wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 04:36 PM JST

PDB ID	:	8GN0 / pdb_00008gn0
Title	:	Crystal structure of DCBQ-bound photosystem II complex
Authors	:	Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on	:	2022-08-22
Resolution	:	2.15 Å(reported)

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

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

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

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

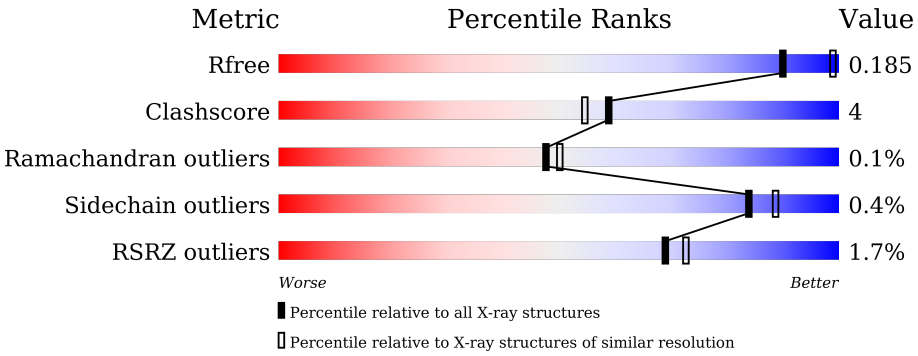
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	344	88% 9%
1	a	344	3% 90% 7%
2	B	505	2% 94% 6%
2	b	505	86% 9%
3	C	455	92% 7%
3	c	455	92% 8%

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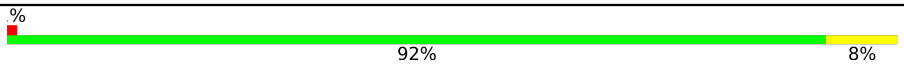
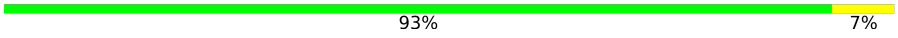
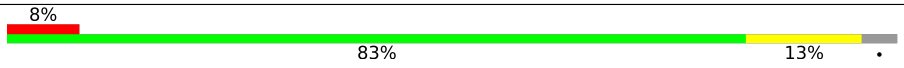
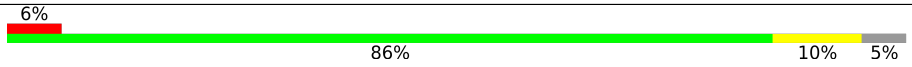
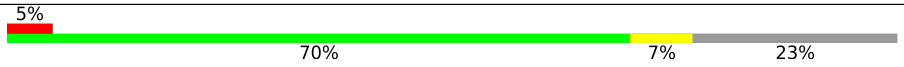
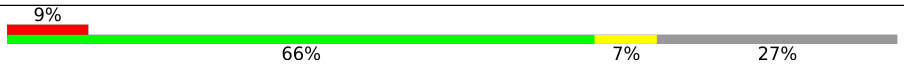
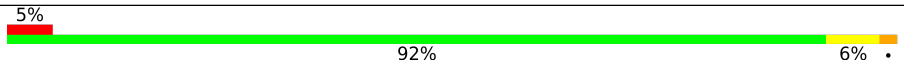
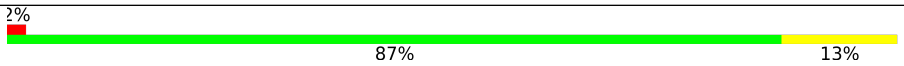
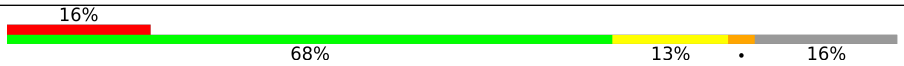
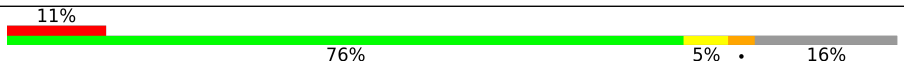
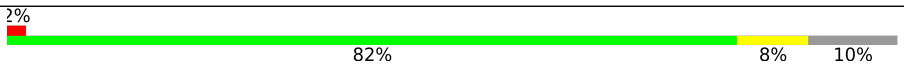
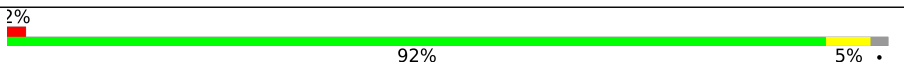
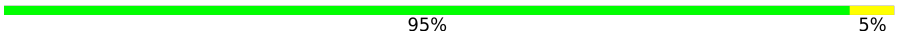
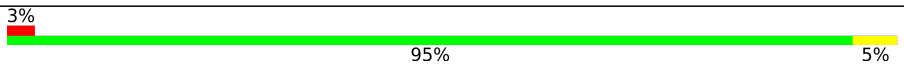
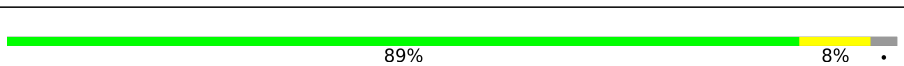
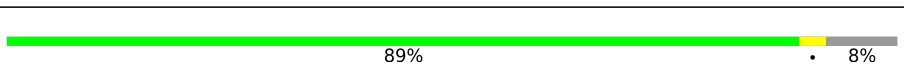
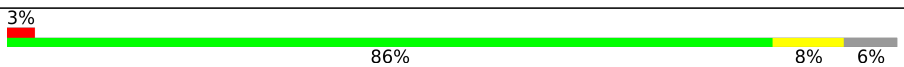
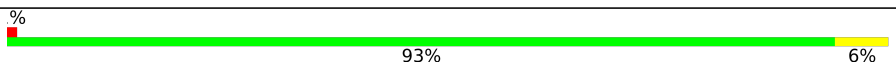
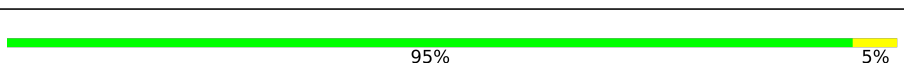
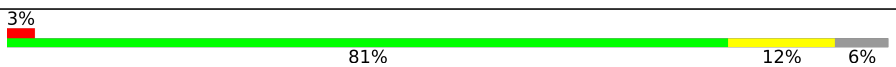
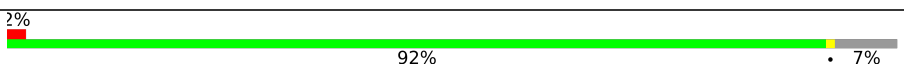
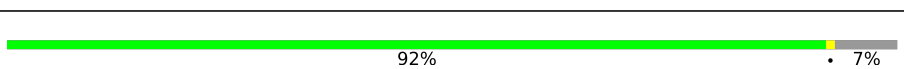
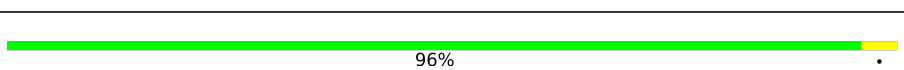
Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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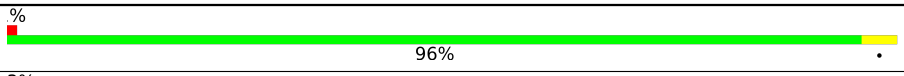
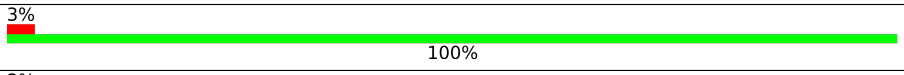
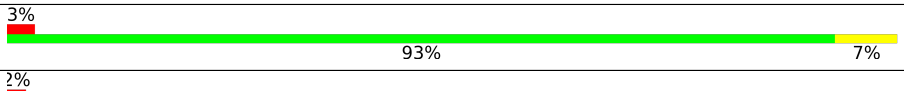
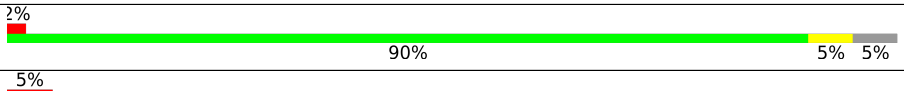
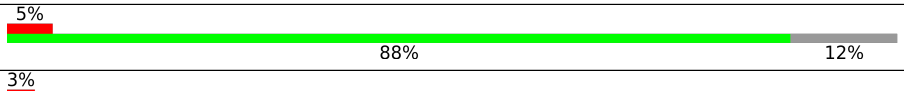
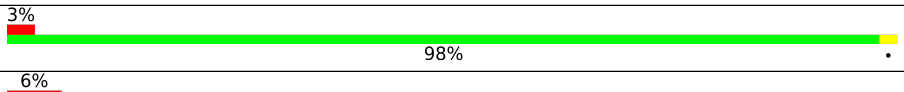
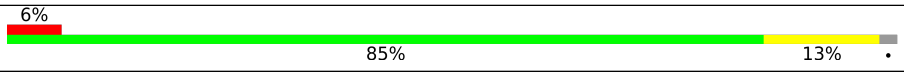
Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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
31	JOX	a	2617	-	X	-	-
42	HEC	V	201	X	-	-	-
42	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 53814 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2614	1715	428	456	15			
1	a	334	Total	C	N	O	S	0	4	0
			2629	1722	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	7	0
			4005	2628	667	697	13			
2	b	483	Total	C	N	O	S	0	9	0
			3833	2520	637	663	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	0	0
			3518	2303	589	613	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	342	Total	C	N	O	S	0	3	0
			2738	1815	447	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			643	422	101	120			
5	e	79	Total	C	N	O	0	1	0
			630	417	99	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			271	184	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	32	Total	C	N	O	S	0	0	0
			256	177	37	41	1			
8	i	32	Total	C	N	O	S	0	0	0
			259	178	37	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			274	184	40	48	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			297	208	43	46			
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			303	204	45	53	1			
11	l	36	Total	C	N	O		0	2	0
			305	206	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	2	0
			267	180	38	48	1			

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	3	0
			1870	1171	314	380	5			
13	o	243	Total	C	N	O	S	0	4	0
			1874	1174	312	382	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			776	493	130	153			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1063	677	177	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			216	139	38	36	3			

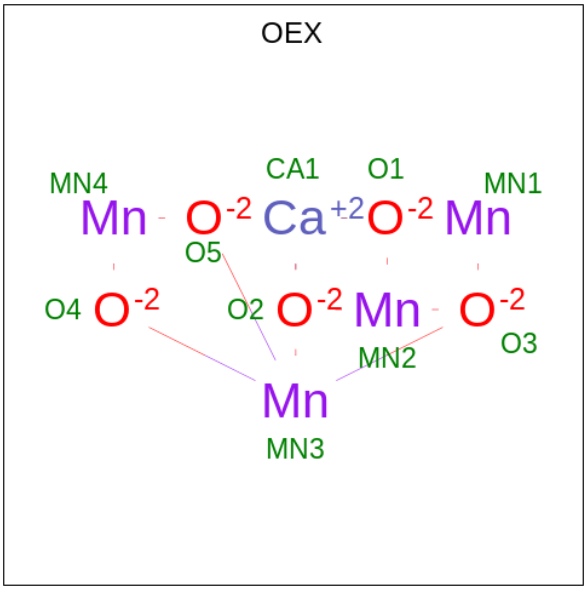
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			275	185	44	46			
18	x	35	Total	C	N	O	0	1	0
			257	176	38	43			

- 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
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			456	312	70	72	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

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

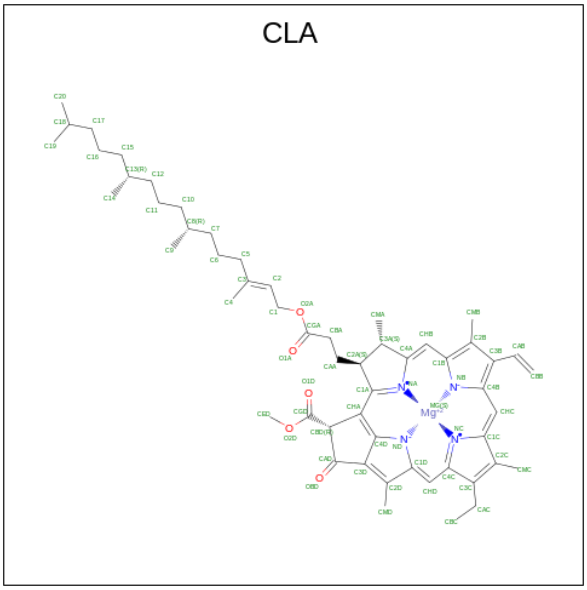
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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

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

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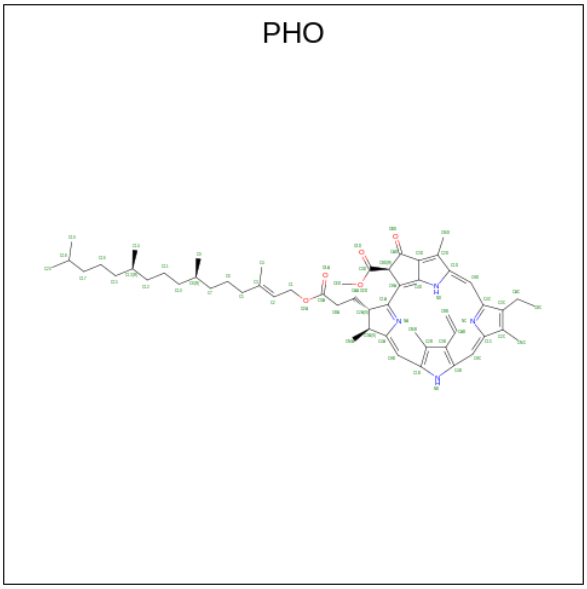
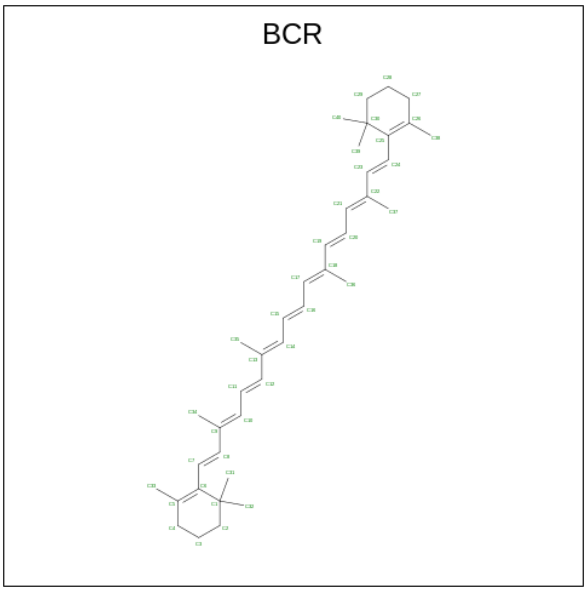
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



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

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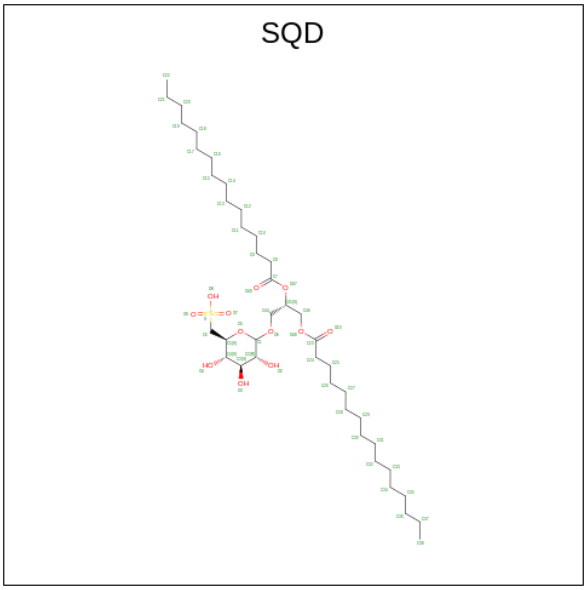
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	z	1	Total C 40 40	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 46 33 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0

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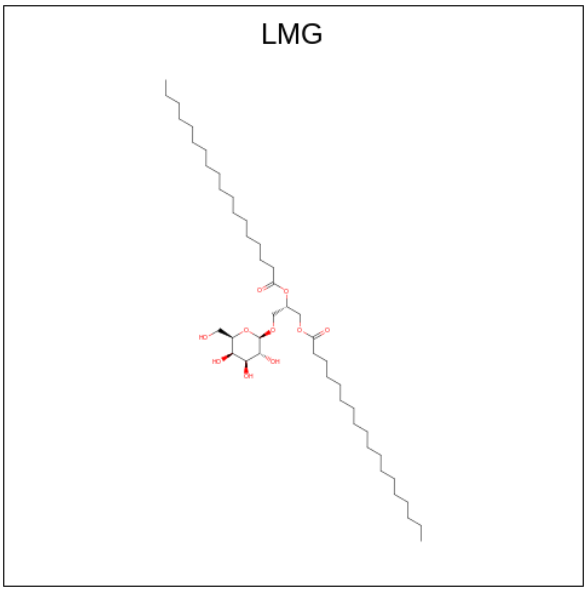
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	a	1	Total C O S 48 35 12 1	0	0
26	b	1	Total C O S 48 35 12 1	0	0
26	d	1	Total C O S 33 23 9 1	0	0
26	l	1	Total C O S 54 41 12 1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	B	1	Total C O 51 41 10	0	0
27	C	1	Total C O 51 41 10	0	0
27	C	1	Total C O 51 41 10	0	0
27	D	1	Total C O 47 37 10	0	0
27	c	1	Total C O 51 41 10	0	0
27	c	1	Total C O 49 39 10	0	0

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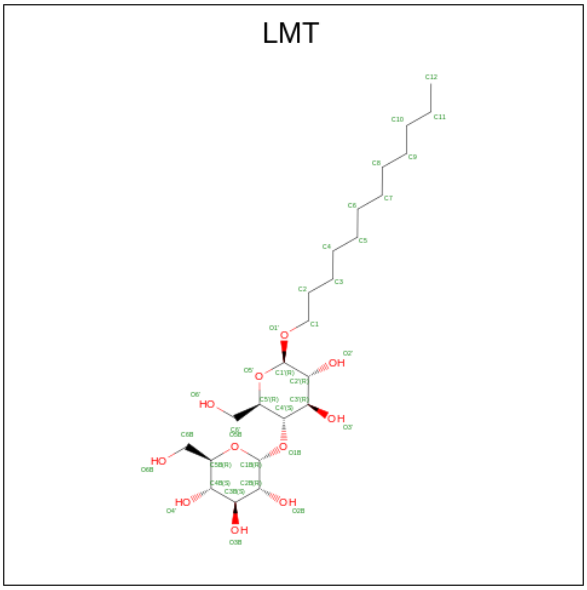
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 51 41 10	0	0
27	d	1	Total C O 51 41 10	0	0
27	m	1	Total C O 51 41 10	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 33 22 11	0	0
28	A	1	Total C O 24 18 6	0	0
28	B	1	Total C O 35 24 11	0	0
28	B	1	Total C O 35 24 11	0	0
28	F	1	Total C O 24 18 6	0	0
28	J	1	Total C O 24 18 6	0	0
28	M	1	Total C O 35 24 11	0	0
28	M	1	Total C O 35 24 11	0	0

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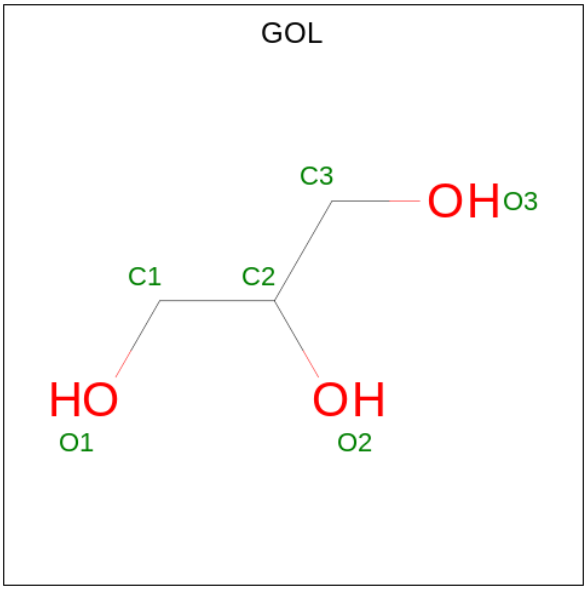
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	T	1	Total C O 24 18 6	0	0
28	Z	1	Total C O 35 24 11	0	0
28	d	1	Total C O 35 24 11	0	0
28	d	1	Total C O 25 19 6	0	0
28	f	1	Total C O 24 18 6	0	0
28	i	1	Total C O 24 18 6	0	0
28	j	1	Total C O 34 23 11	0	0
28	m	1	Total C O 35 24 11	0	0
28	m	1	Total C O 35 24 11	0	0
28	z	1	Total C O 33 22 11	0	0

- Molecule 29 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			6	3	3		
29	B	1	Total	C	O	0	0
			6	3	3		
29	B	1	Total	C	O	0	0
			6	3	3		
29	B	1	Total	C	O	0	0
			6	3	3		
29	C	1	Total	C	O	0	0
			6	3	3		
29	C	1	Total	C	O	0	0
			6	3	3		
29	D	1	Total	C	O	0	0
			6	3	3		
29	E	1	Total	C	O	0	0
			6	3	3		
29	J	1	Total	C	O	0	0
			6	3	3		
29	O	1	Total	C	O	0	0
			6	3	3		
29	O	1	Total	C	O	0	0
			6	3	3		
29	O	1	Total	C	O	0	0
			6	3	3		
29	O	1	Total	C	O	0	0
			6	3	3		
29	U	1	Total	C	O	0	0
			6	3	3		
29	U	1	Total	C	O	0	0
			6	3	3		
29	V	1	Total	C	O	0	0
			6	3	3		
29	a	1	Total	C	O	0	0
			6	3	3		
29	a	1	Total	C	O	0	0
			6	3	3		
29	b	1	Total	C	O	0	0
			6	3	3		
29	b	1	Total	C	O	0	0
			6	3	3		
29	c	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 6 3 3	0	0
29	c	1	Total C O 6 3 3	0	0
29	d	1	Total C O 6 3 3	0	0
29	o	1	Total C O 6 3 3	0	0
29	u	1	Total C O 6 3 3	0	0
29	v	1	Total C O 6 3 3	0	0
29	v	1	Total C O 6 3 3	0	0
29	v	1	Total C O 6 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	2	Total C O 37 32 5	0	0
30	B	3	Total C O 65 58 7	0	0
30	C	2	Total C O 50 45 5	0	0
30	D	3	Total C O 48 44 4	0	0
30	E	2	Total C 15 15	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 5 5	0	0
30	T	1	Total C 13 13	0	0
30	Y	1	Total C 12 12	0	0
30	a	2	Total C O 42 37 5	0	0
30	b	5	Total C O 64 60 4	0	0

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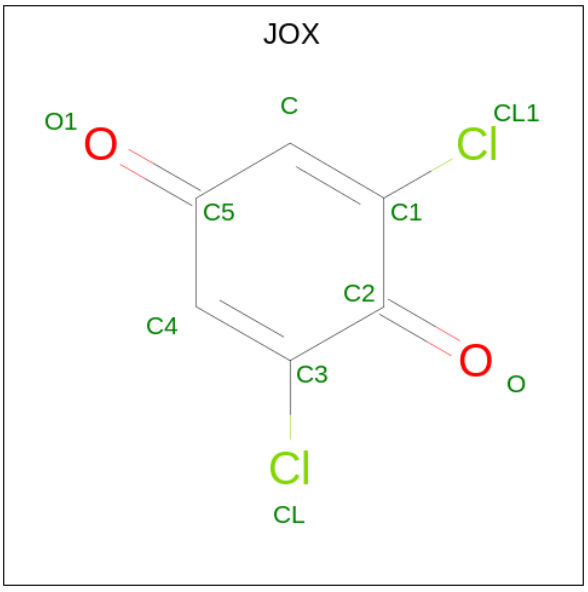
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	4	Total C O 59 54 5	0	0
30	d	2	Total C O 55 48 7	0	0
30	e	1	Total C 15 15	0	0
30	i	1	Total C O 19 15 4	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C 16 16	0	0
30	l	1	Total C O 16 14 2	0	0
30	m	1	Total C O 15 13 2	0	0
30	t	1	Total C 8 8	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is 2,6-bis(chloranyl)cyclohexa-2,5-diene-1,4-dione (CCD ID: JOX) (formula: $C_6H_2Cl_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C Cl O 10 6 2 2	0	0

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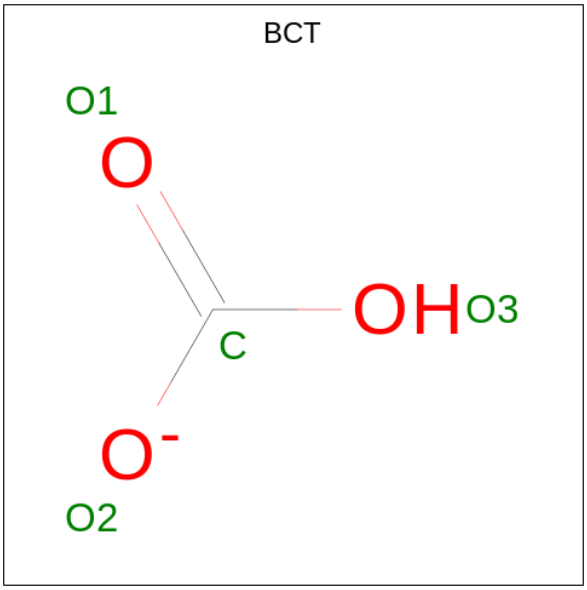
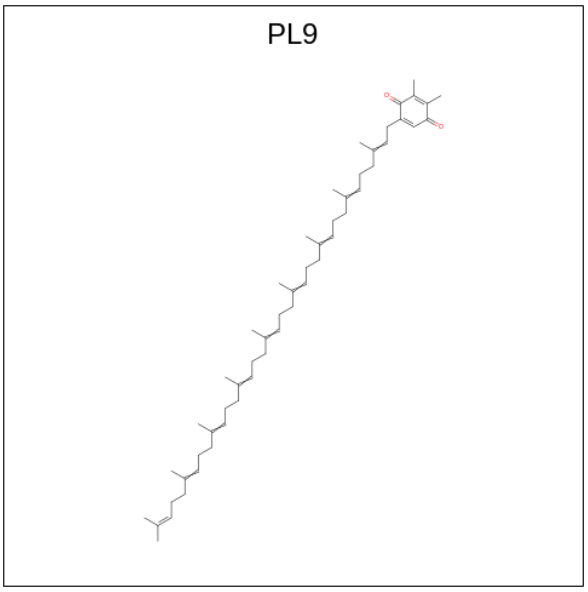
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C Cl O 10 6 2 2	0	0
31	a	1	Total C Cl O 10 6 2 2	0	0
31	a	1	Total C Cl O 10 6 2 2	0	0

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



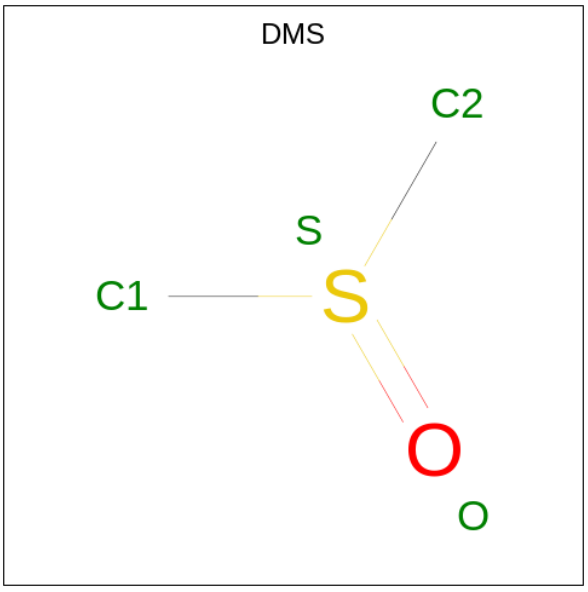
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 4 1 3	0	0
32	a	1	Total C O 4 1 3	0	0

- Molecule 33 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
33	A	1	Total C 39 39	0	0
33	D	1	Total C O 55 53 2	0	0
33	d	1	Total C O 55 53 2	0	0
33	x	1	Total C 39 39	0	0

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



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

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

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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	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	l	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	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		

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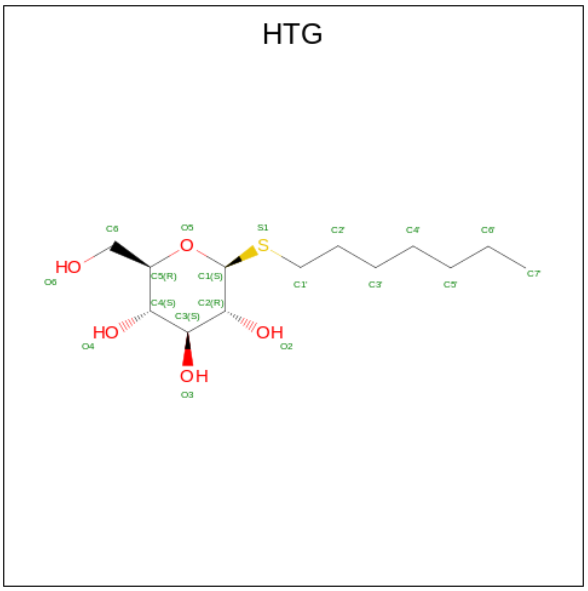
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		

- 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		
35	O	1	Total	Ca	0	0
			1	1		
35	b	1	Total	Ca	0	0
			1	1		
35	c	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

- 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	0	1
			38	26	10	2		
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	H	1	Total	C	O	S	0	0
			17	12	4	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		

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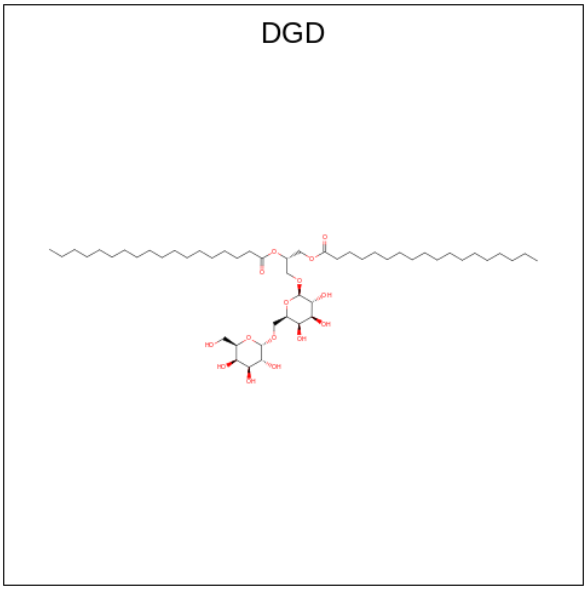
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19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

- 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	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			58	43	15		

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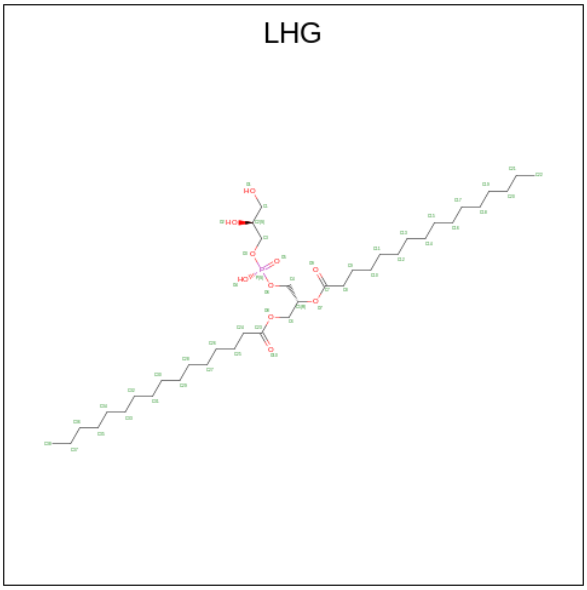
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 53 42 11	0	0
37	H	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	h	1	Total C O 62 47 15	0	0

- 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 39 28 10 1	0	0
38	E	1	Total C O P 40 29 10 1	0	0
38	L	1	Total C O P 49 38 10 1	0	0

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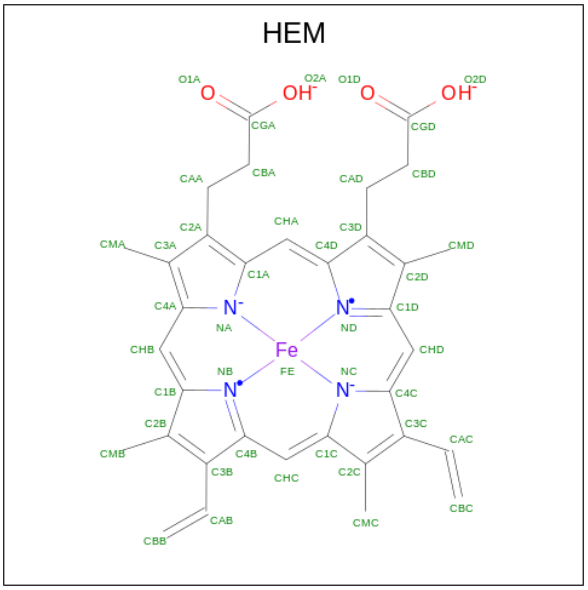
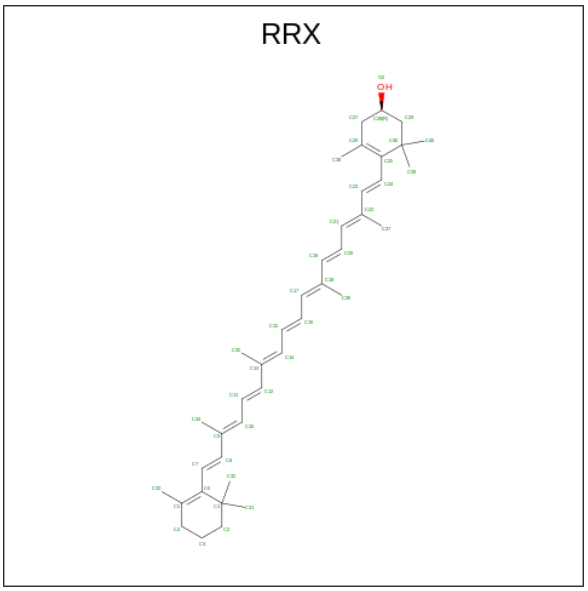
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	d	1	Total C O P 43 32 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	e	1	Total C O P 40 29 10 1	0	0
38	l	1	Total C O P 49 38 10 1	0	0

