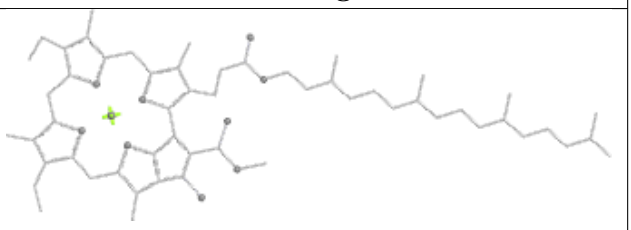
Bond lengths



Bond angles

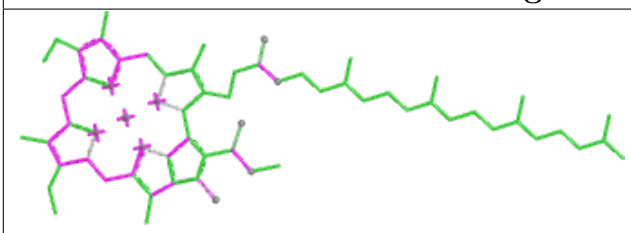


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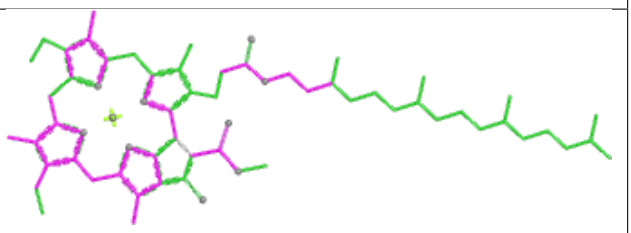


Rings

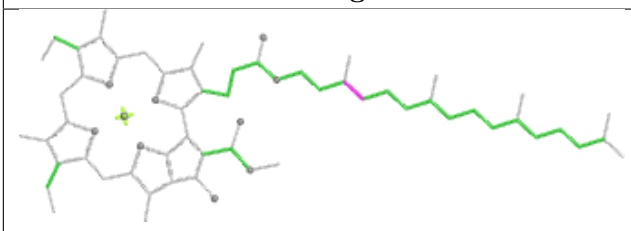
Ligand CLA C 505



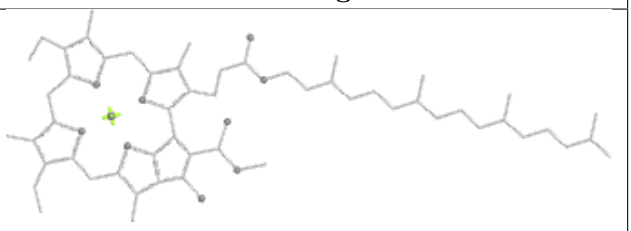
Bond lengths



Bond angles

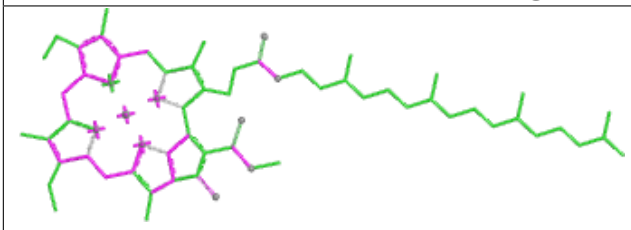


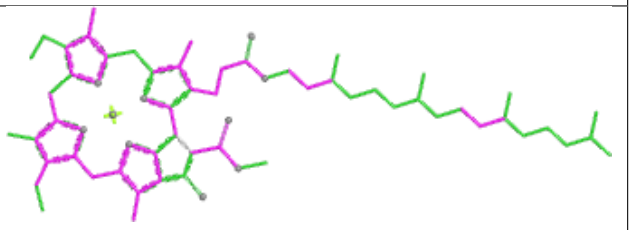
Torsions

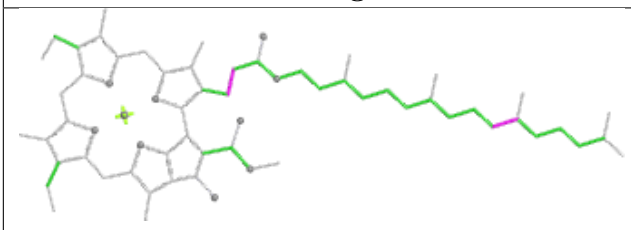


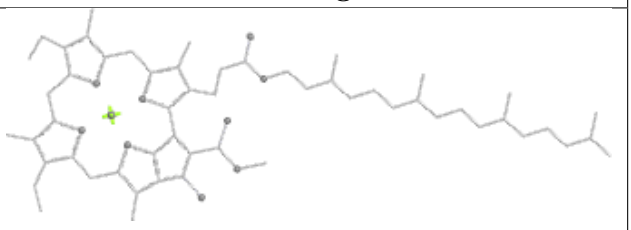
Rings

Ligand CLA b 614

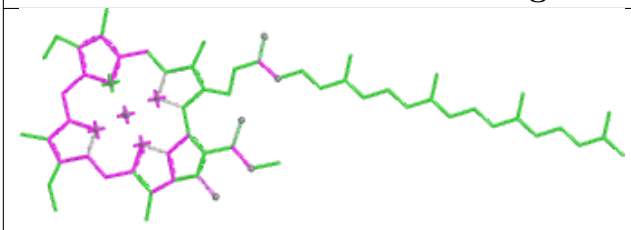

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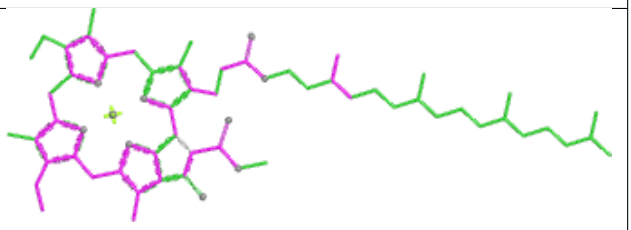

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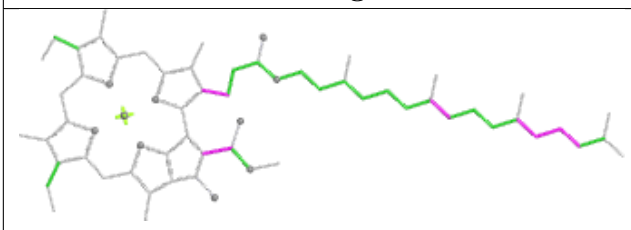

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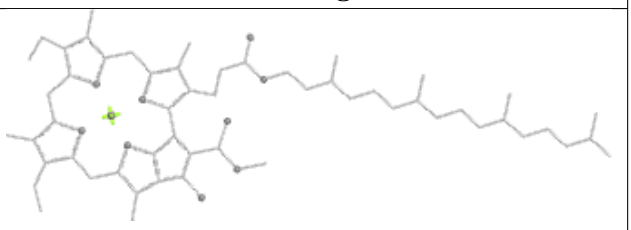

Rings

Ligand CLA c 907

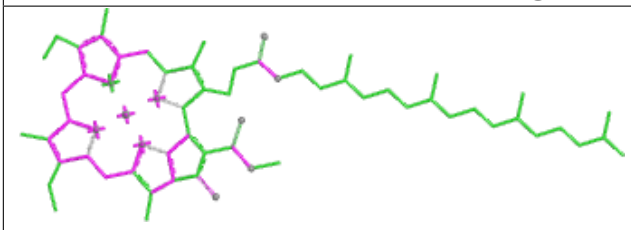

Bond lengths

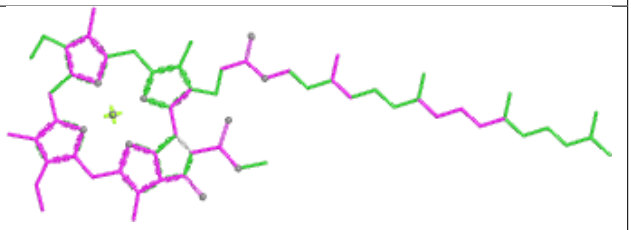

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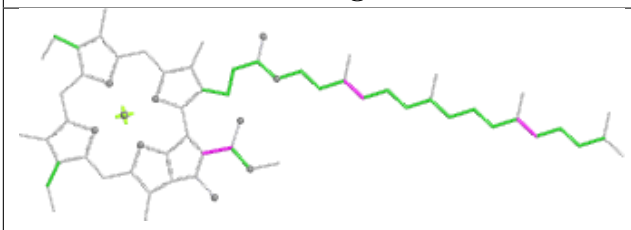

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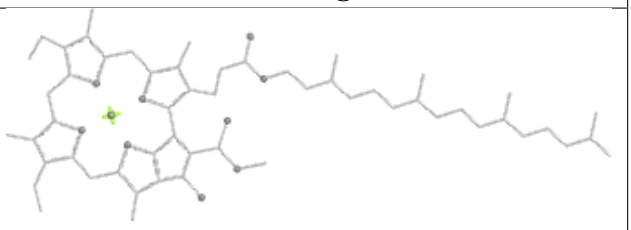

Rings

Ligand CLA c 905

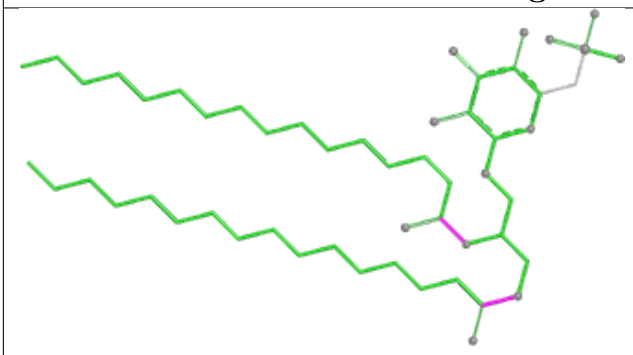

Bond lengths


Bond angles

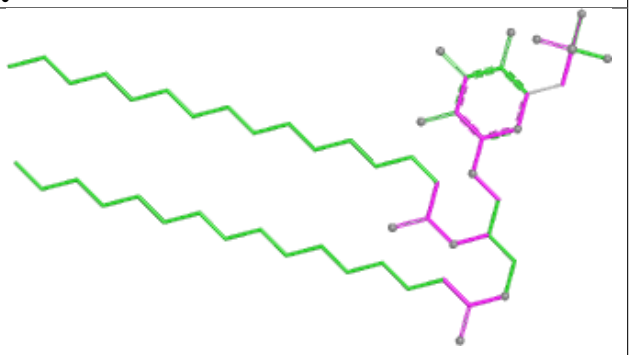

Torsions


Rings

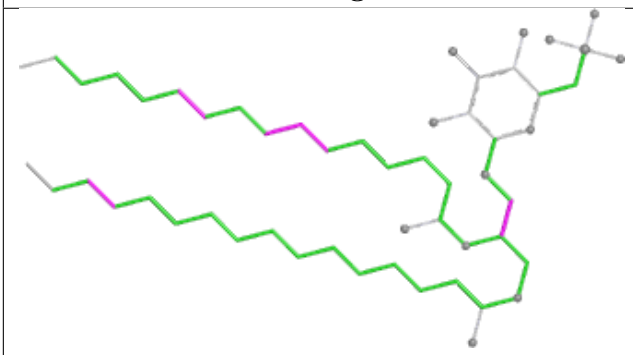
Ligand SQD a 415



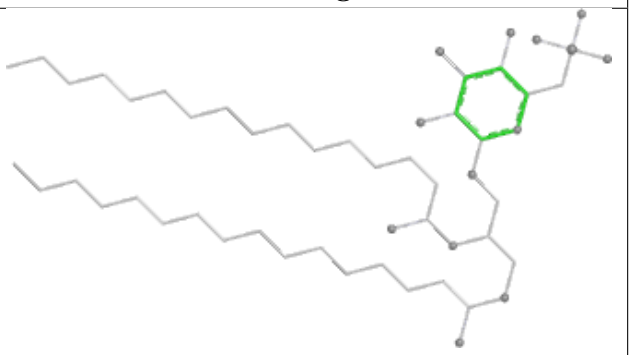
Bond lengths



Bond angles

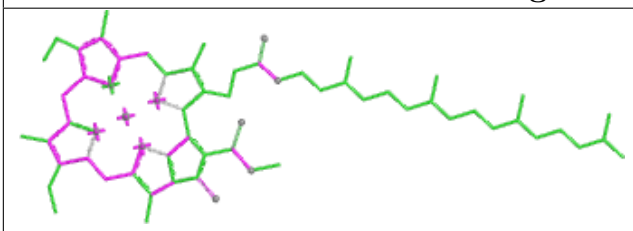


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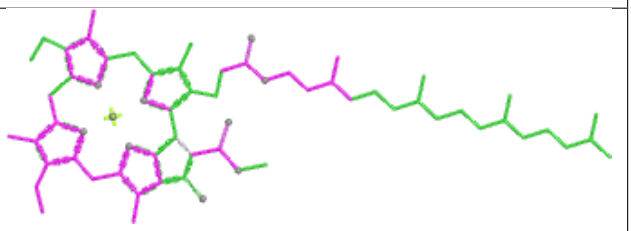


Rings

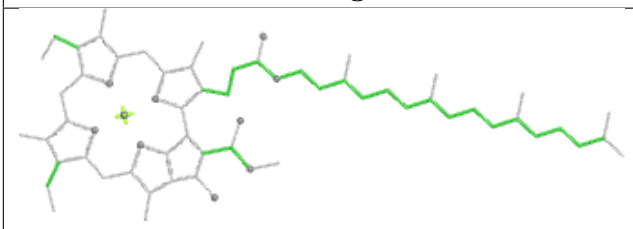
Ligand CLA c 912



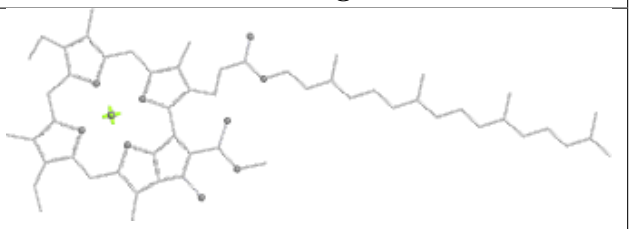
Bond lengths



Bond angles

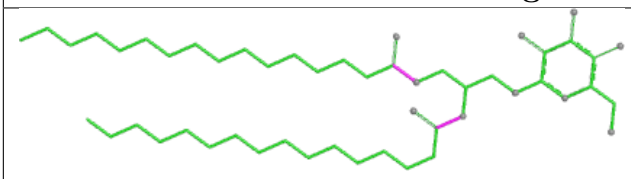


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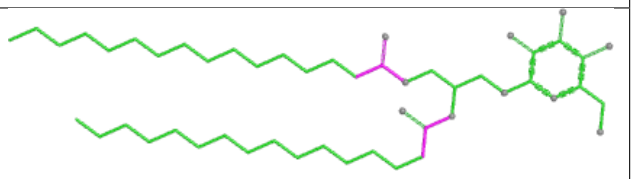


Rings

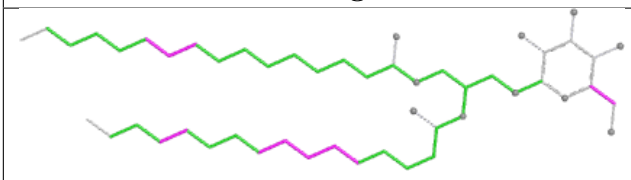
Ligand LMG d 412



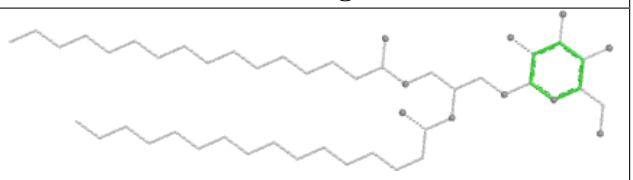
Bond lengths



Bond angles

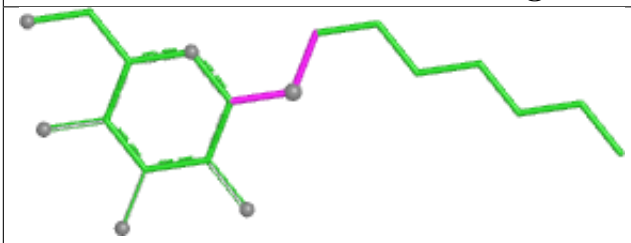


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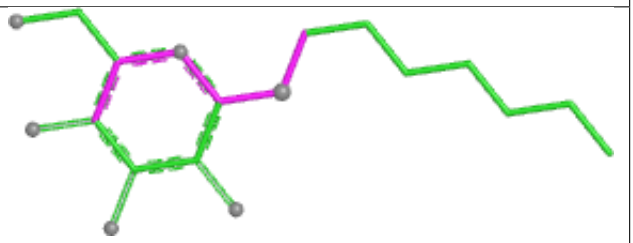


Rings

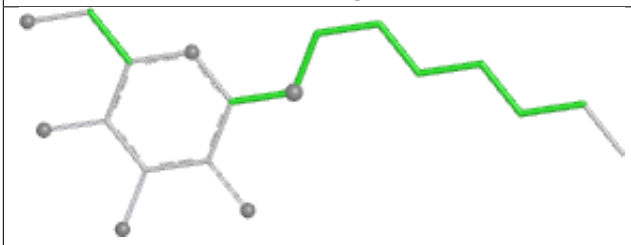
Ligand HTG c 923



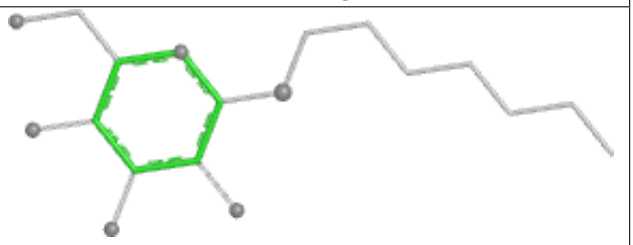
Bond lengths



Bond angles

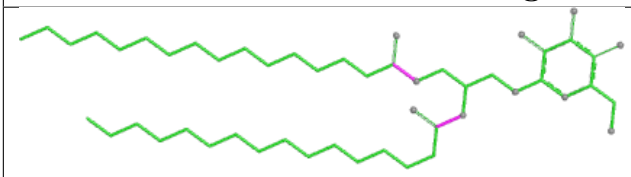


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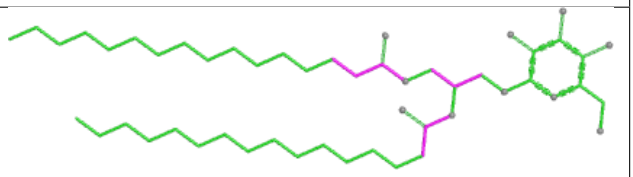


Rings

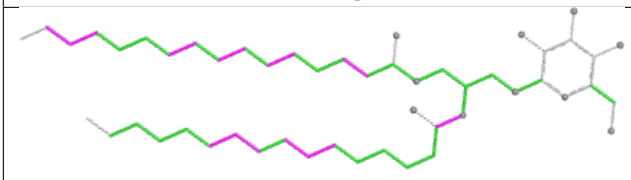
Ligand LMG b 624



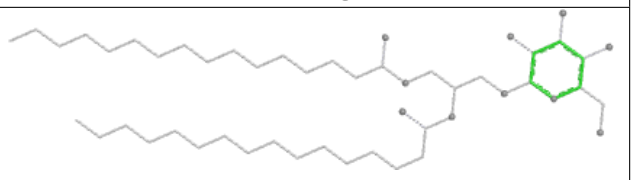
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Bond angles

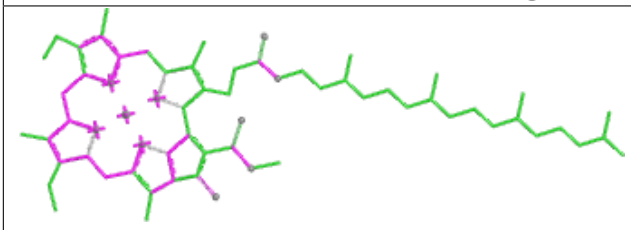


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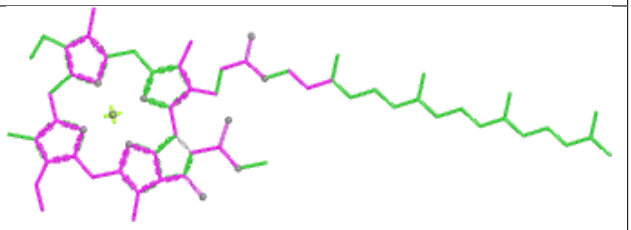


Rings

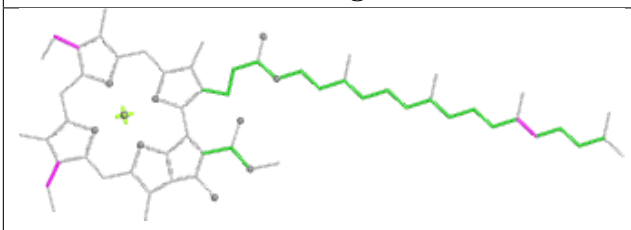
Ligand CLA D 401



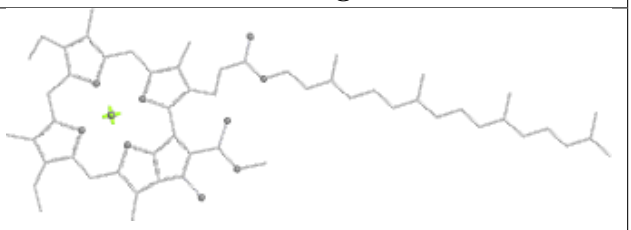
Bond lengths



Bond angles

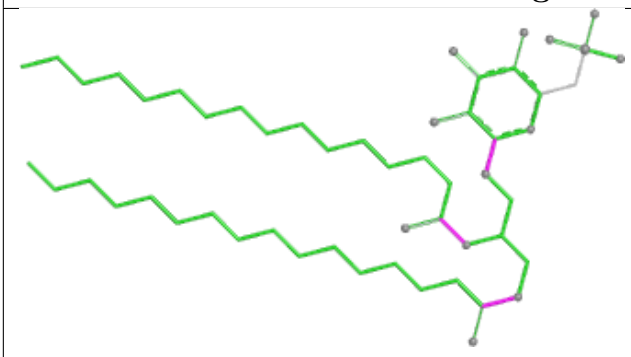


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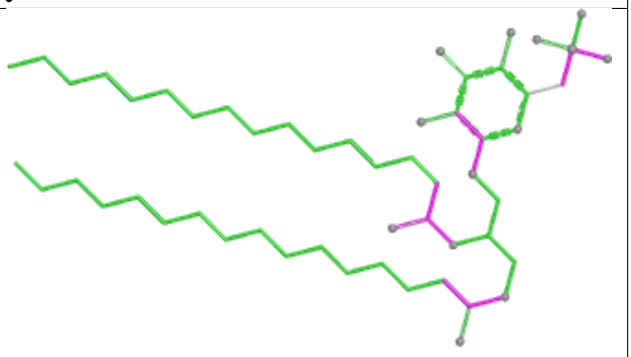


Rings

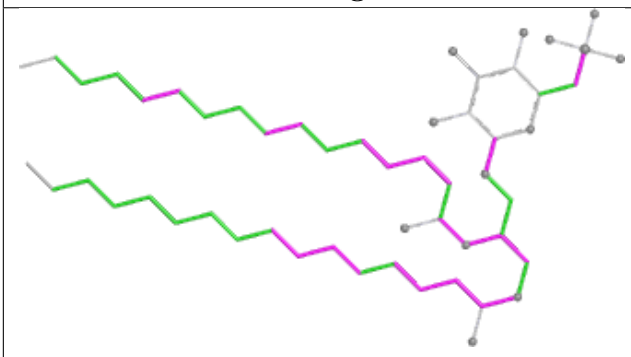
Ligand SQD l 101



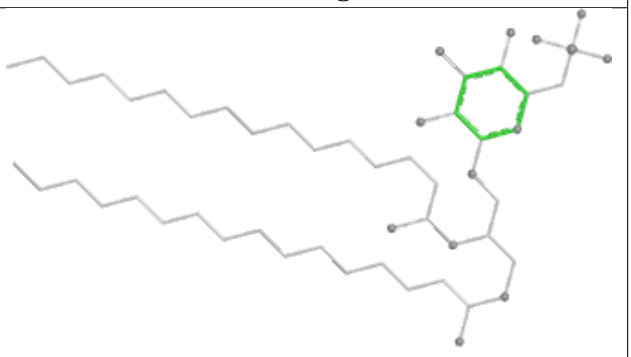
Bond lengths



Bond angles

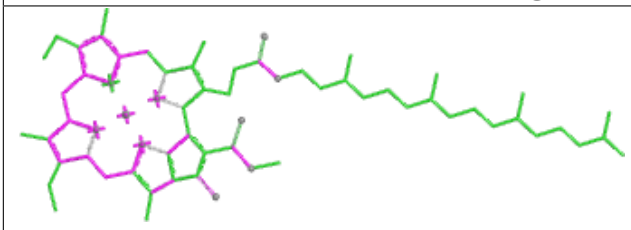


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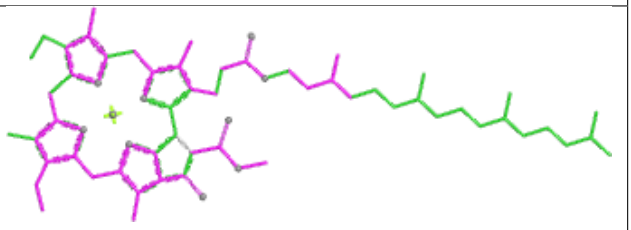


Rings

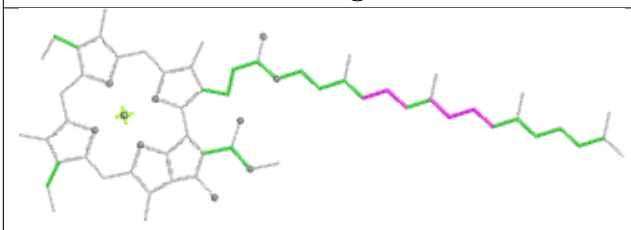
Ligand CLA a 413



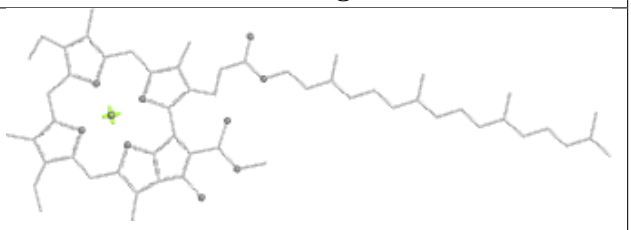
Bond lengths



Bond angles

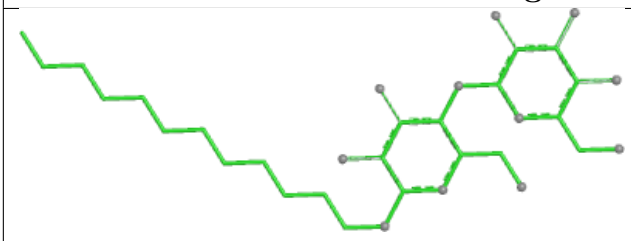


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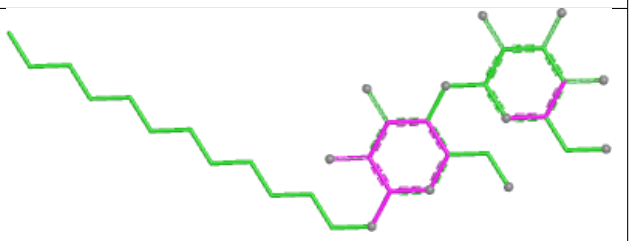


Rings

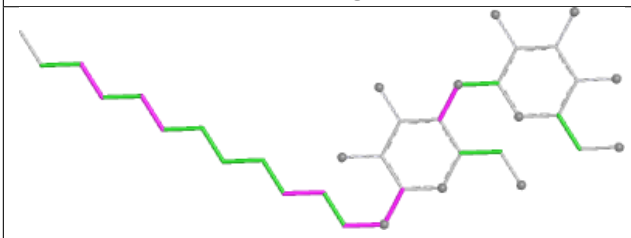
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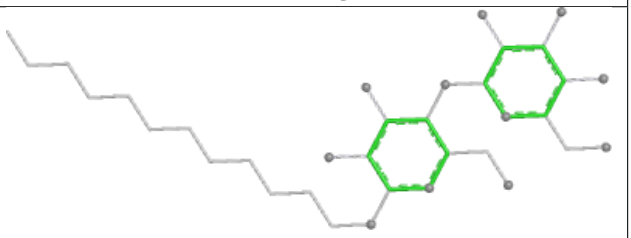
Bond lengths



Bond angles

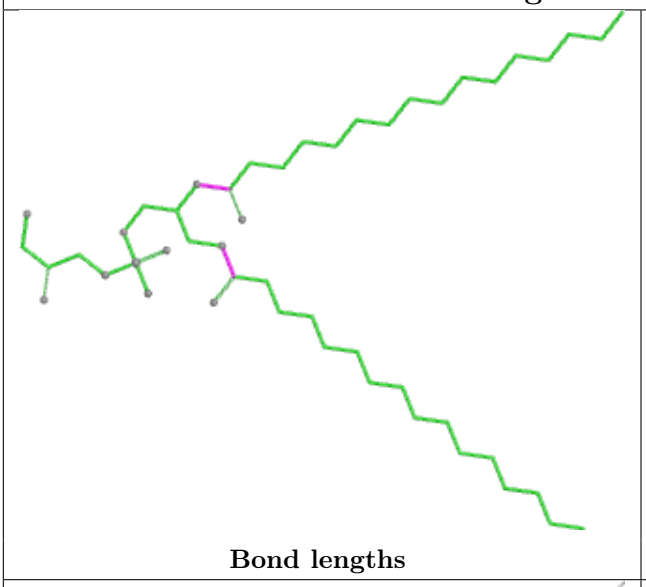


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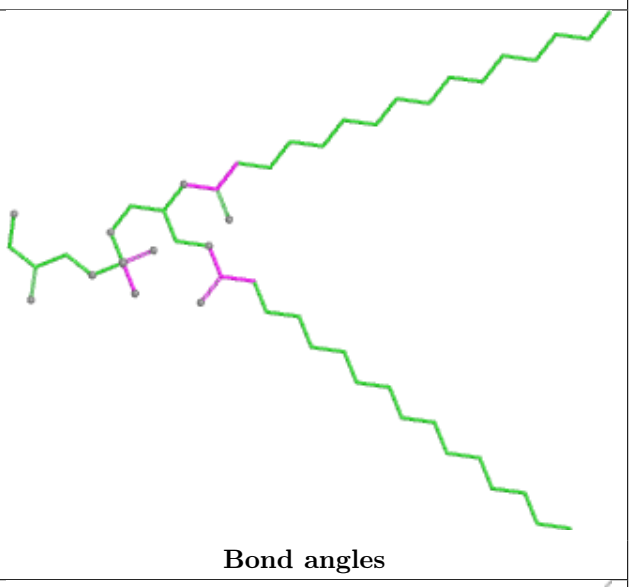


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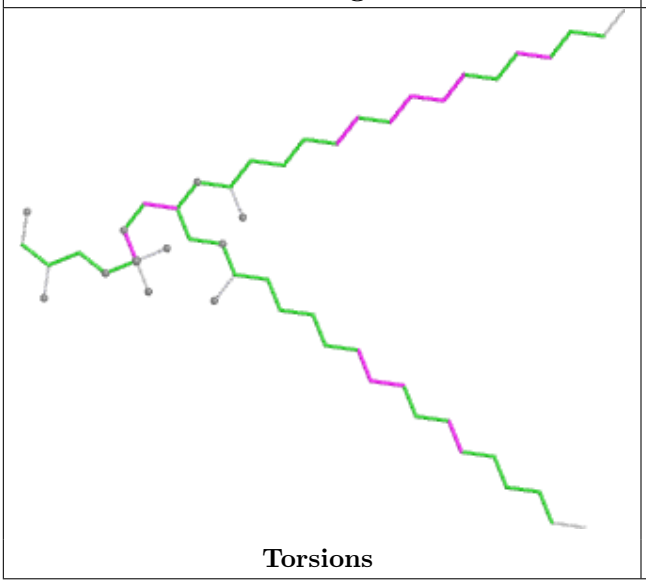
Ligand LHG L 101



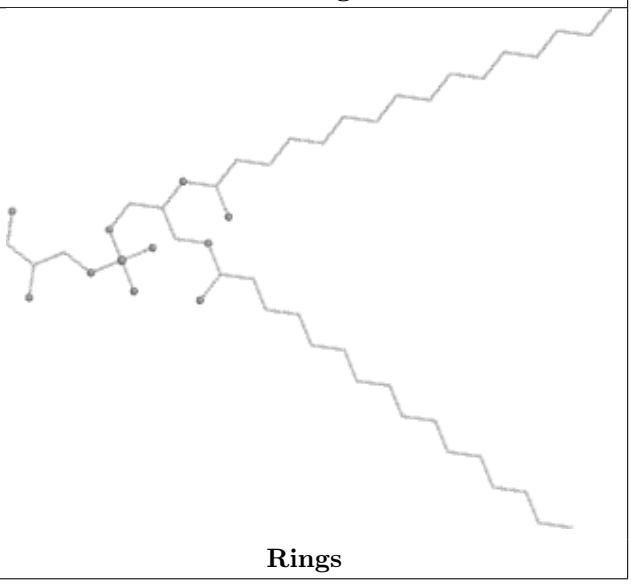
Bond lengths



Bond angles



Torsions

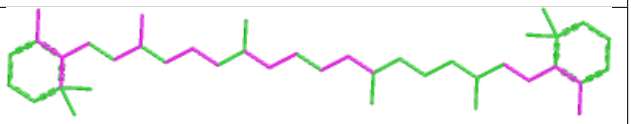


Rings

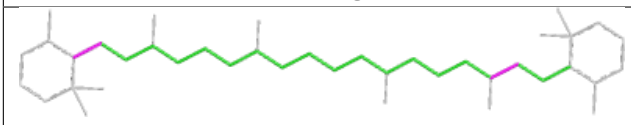
Ligand BCR k 102



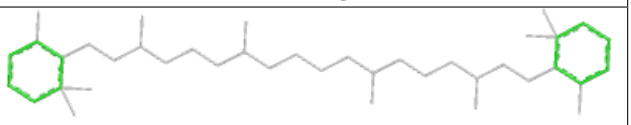
Bond lengths



Bond angles

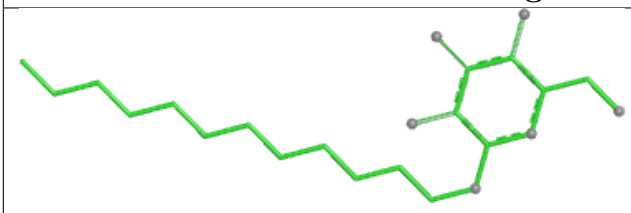


Torsions

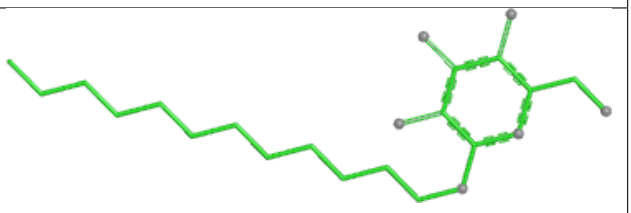


Rings

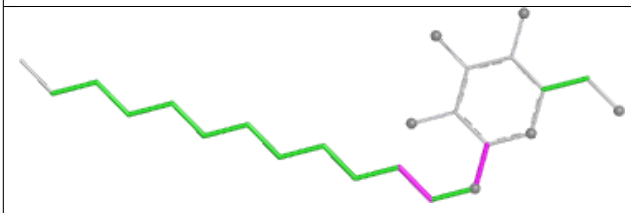
Ligand LMT J 102



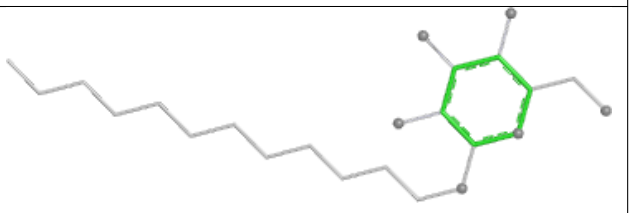
Bond lengths



Bond angles

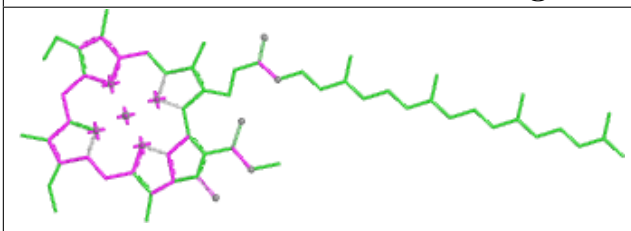


Torsions

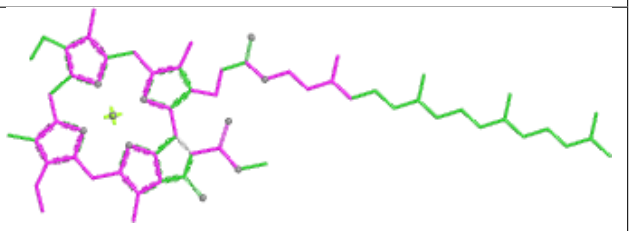


Rings

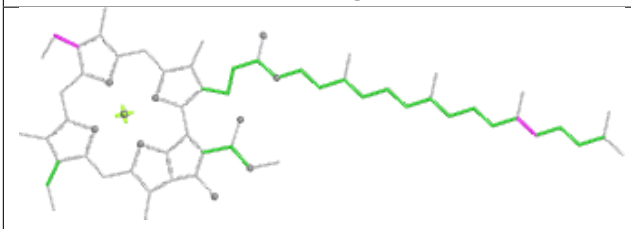
Ligand CLA c 913



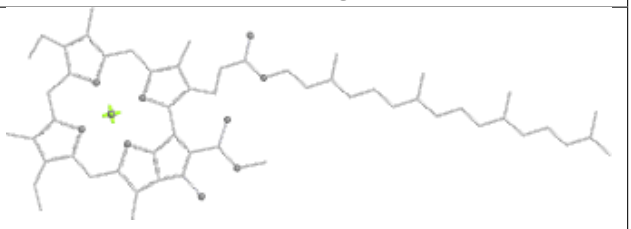
Bond lengths



Bond angles

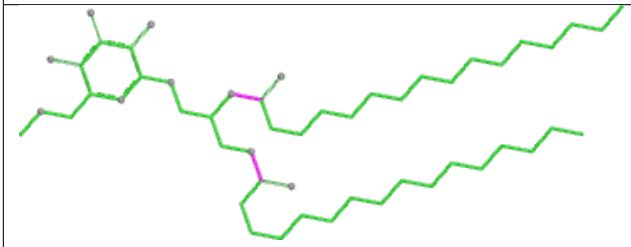


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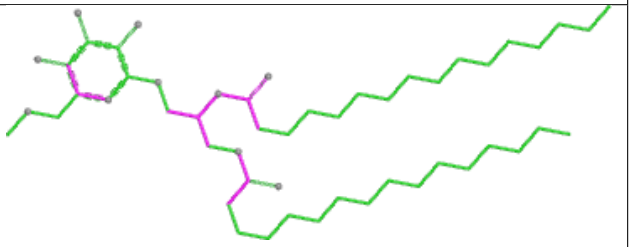


Rings

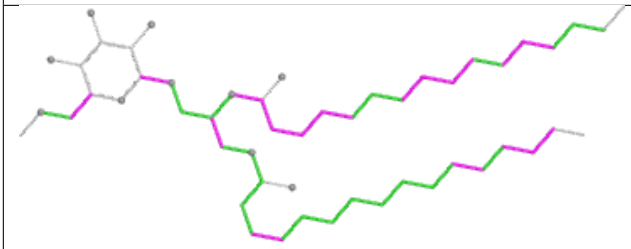
Ligand DGD D 405



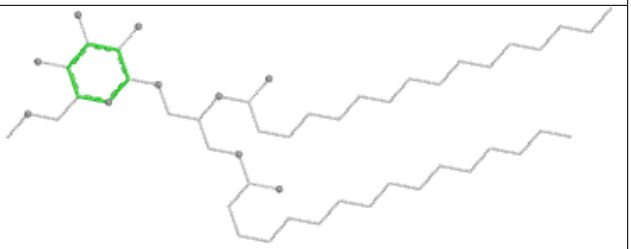
Bond lengths



Bond angles

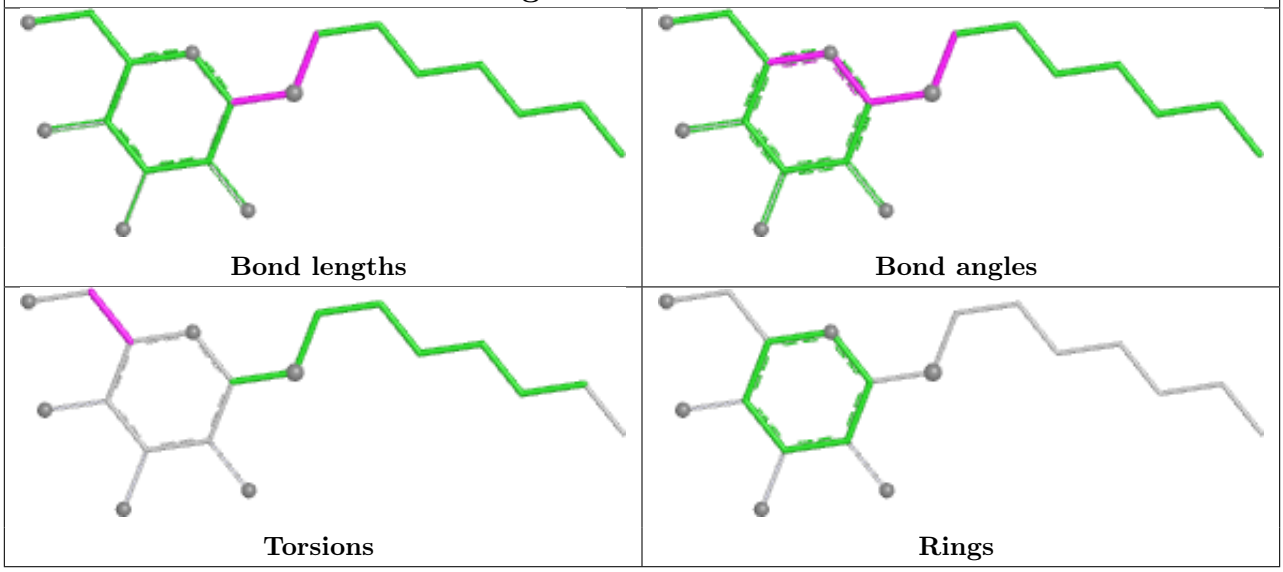


Torsions

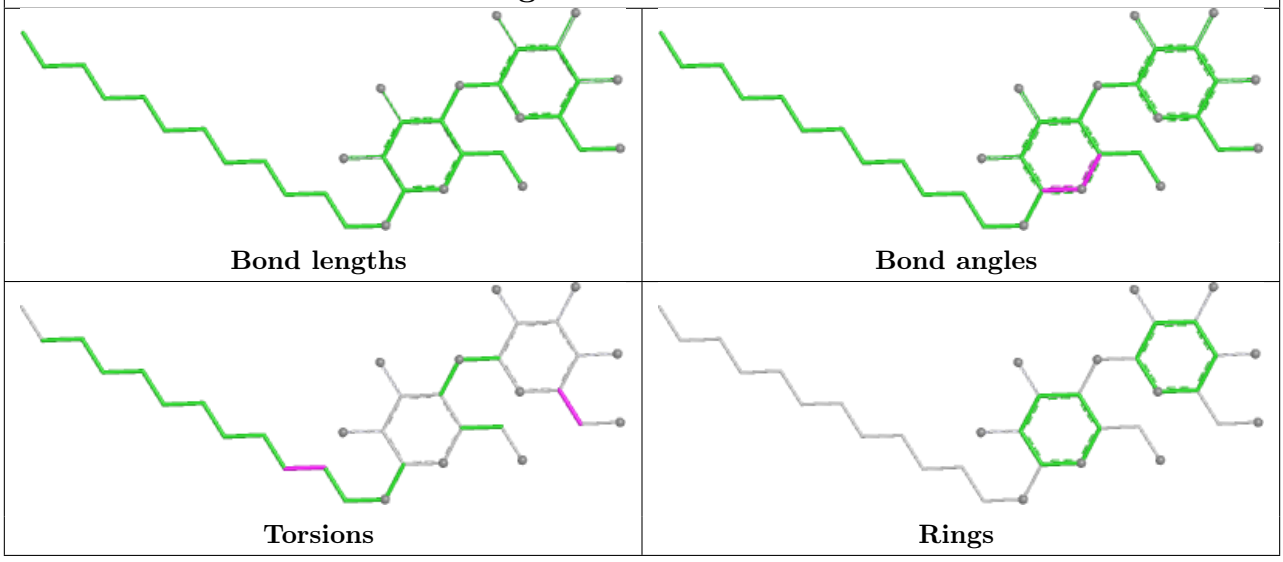


Rings

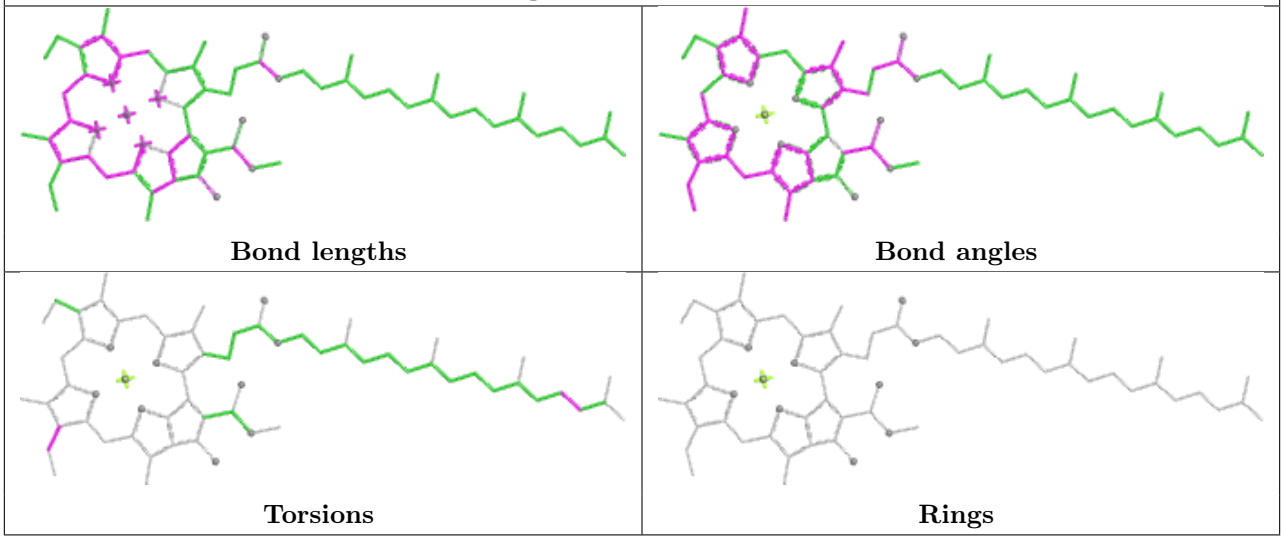
Ligand HTG B 630



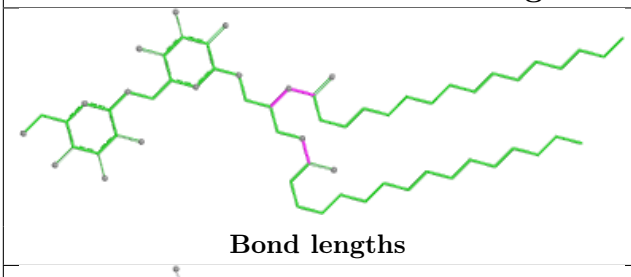
Ligand LMT M 101



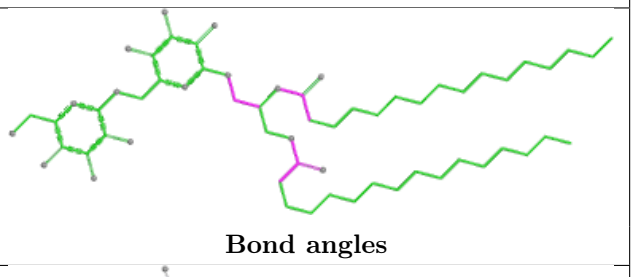
Ligand CLA A 406



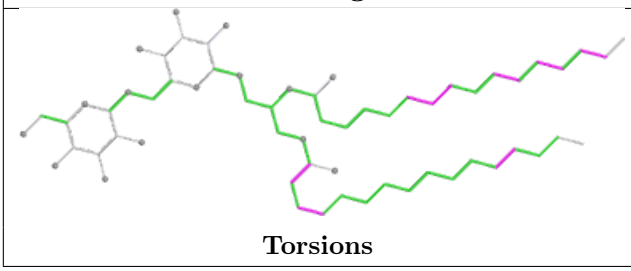
Ligand DGD c 919



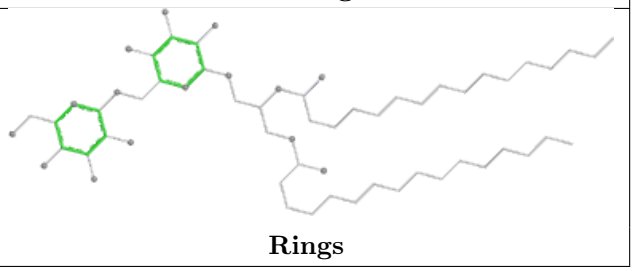
Bond lengths



Bond angles

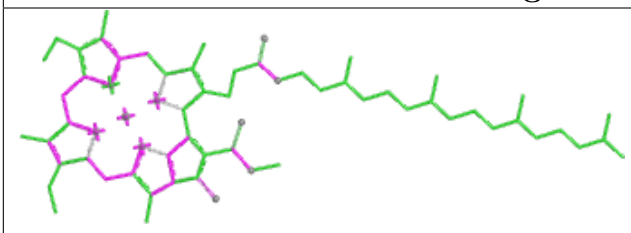


Torsions

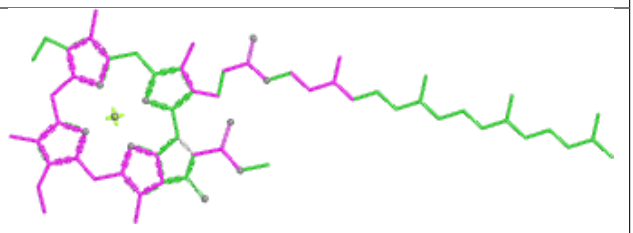


Rings

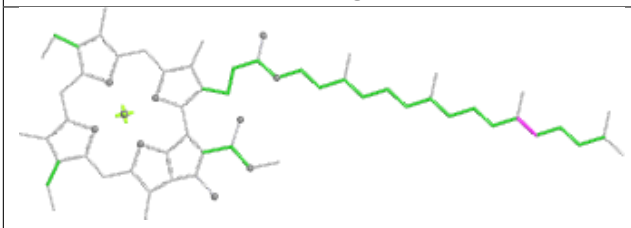
Ligand CLA A 407



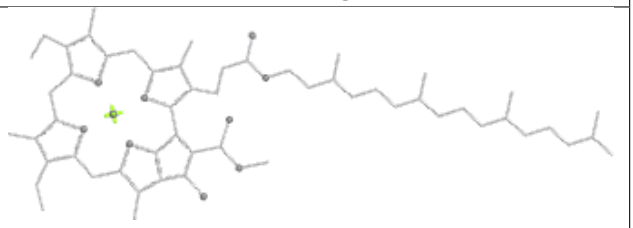
Bond lengths



Bond angles

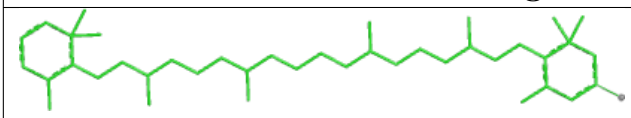


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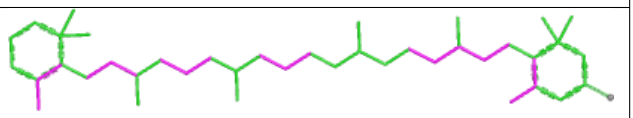


Rings

Ligand RRX h 101



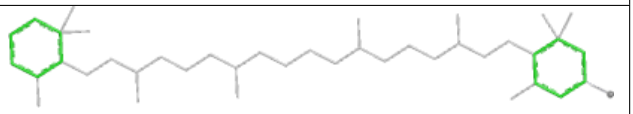
Bond lengths



Bond angles

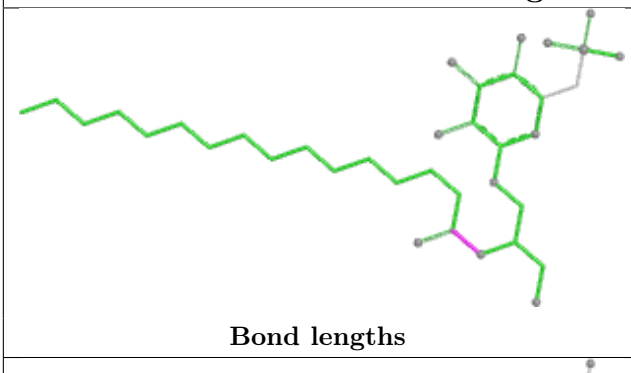


Torsions

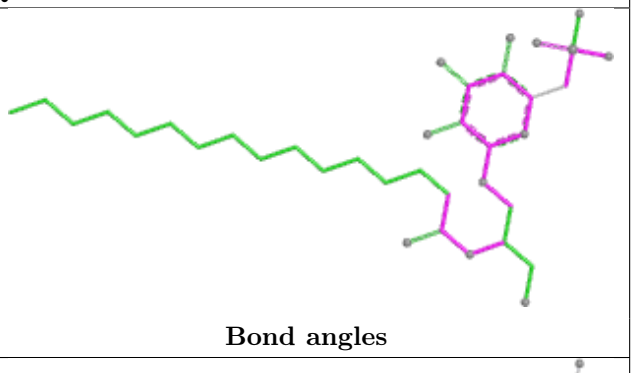


Rings

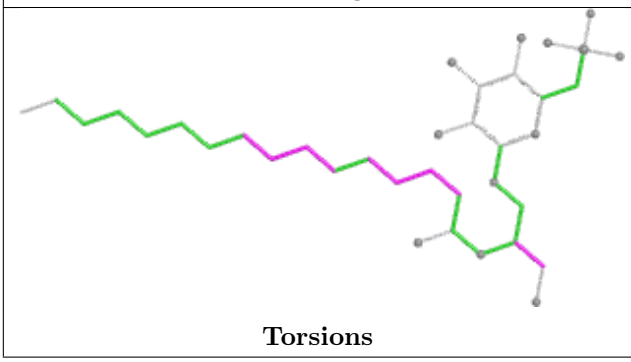
Ligand SQD F 101



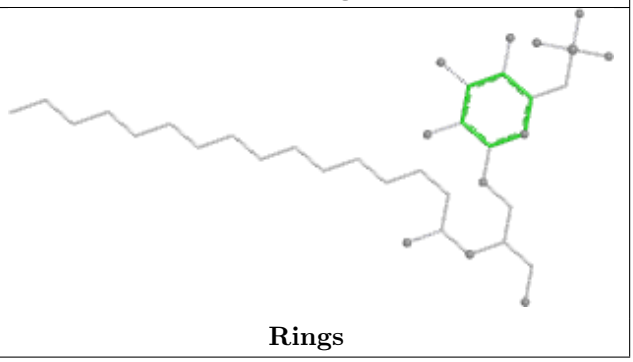
Bond lengths



Bond angles

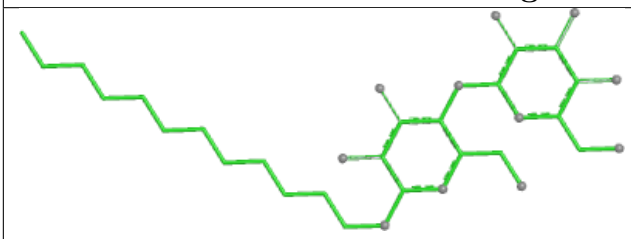


Torsions

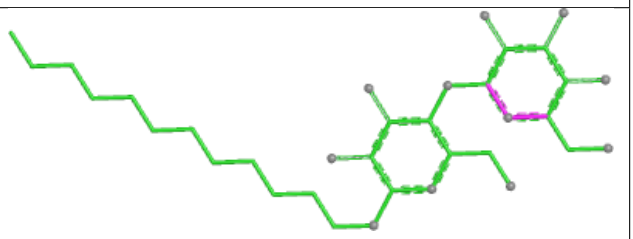


Rings

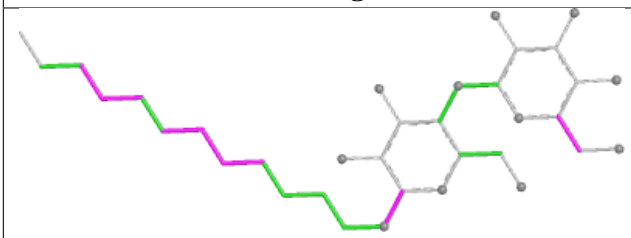
Ligand LMT A 421



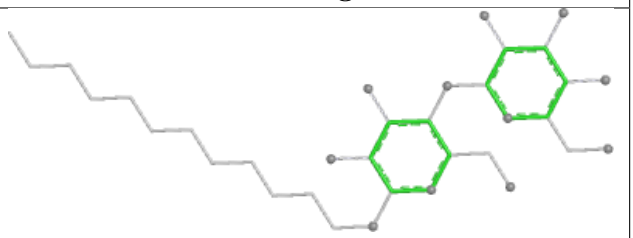
Bond lengths



Bond angles

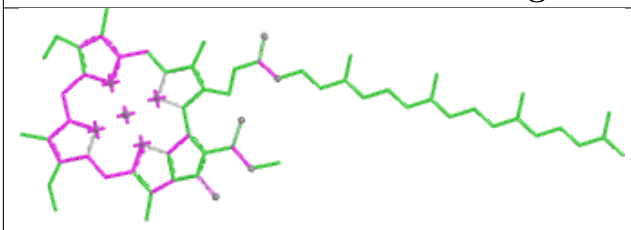


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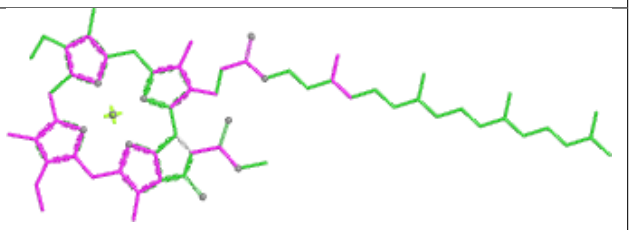