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



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

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

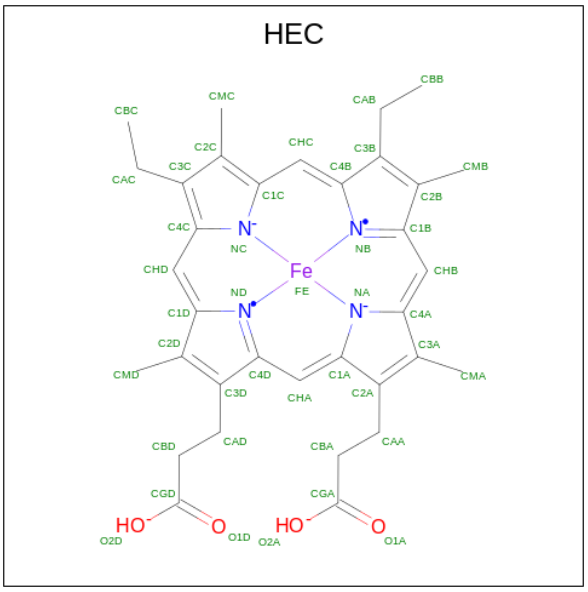


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	H	1	Total C O 41 40 1	0	0
40	h	1	Total C O 41 40 1	0	0

- 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	K	1	Total Mg 1 1	0	0
41	j	1	Total Mg 1 1	0	0
41	k	1	Total Mg 1 1	0	0

- Molecule 42 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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	133	Total	O	0	0
			133	133		
43	B	302	Total	O	0	0
			302	302		
43	C	192	Total	O	0	0
			192	192		
43	D	146	Total	O	0	1
			147	147		
43	E	25	Total	O	0	0
			25	25		
43	F	9	Total	O	0	0
			9	9		
43	H	41	Total	O	0	0
			41	41		
43	I	8	Total	O	0	0
			8	8		
43	J	10	Total	O	0	0
			10	10		
43	K	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	15	Total O 15 15	0	0
43	M	12	Total O 12 12	0	0
43	O	144	Total O 145 145	0	1
43	T	12	Total O 12 12	0	0
43	U	79	Total O 79 79	0	0
43	V	113	Total O 113 113	0	0
43	Y	4	Total O 4 4	0	0
43	X	15	Total O 15 15	0	0
43	Z	8	Total O 8 8	0	0
43	a	122	Total O 122 122	0	0
43	b	250	Total O 251 251	0	1
43	c	211	Total O 211 211	0	0
43	d	146	Total O 147 147	0	1
43	e	19	Total O 19 19	0	0
43	f	7	Total O 7 7	0	0
43	h	27	Total O 27 27	0	0
43	i	8	Total O 8 8	0	0
43	j	10	Total O 10 10	0	0
43	k	5	Total O 5 5	0	0
43	l	20	Total O 20 20	0	0
43	m	11	Total O 11 11	0	0

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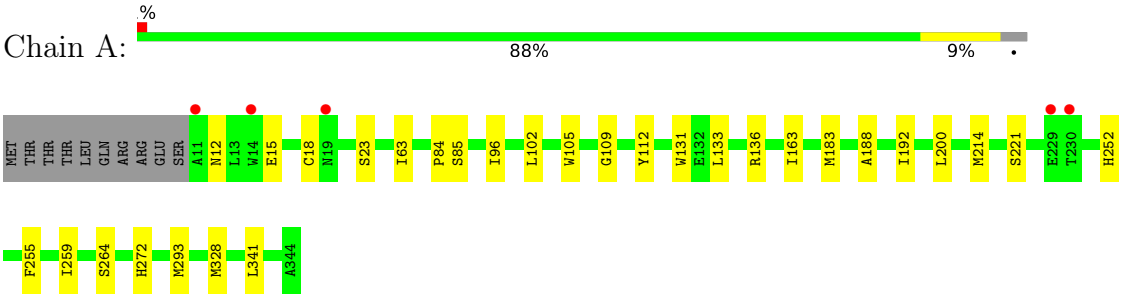
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	o	143	Total O 144 144	0	1
43	t	10	Total O 10 10	0	0
43	u	78	Total O 78 78	0	0
43	v	93	Total O 93 93	0	0
43	y	6	Total O 6 6	0	0
43	x	4	Total O 4 4	0	0
43	z	6	Total O 6 6	0	0

3 Residue-property plots

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

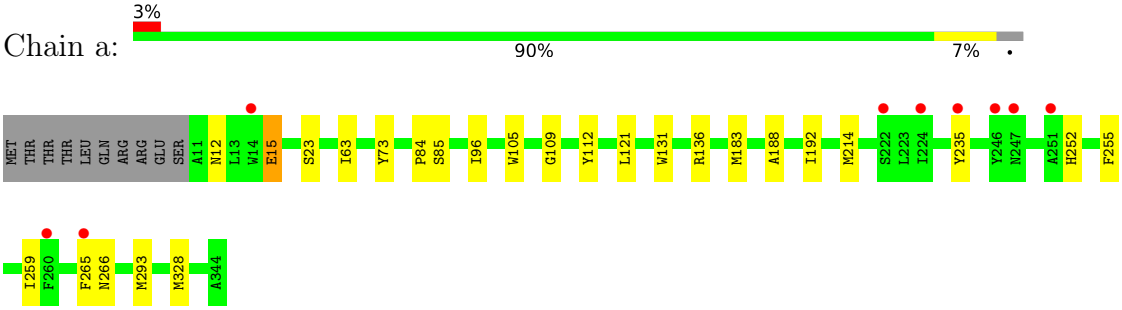
• Molecule 1: Photosystem II protein D1

Chain A:



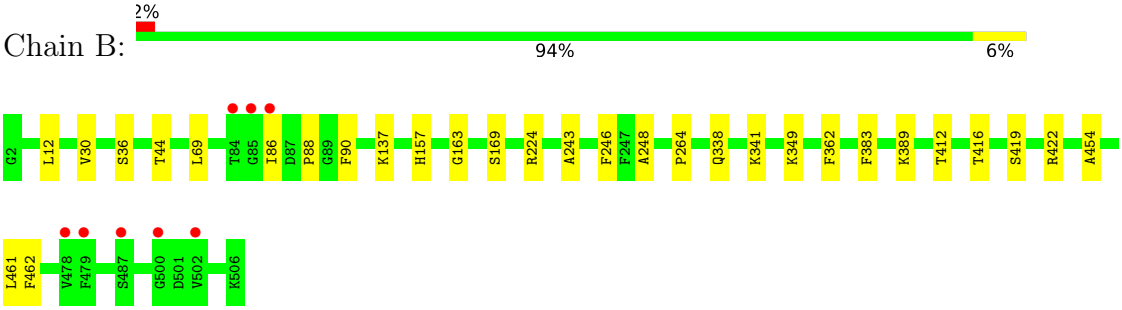
• Molecule 1: Photosystem II protein D1

Chain a:



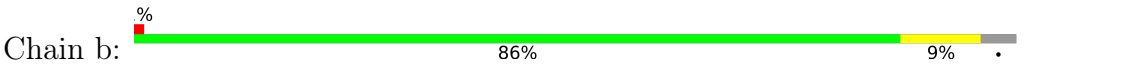
• Molecule 2: Photosystem II CP47 reaction center protein

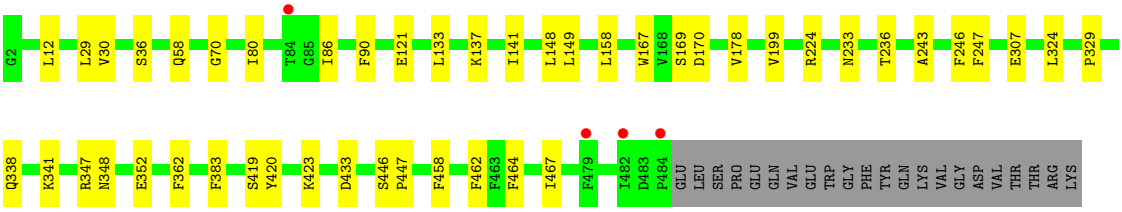
Chain B:



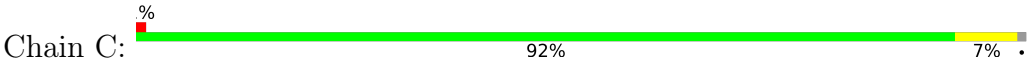
• Molecule 2: Photosystem II CP47 reaction center protein

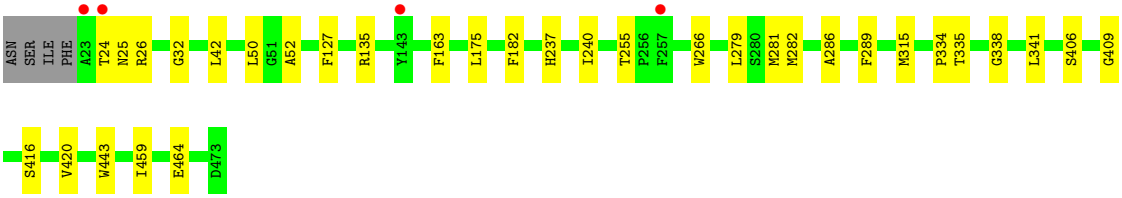
Chain b:



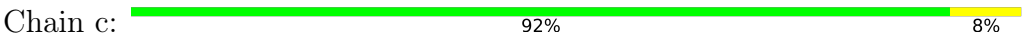


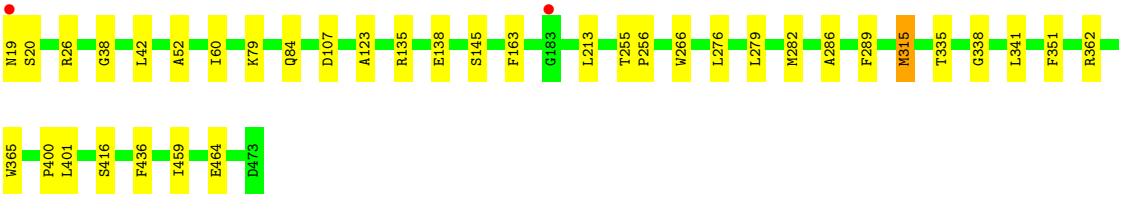
• Molecule 3: Photosystem II CP43 reaction center protein



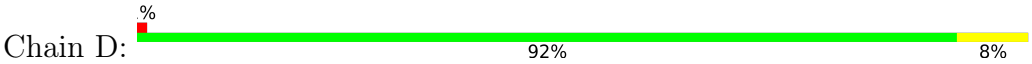


• Molecule 3: Photosystem II CP43 reaction center protein





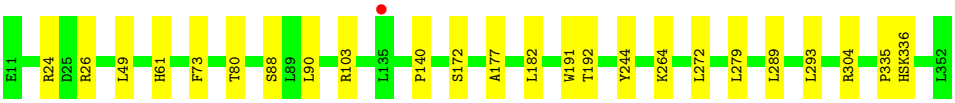
• Molecule 4: Photosystem II D2 protein



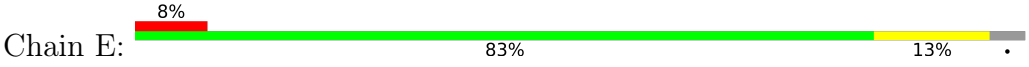


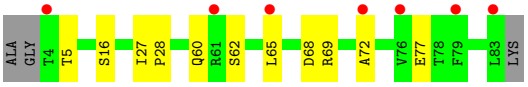
• Molecule 4: Photosystem II D2 protein



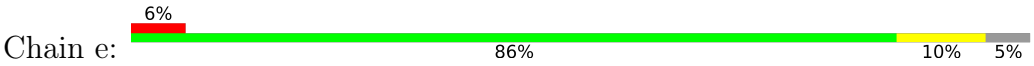


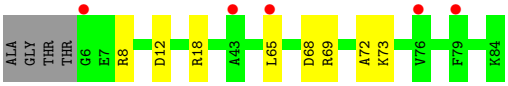
• Molecule 5: Cytochrome b559 subunit alpha





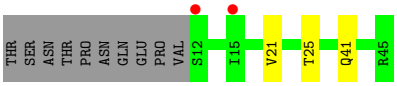
• Molecule 5: Cytochrome b559 subunit alpha





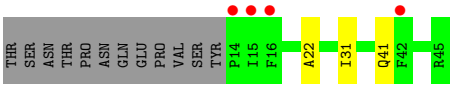
• Molecule 6: Cytochrome b559 subunit beta



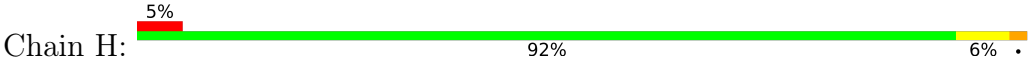


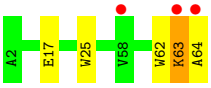
• Molecule 6: Cytochrome b559 subunit beta



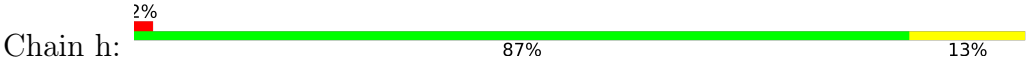


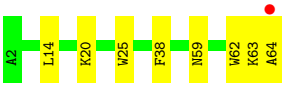
• Molecule 7: Photosystem II reaction center protein H





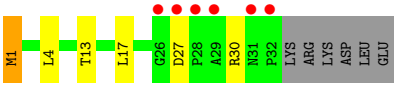
• Molecule 7: Photosystem II reaction center protein H





• Molecule 8: Photosystem II reaction center protein I

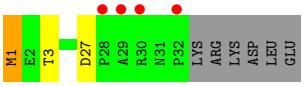




• Molecule 8: Photosystem II reaction center protein I

Chain i:

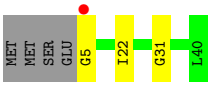




• Molecule 9: Photosystem II reaction center protein J

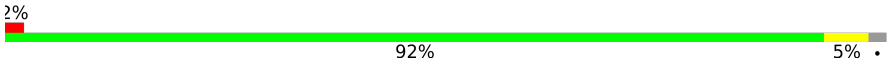
Chain J:

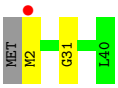




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

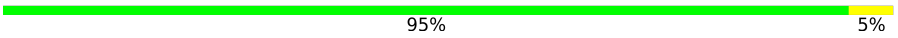
Chain K:

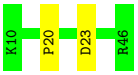


There are no outlier residues recorded for this chain.

• Molecule 10: Photosystem II reaction center protein K

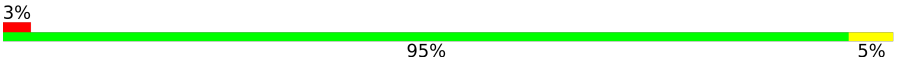
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

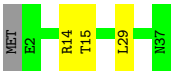




• Molecule 11: Photosystem II reaction center protein L

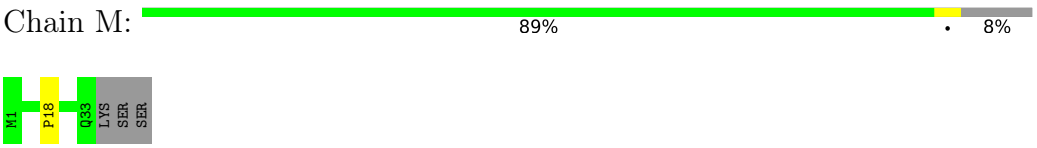
Chain l:





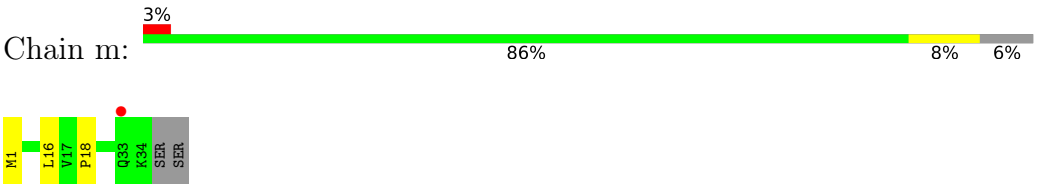
• Molecule 12: Photosystem II reaction center protein M

Chain M:



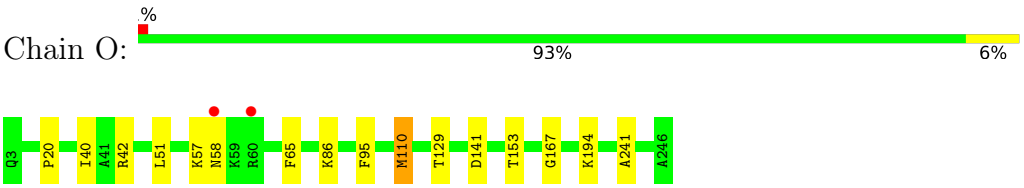
• Molecule 12: Photosystem II reaction center protein M

Chain m:



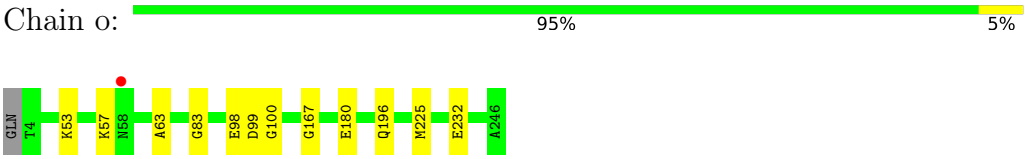
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



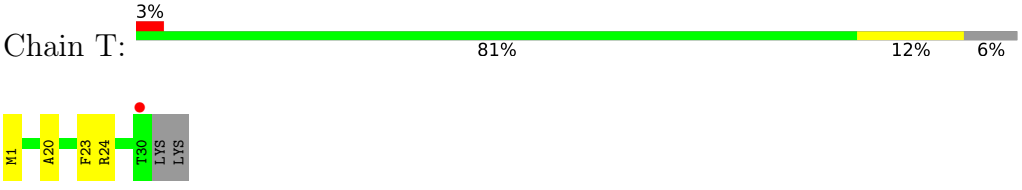
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



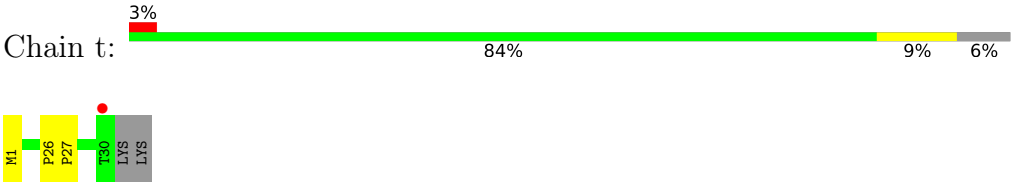
• Molecule 14: Photosystem II reaction center protein T

Chain T:



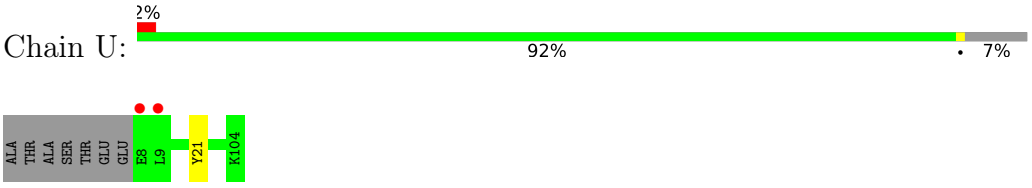
• Molecule 14: Photosystem II reaction center protein T

Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

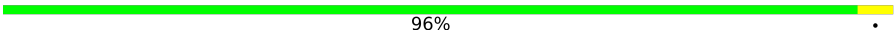
Chain u:





• Molecule 16: Cytochrome c-550

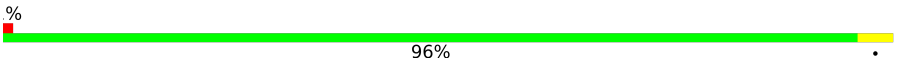
Chain V:





• Molecule 16: Cytochrome c-550

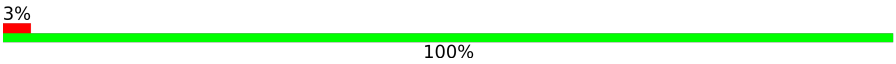
Chain v:





• Molecule 17: Photosystem II reaction center protein Ycf12

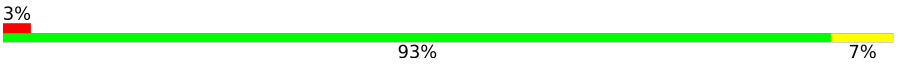
Chain Y:

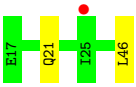




• Molecule 17: Photosystem II reaction center protein Ycf12

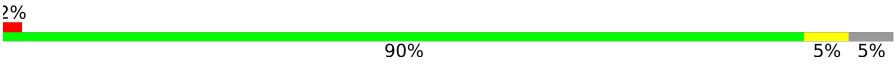
Chain y:

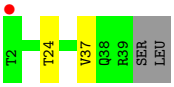




• Molecule 18: Photosystem II reaction center protein X

Chain X:

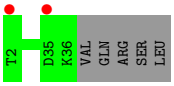




• Molecule 18: Photosystem II reaction center protein X

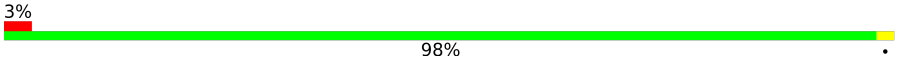
Chain x:





• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

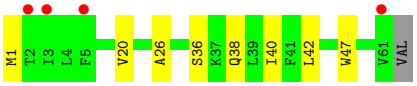




• Molecule 19: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.22Å 228.21Å 287.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.15 49.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.15) 91.1 (49.00-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.151 , 0.185 0.153 , 0.185	Depositor DCC
R_{free} test set	21442 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 69.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53814	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/2708	0.51	0/3695
1	a	0.35	0/2725	0.53	0/3716
2	B	0.35	0/4163	0.48	0/5672
2	b	0.33	0/3994	0.48	0/5442
3	C	0.29	0/3613	0.45	0/4919
3	c	0.29	0/3632	0.46	0/4945
4	D	0.37	0/2804	0.49	0/3820
4	d	0.35	0/2819	0.47	0/3840
5	E	0.23	0/665	0.41	0/911
5	e	0.23	0/652	0.43	0/893
6	F	0.23	0/280	0.43	0/382
6	f	0.24	0/262	0.42	0/356
7	H	0.25	0/511	0.41	0/697
7	h	0.24	0/522	0.41	0/711
8	I	0.21	0/253	0.37	0/345
8	i	0.21	0/256	0.36	0/349
9	J	0.25	0/257	0.37	0/349
9	j	0.24	0/280	0.37	0/379
10	K	0.23	0/310	0.39	0/426
10	k	0.29	0/299	0.42	0/412
11	L	0.41	0/313	0.41	0/426
11	l	0.36	0/318	0.47	0/433
12	M	0.31	0/266	0.47	0/364
12	m	0.36	0/266	0.49	0/363
13	O	0.31	0/1910	0.50	0/2592
13	o	0.30	0/1917	0.50	0/2599
14	T	0.36	0/257	0.41	0/349
14	t	0.36	0/257	0.44	0/349
15	U	0.34	0/790	0.48	0/1071
15	u	0.33	0/785	0.50	0/1064
16	V	0.32	0/1087	0.46	0/1475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.27	0/1082	0.43	0/1472
17	Y	0.20	0/219	0.32	0/293
17	y	0.18	0/217	0.32	0/290
18	X	0.18	0/278	0.29	0/376
18	x	0.17	0/263	0.27	0/356
19	Z	0.18	0/472	0.37	0/646
19	z	0.18	0/457	0.36	0/626
All	All	0.32	0/42159	0.47	0/57403

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2614	0	2510	21	0
1	a	2629	0	2537	18	0
2	B	4005	0	3863	26	0
2	b	3833	0	3711	39	0
3	C	3494	0	3418	24	0
3	c	3518	0	3434	30	0
4	D	2726	0	2629	22	0
4	d	2738	0	2643	20	0
5	E	643	0	618	8	0
5	e	630	0	607	7	0
6	F	271	0	270	2	0
6	f	255	0	263	3	0
7	H	498	0	518	7	0
7	h	506	0	531	8	0
8	I	256	0	266	6	0
8	i	259	0	268	3	0
9	J	251	0	257	3	0
9	j	274	0	277	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	297	0	314	0	0
10	k	289	0	294	2	0
11	L	303	0	316	2	0
11	l	305	0	324	3	0
12	M	267	0	288	1	0
12	m	270	0	293	2	0
13	O	1870	0	1843	13	0
13	o	1874	0	1852	9	0
14	T	258	0	261	2	0
14	t	258	0	261	1	0
15	U	776	0	777	1	0
15	u	774	0	773	0	0
16	V	1063	0	1078	4	0
16	v	1058	0	1053	3	0
17	Y	218	0	238	0	0
17	y	216	0	227	3	0
18	X	275	0	301	2	0
18	x	257	0	288	0	0
19	Z	471	0	498	0	0
19	z	456	0	468	7	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	10	0
23	B	1040	0	1152	23	0
23	C	845	0	936	40	0
23	D	130	0	144	4	0
23	a	195	0	216	6	0
23	b	1040	0	1152	27	0
23	c	845	0	936	31	0
23	d	195	0	216	6	0
24	A	128	0	148	4	0
24	a	128	0	148	2	0
25	A	40	0	56	0	0
25	B	160	0	224	9	0
25	C	80	0	112	5	0
25	D	40	0	56	2	0
25	K	40	0	56	1	0
25	T	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	40	0	56	2	0
25	a	40	0	56	2	0
25	b	120	0	168	7	0
25	c	40	0	56	2	0
25	d	40	0	56	2	0
25	k	40	0	56	1	0
25	y	40	0	56	2	0
25	z	40	0	56	2	0
26	A	46	0	59	2	0
26	B	54	0	78	2	0
26	D	99	0	135	4	0
26	a	102	0	138	3	0
26	b	48	0	63	1	0
26	d	33	0	39	2	0
26	l	54	0	78	4	0
27	A	51	0	72	3	0
27	B	51	0	72	1	0
27	C	102	0	144	2	0
27	D	47	0	64	2	0
27	c	151	0	212	9	0
27	d	51	0	72	4	0
27	m	51	0	72	1	0
28	A	57	0	74	9	0
28	B	70	0	92	2	0
28	F	24	0	35	0	0
28	J	24	0	35	0	0
28	M	70	0	92	1	0
28	T	24	0	35	0	0
28	Z	35	0	46	2	0
28	d	60	0	81	7	0
28	f	24	0	35	0	0
28	i	24	0	35	1	0
28	j	34	0	40	1	0
28	m	70	0	92	1	0
28	z	33	0	35	4	0
29	A	12	0	16	0	0
29	B	18	0	24	5	0
29	C	12	0	16	2	0
29	D	6	0	8	0	0
29	E	6	0	8	0	0
29	J	6	0	8	0	0
29	O	24	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	U	12	0	15	0	0
29	V	6	0	8	0	0
29	a	12	0	16	1	0
29	b	12	0	16	4	0
29	c	18	0	24	1	0
29	d	6	0	8	0	0
29	o	6	0	8	0	0
29	u	6	0	8	0	0
29	v	18	0	24	0	0
30	A	37	0	0	0	0
30	B	65	0	0	0	0
30	C	50	0	0	0	0
30	D	48	0	0	0	0
30	E	15	0	0	0	0
30	I	40	0	0	0	0
30	J	5	0	0	0	0
30	T	13	0	0	0	0
30	Y	12	0	0	0	0
30	a	42	0	0	0	0
30	b	64	0	0	0	0
30	c	59	0	0	0	0
30	d	55	0	0	0	0
30	e	15	0	0	0	0
30	i	19	0	0	0	0
30	j	16	0	0	0	0
30	k	16	0	0	0	0
30	l	16	0	0	0	0
30	m	15	0	0	0	0
30	t	8	0	0	0	0
30	x	18	0	0	0	0
31	A	20	0	0	0	0
31	a	20	0	0	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	A	39	0	59	4	0
33	D	55	0	80	0	0
33	d	55	0	80	1	0
33	x	39	0	59	2	0
34	A	28	0	42	1	0
34	B	52	0	78	6	0
34	C	40	0	60	1	0
34	D	20	0	30	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	O	56	0	84	1	0
34	T	8	0	12	0	0
34	U	12	0	18	1	0
34	V	40	0	60	2	0
34	X	4	0	6	0	0
34	a	20	0	30	1	0
34	b	44	0	66	1	0
34	c	72	0	108	3	0
34	d	24	0	36	1	0
34	l	4	0	6	0	0
34	o	52	0	78	3	0
34	t	4	0	6	0	0
34	u	12	0	18	0	0
34	v	40	0	60	1	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	o	1	0	0	0	0
36	B	95	0	130	4	0
36	C	57	0	78	3	0
36	H	17	0	22	2	0
36	I	19	0	26	2	0
36	V	19	0	26	0	0
36	b	95	0	130	10	0
36	c	57	0	78	0	0
36	d	38	0	52	3	0
36	i	19	0	26	1	0
36	o	19	0	26	2	0
37	C	182	0	238	6	0
37	D	53	0	71	3	0
37	H	62	0	82	0	0
37	c	186	0	246	2	0
37	h	62	0	82	0	0
38	D	137	0	196	4	0
38	E	40	0	53	0	0
38	L	49	0	74	1	0
38	d	141	0	207	6	0
38	e	40	0	53	1	0
38	l	49	0	74	2	0
39	F	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	e	43	0	30	2	0
40	H	41	0	56	3	0
40	h	41	0	56	3	0
41	J	1	0	0	0	0
41	K	1	0	0	0	0
41	j	1	0	0	0	0
41	k	1	0	0	0	0
42	V	43	0	30	0	0
42	v	43	0	30	0	0
43	A	133	0	0	0	0
43	B	302	0	0	3	0
43	C	192	0	0	0	0
43	D	147	0	0	1	0
43	E	25	0	0	0	0
43	F	9	0	0	0	0
43	H	41	0	0	1	0
43	I	8	0	0	0	0
43	J	10	0	0	0	0
43	K	10	0	0	0	0
43	L	15	0	0	0	0
43	M	12	0	0	0	0
43	O	145	0	0	2	0
43	T	12	0	0	0	0
43	U	79	0	0	0	0
43	V	113	0	0	0	0
43	X	15	0	0	0	0
43	Y	4	0	0	0	0
43	Z	8	0	0	0	0
43	a	122	0	0	1	0
43	b	251	0	0	1	0
43	c	211	0	0	2	0
43	d	147	0	0	1	0
43	e	19	0	0	0	0
43	f	7	0	0	0	0
43	h	27	0	0	0	0
43	i	8	0	0	0	0
43	j	10	0	0	0	0
43	k	5	0	0	0	0
43	l	20	0	0	0	0
43	m	11	0	0	0	0
43	o	144	0	0	1	0
43	t	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	u	78	0	0	0	0
43	v	93	0	0	0	0
43	x	4	0	0	0	0
43	y	6	0	0	0	0
43	z	6	0	0	0	0
All	All	53814	0	52371	454	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 454 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)
13:O:20:PRO:HG3	29:O:302:GOL:H12	1.64	0.79
2:b:433:ASP:HB2	29:b:631:GOL:H11	1.66	0.77
28:d:401:LMT:H22	36:o:301:HTG:H1	1.66	0.76
4:d:192:THR:HG23	23:d:408:CLA:HBC2	1.71	0.73
13:O:194:LYS:NZ	43:O:401:HOH:O	2.23	0.70

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36 34
1	a	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	36 34
2	B	510/505 (101%)	501 (98%)	9 (2%)	0	100 100
2	b	490/505 (97%)	484 (99%)	6 (1%)	0	100 100
3	C	451/455 (99%)	441 (98%)	8 (2%)	2 (0%)	30 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	c	453/455 (100%)	444 (98%)	8 (2%)	1 (0%)	43 44
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100 100
4	d	341/342 (100%)	335 (98%)	6 (2%)	0	100 100
5	E	79/83 (95%)	79 (100%)	0	0	100 100
5	e	78/83 (94%)	78 (100%)	0	0	100 100
6	F	32/44 (73%)	32 (100%)	0	0	100 100
6	f	30/44 (68%)	30 (100%)	0	0	100 100
7	H	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7 3
7	h	62/63 (98%)	59 (95%)	2 (3%)	1 (2%)	7 3
8	I	30/38 (79%)	29 (97%)	1 (3%)	0	100 100
8	i	30/38 (79%)	30 (100%)	0	0	100 100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100 100
9	j	37/40 (92%)	37 (100%)	0	0	100 100
10	K	36/37 (97%)	36 (100%)	0	0	100 100
10	k	35/37 (95%)	35 (100%)	0	0	100 100
11	L	36/37 (97%)	36 (100%)	0	0	100 100
11	l	36/37 (97%)	36 (100%)	0	0	100 100
12	M	33/36 (92%)	33 (100%)	0	0	100 100
12	m	33/36 (92%)	33 (100%)	0	0	100 100
13	O	245/244 (100%)	240 (98%)	5 (2%)	0	100 100
13	o	245/244 (100%)	240 (98%)	5 (2%)	0	100 100
14	T	28/32 (88%)	28 (100%)	0	0	100 100
14	t	28/32 (88%)	28 (100%)	0	0	100 100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100 100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100 100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100 100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100 100
17	Y	28/30 (93%)	28 (100%)	0	0	100 100
17	y	28/30 (93%)	28 (100%)	0	0	100 100
18	X	36/40 (90%)	36 (100%)	0	0	100 100
18	x	34/40 (85%)	34 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	5191/5346 (97%)	5103 (98%)	81 (2%)	7 (0%)	48	50

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ASN
3	C	416	SER
3	c	416	SER
7	H	63	LYS
7	h	63	LYS

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	268/279 (96%)	268 (100%)	0	100	100
1	a	272/279 (98%)	271 (100%)	1 (0%)	84	89
2	B	406/403 (101%)	405 (100%)	1 (0%)	87	92
2	b	389/403 (96%)	386 (99%)	3 (1%)	73	79
3	C	354/356 (99%)	351 (99%)	3 (1%)	73	79
3	c	355/356 (100%)	352 (99%)	3 (1%)	73	79
4	D	275/276 (100%)	274 (100%)	1 (0%)	84	89
4	d	277/276 (100%)	275 (99%)	2 (1%)	76	82
5	E	69/72 (96%)	67 (97%)	2 (3%)	37	39
5	e	66/72 (92%)	66 (100%)	0	100	100
6	F	26/38 (68%)	26 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	54/53 (102%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	27/34 (79%)	27 (100%)	0	100	100
8	i	28/34 (82%)	28 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	31/30 (103%)	31 (100%)	0	100	100
10	k	29/30 (97%)	29 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	206/207 (100%)	205 (100%)	1 (0%)	81	87
13	o	208/207 (100%)	208 (100%)	0	100	100
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	84 (100%)	0	100	100
15	u	84/89 (94%)	83 (99%)	1 (1%)	63	70
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100
17	Y	21/23 (91%)	21 (100%)	0	100	100
17	y	20/23 (87%)	20 (100%)	0	100	100
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	28/33 (85%)	28 (100%)	0	100	100
19	Z	48/51 (94%)	48 (100%)	0	100	100
19	z	44/51 (86%)	44 (100%)	0	100	100
All	All	4239/4368 (97%)	4221 (100%)	18 (0%)	84	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	315	MET
15	u	9	LEU
4	d	90	LEU
1	a	15	GLU
3	c	289	PHE

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

Mol	Chain	Res	Type
1	a	296	ASN
3	c	19	ASN
2	b	394	GLN
3	c	201	ASN
3	C	418	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.53	0	7,9,11	1.36	1 (14%)
4	HSK	d	336[A]	-	9,10,12	13.41	1 (11%)	6,12,16	2.04	3 (50%)
4	HSK	d	336[B]	-	9,11,12	1.76	2 (22%)	6,14,16	4.06	4 (66%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.72	3 (42%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.15	0
19	FME	Z	1	19	8,9,10	0.62	0	7,9,11	1.80	3 (42%)
14	FME	T	1	14	8,9,10	0.79	0	7,9,11	1.73	2 (28%)
8	FME	i	1	8	8,9,10	0.64	0	7,9,11	1.69	3 (42%)
4	HSK	D	336[A]	-	9,10,12	13.04	1 (11%)	6,12,16	1.78	2 (33%)
14	FME	t	1	14	8,9,10	0.69	0	7,9,11	1.76	4 (57%)
4	HSK	D	336[B]	-	9,11,12	1.79	2 (22%)	6,14,16	3.83	4 (66%)
19	FME	z	1	19	8,9,10	0.58	0	7,9,11	1.70	3 (42%)

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

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

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[A]	HSK	OM-ND1	-40.09	0.86	1.38
4	D	336[A]	HSK	OM-ND1	-38.97	0.87	1.38
4	D	336[B]	HSK	OM-ND1	3.84	1.43	1.38
4	d	336[B]	HSK	OM-ND1	3.69	1.43	1.38
4	d	336[B]	HSK	CE1-ND1	-2.36	1.33	1.37

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	336[B]	HSK	ND1-CE1-NE2	-6.13	104.09	111.75
4	d	336[B]	HSK	CE1-ND1-CG	6.00	115.05	107.37
4	D	336[B]	HSK	ND1-CE1-NE2	-5.91	104.35	111.75
4	D	336[B]	HSK	CE1-ND1-CG	5.68	114.64	107.37
4	d	336[B]	HSK	CD2-NE2-CE1	3.53	109.51	105.22

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
19	Z	1	FME	CA-CB-CG-SD
8	i	1	FME	O1-CN-N-CA
19	z	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0
8	i	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 407 ligands modelled in this entry, 15 are monoatomic and 37 are unknown - leaving 355 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	DMS	O	311	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
38	LHG	D	2311	-	38,38,48	0.95	2 (5%)	41,44,54	1.11	3 (7%)
38	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	5 (9%)
23	CLA	b	619	2	69,73,73	2.45	25 (36%)	83,113,113	2.63	32 (38%)
23	CLA	a	2609	1	69,73,73	2.52	24 (34%)	83,113,113	2.47	26 (31%)
34	DMS	c	541	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
25	BCR	b	623	-	41,41,41	0.86	0	56,56,56	1.21	6 (10%)
37	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	6 (7%)
36	HTG	B	627	-	19,19,19	1.02	2 (10%)	23,24,24	1.37	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	O	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	b	637	-	3,3,3	2.74	1 (33%)	3,3,3	0.67	0
36	HTG	c	524	-	19,19,19	1.05	2 (10%)	23,24,24	1.44	2 (8%)
37	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	6 (7%)
29	GOL	C	526	-	5,5,5	1.12	1 (20%)	5,5,5	0.96	0
38	LHG	D	2309	-	48,48,48	0.90	2 (4%)	51,54,54	1.15	5 (9%)
23	CLA	b	615	43	69,73,73	2.52	25 (36%)	83,113,113	2.47	28 (33%)
23	CLA	b	616	2	69,73,73	2.35	25 (36%)	83,113,113	2.46	30 (36%)
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
36	HTG	C	525	-	19,19,19	1.10	2 (10%)	23,24,24	1.69	4 (17%)
42	HEC	V	201	16	50,50,50	1.90	10 (20%)	68,82,82	1.49	8 (11%)
28	LMT	J	303	-	24,24,36	0.54	0	29,29,47	0.94	1 (3%)
34	DMS	o	305	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
23	CLA	B	617	2	69,73,73	2.54	22 (31%)	83,113,113	2.49	29 (34%)
34	DMS	B	646	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
23	CLA	B	612	2	69,73,73	2.56	22 (31%)	83,113,113	2.57	30 (36%)
23	CLA	d	409	4	69,73,73	2.55	24 (34%)	83,113,113	2.48	27 (32%)
33	PL9	D	2306	-	55,55,55	0.69	1 (1%)	68,69,69	1.60	18 (26%)
34	DMS	o	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
34	DMS	o	308	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
23	CLA	C	504	3	69,73,73	2.51	22 (31%)	83,113,113	2.39	27 (32%)
23	CLA	d	402	43	69,73,73	2.48	22 (31%)	83,113,113	2.57	28 (33%)
26	SQD	d	417	-	31,32,54	1.97	4 (12%)	34,36,65	1.57	4 (11%)
36	HTG	b	604	-	19,19,19	1.07	2 (10%)	23,24,24	1.66	4 (17%)
34	DMS	V	211	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
29	GOL	b	631	-	5,5,5	1.07	0	5,5,5	0.60	0
23	CLA	a	2613	1	69,73,73	2.28	22 (31%)	83,113,113	2.52	29 (34%)
26	SQD	a	2615	-	47,48,54	1.01	3 (6%)	56,59,65	1.79	12 (21%)
29	GOL	E	104	-	5,5,5	1.00	0	5,5,5	0.88	0
40	RRX	H	102	-	42,42,42	0.69	0	57,58,58	1.47	9 (15%)
23	CLA	c	506	3	69,73,73	2.56	24 (34%)	83,113,113	2.39	26 (31%)
34	DMS	V	206	-	3,3,3	2.71	1 (33%)	3,3,3	0.73	0
26	SQD	D	2308	-	44,45,54	1.12	3 (6%)	53,56,65	1.31	8 (15%)
34	DMS	B	636	-	3,3,3	2.57	1 (33%)	3,3,3	0.58	0
23	CLA	B	602	43	69,73,73	2.66	26 (37%)	83,113,113	2.28	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	JOX	A	419	-	10,10,10	1.98	4 (40%)	14,14,14	4.84	11 (78%)
34	DMS	c	543	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
25	BCR	c	517	-	41,41,41	0.75	0	56,56,56	1.57	9 (16%)
34	DMS	C	535	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
36	HTG	i	102	-	19,19,19	1.13	2 (10%)	23,24,24	1.92	3 (13%)
23	CLA	C	513	3	69,73,73	2.86	24 (34%)	83,113,113	2.45	28 (33%)
36	HTG	B	624[A]	-	19,19,19	0.90	1 (5%)	23,24,24	1.25	4 (17%)
34	DMS	O	313	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
34	DMS	c	547	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
34	DMS	A	427	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
34	DMS	d	422	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
28	LMT	M	101	-	36,36,36	0.47	0	47,47,47	1.27	7 (14%)
24	PHO	a	2611	-	58,69,69	2.62	11 (18%)	56,99,99	2.76	17 (30%)
25	BCR	k	302	-	41,41,41	0.69	0	56,56,56	1.47	12 (21%)
34	DMS	c	539	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
36	HTG	b	625	-	19,19,19	0.89	1 (5%)	23,24,24	1.54	4 (17%)
29	GOL	V	203	-	5,5,5	0.90	0	5,5,5	0.92	0
31	JOX	a	2619	1	10,10,10	1.91	6 (60%)	14,14,14	2.29	5 (35%)
25	BCR	d	410	-	41,41,41	0.80	0	56,56,56	1.65	5 (8%)
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
34	DMS	a	2624	-	3,3,3	2.74	1 (33%)	3,3,3	0.70	0
25	BCR	b	624	-	41,41,41	0.72	0	56,56,56	1.59	12 (21%)
34	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.35	0
27	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.05	3 (5%)
34	DMS	O	314	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	b	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.35	0
34	DMS	C	532	-	3,3,3	2.63	1 (33%)	3,3,3	0.72	0
23	CLA	b	617	2	69,73,73	2.36	22 (31%)	83,113,113	2.58	26 (31%)
34	DMS	O	312	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
34	DMS	c	544	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
38	LHG	D	2310	-	48,48,48	0.87	2 (4%)	51,54,54	0.95	3 (5%)
23	CLA	c	516	3	69,73,73	2.52	25 (36%)	83,113,113	2.39	26 (31%)
34	DMS	D	2316	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
23	CLA	b	606	43	69,73,73	2.67	26 (37%)	83,113,113	2.28	27 (32%)
27	LMG	d	414	41	51,51,55	0.90	2 (3%)	59,59,63	0.86	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	BCT	a	2608	21	2,3,3	0.67	0	2,3,3	1.05	0
29	GOL	O	305	-	5,5,5	0.88	0	5,5,5	0.90	0
34	DMS	o	312	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
34	DMS	v	210	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
28	LMT	Z	101	-	36,36,36	0.45	0	47,47,47	0.91	2 (4%)
23	CLA	B	614	2	69,73,73	2.37	22 (31%)	83,113,113	2.54	28 (33%)
23	CLA	A	406	43	69,73,73	2.32	23 (33%)	83,113,113	2.74	30 (36%)
23	CLA	b	609	2	69,73,73	2.78	23 (33%)	83,113,113	2.44	27 (32%)
34	DMS	V	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
36	HTG	d	415	-	19,19,19	1.05	2 (10%)	23,24,24	1.52	1 (4%)
29	GOL	B	632	-	5,5,5	0.95	0	5,5,5	0.91	0
24	PHO	A	409	-	58,69,69	2.79	16 (27%)	56,99,99	2.88	13 (23%)
23	CLA	A	407	43	69,73,73	2.24	23 (33%)	83,113,113	2.58	32 (38%)
31	JOX	A	418	-	10,10,10	2.05	4 (40%)	14,14,14	3.36	10 (71%)
23	CLA	a	2610	43	69,73,73	2.37	22 (31%)	83,113,113	2.62	29 (34%)
29	GOL	O	302	-	5,5,5	0.92	0	5,5,5	1.03	0
34	DMS	a	2622	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
23	CLA	c	508	3	69,73,73	2.56	25 (36%)	83,113,113	2.50	23 (27%)
23	CLA	b	611	2	69,73,73	2.65	23 (33%)	83,113,113	2.41	26 (31%)
27	LMG	C	527	-	51,51,55	0.96	2 (3%)	59,59,63	1.27	5 (8%)
23	CLA	A	405	1	69,73,73	2.36	23 (33%)	83,113,113	2.49	29 (34%)
23	CLA	D	2303	4	69,73,73	2.14	22 (31%)	83,113,113	2.66	27 (32%)
23	CLA	B	608	43	69,73,73	2.42	22 (31%)	83,113,113	2.45	28 (33%)
29	GOL	v	203	-	5,5,5	0.93	0	5,5,5	1.14	1 (20%)
29	GOL	U	502	-	5,5,5	1.29	1 (20%)	5,5,5	0.80	0
34	DMS	d	423	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
23	CLA	c	512	3	69,73,73	2.57	24 (34%)	83,113,113	2.47	26 (31%)
28	LMT	i	103	-	24,24,36	0.51	0	29,29,47	1.08	2 (6%)
23	CLA	b	614	2	69,73,73	2.61	24 (34%)	83,113,113	2.33	27 (32%)
25	BCR	y	101	-	41,41,41	0.76	0	56,56,56	1.56	12 (21%)
27	LMG	c	522	-	51,51,55	0.98	2 (3%)	59,59,63	1.34	6 (10%)
34	DMS	U	505	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
34	DMS	d	418	-	3,3,3	2.65	1 (33%)	3,3,3	0.62	0
34	DMS	B	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
23	CLA	C	511	3	69,73,73	2.64	25 (36%)	83,113,113	2.47	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	B	642	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
37	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	0.86	5 (6%)
38	LHG	l	103	-	48,48,48	0.87	2 (4%)	51,54,54	1.02	3 (5%)
28	LMT	z	102	-	33,33,36	0.54	0	43,43,47	1.06	4 (9%)
34	DMS	A	428	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
29	GOL	c	531	-	5,5,5	0.95	0	5,5,5	0.86	0
28	LMT	B	634	-	36,36,36	0.53	1 (2%)	47,47,47	0.85	0
23	CLA	B	603	2	69,73,73	2.55	24 (34%)	83,113,113	2.48	29 (34%)
27	LMG	c	521	-	49,49,55	0.91	2 (4%)	57,57,63	1.13	5 (8%)
36	HTG	c	526	-	19,19,19	1.00	2 (10%)	23,24,24	1.24	1 (4%)
34	DMS	O	317	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
37	DGD	h	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.03	5 (6%)
36	HTG	b	626	-	19,19,19	1.14	2 (10%)	23,24,24	1.46	2 (8%)
25	BCR	T	102	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
28	LMT	j	2701	41	34,34,36	0.56	1 (2%)	44,44,47	1.05	3 (6%)
34	DMS	U	504	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
38	LHG	d	412	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
34	DMS	C	536	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
23	CLA	b	621	2	69,73,73	2.57	23 (33%)	83,113,113	2.63	28 (33%)
25	BCR	a	2614	-	41,41,41	0.80	0	56,56,56	1.31	6 (10%)
36	HTG	B	625	-	19,19,19	1.05	1 (5%)	23,24,24	2.09	4 (17%)
23	CLA	c	513	3	69,73,73	2.61	25 (36%)	83,113,113	2.35	28 (33%)
34	DMS	c	534	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
34	DMS	B	644	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
25	BCR	K	101	-	41,41,41	0.68	0	56,56,56	1.33	9 (16%)
34	DMS	O	308	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
33	PL9	A	422	-	38,38,55	0.42	0	45,45,69	1.86	14 (31%)
34	DMS	U	503	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
23	CLA	c	507	43	69,73,73	2.28	22 (31%)	83,113,113	2.64	25 (30%)
38	LHG	d	403	-	42,42,48	0.98	2 (4%)	45,48,54	0.91	3 (6%)
26	SQD	D	2302	-	53,54,54	1.05	4 (7%)	62,65,65	1.42	9 (14%)
34	DMS	B	647	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	O	319	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
34	DMS	o	316	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
34	DMS	d	420	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HTG	b	602	-	19,19,19	1.04	1 (5%)	23,24,24	1.04	2 (8%)
23	CLA	b	608	2	69,73,73	2.55	24 (34%)	83,113,113	2.50	28 (33%)
25	BCR	Y	302	-	41,41,41	0.81	0	56,56,56	1.76	11 (19%)
34	DMS	A	424	-	3,3,3	2.61	1 (33%)	3,3,3	0.62	0
25	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.53	7 (12%)
27	LMG	m	2802	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	2 (3%)
23	CLA	b	618	2	69,73,73	2.43	24 (34%)	83,113,113	2.44	26 (31%)
28	LMT	A	420	-	24,24,36	0.42	0	29,29,47	0.96	0
34	DMS	D	2319	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
25	BCR	D	2305	-	41,41,41	0.82	1 (2%)	56,56,56	1.63	8 (14%)
28	LMT	d	404	-	25,25,36	0.52	0	30,30,47	0.90	2 (6%)
34	DMS	c	540	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
26	SQD	a	2603	-	53,54,54	1.03	3 (5%)	62,65,65	1.14	3 (4%)
31	JOX	a	2617	-	10,10,10	1.85	4 (40%)	14,14,14	4.93	14 (100%)
28	LMT	A	414	-	34,34,36	0.49	0	45,45,47	1.17	4 (8%)
29	GOL	A	417	-	5,5,5	0.89	0	5,5,5	1.02	0
25	BCR	B	619	-	41,41,41	0.81	0	56,56,56	1.20	5 (8%)
34	DMS	V	213	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
34	DMS	o	310	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
25	BCR	B	620	-	41,41,41	0.74	0	56,56,56	1.17	6 (10%)
20	OEX	A	401	3,43,1	0,14,14	-	-	-		
24	PHO	A	408	-	58,69,69	2.70	12 (20%)	56,99,99	2.73	14 (25%)
34	DMS	c	537	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
34	DMS	O	315	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
23	CLA	b	620	2	69,73,73	2.49	24 (34%)	83,113,113	2.27	31 (37%)
36	HTG	o	301	-	19,19,19	0.88	1 (5%)	23,24,24	1.15	2 (8%)
29	GOL	C	524	-	5,5,5	0.83	0	5,5,5	0.97	0
34	DMS	b	642	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
25	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.28	5 (8%)
23	CLA	b	613	2	69,73,73	2.52	25 (36%)	83,113,113	2.51	31 (37%)
34	DMS	o	314	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
29	GOL	v	204	-	5,5,5	0.88	0	5,5,5	0.96	0
34	DMS	A	429	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	D	2317	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
25	BCR	B	633	-	41,41,41	0.69	0	56,56,56	1.72	12 (21%)
23	CLA	c	515	3	69,73,73	2.65	25 (36%)	83,113,113	2.52	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	609	2	69,73,73	2.50	24 (34%)	83,113,113	2.38	28 (33%)
34	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
29	GOL	c	530	-	5,5,5	0.92	0	5,5,5	0.80	0
34	DMS	C	530	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
34	DMS	v	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	l	104	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
23	CLA	B	611	43	69,73,73	2.37	25 (36%)	83,113,113	2.59	30 (36%)
23	CLA	d	408	4	69,73,73	2.41	24 (34%)	83,113,113	2.55	27 (32%)
36	HTG	C	521	-	19,19,19	0.99	2 (10%)	23,24,24	1.04	1 (4%)
36	HTG	C	522	-	19,19,19	0.97	2 (10%)	23,24,24	2.32	4 (17%)
34	DMS	B	635	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
23	CLA	C	502	3	69,73,73	2.69	26 (37%)	83,113,113	2.28	24 (28%)
23	CLA	c	504	3	69,73,73	2.41	23 (33%)	83,113,113	2.64	25 (30%)
26	SQD	l	101	-	53,54,54	1.05	4 (7%)	62,65,65	1.69	10 (16%)
25	BCR	b	622	-	41,41,41	0.78	0	56,56,56	1.39	9 (16%)
33	PL9	d	411	-	55,55,55	0.69	1 (1%)	68,69,69	1.60	15 (22%)
34	DMS	C	534	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	O	310	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
23	CLA	C	507	3	69,73,73	2.58	23 (33%)	83,113,113	2.61	29 (34%)
23	CLA	C	510	3	69,73,73	2.57	26 (37%)	83,113,113	2.49	27 (32%)
23	CLA	c	505	3	69,73,73	2.45	25 (36%)	83,113,113	2.38	24 (28%)
27	LMG	c	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	3 (5%)
34	DMS	B	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
32	BCT	A	421	21	2,3,3	0.65	0	2,3,3	1.06	0
29	GOL	c	529	-	5,5,5	0.91	0	5,5,5	0.98	0
29	GOL	a	2602	-	5,5,5	0.85	0	5,5,5	1.03	0
24	PHO	a	2612	-	58,69,69	2.69	13 (22%)	56,99,99	3.01	15 (26%)
34	DMS	b	639	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	V	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
29	GOL	O	303	-	5,5,5	0.93	0	5,5,5	0.94	0
34	DMS	u	502	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
36	HTG	b	603	-	19,19,19	0.95	2 (10%)	23,24,24	2.00	4 (17%)
23	CLA	c	514	3	69,73,73	2.47	23 (33%)	83,113,113	2.40	28 (33%)
34	DMS	u	504	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
23	CLA	C	508	43	69,73,73	2.67	24 (34%)	83,113,113	2.54	28 (33%)
34	DMS	o	307	-	3,3,3	2.63	1 (33%)	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HTG	H	101	-	17,17,19	1.23	2 (11%)	19,21,24	1.61	4 (21%)
34	DMS	b	638	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	v	208	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	v	213	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
34	DMS	c	548	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
34	DMS	d	421	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
37	DGD	C	519	-	59,59,67	0.92	2 (3%)	73,73,81	1.28	6 (8%)
28	LMT	T	103	-	24,24,36	0.60	1 (4%)	29,29,47	0.94	2 (6%)
42	HEC	v	201	16	50,50,50	1.92	9 (18%)	68,82,82	1.53	11 (16%)
28	LMT	d	401	-	36,36,36	0.47	0	47,47,47	0.81	1 (2%)
34	DMS	v	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
34	DMS	H	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
37	DGD	D	2307	-	53,53,67	0.96	2 (3%)	60,61,81	1.20	5 (8%)
34	DMS	c	549	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
34	DMS	V	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
34	DMS	o	304	-	3,3,3	2.54	1 (33%)	3,3,3	0.32	0
23	CLA	C	506	3	69,73,73	2.70	25 (36%)	83,113,113	2.27	27 (32%)
34	DMS	c	545	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
28	LMT	f	101	-	24,24,36	0.46	0	29,29,47	0.76	0
34	DMS	O	316	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
39	HEM	e	103	5,6	50,50,50	1.95	8 (16%)	66,82,82	1.52	7 (10%)
29	GOL	D	2301	-	5,5,5	1.00	0	5,5,5	0.79	0
23	CLA	A	410	1	69,73,73	2.34	24 (34%)	83,113,113	2.59	28 (33%)
36	HTG	V	204	-	19,19,19	0.96	1 (5%)	23,24,24	1.84	4 (17%)
34	DMS	a	2623	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
34	DMS	B	643	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
27	LMG	D	2312	41	47,47,55	0.90	2 (4%)	55,55,63	0.88	3 (5%)
23	CLA	C	512	3	69,73,73	2.58	23 (33%)	83,113,113	2.39	27 (32%)
40	RRX	h	101	-	42,42,42	0.69	0	57,58,58	1.41	8 (14%)
34	DMS	c	532	-	3,3,3	2.76	1 (33%)	3,3,3	0.80	0
27	LMG	A	413	-	51,51,55	0.93	2 (3%)	59,59,63	1.24	6 (10%)
34	DMS	o	311	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
36	HTG	I	101	-	19,19,19	1.10	2 (10%)	23,24,24	1.81	4 (17%)
25	BCR	z	101	-	41,41,41	0.74	0	56,56,56	1.52	12 (21%)
34	DMS	C	529	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	GOL	a	2618	-	5,5,5	0.87	0	5,5,5	1.04	0
23	CLA	B	613	2	69,73,73	2.35	23 (33%)	83,113,113	2.53	25 (30%)
29	GOL	J	301	-	5,5,5	0.96	0	5,5,5	0.89	0
34	DMS	c	538	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
37	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
34	DMS	o	313	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
34	DMS	c	533	-	3,3,3	2.61	1 (33%)	3,3,3	0.39	0
23	CLA	c	511	3	69,73,73	2.76	24 (34%)	83,113,113	2.42	24 (28%)
36	HTG	d	407	-	19,19,19	1.15	2 (10%)	23,24,24	1.64	5 (21%)
28	LMT	F	102	-	24,24,36	0.47	0	29,29,47	0.73	0
29	GOL	B	630	-	5,5,5	0.98	0	5,5,5	0.93	0
34	DMS	T	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
38	LHG	d	413	-	48,48,48	0.82	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	604	2	69,73,73	2.56	23 (33%)	83,113,113	2.56	28 (33%)
34	DMS	T	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	c	535	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
23	CLA	B	605	2	69,73,73	2.45	23 (33%)	83,113,113	2.45	28 (33%)
37	DGD	H	103	-	63,63,67	0.90	2 (3%)	77,77,81	1.09	7 (9%)
34	DMS	V	208	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	a	2620	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	t	102	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
38	LHG	e	101	-	39,39,48	1.08	2 (5%)	42,45,54	1.07	3 (7%)
27	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
29	GOL	O	304	-	5,5,5	0.86	0	5,5,5	0.99	0
29	GOL	b	644	-	5,5,5	0.69	0	5,5,5	1.21	1 (20%)
34	DMS	C	531	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
34	DMS	v	207	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
26	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.45	9 (14%)
34	DMS	V	207	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
28	LMT	m	2804	-	36,36,36	0.45	0	47,47,47	1.13	6 (12%)
33	PL9	x	1301	-	38,38,55	0.44	0	45,45,69	1.72	11 (24%)
36	HTG	B	626	-	19,19,19	1.01	2 (10%)	23,24,24	1.49	1 (4%)
36	HTG	c	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.49	2 (8%)
23	CLA	b	612	43	69,73,73	2.38	24 (34%)	83,113,113	2.45	28 (33%)
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.81	0
23	CLA	B	606	2	69,73,73	2.35	23 (33%)	83,113,113	2.48	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	509	3	69,73,73	2.63	25 (36%)	83,113,113	2.46	30 (36%)
34	DMS	O	306	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
25	BCR	C	515	-	41,41,41	0.76	0	56,56,56	1.49	8 (14%)
34	DMS	B	638	-	3,3,3	2.54	1 (33%)	3,3,3	0.34	0
29	GOL	A	415	-	5,5,5	0.82	0	5,5,5	1.08	0
34	DMS	A	426	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	b	641	-	3,3,3	2.68	1 (33%)	3,3,3	0.40	0
34	DMS	a	2621	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
34	DMS	o	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
34	DMS	c	542	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	b	643	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	A	430	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0
34	DMS	v	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	c	536	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
34	DMS	O	318	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
29	GOL	o	303	-	5,5,5	0.98	0	5,5,5	0.94	0
23	CLA	C	505	43	69,73,73	2.39	25 (36%)	83,113,113	2.46	27 (32%)
23	CLA	C	514	3	69,73,73	2.50	25 (36%)	83,113,113	2.42	24 (28%)
28	LMT	m	2803	-	36,36,36	0.42	0	47,47,47	0.83	0
29	GOL	v	202	-	5,5,5	1.01	0	5,5,5	0.89	0
34	DMS	d	419	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
23	CLA	B	607	2	69,73,73	2.48	22 (31%)	83,113,113	2.41	26 (31%)
23	CLA	B	610	2	69,73,73	2.65	22 (31%)	83,113,113	2.43	26 (31%)
37	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	4 (5%)
34	DMS	b	636	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
34	DMS	D	2320	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
34	DMS	b	633	-	3,3,3	2.50	1 (33%)	3,3,3	0.35	0
25	BCR	A	411	-	41,41,41	0.75	0	56,56,56	1.39	8 (14%)
34	DMS	o	315	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
38	LHG	E	101	-	39,39,48	1.06	2 (5%)	42,45,54	1.12	3 (7%)
23	CLA	B	615	2	69,73,73	2.39	22 (31%)	83,113,113	2.60	30 (36%)
23	CLA	B	616	2	69,73,73	2.44	22 (31%)	83,113,113	2.61	30 (36%)
29	GOL	B	648	-	5,5,5	0.89	0	5,5,5	0.94	0
34	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	V	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
34	DMS	B	639	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	u	503	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
34	DMS	D	2318	-	3,3,3	2.57	1 (33%)	3,3,3	0.47	0
23	CLA	C	503	3	69,73,73	2.62	25 (36%)	83,113,113	2.47	27 (32%)
26	SQD	b	601	-	47,48,54	1.04	3 (6%)	56,59,65	1.46	9 (16%)
34	DMS	A	425	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
28	LMT	B	623	-	36,36,36	0.41	0	47,47,47	1.35	4 (8%)
34	DMS	X	101	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
34	DMS	V	202	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
26	SQD	A	412	-	45,46,54	1.05	3 (6%)	54,57,65	1.55	11 (20%)
34	DMS	b	635	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
29	GOL	d	416	-	5,5,5	0.89	0	5,5,5	0.99	0
34	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
39	HEM	F	101	5,6	50,50,50	1.88	9 (18%)	66,82,82	1.47	7 (10%)
36	HTG	B	624[B]	-	19,19,19	0.96	1 (5%)	23,24,24	1.86	6 (26%)
23	CLA	C	509	3	69,73,73	2.52	23 (33%)	83,113,113	2.44	27 (32%)
34	DMS	C	537	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
23	CLA	c	510	43	69,73,73	2.54	23 (33%)	83,113,113	2.62	32 (38%)
34	DMS	v	214	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
23	CLA	D	2304	4	69,73,73	2.23	22 (31%)	83,113,113	2.55	28 (33%)
20	OEX	a	2604	3,43,1	0,14,14	-	-	-		
29	GOL	U	501	-	5,5,5	1.02	0	5,5,5	0.93	0
34	DMS	v	211	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
34	DMS	c	546	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
29	GOL	u	501	-	5,5,5	1.25	0	5,5,5	0.83	0
23	CLA	b	607	2	69,73,73	2.52	24 (34%)	83,113,113	2.46	26 (31%)
23	CLA	b	610	2	69,73,73	2.36	23 (33%)	83,113,113	2.73	27 (32%)
34	DMS	B	641	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	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
38	LHG	D	2311	-	-	9/43/43/53	-
38	LHG	L	101	-	-	15/53/53/53	-
29	GOL	v	203	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	e	101	-	-	14/44/44/53	-
23	CLA	b	619	2	-	8/39/115/115	-
23	CLA	a	2609	1	-	4/39/115/115	-
27	LMG	C	520	-	-	13/46/66/70	0/1/1/1
29	GOL	O	304	-	-	2/4/4/4	-
29	GOL	U	502	-	-	2/4/4/4	-
29	GOL	b	644	-	-	2/4/4/4	-
23	CLA	B	611	43	-	5/39/115/115	-
26	SQD	B	621	-	-	22/49/69/69	0/1/1/1
23	CLA	d	408	4	-	3/39/115/115	-
28	LMT	m	2804	-	-	10/21/61/61	0/2/2/2
25	BCR	b	623	-	-	1/29/63/63	0/2/2/2
37	DGD	c	519	-	-	18/51/91/95	0/2/2/2
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1
23	CLA	c	512	3	-	5/39/115/115	-
33	PL9	x	1301	-	-	12/42/42/73	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
36	HTG	C	521	-	-	2/10/30/30	0/1/1/1
36	HTG	C	522	-	-	2/10/30/30	0/1/1/1
37	DGD	C	518	-	-	17/51/91/95	0/2/2/2
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
23	CLA	C	502	3	-	4/39/115/115	-
23	CLA	b	612	43	-	1/39/115/115	-
28	LMT	i	103	-	-	8/15/35/61	0/1/1/2
29	GOL	C	526	-	-	2/4/4/4	-
38	LHG	D	2309	-	-	13/53/53/53	-
23	CLA	b	615	43	-	6/39/115/115	-
23	CLA	b	616	2	-	4/39/115/115	-
28	LMT	M	102	-	-	4/21/61/61	0/2/2/2
23	CLA	B	606	2	-	9/39/115/115	-
23	CLA	b	614	2	-	7/39/115/115	-
23	CLA	c	504	3	-	4/39/115/115	-
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
36	HTG	C	525	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	522	-	-	5/46/66/70	0/1/1/1
42	HEC	V	201	16	1/1/3/7	6/14/54/54	-
26	SQD	l	101	-	-	23/49/69/69	0/1/1/1
28	LMT	J	303	-	-	5/15/35/61	0/1/1/2
23	CLA	c	509	3	-	11/39/115/115	-
23	CLA	B	617	2	-	9/39/115/115	-
25	BCR	b	622	-	-	2/29/63/63	0/2/2/2
33	PL9	d	411	-	-	4/53/73/73	0/1/1/1
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	CLA	B	612	2	-	3/39/115/115	-
29	GOL	A	415	-	-	2/4/4/4	-
23	CLA	C	507	3	-	14/39/115/115	-
23	CLA	C	510	3	-	6/39/115/115	-
23	CLA	d	409	4	-	6/39/115/115	-
23	CLA	C	511	3	-	6/39/115/115	-
33	PL9	D	2306	-	-	3/53/73/73	0/1/1/1
37	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	C	504	3	-	5/39/115/115	-
38	LHG	l	103	-	-	13/53/53/53	-
23	CLA	c	505	3	-	6/39/115/115	-
23	CLA	d	402	43	-	5/39/115/115	-
27	LMG	c	501	-	-	12/46/66/70	0/1/1/1
28	LMT	z	102	-	-	12/16/56/61	0/2/2/2
26	SQD	d	417	-	-	13/33/33/69	-
29	GOL	c	531	-	-	2/4/4/4	-
28	LMT	B	634	-	-	8/21/61/61	0/2/2/2
23	CLA	B	603	2	-	3/39/115/115	-
27	LMG	c	521	-	-	14/44/64/70	0/1/1/1
29	GOL	c	529	-	-	0/4/4/4	-
29	GOL	a	2602	-	-	4/4/4/4	-
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
29	GOL	o	303	-	-	0/4/4/4	-
23	CLA	C	505	43	-	8/39/115/115	-
24	PHO	a	2612	-	-	1/37/103/103	0/5/6/6
36	HTG	b	604	-	-	1/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	h	102	-	-	12/51/91/95	0/2/2/2
23	CLA	C	514	3	-	8/39/115/115	-
36	HTG	b	626	-	-	6/10/30/30	0/1/1/1
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
28	LMT	j	2701	41	-	3/17/57/61	0/2/2/2
29	GOL	O	303	-	-	0/4/4/4	-
28	LMT	m	2803	-	-	3/21/61/61	0/2/2/2
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
38	LHG	d	412	-	-	13/53/53/53	-
23	CLA	c	514	3	-	3/39/115/115	-
29	GOL	b	631	-	-	0/4/4/4	-
23	CLA	a	2613	1	-	7/39/115/115	-
29	GOL	v	202	-	-	2/4/4/4	-
26	SQD	a	2615	-	-	8/43/63/69	0/1/1/1
29	GOL	E	104	-	-	0/4/4/4	-
23	CLA	C	508	43	-	9/39/115/115	-
36	HTG	H	101	-	-	2/8/25/30	0/1/1/1
23	CLA	B	607	2	-	6/39/115/115	-
23	CLA	B	610	2	-	5/39/115/115	-
23	CLA	b	621	2	-	12/39/115/115	-
25	BCR	a	2614	-	-	3/29/63/63	0/2/2/2
37	DGD	c	518	-	-	17/51/91/95	0/2/2/2
36	HTG	B	625	-	-	1/10/30/30	0/1/1/1
40	RRX	H	102	-	-	1/29/65/65	0/2/2/2
23	CLA	c	506	3	-	5/39/115/115	-
23	CLA	c	513	3	-	8/39/115/115	-
37	DGD	C	519	-	-	14/47/87/95	0/2/2/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	SQD	D	2308	-	-	16/40/60/69	0/1/1/1
23	CLA	B	602	43	-	10/39/115/115	-
28	LMT	T	103	-	-	9/15/35/61	0/1/1/2
31	JOX	A	419	-	-	-	0/1/1/1
42	HEC	v	201	16	1/1/3/7	6/14/54/54	-
28	LMT	d	401	-	-	8/21/61/61	0/2/2/2
33	PL9	A	422	-	-	10/42/42/73	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	D	2307	-	-	23/47/68/95	0/1/1/2
23	CLA	c	507	43	-	6/39/115/115	-
25	BCR	c	517	-	-	3/29/63/63	0/2/2/2
38	LHG	d	403	-	-	7/47/47/53	-
38	LHG	E	101	-	-	13/44/44/53	-
26	SQD	D	2302	-	-	14/49/69/69	0/1/1/1
36	HTG	i	102	-	-	6/10/30/30	0/1/1/1
23	CLA	C	513	3	-	9/39/115/115	-
23	CLA	C	506	3	-	8/39/115/115	-
36	HTG	B	624[A]	-	-	2/10/30/30	0/1/1/1
28	LMT	f	101	-	-	4/15/35/61	0/1/1/2
23	CLA	B	615	2	-	12/39/115/115	-
23	CLA	B	616	2	-	7/39/115/115	-
29	GOL	B	648	-	-	0/4/4/4	-
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
23	CLA	b	608	2	-	4/39/115/115	-
25	BCR	Y	302	-	-	5/29/63/63	0/2/2/2
39	HEM	e	103	5,6	-	4/14/54/54	-
25	BCR	C	516	-	-	3/29/63/63	0/2/2/2
29	GOL	D	2301	-	-	2/4/4/4	-
23	CLA	A	410	1	-	10/39/115/115	-
28	LMT	M	101	-	-	6/21/61/61	0/2/2/2
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
27	LMG	m	2802	-	-	10/46/66/70	0/1/1/1
24	PHO	a	2611	-	-	3/37/103/103	0/5/6/6
25	BCR	k	302	-	-	0/29/63/63	0/2/2/2
36	HTG	b	625	-	-	2/10/30/30	0/1/1/1
29	GOL	V	203	-	-	0/4/4/4	-
31	JOX	a	2619	1	-	-	0/1/1/1
25	BCR	d	410	-	-	8/29/63/63	0/2/2/2
23	CLA	b	618	2	-	6/39/115/115	-
28	LMT	A	420	-	-	6/15/35/61	0/1/1/2
25	BCR	D	2305	-	-	8/29/63/63	0/2/2/2
25	BCR	b	624	-	-	4/29/63/63	0/2/2/2
27	LMG	D	2312	41	-	6/42/62/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	d	404	-	-	5/17/37/61	0/1/1/2
23	CLA	C	503	3	-	6/39/115/115	-
27	LMG	B	622	-	-	16/46/66/70	0/1/1/1
26	SQD	a	2603	-	-	16/49/69/69	0/1/1/1
23	CLA	C	512	3	-	2/39/115/115	-
26	SQD	b	601	-	-	16/43/63/69	0/1/1/1
40	RRX	h	101	-	-	2/29/65/65	0/2/2/2
31	JOX	a	2617	-	-	-	0/1/1/1
28	LMT	B	623	-	-	12/21/61/61	0/2/2/2
28	LMT	A	414	-	-	8/19/59/61	0/2/2/2
27	LMG	A	413	-	-	20/46/66/70	0/1/1/1
29	GOL	A	417	-	-	3/4/4/4	-
36	HTG	I	101	-	-	6/10/30/30	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	SQD	A	412	-	-	8/41/61/69	0/1/1/1
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
23	CLA	b	617	2	-	2/39/115/115	-
38	LHG	D	2310	-	-	8/53/53/53	-
29	GOL	d	416	-	-	2/4/4/4	-
23	CLA	c	516	3	-	10/39/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	PHO	A	408	-	-	4/37/103/103	0/5/6/6
23	CLA	b	606	43	-	10/39/115/115	-
29	GOL	a	2618	-	-	1/4/4/4	-
27	LMG	d	414	41	-	11/46/66/70	0/1/1/1
23	CLA	b	620	2	-	5/39/115/115	-
36	HTG	o	301	-	-	6/10/30/30	0/1/1/1
29	GOL	C	524	-	-	2/4/4/4	-
29	GOL	O	305	-	-	2/4/4/4	-
23	CLA	B	613	2	-	5/39/115/115	-
29	GOL	J	301	-	-	4/4/4/4	-
37	DGD	C	517	-	-	18/51/91/95	0/2/2/2
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
23	CLA	B	614	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	511	3	-	5/39/115/115	-
23	CLA	A	406	43	-	4/39/115/115	-
23	CLA	b	609	2	-	2/39/115/115	-
39	HEM	F	101	5,6	-	4/14/54/54	-
23	CLA	b	613	2	-	1/39/115/115	-
36	HTG	B	624[B]	-	-	4/10/30/30	0/1/1/1
36	HTG	d	415	-	-	2/10/30/30	0/1/1/1
36	HTG	d	407	-	-	7/10/30/30	0/1/1/1
29	GOL	B	632	-	-	3/4/4/4	-
24	PHO	A	409	-	-	3/37/103/103	0/5/6/6
23	CLA	C	509	3	-	6/39/115/115	-
29	GOL	v	204	-	-	1/4/4/4	-
23	CLA	A	407	43	-	6/39/115/115	-
23	CLA	c	510	43	-	10/39/115/115	-
25	BCR	B	633	-	-	3/29/63/63	0/2/2/2
28	LMT	F	102	-	-	5/15/35/61	0/1/1/2
31	JOX	A	418	-	-	-	0/1/1/1
23	CLA	a	2610	43	-	13/39/115/115	-
23	CLA	c	515	3	-	8/39/115/115	-
23	CLA	D	2304	4	-	7/39/115/115	-
29	GOL	O	302	-	-	2/4/4/4	-
23	CLA	B	609	2	-	1/39/115/115	-
29	GOL	B	630	-	-	0/4/4/4	-
29	GOL	U	501	-	-	0/4/4/4	-
38	LHG	d	413	-	-	10/53/53/53	-
23	CLA	c	508	3	-	9/39/115/115	-
23	CLA	B	604	2	-	7/39/115/115	-
23	CLA	B	605	2	-	6/39/115/115	-
29	GOL	u	501	-	-	1/4/4/4	-
23	CLA	b	611	2	-	11/39/115/115	-
27	LMG	C	527	-	-	14/46/66/70	0/1/1/1
23	CLA	A	405	1	-	2/39/115/115	-
23	CLA	D	2303	4	-	3/39/115/115	-
23	CLA	b	607	2	-	4/39/115/115	-
23	CLA	B	608	43	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	610	2	-	3/39/115/115	-
29	GOL	c	530	-	-	4/4/4/4	-
37	DGD	H	103	-	-	12/51/91/95	0/2/2/2