Rings

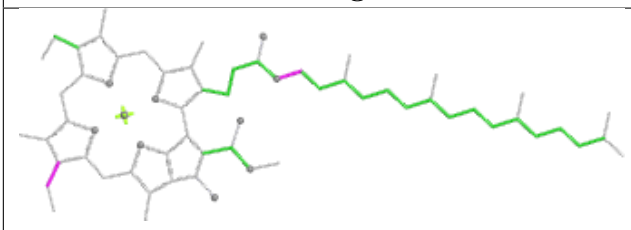
Ligand CLA a 409



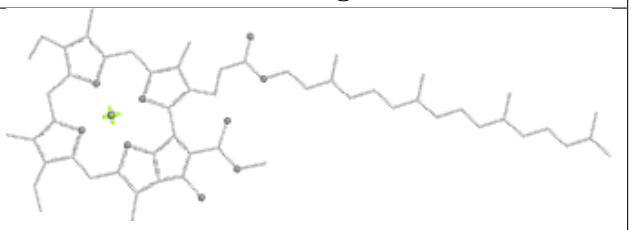
Bond lengths



Bond angles

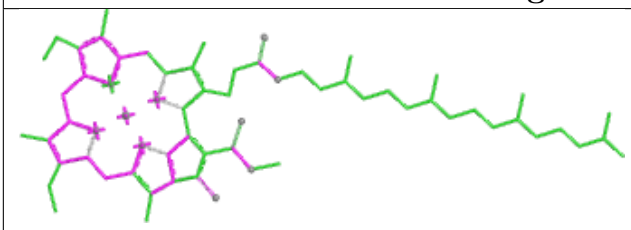


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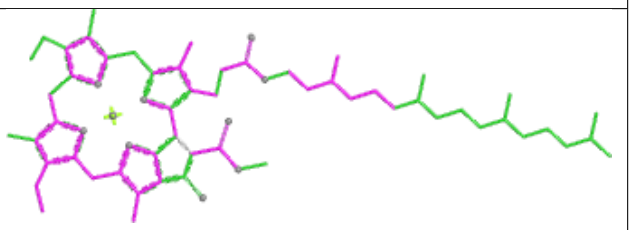


Rings

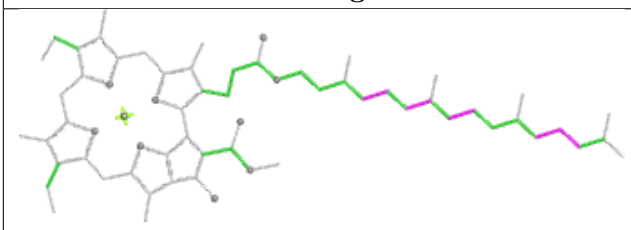
Ligand CLA b 606



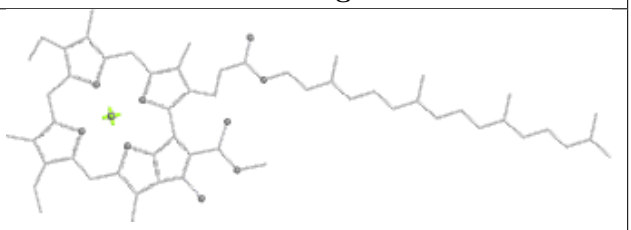
Bond lengths



Bond angles

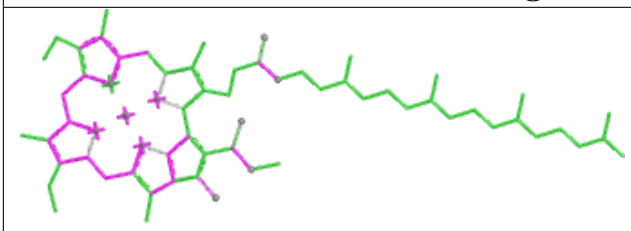


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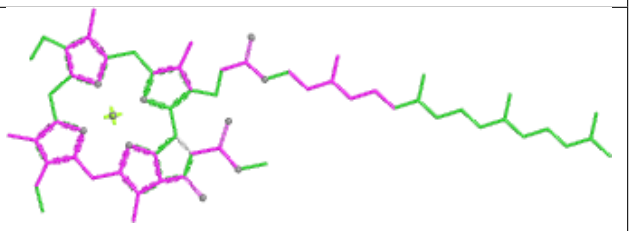


Rings

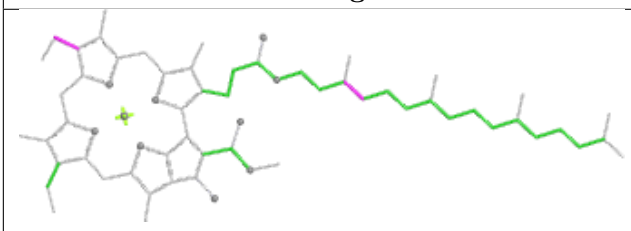
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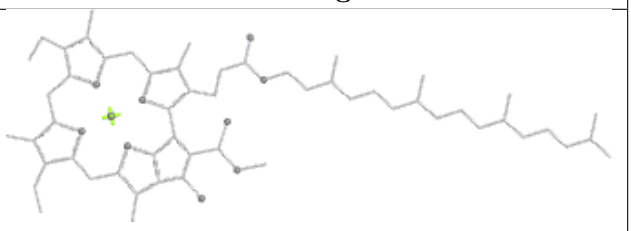
Bond lengths



Bond angles

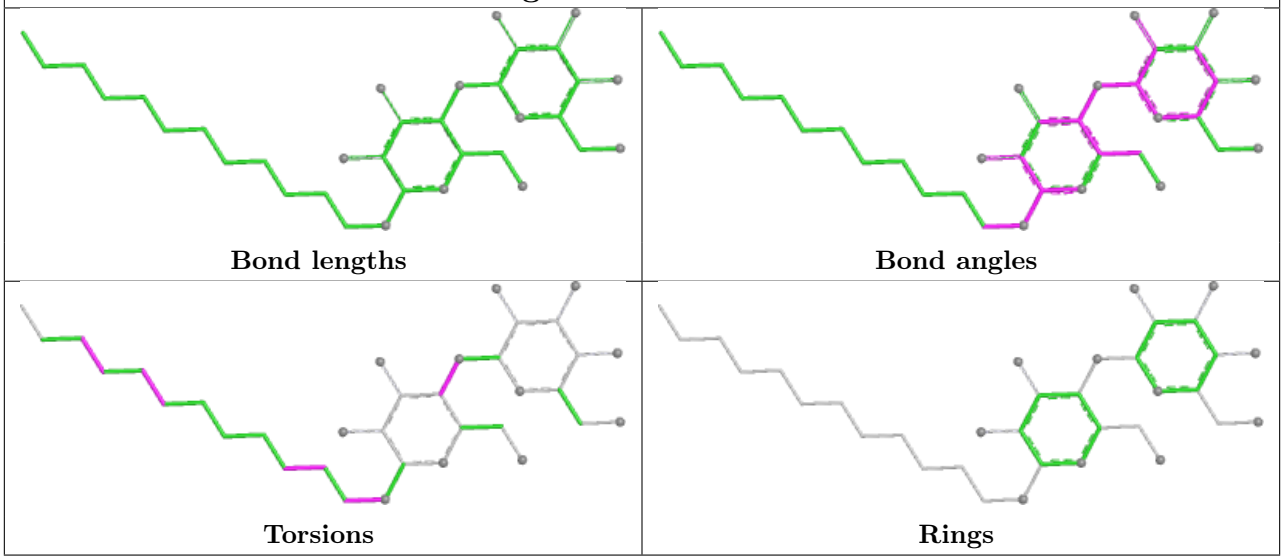


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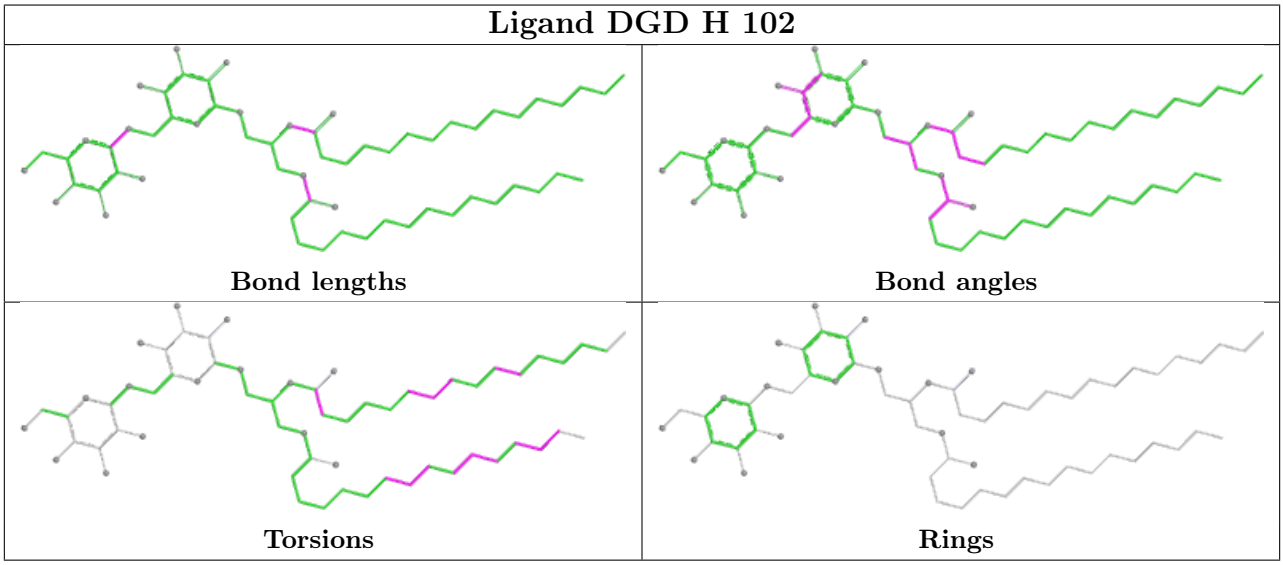


Rings

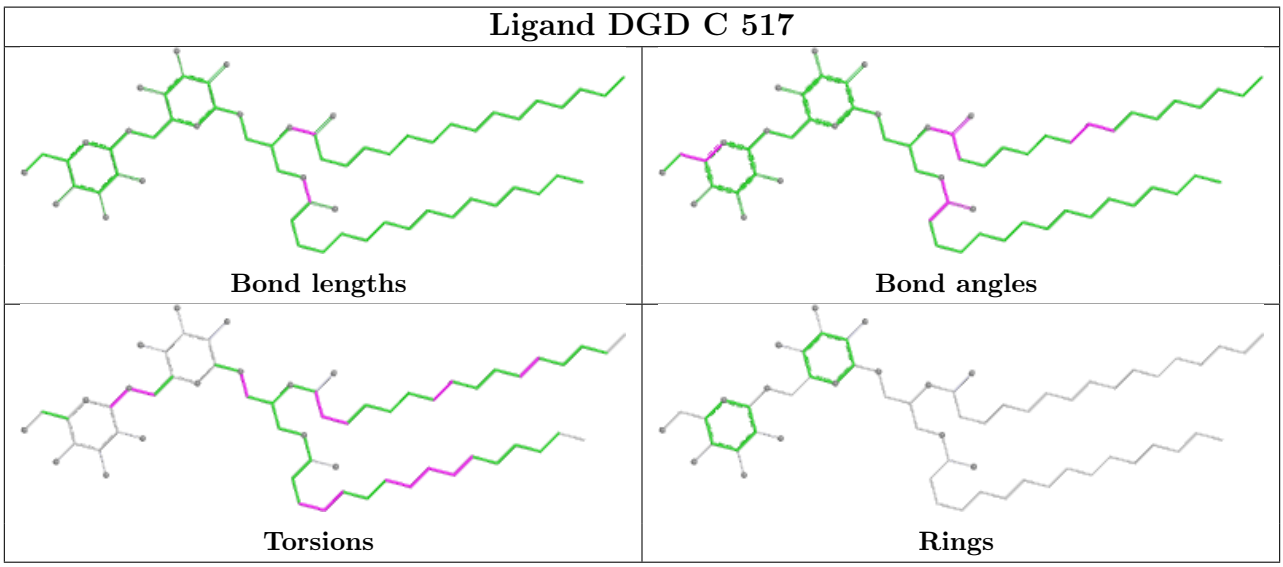
Ligand LMT B 622



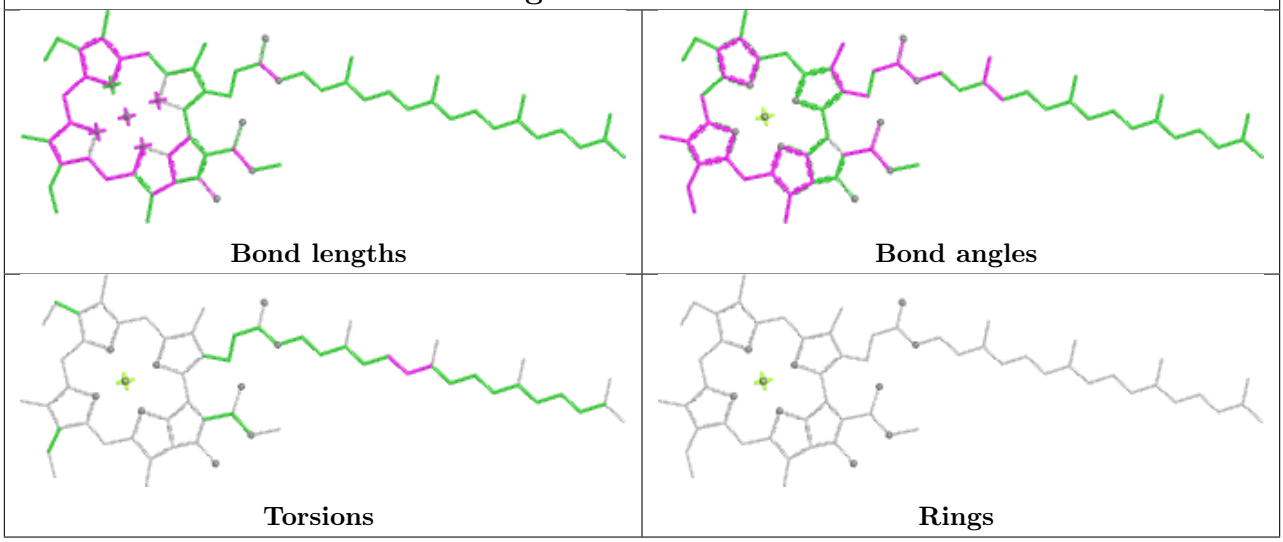
Ligand DGD H 102



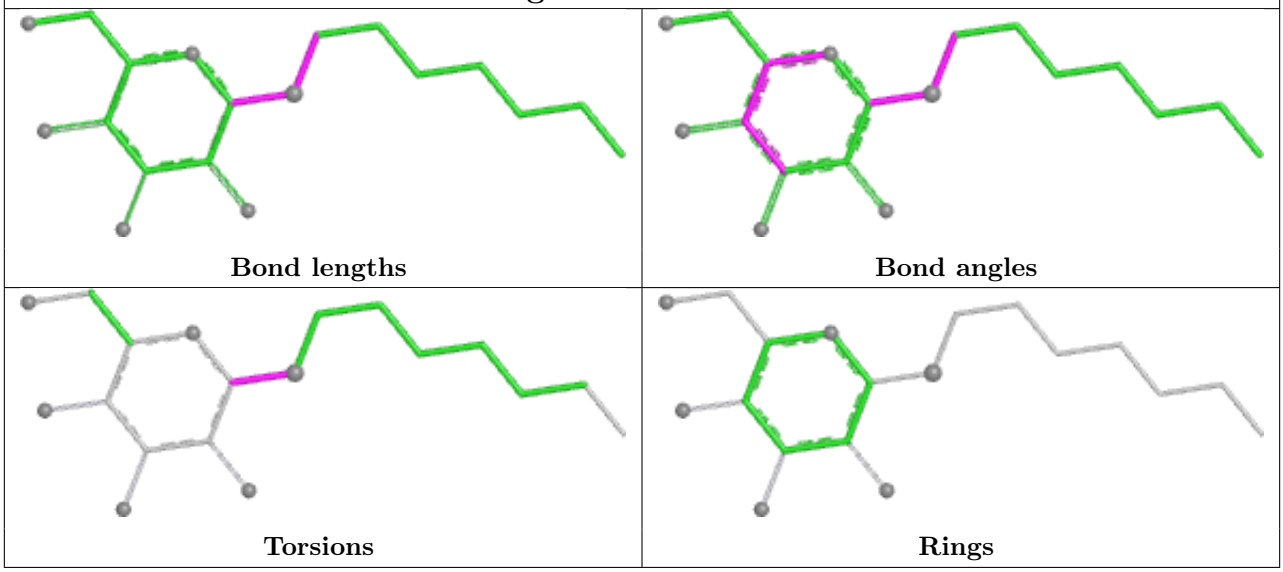
Ligand DGD C 517



Ligand CLA B 604



Ligand HTG c 942



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/360 (92%)	-0.64	2 (0%) 85 87	19, 30, 52, 108	2 (0%)
1	a	336/360 (93%)	-0.52	3 (0%) 81 83	24, 32, 66, 131	3 (0%)
2	B	505/510 (99%)	-0.52	1 (0%) 91 92	18, 35, 61, 93	8 (1%)
2	b	504/510 (98%)	-0.39	15 (2%) 52 56	19, 37, 70, 153	9 (1%)
3	C	451/461 (97%)	-0.49	2 (0%) 88 90	25, 40, 56, 104	6 (1%)
3	c	456/461 (98%)	-0.42	2 (0%) 88 90	25, 43, 59, 112	3 (0%)
4	D	342/352 (97%)	-0.70	1 (0%) 90 91	18, 31, 48, 116	1 (0%)
4	d	342/352 (97%)	-0.62	0 100 100	19, 34, 52, 104	2 (0%)
5	E	80/84 (95%)	0.33	5 (6%) 26 27	33, 53, 100, 124	1 (1%)
5	e	79/84 (94%)	0.12	2 (2%) 58 62	31, 52, 98, 121	2 (2%)
6	F	34/45 (75%)	-0.31	0 100 100	35, 42, 64, 94	0
6	f	32/45 (71%)	-0.23	1 (3%) 51 55	33, 43, 82, 101	1 (3%)
7	H	65/66 (98%)	-0.16	3 (4%) 37 40	32, 43, 64, 121	0
7	h	65/66 (98%)	-0.15	3 (4%) 37 40	34, 47, 62, 133	1 (1%)
8	I	36/38 (94%)	0.14	1 (2%) 55 59	39, 46, 115, 133	0
8	i	36/38 (94%)	-0.18	1 (2%) 55 59	37, 45, 86, 108	0
9	J	36/40 (90%)	-0.19	1 (2%) 55 59	33, 46, 85, 103	0
9	j	39/40 (97%)	-0.15	0 100 100	38, 49, 64, 71	0
10	K	37/46 (80%)	-0.39	0 100 100	40, 46, 61, 68	0
10	k	37/46 (80%)	0.02	0 100 100	40, 50, 69, 82	0
11	L	37/37 (100%)	-0.58	0 100 100	15, 29, 75, 116	2 (5%)
11	l	37/37 (100%)	-0.49	1 (2%) 56 60	17, 30, 83, 121	1 (2%)
12	M	33/36 (91%)	-0.51	0 100 100	19, 32, 75, 105	1 (3%)
12	m	33/36 (91%)	-0.51	0 100 100	18, 33, 73, 86	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	-0.32	2 (0%)	82	85	22, 41, 69, 115	10 (4%)
13	o	243/272 (89%)	-0.25	4 (1%)	70	74	24, 44, 80, 109	5 (2%)
14	T	29/32 (90%)	-0.55	1 (3%)	48	51	25, 30, 51, 120	1 (3%)
14	t	29/32 (90%)	-0.46	1 (3%)	48	51	25, 31, 59, 101	1 (3%)
15	U	98/134 (73%)	-0.41	2 (2%)	65	69	30, 38, 61, 115	0
15	u	97/134 (72%)	-0.38	0	100	100	34, 44, 61, 123	0
16	V	137/163 (84%)	-0.52	0	100	100	20, 37, 55, 70	4 (2%)
16	v	137/163 (84%)	-0.31	1 (0%)	84	86	25, 50, 70, 87	2 (1%)
17	Y	30/46 (65%)	0.40	3 (10%)	12	13	47, 60, 102, 111	0
17	y	30/46 (65%)	0.55	2 (6%)	24	25	35, 64, 96, 105	1 (3%)
18	X	40/41 (97%)	0.04	1 (2%)	58	62	41, 50, 92, 125	0
18	x	39/41 (95%)	0.27	3 (7%)	19	21	44, 52, 113, 137	0
19	Z	61/62 (98%)	0.35	3 (4%)	35	37	45, 55, 85, 112	0
19	z	61/62 (98%)	0.52	3 (4%)	35	37	51, 64, 105, 121	0
20	R	34/41 (82%)	1.84	13 (38%)	1	0	60, 94, 119, 124	0
All	All	5294/5691 (93%)	-0.38	83 (1%)	70	74	15, 39, 72, 153	68 (1%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	I	37	LEU	6.8
7	H	65	LEU	5.1
13	o	58	ASN	4.6
18	x	37	VAL	4.6
7	h	65	LEU	4.5

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	0.84	0.10	98,112,120,122	0
19	FME	Z	1	10/11	0.88	0.12	68,82,98,101	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	0.95	0.08	30,39,62,64	0
14	FME	t	1	10/11	0.96	0.07	30,34,59,63	0
12	FME	M	1	10/11	0.97	0.07	31,40,71,76	0
12	FME	m	1	10/11	0.97	0.07	33,42,69,78	0
8	FME	i	1	10/11	0.98	0.07	31,40,44,47	0
8	FME	I	1	10/11	0.98	0.06	34,43,49,50	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
36	HTG	V	215	19/19	0.54	0.19	100,116,127,128	0
30	UNL	h	103	9/-	0.59	0.20	81,86,109,110	0
30	UNL	b	634	9/-	0.60	0.15	99,103,113,114	0
30	UNL	h	106	11/-	0.63	0.18	72,75,78,79	0
30	UNL	C	538	4/-	0.65	0.15	74,76,77,82	0
36	HTG	c	941	19/19	0.65	0.15	67,133,141,142	0
34	DMS	B	646	4/4	0.66	0.20	109,114,115,116	0
34	DMS	c	939	4/4	0.66	0.19	112,114,119,120	0
30	UNL	A	420	9/-	0.66	0.14	85,95,111,112	0
30	UNL	i	105	12/-	0.66	0.15	77,86,88,89	0
34	DMS	i	106	4/4	0.67	0.22	125,125,125,127	0
30	UNL	h	104	9/-	0.67	0.18	68,74,84,85	0
34	DMS	e	103	4/4	0.67	0.22	106,108,108,111	0
30	UNL	I	105	9/-	0.68	0.14	70,73,81,83	0
31	LMT	A	417	35/35	0.68	0.18	55,92,108,115	0
30	UNL	c	947	6/-	0.69	0.19	71,80,83,85	0
30	UNL	J	105	8/-	0.69	0.16	80,94,98,99	0
30	UNL	a	418	40/-	0.69	0.17	79,99,122,125	0
30	UNL	A	415	36/-	0.69	0.17	75,99,113,114	0
37	DGD	d	408	50/66	0.69	0.15	81,99,121,130	0
36	HTG	B	631	19/19	0.70	0.14	71,107,118,120	0
31	LMT	m	103	35/35	0.71	0.16	53,125,136,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	v	210	4/4	0.71	0.20	119,119,120,120	0
37	DGD	D	405	52/66	0.71	0.18	74,102,120,124	0
31	LMT	c	922	35/35	0.71	0.15	85,117,122,126	0
34	DMS	A	425	4/4	0.72	0.19	94,101,101,104	0
30	UNL	y	103	4/-	0.72	0.14	81,82,84,85	0
34	DMS	O	307	4/4	0.72	0.20	113,113,115,121	0
30	UNL	c	944	4/-	0.72	0.16	76,77,78,81	0
30	UNL	b	633	9/-	0.72	0.18	76,81,87,88	0
30	UNL	A	428	4/-	0.72	0.15	64,66,70,71	0
31	LMT	e	101	24/35	0.73	0.15	94,101,125,127	0
34	DMS	U	202	4/4	0.73	0.18	105,108,108,110	0
34	DMS	V	214	4/4	0.73	0.20	102,102,104,106	0
31	LMT	a	402	35/35	0.73	0.16	49,96,119,123	0
31	LMT	b	625	35/35	0.73	0.16	59,119,133,139	0
30	UNL	Z	104	8/-	0.73	0.20	69,83,102,103	0
34	DMS	d	417	4/4	0.74	0.20	106,109,109,110	0
34	DMS	b	646	4/4	0.74	0.22	74,83,84,85	0
31	LMT	A	421	35/35	0.74	0.14	84,100,131,132	0
30	UNL	C	522	34/-	0.75	0.15	68,94,102,106	0
32	GOL	O	304	6/6	0.75	0.12	89,90,92,96	0
32	GOL	V	207	6/6	0.75	0.13	78,85,88,96	0
30	UNL	l	102	13/-	0.75	0.16	55,61,77,83	0
34	DMS	B	645	4/4	0.75	0.21	103,104,107,107	0
36	HTG	c	943	17/19	0.75	0.13	76,122,129,130	0
30	UNL	J	104	16/-	0.75	0.21	75,83,91,91	0
34	DMS	C	532	4/4	0.75	0.19	96,99,100,102	0
30	UNL	b	635	9/-	0.76	0.16	59,82,90,90	0
34	DMS	c	936	4/4	0.76	0.18	119,124,124,124	0
34	DMS	B	642	4/4	0.76	0.21	104,106,109,111	0
34	DMS	O	315	4/4	0.76	0.24	96,96,98,99	0
36	HTG	c	942	19/19	0.76	0.17	52,78,94,100	0
30	UNL	j	105	5/-	0.76	0.14	66,67,73,74	0
31	LMT	j	102	24/35	0.76	0.14	66,84,120,122	0
34	DMS	o	307	4/4	0.76	0.21	89,91,91,93	0
30	UNL	b	636	11/-	0.77	0.18	70,77,83,83	0
36	HTG	B	625	19/19	0.77	0.12	64,112,121,124	0
31	LMT	t	101	23/35	0.77	0.16	60,95,135,138	0
36	HTG	C	520	19/19	0.77	0.13	81,93,101,105	0
34	DMS	B	647	4/4	0.77	0.22	107,108,110,113	0
36	HTG	c	924	19/19	0.77	0.13	69,99,118,118	0
30	UNL	I	106	9/-	0.77	0.17	76,80,87,87	0
34	DMS	D	415	4/4	0.77	0.22	83,93,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	I	107	11/-	0.77	0.17	65,78,88,88	0
36	HTG	y	102	19/19	0.77	0.14	84,115,122,124	0
30	UNL	B	627	8/-	0.77	0.14	63,68,78,83	0
31	LMT	F	103	24/35	0.77	0.13	85,90,119,121	0
34	DMS	T	103	4/4	0.78	0.26	112,112,112,112	0
34	DMS	c	926	4/4	0.78	0.20	107,110,110,111	0
30	UNL	c	946	4/-	0.78	0.14	83,83,83,84	0
30	UNL	e	106	11/-	0.78	0.13	83,87,92,94	0
34	DMS	b	639	4/4	0.78	0.19	90,100,102,102	0
30	UNL	c	945	4/-	0.79	0.14	77,77,77,78	0
36	HTG	C	521	19/19	0.79	0.12	58,93,110,117	0
30	UNL	A	418	8/-	0.79	0.12	70,75,82,82	0
36	HTG	b	603	19/19	0.79	0.12	64,103,118,120	0
34	DMS	U	204	4/4	0.79	0.15	134,135,136,136	0
34	DMS	C	533	4/4	0.79	0.14	121,122,123,125	0
34	DMS	C	534	4/4	0.79	0.18	112,116,117,120	0
27	SQD	b	601	54/54	0.79	0.13	46,73,108,111	0
34	DMS	y	101	4/4	0.79	0.20	116,122,123,124	0
30	UNL	x	104	9/-	0.79	0.17	93,95,99,102	0
30	UNL	I	103	12/-	0.79	0.14	60,63,84,84	0
38	LHG	E	101	42/49	0.79	0.14	53,100,110,112	0
30	UNL	c	948	18/-	0.80	0.16	79,89,113,114	0
30	UNL	b	628	18/-	0.80	0.14	51,61,81,95	0
34	DMS	A	424	4/4	0.80	0.20	95,98,100,101	0
30	UNL	J	103	12/-	0.80	0.16	69,79,83,84	0
31	LMT	J	102	24/35	0.80	0.14	64,86,118,120	0
30	UNL	I	104	12/-	0.80	0.14	70,80,92,93	0
27	SQD	a	401	54/54	0.80	0.12	55,80,106,110	0
30	UNL	T	102	15/-	0.80	0.16	78,86,92,93	0
36	HTG	c	923	19/19	0.80	0.11	84,98,100,102	0
34	DMS	c	935	4/4	0.80	0.13	101,101,101,102	0
34	DMS	C	530	4/4	0.80	0.14	89,96,97,99	0
30	UNL	Z	103	6/-	0.80	0.14	73,84,87,88	0
30	UNL	H	103	6/-	0.80	0.14	65,66,79,81	0
36	HTG	d	419	19/19	0.80	0.12	75,100,110,113	0
36	HTG	v	211	19/19	0.80	0.14	63,84,98,102	0
30	UNL	a	403	5/-	0.80	0.13	73,73,74,75	0
27	SQD	l	101	54/54	0.80	0.14	48,77,116,117	0
32	GOL	B	637	6/6	0.80	0.13	61,67,75,80	0
34	DMS	v	207	4/4	0.80	0.15	111,114,114,114	0
28	LMG	C	523	51/55	0.81	0.13	47,94,109,114	0
34	DMS	o	306	4/4	0.81	0.19	84,85,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	C	535	4/4	0.81	0.19	66,79,83,89	0
34	DMS	v	205	4/4	0.81	0.16	90,95,98,106	0
30	UNL	i	104	16/-	0.81	0.13	65,72,83,83	0
34	DMS	O	302	4/4	0.81	0.22	101,104,107,108	0
30	UNL	d	403	36/-	0.81	0.14	47,67,99,107	0
36	HTG	d	414	19/19	0.81	0.11	67,100,117,120	0
34	DMS	C	524	4/4	0.81	0.15	105,107,108,108	0
36	HTG	B	630	19/19	0.81	0.11	56,109,116,118	0
30	UNL	I	102	12/-	0.81	0.17	70,82,95,98	0
30	UNL	D	417	4/-	0.81	0.21	57,66,66,70	0
30	UNL	E	104	5/-	0.81	0.16	59,64,67,69	0
36	HTG	D	412	19/19	0.81	0.13	68,112,130,130	0
34	DMS	c	938	4/4	0.82	0.14	97,97,100,104	0
30	UNL	t	103	12/-	0.82	0.12	64,74,83,86	0
34	DMS	A	427	4/4	0.82	0.16	82,88,89,89	0
31	LMT	B	622	35/35	0.82	0.12	48,85,97,99	0
30	UNL	b	648	5/-	0.82	0.16	73,74,76,77	0
29	PL9	a	417	55/55	0.82	0.15	50,78,101,105	0
32	GOL	b	637	6/6	0.82	0.12	92,92,94,96	0
36	HTG	O	316	19/19	0.82	0.15	47,71,81,84	0
32	GOL	c	929	6/6	0.82	0.16	77,89,93,94	0
34	DMS	O	312	4/4	0.82	0.14	101,103,104,106	0
30	UNL	b	629	16/-	0.82	0.17	59,83,97,99	0
36	HTG	C	537	19/19	0.83	0.11	84,109,123,126	0
30	UNL	i	102	18/-	0.83	0.13	44,68,93,96	0
34	DMS	O	314	4/4	0.83	0.16	81,87,87,88	0
30	UNL	x	102	8/-	0.83	0.13	77,80,86,88	0
34	DMS	C	531	4/4	0.83	0.16	109,111,113,116	0
36	HTG	b	627	19/19	0.83	0.13	69,113,125,128	0
30	UNL	b	630	10/-	0.83	0.16	71,82,85,85	0
30	UNL	D	410	40/-	0.83	0.13	46,67,103,106	0
36	HTG	c	928	19/19	0.83	0.12	74,98,122,126	0
34	DMS	V	212	4/4	0.83	0.15	86,96,99,99	0
30	UNL	C	539	16/-	0.83	0.15	76,79,102,107	0
34	DMS	a	425	4/4	0.83	0.15	116,120,120,121	0
30	UNL	k	101	30/-	0.83	0.13	62,90,106,111	0
36	HTG	B	624	19/19	0.83	0.15	34,53,75,76	0
36	HTG	d	420	19/19	0.83	0.11	85,115,118,118	0
30	UNL	k	104	9/-	0.83	0.15	69,82,89,90	0
30	UNL	E	102	5/-	0.83	0.14	76,76,76,77	0
30	UNL	i	101	8/-	0.83	0.13	63,67,75,81	0
34	DMS	O	309	4/4	0.83	0.18	98,101,102,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	O	311	4/4	0.83	0.16	93,96,97,98	0
29	PL9	A	414	55/55	0.84	0.14	53,68,102,104	0
34	DMS	V	211	4/4	0.84	0.16	94,94,96,99	0
34	DMS	B	643	4/4	0.84	0.12	100,104,106,106	0
34	DMS	H	104	4/4	0.84	0.23	109,109,112,116	0
34	DMS	a	424	4/4	0.84	0.17	102,104,105,105	0
34	DMS	v	209	4/4	0.84	0.20	110,110,110,111	0
34	DMS	L	102	4/4	0.84	0.16	106,110,111,112	0
30	UNL	c	925	11/-	0.84	0.12	74,77,85,85	0
34	DMS	b	640	4/4	0.84	0.14	69,91,92,97	0
30	UNL	i	103	12/-	0.84	0.14	67,75,83,87	0
30	UNL	e	105	4/-	0.84	0.18	74,77,79,82	0
32	GOL	a	419	6/6	0.84	0.12	55,59,59,60	0
27	SQD	A	416	54/54	0.84	0.11	50,70,89,95	0
31	LMT	c	927	35/35	0.84	0.13	49,97,104,111	0
30	UNL	E	105	4/-	0.84	0.13	60,62,69,72	0
28	LMG	a	416	51/55	0.84	0.12	54,73,92,98	0
28	LMG	c	921	51/55	0.84	0.12	47,94,101,104	0
30	UNL	m	101	11/-	0.85	0.13	56,67,78,84	0
34	DMS	D	416	4/4	0.85	0.18	93,94,97,98	0
30	UNL	B	628	6/-	0.85	0.14	68,69,79,82	0
30	UNL	H	105	18/-	0.85	0.12	51,67,98,103	0
34	DMS	o	305	4/4	0.85	0.18	94,102,106,107	0
31	LMT	m	102	35/35	0.85	0.11	34,64,85,88	0
34	DMS	b	645	4/4	0.85	0.17	103,110,111,111	0
34	DMS	U	203	4/4	0.85	0.19	40,60,64,66	0
30	UNL	Z	102	6/-	0.85	0.14	61,72,75,77	0
34	DMS	v	208	4/4	0.85	0.13	86,89,94,98	0
31	LMT	B	626	24/35	0.85	0.12	47,73,114,118	0
31	LMT	t	102	35/35	0.85	0.11	43,91,116,118	0
34	DMS	V	213	4/4	0.85	0.14	76,84,85,86	0
36	HTG	b	626	19/19	0.86	0.15	41,52,95,99	0
30	UNL	B	648	4/-	0.86	0.13	66,70,70,71	0
34	DMS	a	422	4/4	0.86	0.15	91,94,96,98	0
36	HTG	B	623	19/19	0.86	0.13	46,59,69,72	0
30	UNL	E	103	8/-	0.86	0.15	65,78,79,79	0
34	DMS	K	102	4/4	0.86	0.16	95,106,107,109	0
34	DMS	e	104	4/4	0.86	0.15	88,94,96,98	0
34	DMS	B	641	4/4	0.86	0.18	107,108,110,110	0
30	UNL	j	103	6/-	0.86	0.12	72,80,86,88	0
30	UNL	j	104	4/-	0.86	0.12	74,75,76,78	0
36	HTG	C	536	19/19	0.86	0.10	66,106,124,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	V	205	4/4	0.86	0.19	94,98,98,100	0
28	LMG	A	413	51/55	0.86	0.12	49,74,97,102	0
34	DMS	c	934	4/4	0.86	0.13	73,80,82,84	0
33	BCT	a	408[A]	4/4	0.86	0.11	31,38,39,41	4
30	UNL	B	635	6/-	0.86	0.14	70,73,75,79	0
34	DMS	b	638	4/4	0.87	0.14	58,80,83,83	0
31	LMT	Z	101	35/35	0.87	0.13	52,104,121,123	0
34	DMS	O	313	4/4	0.87	0.12	101,106,108,111	0
34	DMS	b	641	4/4	0.87	0.18	89,91,92,95	0
34	DMS	b	643	4/4	0.87	0.20	113,118,118,120	0
34	DMS	B	639	4/4	0.87	0.15	87,90,93,95	0
27	SQD	f	102	43/54	0.87	0.13	50,91,111,117	0
31	LMT	M	101	35/35	0.87	0.11	42,70,85,89	0
34	DMS	D	414	4/4	0.87	0.16	102,104,106,107	0
31	LMT	M	102	25/35	0.87	0.12	40,67,106,110	0
34	DMS	B	644	4/4	0.87	0.16	56,75,78,78	0
30	UNL	d	421	11/-	0.88	0.13	77,88,95,95	0
34	DMS	d	418	4/4	0.88	0.15	74,75,76,78	0
34	DMS	c	933	4/4	0.88	0.15	108,111,113,114	0
34	DMS	C	529	4/4	0.88	0.20	100,103,104,105	0
30	UNL	x	103	4/-	0.88	0.13	74,75,83,84	0
34	DMS	o	304	4/4	0.88	0.12	83,88,90,94	0
35	CA	v	201	1/1	0.88	0.09	104,104,104,104	0
34	DMS	O	306	4/4	0.88	0.14	78,82,86,86	0
32	GOL	A	419	6/6	0.88	0.14	59,61,62,66	0
34	DMS	b	647	4/4	0.88	0.16	72,73,79,79	0
34	DMS	u	202	4/4	0.88	0.16	68,80,81,86	0
34	DMS	v	203	4/4	0.88	0.17	87,94,95,96	0
32	GOL	C	525	6/6	0.89	0.12	89,91,92,93	0
36	HTG	V	204	13/19	0.89	0.09	49,59,79,86	0
30	UNL	I	101	14/-	0.89	0.10	46,53,70,73	0
36	HTG	O	303	19/19	0.89	0.12	46,56,64,64	0
36	HTG	B	629	19/19	0.90	0.10	46,70,92,97	0
28	LMG	B	621	51/55	0.90	0.10	39,54,71,82	0
32	GOL	V	206	6/6	0.90	0.09	58,69,71,83	0
34	DMS	a	423	4/4	0.90	0.13	63,76,79,85	0
26	BCR	B	636	40/40	0.90	0.08	29,41,59,59	0
34	DMS	e	102	4/4	0.90	0.12	95,95,96,99	0
34	DMS	V	201	4/4	0.90	0.13	75,76,79,88	0
30	UNL	d	413	18/-	0.90	0.11	42,57,77,85	0
26	BCR	T	101	40/40	0.90	0.07	29,42,60,63	0
34	DMS	o	302	4/4	0.90	0.14	71,74,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	HTG	U	201	4/19	0.90	0.19	49,51,51,56	0
34	DMS	o	303	4/4	0.90	0.11	92,94,95,101	0
30	UNL	D	411	16/-	0.90	0.10	44,51,73,74	0
28	LMG	b	624	51/55	0.90	0.10	44,56,78,89	0
38	LHG	D	406	49/49	0.90	0.11	36,50,67,81	0
34	DMS	c	937	4/4	0.90	0.11	99,101,103,103	0
38	LHG	d	409	49/49	0.90	0.10	38,50,61,67	0
28	LMG	C	519	51/55	0.91	0.11	36,80,92,97	0
36	HTG	b	602	19/19	0.91	0.09	51,67,78,83	0
34	DMS	h	105	4/4	0.91	0.13	52,53,61,80	0
34	DMS	v	206	4/4	0.91	0.12	55,68,74,84	0
34	DMS	A	426	4/4	0.91	0.15	81,86,86,88	0
34	DMS	O	305	4/4	0.91	0.13	81,82,85,88	0
34	DMS	a	421	4/4	0.91	0.13	78,84,85,89	0
34	DMS	u	201	4/4	0.92	0.16	52,64,66,70	0
27	SQD	a	415	54/54	0.92	0.10	35,65,85,87	0
34	DMS	B	640	4/4	0.92	0.10	77,78,82,86	0
27	SQD	A	412	54/54	0.92	0.10	35,64,79,85	0
24	CLA	C	506	65/65	0.92	0.09	37,52,90,94	0
34	DMS	O	308	4/4	0.92	0.12	80,83,84,90	0
27	SQD	F	101	37/54	0.92	0.10	45,71,88,92	0
34	DMS	O	310	4/4	0.92	0.12	88,89,90,94	0
30	UNL	x	101	18/-	0.92	0.13	51,65,90,92	0
33	BCT	d	402[B]	4/4	0.92	0.09	34,37,37,40	4
35	CA	V	202	1/1	0.92	0.06	89,89,89,89	0
32	GOL	B	638	6/6	0.92	0.10	39,58,69,73	0
30	UNL	X	101	16/-	0.92	0.11	48,57,70,73	0
26	BCR	c	915	40/40	0.92	0.08	47,58,64,66	0
34	DMS	C	528	4/4	0.92	0.12	81,81,83,83	0
28	LMG	c	920	51/55	0.92	0.09	41,72,98,99	0
26	BCR	Y	101	40/40	0.93	0.07	40,44,48,54	0
34	DMS	V	210	4/4	0.93	0.09	69,71,76,76	0
26	BCR	b	622	40/40	0.93	0.07	31,39,57,64	0
26	BCR	B	619	40/40	0.93	0.07	28,37,54,62	0
26	BCR	d	406	40/40	0.93	0.08	34,41,69,72	0
24	CLA	c	907	65/65	0.93	0.08	39,48,81,85	0
26	BCR	K	101	40/40	0.93	0.08	34,43,48,49	0
24	CLA	c	914	65/65	0.93	0.09	41,53,89,96	0
34	DMS	b	644	4/4	0.93	0.15	63,65,67,78	0
34	DMS	c	940	4/4	0.94	0.20	58,63,64,66	0
34	DMS	d	415	4/4	0.94	0.14	63,66,70,74	0
24	CLA	b	618	65/65	0.94	0.08	24,33,88,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	a	414	40/40	0.94	0.06	27,33,39,41	0
24	CLA	B	617	65/65	0.94	0.09	30,36,105,109	0
24	CLA	c	913	65/65	0.94	0.08	40,49,84,89	0
34	DMS	b	642	4/4	0.94	0.09	57,63,69,73	0
24	CLA	B	602	65/65	0.94	0.08	35,52,105,110	0
28	LMG	D	409	51/55	0.94	0.09	32,43,99,106	0
24	CLA	C	512	65/65	0.94	0.08	43,50,90,92	0
33	BCT	A	422	4/4	0.94	0.09	37,37,48,55	0
24	CLA	C	513	65/65	0.94	0.08	43,54,86,88	0
26	BCR	C	514	40/40	0.94	0.07	41,49,57,57	0
34	DMS	c	931	4/4	0.94	0.16	88,88,89,92	0
26	BCR	C	515	40/40	0.94	0.06	33,42,50,54	0
28	LMG	d	412	51/55	0.94	0.09	35,45,89,94	0
37	DGD	C	517	62/66	0.94	0.08	31,43,92,101	0
26	BCR	D	403	40/40	0.94	0.07	33,41,69,73	0
37	DGD	H	102	62/66	0.94	0.07	27,40,51,53	0
24	CLA	b	605	65/65	0.94	0.08	40,54,102,107	0
37	DGD	h	102	62/66	0.94	0.08	34,42,51,63	0
34	DMS	B	633	4/4	0.94	0.13	48,49,56,58	0
34	DMS	B	634	4/4	0.94	0.11	63,64,64,65	0
24	CLA	b	610	65/65	0.94	0.08	29,37,71,80	0
40	RRX	h	101	41/41	0.94	0.07	31,44,61,71	0
24	CLA	c	902	65/65	0.95	0.07	33,42,54,60	0
24	CLA	c	905	65/65	0.95	0.07	32,40,72,81	0
24	CLA	B	607	65/65	0.95	0.07	28,34,65,71	0
34	DMS	V	209	4/4	0.95	0.13	50,59,66,67	0
24	CLA	c	908	65/65	0.95	0.07	32,42,59,61	0
24	CLA	C	503	65/65	0.95	0.06	32,39,46,56	0
24	CLA	B	615	65/65	0.95	0.08	24,32,86,95	0
34	DMS	c	932	4/4	0.95	0.11	80,88,88,89	0
34	DMS	C	527	4/4	0.95	0.11	72,74,75,77	0
24	CLA	d	405	65/65	0.95	0.08	33,39,102,107	0
26	BCR	c	916	40/40	0.95	0.06	38,43,54,57	0
26	BCR	A	411	40/40	0.95	0.06	27,33,41,45	0
37	DGD	C	516	62/66	0.95	0.07	27,38,90,95	0
26	BCR	k	102	40/40	0.95	0.06	40,45,54,55	0
34	DMS	v	204	4/4	0.95	0.10	55,57,58,64	0
26	BCR	B	618	40/40	0.95	0.06	27,35,41,41	0
37	DGD	c	917	62/66	0.95	0.07	28,39,84,88	0
37	DGD	c	918	62/66	0.95	0.08	36,44,99,109	0
24	CLA	C	507	65/65	0.95	0.07	36,42,57,66	0
24	CLA	b	614	65/65	0.95	0.06	30,36,42,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	508	65/65	0.95	0.07	28,37,95,108	0
29	PL9	D	404	55/55	0.95	0.06	23,29,38,51	0
38	LHG	L	101	49/49	0.95	0.07	30,41,64,71	0
24	CLA	b	620	65/65	0.95	0.08	30,41,98,102	0
38	LHG	l	103	49/49	0.95	0.07	32,42,66,69	0
29	PL9	d	407	55/55	0.95	0.06	22,29,43,56	0
24	CLA	C	505	65/65	0.96	0.06	32,39,57,63	0
26	BCR	b	623	40/40	0.96	0.06	32,41,55,58	0
24	CLA	B	610	65/65	0.96	0.06	30,36,43,46	0
24	CLA	c	904	65/65	0.96	0.06	35,44,50,62	0
24	CLA	B	611	65/65	0.96	0.06	26,35,43,50	0
24	CLA	B	604	65/65	0.96	0.06	28,33,40,42	0
26	BCR	k	103	40/40	0.96	0.06	37,46,54,59	0
24	CLA	C	510	65/65	0.96	0.06	31,39,51,58	0
24	CLA	c	909	65/65	0.96	0.06	31,37,91,96	0
24	CLA	c	910	65/65	0.96	0.07	34,40,58,64	0
24	CLA	c	912	65/65	0.96	0.07	34,43,52,58	0
24	CLA	C	511	65/65	0.96	0.07	33,44,51,54	0
24	CLA	B	616	65/65	0.96	0.06	26,35,53,65	0
24	CLA	A	410	65/65	0.96	0.08	26,35,99,104	0
34	DMS	C	526	4/4	0.96	0.09	44,46,46,50	0
25	PHO	A	409	64/64	0.96	0.05	24,30,37,42	0
24	CLA	D	402	65/65	0.96	0.07	29,37,102,104	0
24	CLA	a	413	65/65	0.96	0.08	26,34,107,111	0
24	CLA	C	501	65/65	0.96	0.06	30,39,53,61	0
37	DGD	C	518	62/66	0.96	0.07	28,37,80,85	0
26	BCR	B	620	40/40	0.96	0.06	30,37,52,55	0
24	CLA	b	606	65/65	0.96	0.06	31,36,46,56	0
24	CLA	C	502	65/65	0.96	0.06	29,36,48,63	0
24	CLA	b	611	65/65	0.96	0.05	23,31,44,50	0
37	DGD	c	919	62/66	0.96	0.07	32,40,76,82	0
24	CLA	b	613	65/65	0.96	0.06	32,38,44,57	0
34	DMS	D	413	4/4	0.96	0.13	62,65,67,73	0
24	CLA	B	608	65/65	0.96	0.06	23,29,44,50	0
38	LHG	D	408	46/49	0.96	0.07	32,39,72,77	0
24	CLA	b	616	65/65	0.96	0.06	25,33,41,42	0
24	CLA	b	617	65/65	0.96	0.06	25,31,71,77	0
24	CLA	C	504	65/65	0.96	0.07	27,35,80,83	0
38	LHG	d	410	49/49	0.96	0.07	27,33,53,64	0
38	LHG	d	411	47/49	0.96	0.08	32,39,87,92	0
26	BCR	b	621	40/40	0.96	0.05	31,37,48,53	0
40	RRX	H	101	41/41	0.96	0.06	30,41,56,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	b	632	4/4	0.96	0.12	61,63,64,65	0
24	CLA	a	409	65/65	0.97	0.05	23,28,37,50	0
24	CLA	a	410	65/65	0.97	0.06	26,32,89,95	0
24	CLA	c	903	65/65	0.97	0.06	29,38,50,61	0
24	CLA	B	613	65/65	0.97	0.05	24,31,37,41	0
35	CA	b	604	1/1	0.97	0.06	52,52,52,52	0
35	CA	c	901	1/1	0.97	0.05	52,52,52,52	0
24	CLA	B	614	65/65	0.97	0.06	21,30,67,76	0
34	DMS	d	416	4/4	0.97	0.09	62,64,65,72	0
24	CLA	c	906	65/65	0.97	0.06	30,37,66,74	0
24	CLA	B	606	65/65	0.97	0.06	25,30,43,46	0
24	CLA	b	607	65/65	0.97	0.05	28,35,41,44	0
24	CLA	b	608	65/65	0.97	0.06	25,31,69,74	0
24	CLA	b	609	65/65	0.97	0.06	25,33,44,49	0
24	CLA	c	911	65/65	0.97	0.06	30,39,51,61	0
24	CLA	A	407	65/65	0.97	0.06	21,29,89,95	0
24	CLA	C	509	65/65	0.97	0.07	34,41,63,67	0
24	CLA	b	612	65/65	0.97	0.05	28,35,42,45	0
24	CLA	d	401	65/65	0.97	0.05	21,27,41,51	0
24	CLA	d	404	65/65	0.97	0.05	23,28,50,57	0
24	CLA	B	603	65/65	0.97	0.05	27,34,44,49	0
38	LHG	D	407	49/49	0.97	0.06	25,34,48,65	0
24	CLA	B	609	65/65	0.97	0.05	27,33,40,44	0
25	PHO	a	411	64/64	0.97	0.05	24,28,33,38	0
25	PHO	a	412	64/64	0.97	0.05	26,33,41,43	0
24	CLA	b	615	65/65	0.97	0.05	25,31,51,55	0
24	CLA	A	406	65/65	0.97	0.04	20,26,38,53	0
34	DMS	V	208	4/4	0.97	0.08	50,53,56,57	0
24	CLA	B	605	65/65	0.97	0.06	23,29,61,62	0
39	HEM	f	101	43/43	0.97	0.08	42,50,65,84	0
24	CLA	B	612	65/65	0.97	0.05	25,30,46,54	0
24	CLA	b	619	65/65	0.97	0.06	29,37,58,65	0
25	PHO	A	408	64/64	0.98	0.04	21,28,33,36	0
24	CLA	A	405	65/65	0.98	0.04	22,26,33,54	0
34	DMS	a	420	4/4	0.98	0.07	34,35,35,42	0
34	DMS	b	631	4/4	0.98	0.07	34,34,37,43	0
34	DMS	c	930	4/4	0.98	0.07	46,49,49,50	0
39	HEM	F	102	43/43	0.98	0.06	38,48,56,60	0
24	CLA	D	401	65/65	0.98	0.05	20,26,41,46	0
35	CA	B	601	1/1	0.98	0.09	51,51,51,51	0
34	DMS	B	632	4/4	0.98	0.07	28,31,33,34	0
41	MG	j	101	1/1	0.98	0.12	44,44,44,44	0

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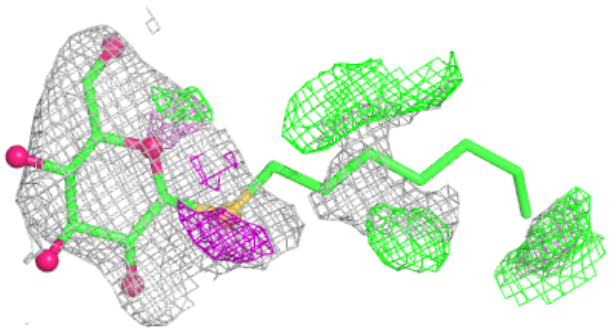
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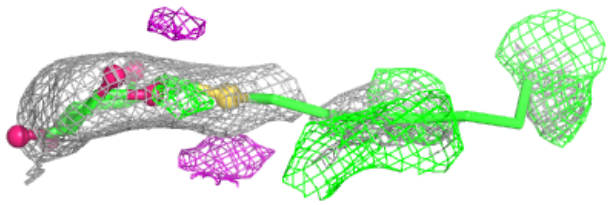
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
42	HEC	v	202	43/43	0.98	0.06	35,41,47,48	0
23	CL	A	403	1/1	0.99	0.03	26,26,26,26	0
21	OEX	a	404	10/10	0.99	0.03	29,32,33,34	0
35	CA	o	301	1/1	0.99	0.03	55,55,55,55	0
41	MG	J	101	1/1	0.99	0.09	36,36,36,36	0
35	CA	O	301	1/1	0.99	0.06	56,56,56,56	0
42	HEC	V	203	43/43	0.99	0.05	27,31,37,40	0
34	DMS	A	423	4/4	0.99	0.06	31,34,37,48	0
23	CL	a	406	1/1	1.00	0.02	29,29,29,29	0
23	CL	a	407	1/1	1.00	0.03	34,34,34,34	0
22	FE2	A	402	1/1	1.00	0.01	33,33,33,33	0
22	FE2	a	405	1/1	1.00	0.02	33,33,33,33	0
21	OEX	A	401	10/10	1.00	0.03	25,28,31,31	0
23	CL	A	404	1/1	1.00	0.02	29,29,29,29	0

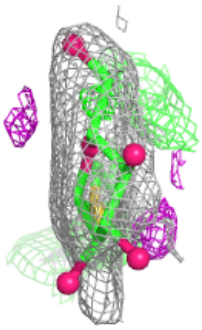
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG V 215:

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

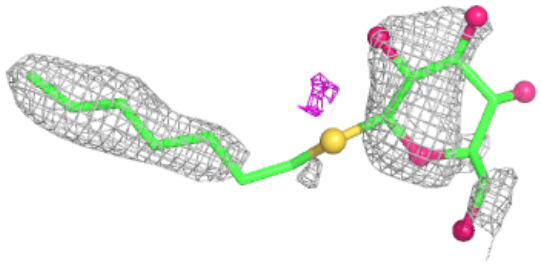


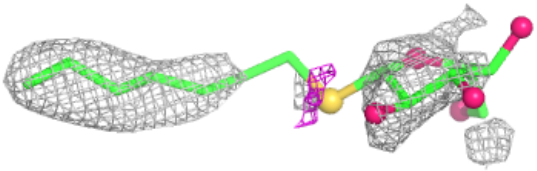


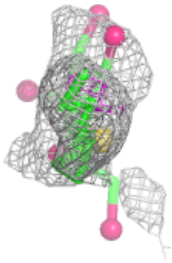


Electron density around HTG c 941:

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

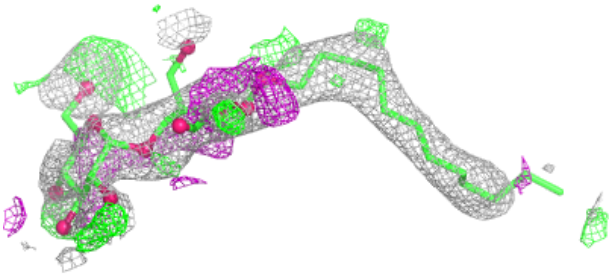


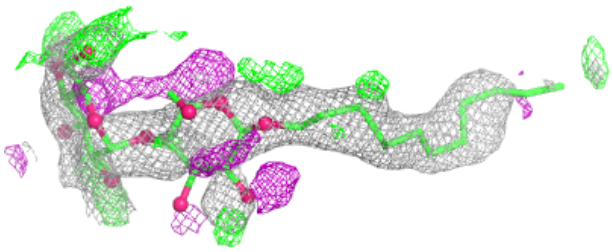


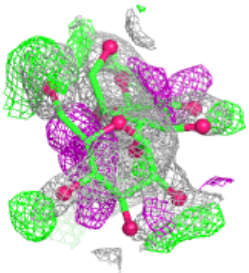


Electron density around LMT A 417:

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

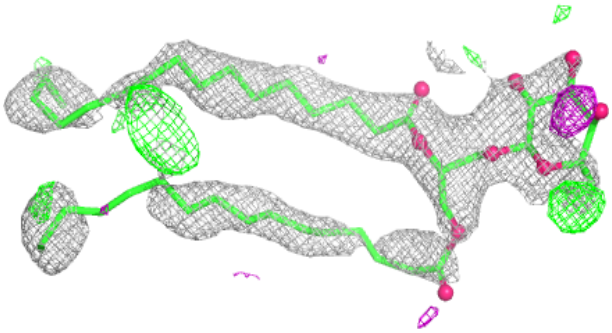


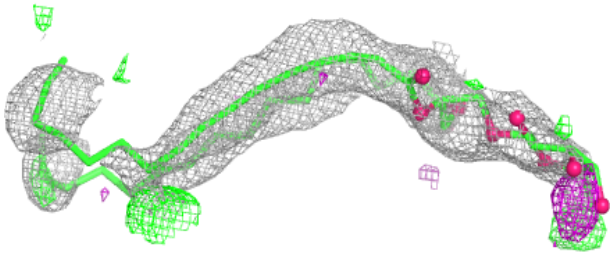


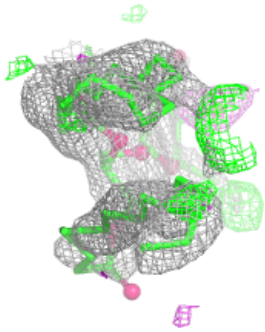


Electron density around DGD d 408:

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

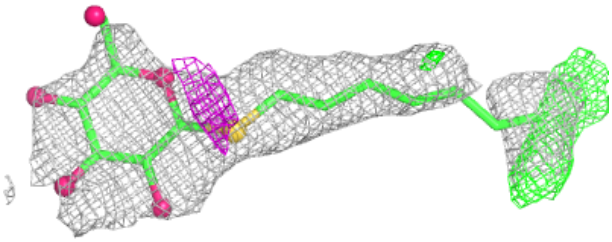


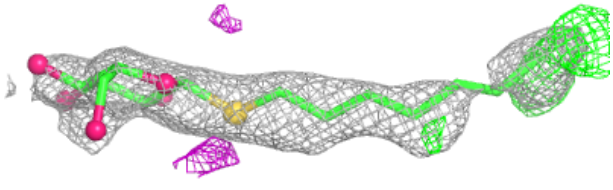


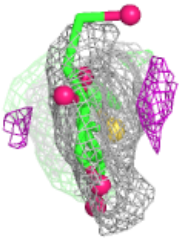


Electron density around HTG B 631:

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

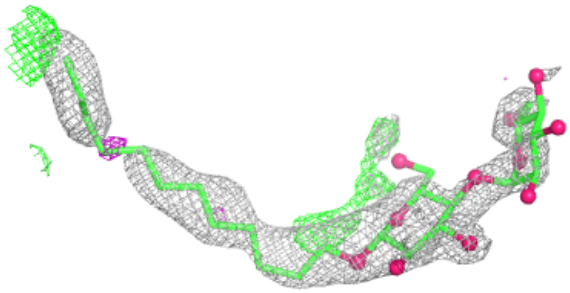


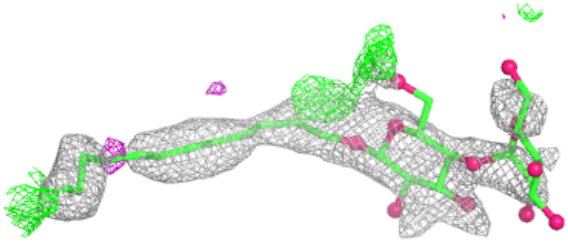


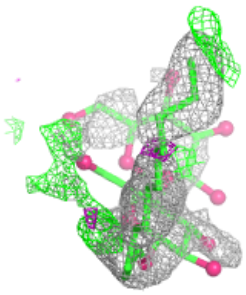


Electron density around LMT m 103:

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

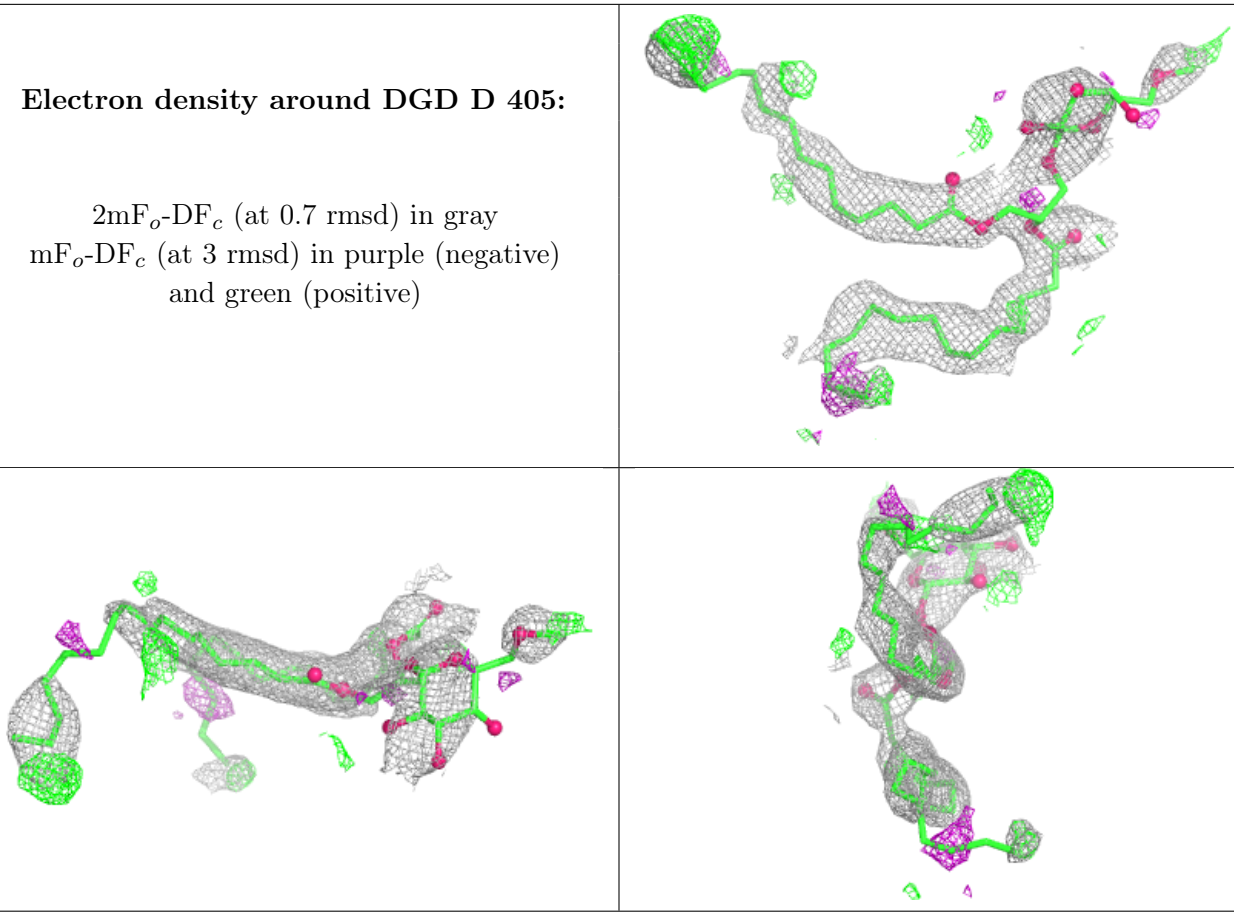






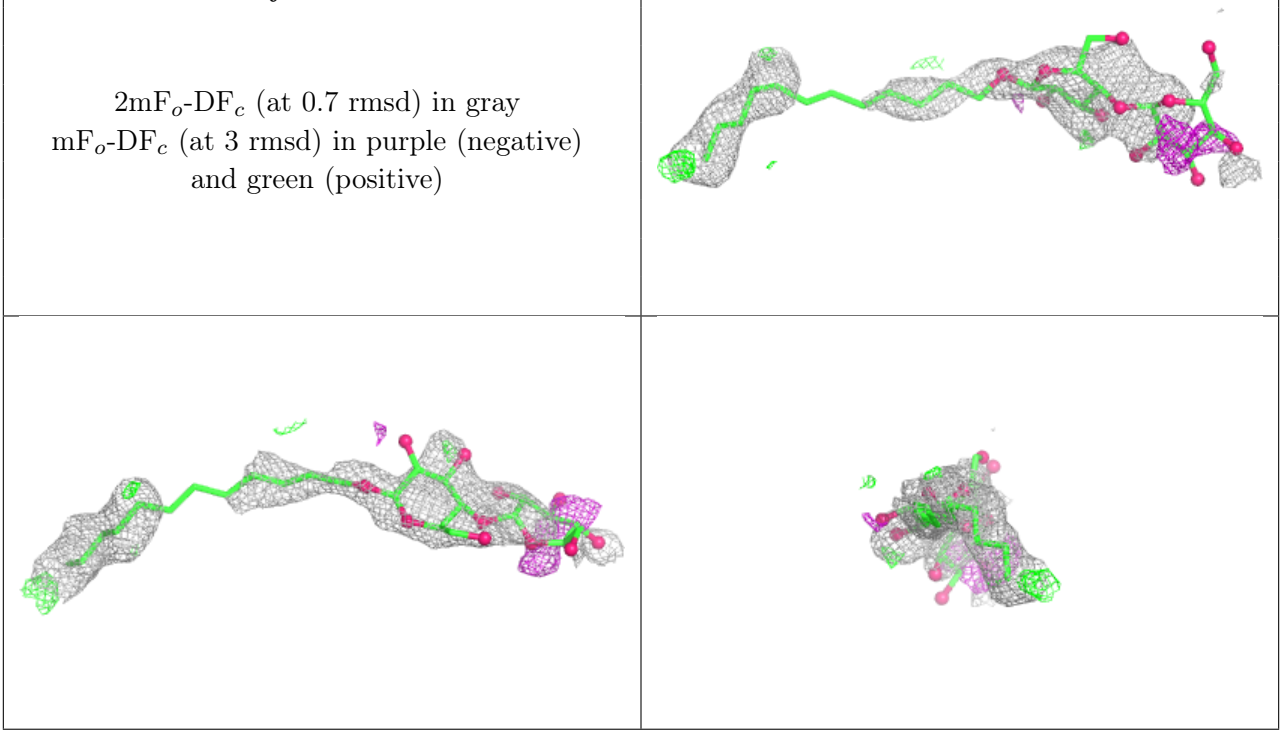
Electron density around DGD D 405:

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



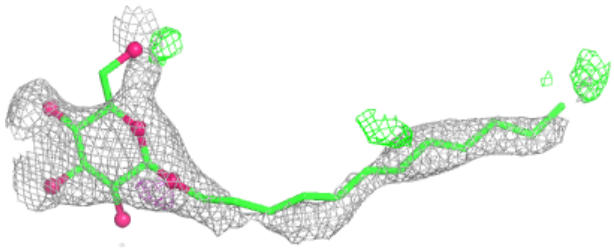
Electron density around LMT c 922:

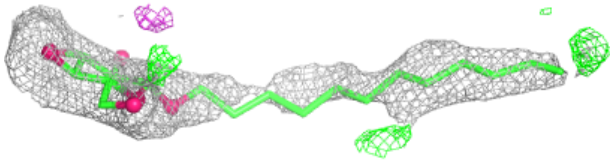
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

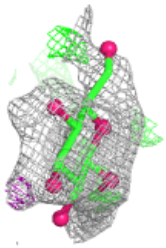


Electron density around LMT e 101:

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

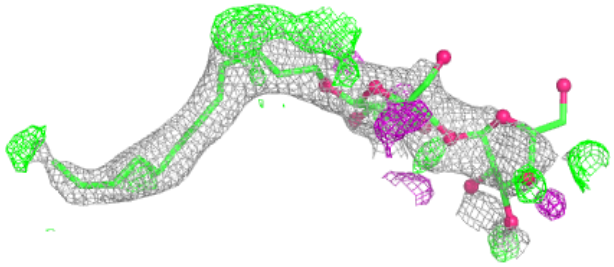


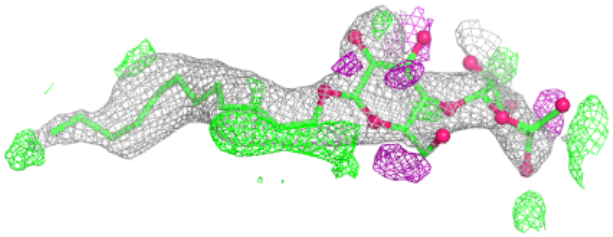


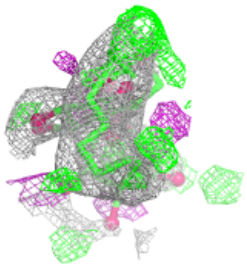


Electron density around LMT a 402:

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

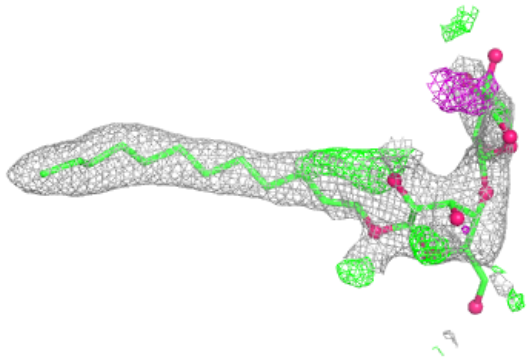


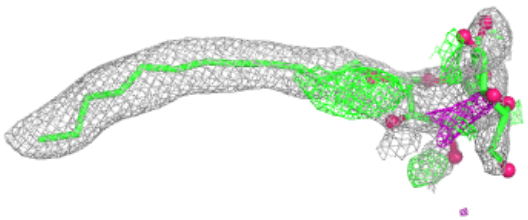


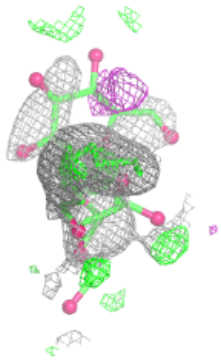


Electron density around LMT b 625:

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

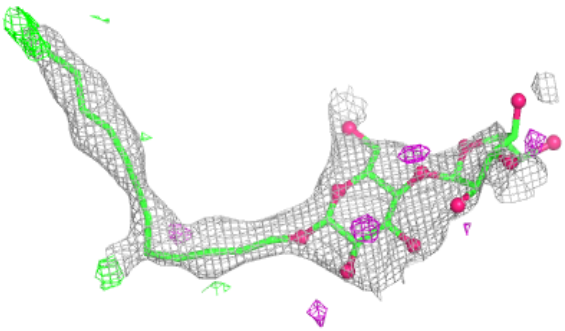


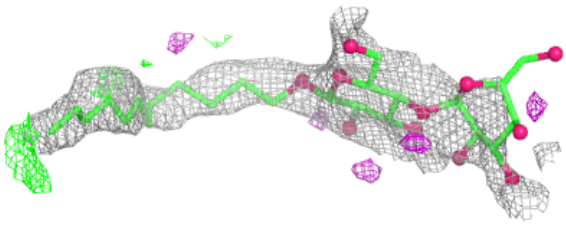


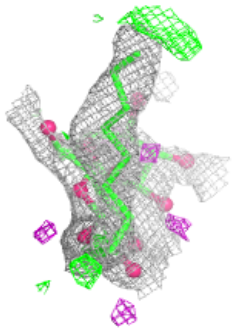


Electron density around LMT A 421:

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

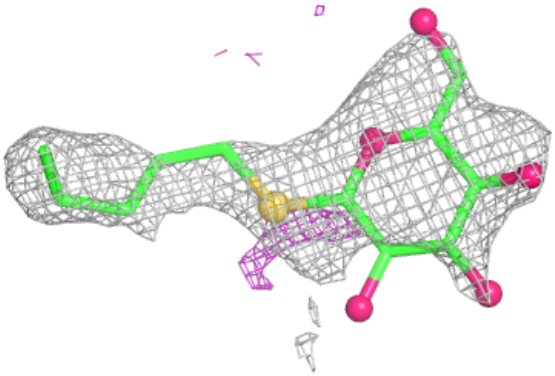


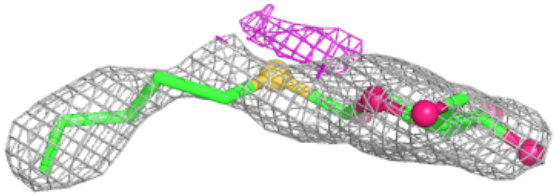


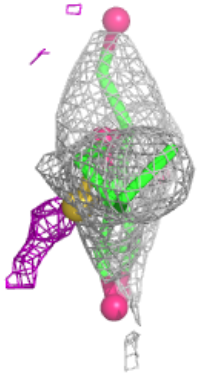


Electron density around HTG c 943:

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

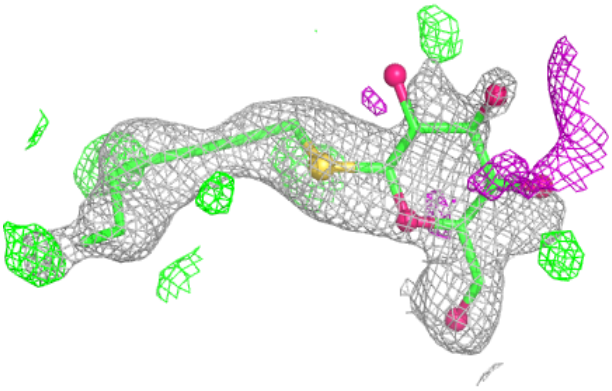


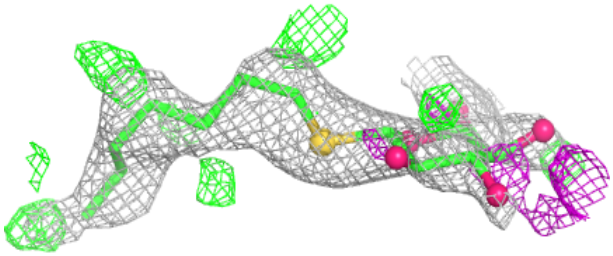


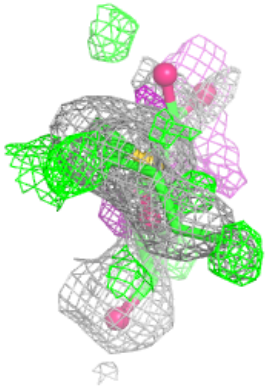


Electron density around HTG c 942:

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

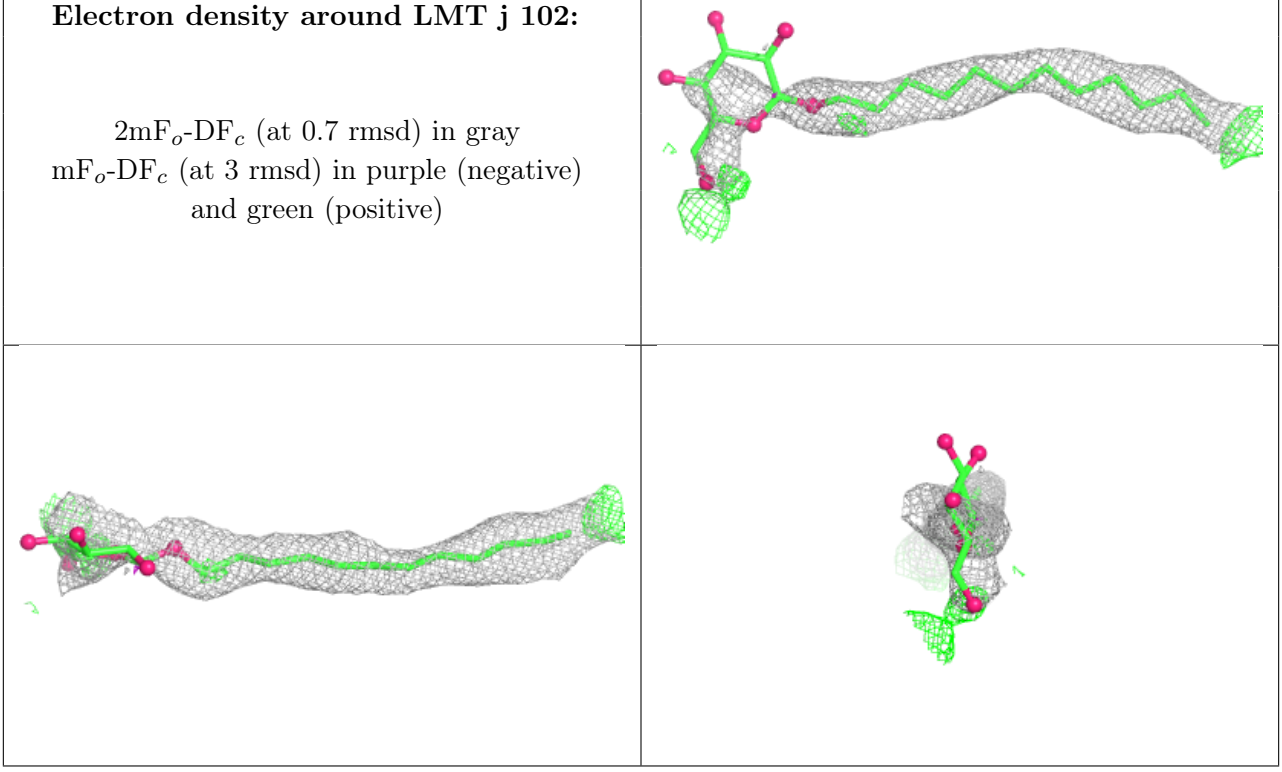






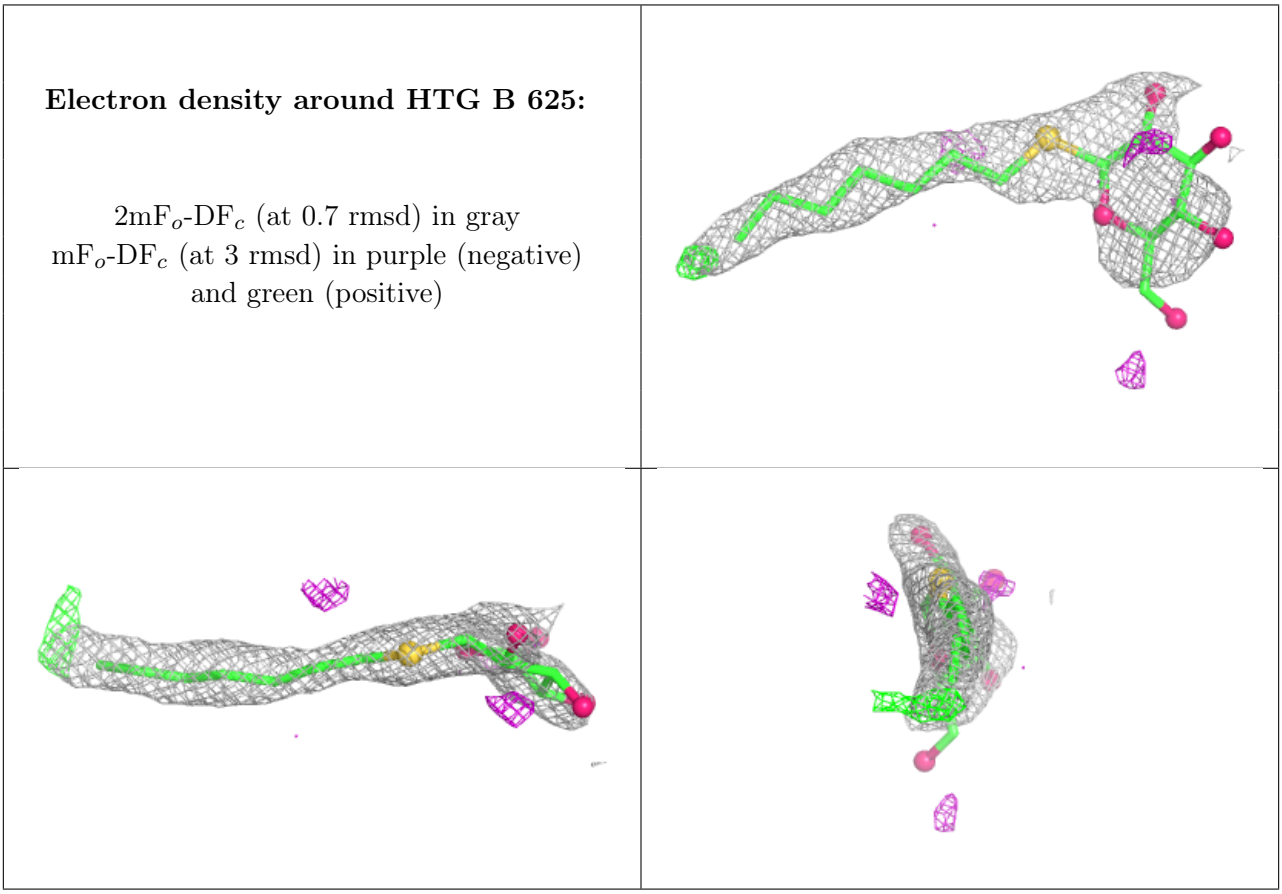
Electron density around LMT j 102:

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



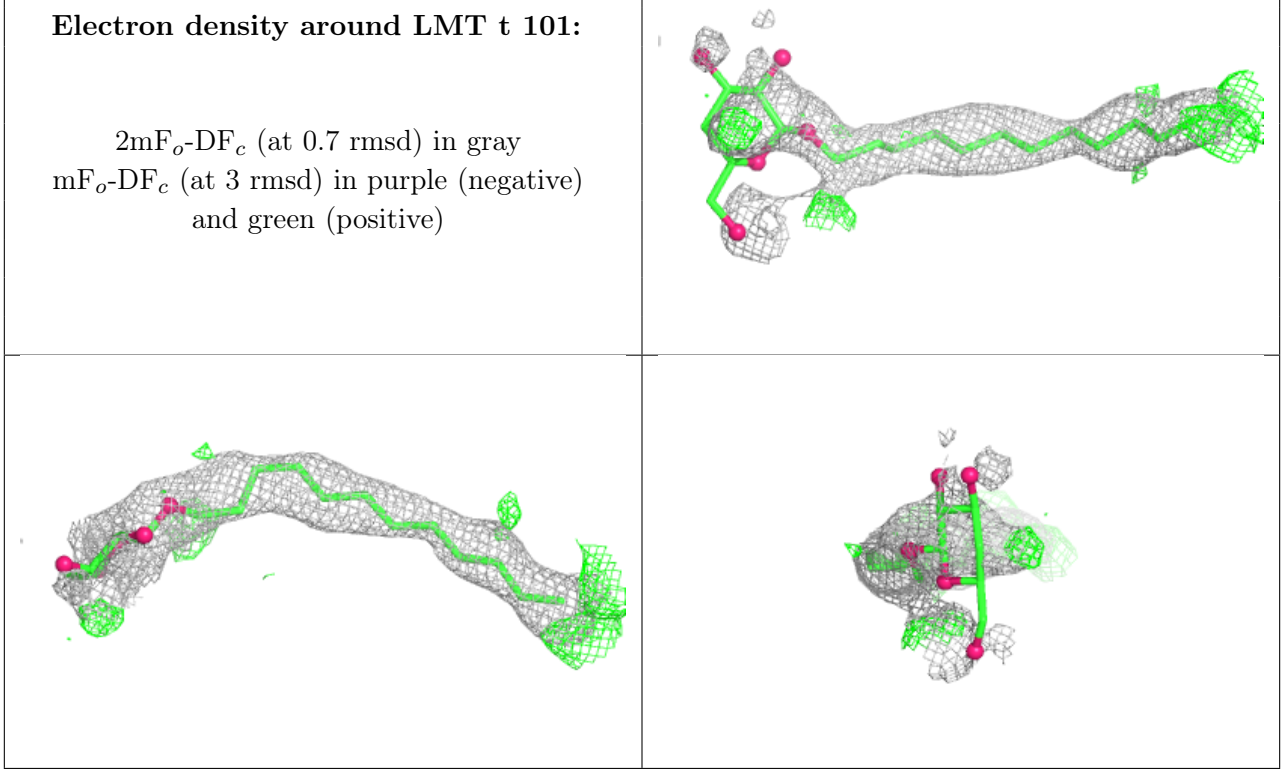
Electron density around HTG B 625:

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



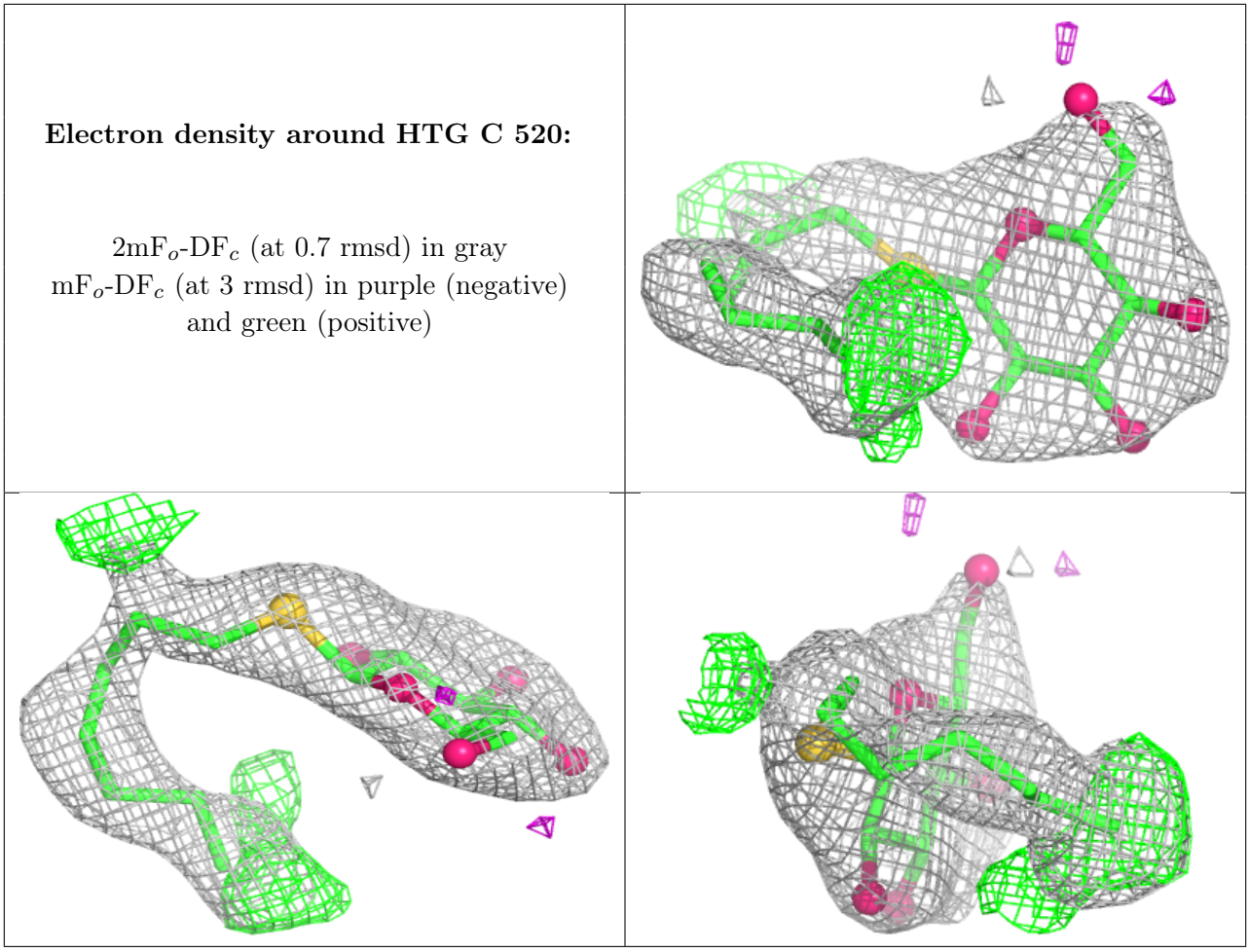
Electron density around LMT t 101:

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



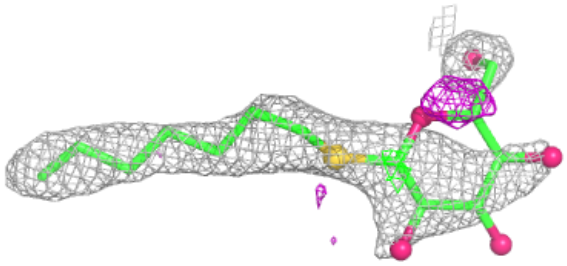
Electron density around HTG C 520:

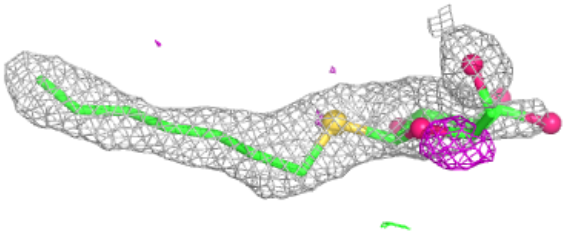
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

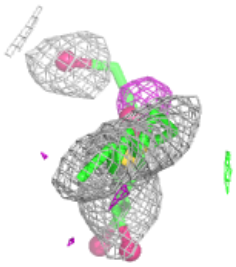


Electron density around HTG c 924:

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

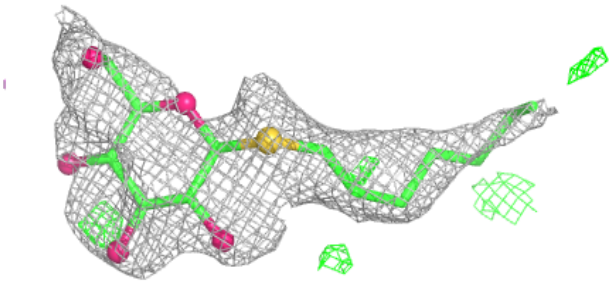


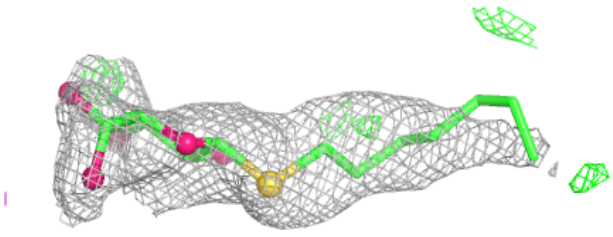


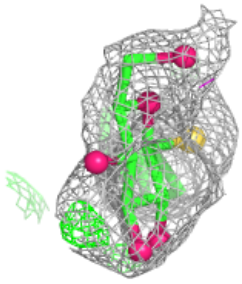


Electron density around HTG y 102:

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

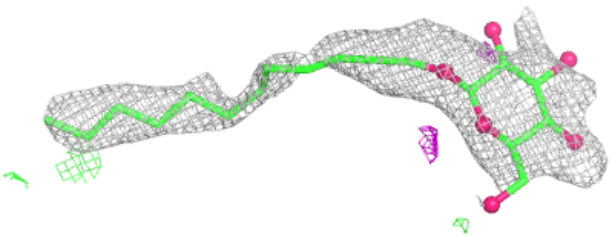


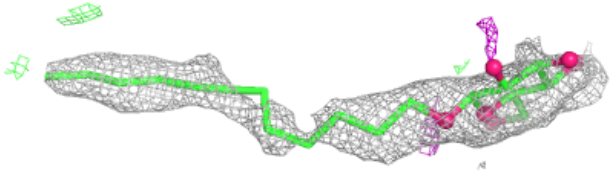


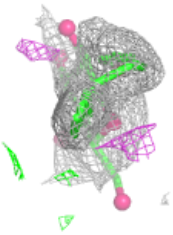


Electron density around LMT F 103:

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

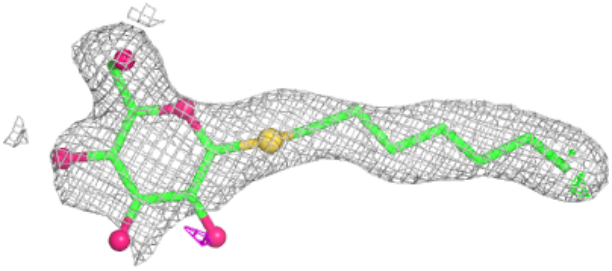


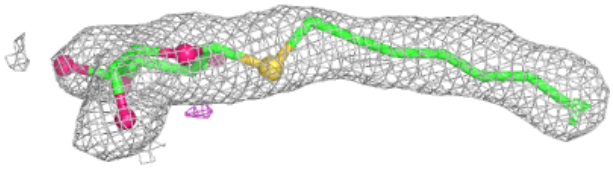


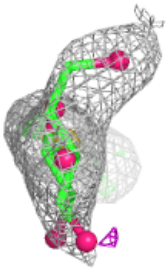


Electron density around HTG C 521:

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

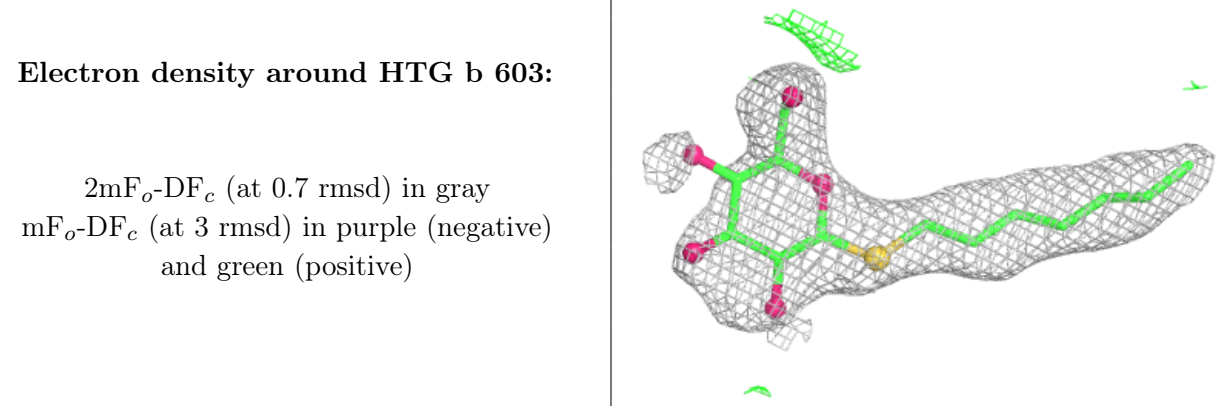


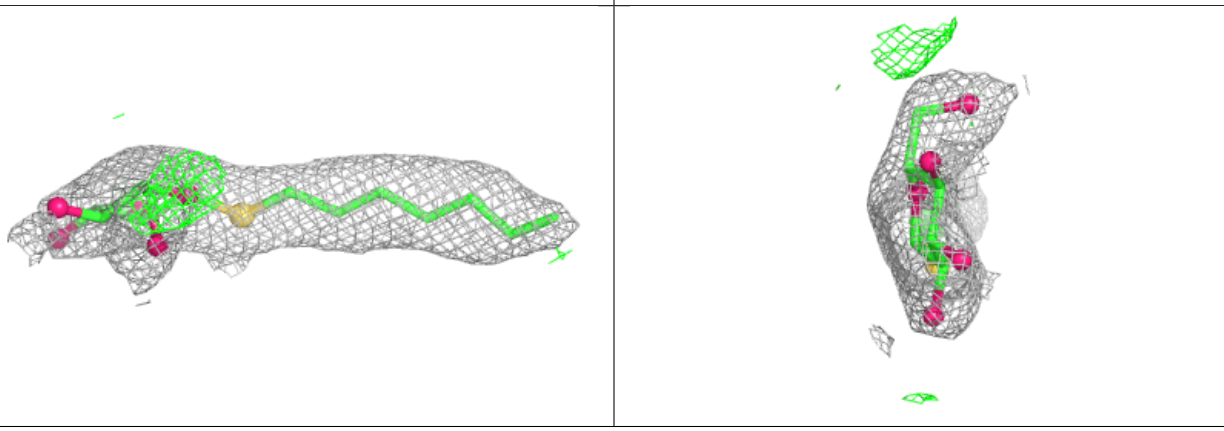




Electron density around HTG b 603:

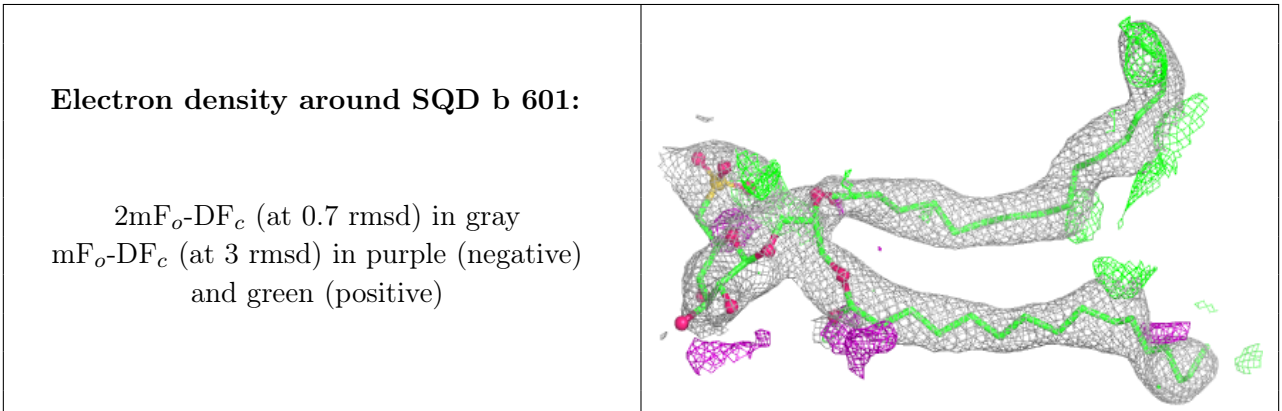
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

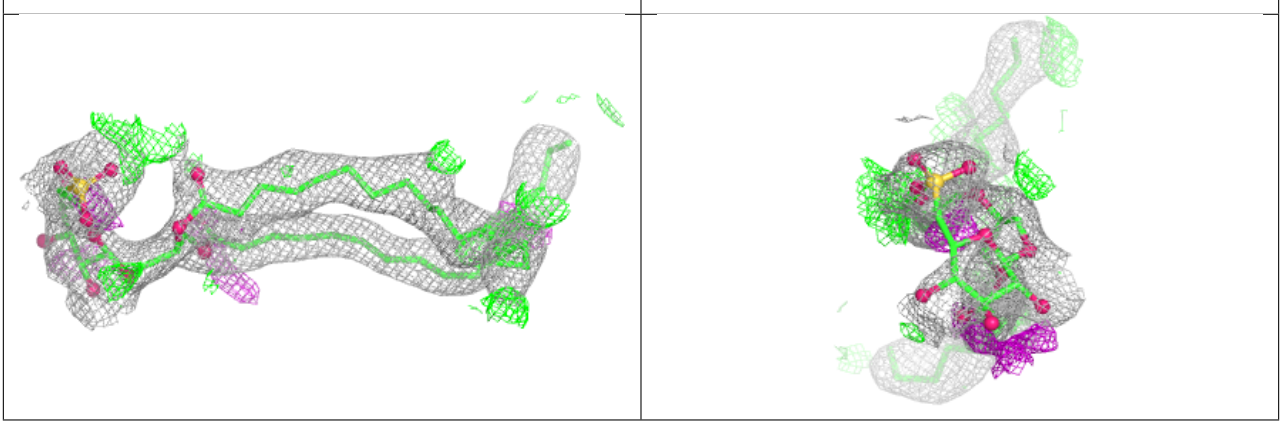




Electron density around SQD b 601:

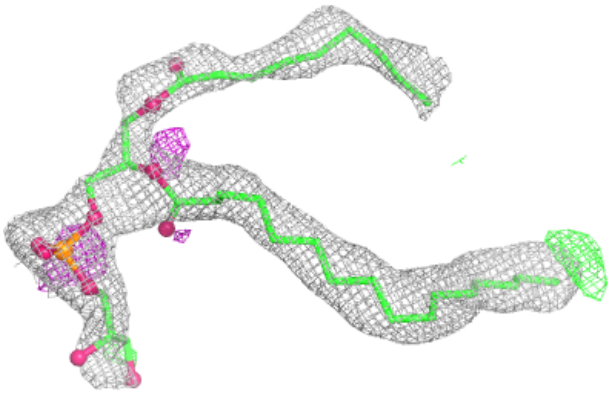
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

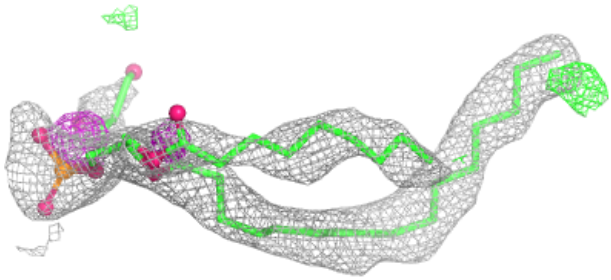


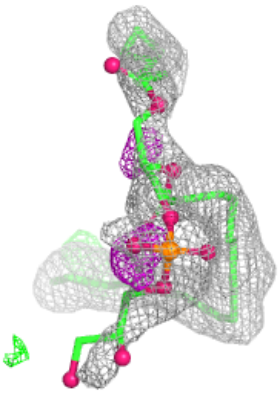


Electron density around LHG E 101:

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

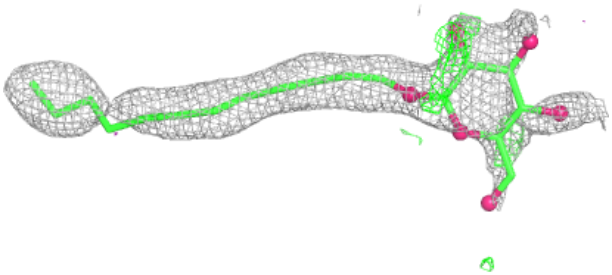


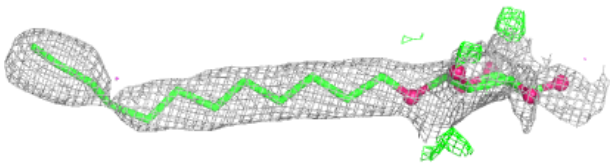


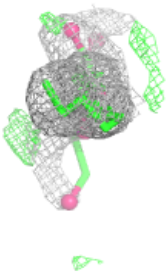


Electron density around LMT J 102:

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

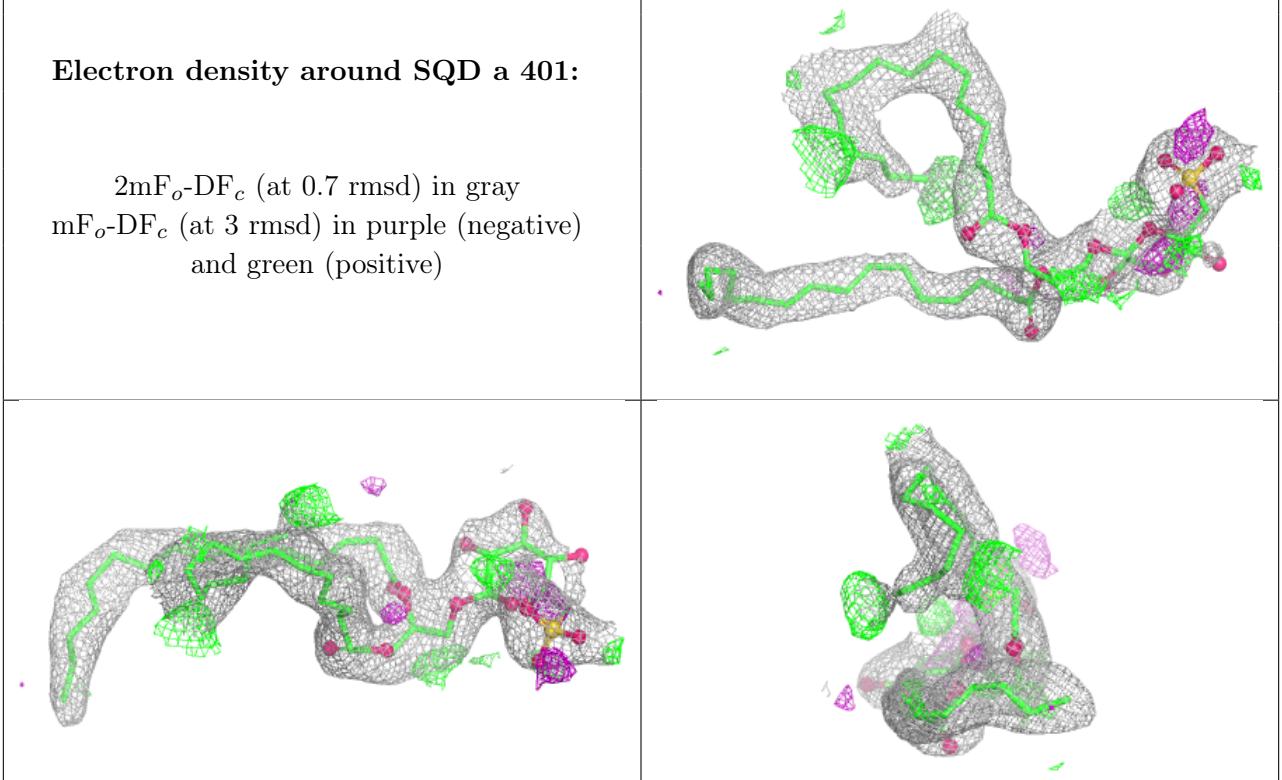






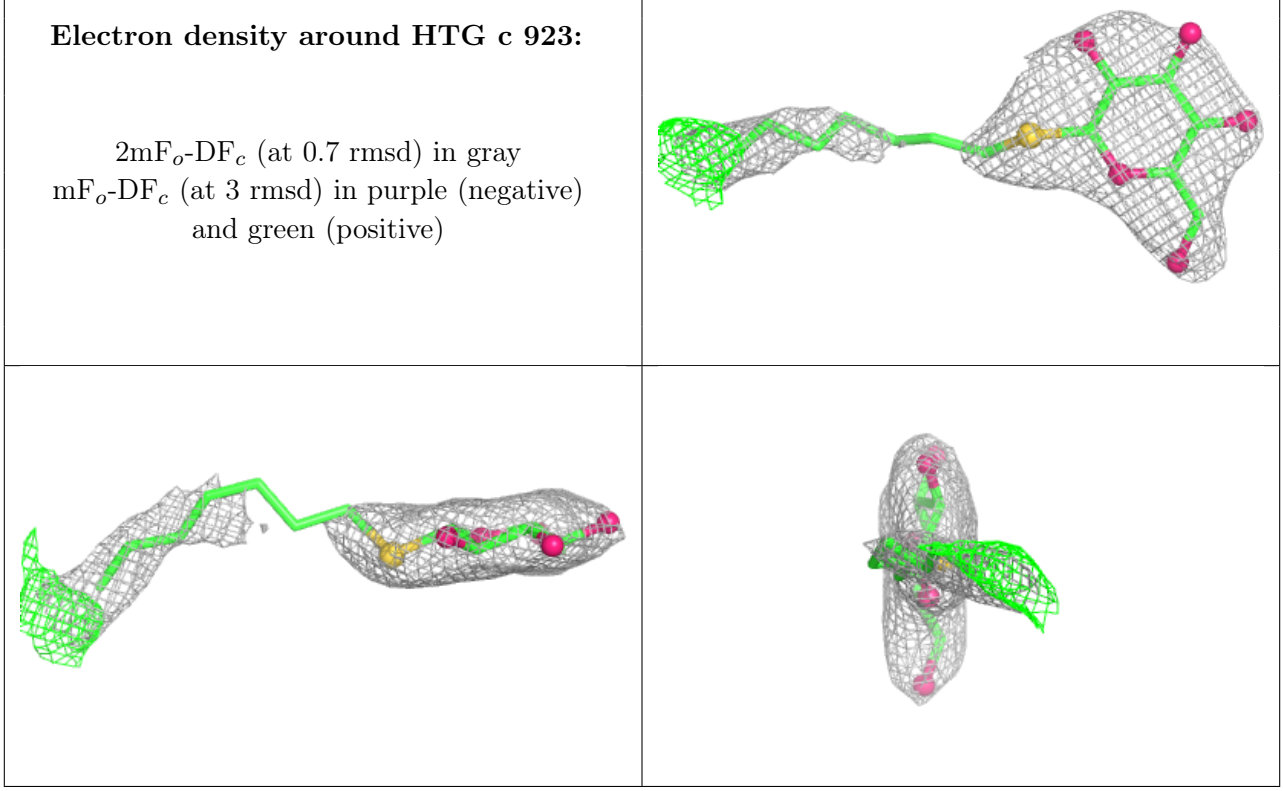
Electron density around SQD a 401:

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



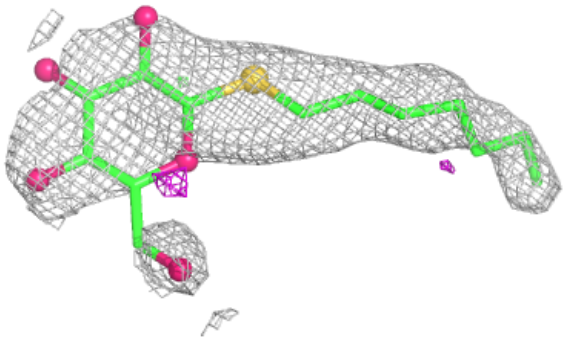
Electron density around HTG c 923:

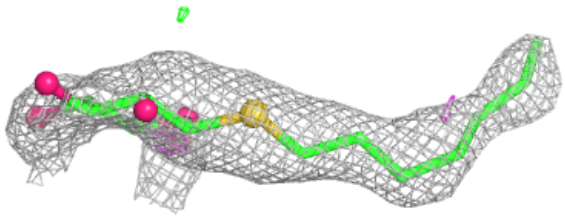
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

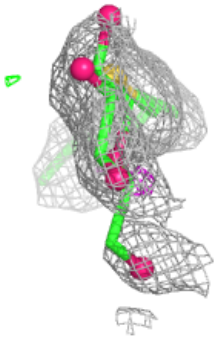


Electron density around HTG d 419:

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

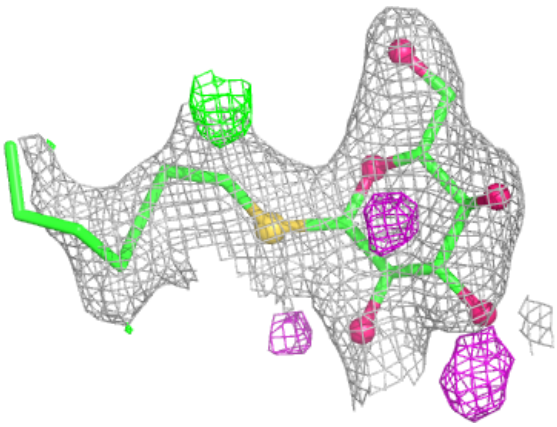


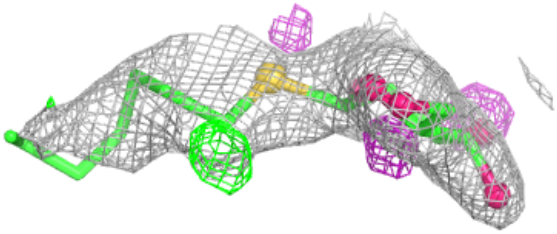


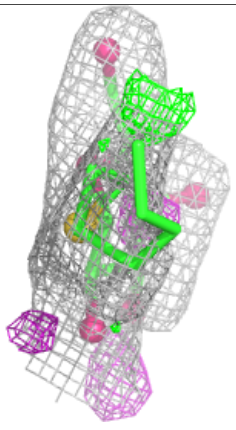


Electron density around HTG v 211:

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

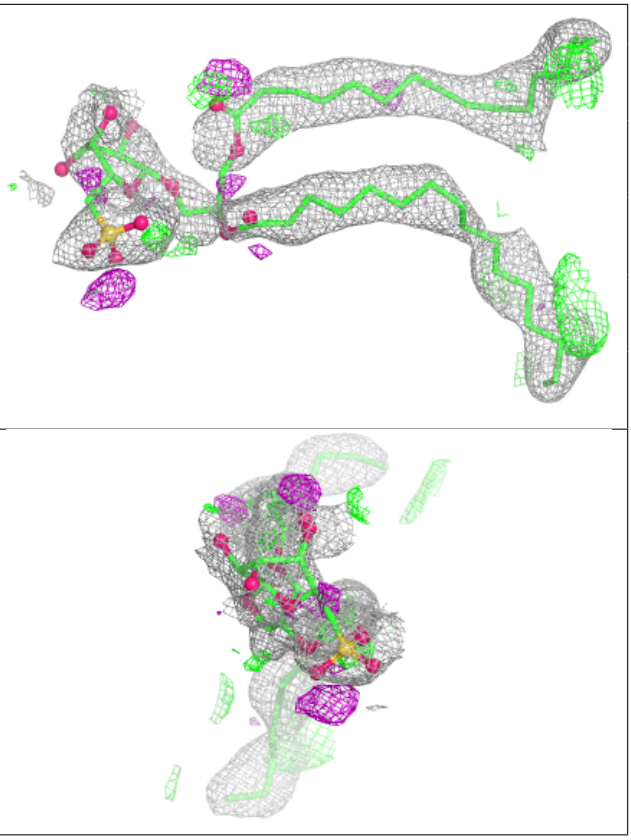






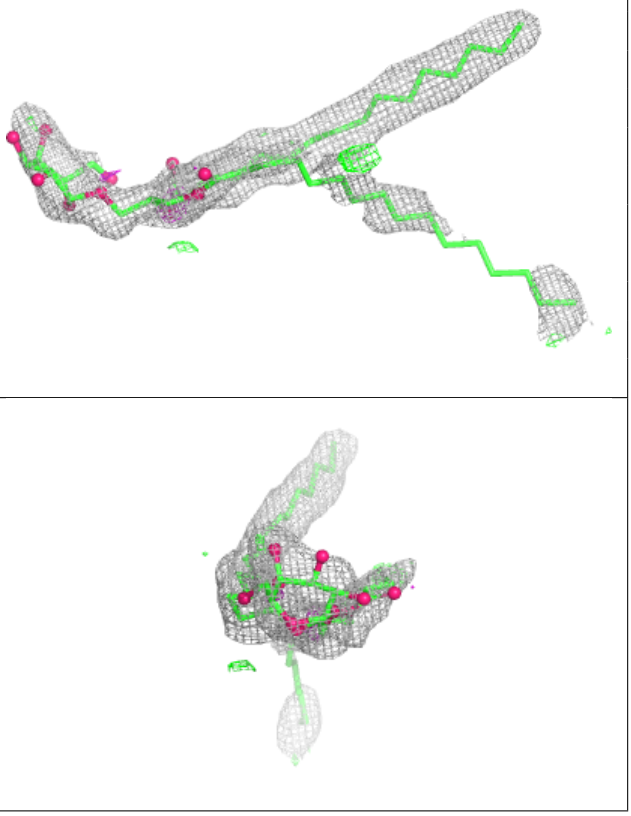
Electron density around SQD l 101:

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



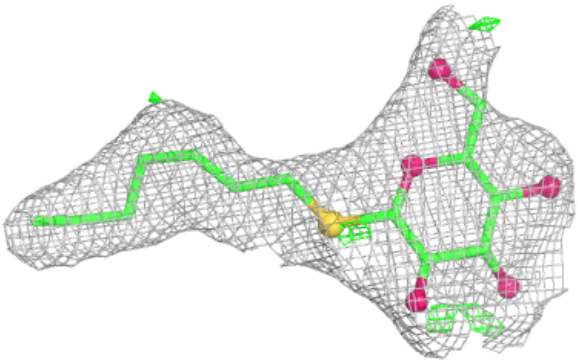
Electron density around LMG C 523:

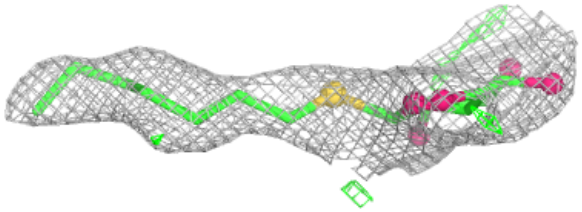
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

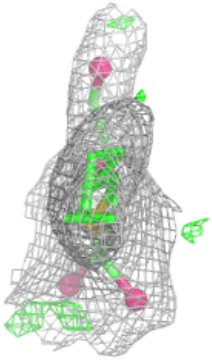


Electron density around HTG d 414:

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

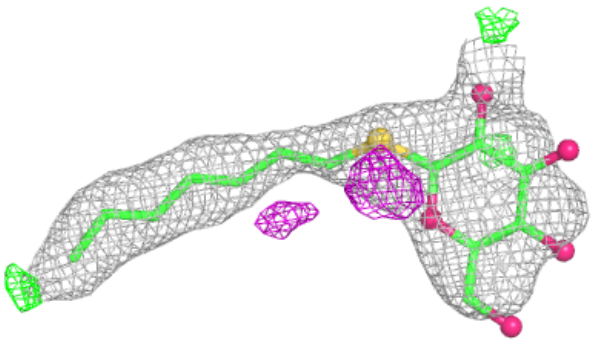


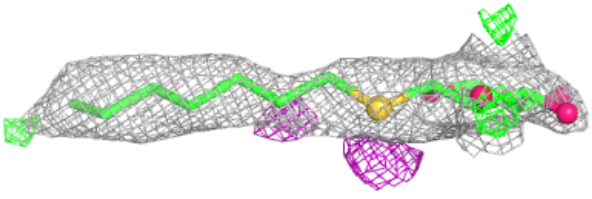


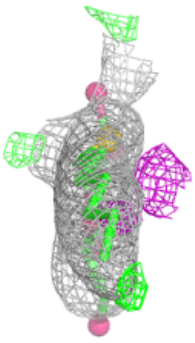


Electron density around HTG B 630:

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

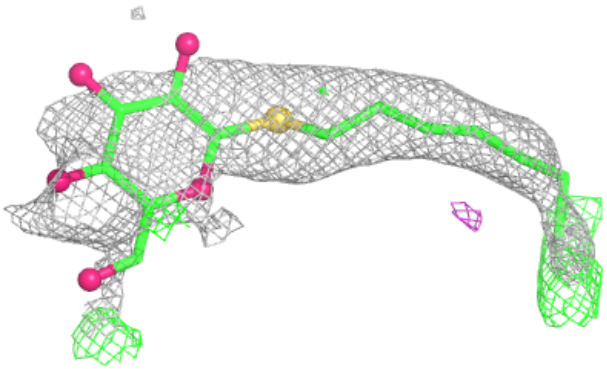


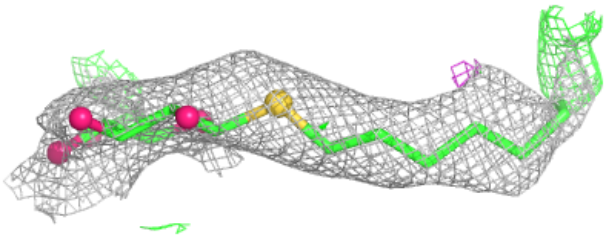


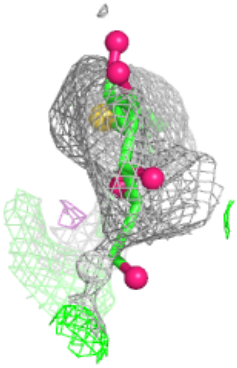


Electron density around HTG D 412:

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

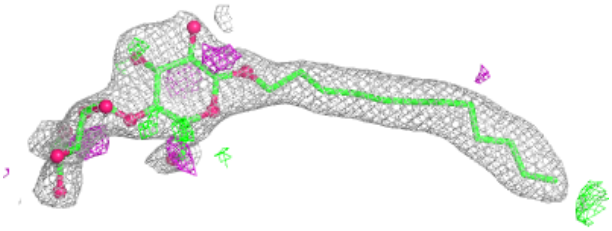


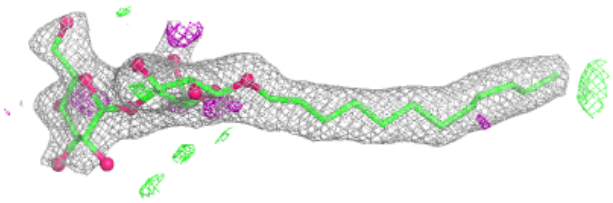


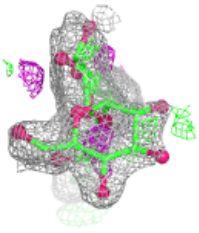


Electron density around LMT B 622:

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

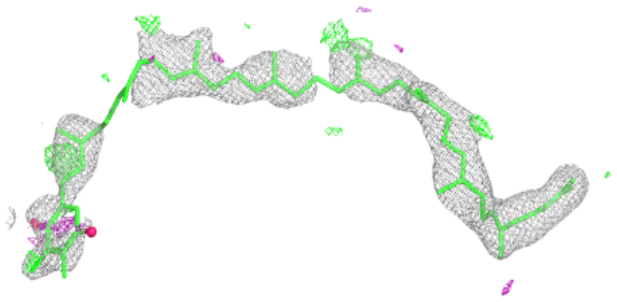


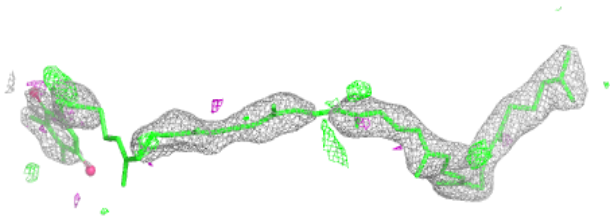


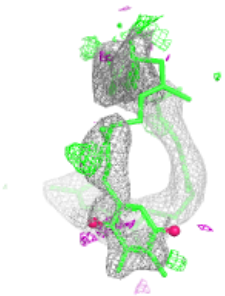


Electron density around PL9 a 417:

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

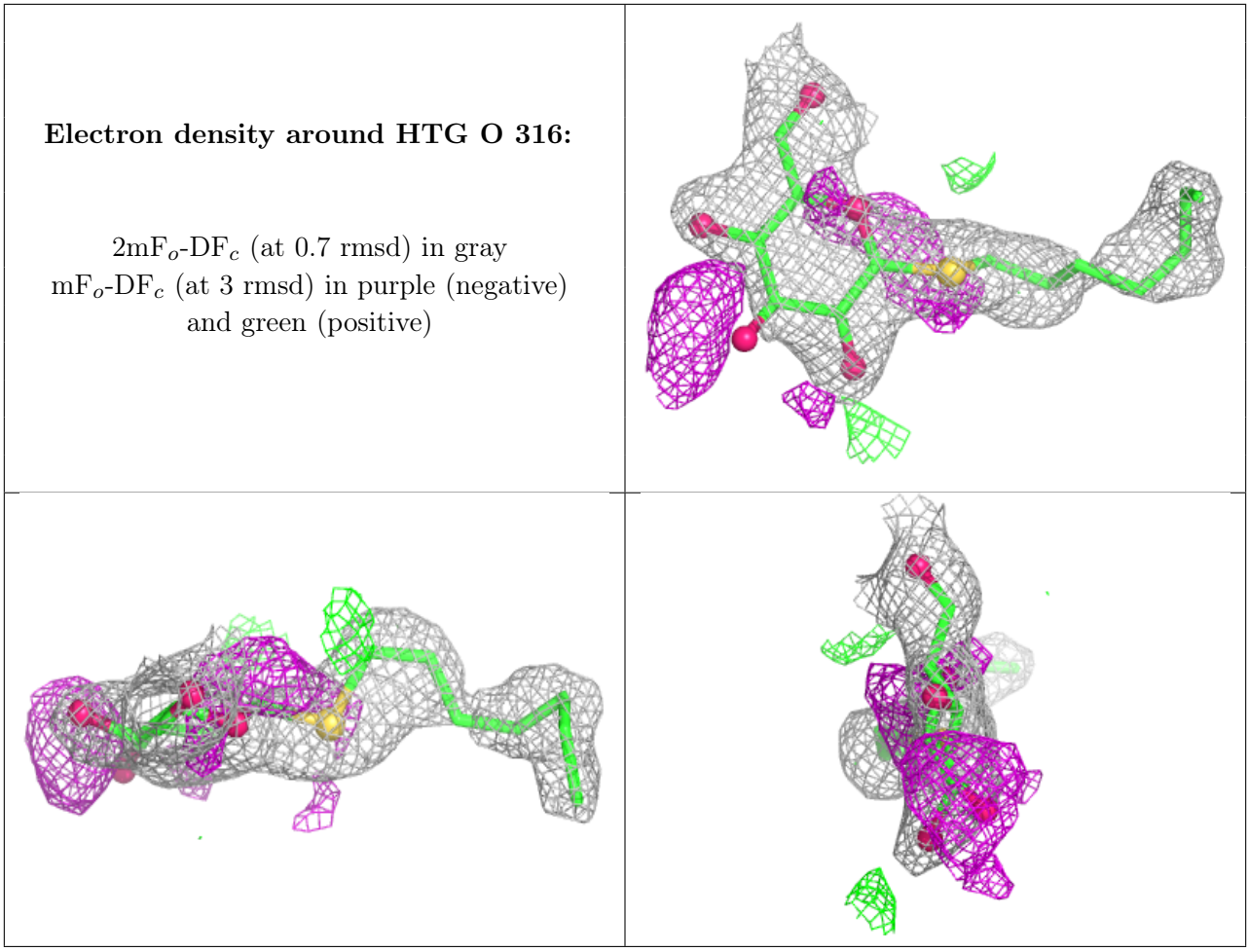






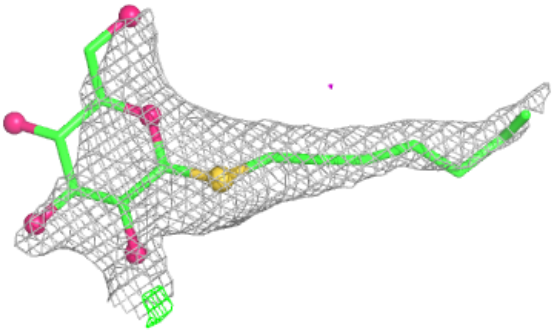
Electron density around HTG O 316:

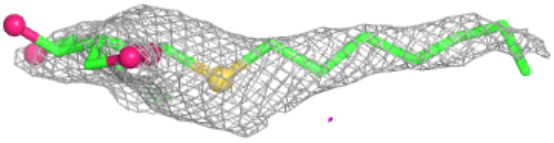
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HTG C 537:

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

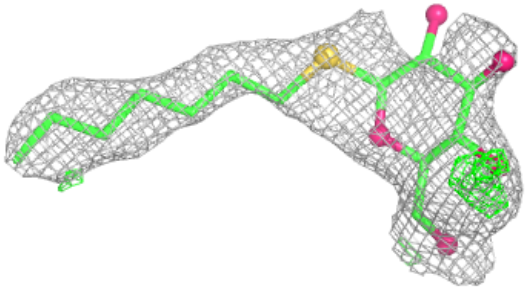


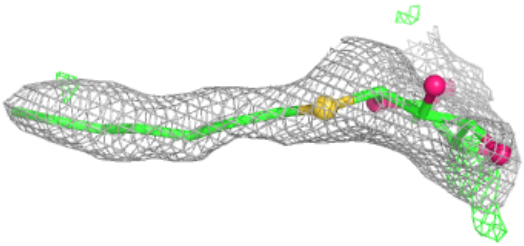


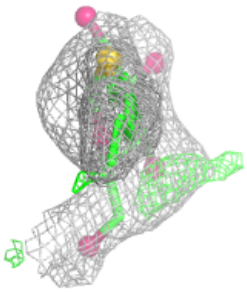


Electron density around HTG b 627:

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

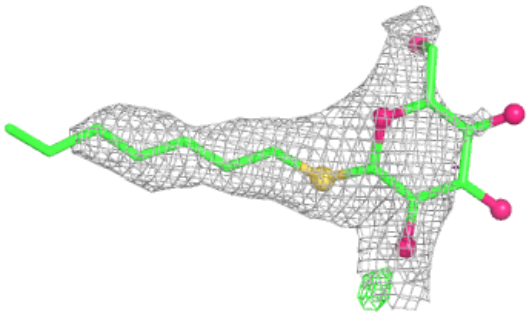


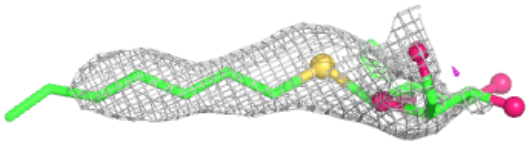


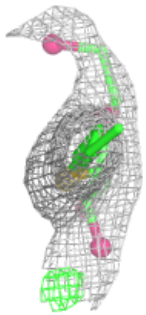


Electron density around HTG c 928:

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

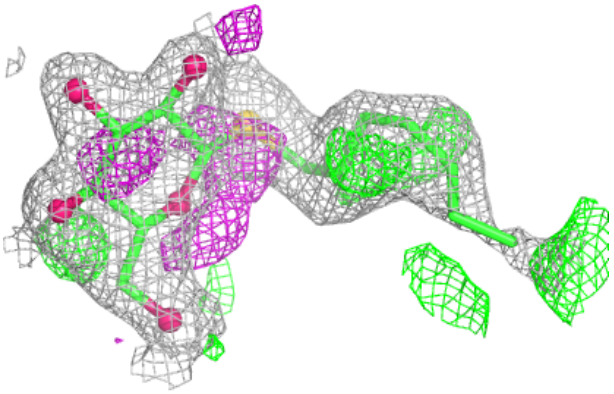


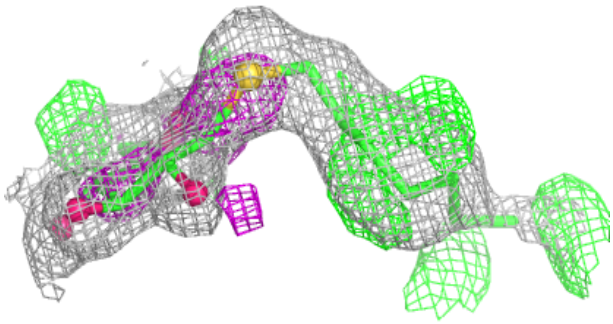


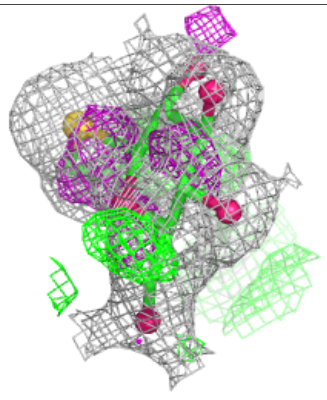


Electron density around HTG B 624:

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

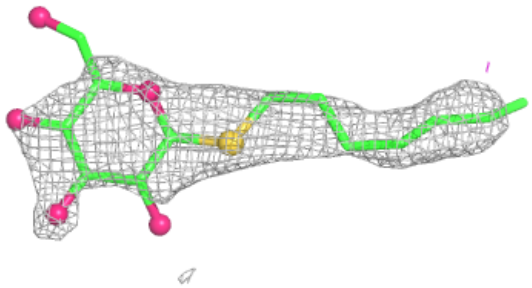


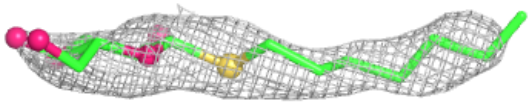


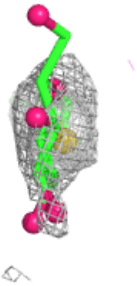


Electron density around HTG d 420:

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

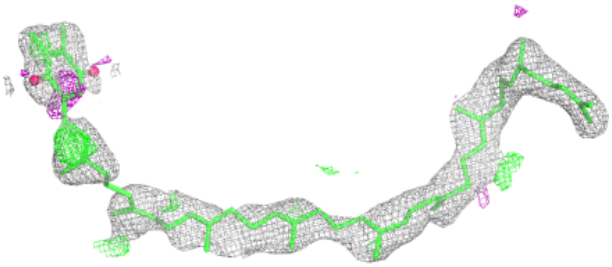


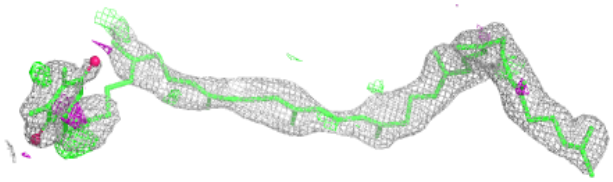


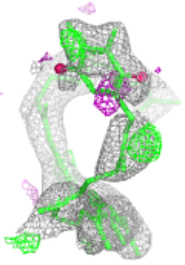


Electron density around PL9 A 414:

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

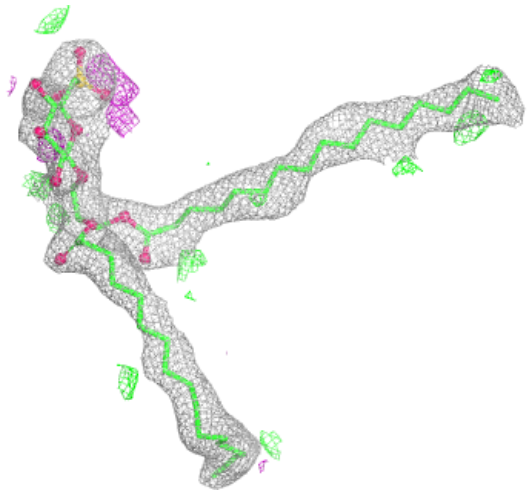


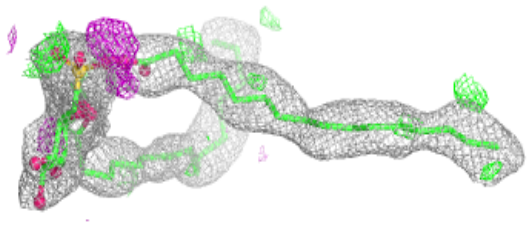


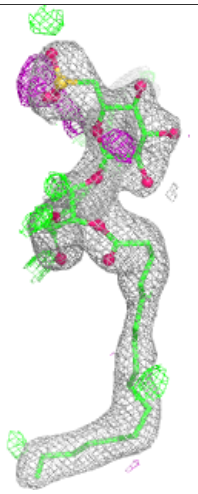


Electron density around SQD A 416:

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

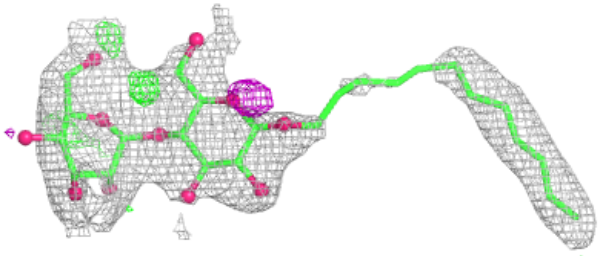


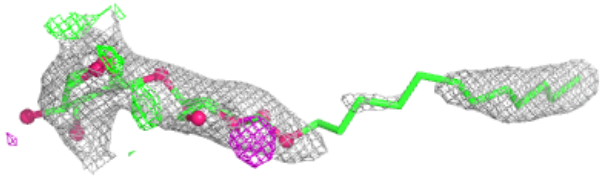


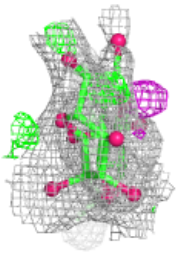


Electron density around LMT c 927:

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

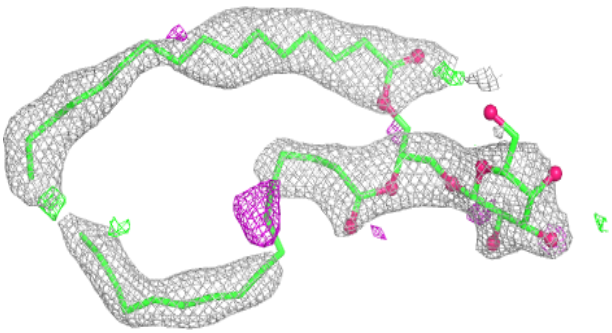


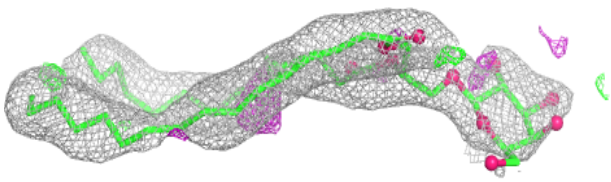


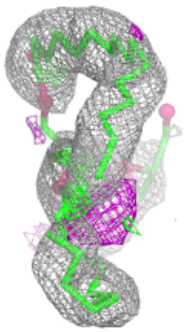


Electron density around LMG a 416:

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

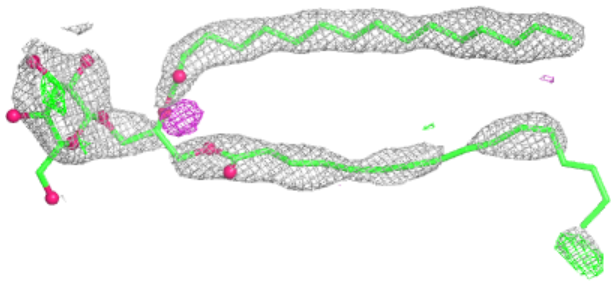


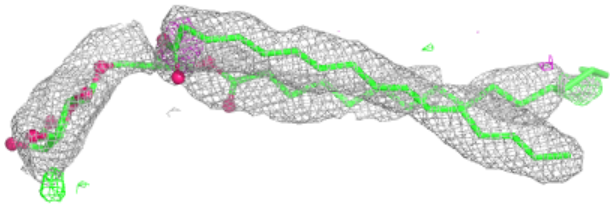


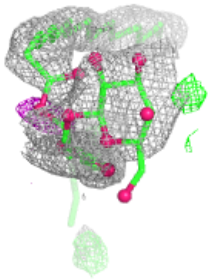


Electron density around LMG c 921:

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

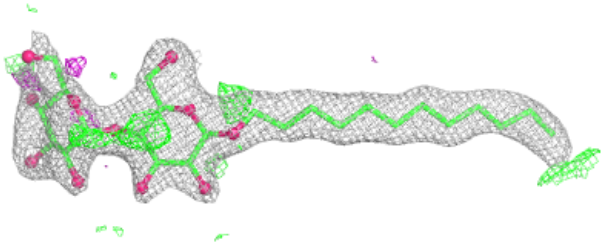


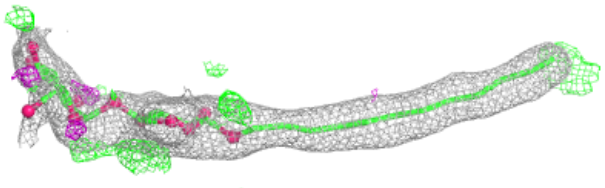


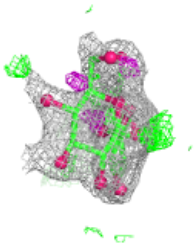


Electron density around LMT m 102:

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

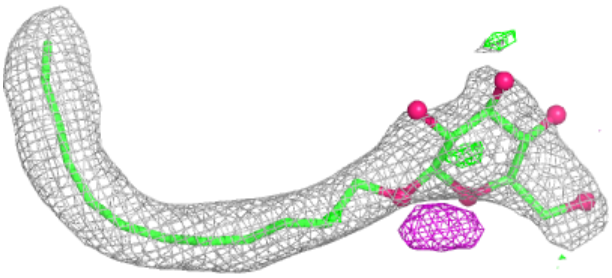


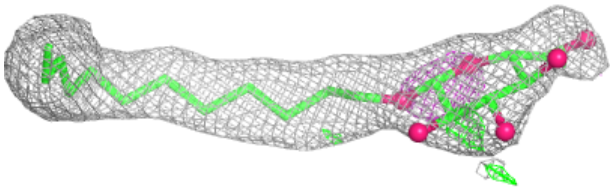


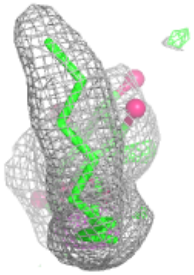


Electron density around LMT B 626:

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

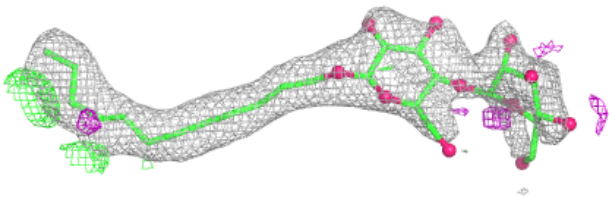


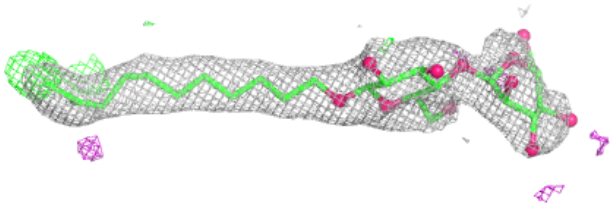


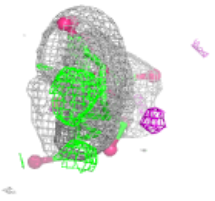


Electron density around LMT t 102:

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

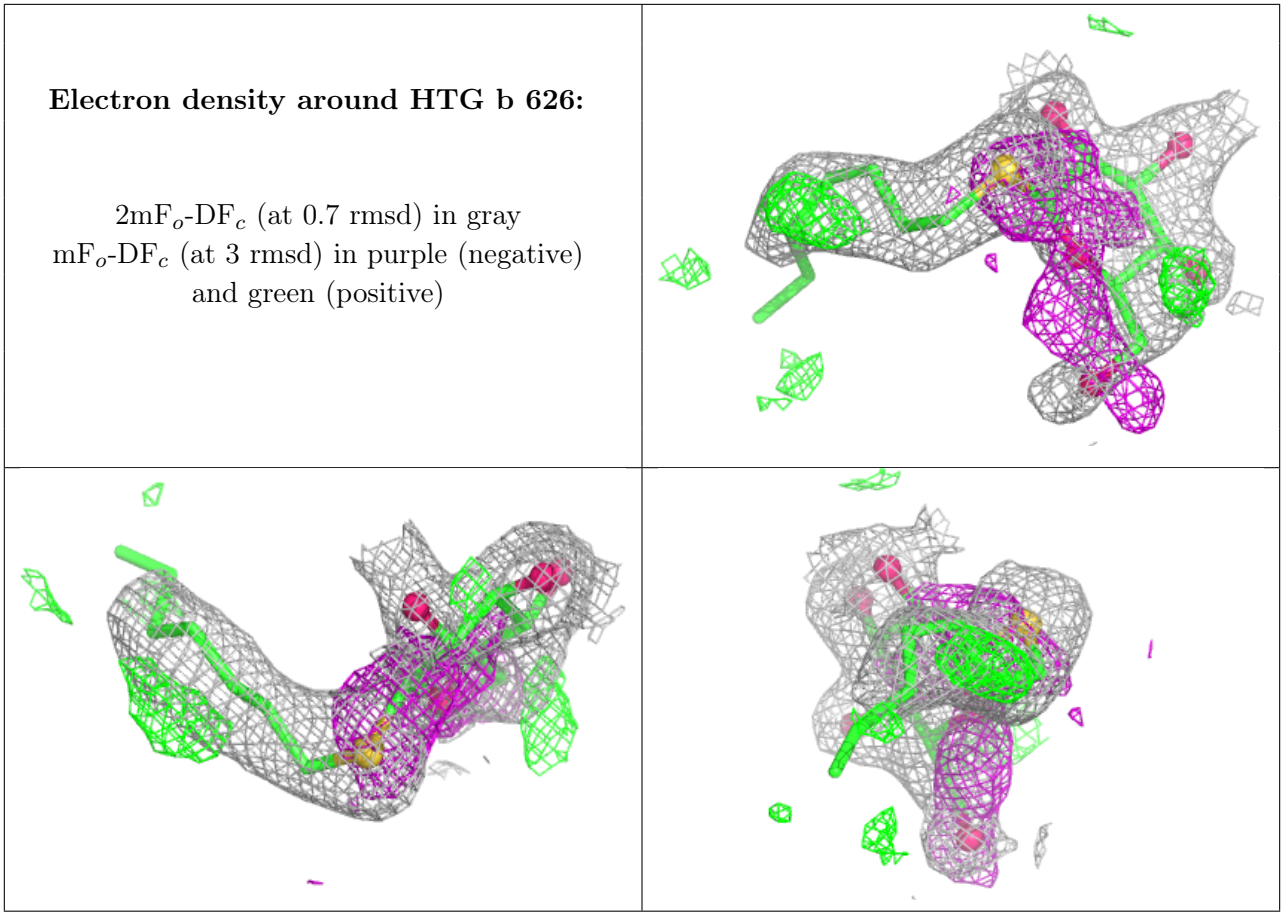






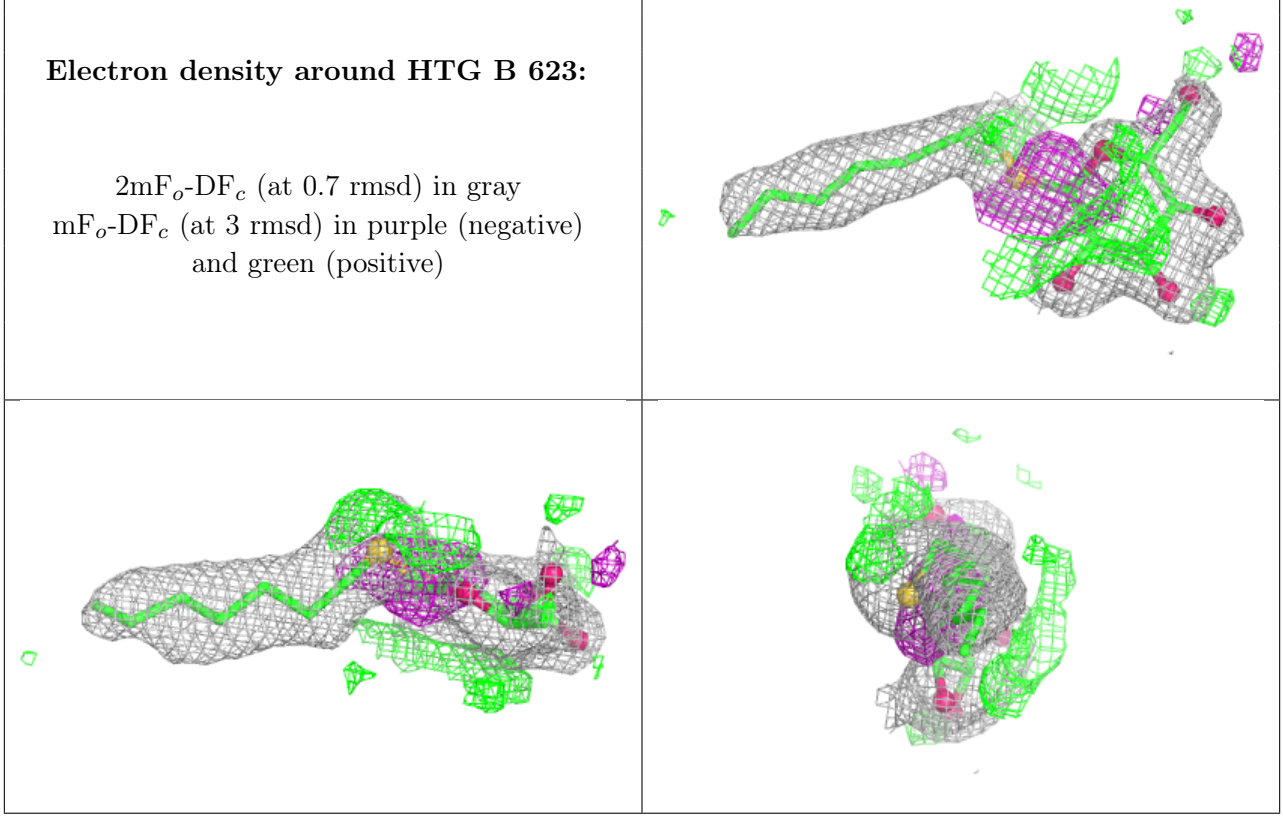
Electron density around HTG b 626:

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



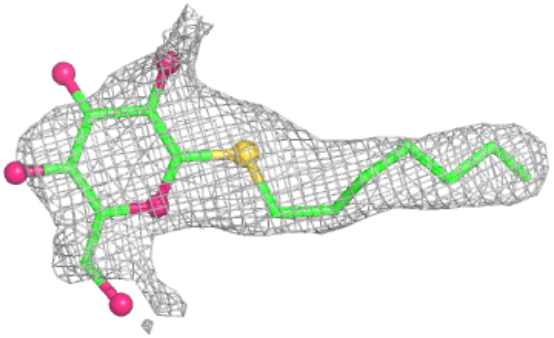
Electron density around HTG B 623:

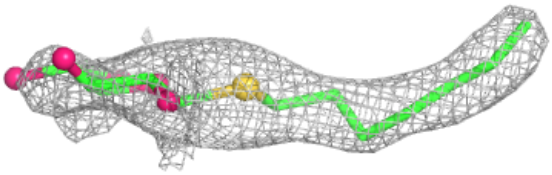
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

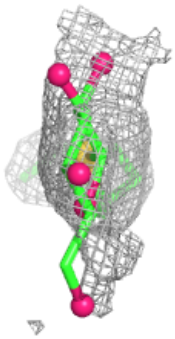


Electron density around HTG C 536:

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

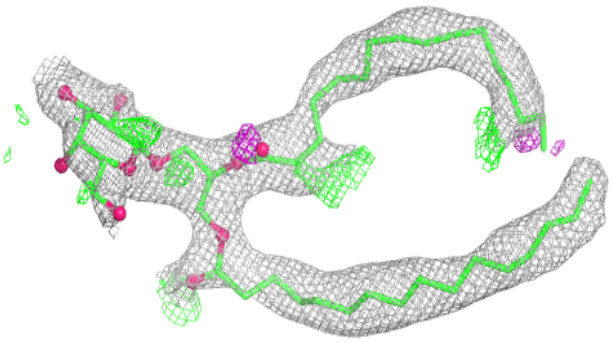


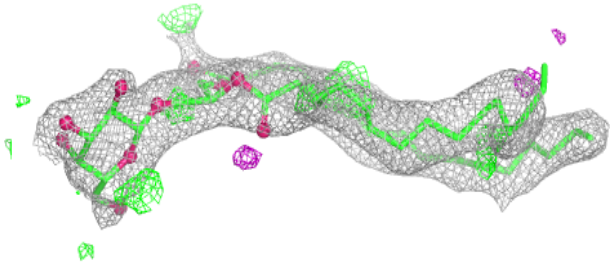


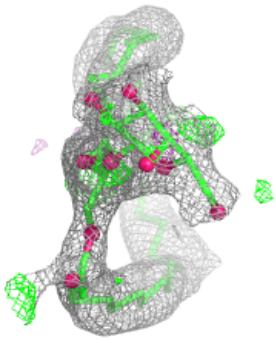


Electron density around LMG A 413:

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

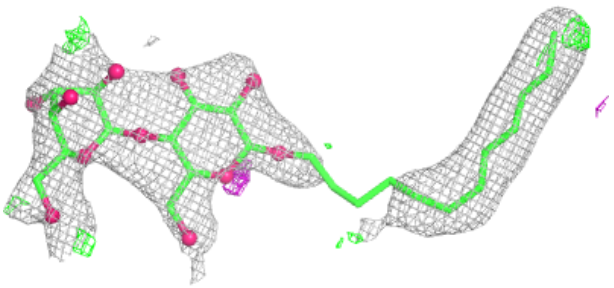


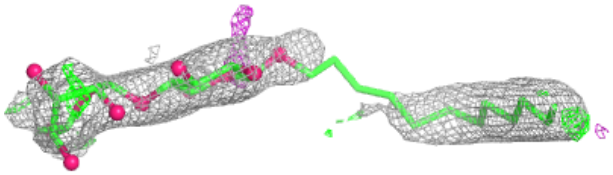


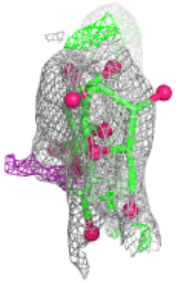


Electron density around LMT Z 101:

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

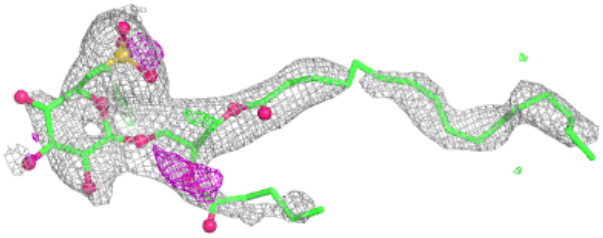


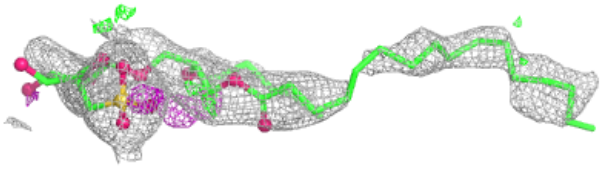


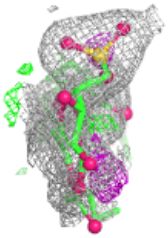


Electron density around SQD f 102:

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

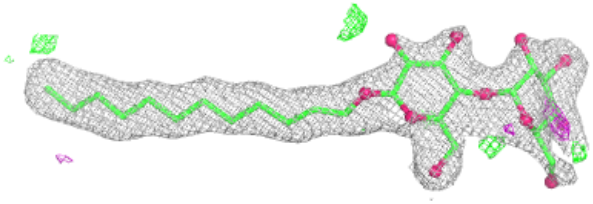


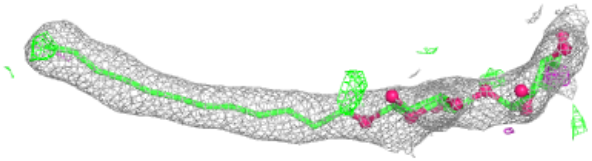


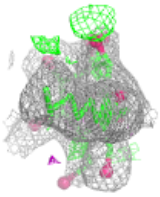


Electron density around LMT M 101:

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

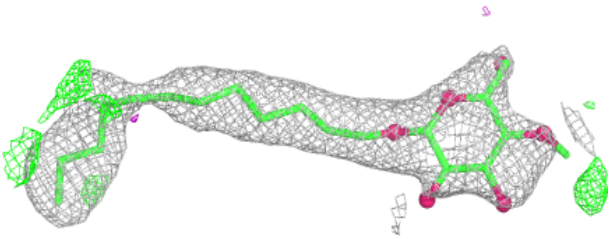


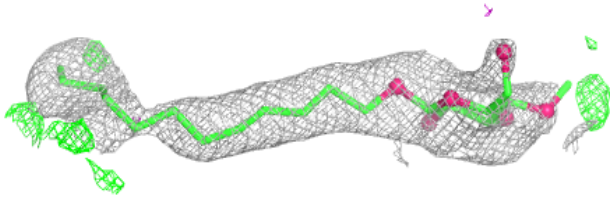


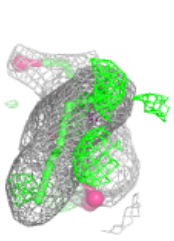


Electron density around LMT M 102:

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

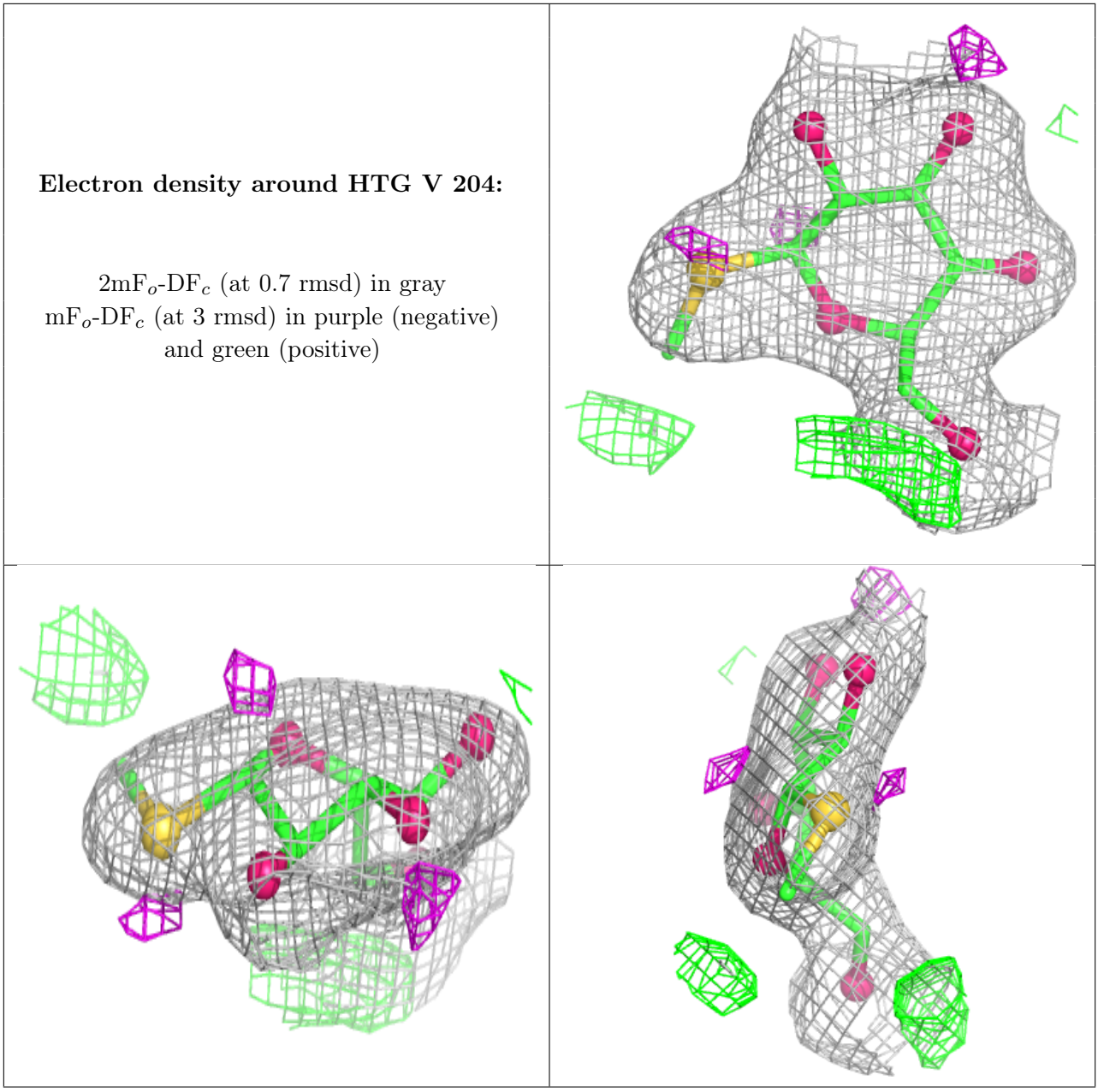






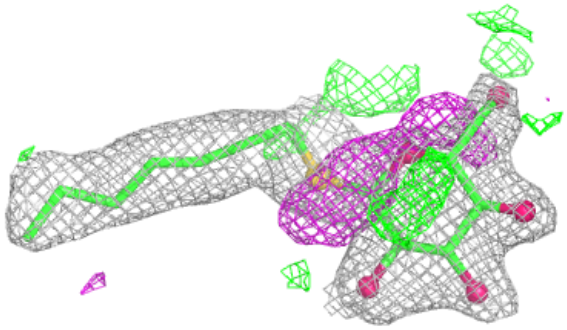
Electron density around HTG V 204:

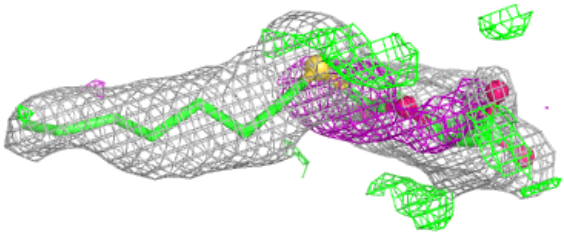
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

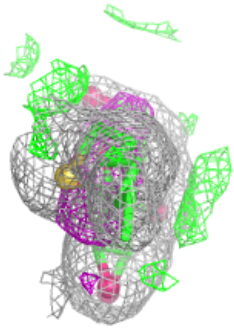


Electron density around HTG O 303:

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

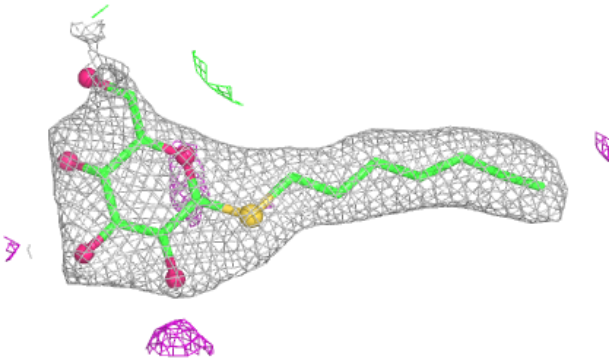


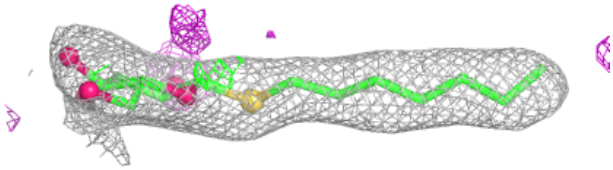


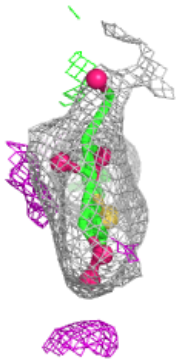


Electron density around HTG B 629:

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

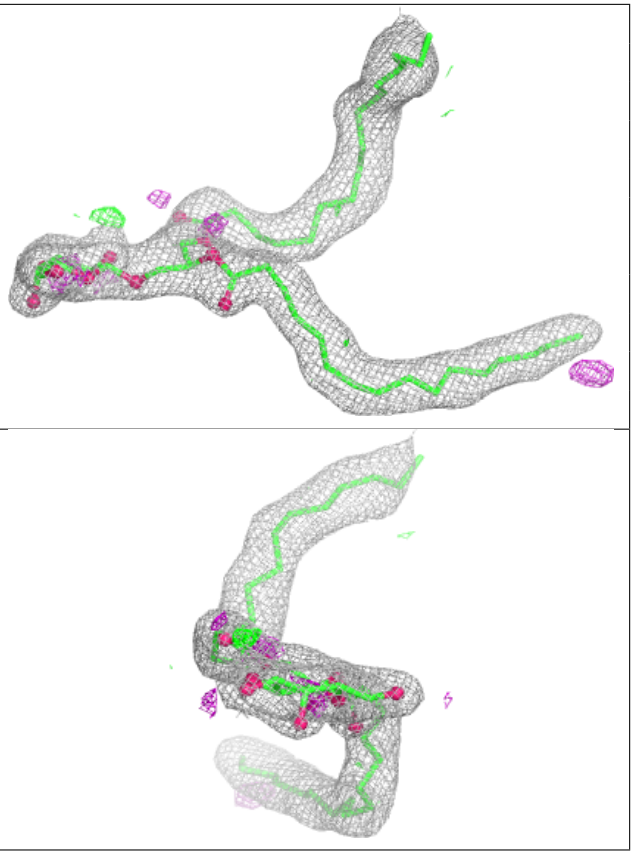






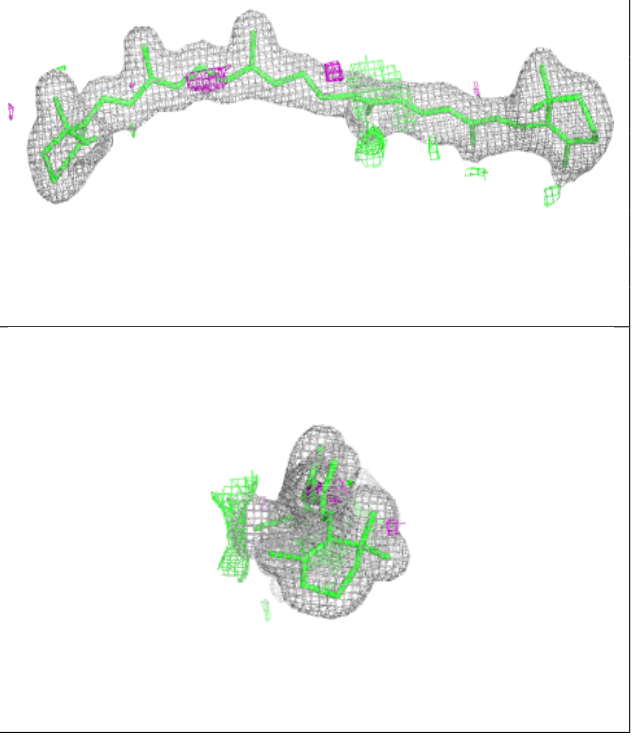
Electron density around LMG B 621:

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



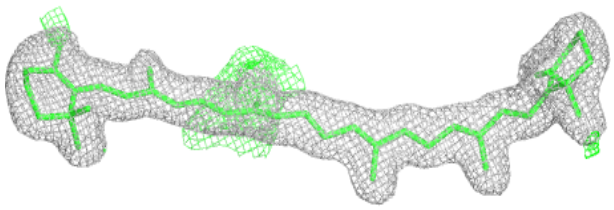
Electron density around BCR B 636:

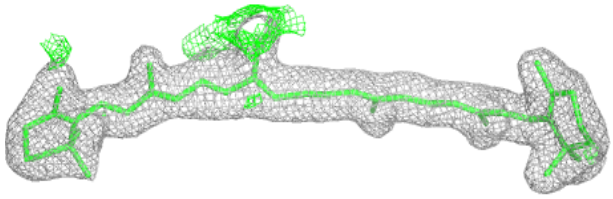
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

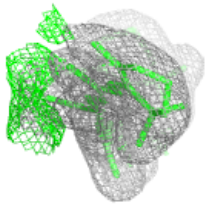


Electron density around BCR T 101:

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

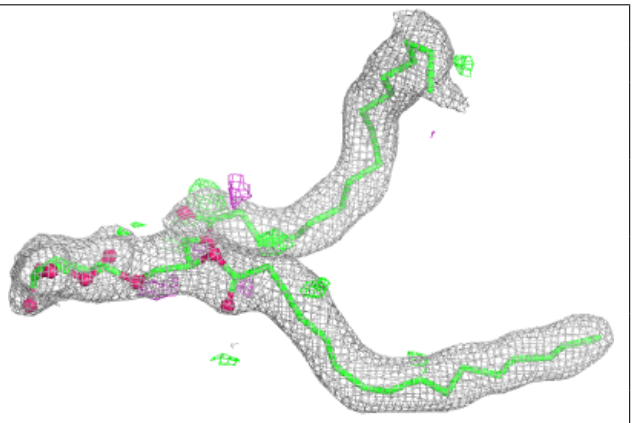


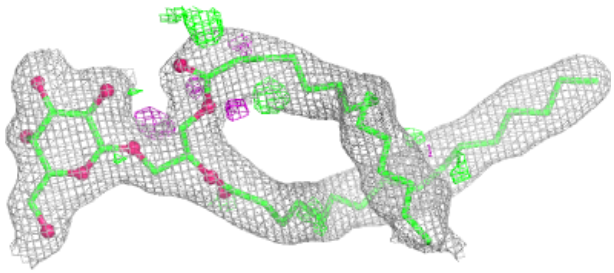


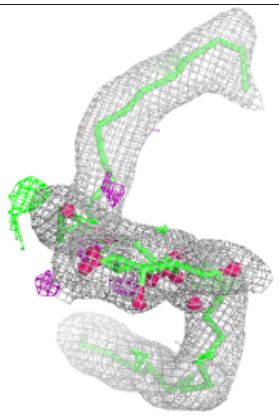


Electron density around LMG b 624:

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

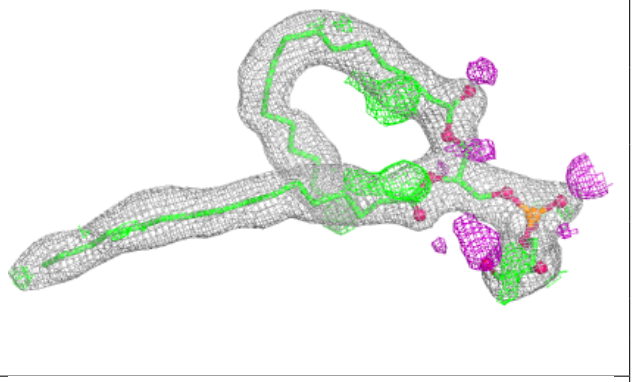


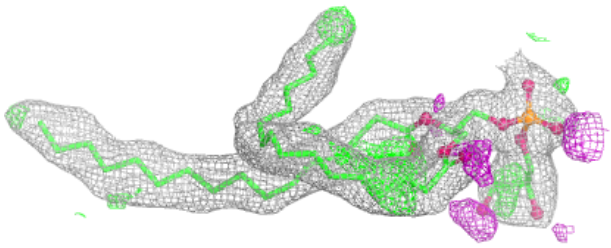




Electron density around LHG D 406:

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

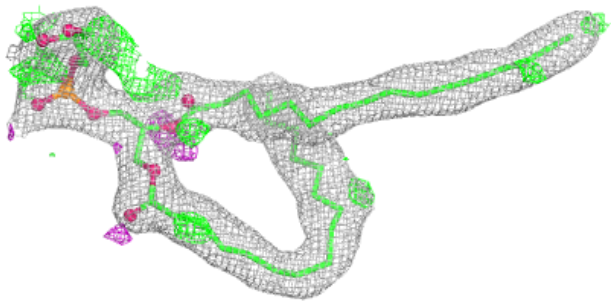


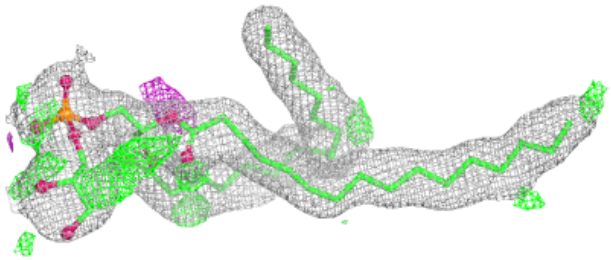


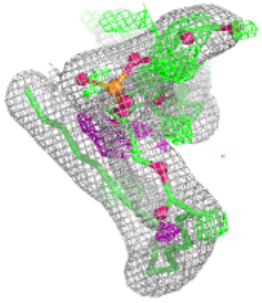


Electron density around LHG d 409:

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

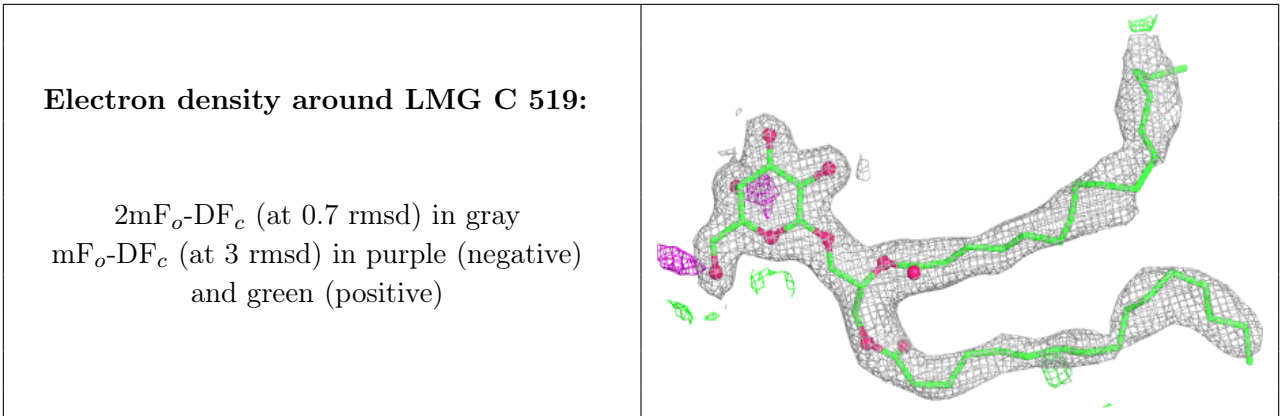






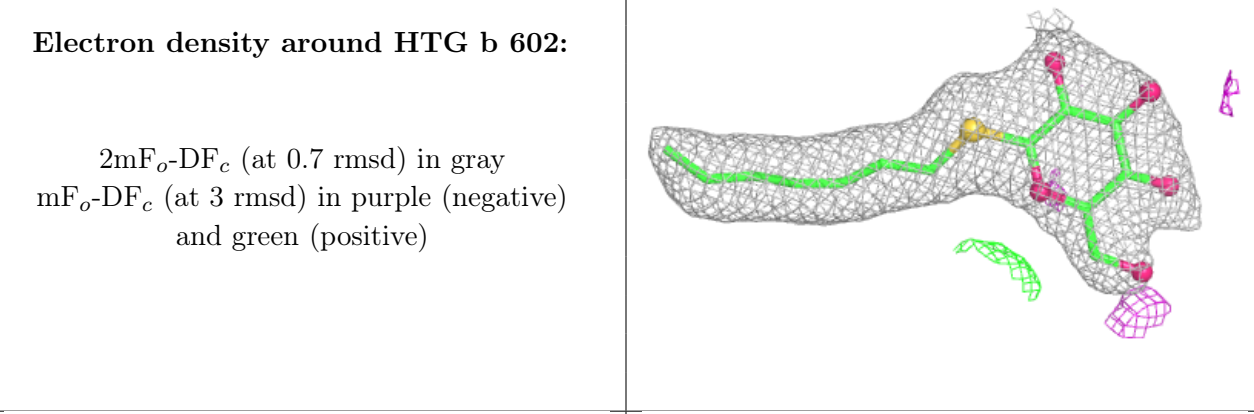
Electron density around LMG C 519:

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



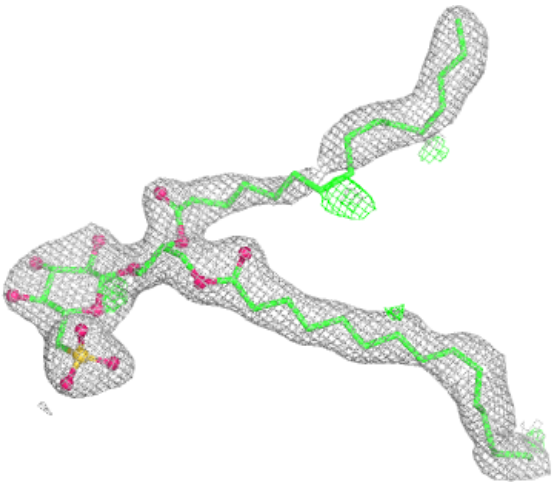
Electron density around HTG b 602:

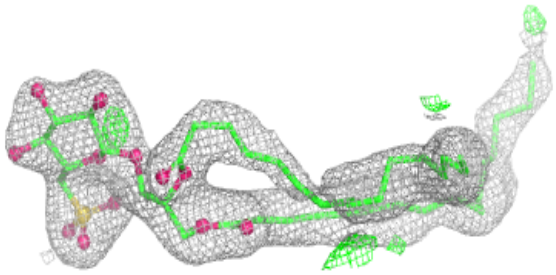
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

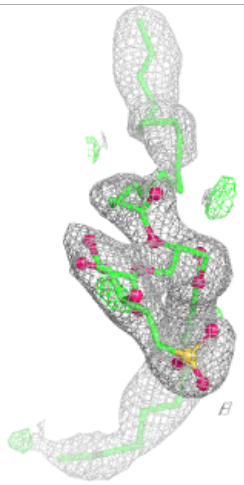


Electron density around SQD a 415:

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

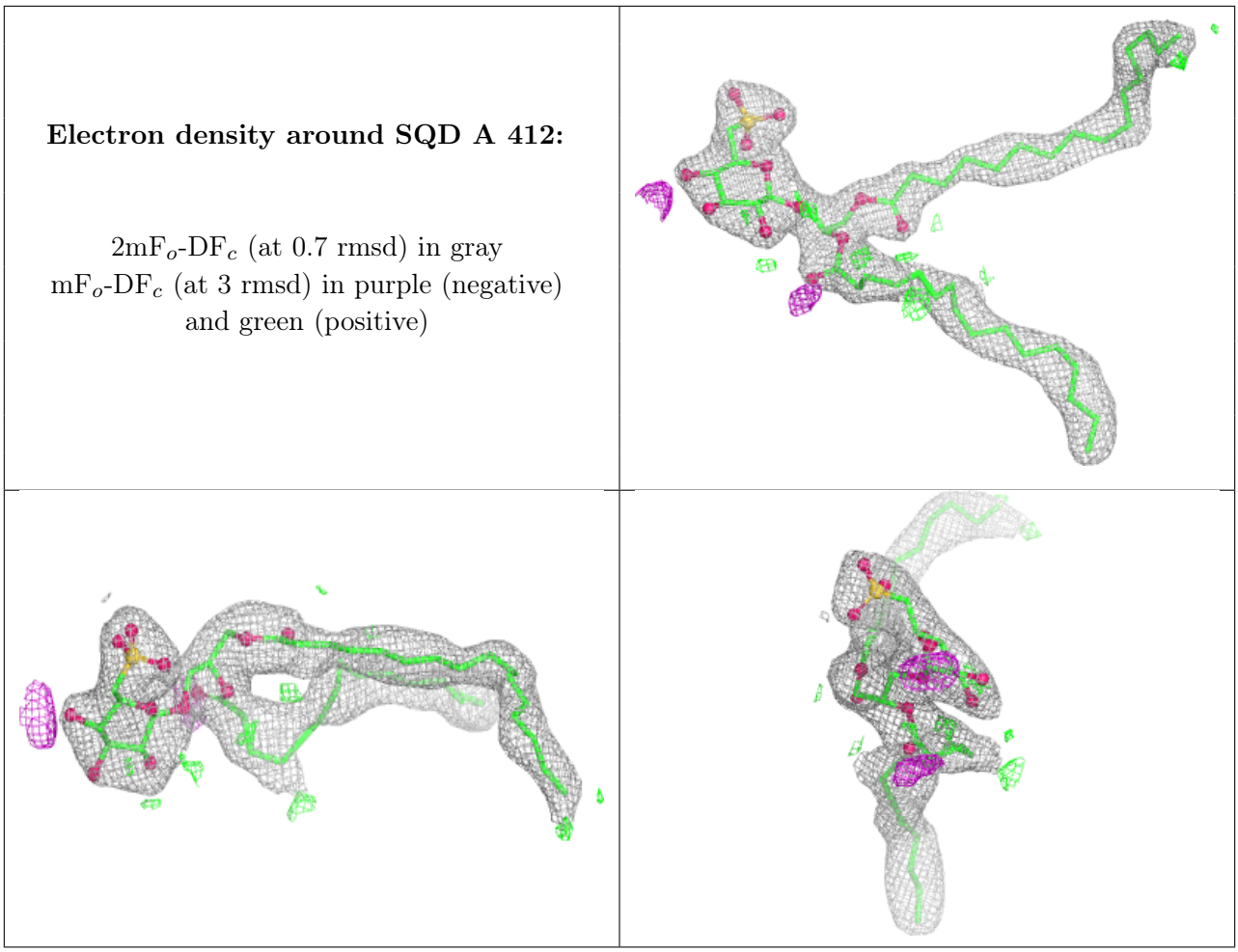






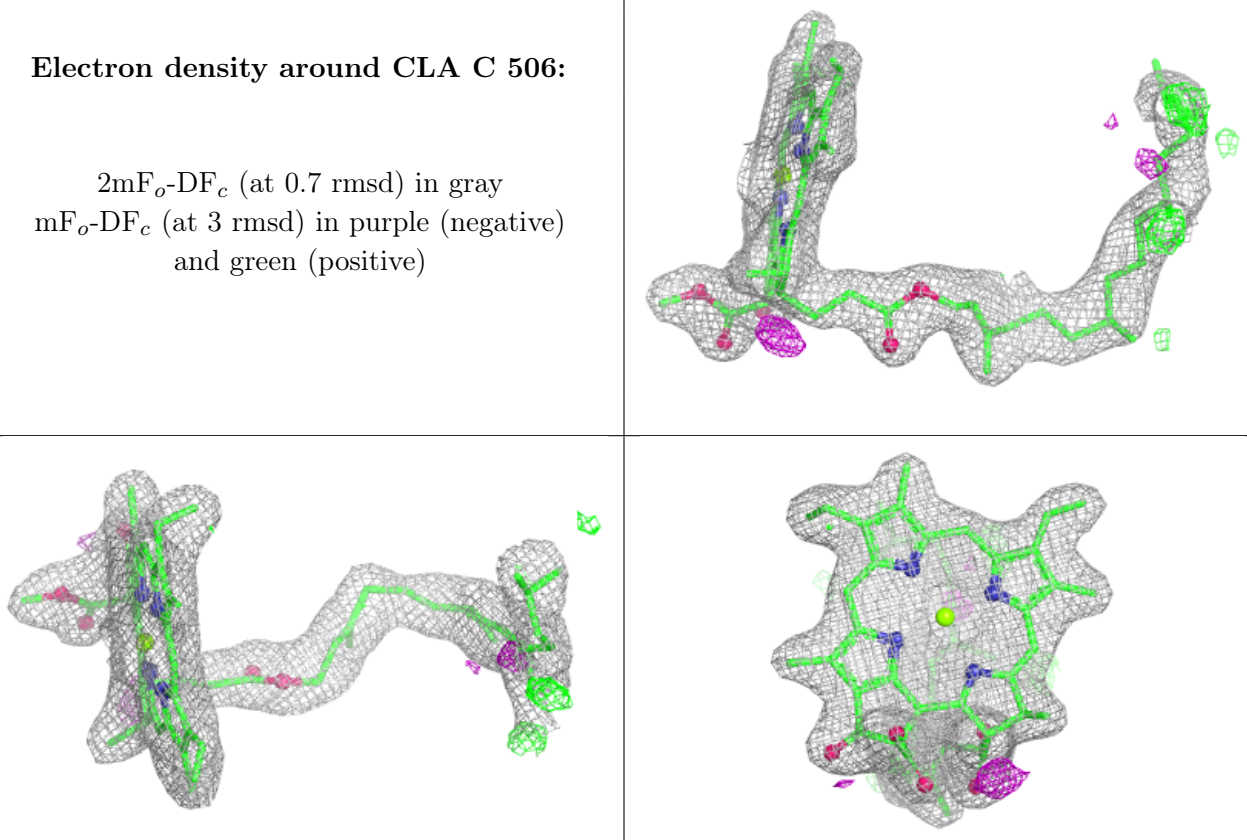
Electron density around SQD A 412:

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



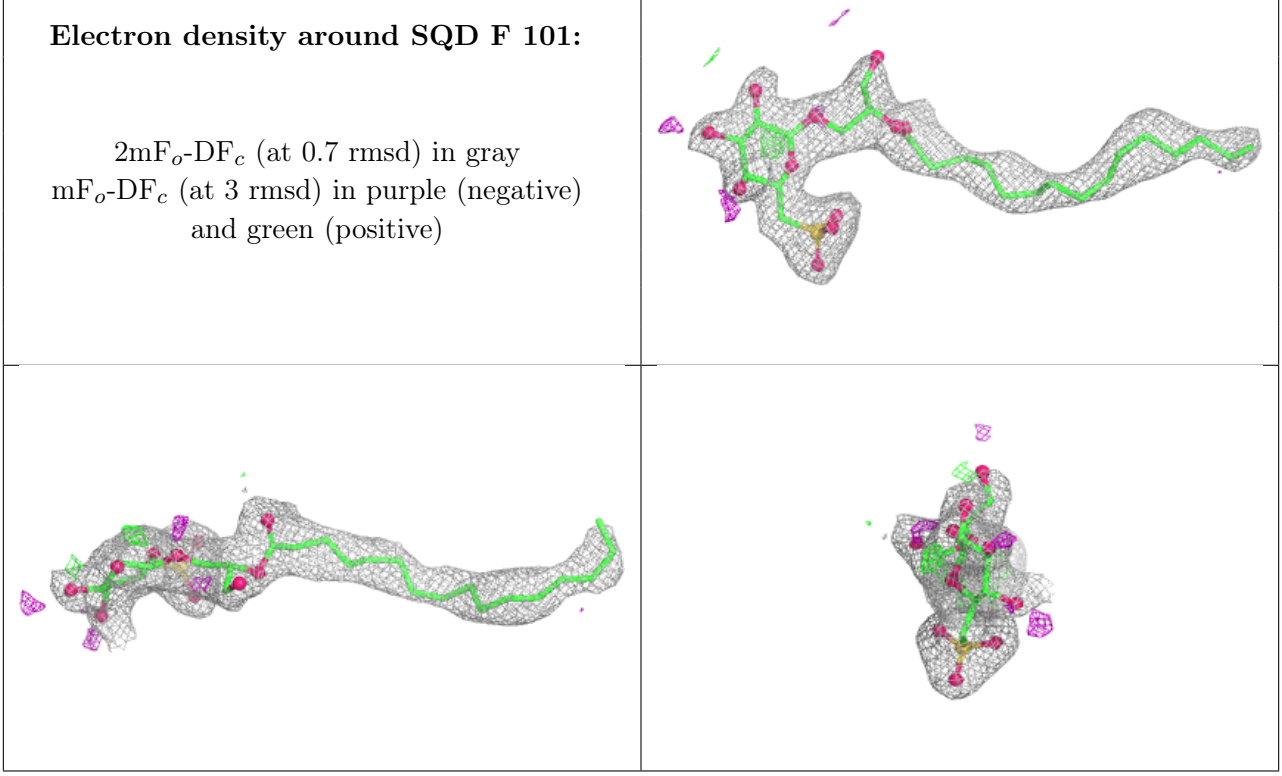
Electron density around CLA C 506:

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



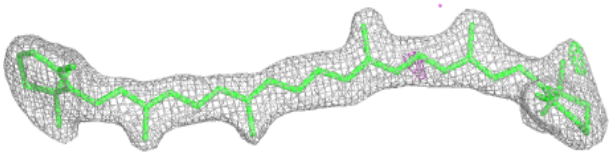
Electron density around SQD F 101:

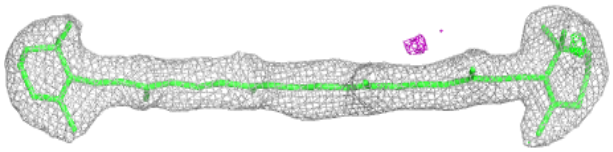
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

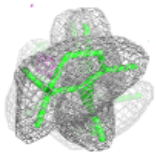


Electron density around BCR c 915:

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

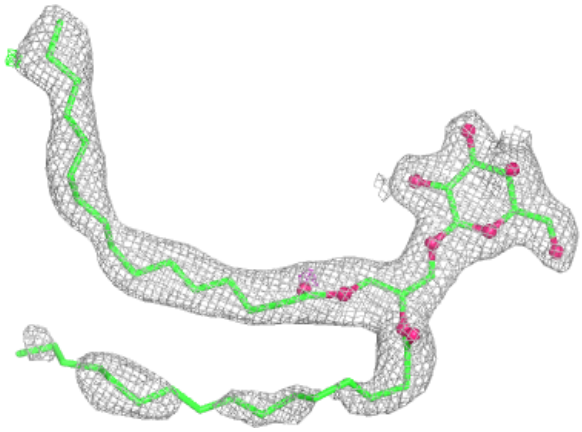


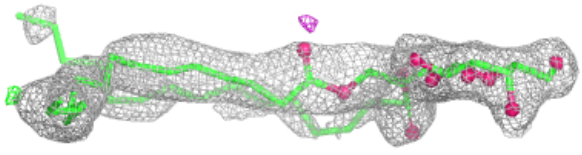




Electron density around LMG c 920:

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

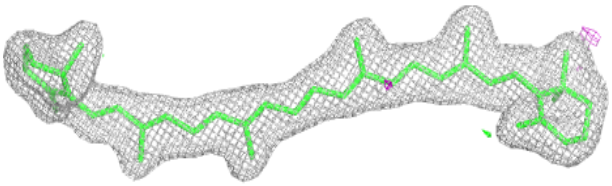


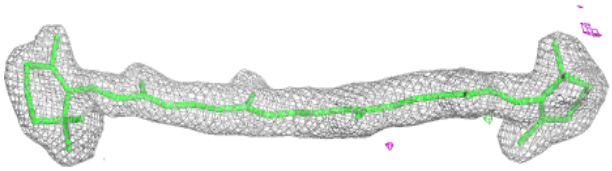


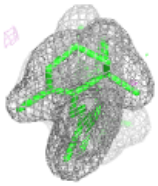


Electron density around BCR Y 101:

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

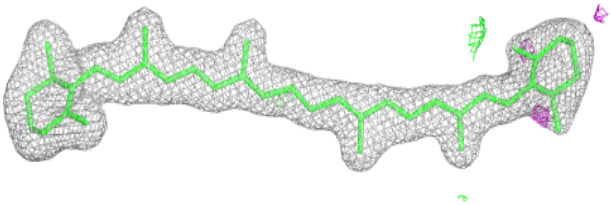


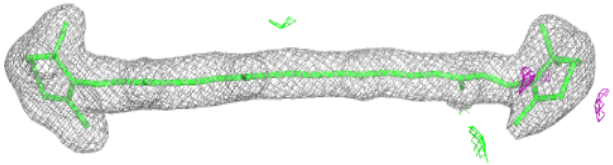


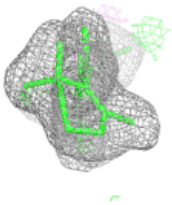


Electron density around BCR b 622:

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

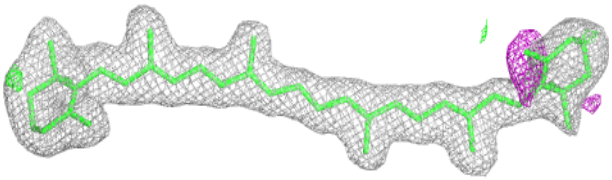


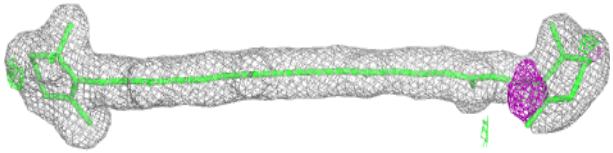


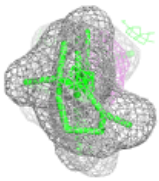


Electron density around BCR B 619:

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

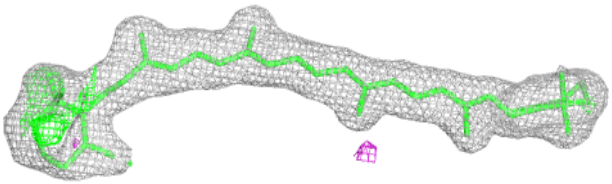


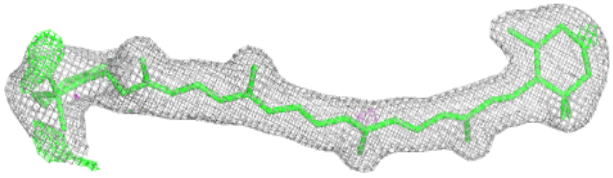


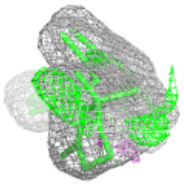


Electron density around BCR d 406:

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

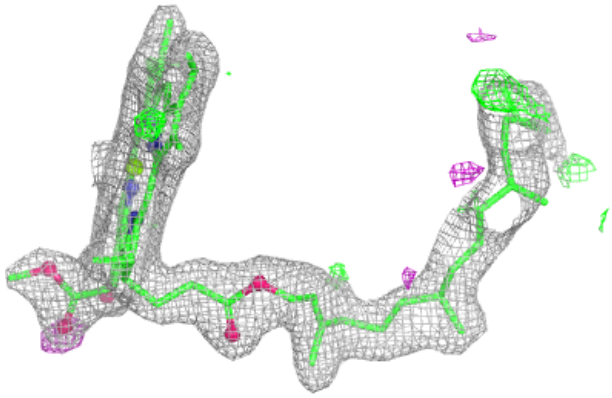


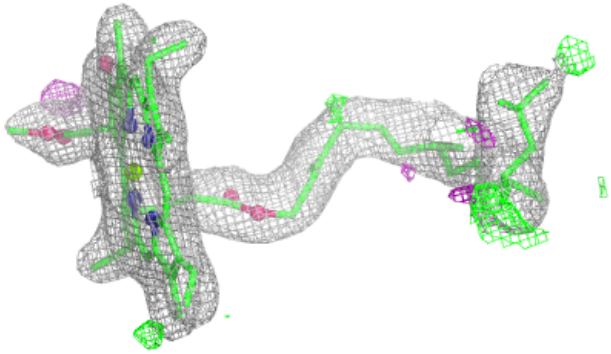


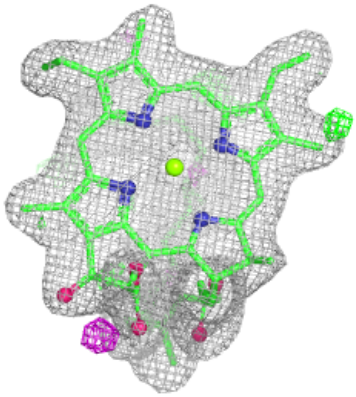


Electron density around CLA c 907:

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

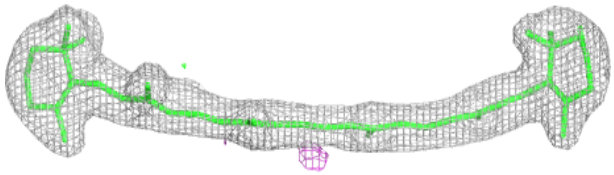


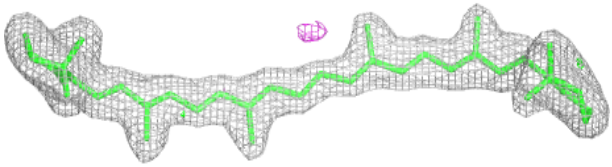


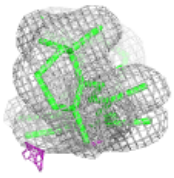


Electron density around BCR K 101:

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

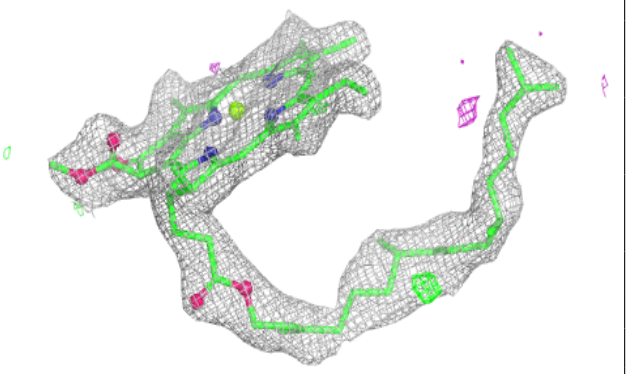


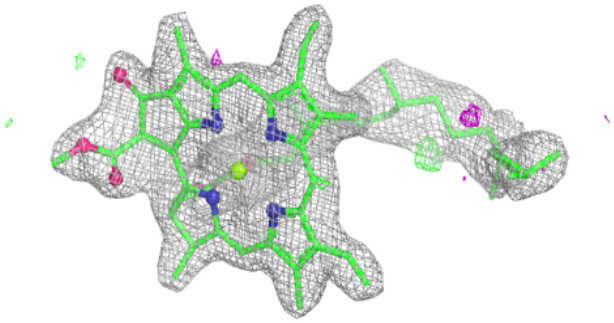


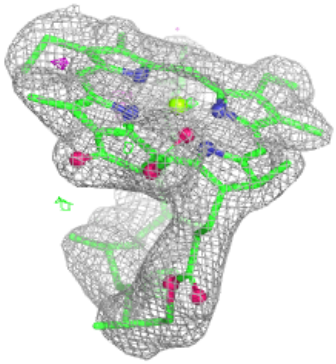


Electron density around CLA c 914:

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

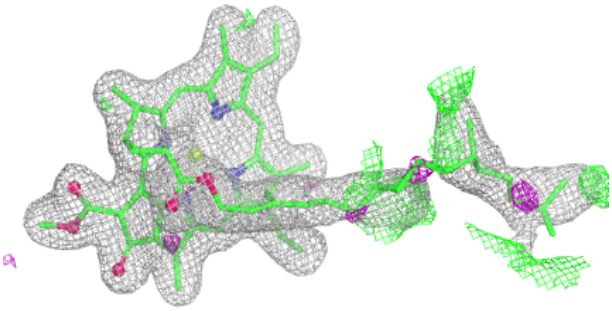


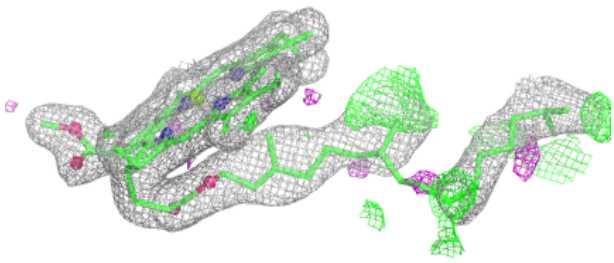


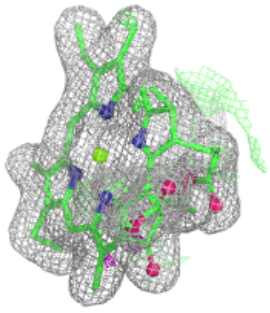


Electron density around CLA b 618:

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

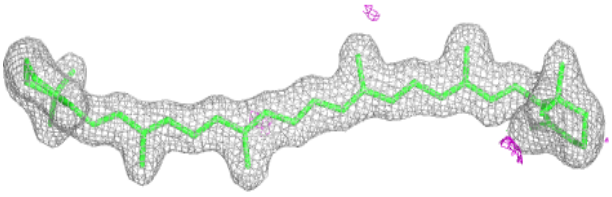


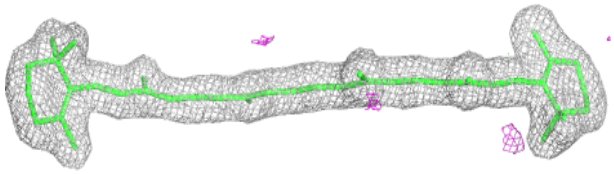


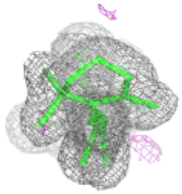


Electron density around BCR a 414:

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

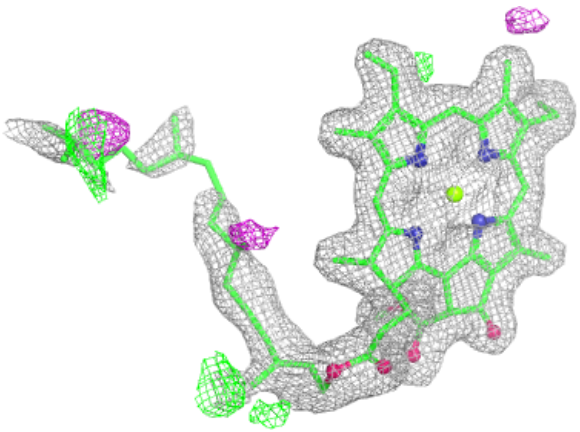


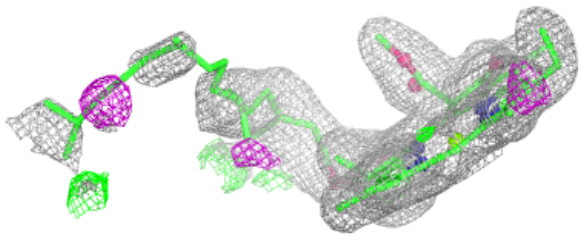


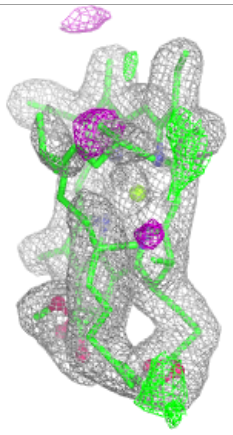


Electron density around CLA B 617:

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

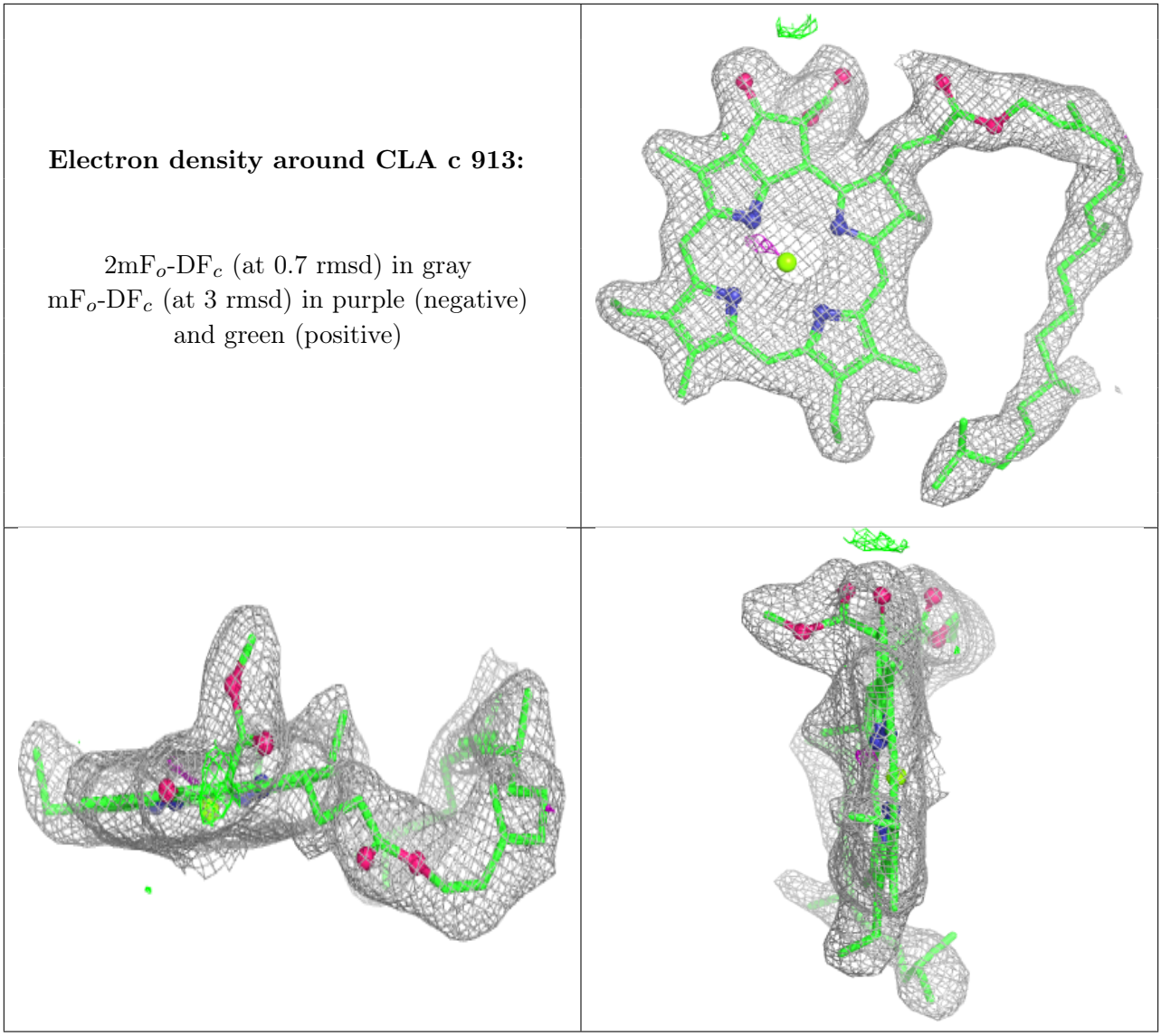






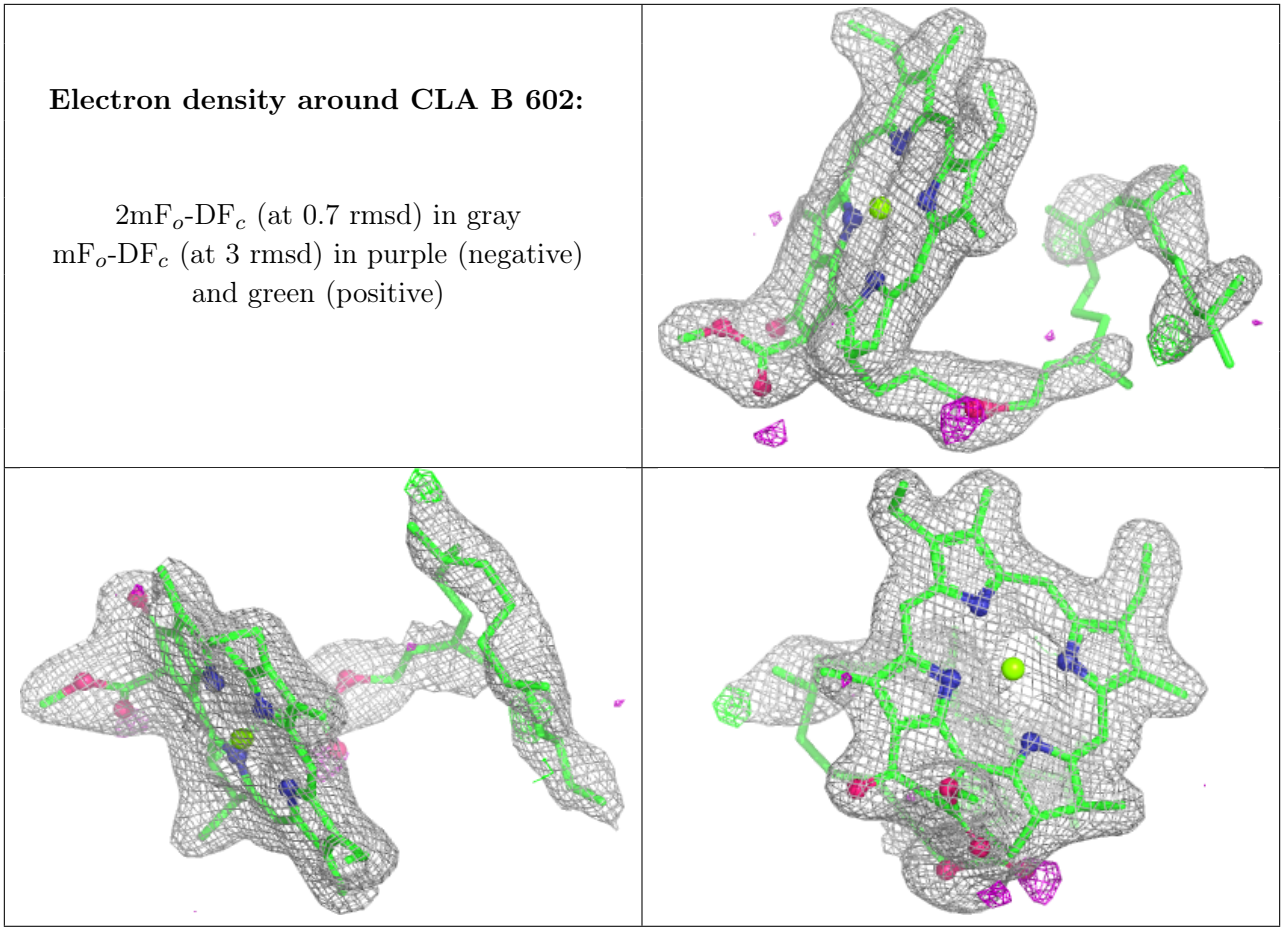
Electron density around CLA c 913:

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



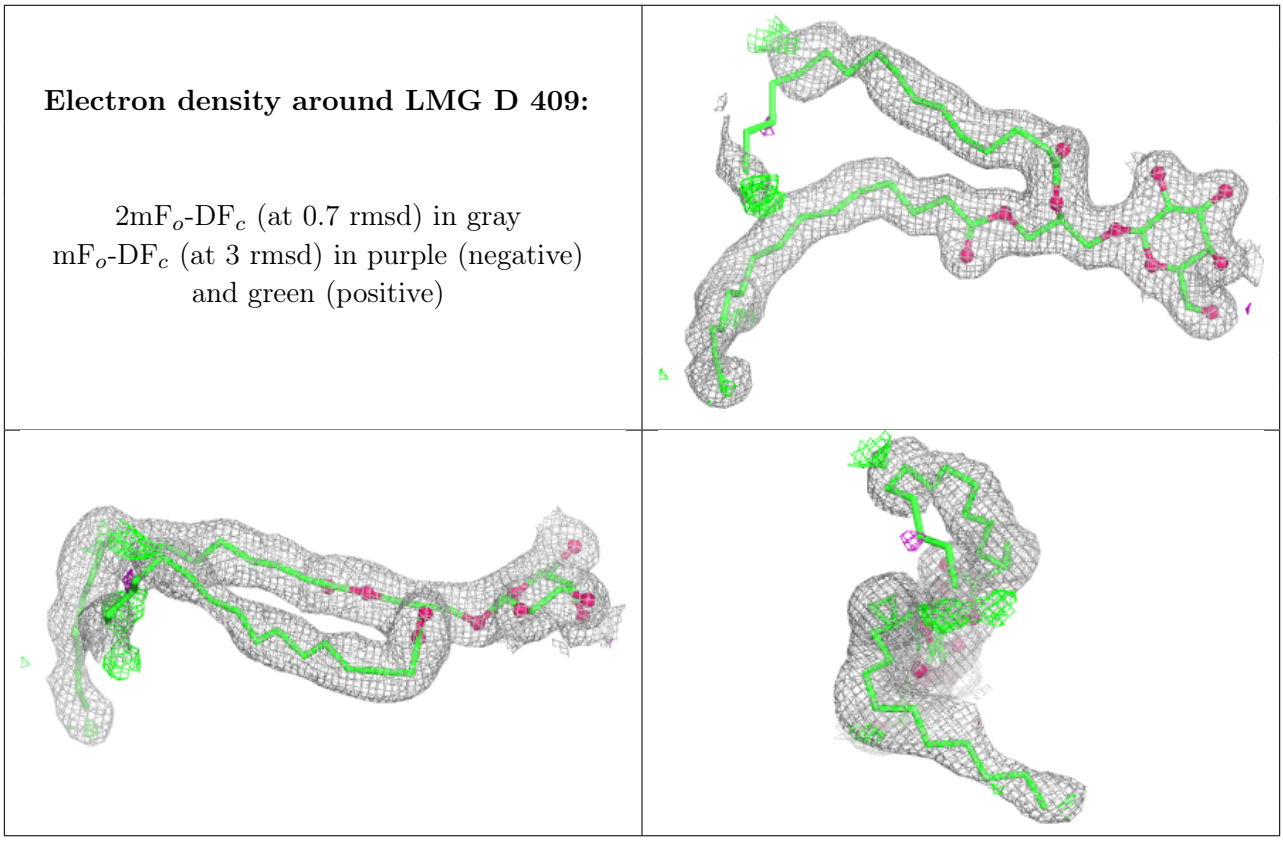
Electron density around CLA B 602:

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



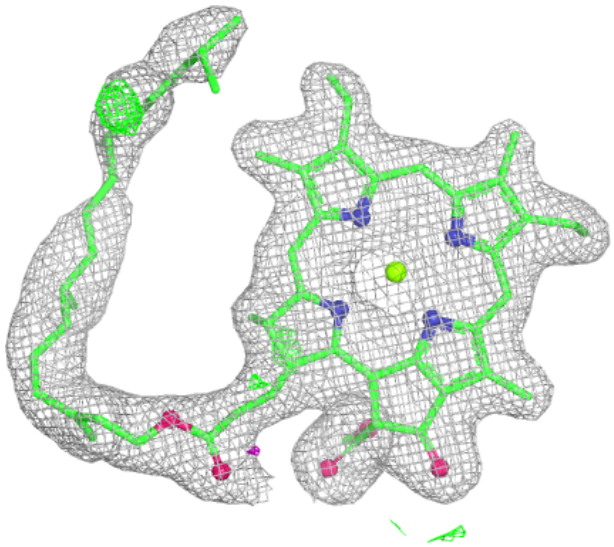
Electron density around LMG D 409:

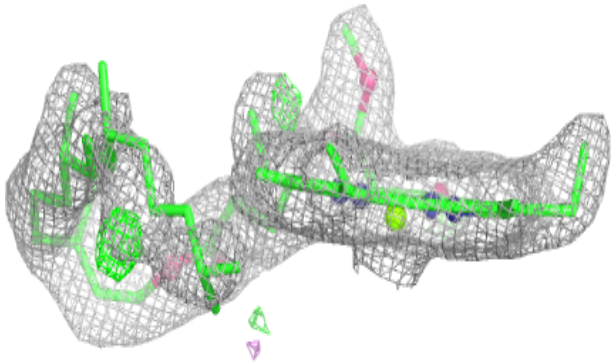
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

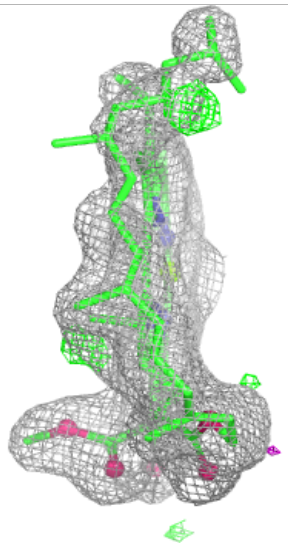


Electron density around CLA C 512:

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

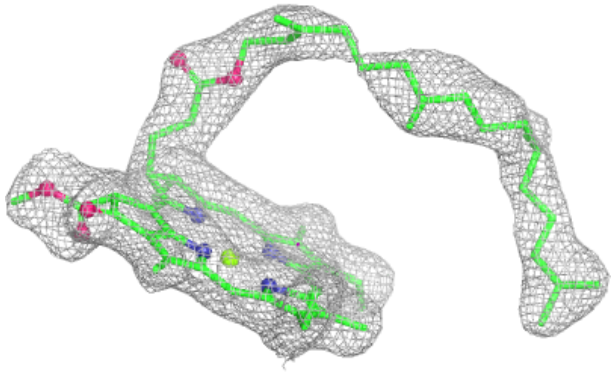


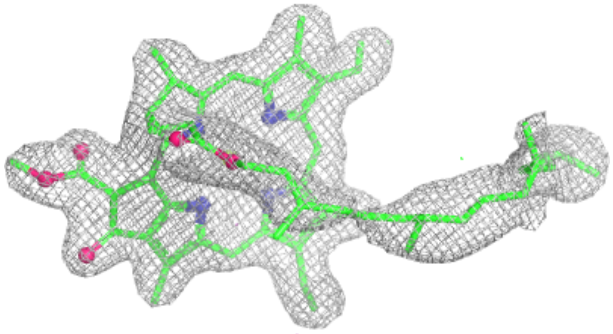


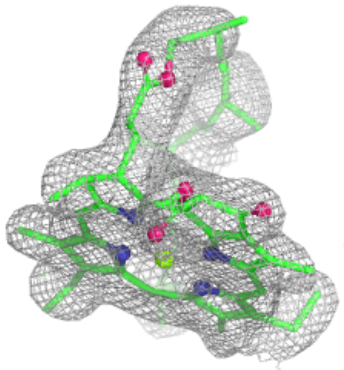


Electron density around CLA C 513:

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

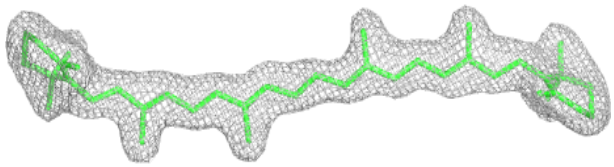


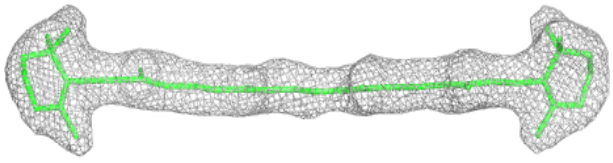


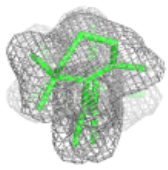


Electron density around BCR C 514:

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

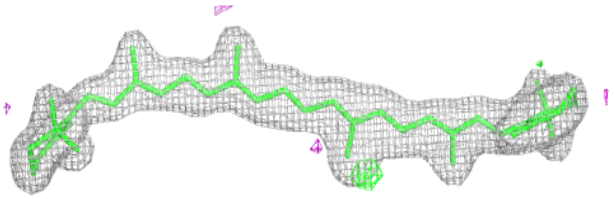


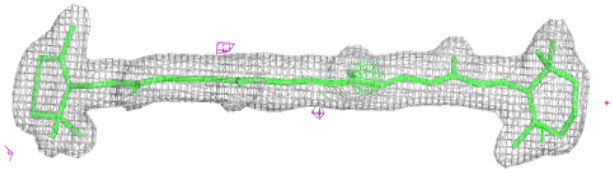


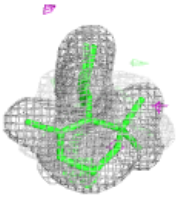


Electron density around BCR C 515:

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

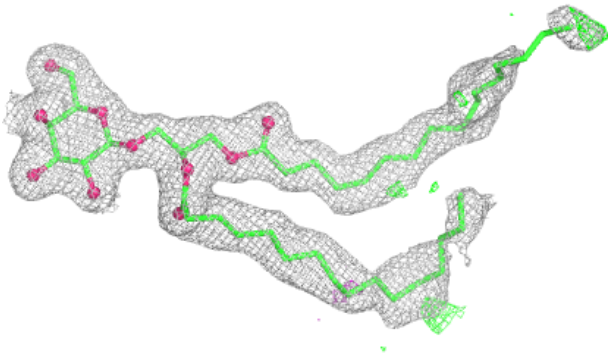


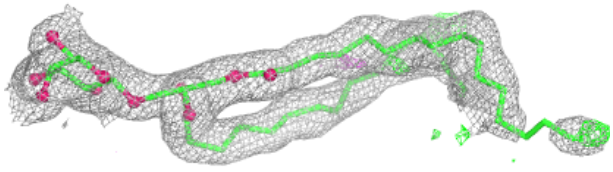


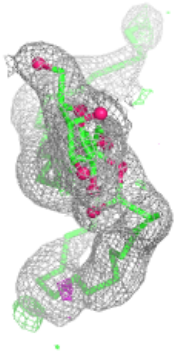


Electron density around LMG d 412:

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

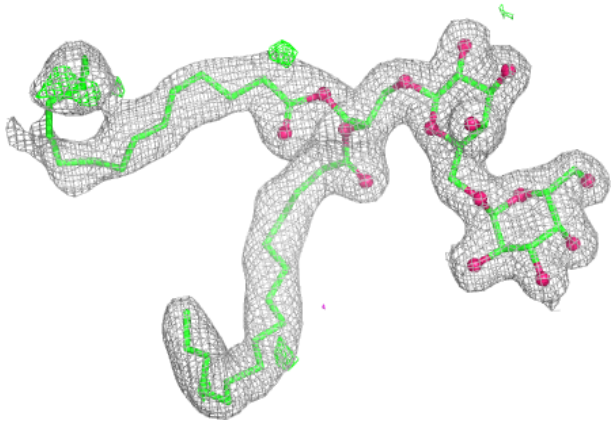


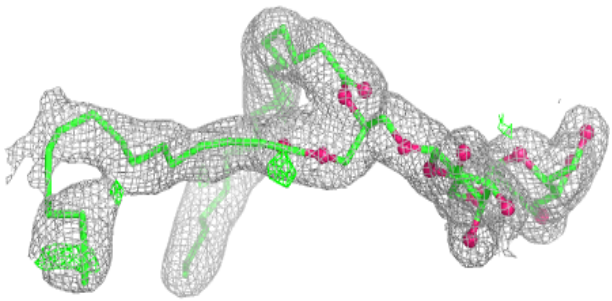




Electron density around DGD C 517:

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

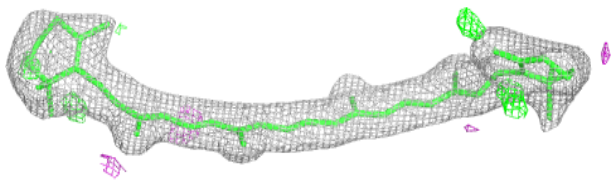


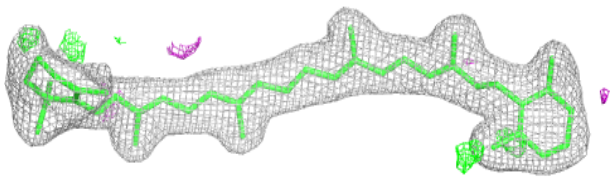


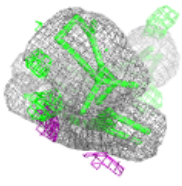


Electron density around BCR D 403:

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

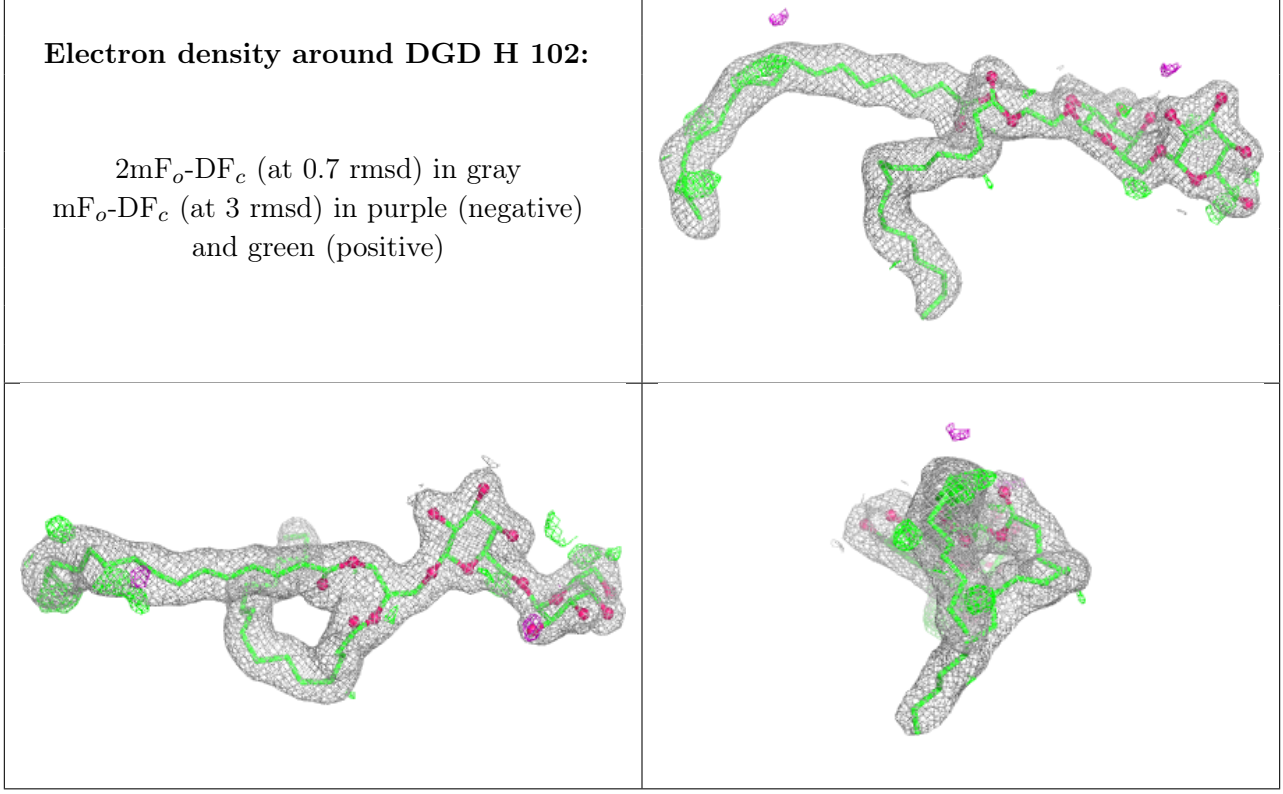






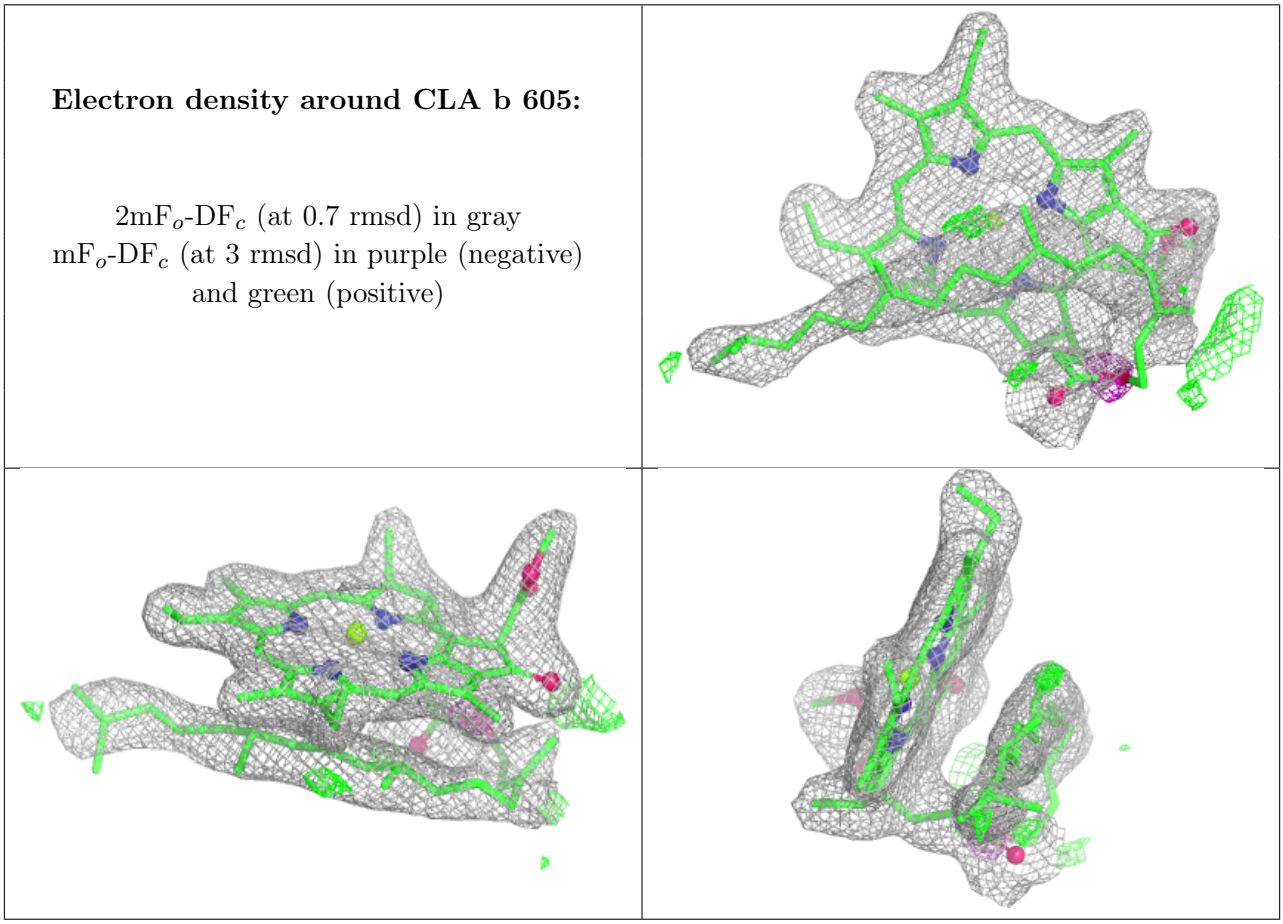
Electron density around DGD H 102:

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



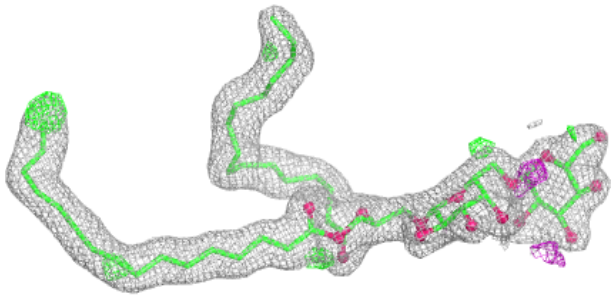
Electron density around CLA b 605:

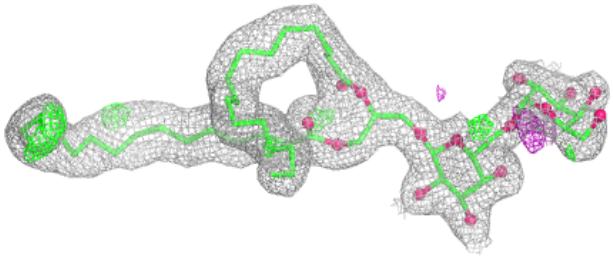
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD h 102:

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

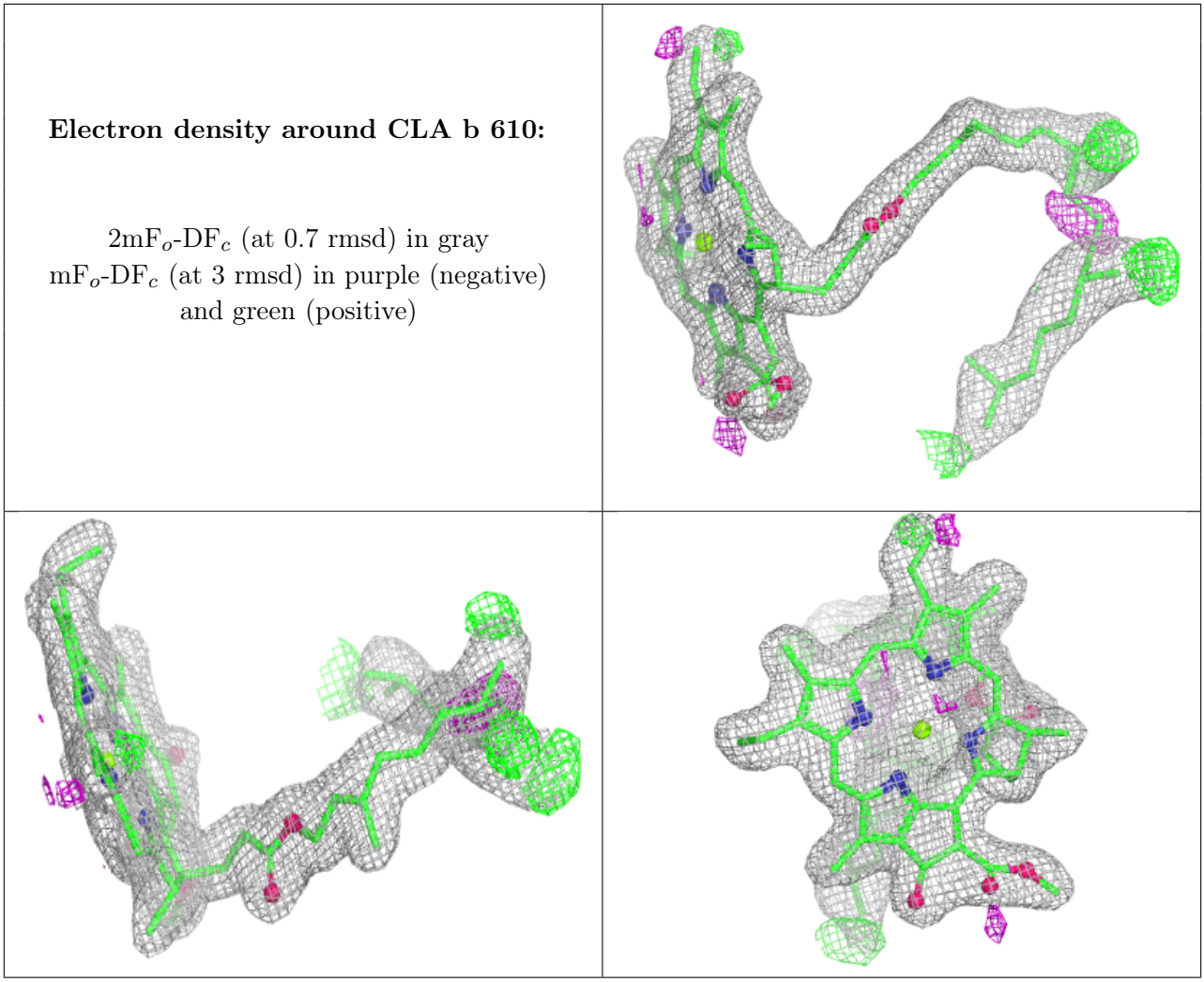






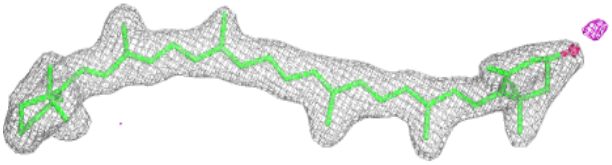
Electron density around CLA b 610:

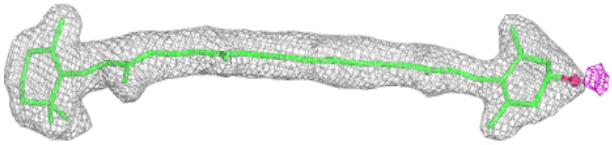
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

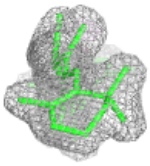


Electron density around RRX h 101:

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

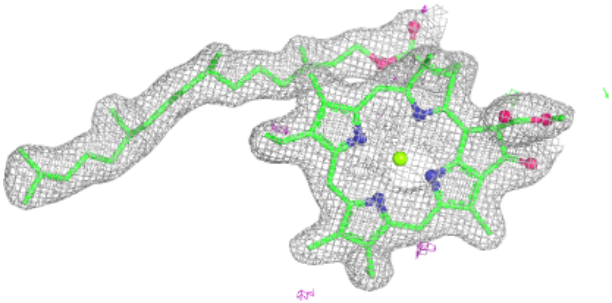


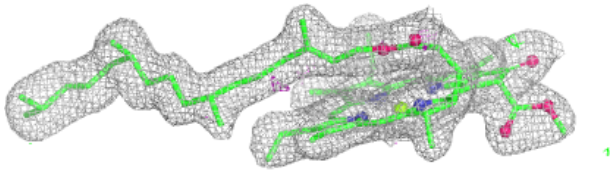


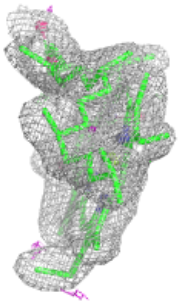


Electron density around CLA c 902:

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

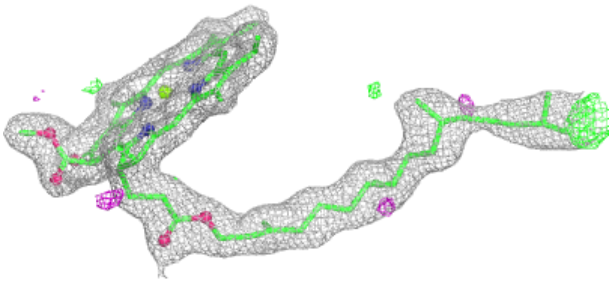


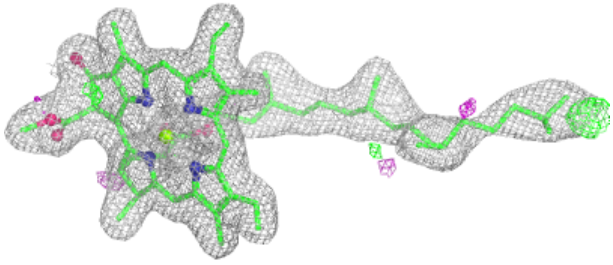


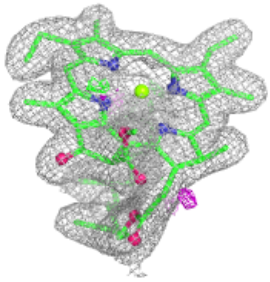


Electron density around CLA c 905:

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

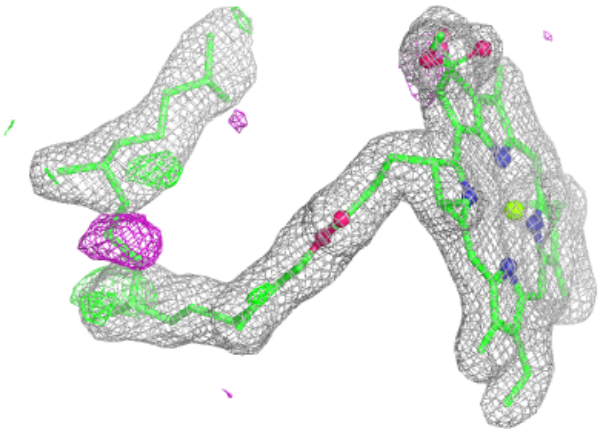


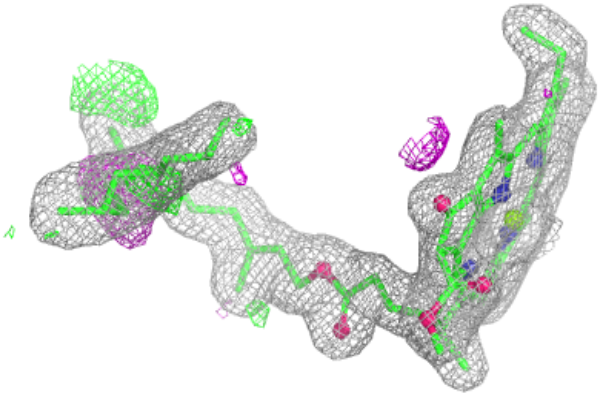


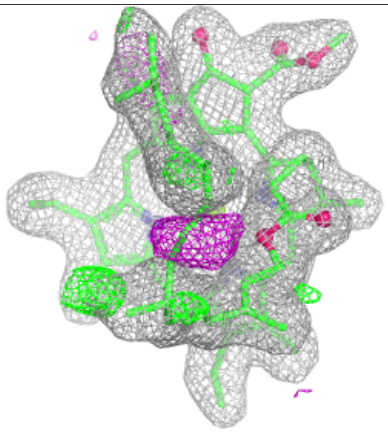


Electron density around CLA B 607:

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

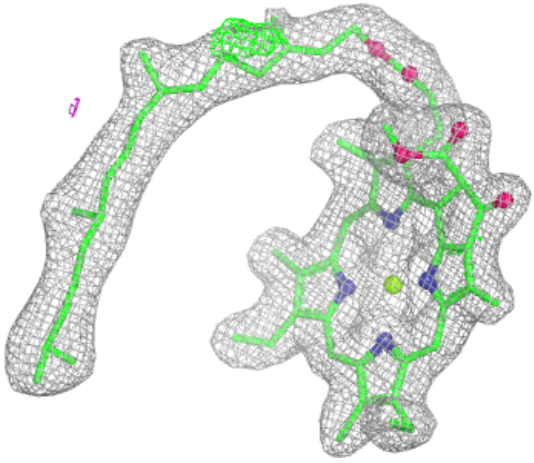


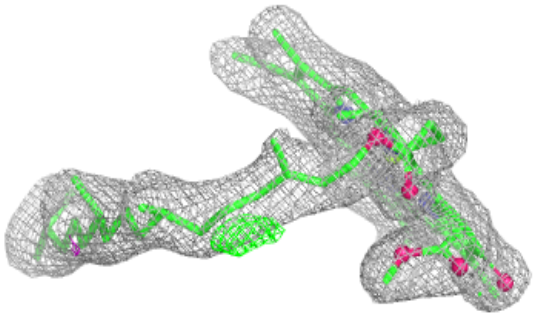


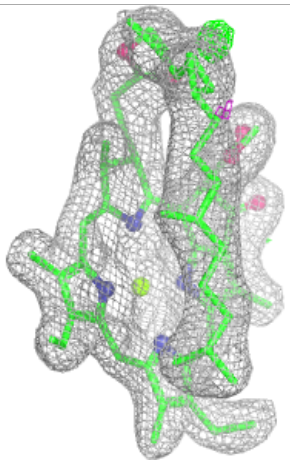


Electron density around CLA c 908:

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

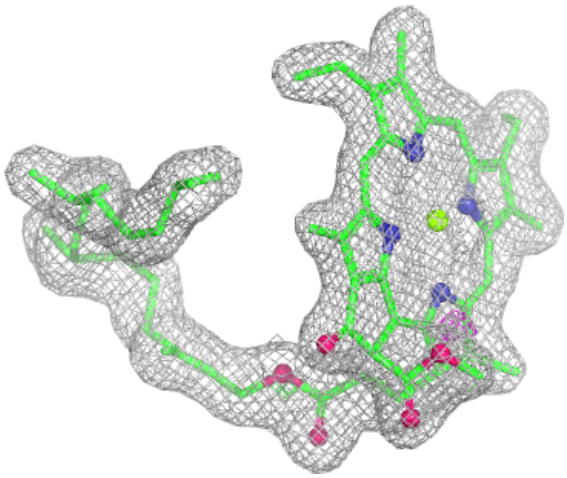


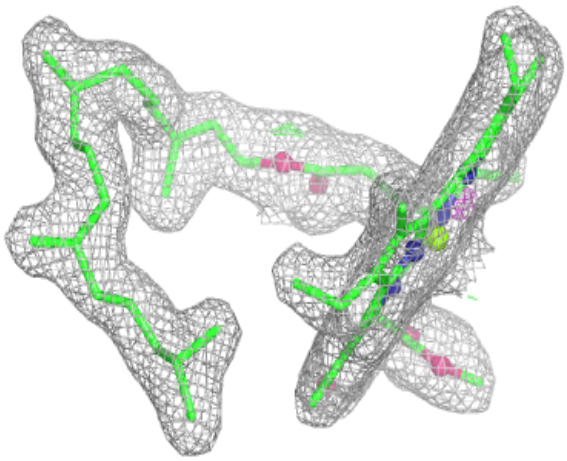


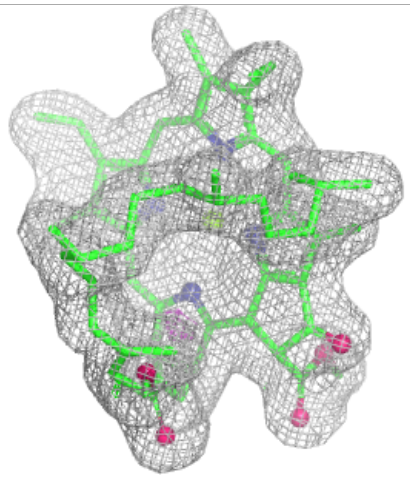


Electron density around CLA C 503:

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

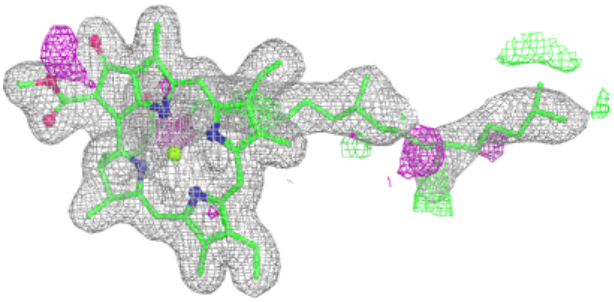


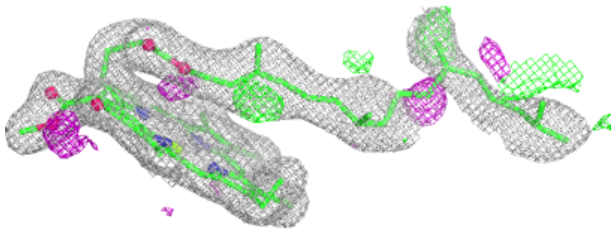


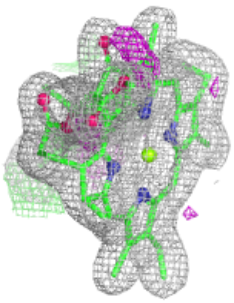


Electron density around CLA B 615:

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

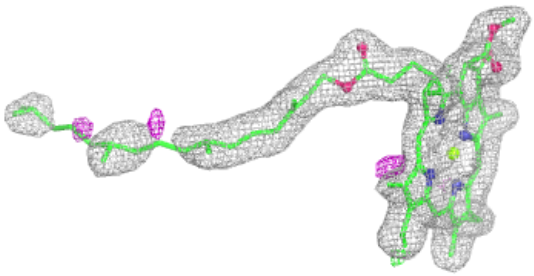


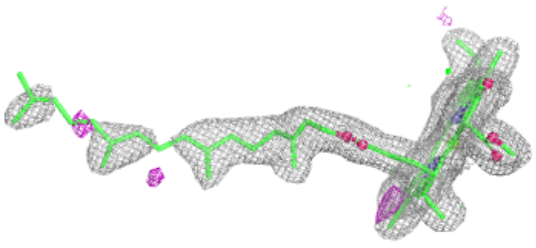


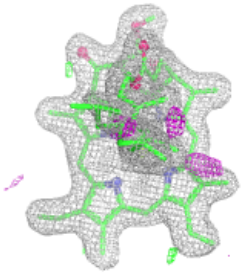


Electron density around CLA d 405:

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

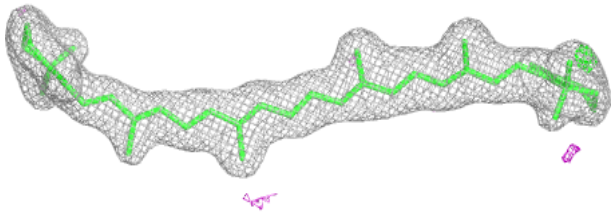


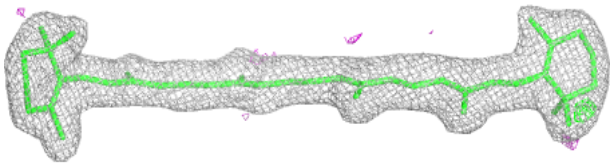




Electron density around BCR c 916:

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

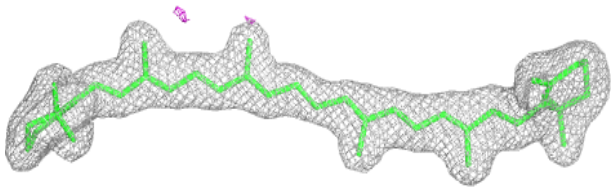


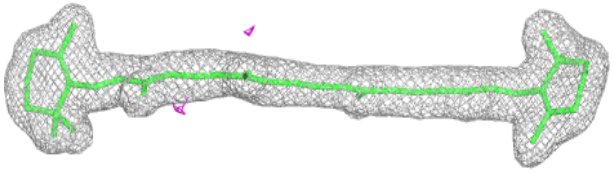


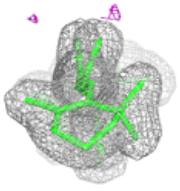


Electron density around BCR A 411:

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

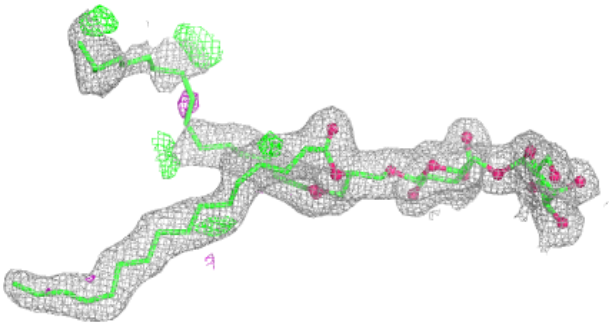


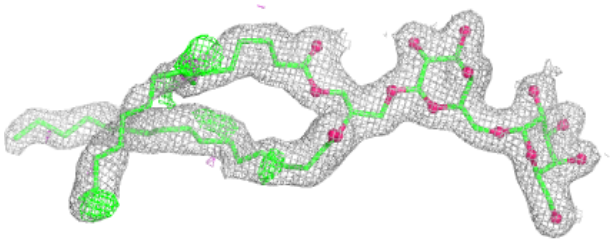


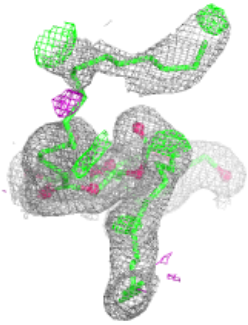


Electron density around DGD C 516:

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

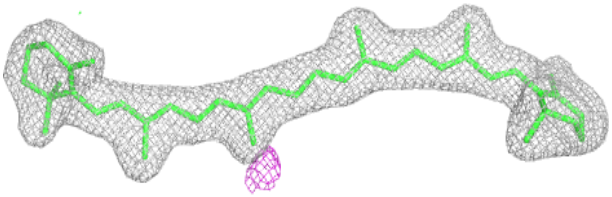


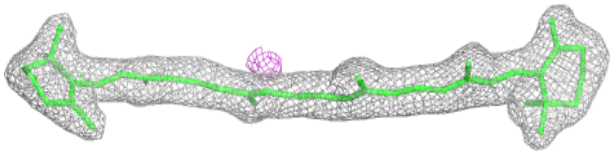


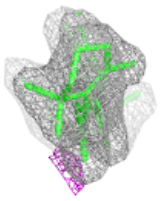


Electron density around BCR k 102:

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

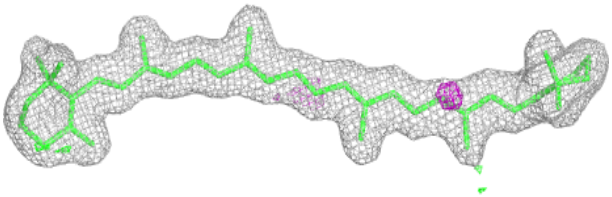


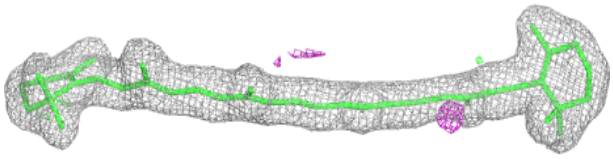


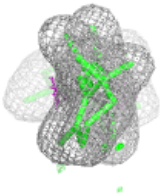


Electron density around BCR B 618:

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

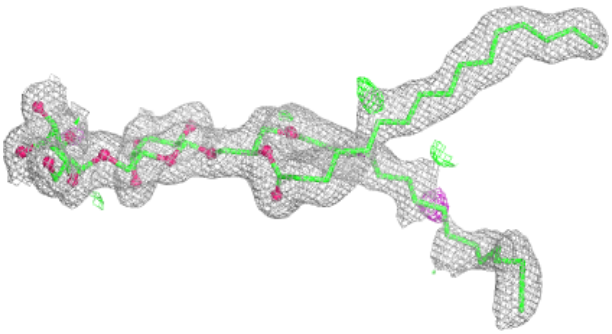


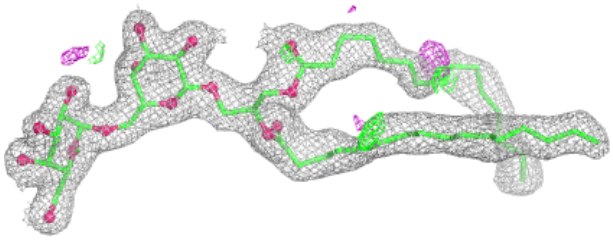


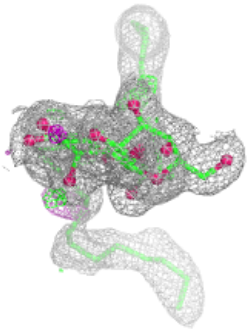


Electron density around DGD c 917:

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

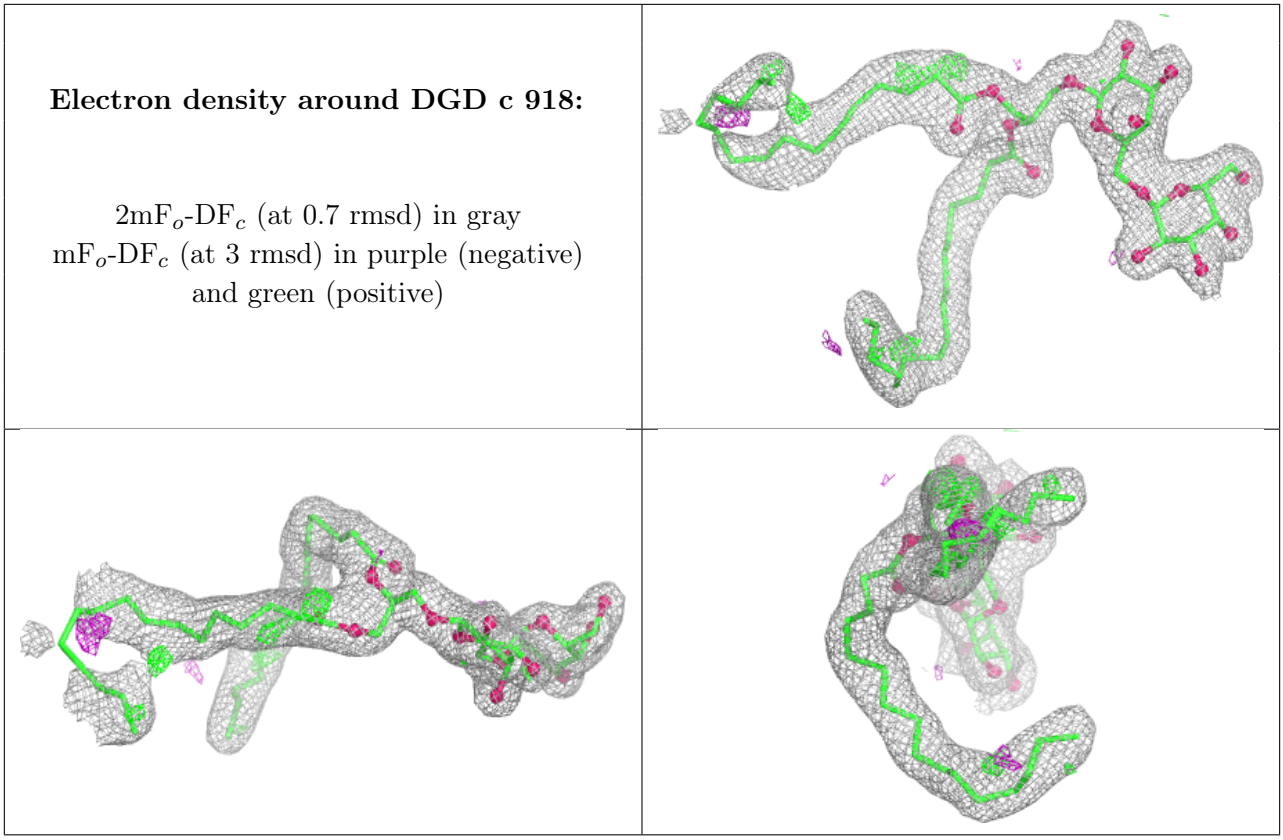






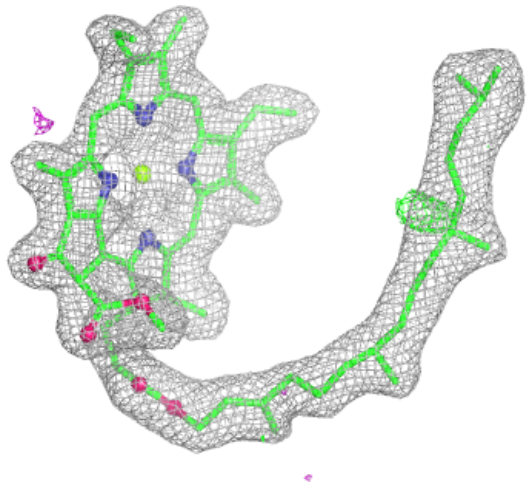
Electron density around DGD c 918:

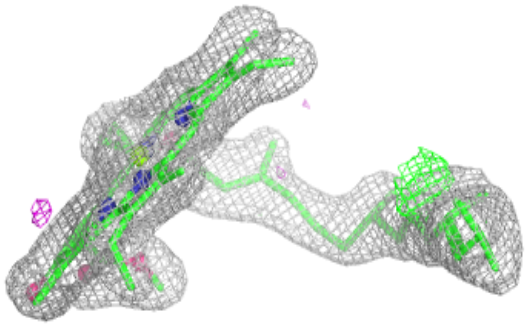
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

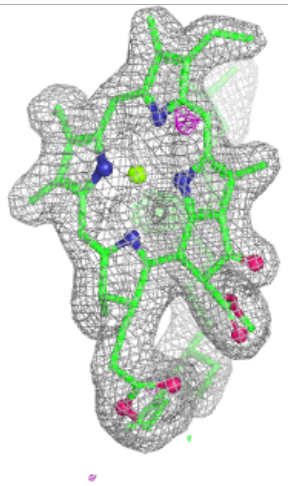


Electron density around CLA C 507:

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

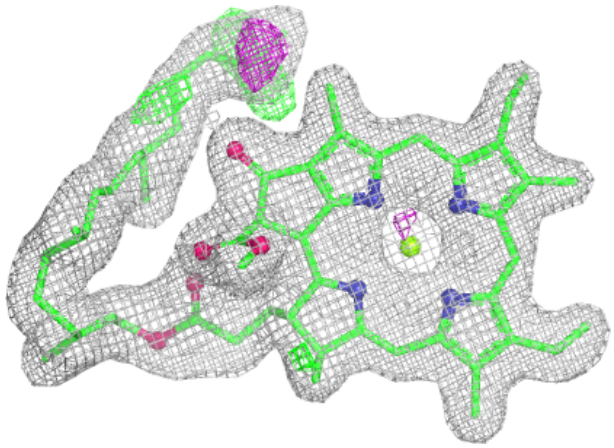


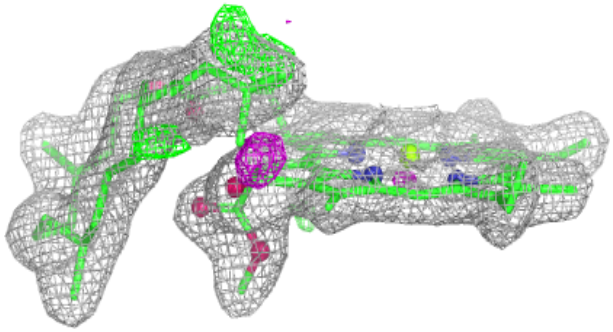


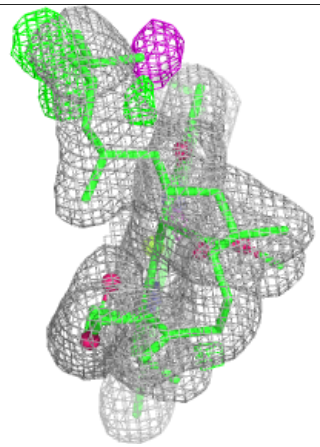


Electron density around CLA b 614:

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

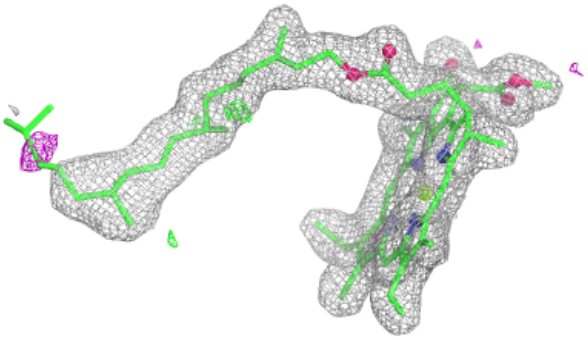


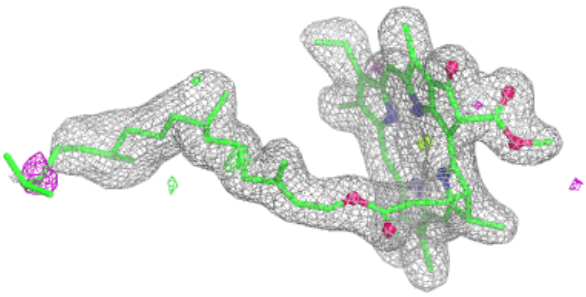


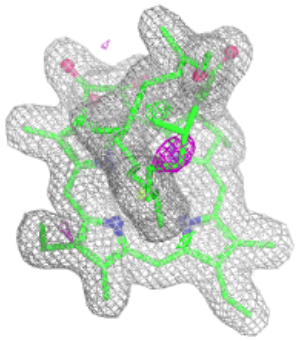


Electron density around CLA C 508:

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

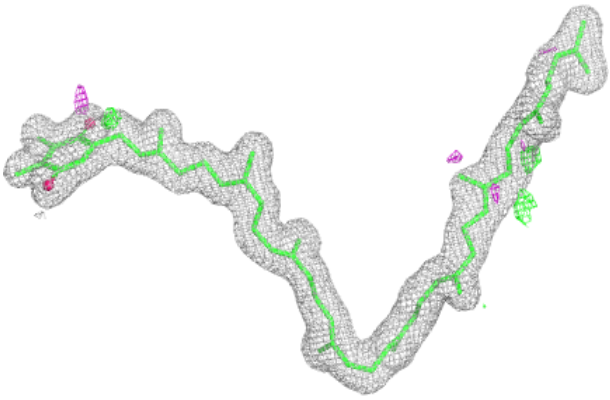


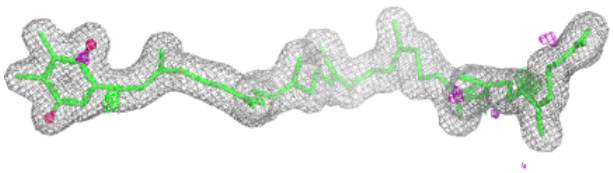


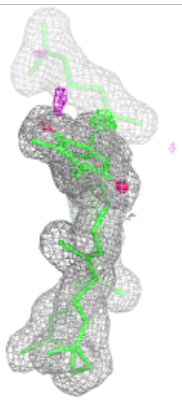


Electron density around PL9 D 404:

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

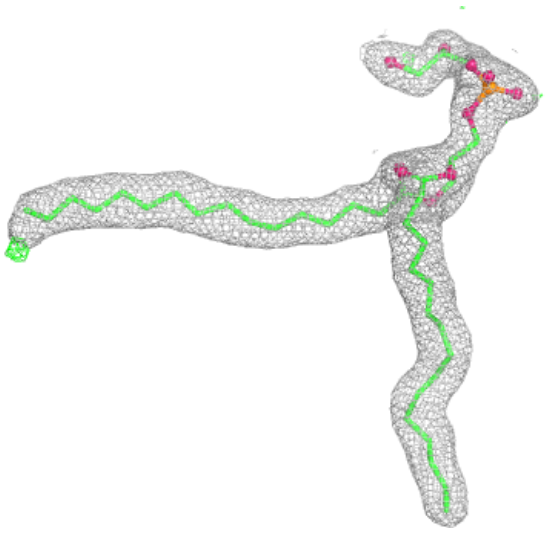


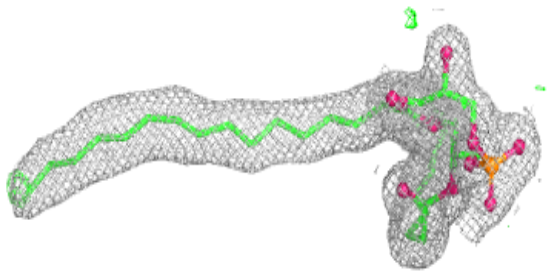


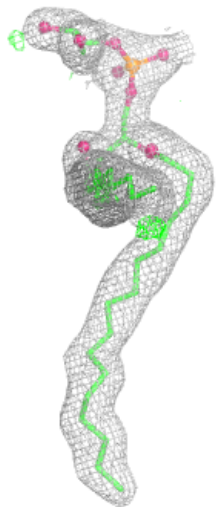


Electron density around LHG L 101:

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

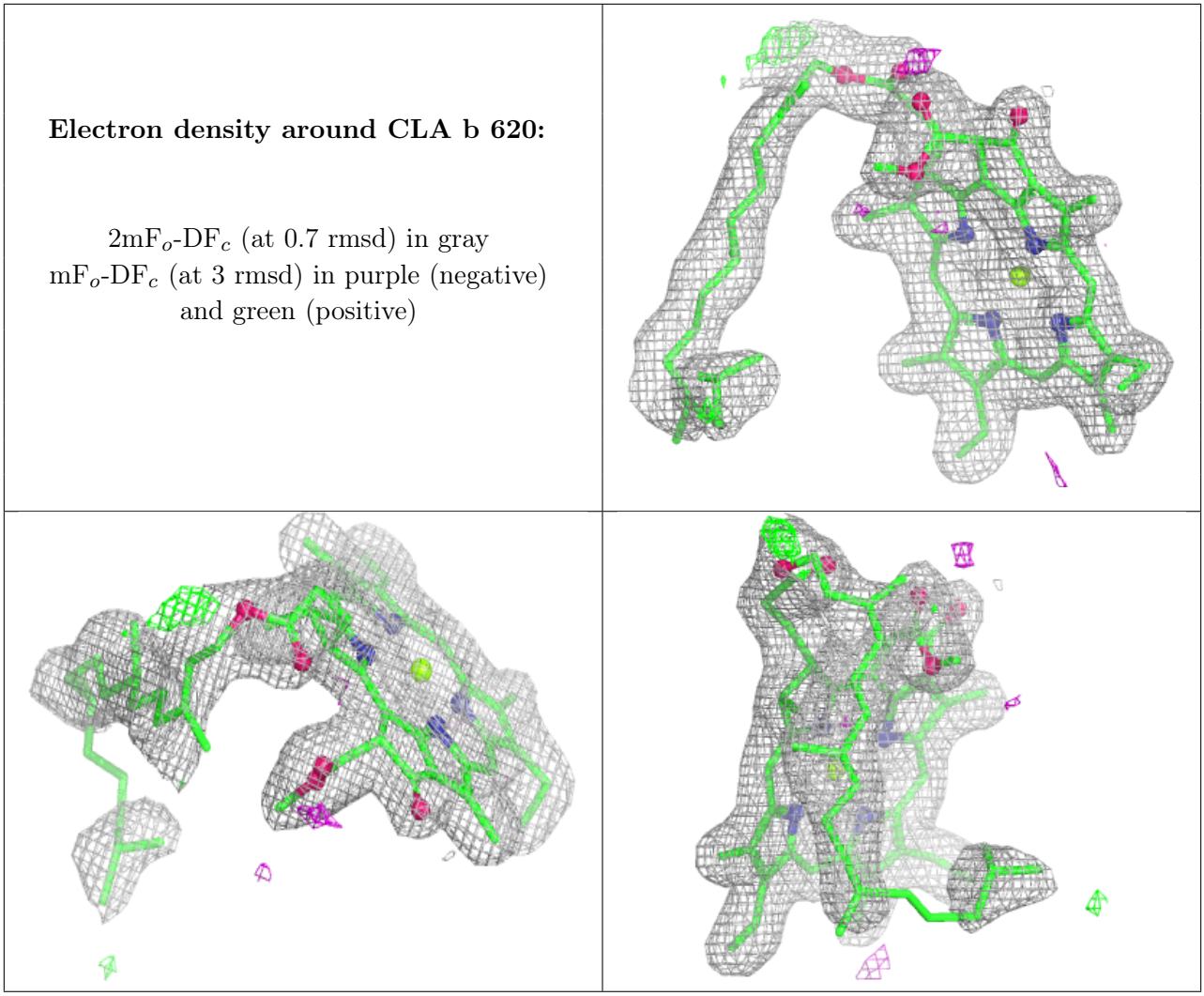






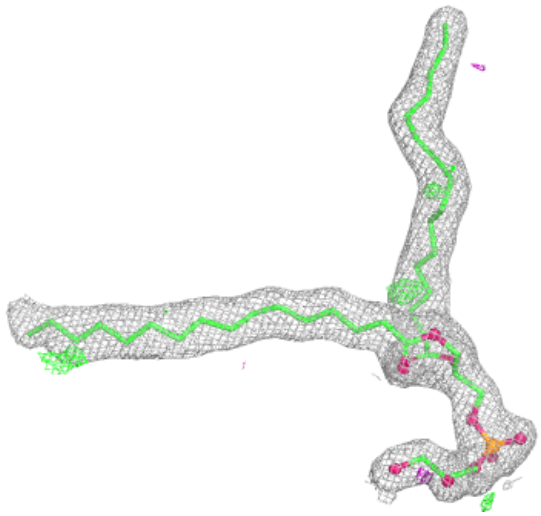
Electron density around CLA b 620:

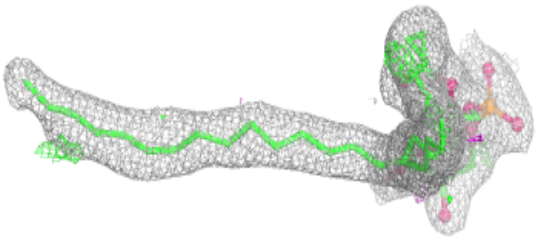
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

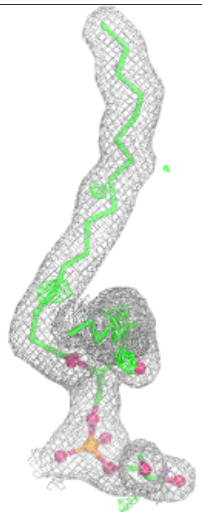


Electron density around LHG l 103:

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

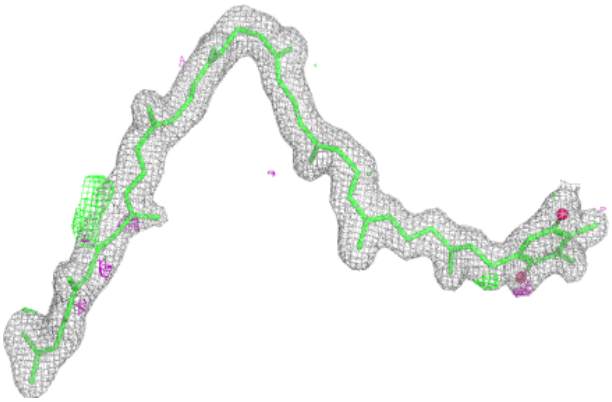


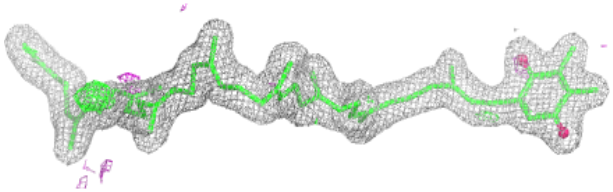


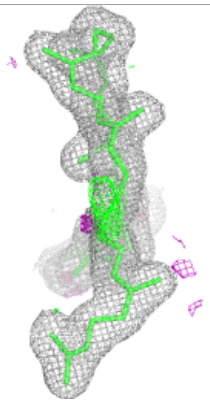


Electron density around PL9 d 407:

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

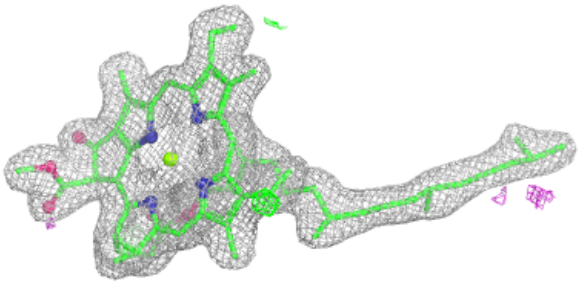


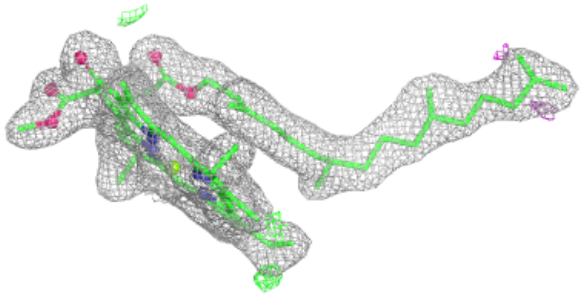


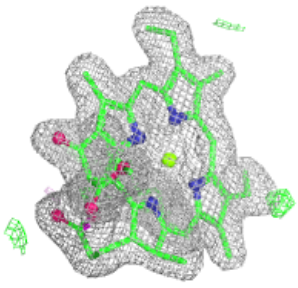


Electron density around CLA C 505:

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

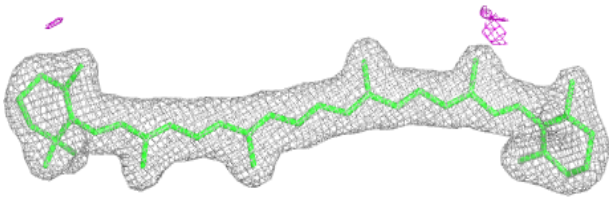


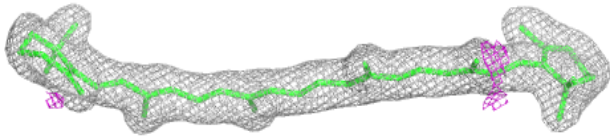


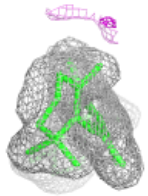


Electron density around BCR b 623:

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

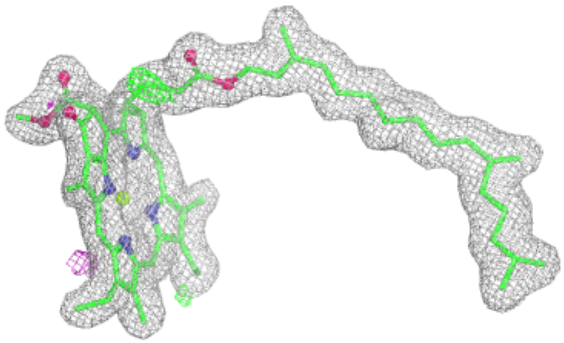


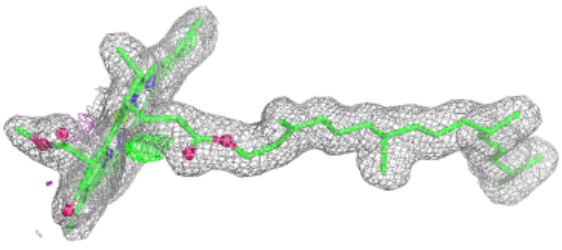


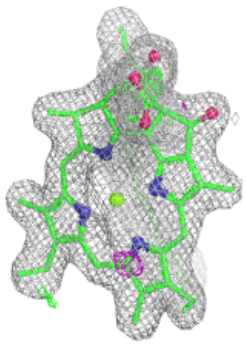


Electron density around CLA B 610:

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

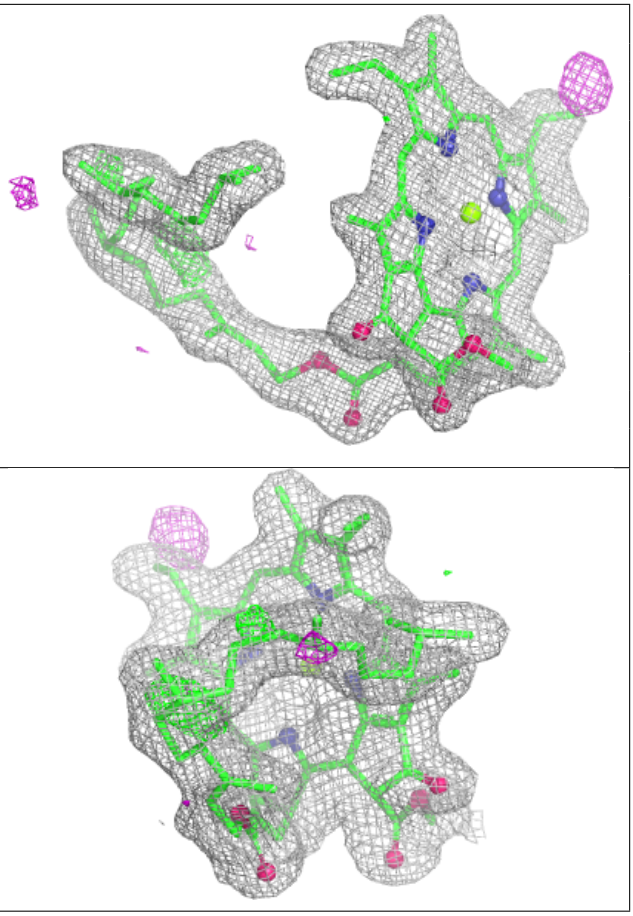






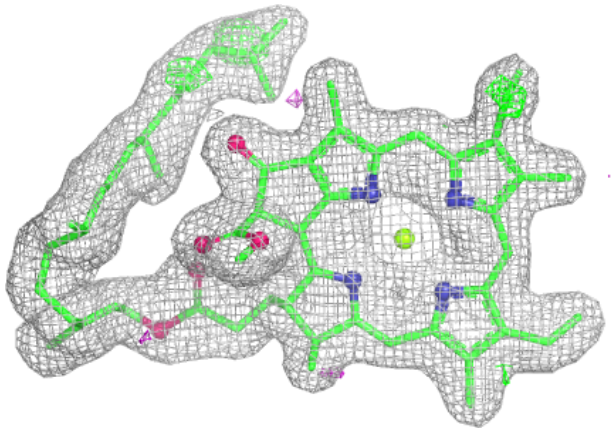
Electron density around CLA c 904:

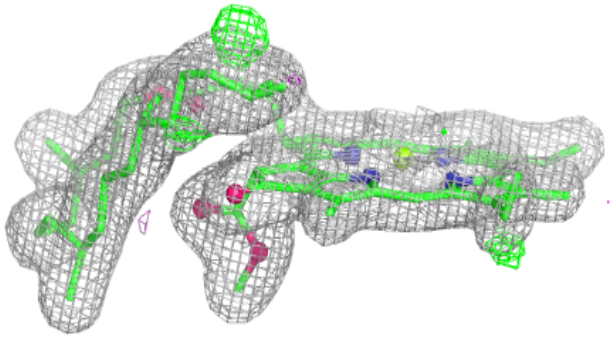
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

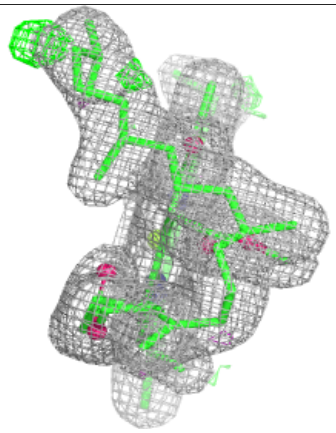


Electron density around CLA B 611:

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

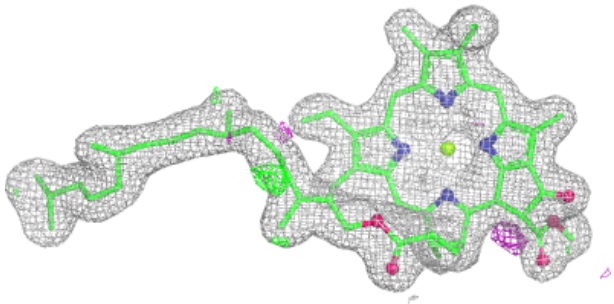


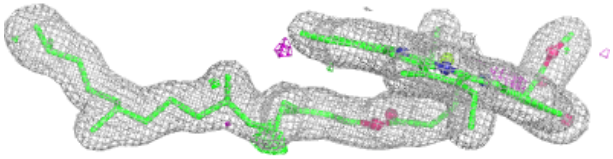


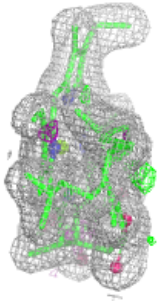


Electron density around CLA B 604:

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

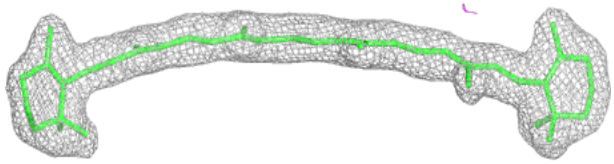


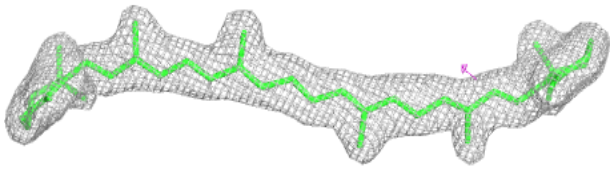


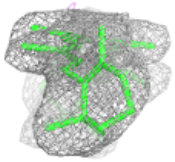


Electron density around BCR k 103:

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

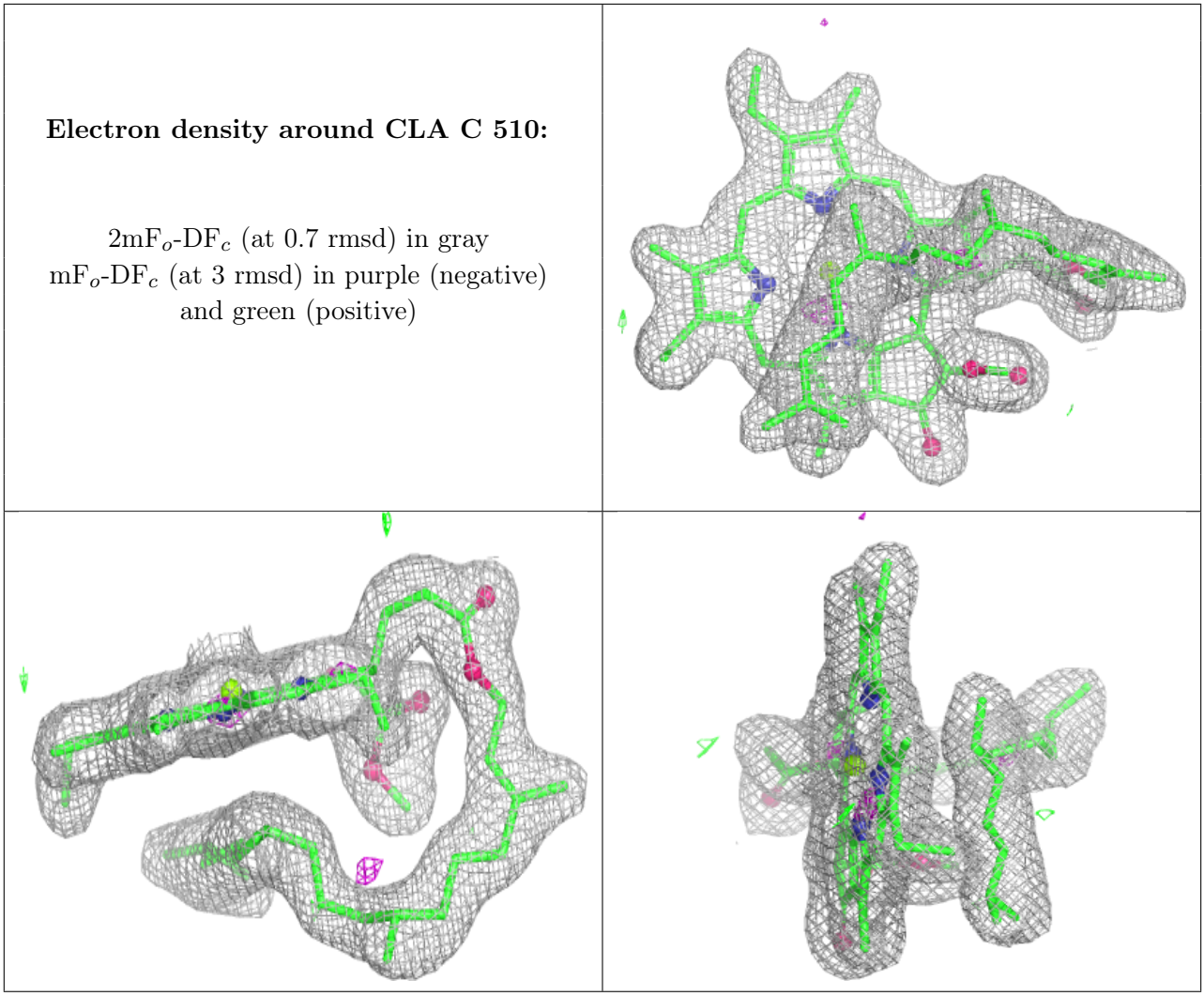






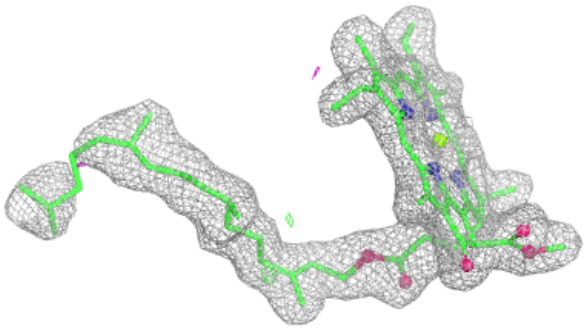
Electron density around CLA C 510:

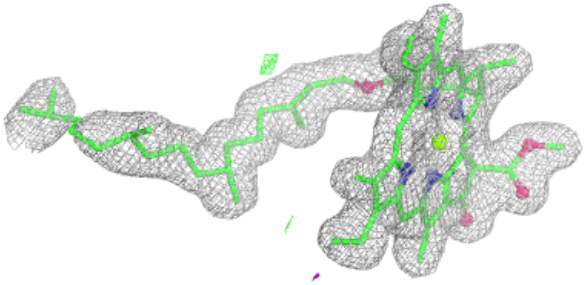
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

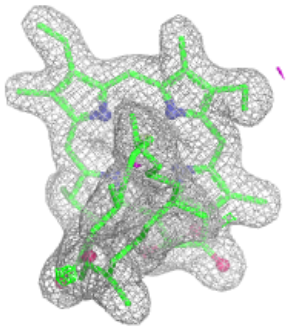


Electron density around CLA c 909:

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

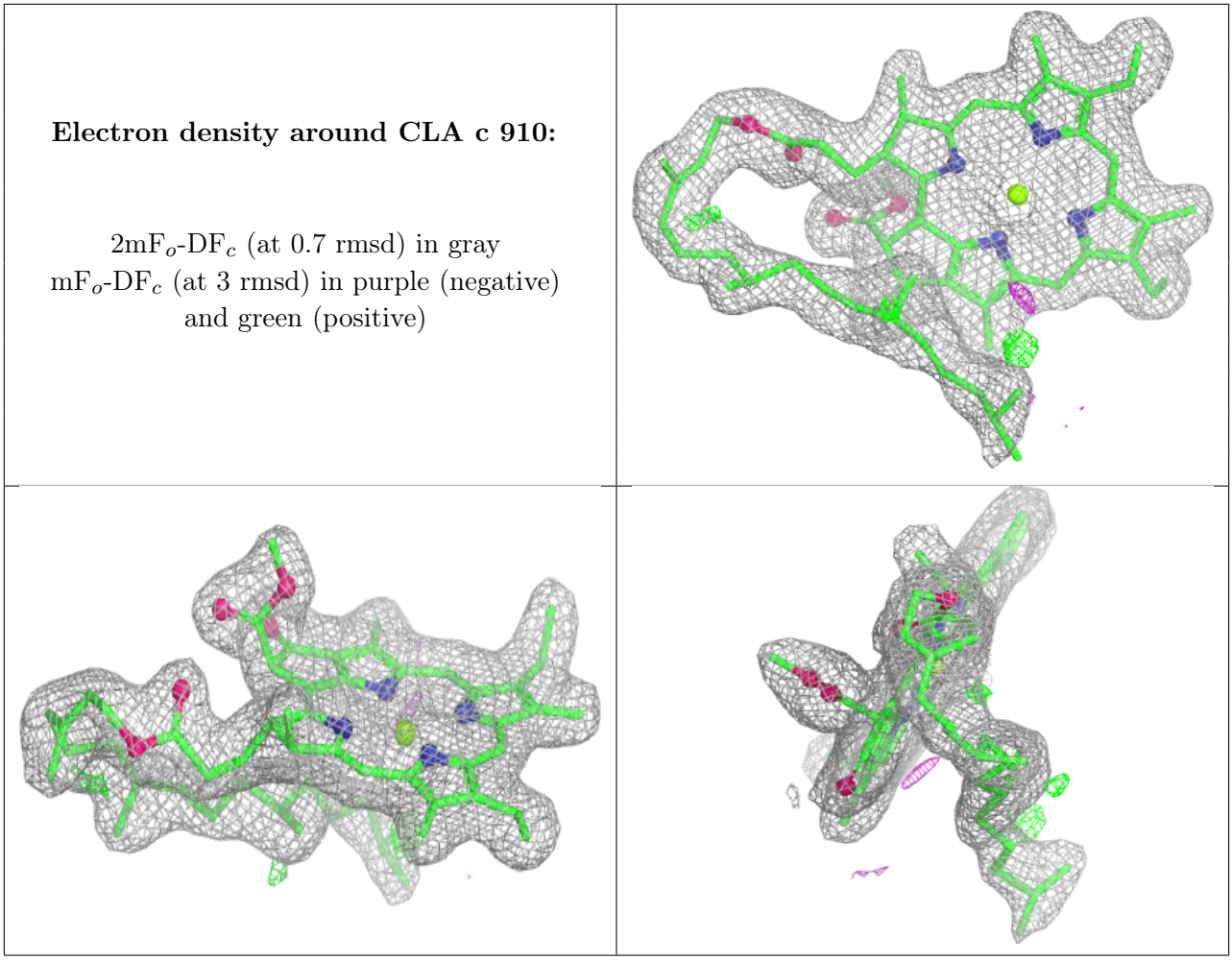






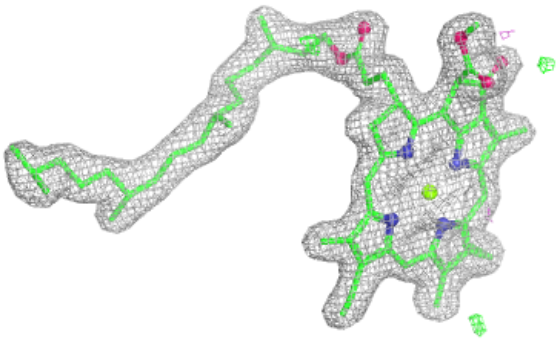
Electron density around CLA c 910:

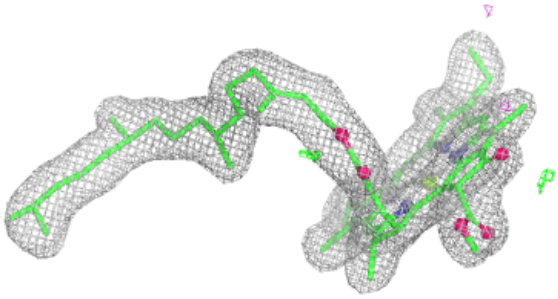
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

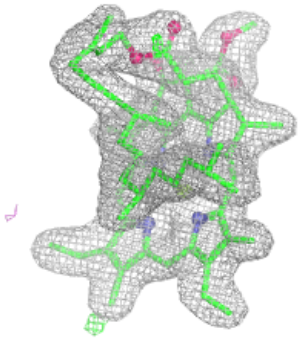


Electron density around CLA c 912:

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

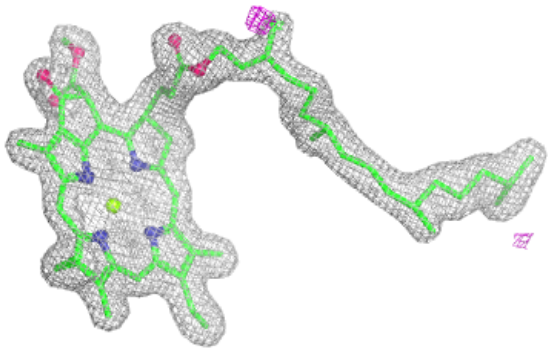


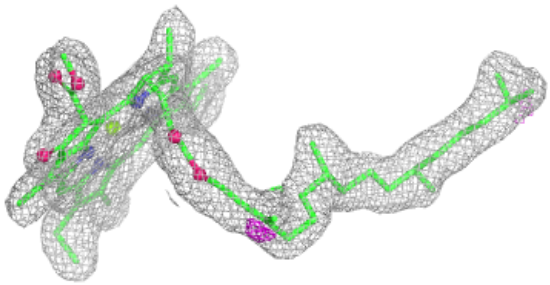


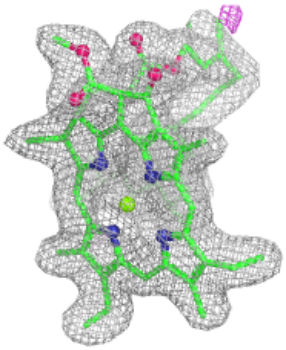


Electron density around CLA C 511:

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

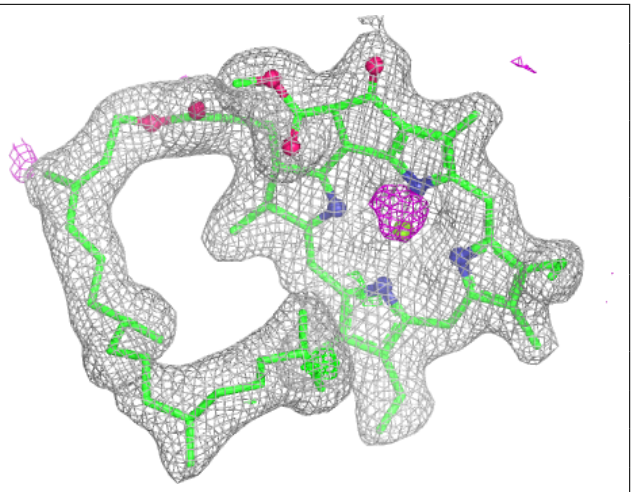


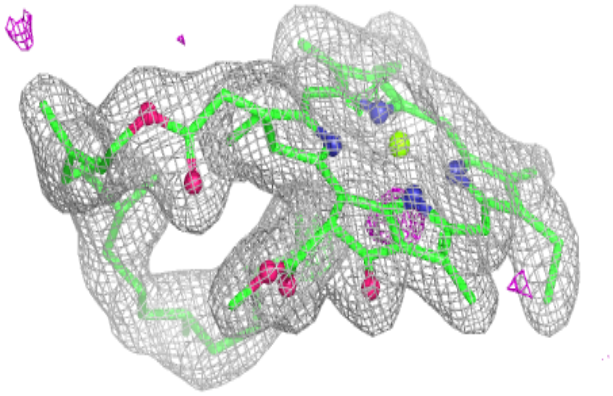


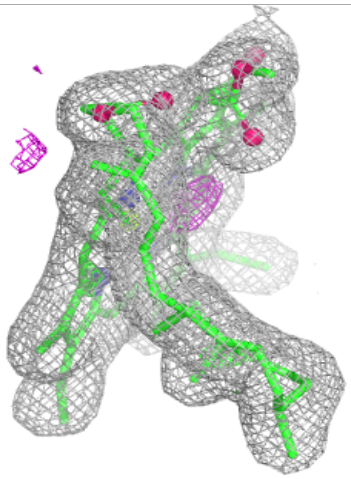


Electron density around CLA B 616:

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

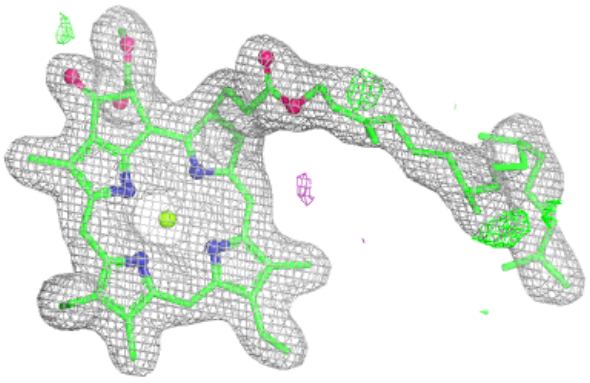


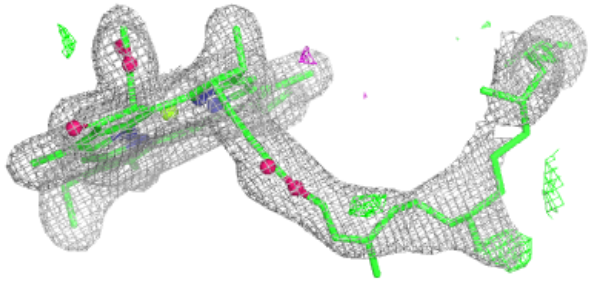


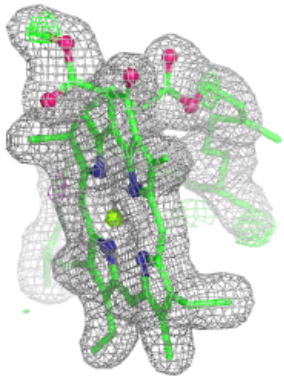


Electron density around CLA A 410:

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

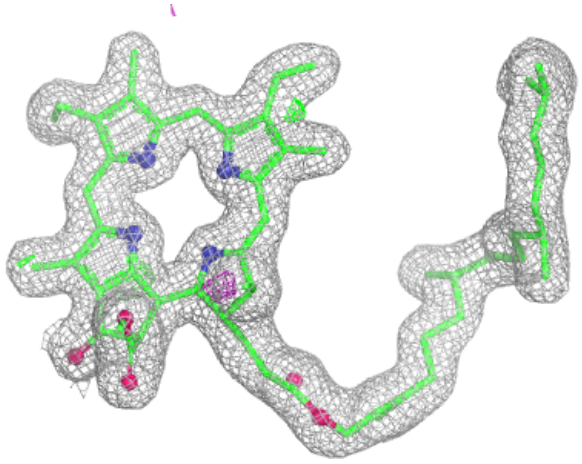


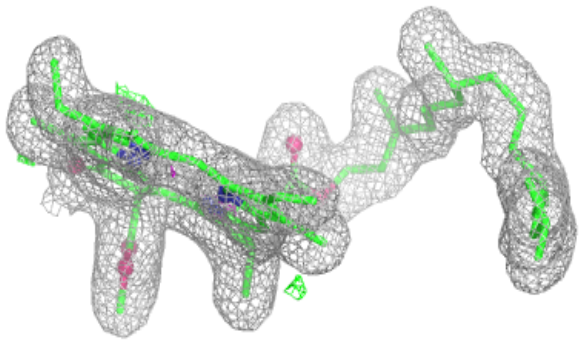


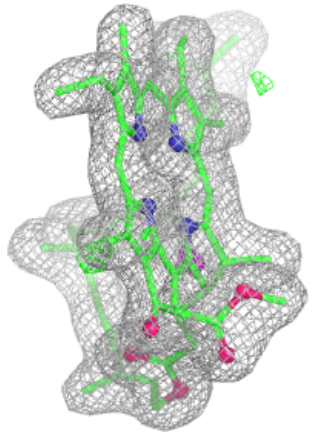


Electron density around PHO A 409:

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

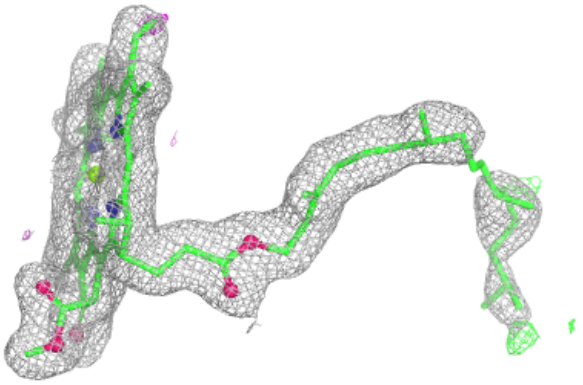


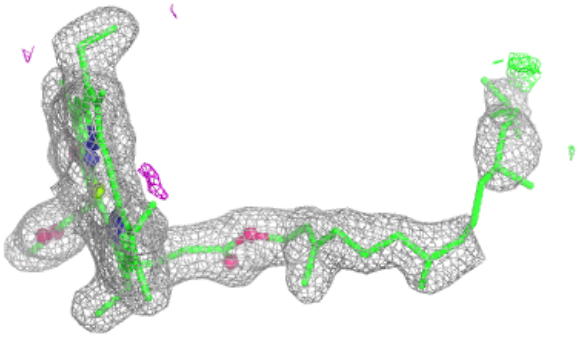


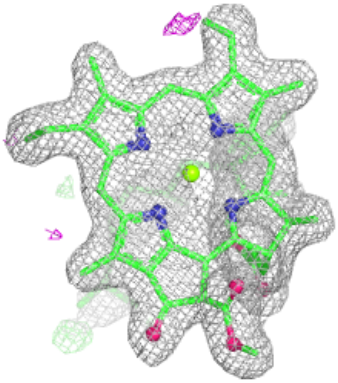


Electron density around CLA D 402:

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

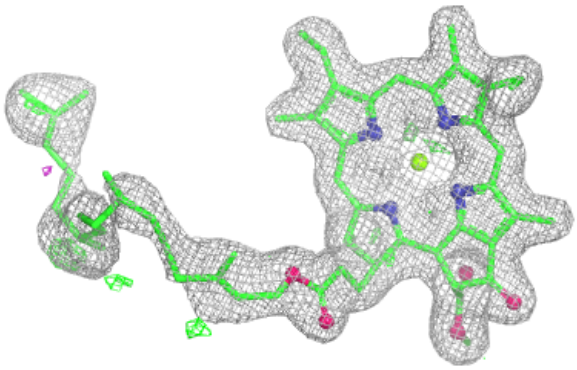


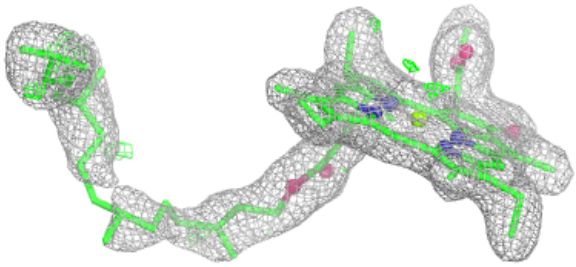


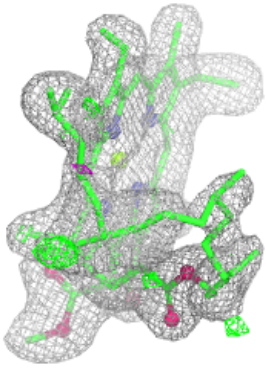


Electron density around CLA a 413:

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

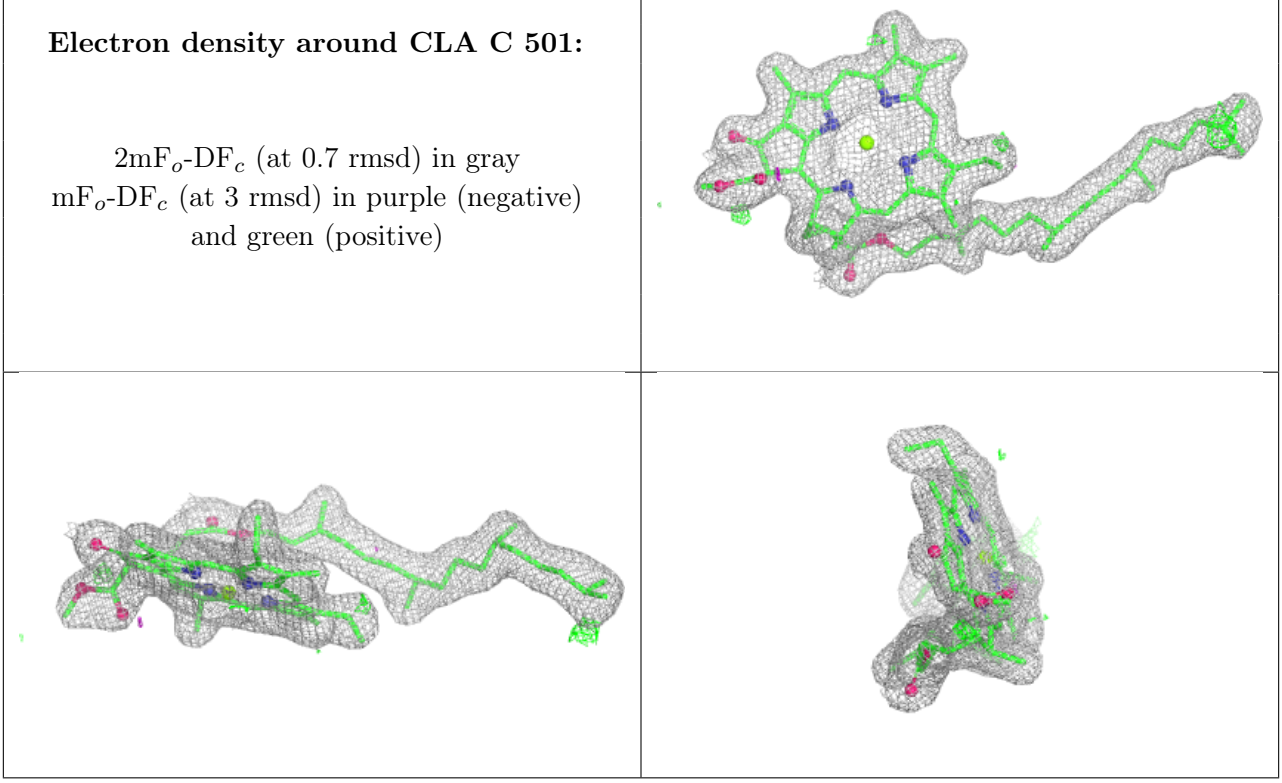






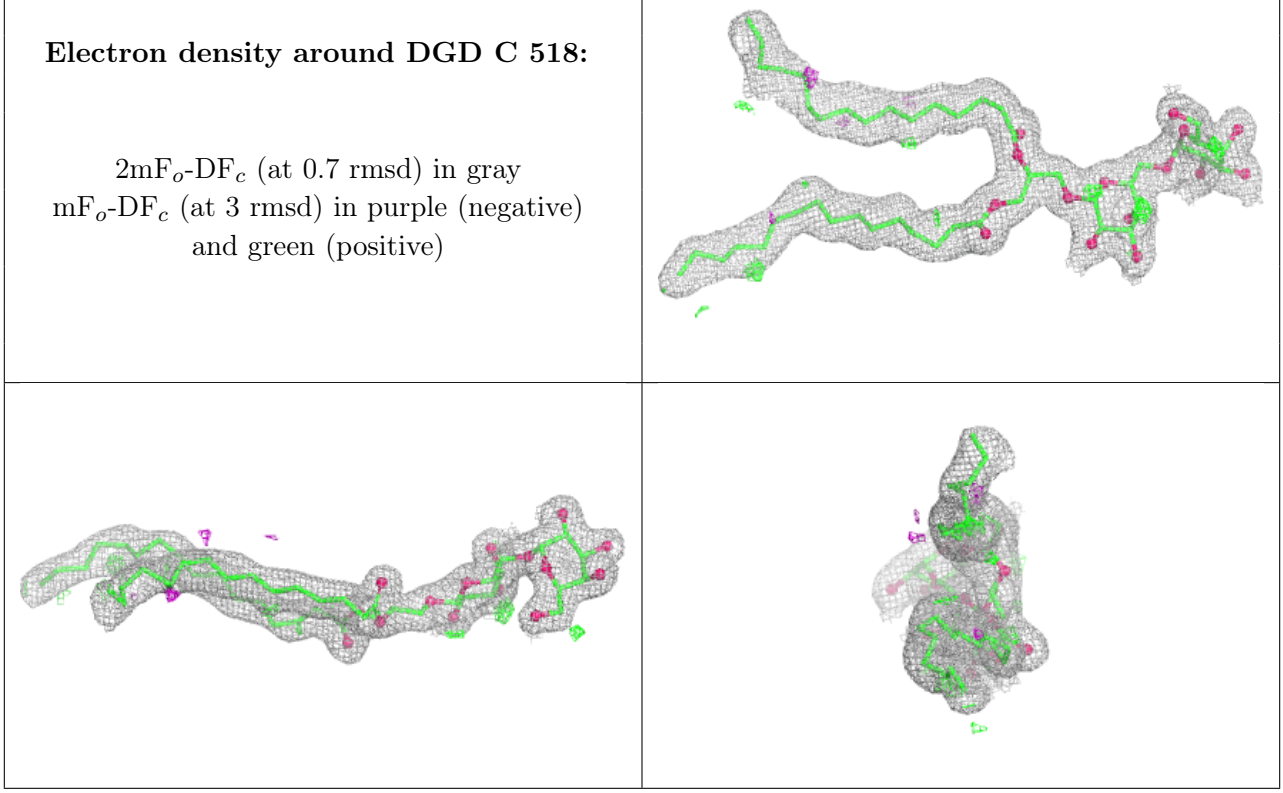
Electron density around CLA C 501:

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



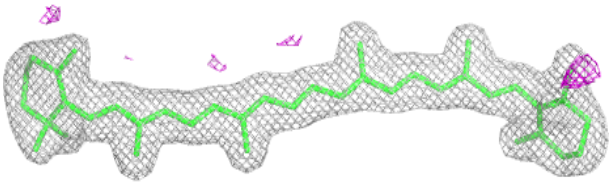
Electron density around DGD C 518:

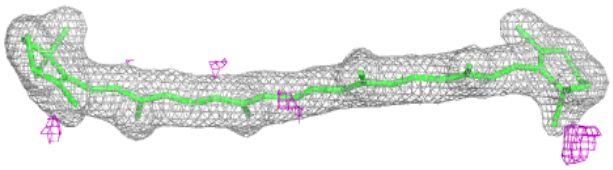
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

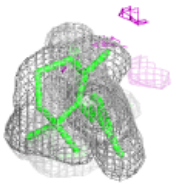


Electron density around BCR B 620:

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

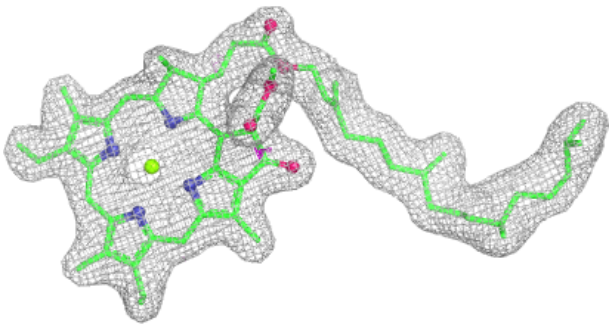


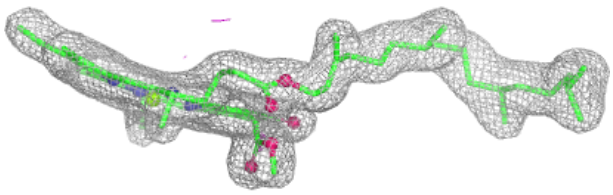


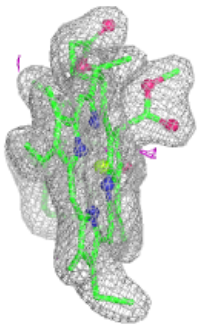


Electron density around CLA b 606:

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

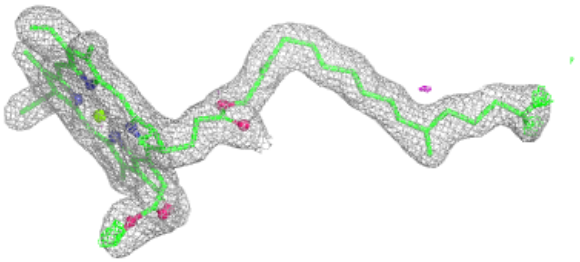


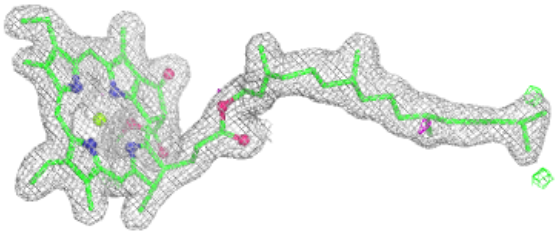


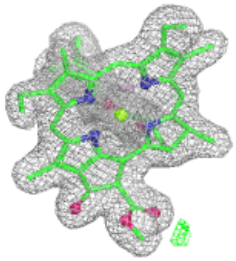


Electron density around CLA C 502:

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

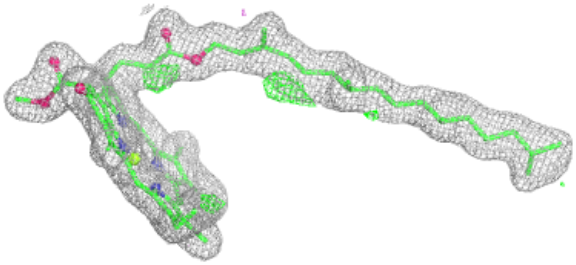


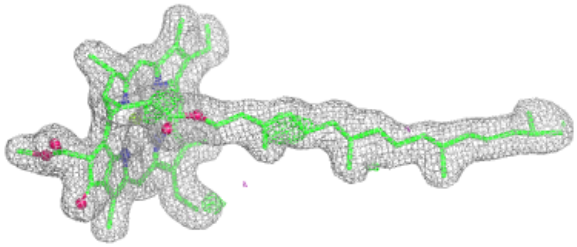


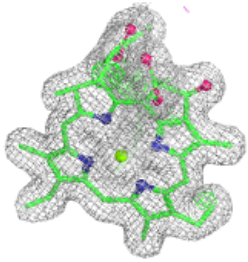


Electron density around CLA b 611:

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

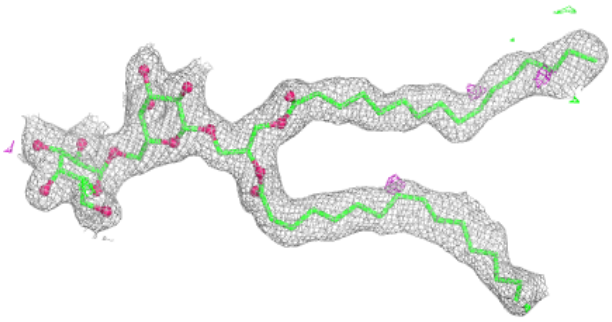


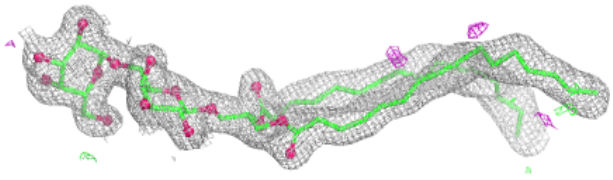


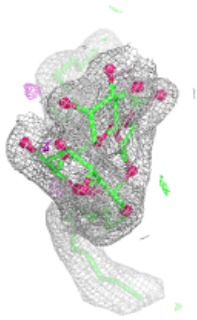


Electron density around DGD c 919:

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

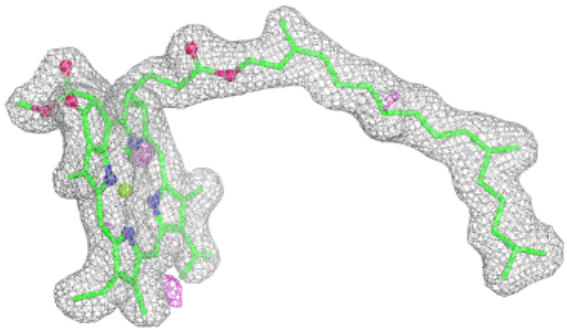


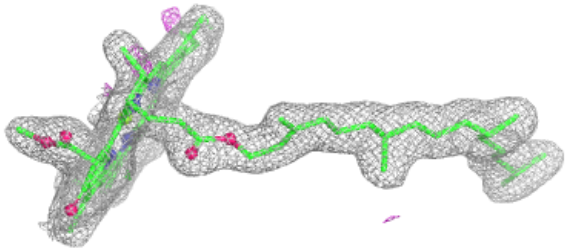


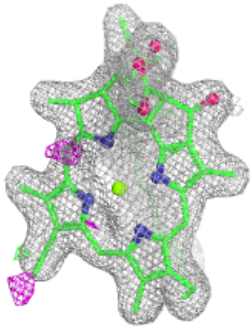


Electron density around CLA b 613:

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

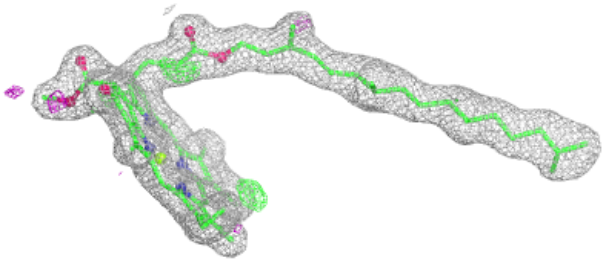


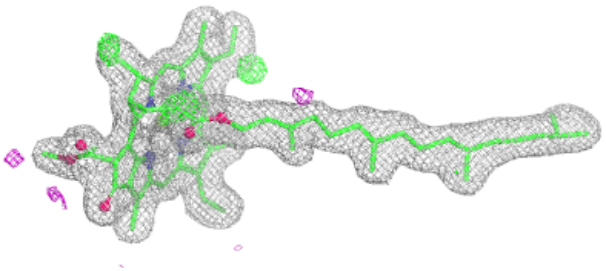


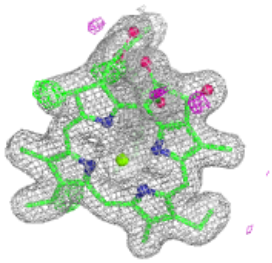


Electron density around CLA B 608:

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

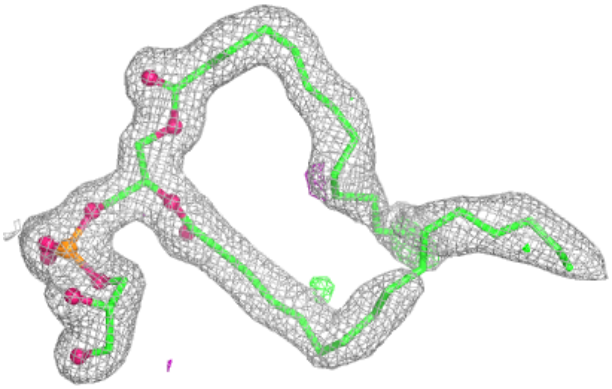


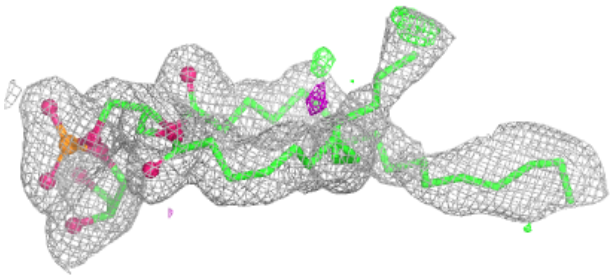


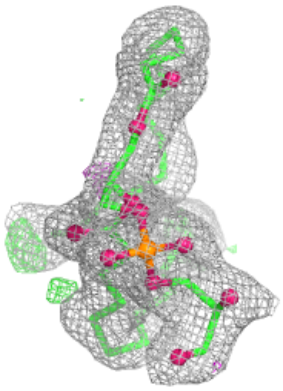


Electron density around LHG D 408:

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

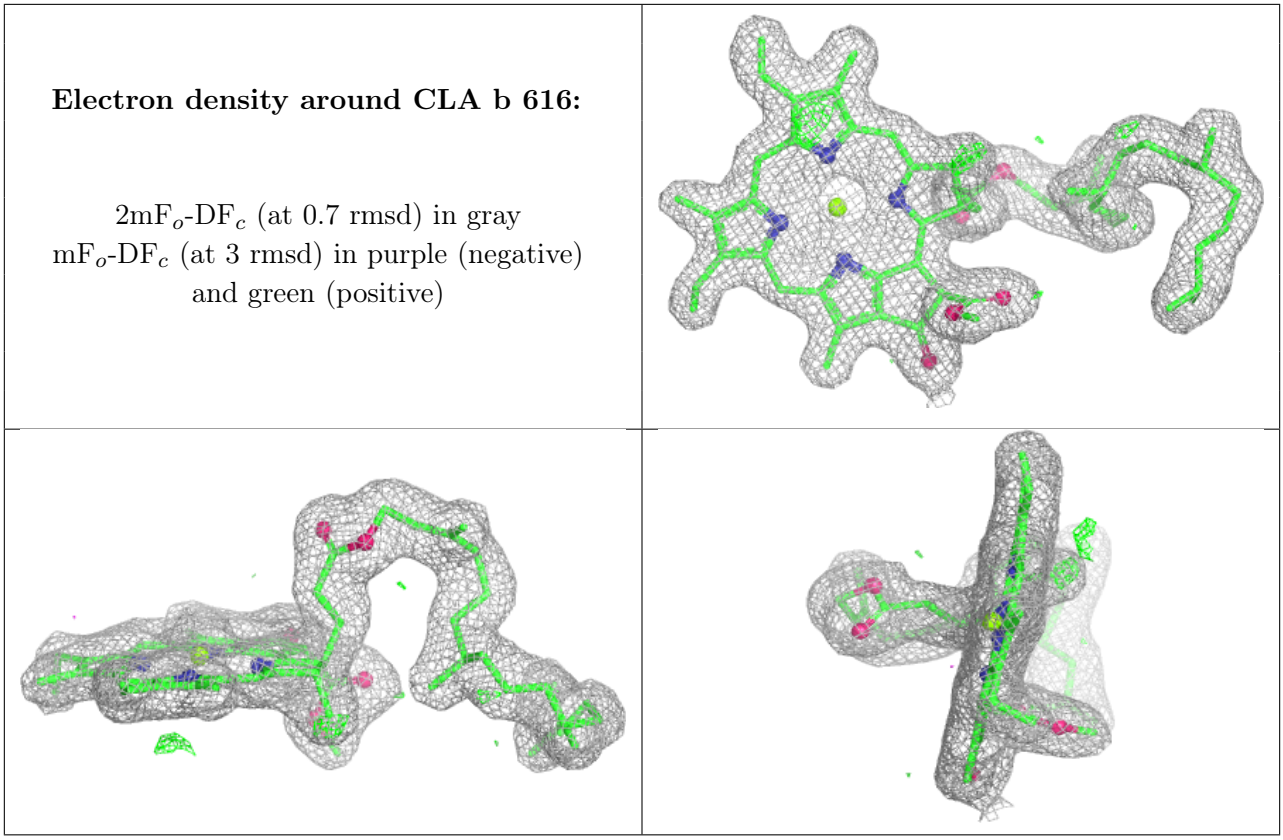






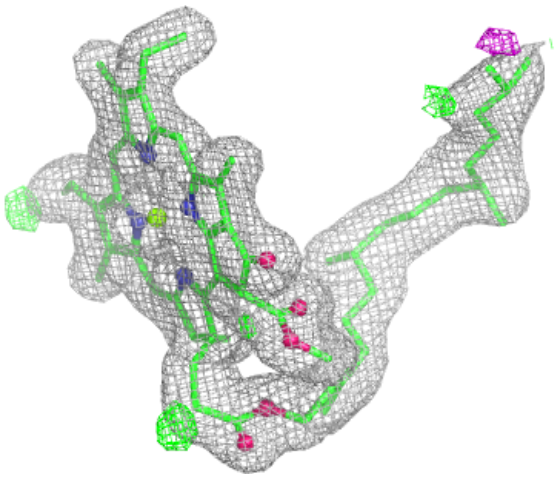
Electron density around CLA b 616:

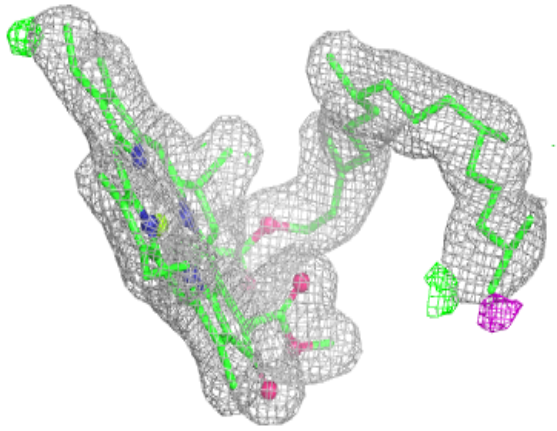
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

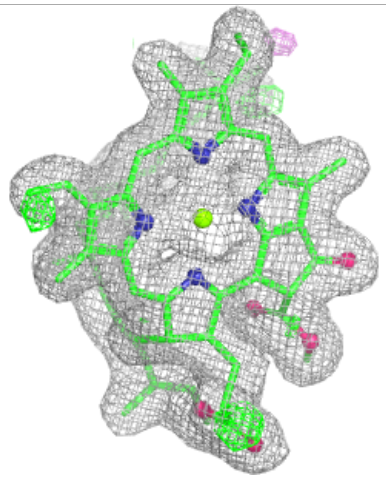


Electron density around CLA b 617:

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

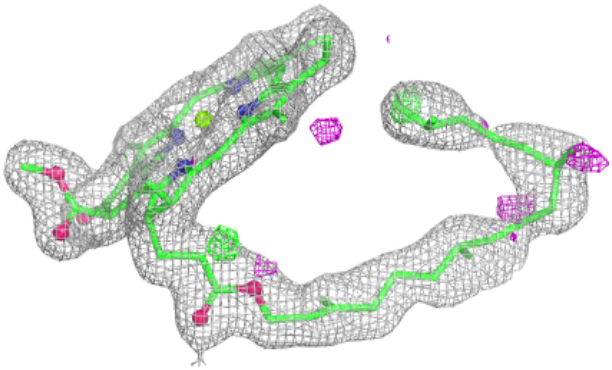


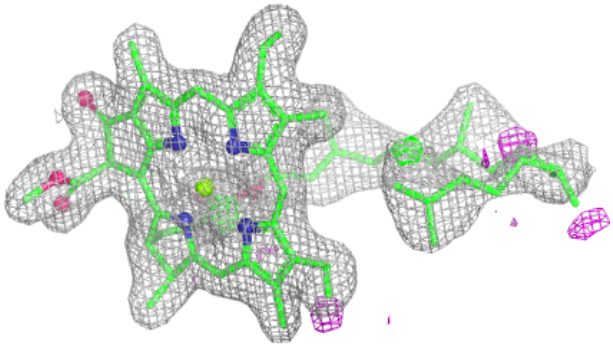


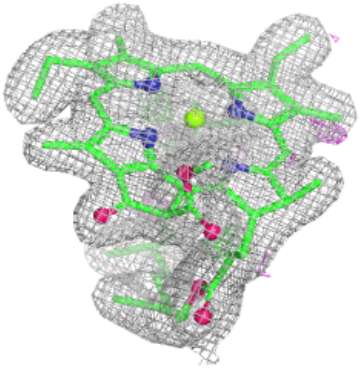


Electron density around CLA C 504:

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

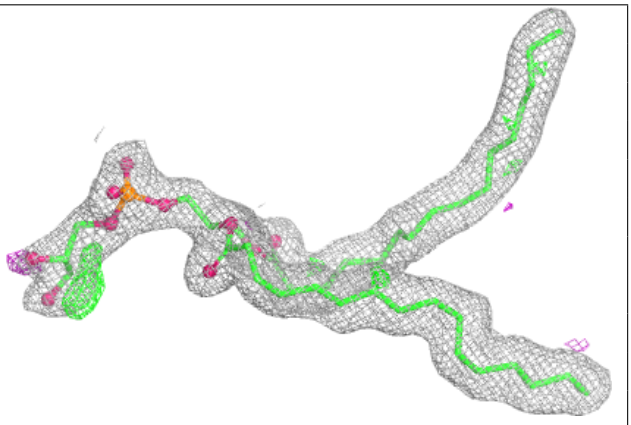


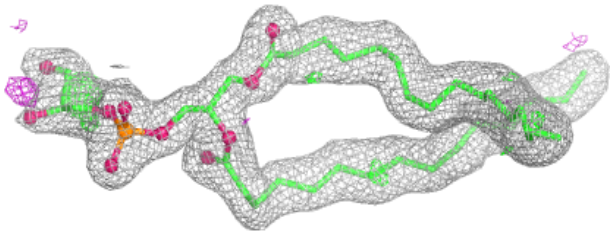


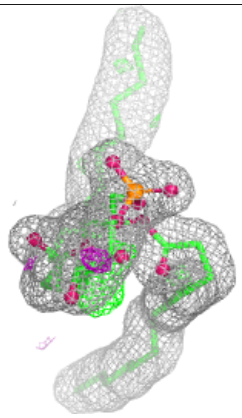


Electron density around LHG d 410:

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

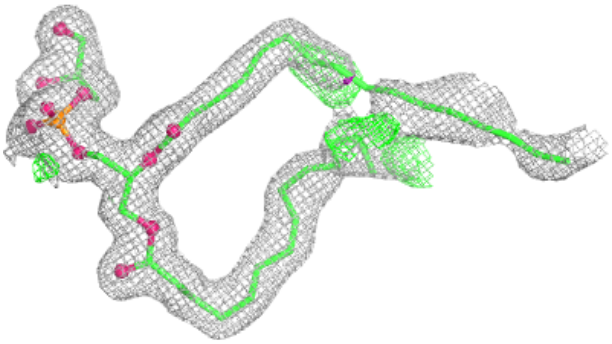


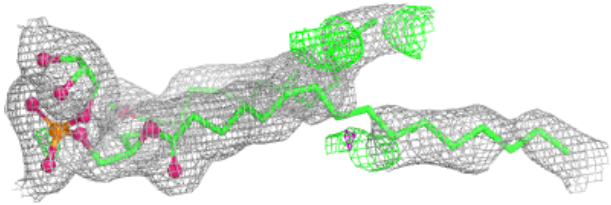


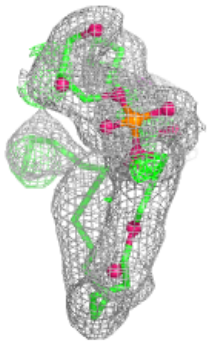


Electron density around LHG d 411:

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

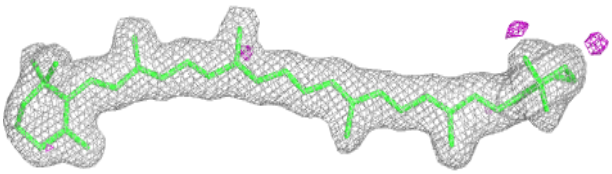


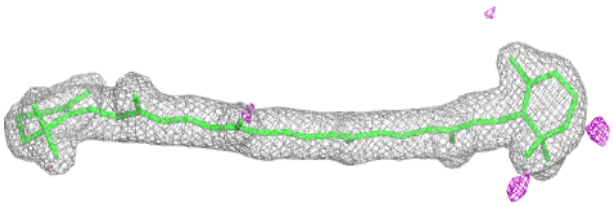


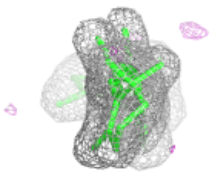


Electron density around BCR b 621:

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

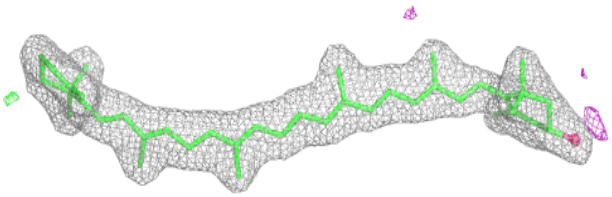


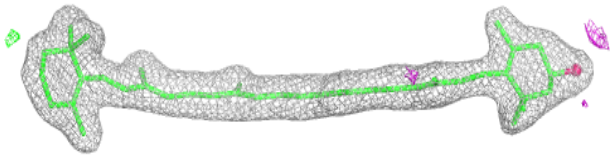


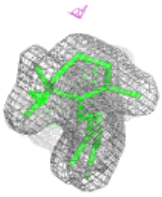


Electron density around RRX H 101:

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

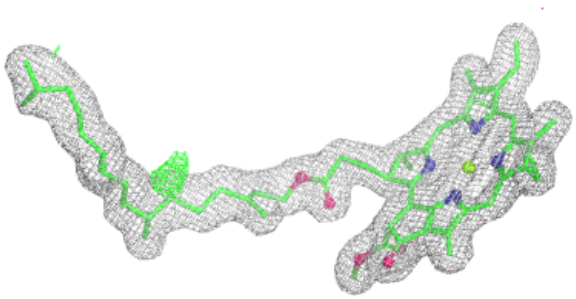


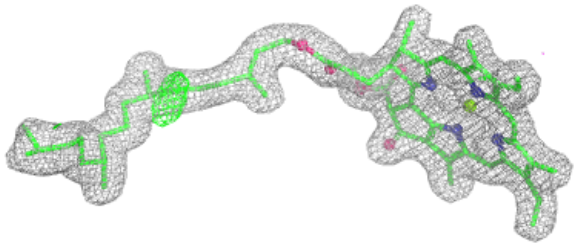


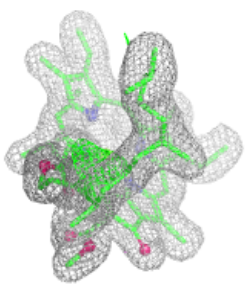


Electron density around CLA a 409:

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

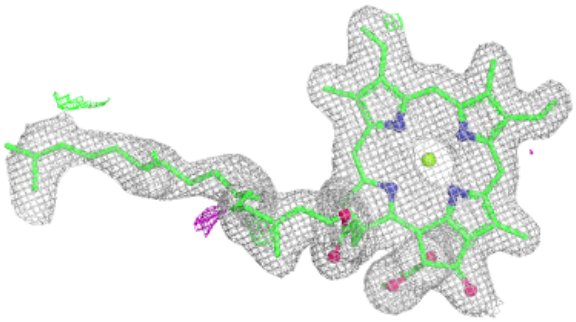


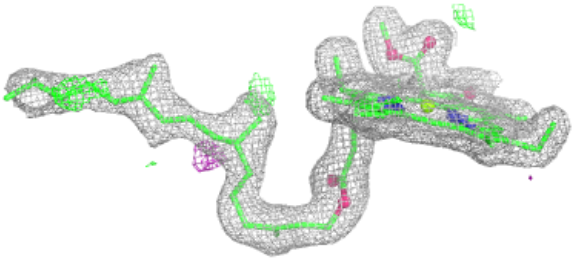


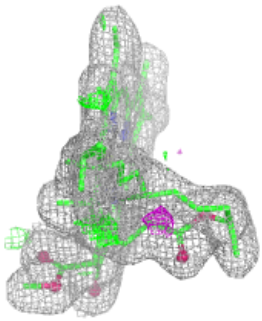


Electron density around CLA a 410:

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

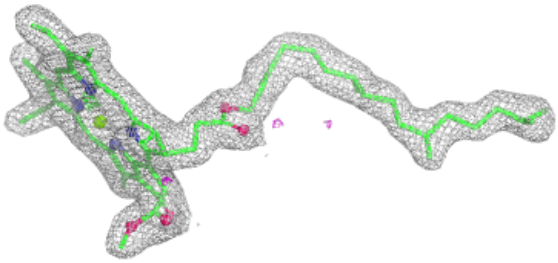


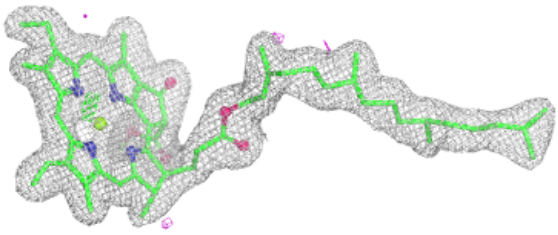


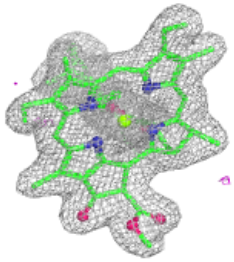


Electron density around CLA c 903:

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

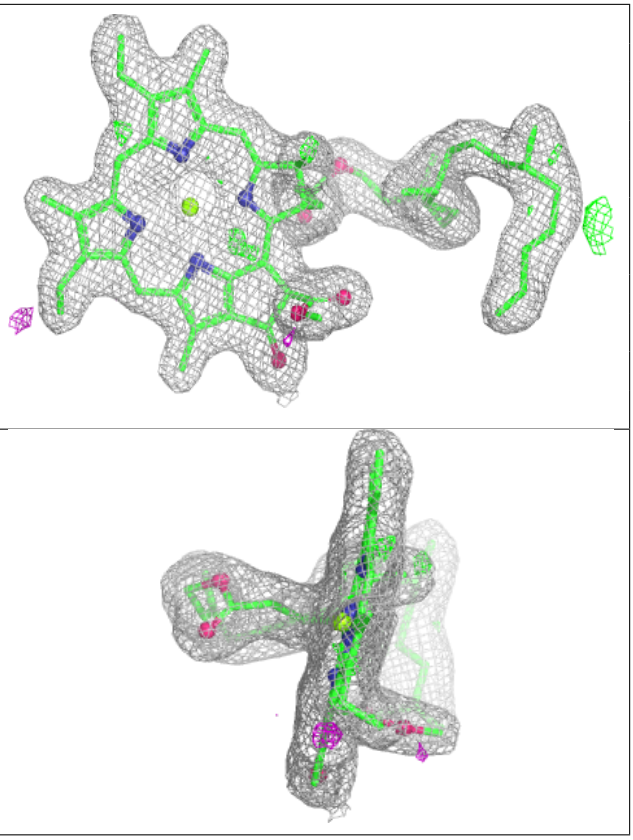






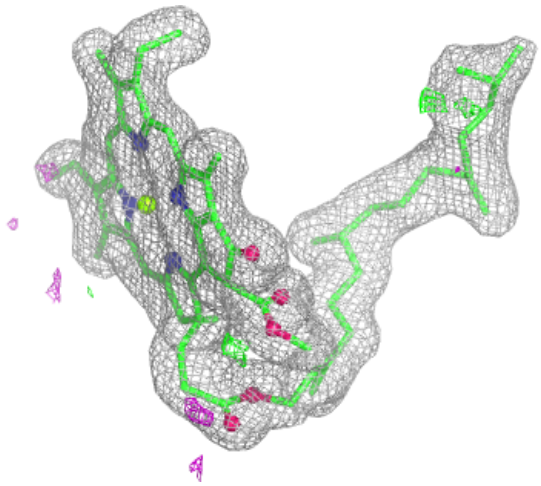
Electron density around CLA B 613:

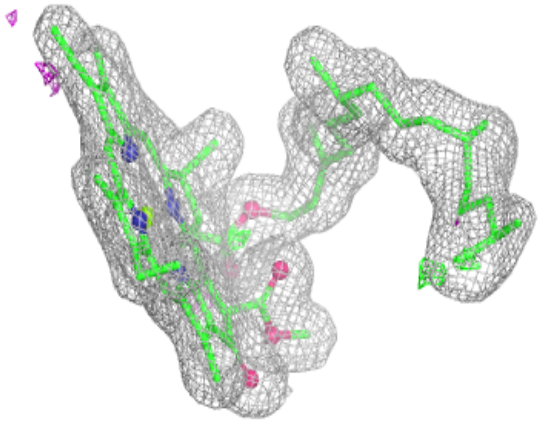
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

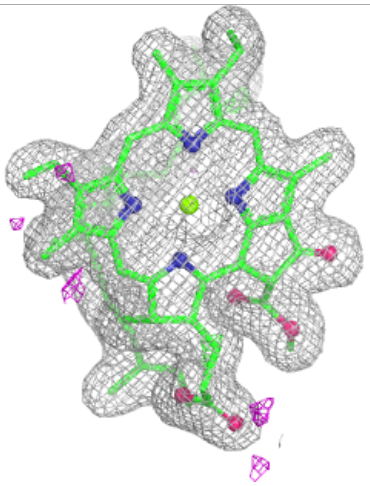


Electron density around CLA B 614:

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

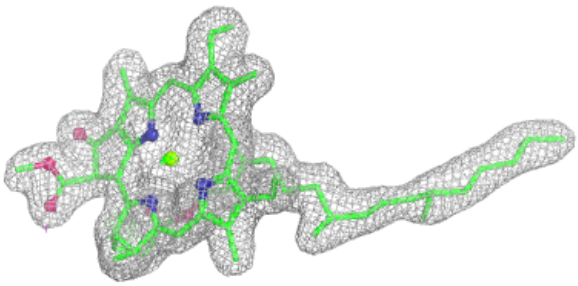


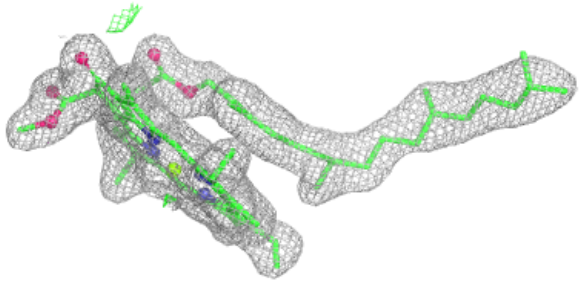


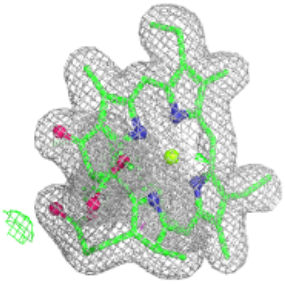


Electron density around CLA c 906:

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

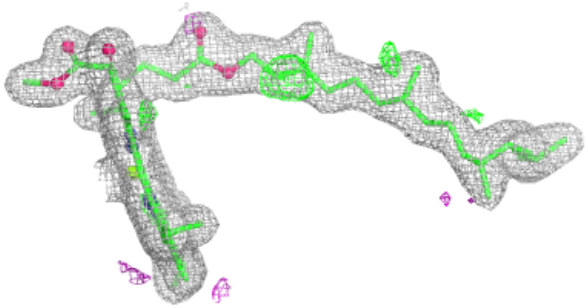


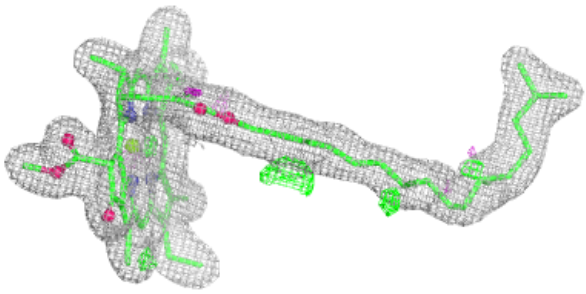


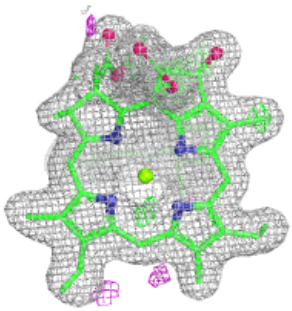


Electron density around CLA B 606:

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

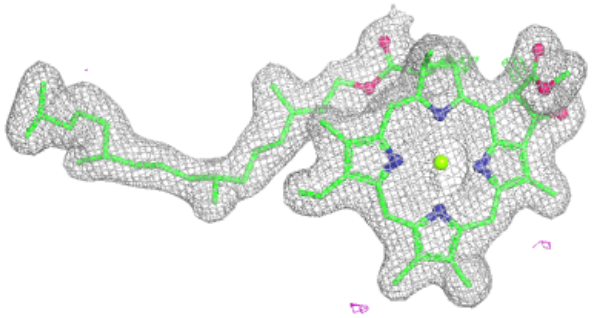


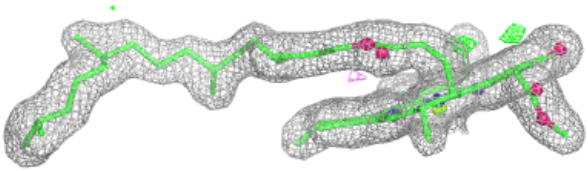


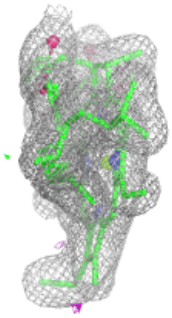


Electron density around CLA b 607:

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

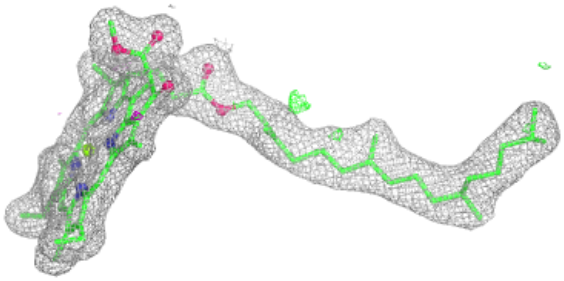


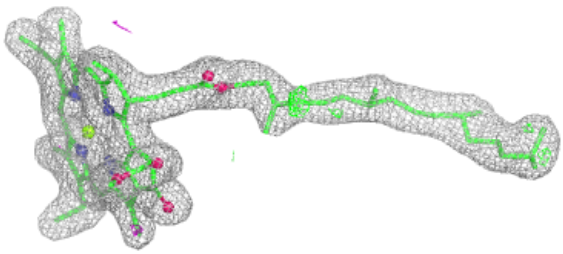


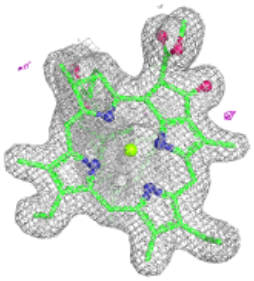


Electron density around CLA b 608:

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

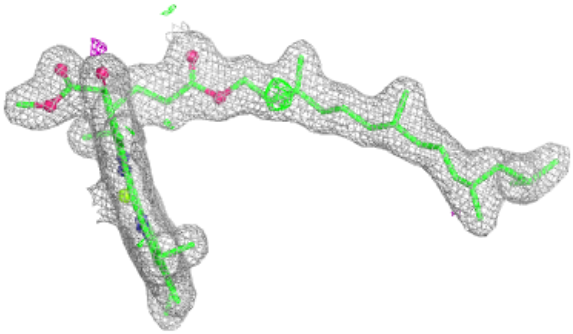


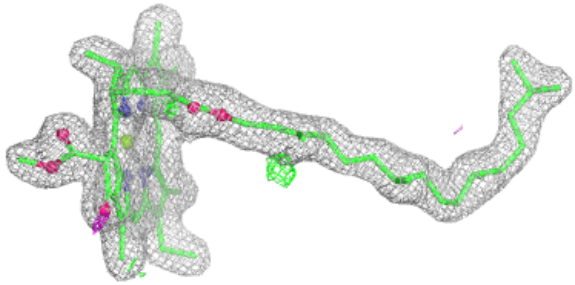


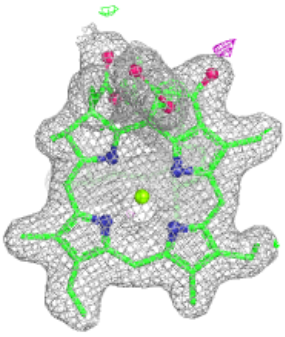


Electron density around CLA b 609:

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

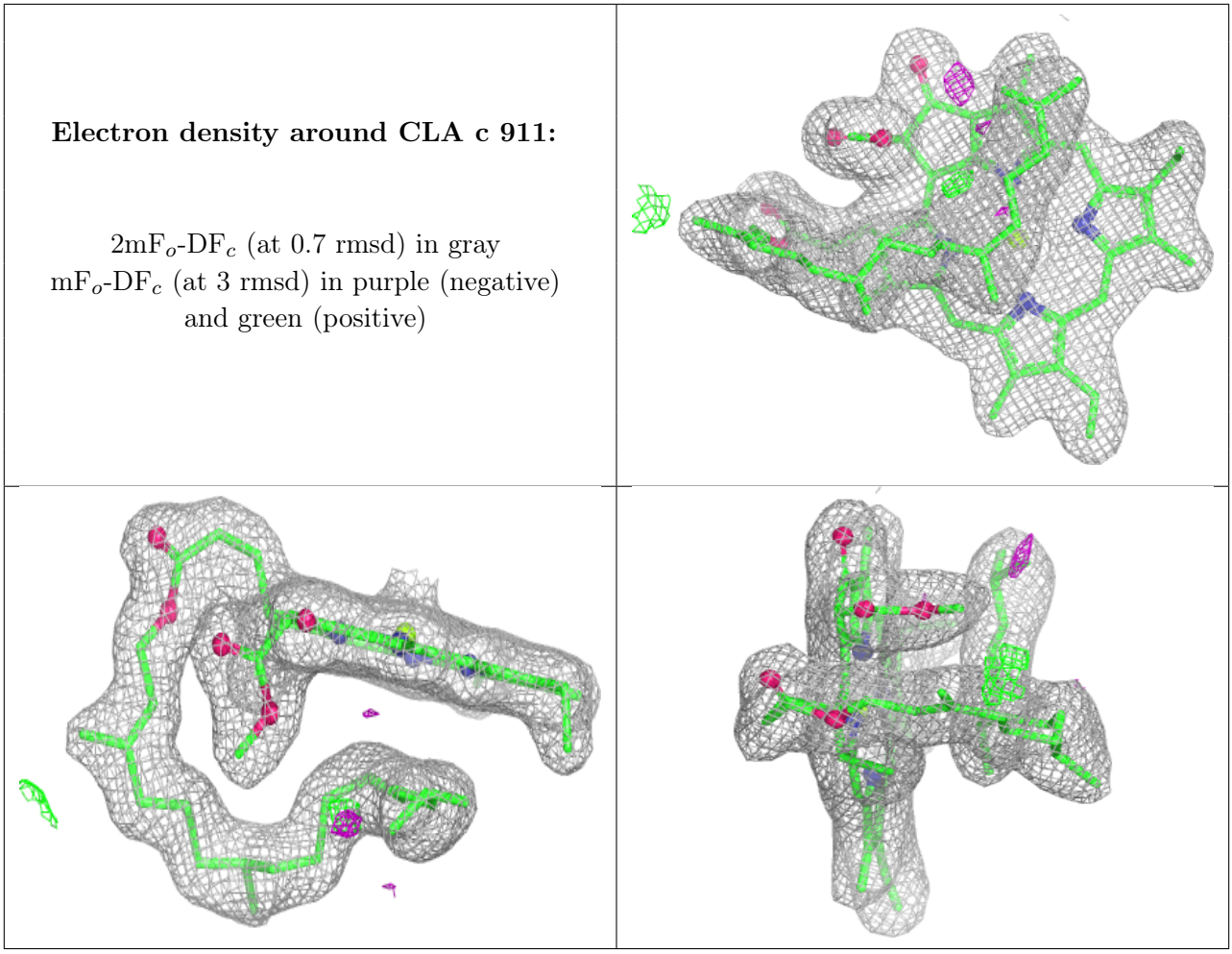






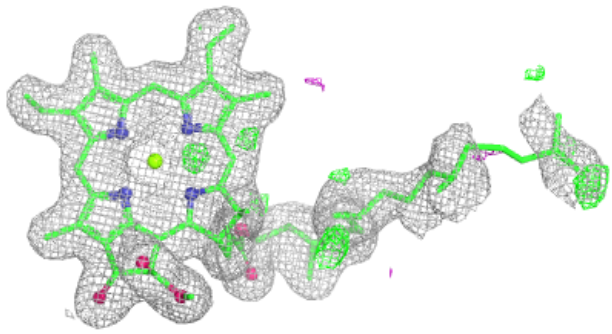
Electron density around CLA c 911:

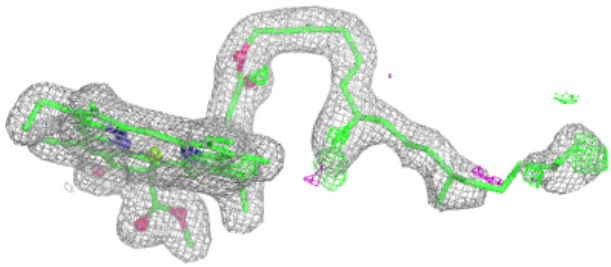
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

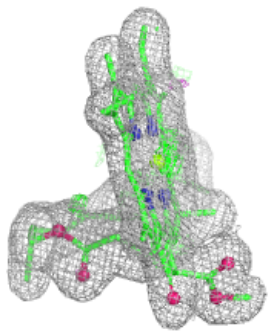


Electron density around CLA A 407:

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

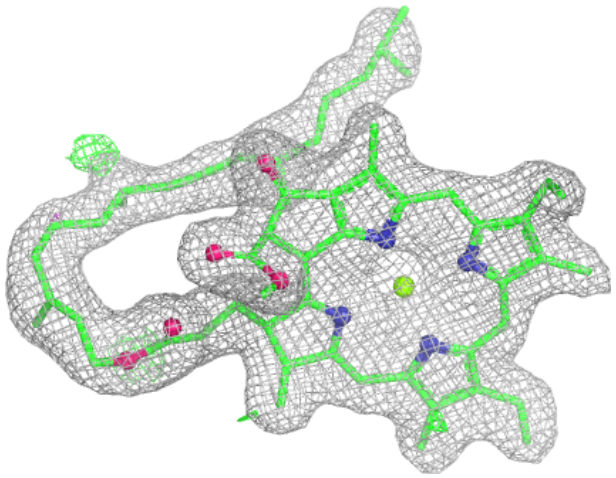


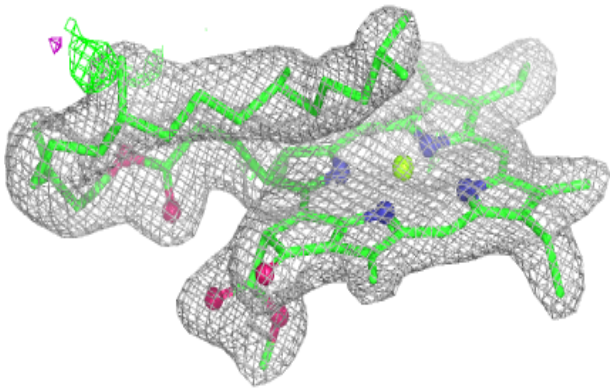


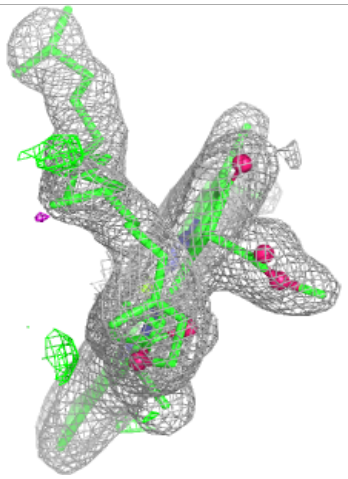


Electron density around CLA C 509:

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

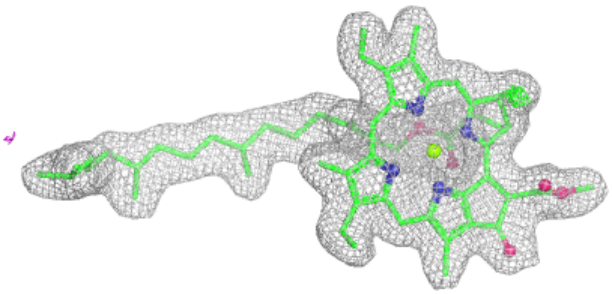


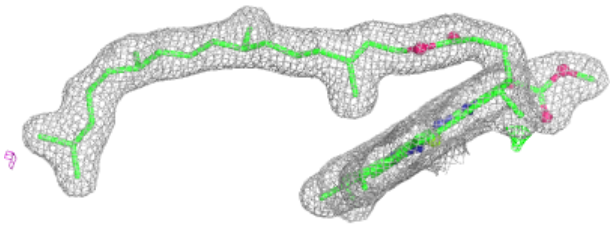


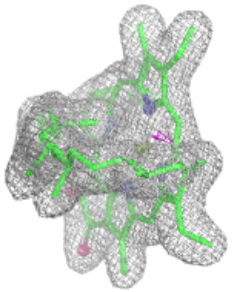


Electron density around CLA b 612:

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

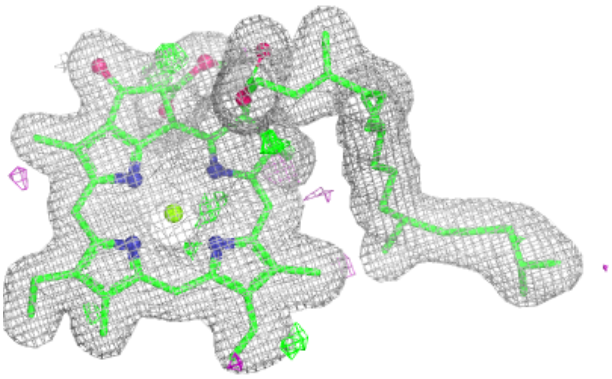


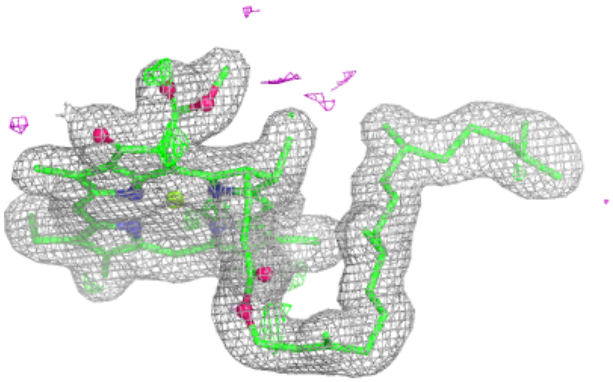


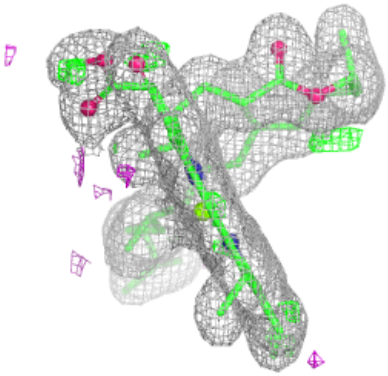


Electron density around CLA d 401:

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

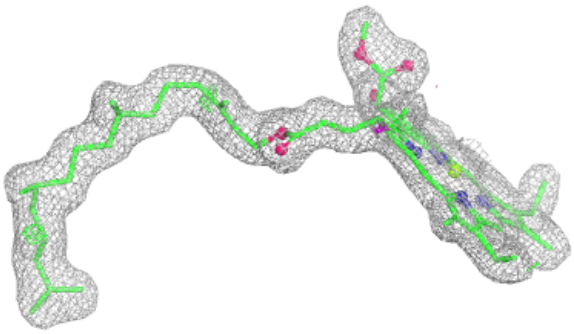


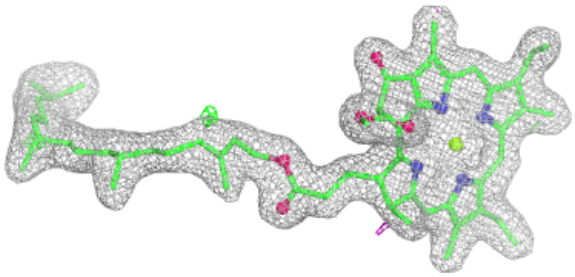


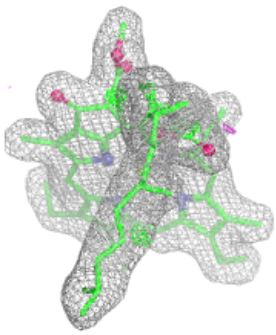


Electron density around CLA d 404:

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

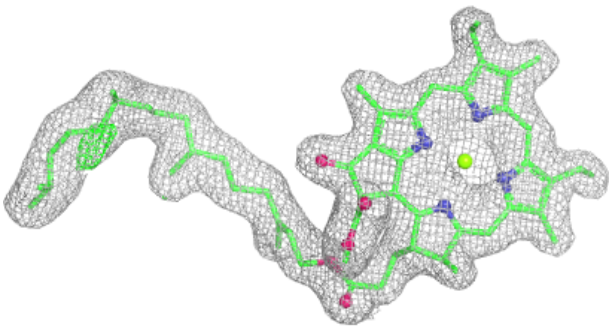


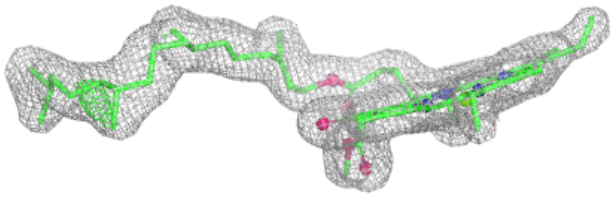


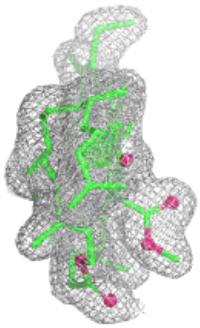


Electron density around CLA B 603:

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

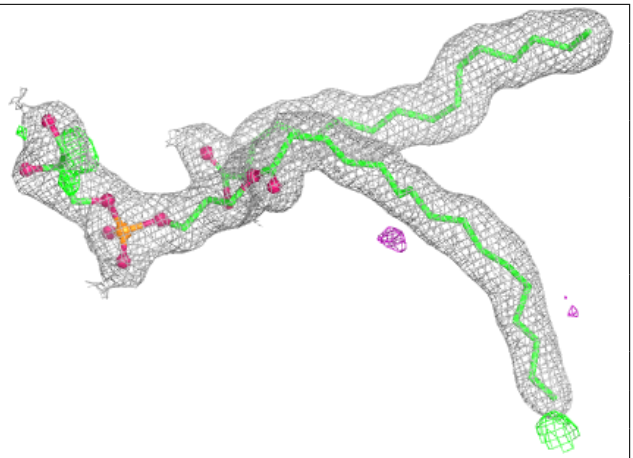


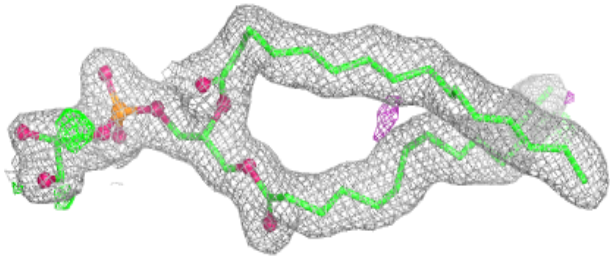


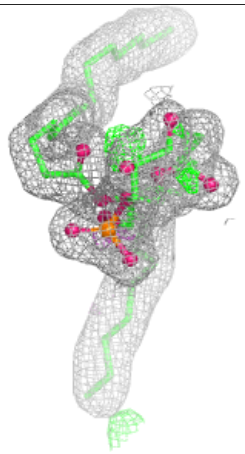


Electron density around LHG D 407:

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

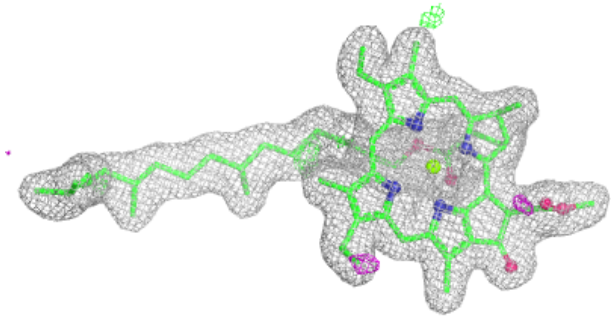


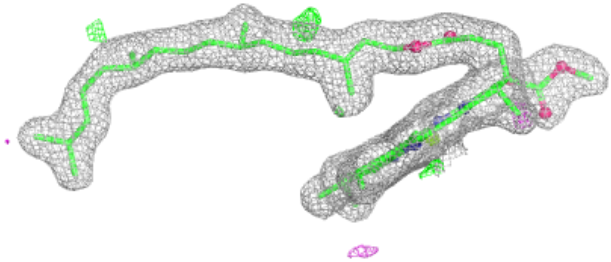




Electron density around CLA B 609:

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

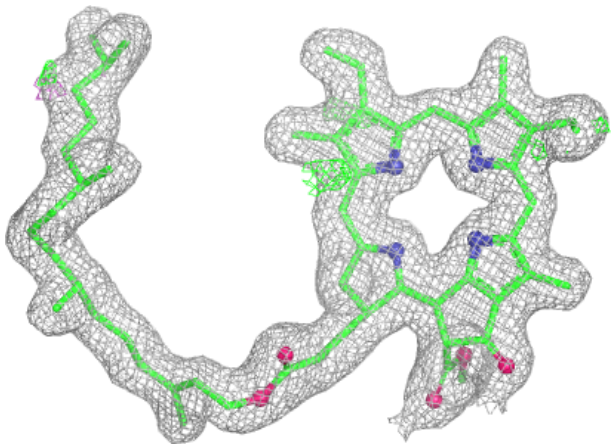


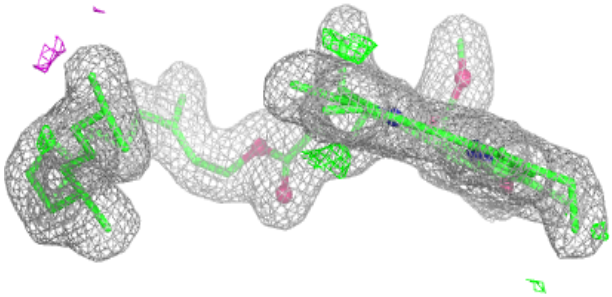


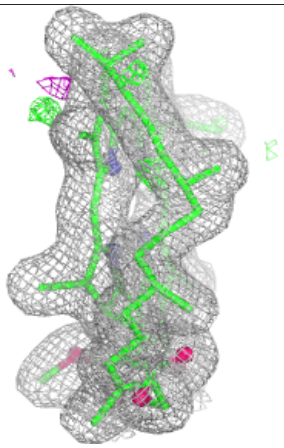


Electron density around PHO a 411:

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

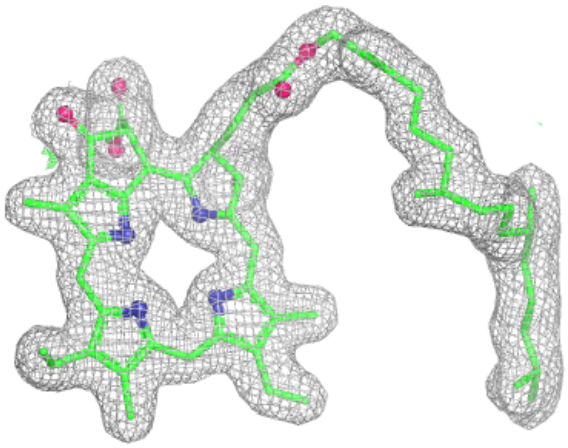


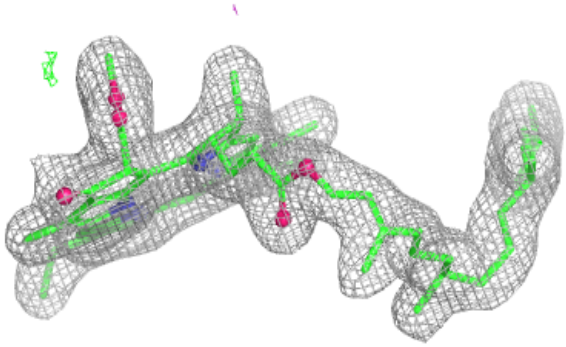


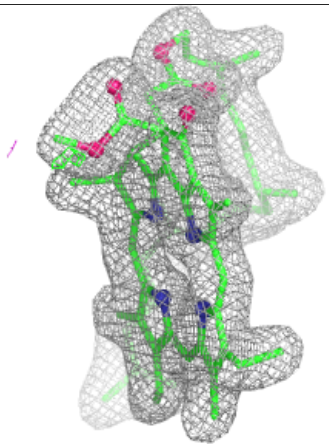


Electron density around PHO a 412:

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

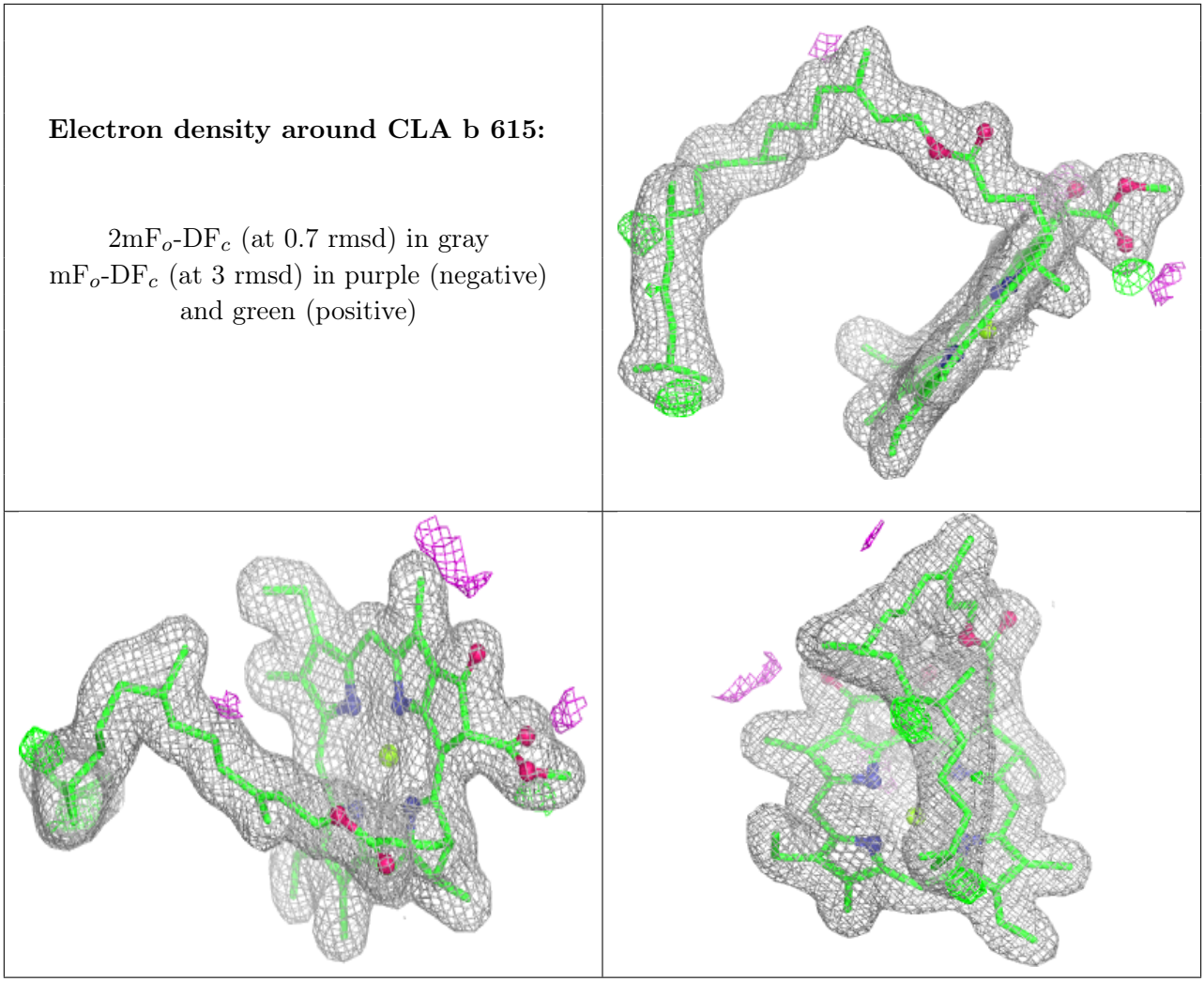






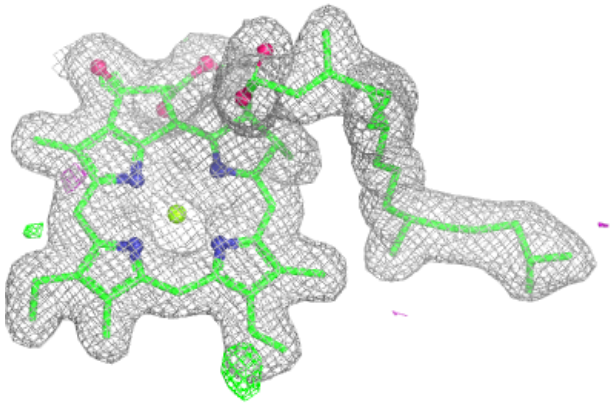
Electron density around CLA b 615:

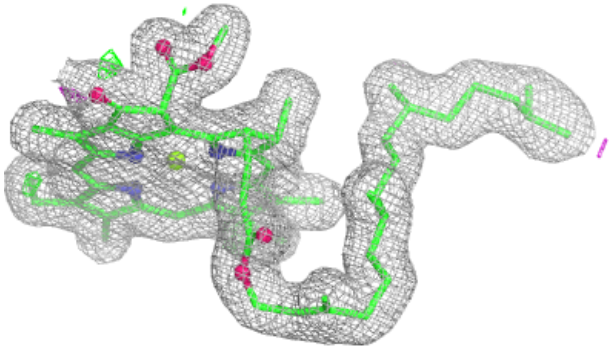
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

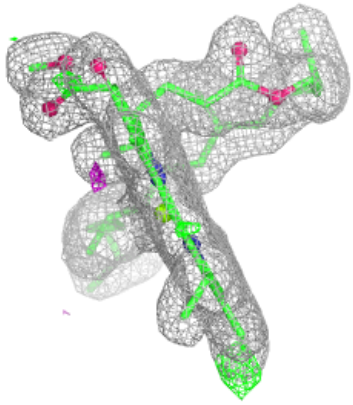


Electron density around CLA A 406:

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

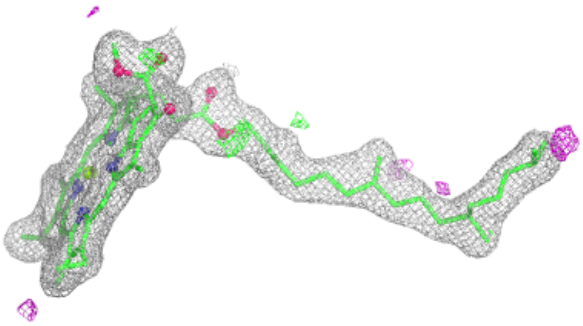


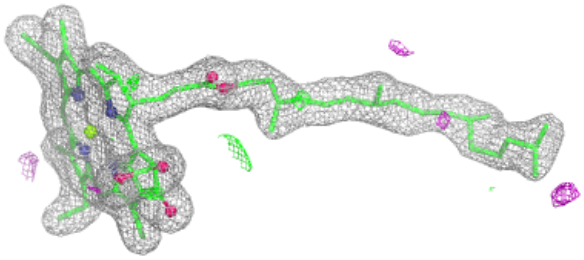


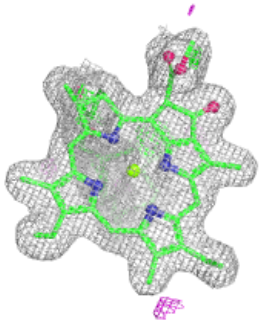


Electron density around CLA B 605:

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

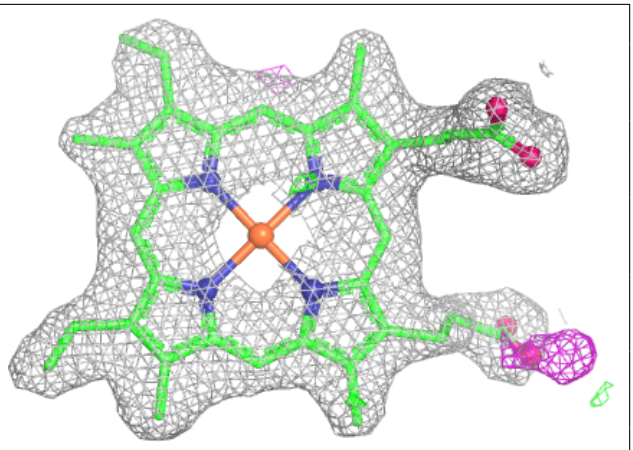


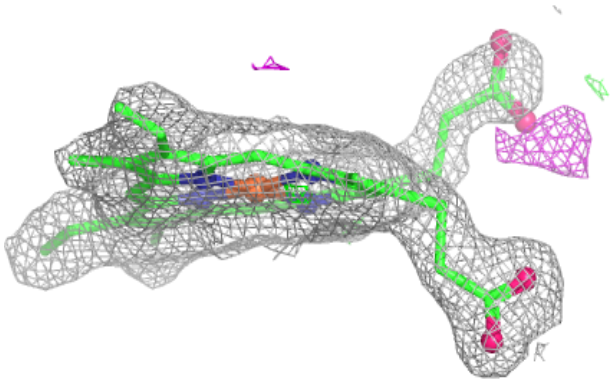


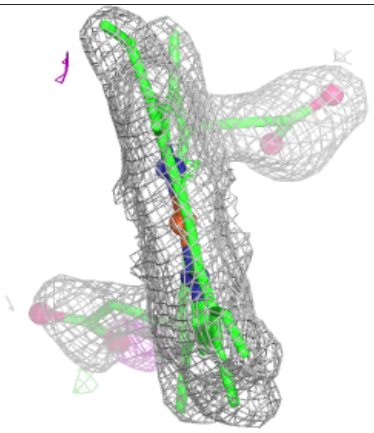


Electron density around HEM f 101:

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

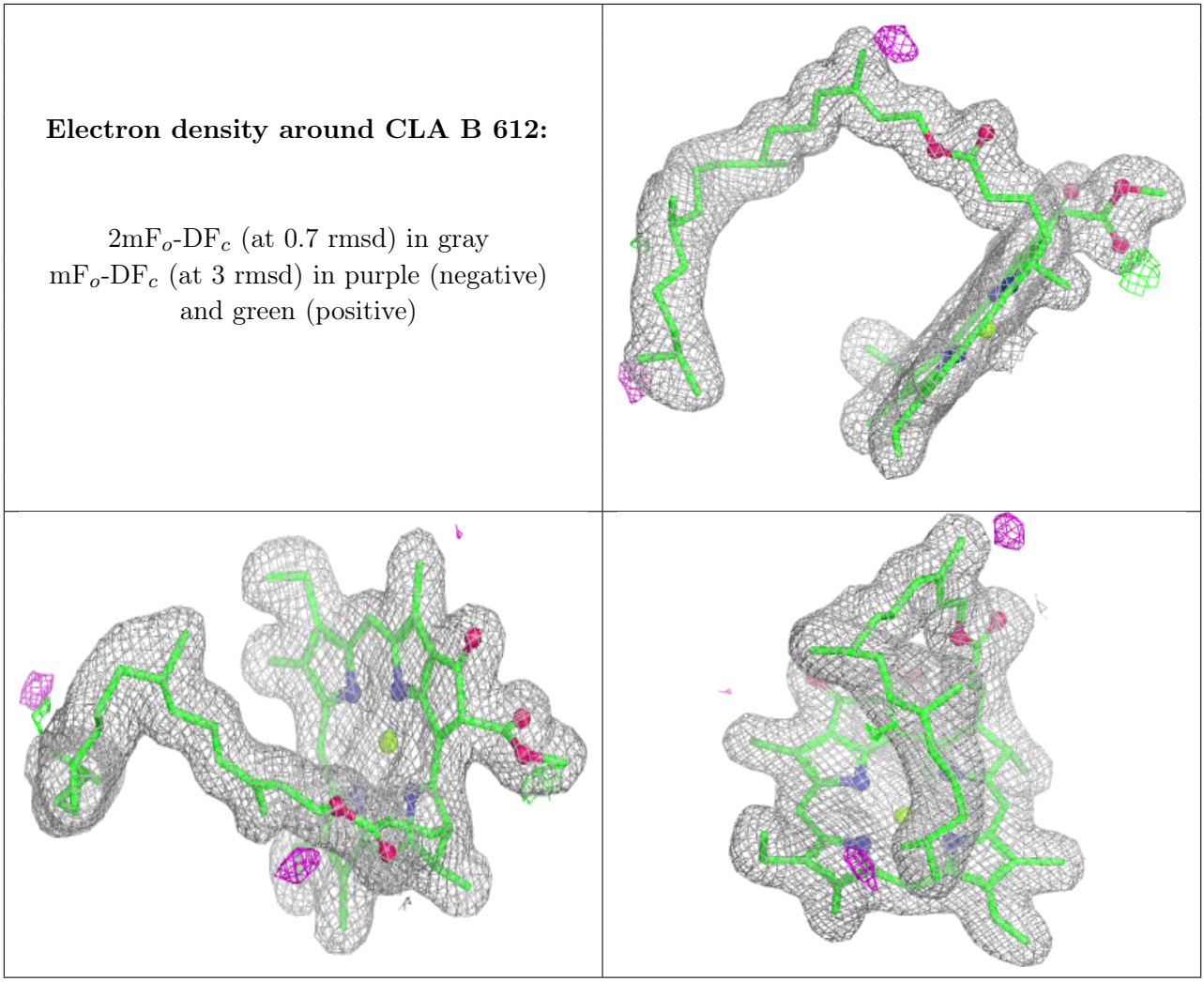






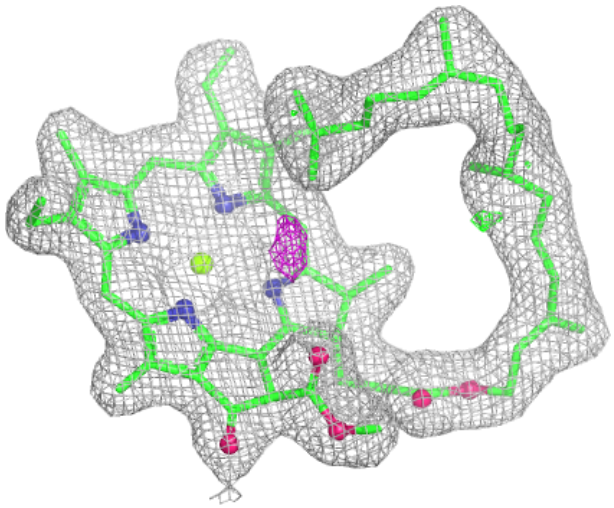
Electron density around CLA B 612:

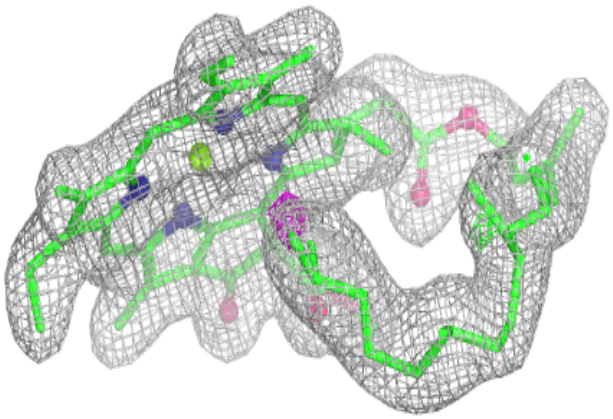
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

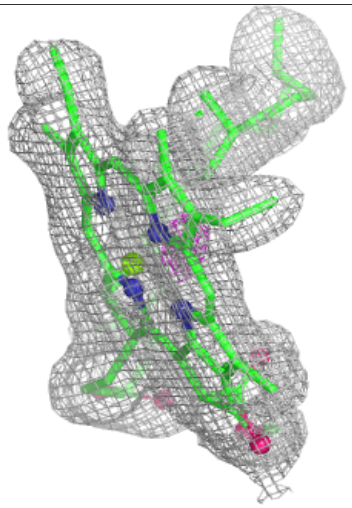


Electron density around CLA b 619:

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

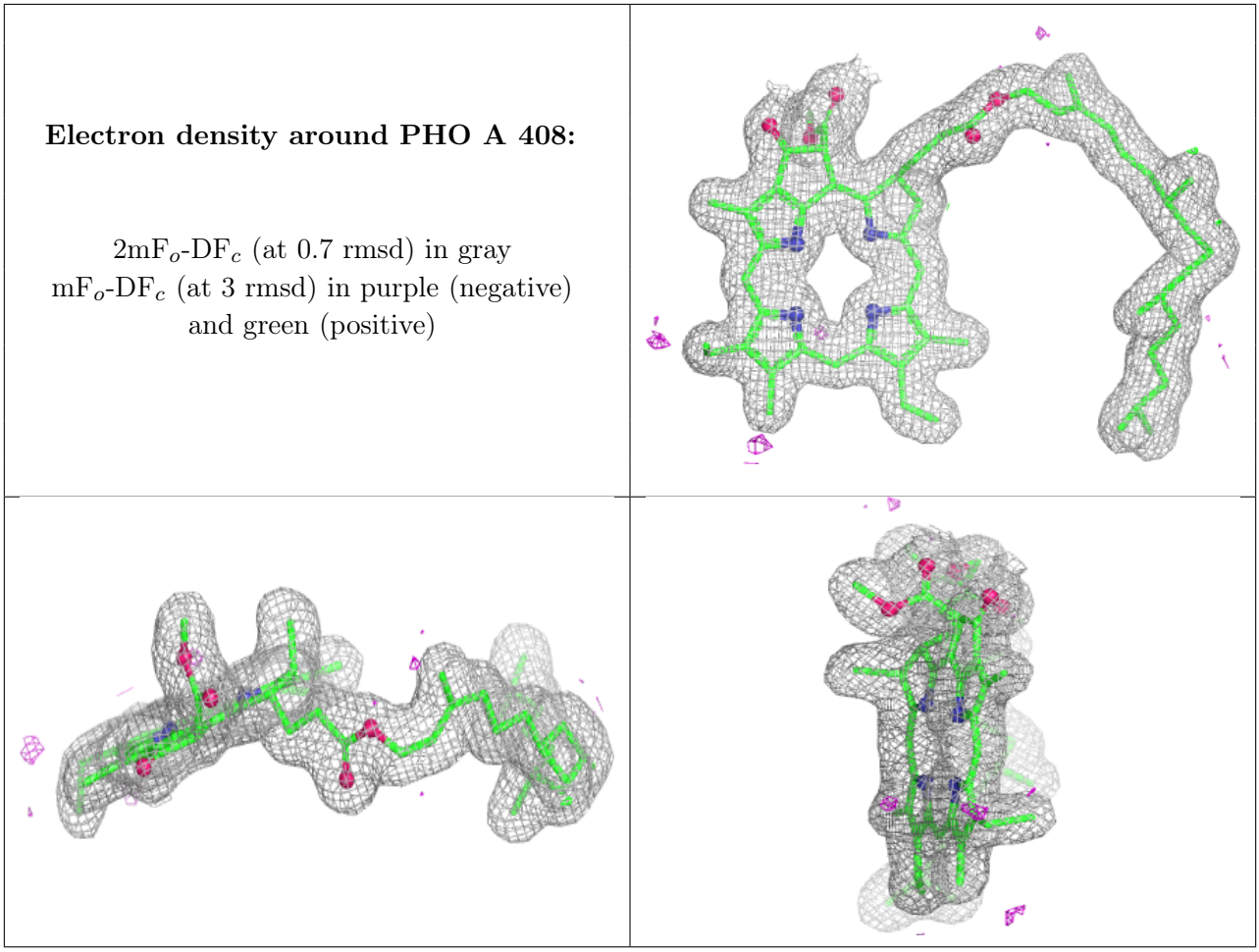






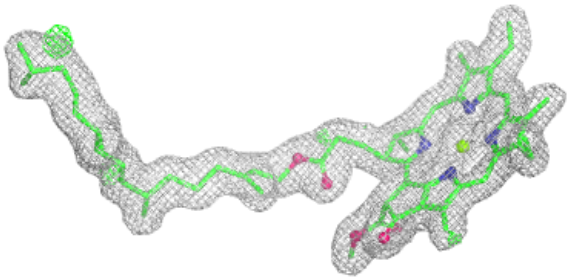
Electron density around PHO A 408:

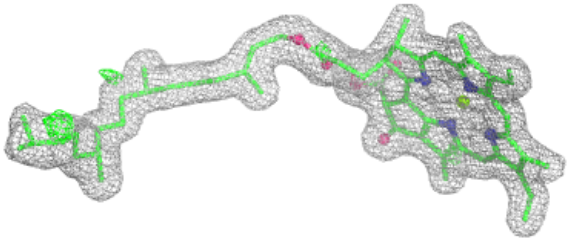
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

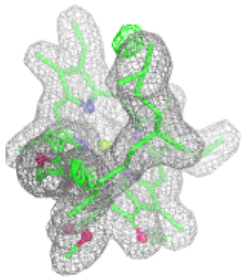


Electron density around CLA A 405:

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

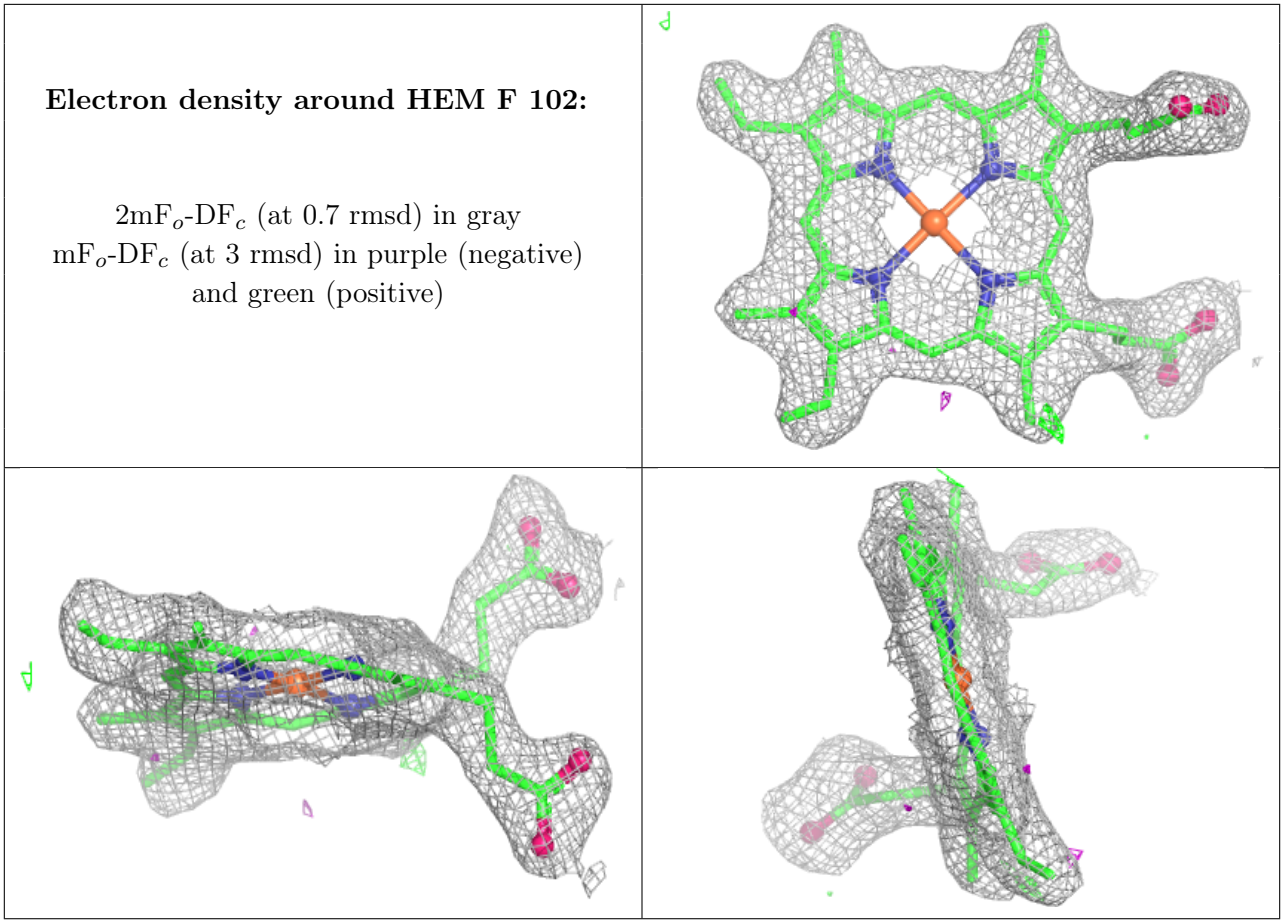






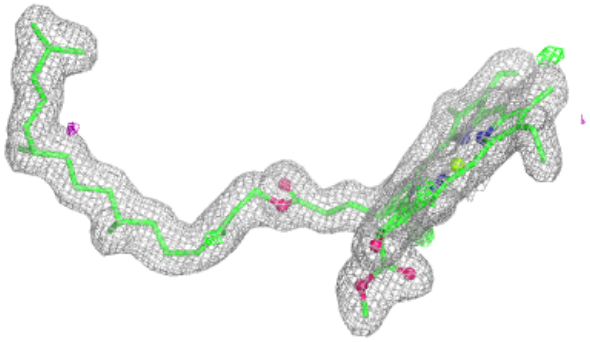
Electron density around HEM F 102:

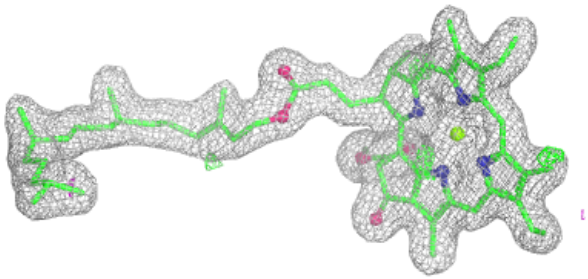
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

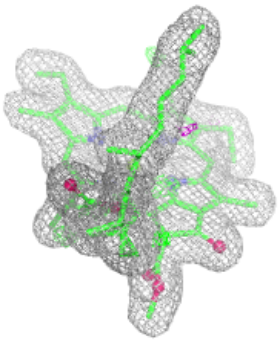


Electron density around CLA D 401:

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

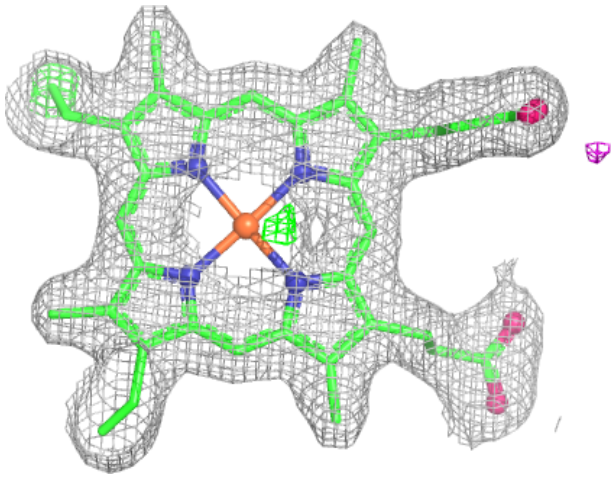


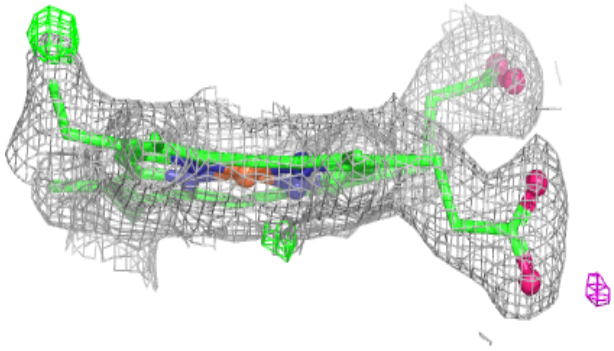


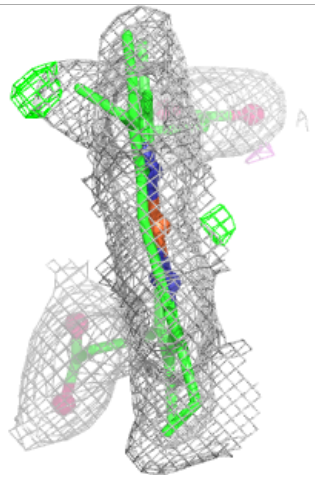


Electron density around HEC v 202:

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

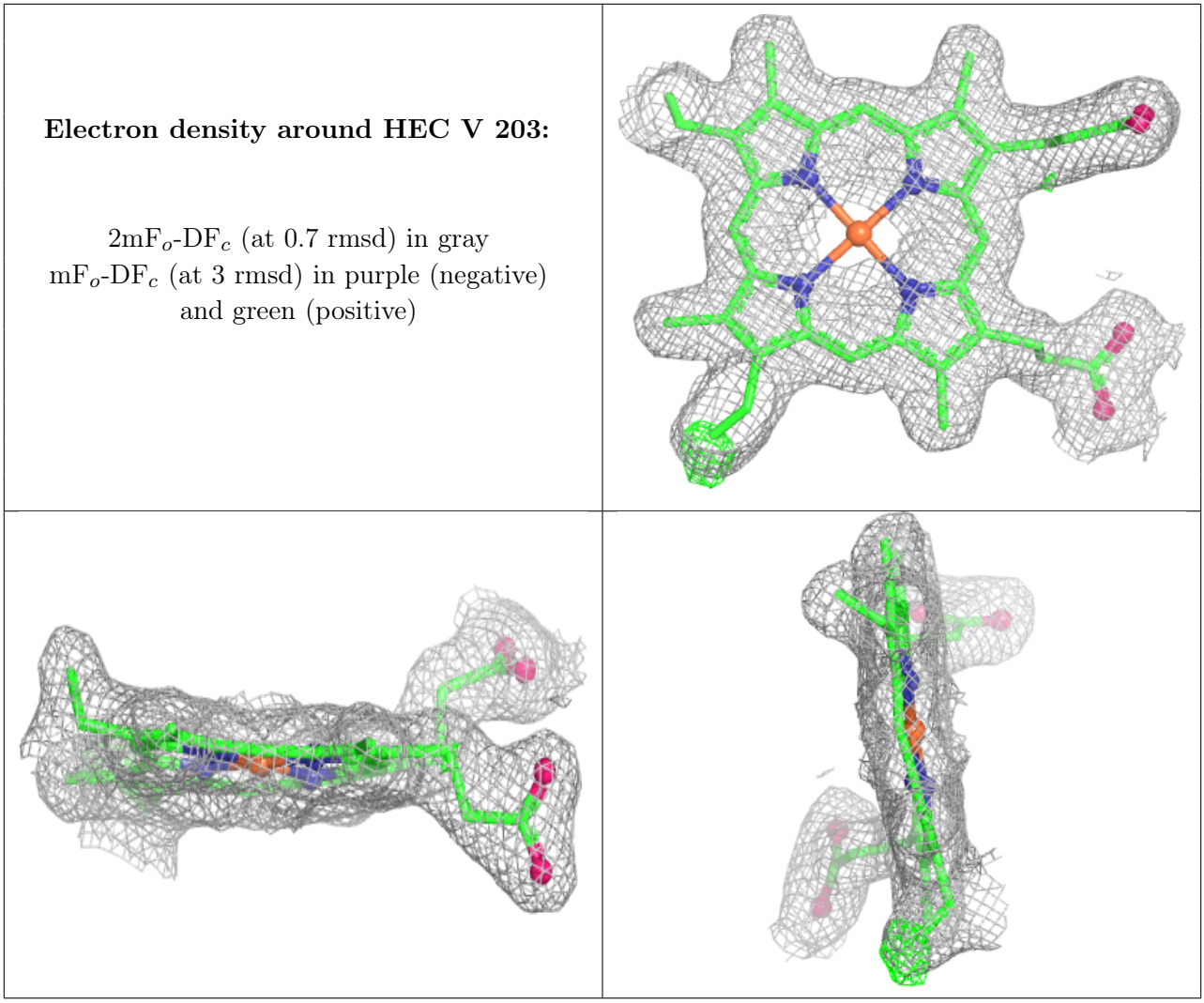






Electron density around HEC V 203:

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



6.5 Other polymers (i)

There are no such residues in this entry.