The worst 5 of 2032 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	MG-NA	10.59	2.31	2.06
23	C	512	CLA	MG-NA	10.29	2.30	2.06
23	c	506	CLA	MG-NA	10.17	2.30	2.06
23	c	511	CLA	MG-ND	-9.74	1.86	2.05
23	b	609	CLA	MG-ND	-9.39	1.87	2.05

The worst 5 of 2621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	408	PHO	C2D-C1D-ND	11.71	117.61	109.53
24	A	409	PHO	C2D-C1D-ND	11.34	117.35	109.53
24	a	2612	PHO	C2D-C1D-ND	11.01	117.13	109.53
23	c	504	CLA	C1D-ND-C4D	-10.80	98.66	106.33
24	a	2611	PHO	C2D-C1D-ND	10.60	116.84	109.53

All (2) chirality outliers are listed below:

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

5 of 1308 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

180 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	D	2311	LHG	2	0
38	L	101	LHG	1	0
23	a	2609	CLA	3	0
25	b	623	BCR	3	0
37	c	519	DGD	1	0
36	B	627	HTG	1	0
34	O	307	DMS	1	0
37	C	518	DGD	2	0
29	C	526	GOL	2	0
38	D	2309	LHG	1	0
23	b	615	CLA	4	0
23	b	616	CLA	1	0
36	C	525	HTG	1	0
23	B	617	CLA	2	0
23	C	504	CLA	6	0
23	d	402	CLA	5	0
26	d	417	SQD	2	0
36	b	604	HTG	1	0
29	b	631	GOL	1	0
23	a	2613	CLA	1	0
26	a	2615	SQD	1	0
40	H	102	RRX	3	0
23	c	506	CLA	7	0
34	V	206	DMS	1	0
26	D	2308	SQD	1	0
23	B	602	CLA	1	0
34	c	543	DMS	1	0
25	c	517	BCR	2	0
36	i	102	HTG	1	0
23	C	513	CLA	5	0
28	M	101	LMT	1	0
25	k	302	BCR	1	0
36	b	625	HTG	6	0
25	d	410	BCR	2	0
34	a	2624	DMS	1	0
25	b	624	BCR	2	0
27	B	622	LMG	1	0
23	b	617	CLA	1	0
38	D	2310	LHG	1	0
23	c	516	CLA	2	0
23	b	606	CLA	1	0
27	d	414	LMG	4	0
28	Z	101	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	614	CLA	3	0
23	A	406	CLA	2	0
23	b	609	CLA	2	0
29	B	632	GOL	2	0
24	A	409	PHO	3	0
23	A	407	CLA	3	0
23	a	2610	CLA	2	0
29	O	302	GOL	1	0
23	c	508	CLA	4	0
23	b	611	CLA	4	0
27	C	527	LMG	2	0
23	A	405	CLA	2	0
23	D	2303	CLA	3	0
23	c	512	CLA	2	0
28	i	103	LMT	1	0
23	b	614	CLA	2	0
25	y	101	BCR	2	0
27	c	522	LMG	4	0
34	d	418	DMS	1	0
23	C	511	CLA	3	0
34	B	642	DMS	1	0
38	l	103	LHG	2	0
28	z	102	LMT	4	0
28	B	634	LMT	1	0
27	c	521	LMG	1	0
36	b	626	HTG	1	0
25	T	102	BCR	3	0
28	j	2701	LMT	1	0
38	d	412	LHG	4	0
34	C	536	DMS	1	0
23	b	621	CLA	3	0
25	a	2614	BCR	2	0
36	B	625	HTG	1	0
34	B	644	DMS	1	0
25	K	101	BCR	1	0
33	A	422	PL9	4	0
34	U	503	DMS	1	0
23	c	507	CLA	2	0
38	d	403	LHG	1	0
26	D	2302	SQD	3	0
34	B	647	DMS	2	0
36	b	602	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	608	CLA	2	0
25	Y	302	BCR	2	0
25	C	516	BCR	3	0
27	m	2802	LMG	1	0
23	b	618	CLA	4	0
28	A	420	LMT	3	0
25	D	2305	BCR	2	0
28	d	404	LMT	1	0
26	a	2603	SQD	2	0
28	A	414	LMT	6	0
25	B	619	BCR	3	0
25	B	620	BCR	2	0
24	A	408	PHO	1	0
23	b	620	CLA	4	0
36	o	301	HTG	2	0
25	B	618	BCR	1	0
34	o	314	DMS	2	0
25	B	633	BCR	4	0
23	c	515	CLA	2	0
23	B	609	CLA	1	0
29	c	530	GOL	1	0
23	B	611	CLA	4	0
23	d	408	CLA	1	0
36	C	521	HTG	2	0
23	C	502	CLA	5	0
23	c	504	CLA	3	0
26	l	101	SQD	4	0
25	b	622	BCR	2	0
33	d	411	PL9	1	0
23	C	507	CLA	5	0
23	C	510	CLA	3	0
23	c	505	CLA	2	0
27	c	501	LMG	4	0
34	B	637	DMS	1	0
29	a	2602	GOL	1	0
24	a	2612	PHO	2	0
34	b	639	DMS	1	0
36	b	603	HTG	1	0
23	c	514	CLA	5	0
23	C	508	CLA	4	0
34	o	307	DMS	1	0
36	H	101	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	C	519	DGD	2	0
28	d	401	LMT	6	0
34	v	209	DMS	1	0
37	D	2307	DGD	3	0
23	C	506	CLA	4	0
39	e	103	HEM	2	0
23	A	410	CLA	4	0
27	D	2312	LMG	2	0
23	C	512	CLA	2	0
40	h	101	RRX	3	0
27	A	413	LMG	3	0
36	I	101	HTG	2	0
25	z	101	BCR	2	0
23	B	613	CLA	2	0
37	C	517	DGD	2	0
36	d	407	HTG	3	0
38	d	413	LHG	1	0
23	B	604	CLA	3	0
34	c	535	DMS	1	0
23	B	605	CLA	1	0
38	e	101	LHG	1	0
29	b	644	GOL	3	0
26	B	621	SQD	2	0
33	x	1301	PL9	2	0
23	b	612	CLA	1	0
23	B	606	CLA	4	0
23	c	509	CLA	4	0
25	C	515	BCR	2	0
34	B	638	DMS	1	0
34	A	430	DMS	1	0
34	c	536	DMS	1	0
23	C	505	CLA	2	0
23	C	514	CLA	6	0
28	m	2803	LMT	1	0
23	B	607	CLA	1	0
23	B	610	CLA	1	0
37	c	518	DGD	1	0
34	D	2320	DMS	1	0
23	B	615	CLA	2	0
23	B	616	CLA	2	0
29	B	648	GOL	3	0
34	V	212	DMS	1	0

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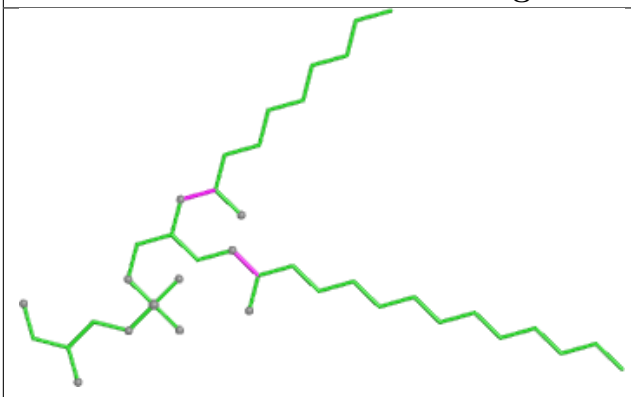
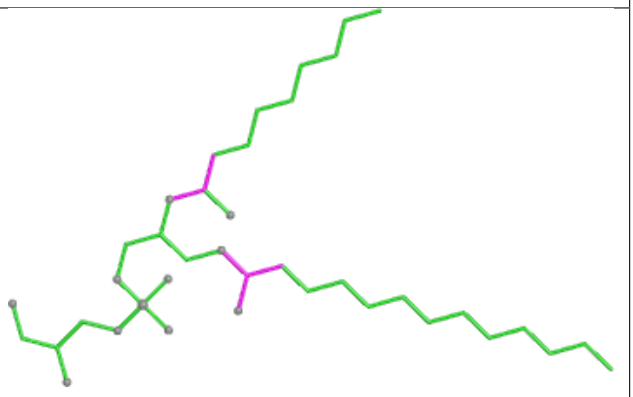
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	503	CLA	4	0
26	b	601	SQD	1	0
28	B	623	LMT	1	0
26	A	412	SQD	2	0
39	F	101	HEM	1	0
36	B	624[B]	HTG	2	0
23	C	509	CLA	3	0
23	c	510	CLA	3	0
23	D	2304	CLA	1	0
23	b	607	CLA	1	0
23	b	610	CLA	2	0

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

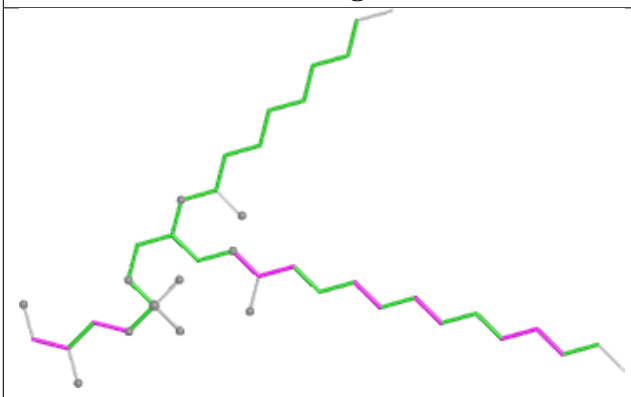
Ligand LHG D 2311



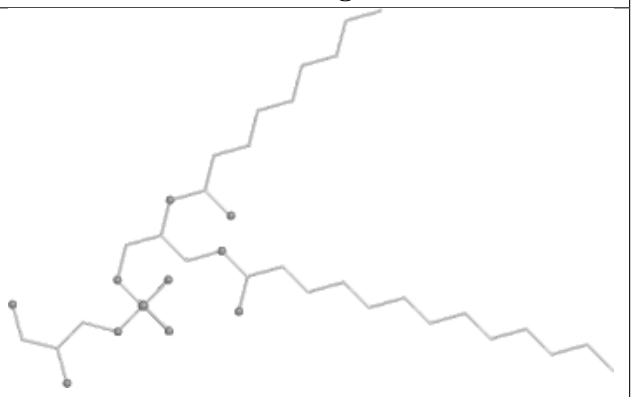
Bond lengths



Bond angles

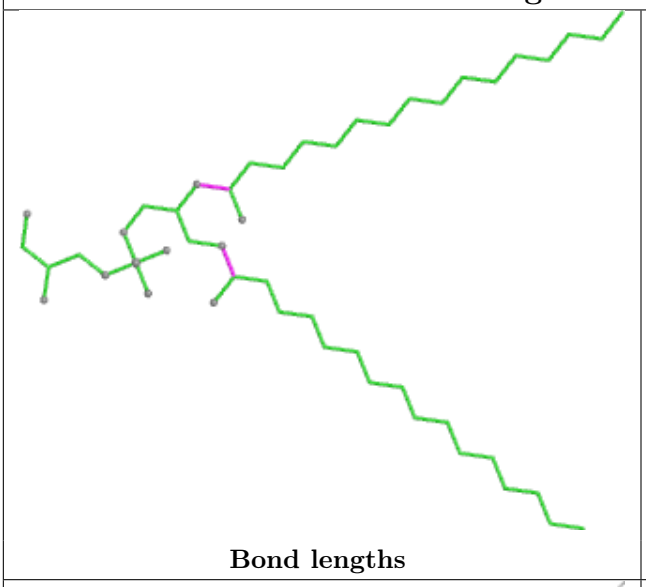


Torsions

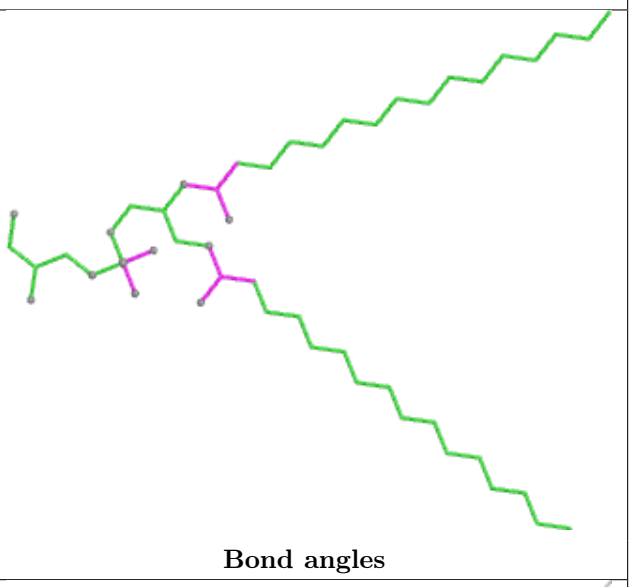


Rings

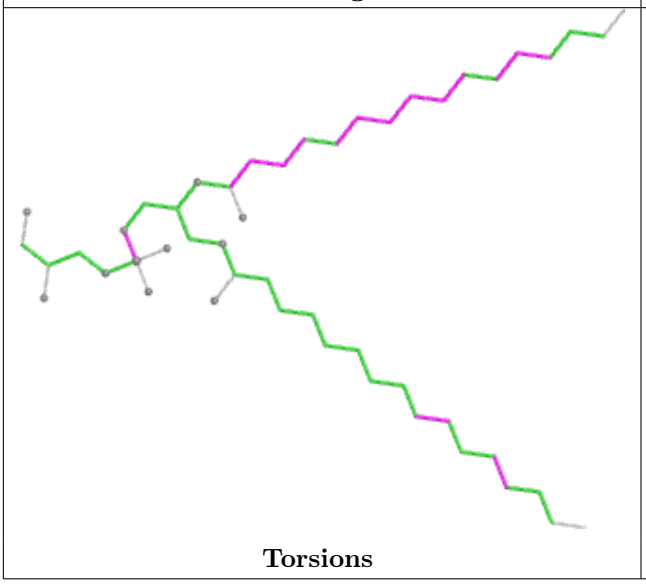
Ligand LHG L 101



Bond lengths



Bond angles



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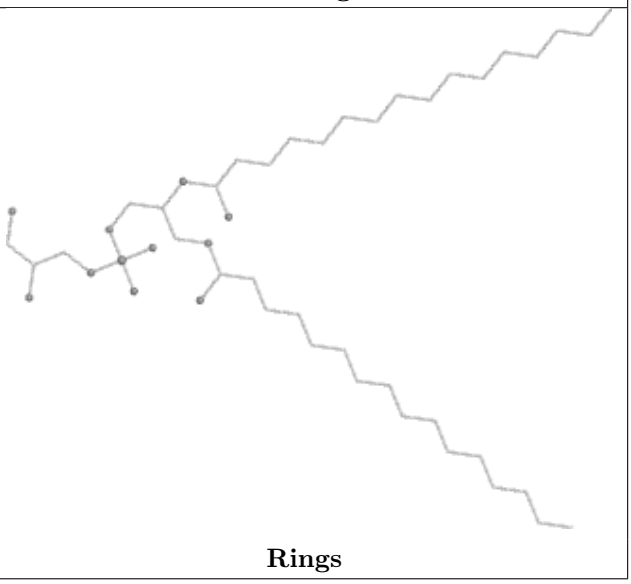
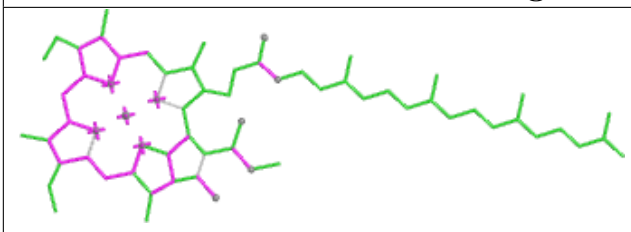
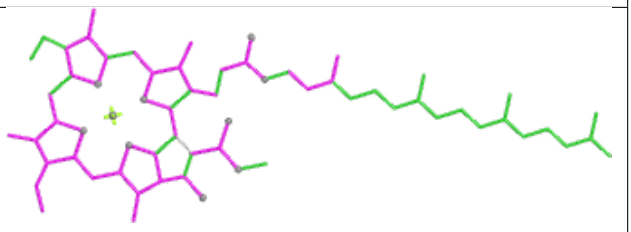


Rings

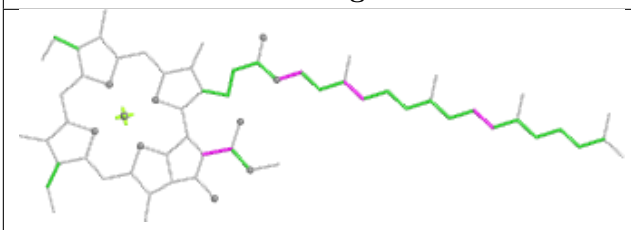
Ligand CLA b 619



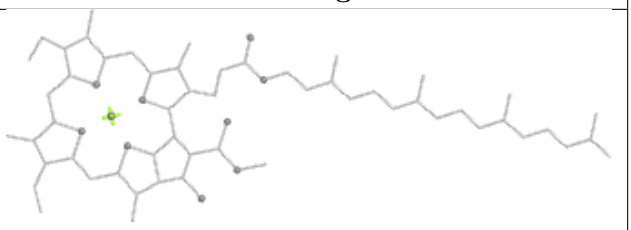
Bond lengths



Bond angles

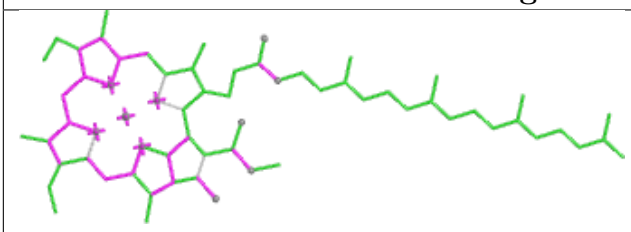


Torsions



Rings

Ligand CLA a 2609



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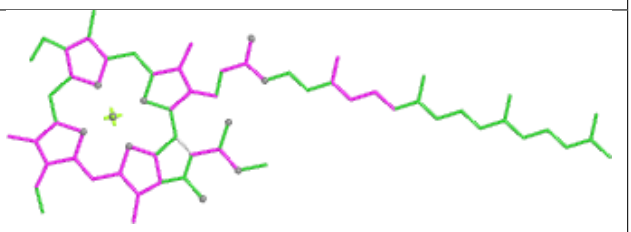

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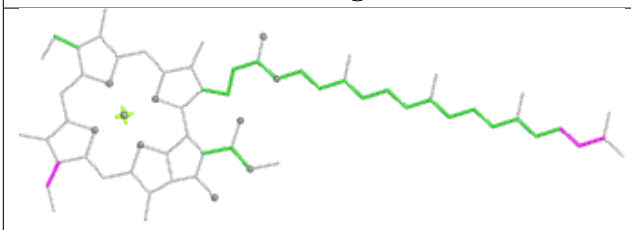

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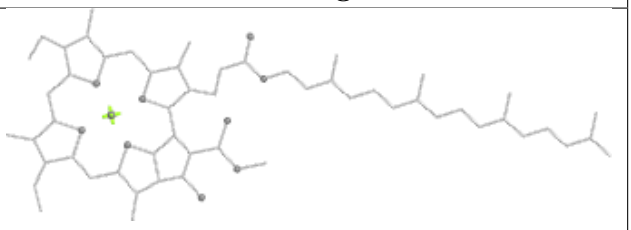
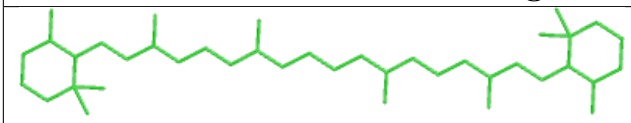


Rings

Ligand BCR b 623



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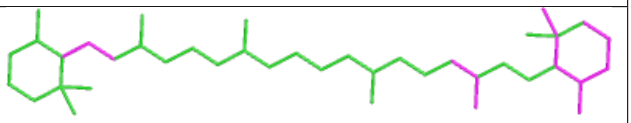
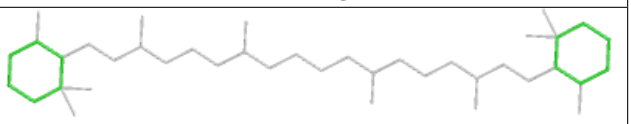


Bond angles

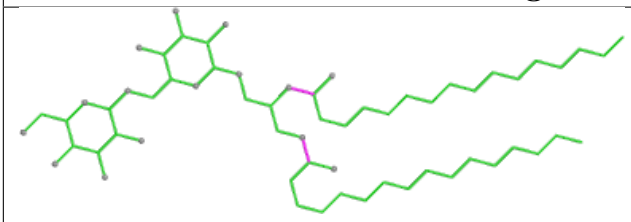


Torsions



Rings

Ligand DGD c 519



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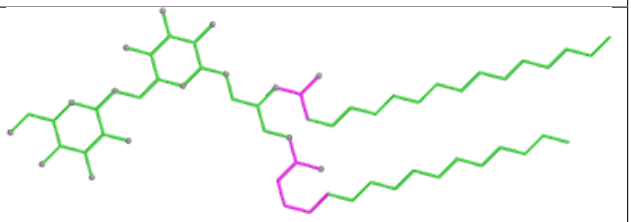

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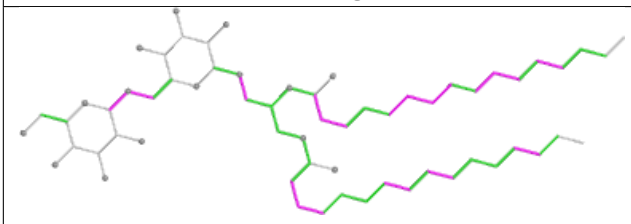

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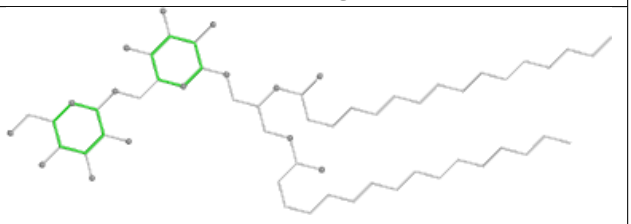
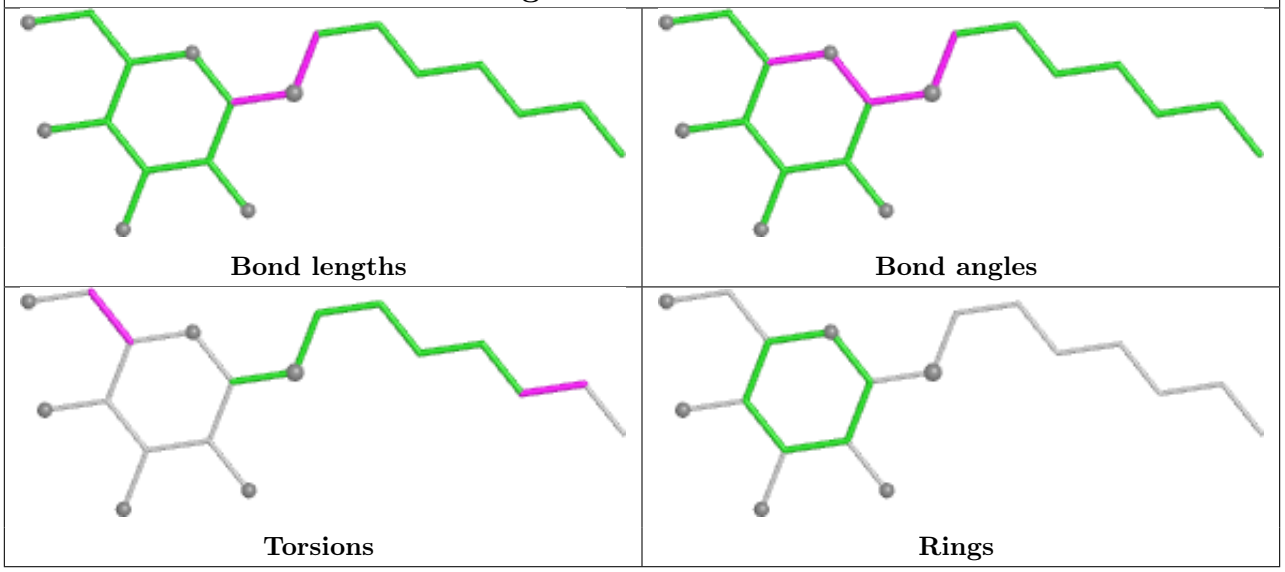
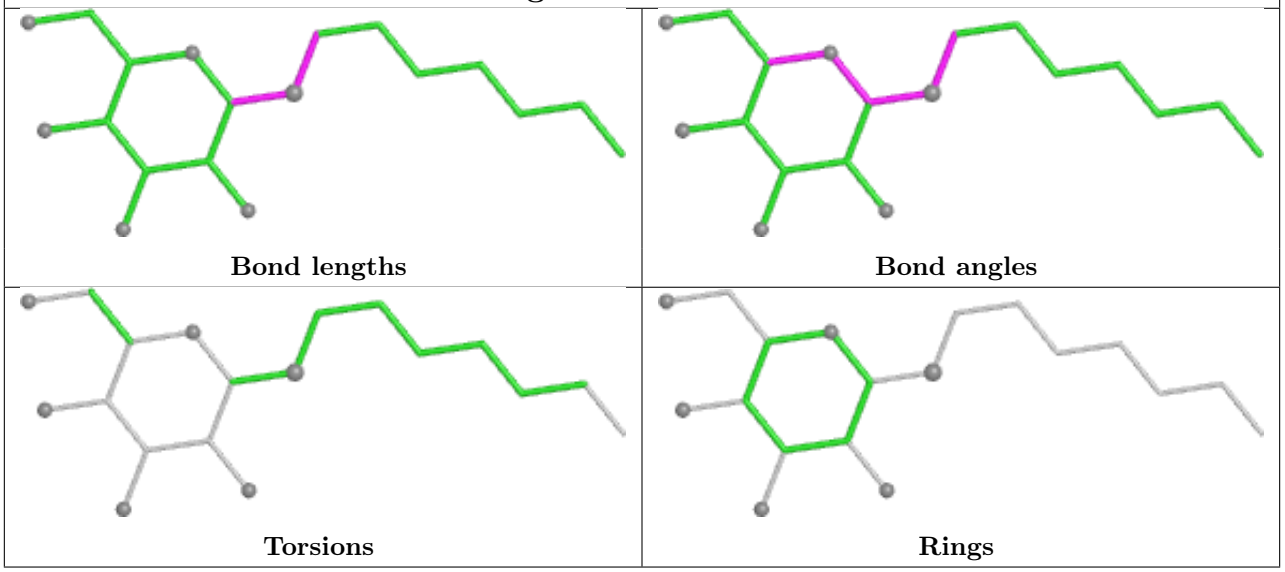


Rings

Ligand HTG B 627



Ligand HTG c 524



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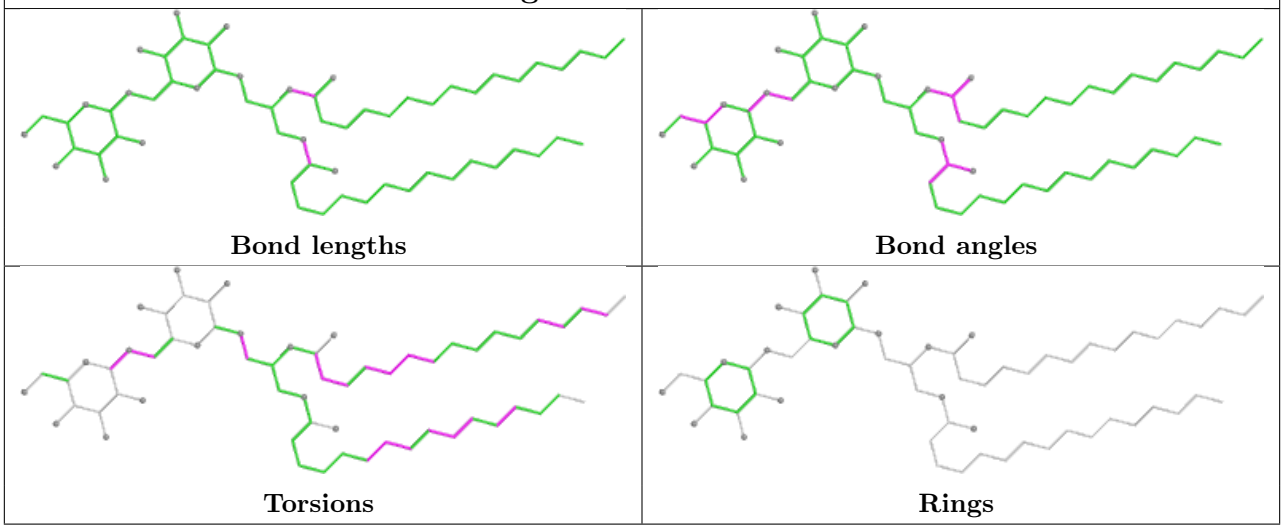
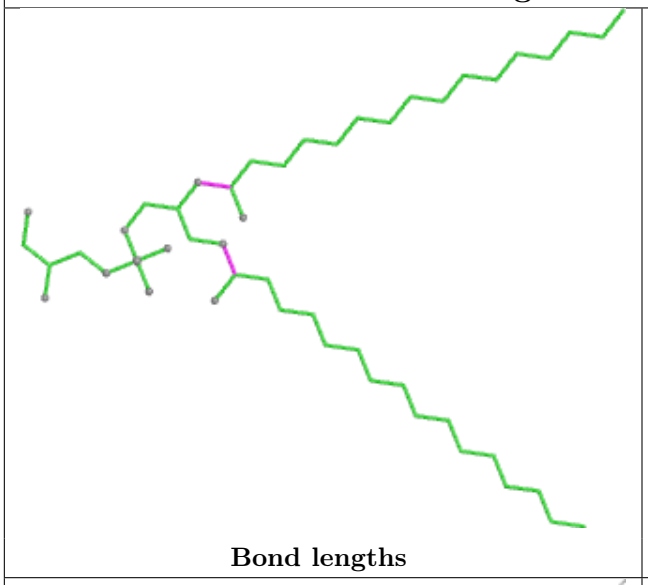


Ligand LHG D 2309



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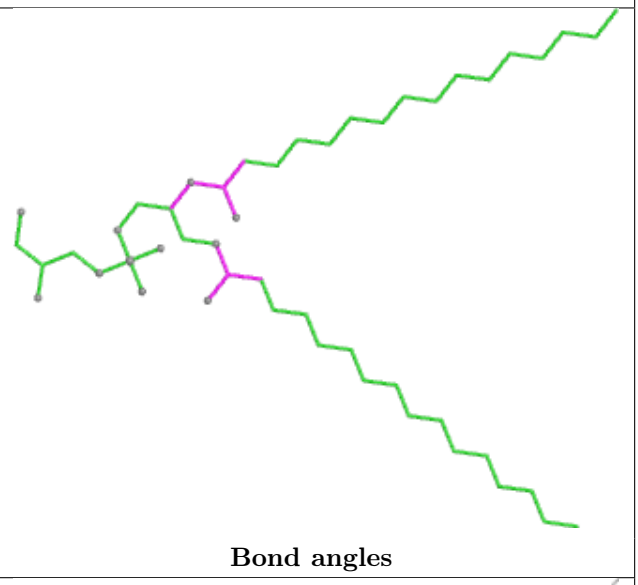
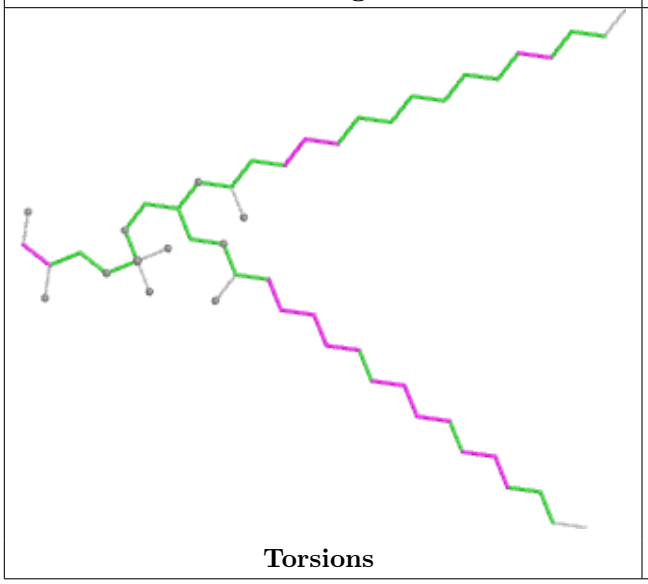
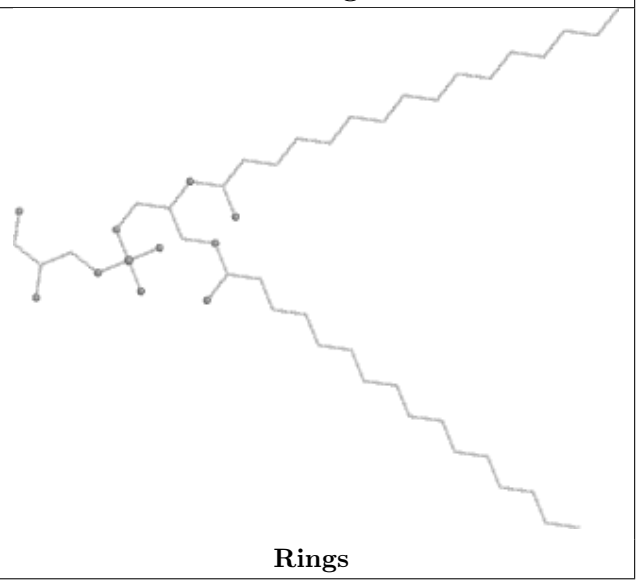


Bond angles

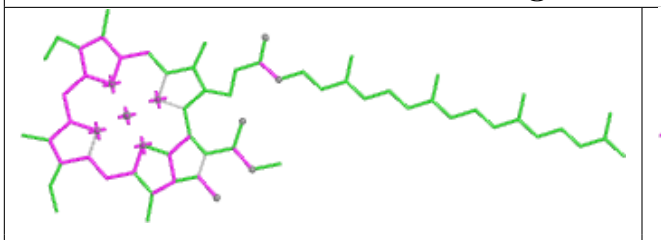


Torsions



Rings

Ligand CLA b 615



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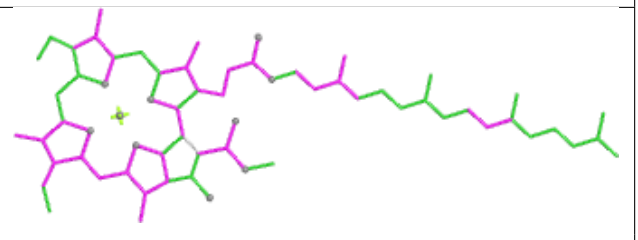

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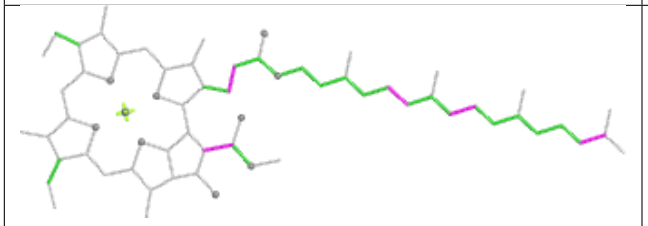

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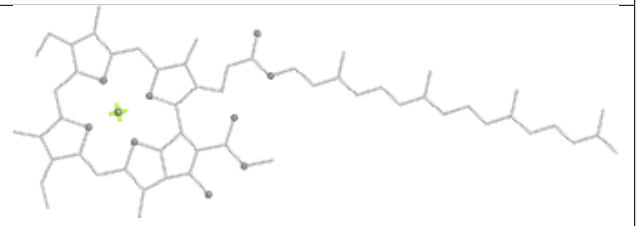
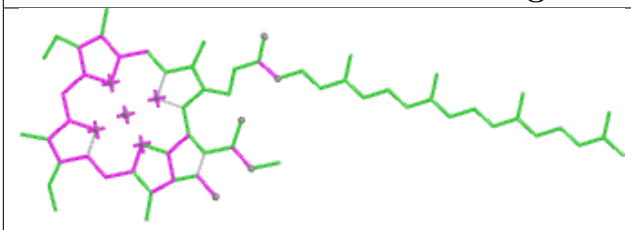


Rings

Ligand CLA b 616



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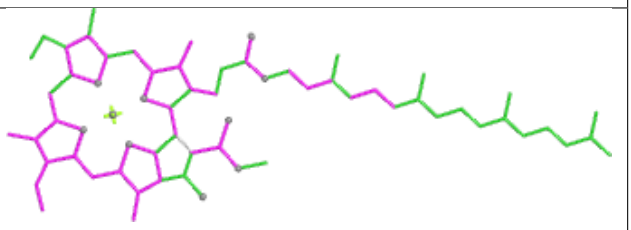
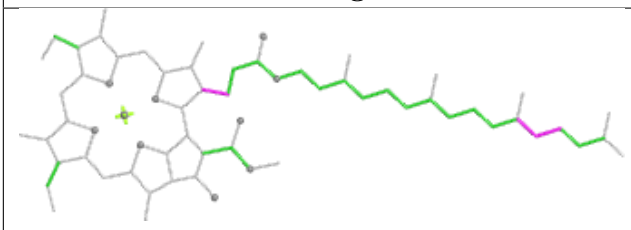


Bond angles



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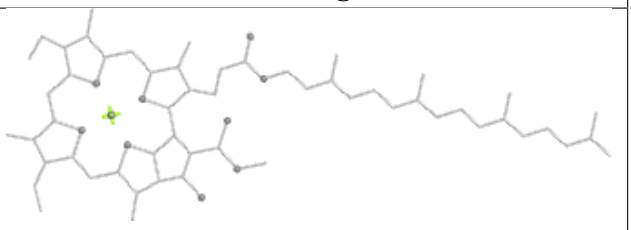
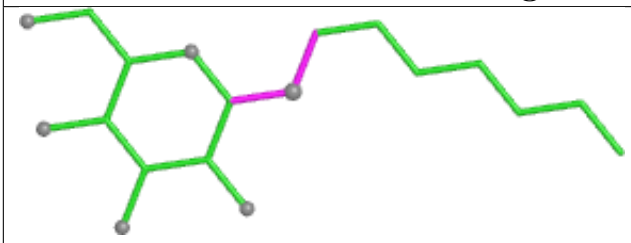


Rings

Ligand HTG C 525



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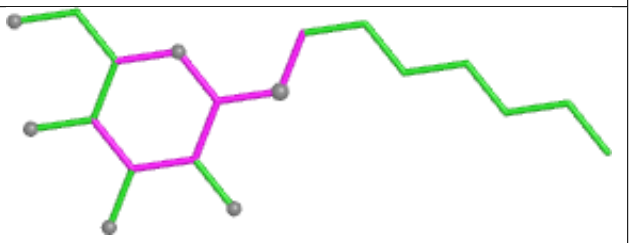
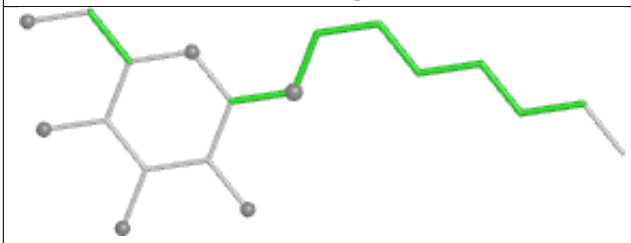


Bond angles



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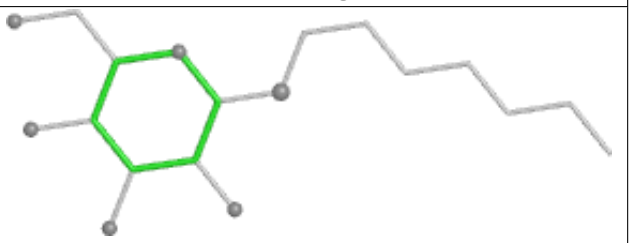
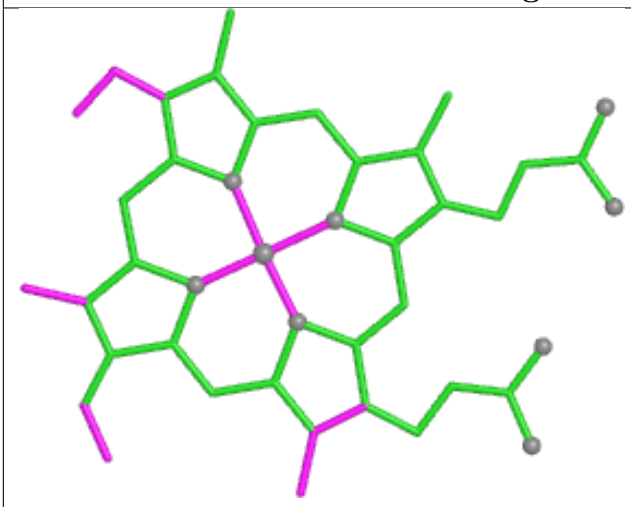


Rings

Ligand HEC V 201



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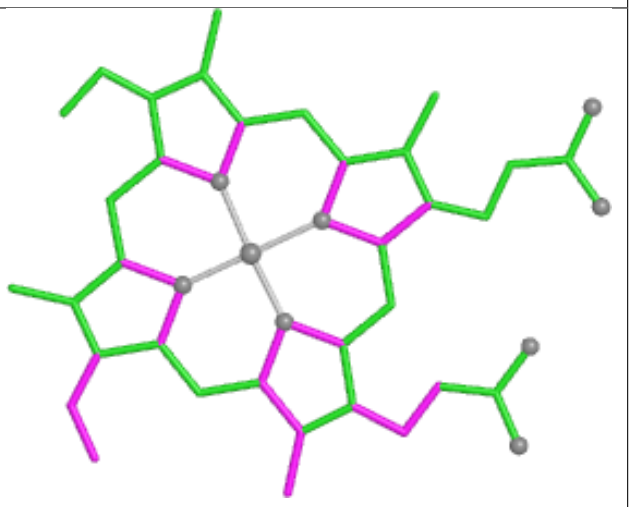
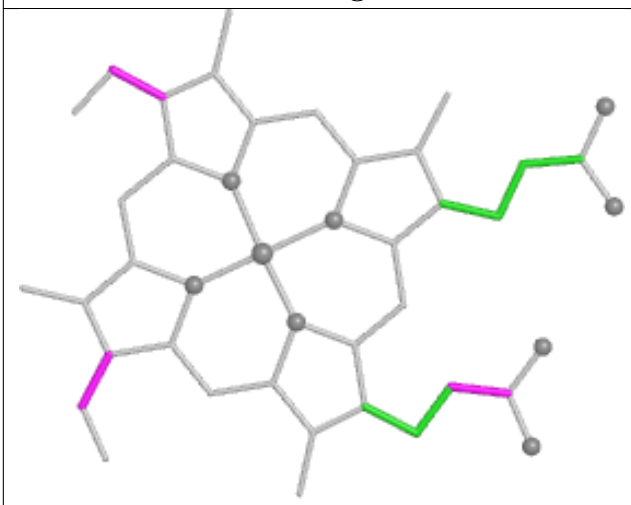


Bond angles



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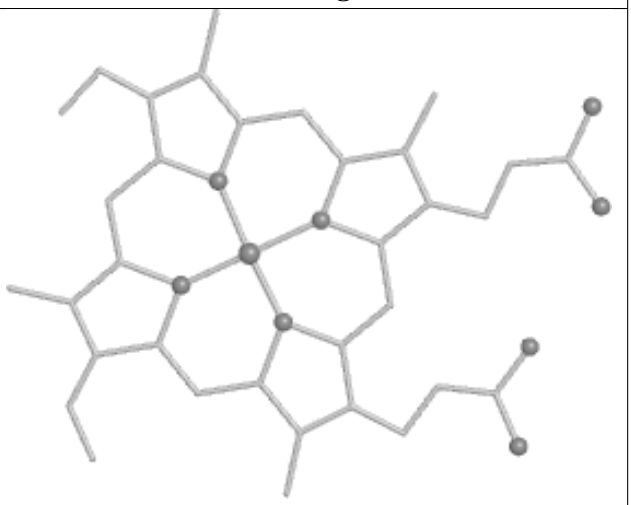
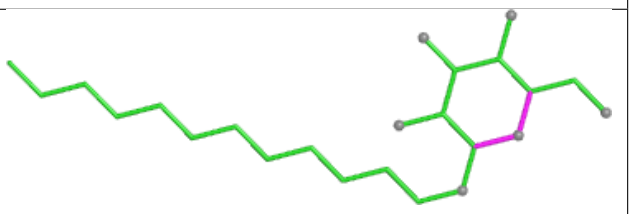


Rings

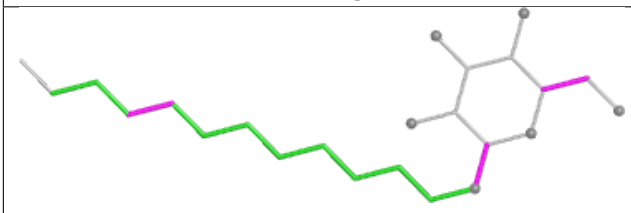
Ligand LMT J 303



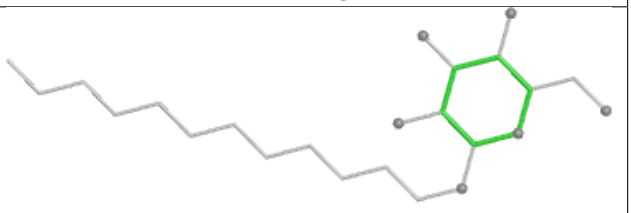
Bond lengths



Bond angles

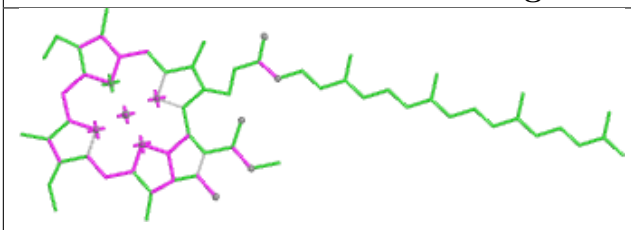


Torsions

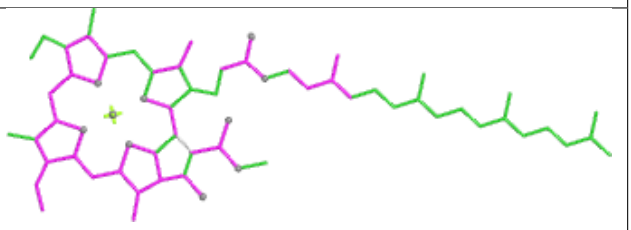


Rings

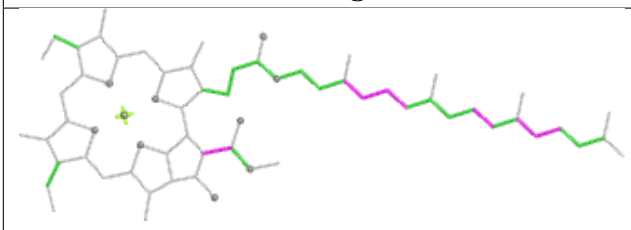
Ligand CLA B 617



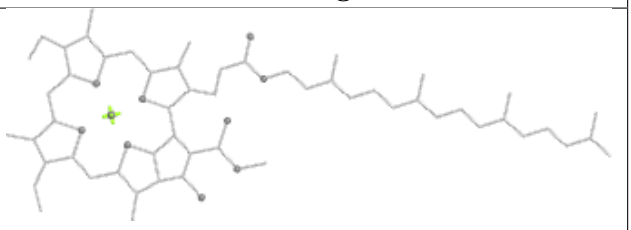
Bond lengths



Bond angles

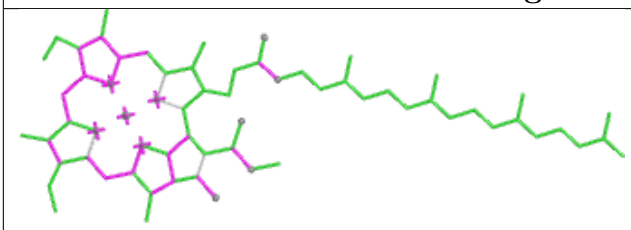


Torsions



Rings

Ligand CLA B 612



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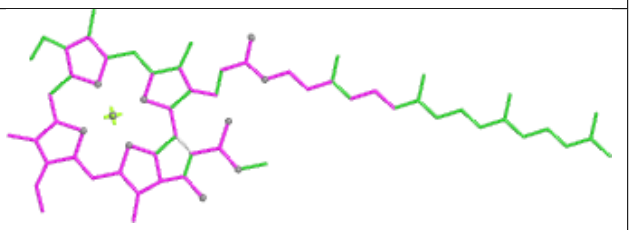

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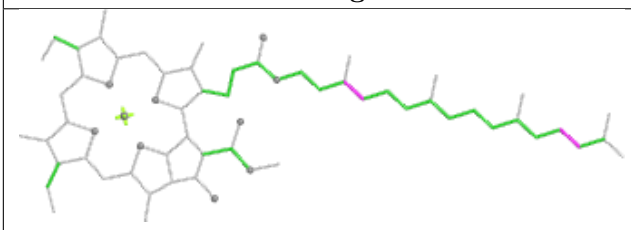

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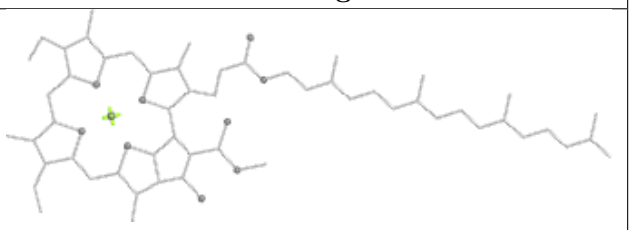
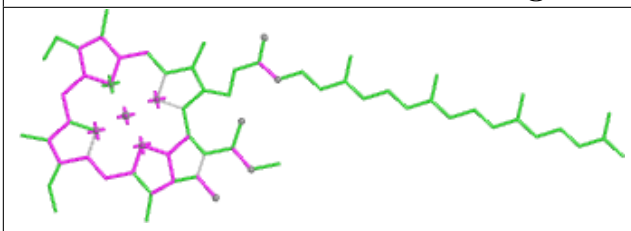


Rings

Ligand CLA d 409



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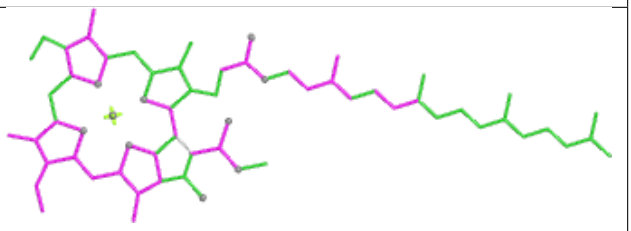

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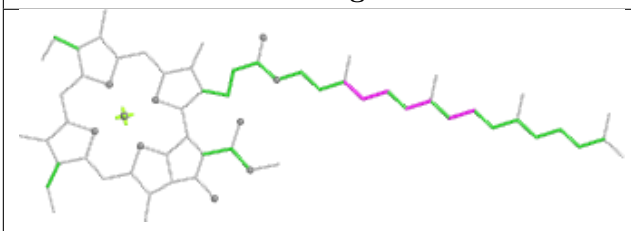

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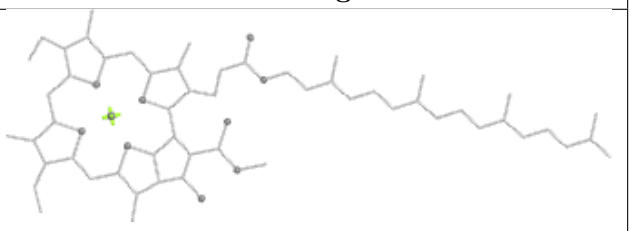
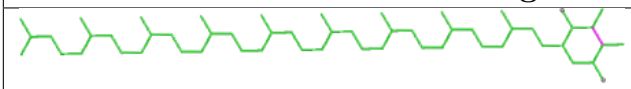


Rings

Ligand PL9 D 2306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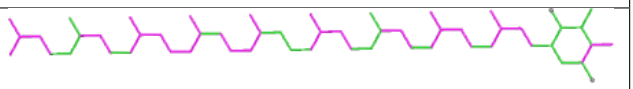
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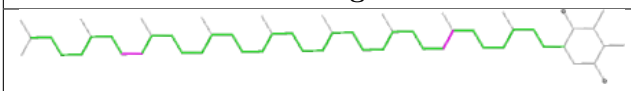
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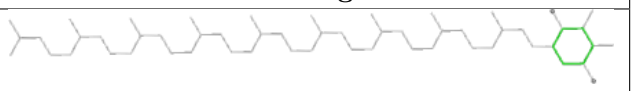
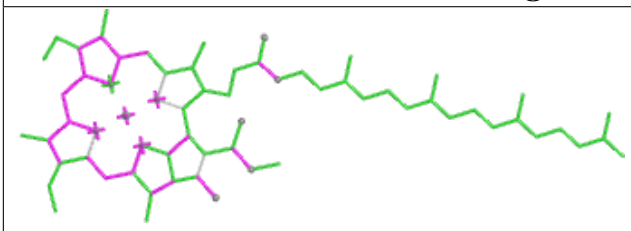

Rings

Ligand CLA C 504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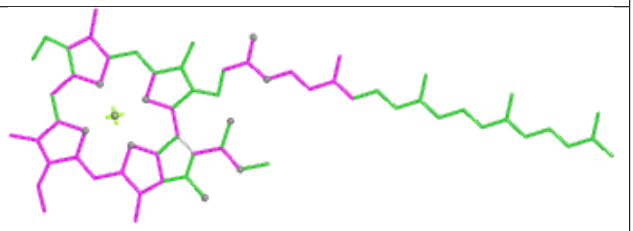
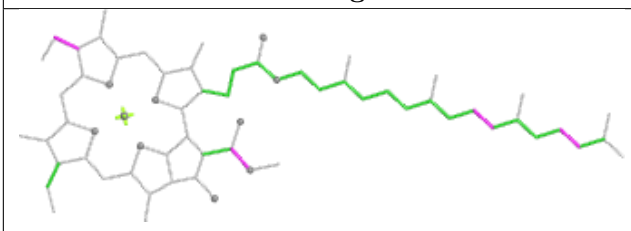

Bond angles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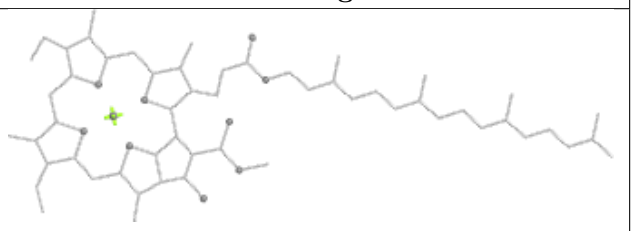
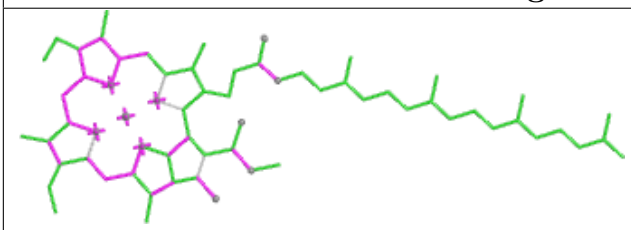

Rings

Ligand CLA d 402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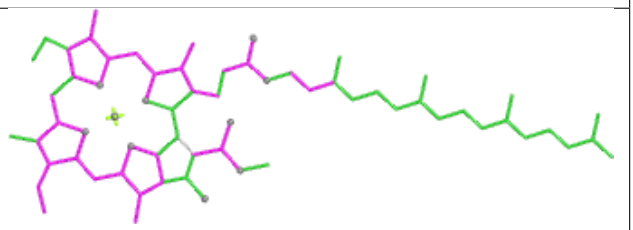
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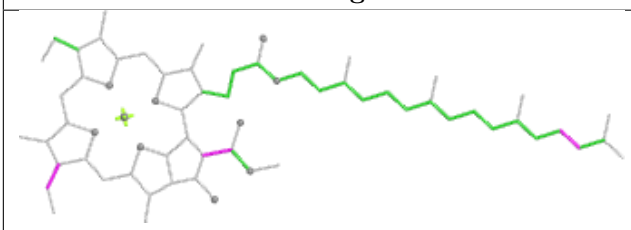
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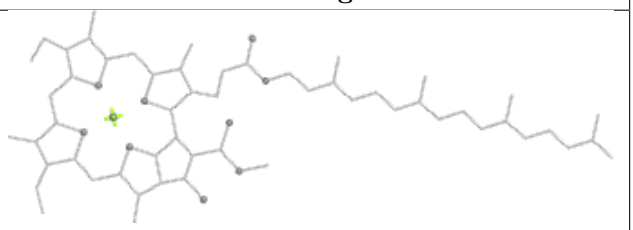
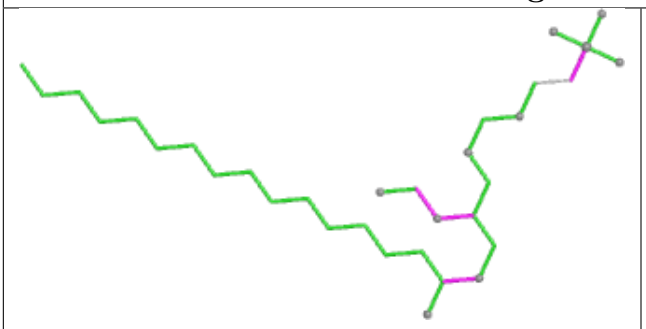

Rings

Ligand SQD d 417



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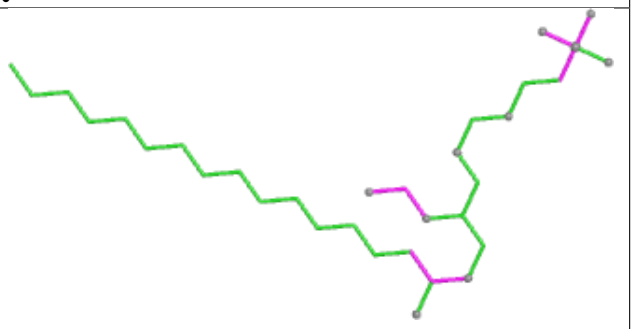
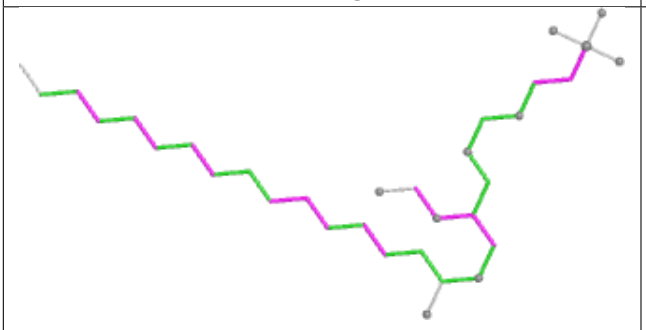


Bond angles



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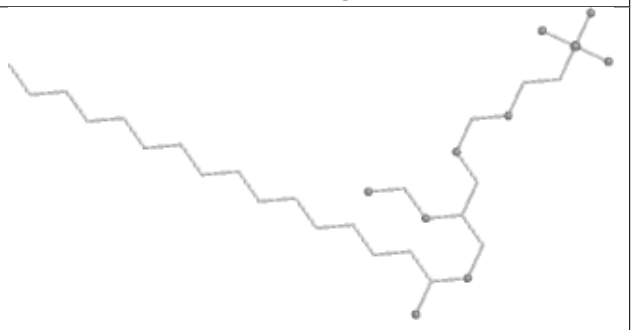
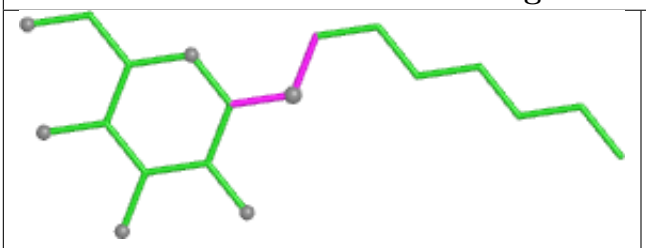


Rings

Ligand HTG b 604



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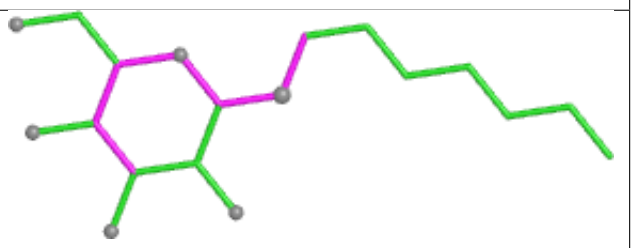

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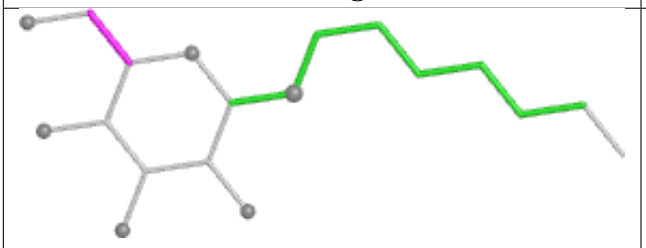

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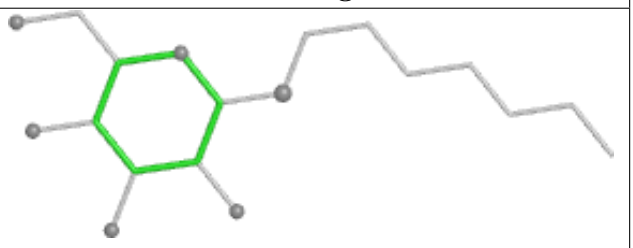
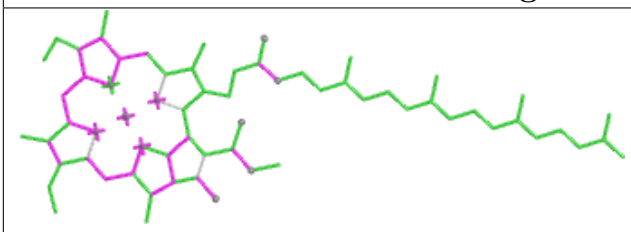


Rings

Ligand CLA a 2613



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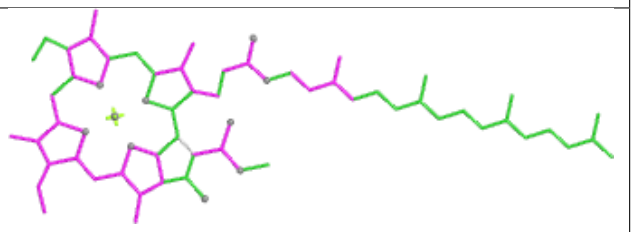
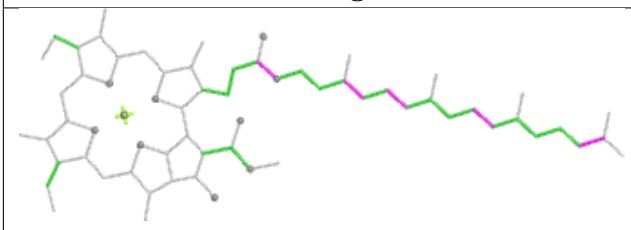


Bond angles



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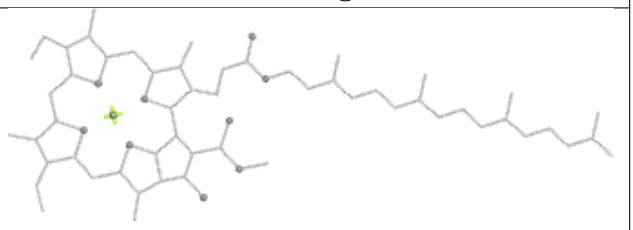
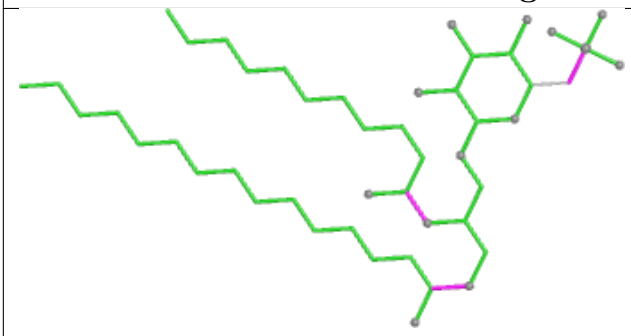


Rings

Ligand SQD a 2615



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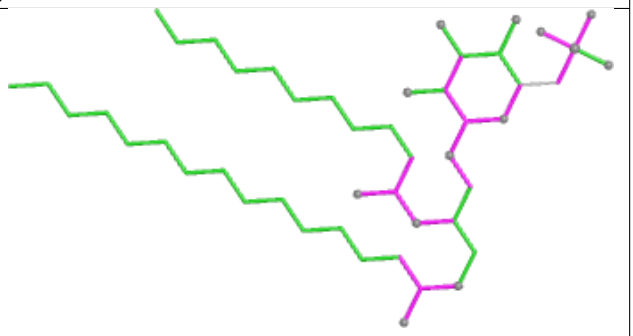
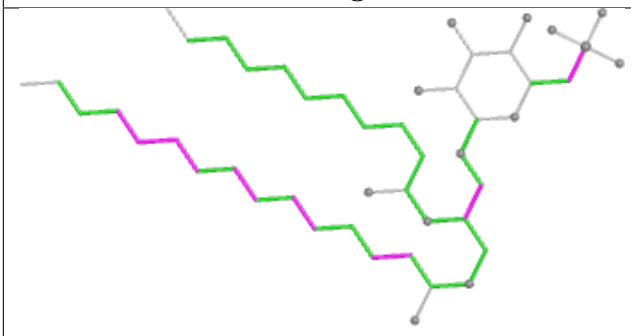


Bond angles



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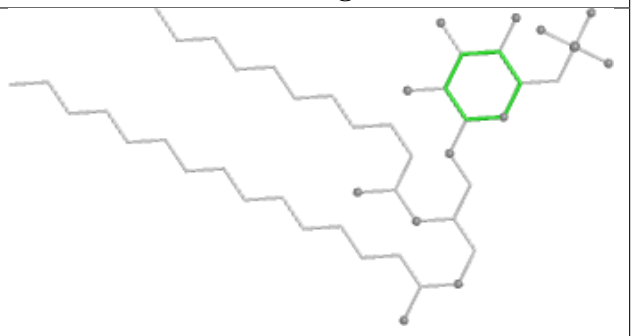
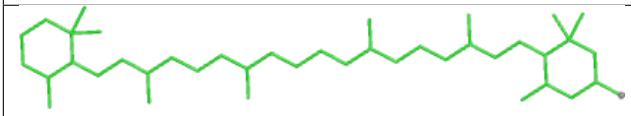


Rings

Ligand RRX H 102



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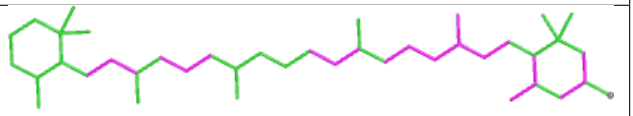
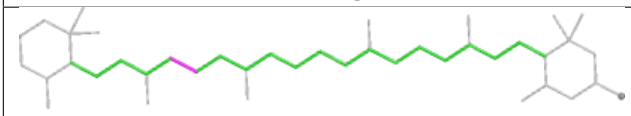


Bond angles



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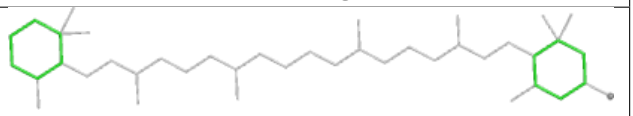
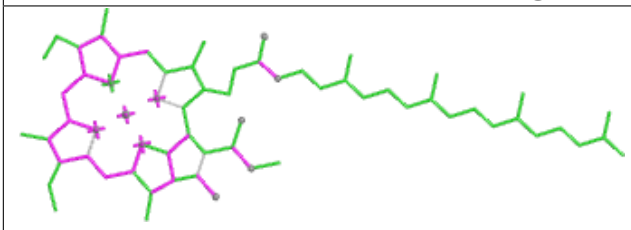


Rings

Ligand CLA c 506



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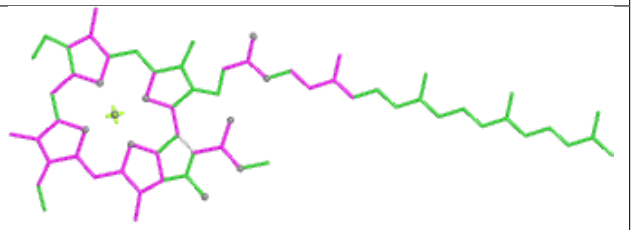
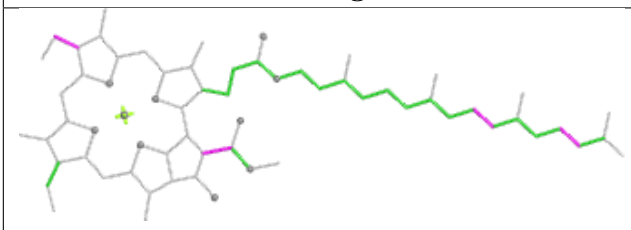


Bond angles



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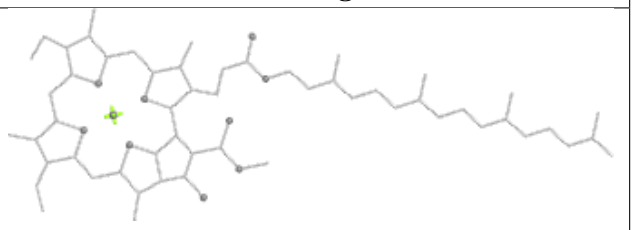
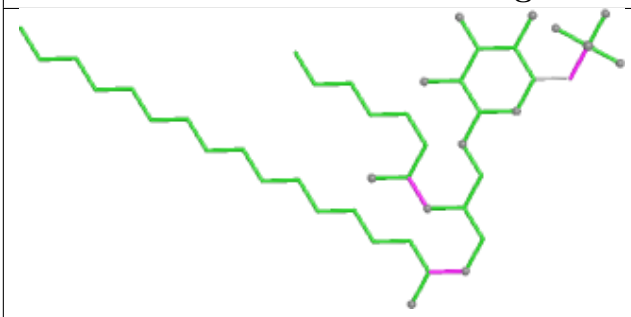


Rings

Ligand SQD D 2308



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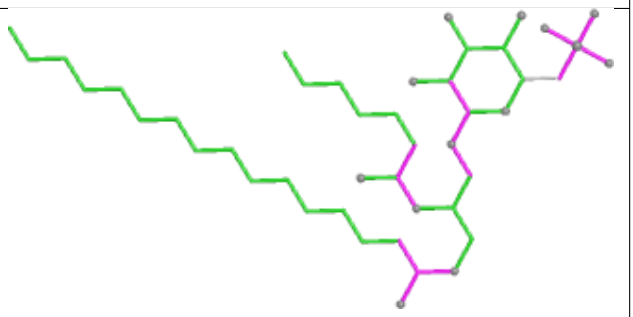
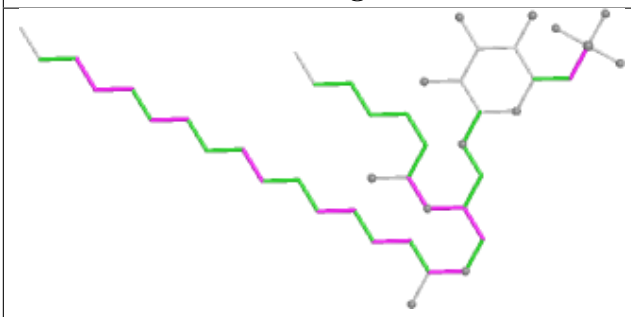


Bond angles



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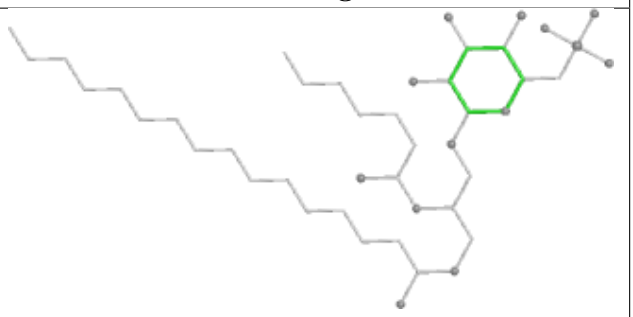
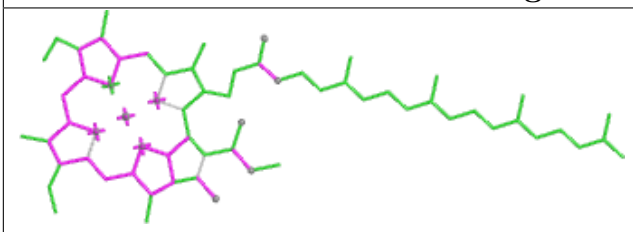


Rings

Ligand CLA B 602



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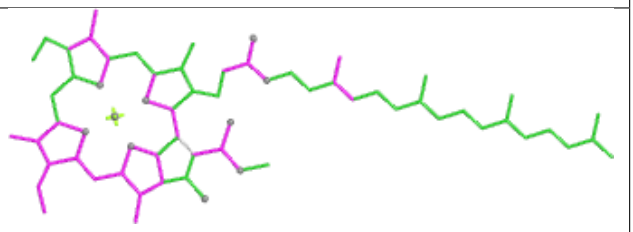
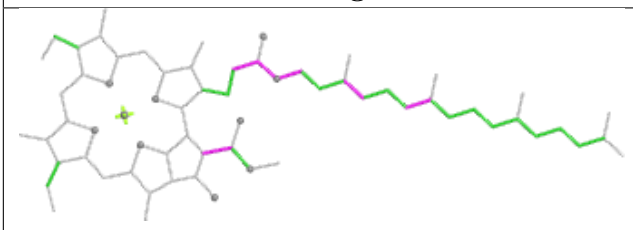


Bond angles



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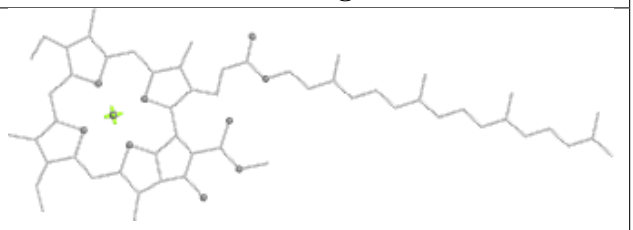
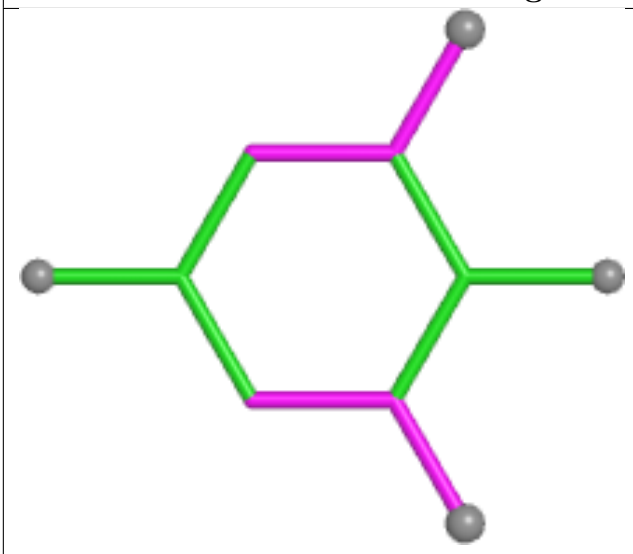


Rings

Ligand JOX A 419



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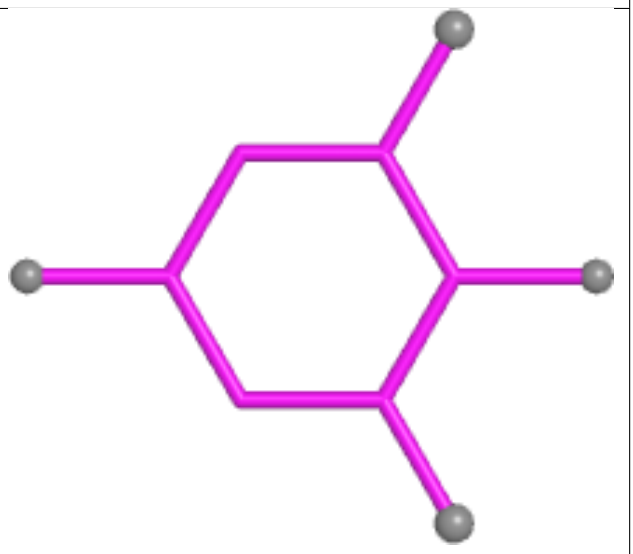
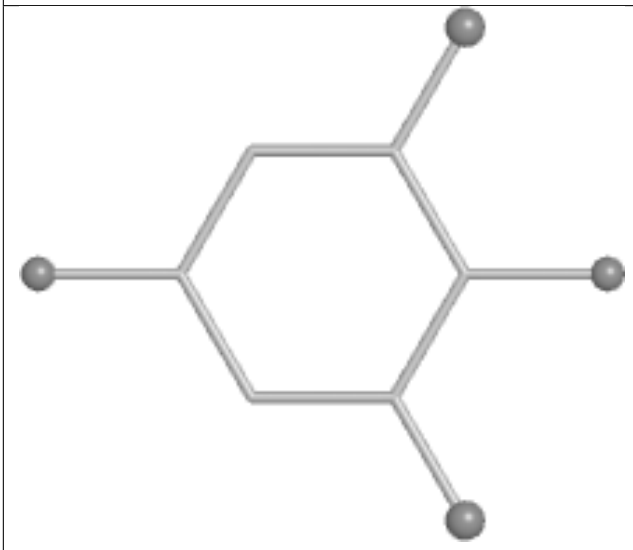


Bond angles



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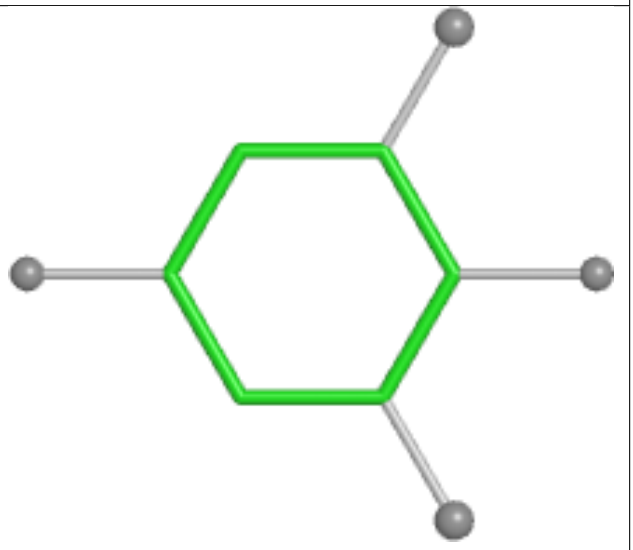
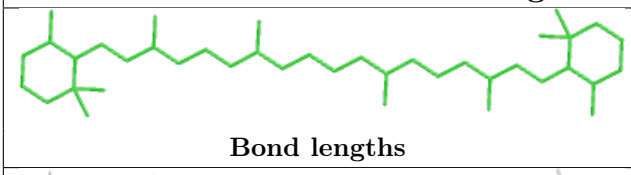
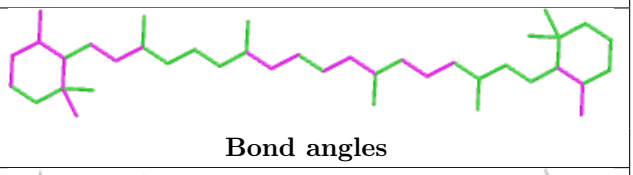


Rings

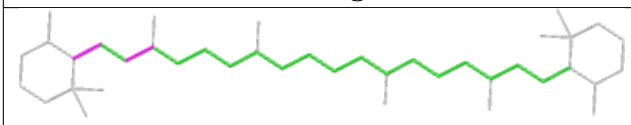
Ligand BCR c 517



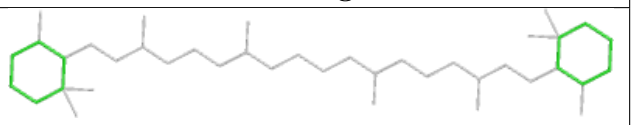
Bond lengths



Bond angles

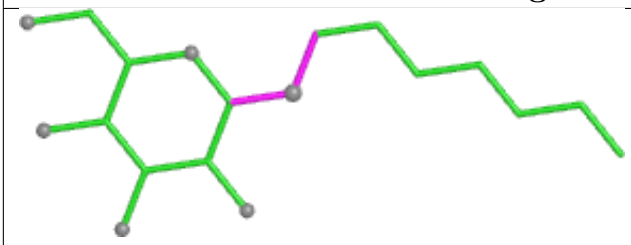


Torsions



Rings

Ligand HTG i 102



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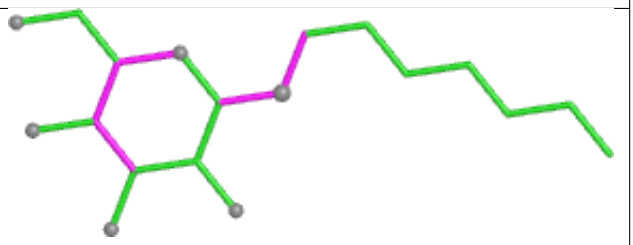

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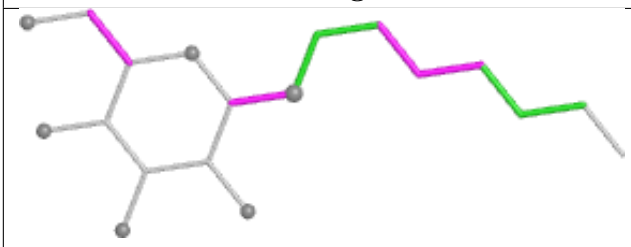

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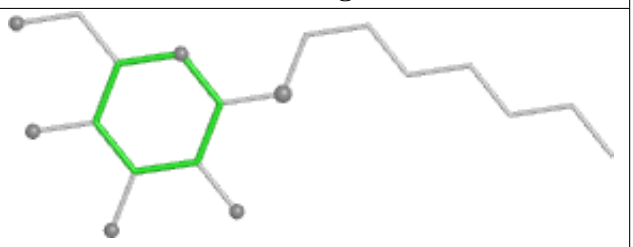
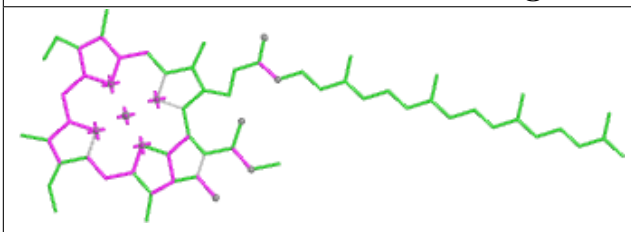


Rings

Ligand CLA C 513



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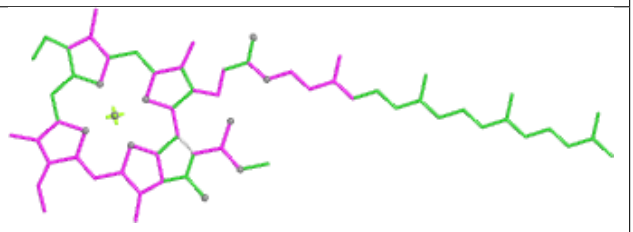

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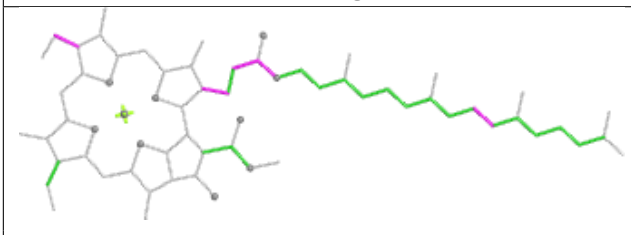

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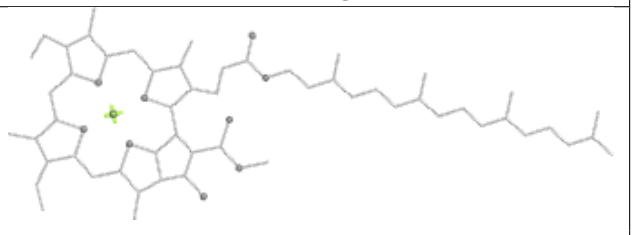
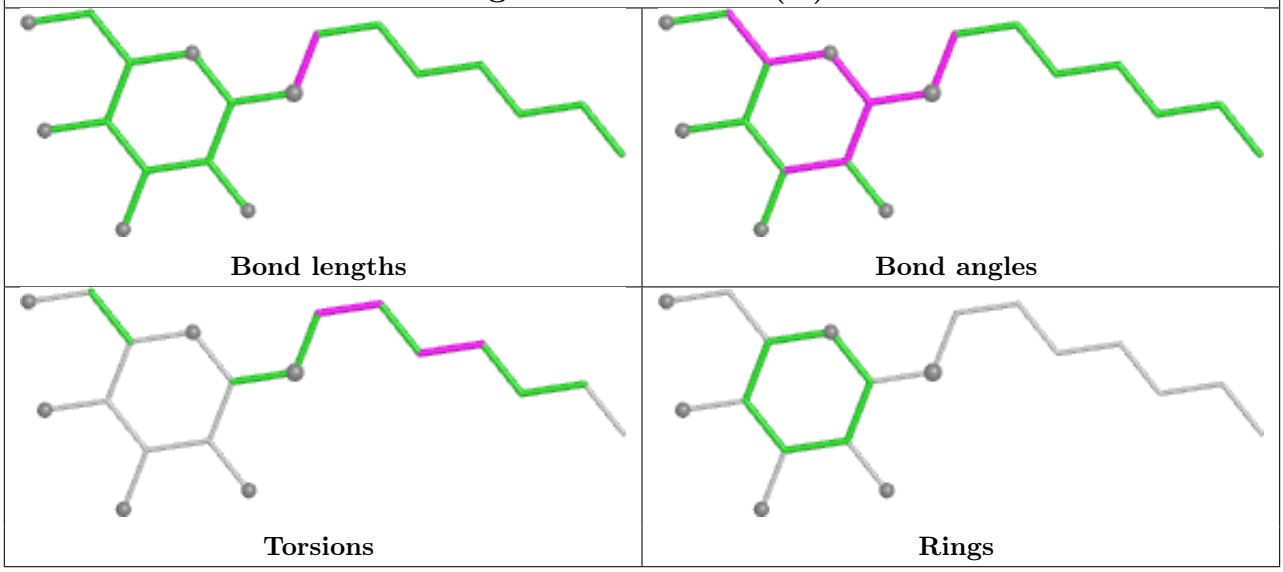
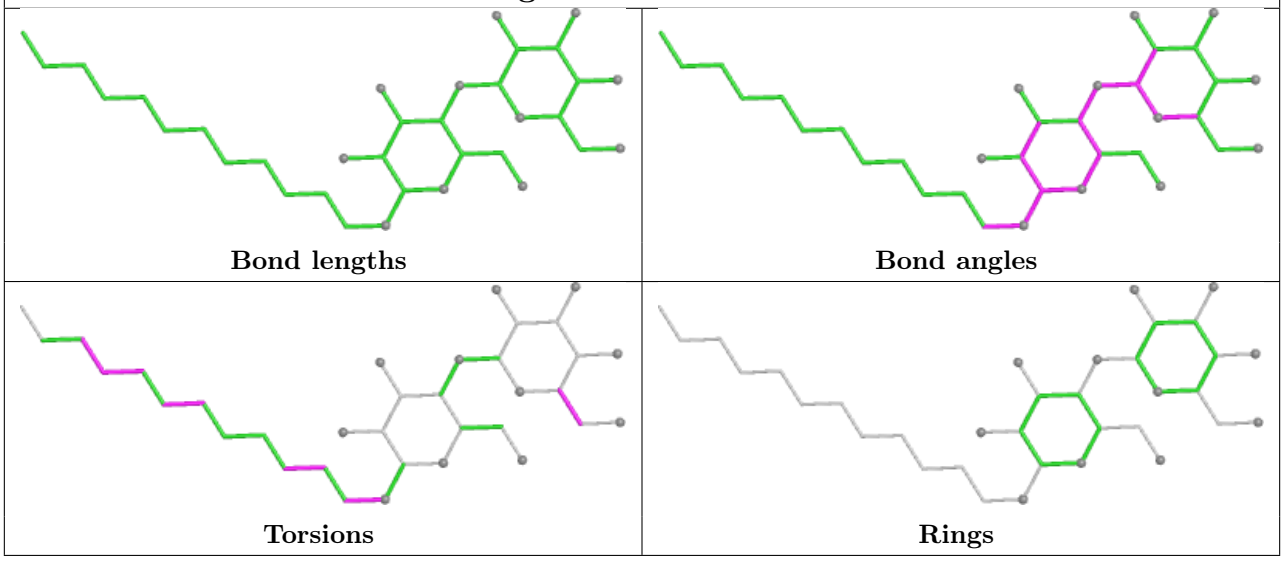


Rings

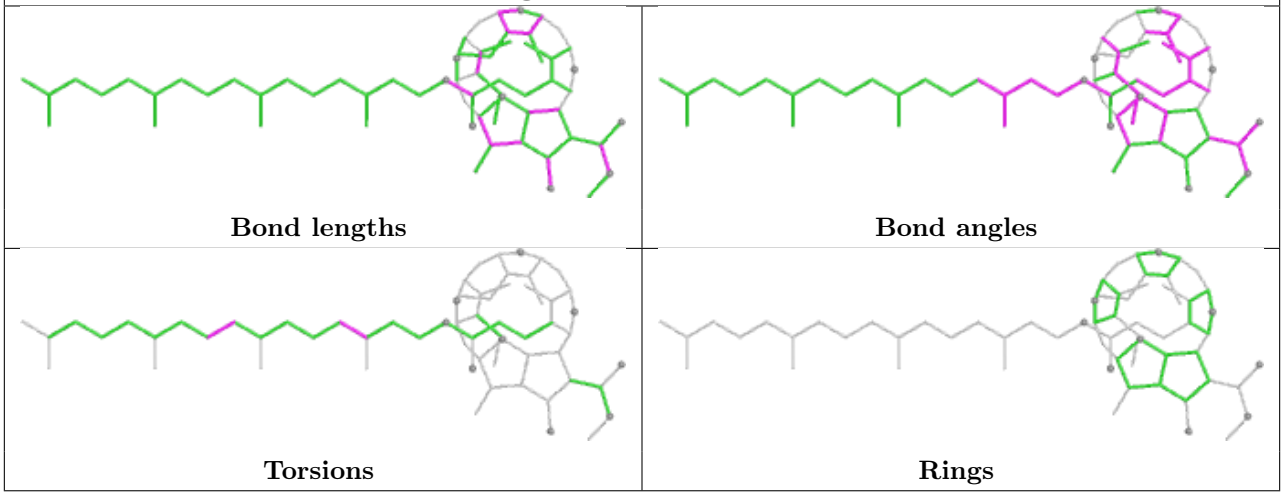
Ligand HTG B 624 (A)



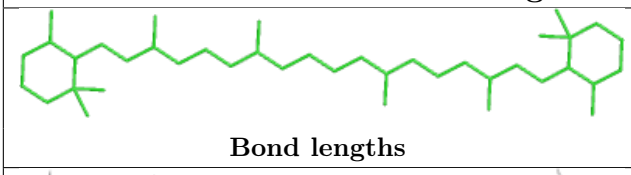
Ligand LMT M 101



Ligand PHO a 2611



Ligand BCR k 302



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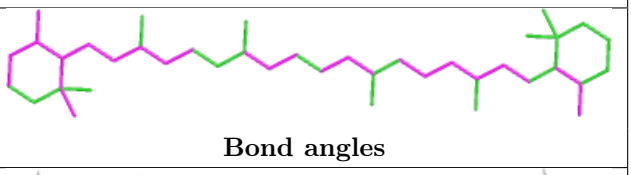
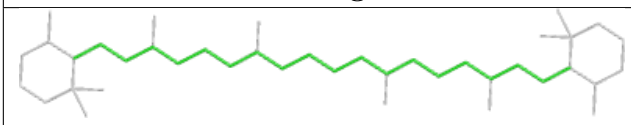


Bond angles



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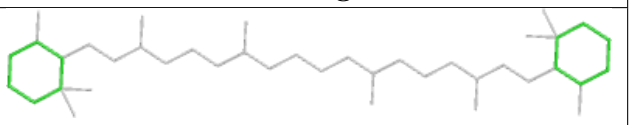
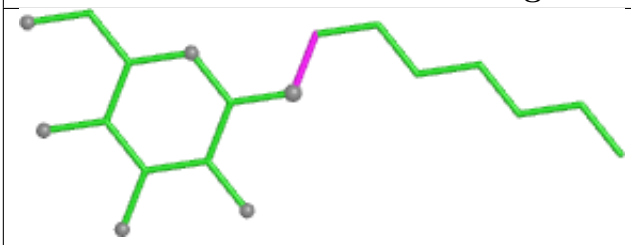


Rings

Ligand HTG b 625



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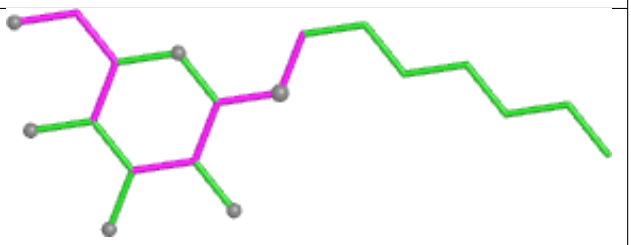
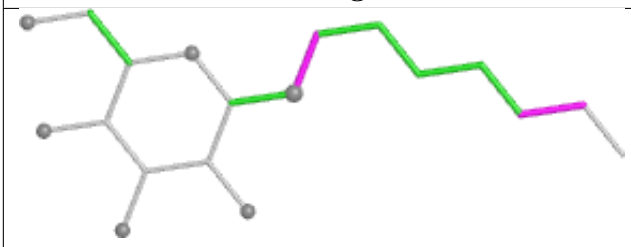


Bond angles



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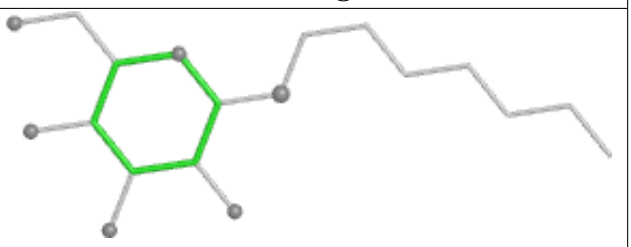
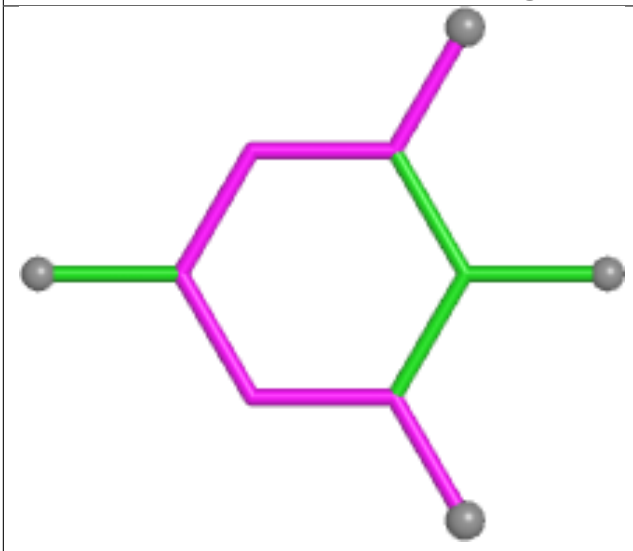


Rings

Ligand JOX a 2619



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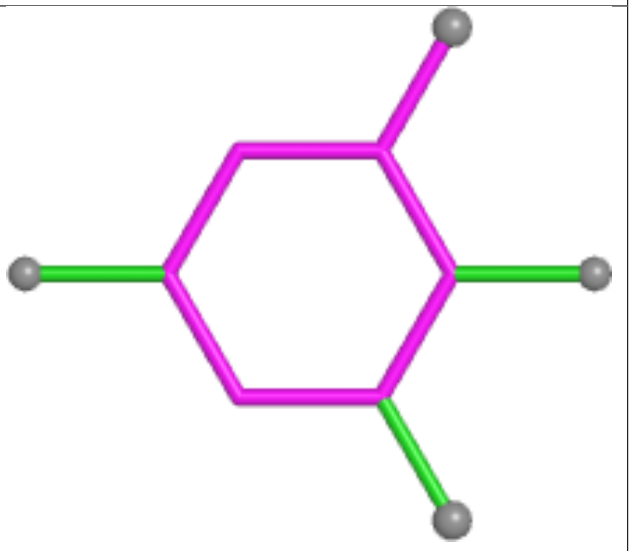
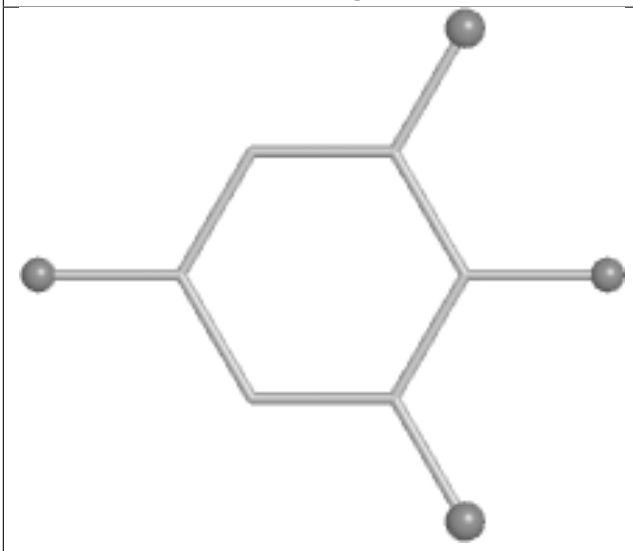


Bond angles



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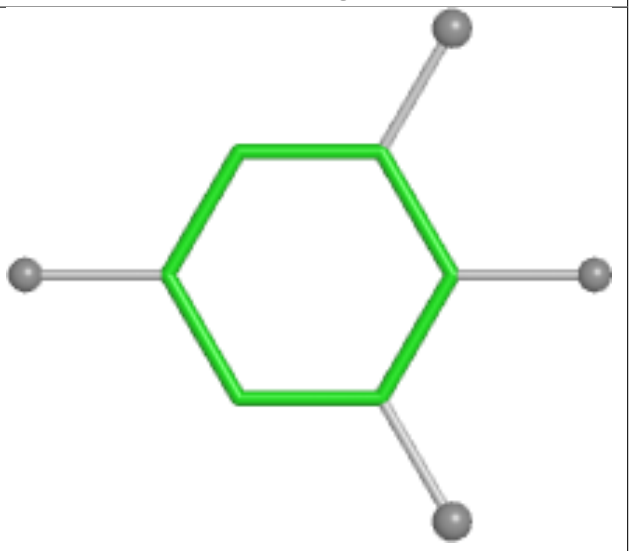
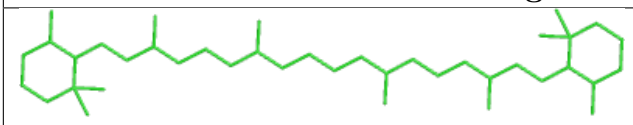


Rings

Ligand BCR d 410



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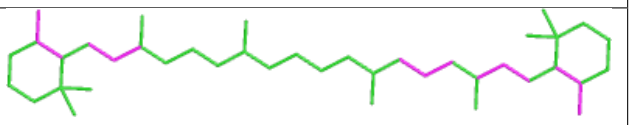

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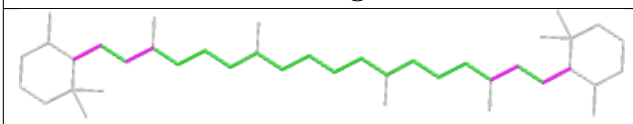

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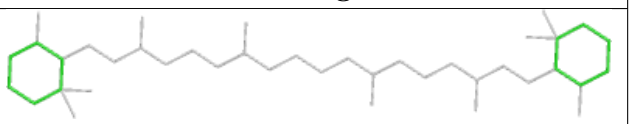
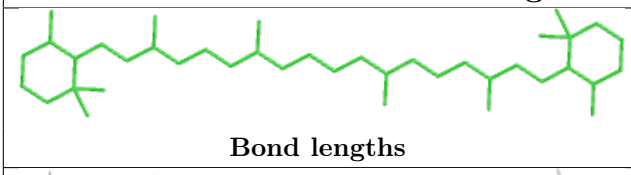


Rings

Ligand BCR b 624



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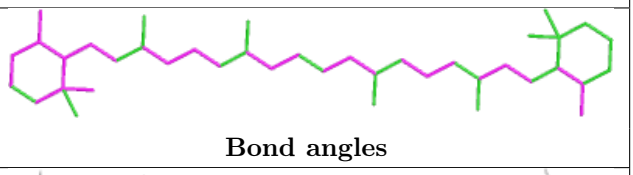
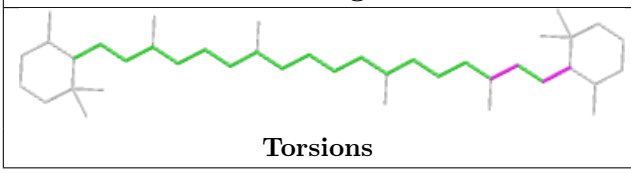


Bond angles



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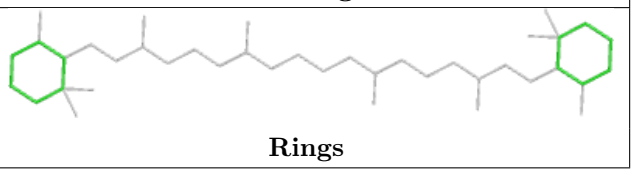
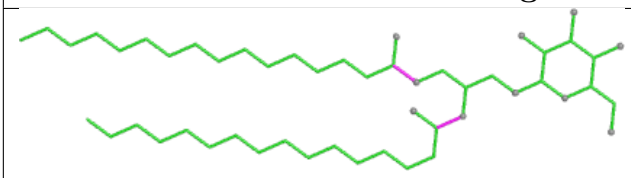


Rings

Ligand LMG B 622



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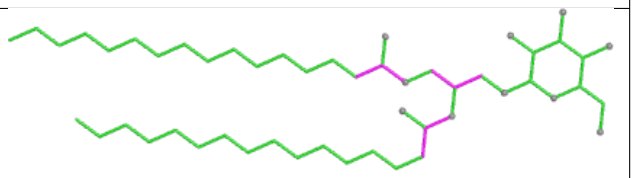

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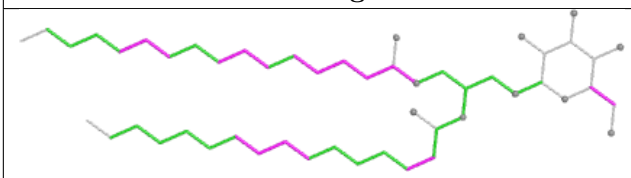

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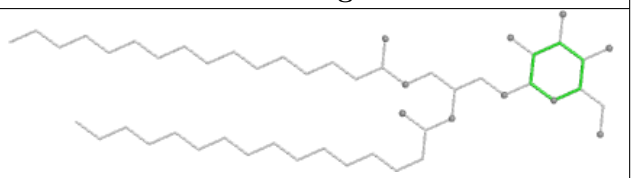
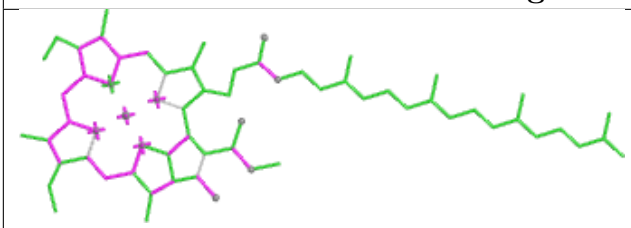


Rings

Ligand CLA b 617



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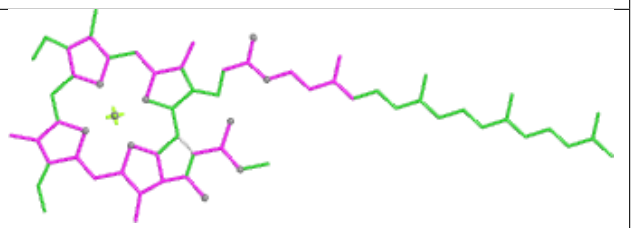
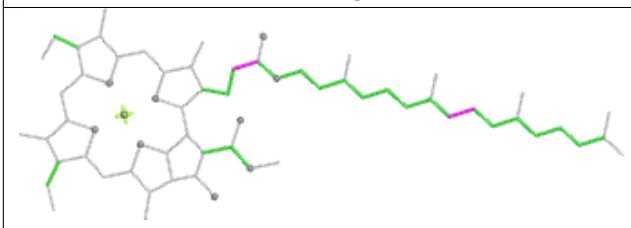


Bond angles



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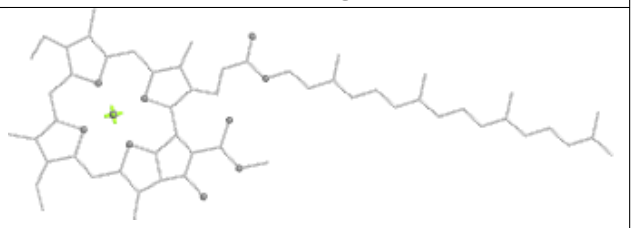
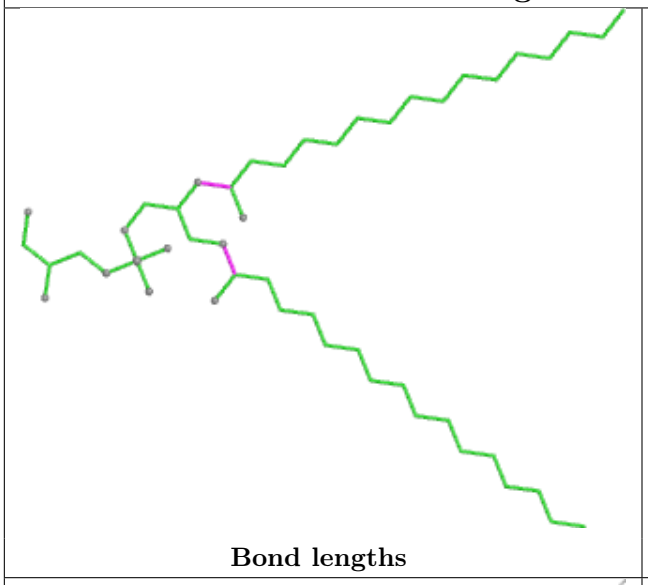


Rings

Ligand LHG D 2310



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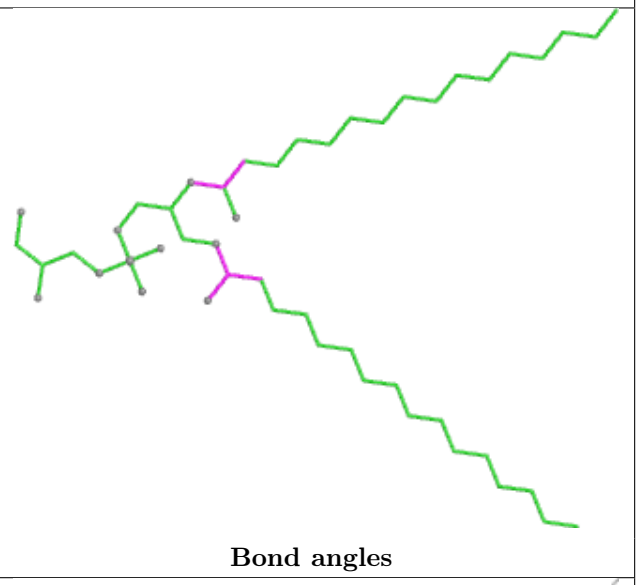
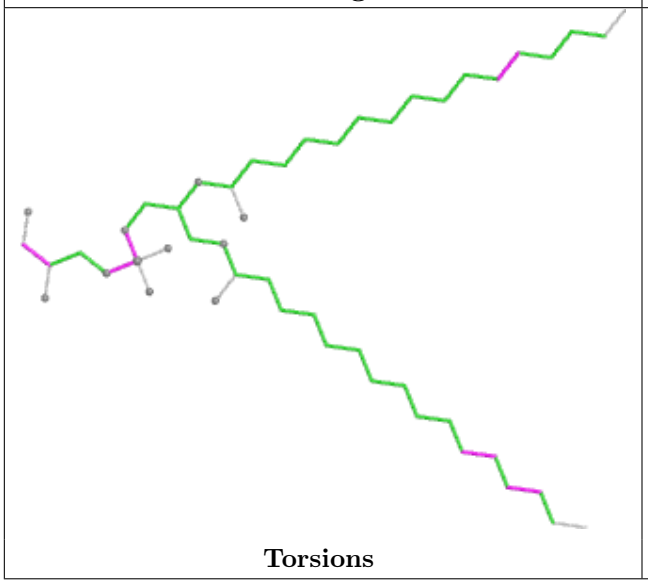


Bond angles



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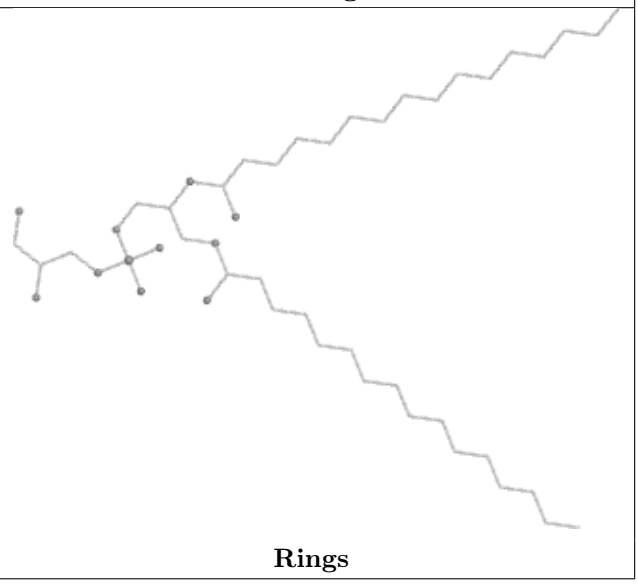
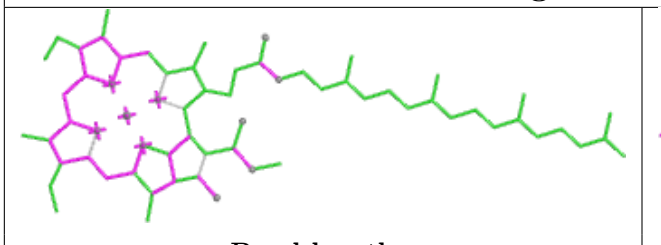


Rings

Ligand CLA c 516



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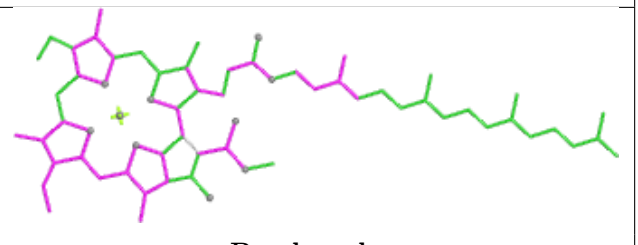
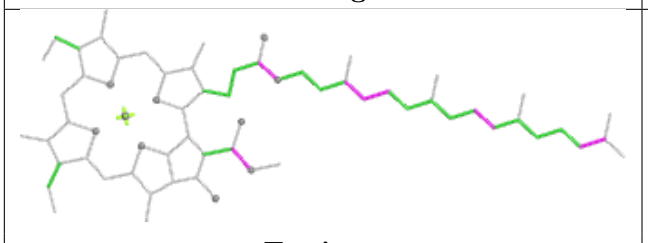


Bond angles



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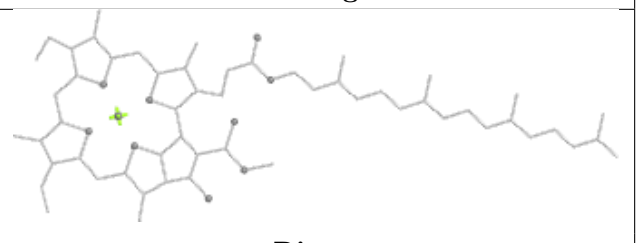
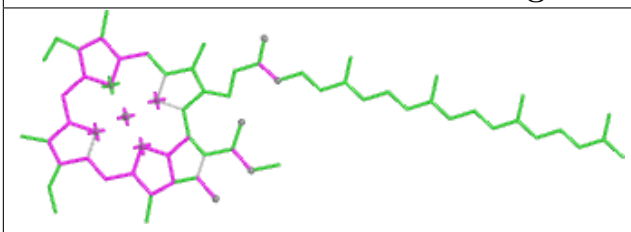


Rings

Ligand CLA b 606



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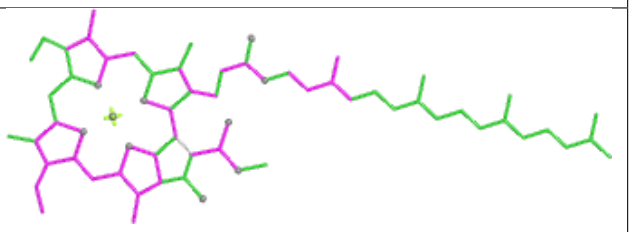
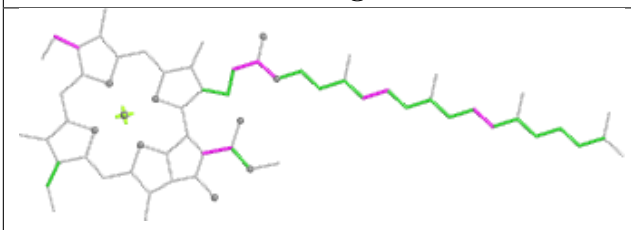


Bond angles



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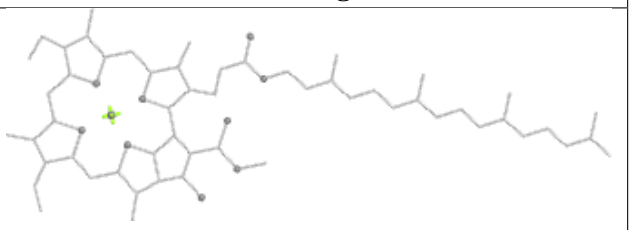
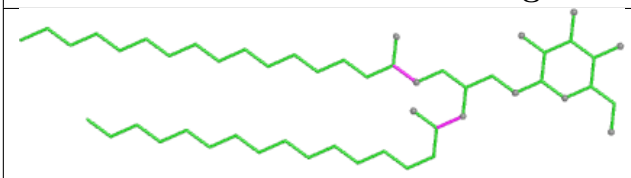


Rings

Ligand LMG d 414



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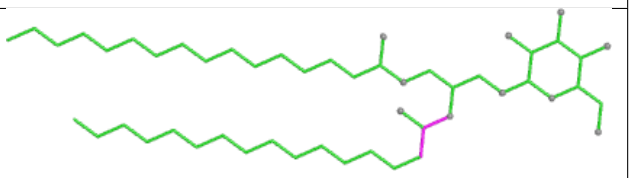
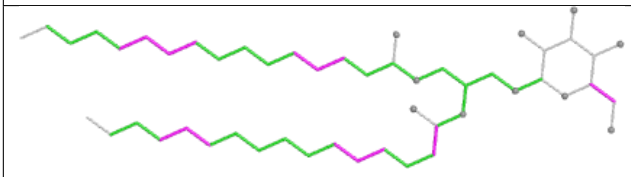


Bond angles



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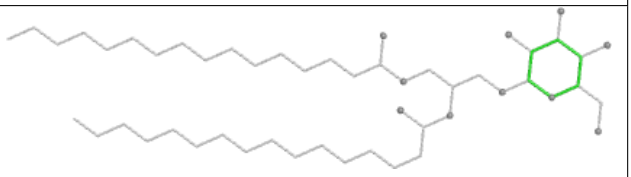
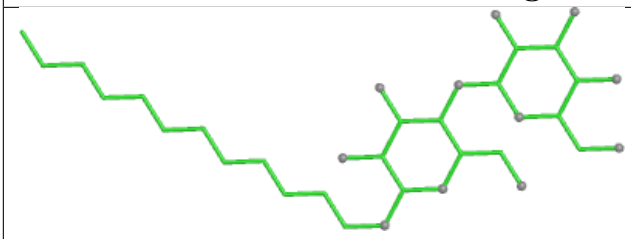
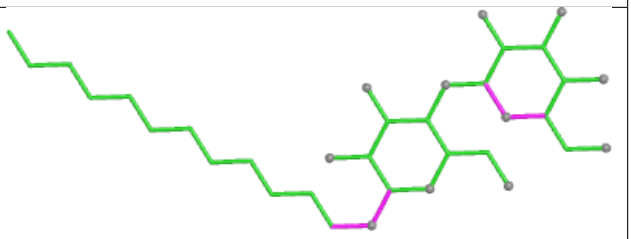


Rings

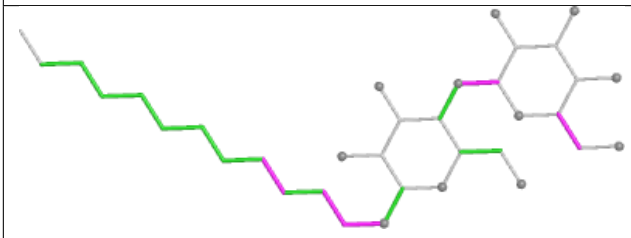
Ligand LMT Z 101



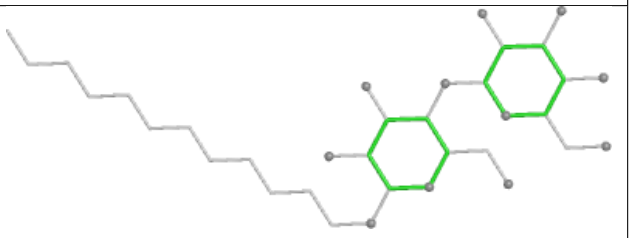
Bond lengths



Bond angles

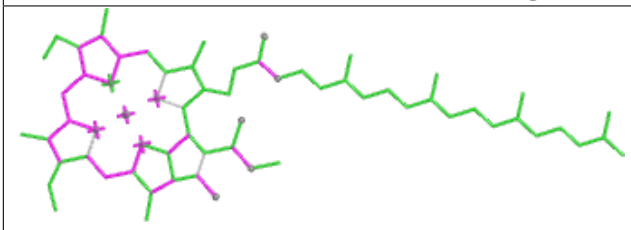


Torsions



Rings

Ligand CLA B 614



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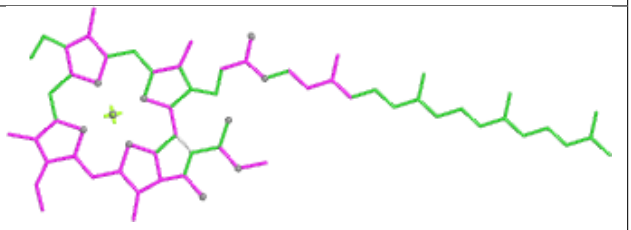

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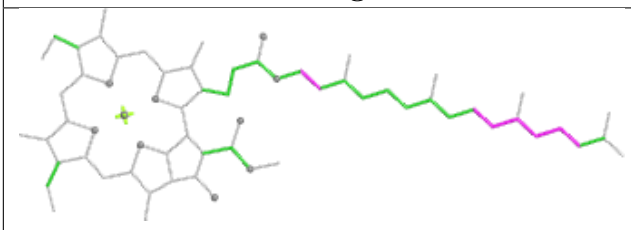

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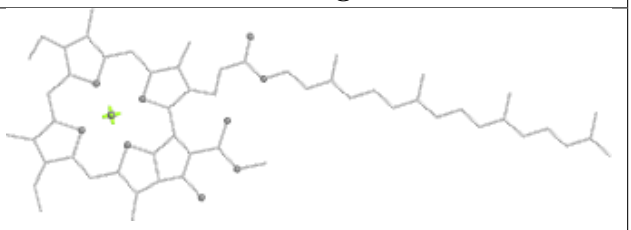
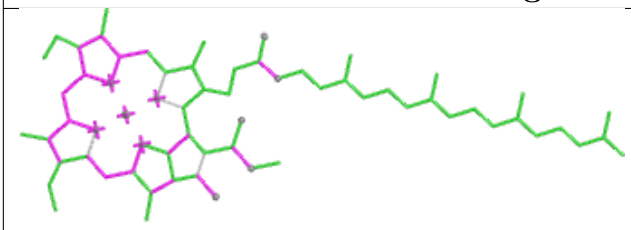


Rings

Ligand CLA A 406



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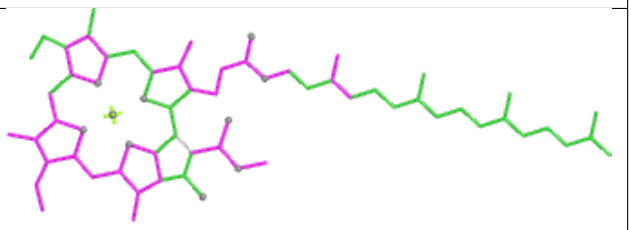

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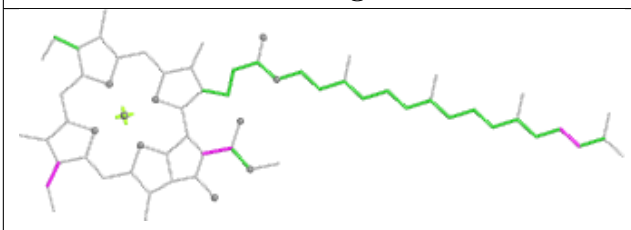

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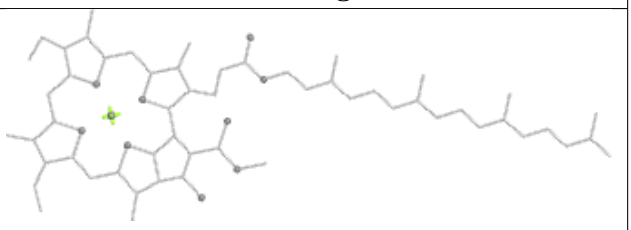
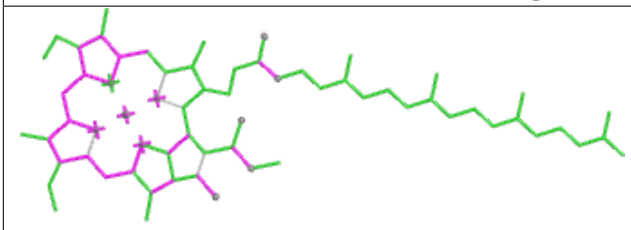


Rings

Ligand CLA b 609



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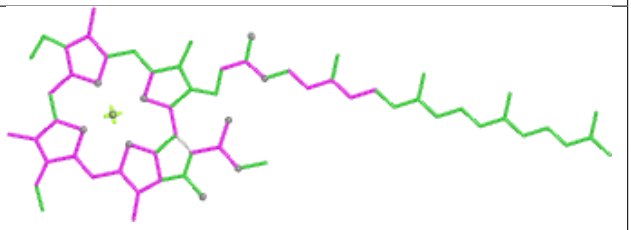

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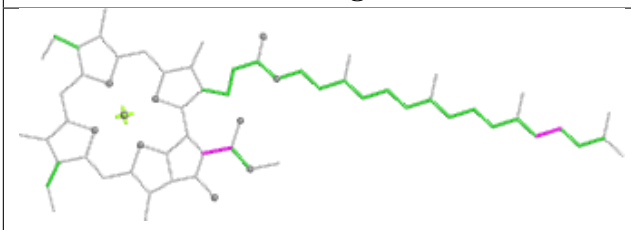

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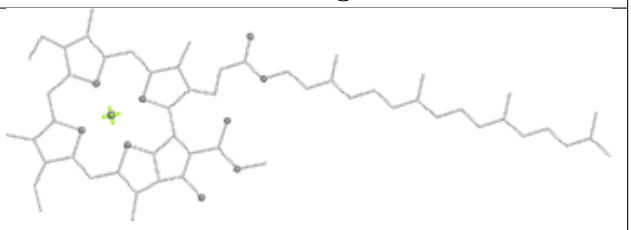
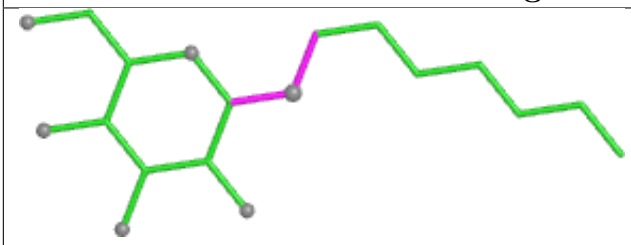


Rings

Ligand HTG d 415



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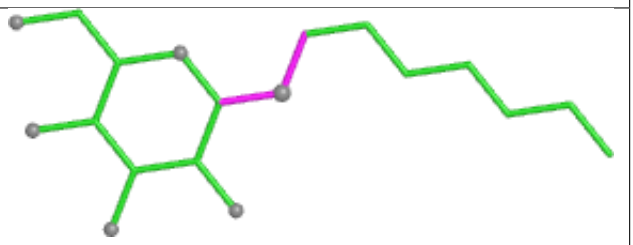

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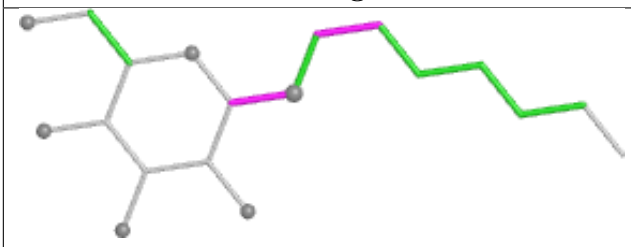

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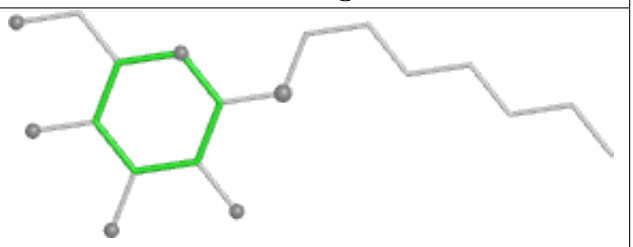
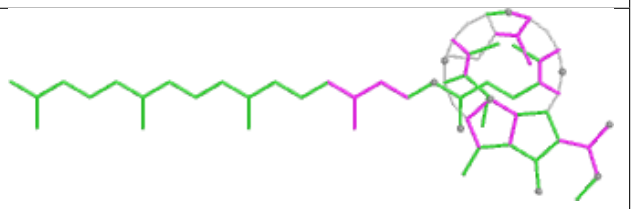


Rings

Ligand PHO A 409



Bond lengths



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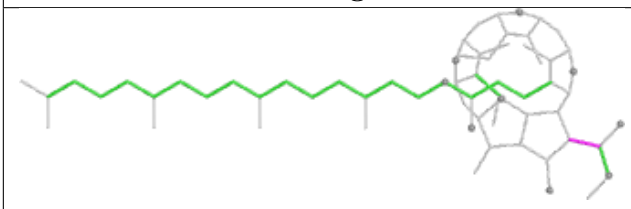

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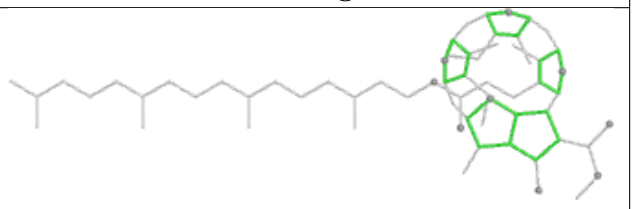
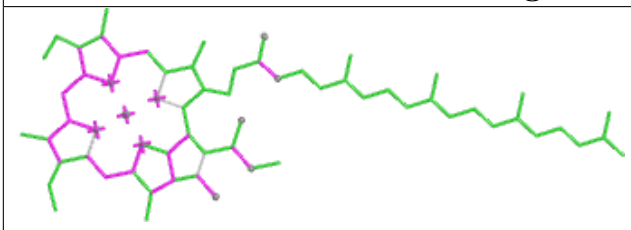


Rings

Ligand CLA A 407



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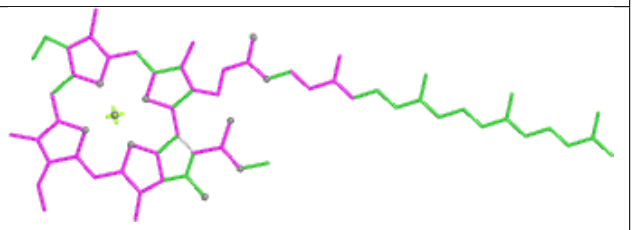

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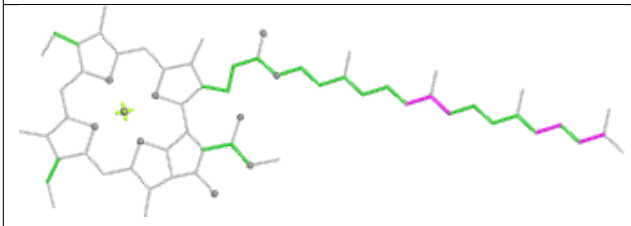

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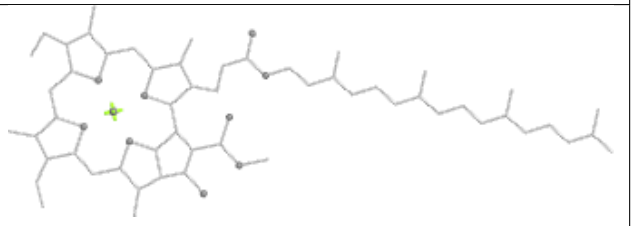
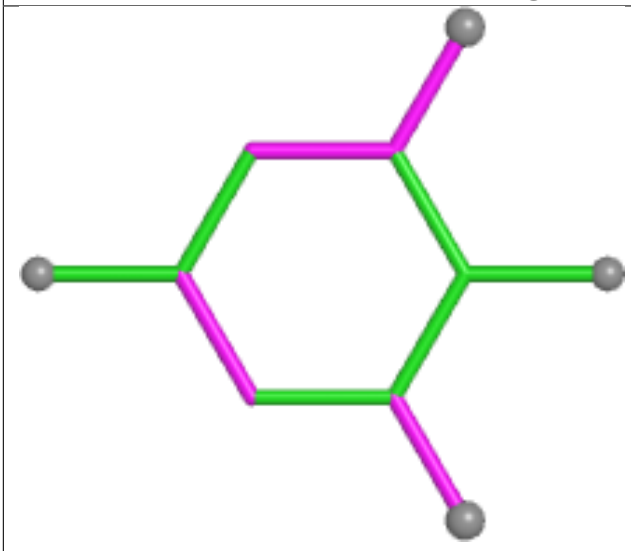


Rings

Ligand JOX A 418



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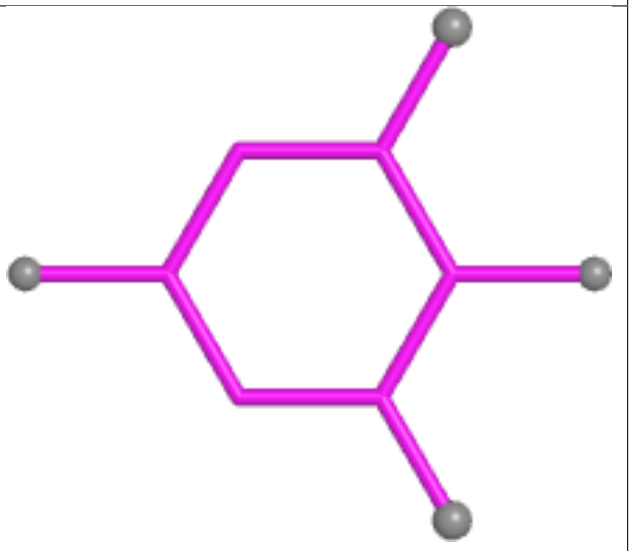
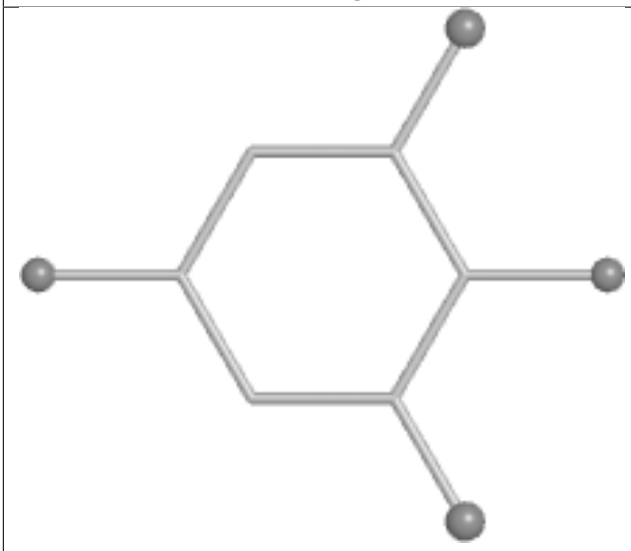


Bond angles



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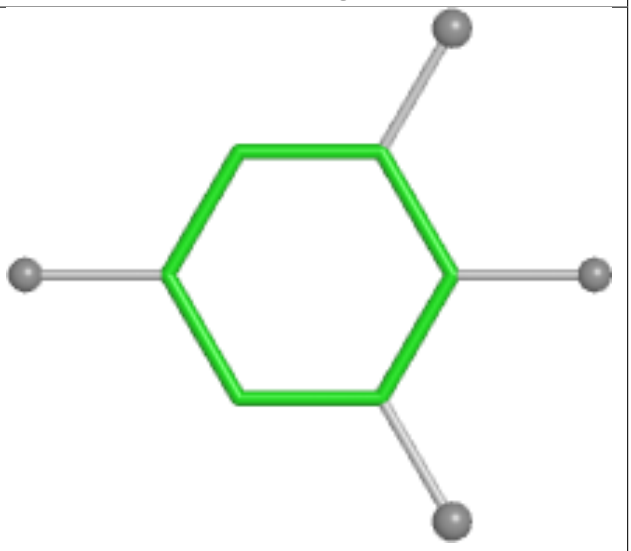
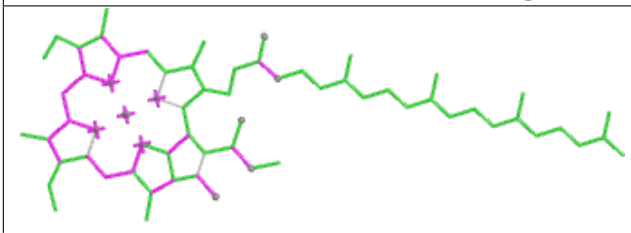


Rings

Ligand CLA a 2610



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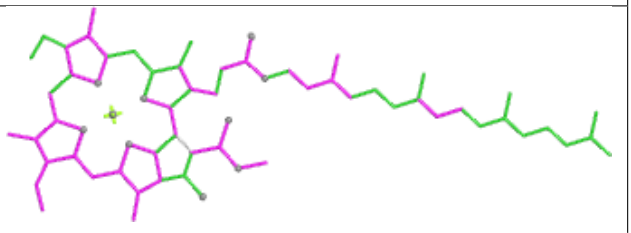
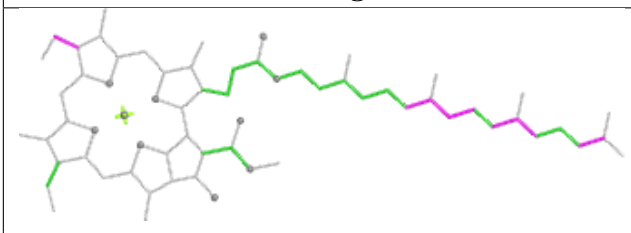


Bond angles



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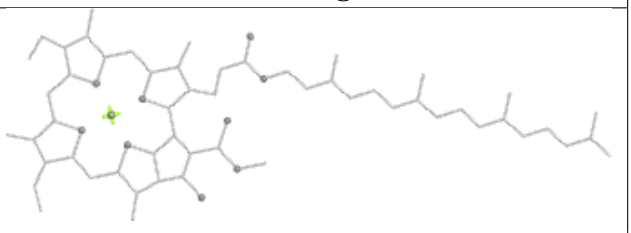
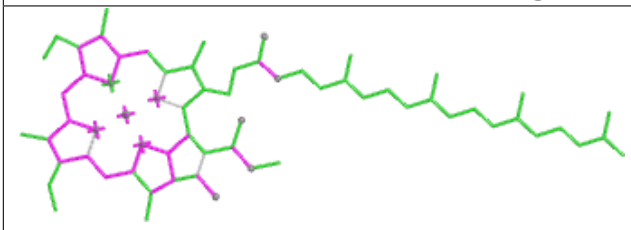


Rings

Ligand CLA c 508



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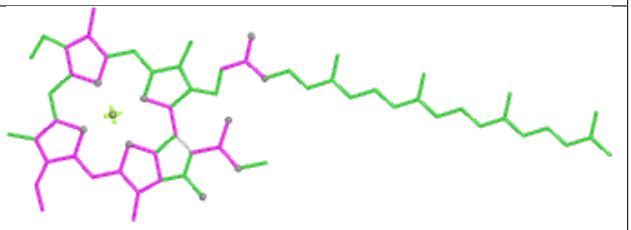
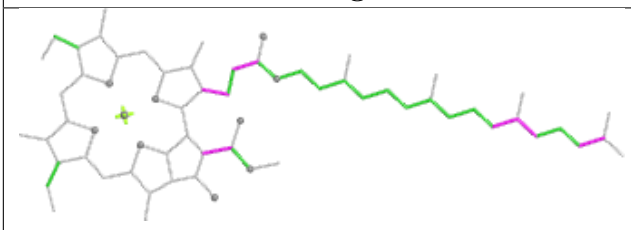


Bond angles



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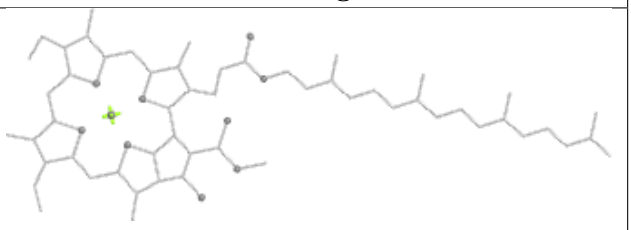
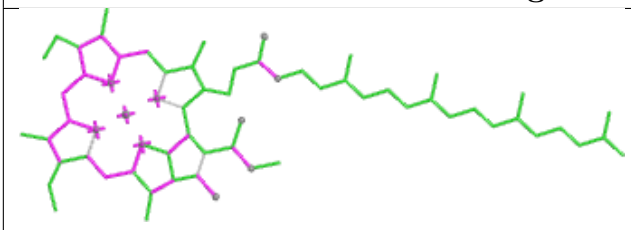


Rings

Ligand CLA b 611



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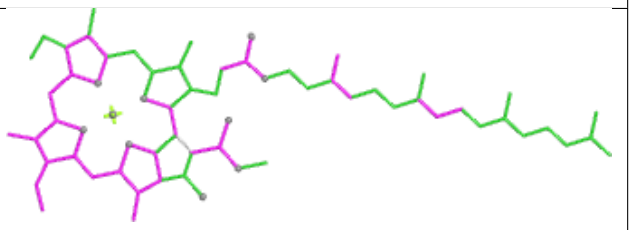

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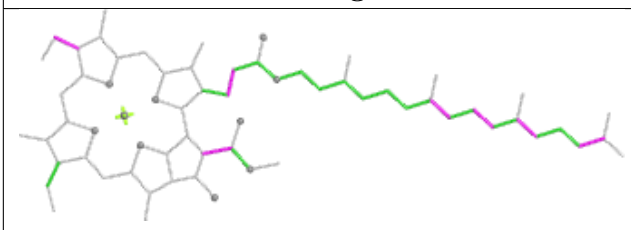

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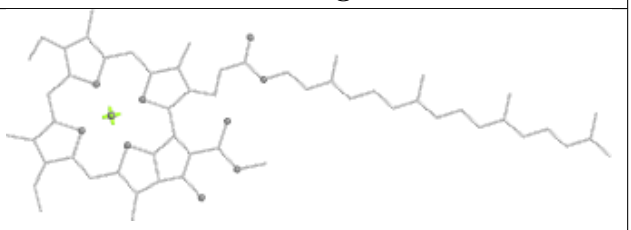
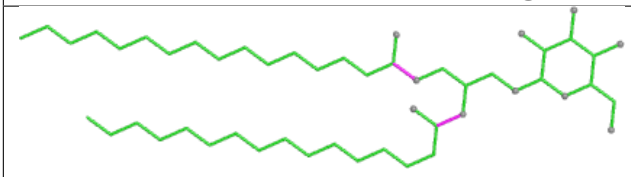


Rings

Ligand LMG C 527



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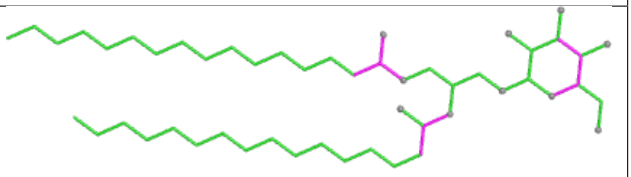
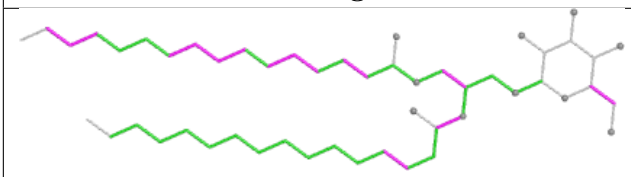


Bond angles



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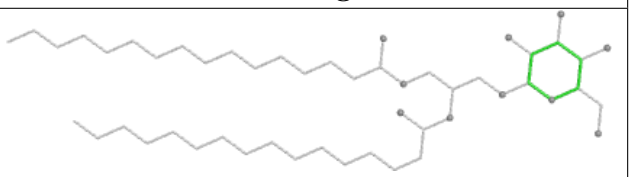
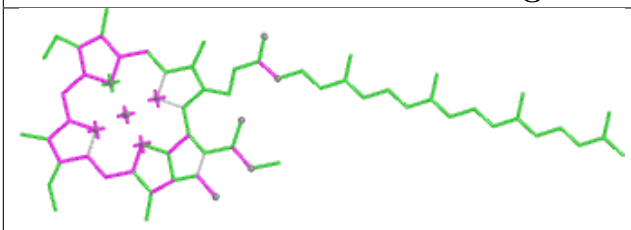


Rings

Ligand CLA A 405



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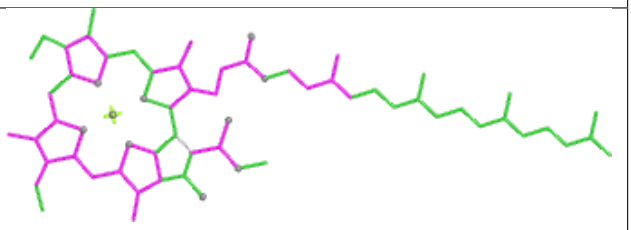
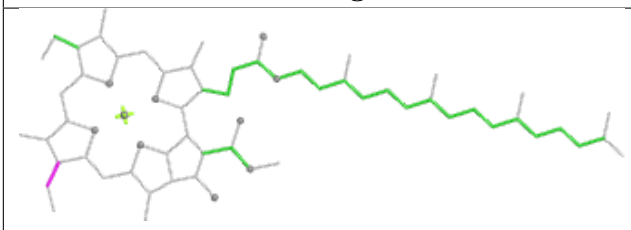


Bond angles



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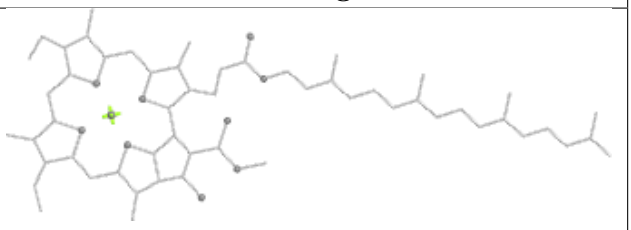
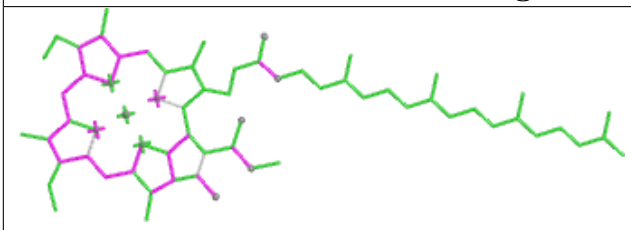


Rings

Ligand CLA D 2303



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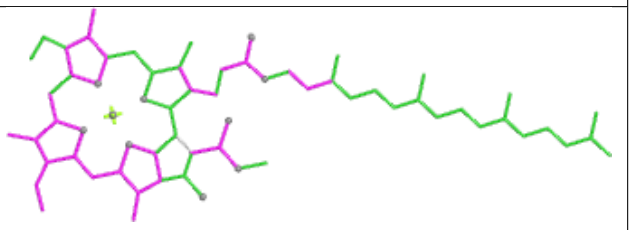
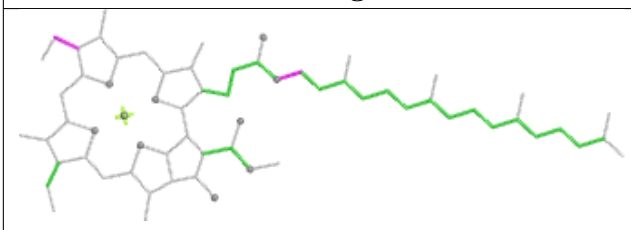


Bond angles



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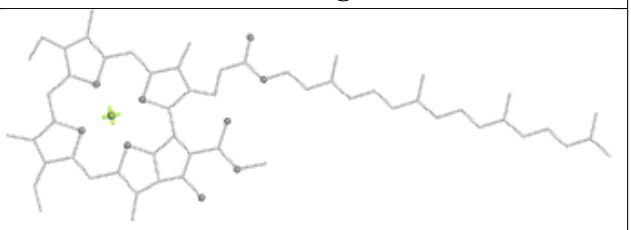
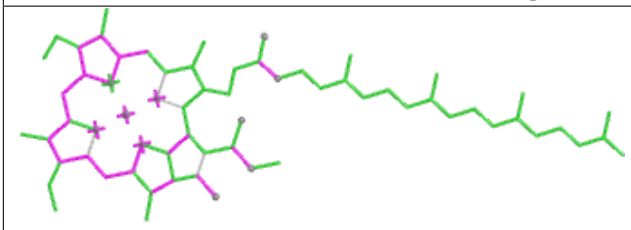


Rings

Ligand CLA B 608



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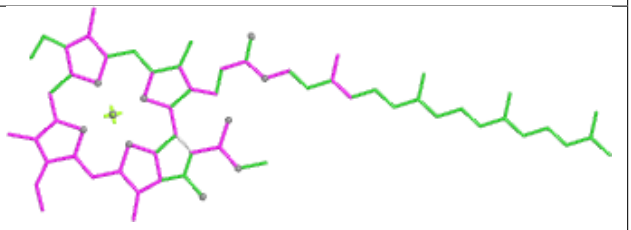
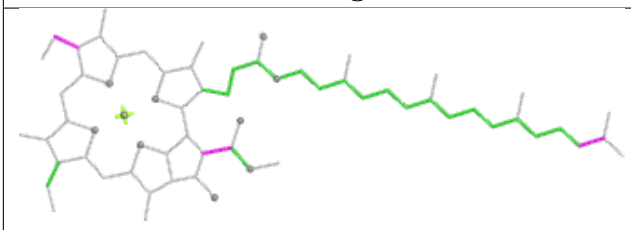


Bond angles



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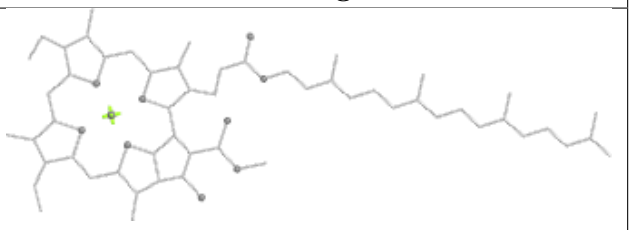
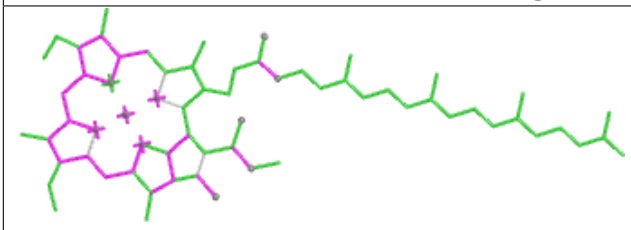
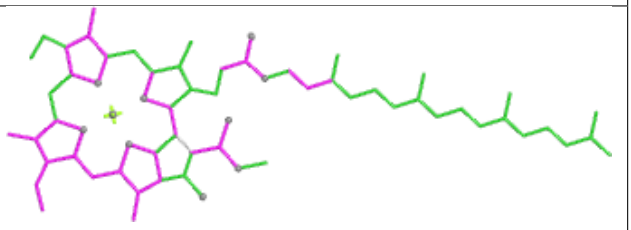


Rings

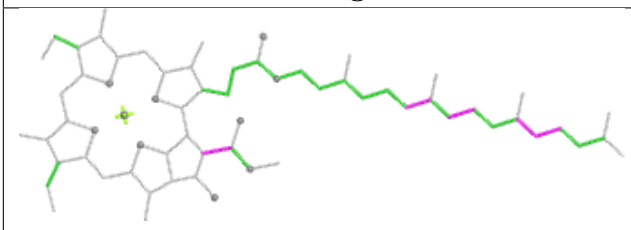
Ligand CLA c 512



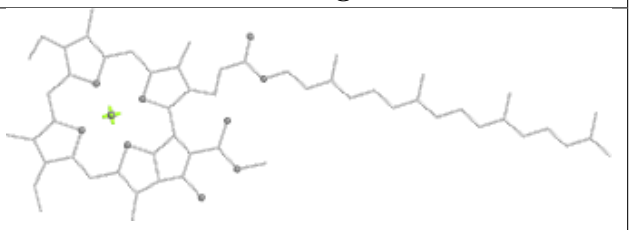
Bond lengths



Bond angles



Torsions



Rings

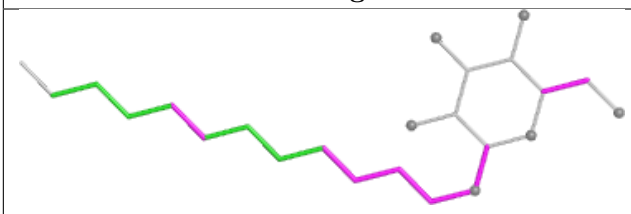
Ligand LMT i 103



Bond lengths



Bond angles



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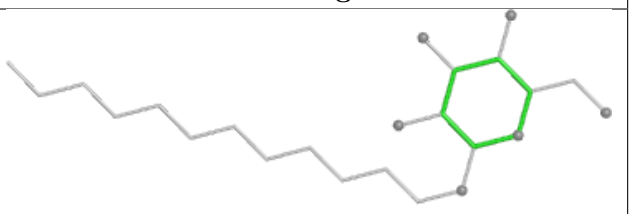
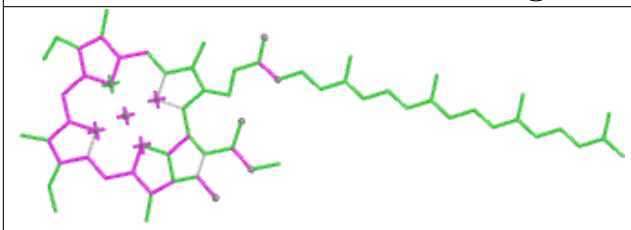
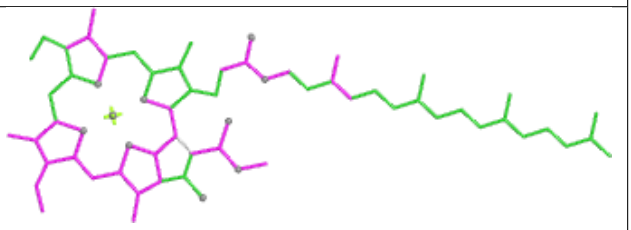


Rings

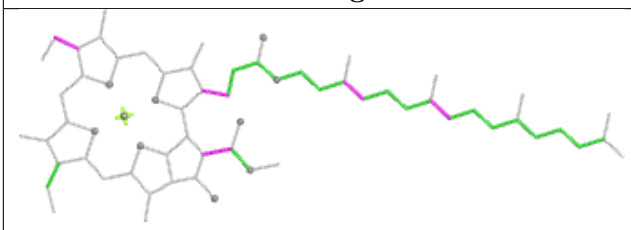
Ligand CLA b 614



Bond lengths



Bond angles



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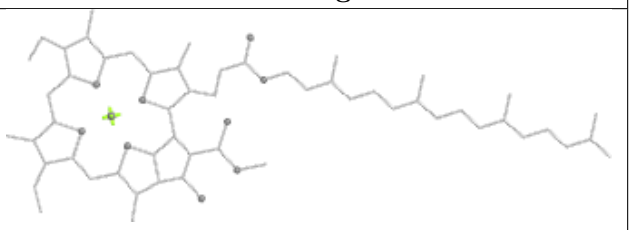
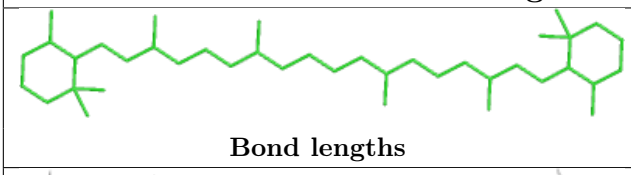
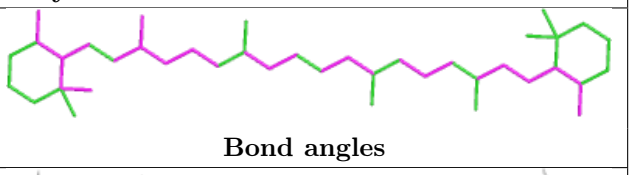


Rings

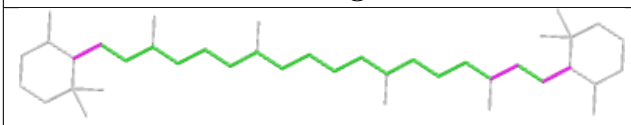
Ligand BCR y 101



Bond lengths



Bond angles



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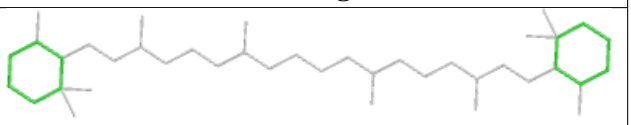
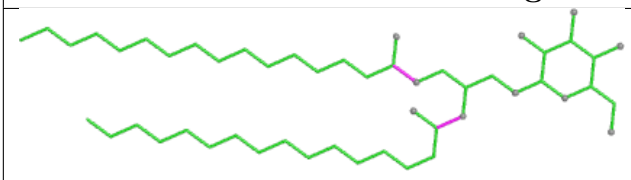


Rings

Ligand LMG c 522



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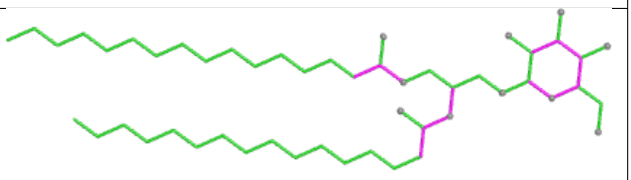
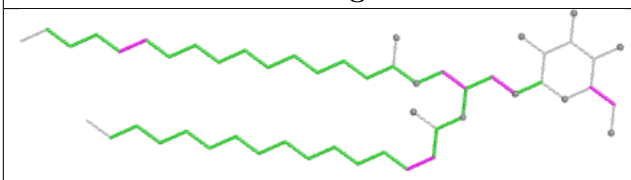
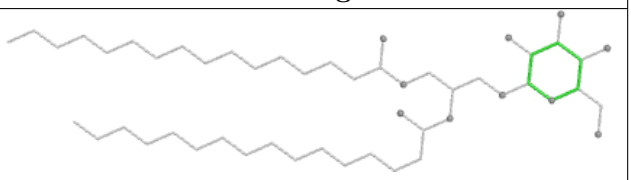


Bond angles

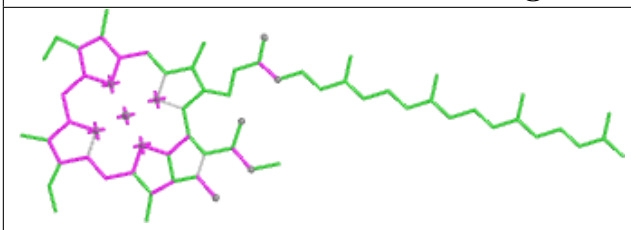


Torsions

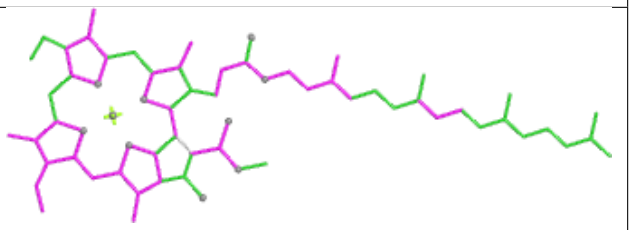


Rings

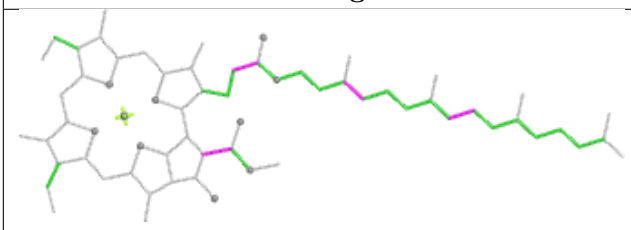
Ligand CLA C 511



Bond lengths



Bond angles



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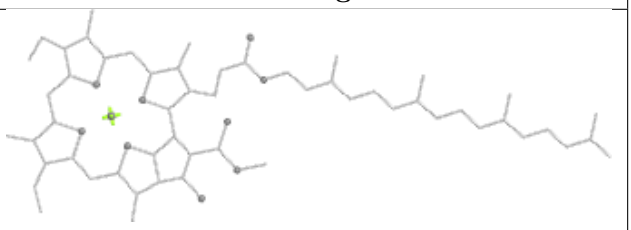
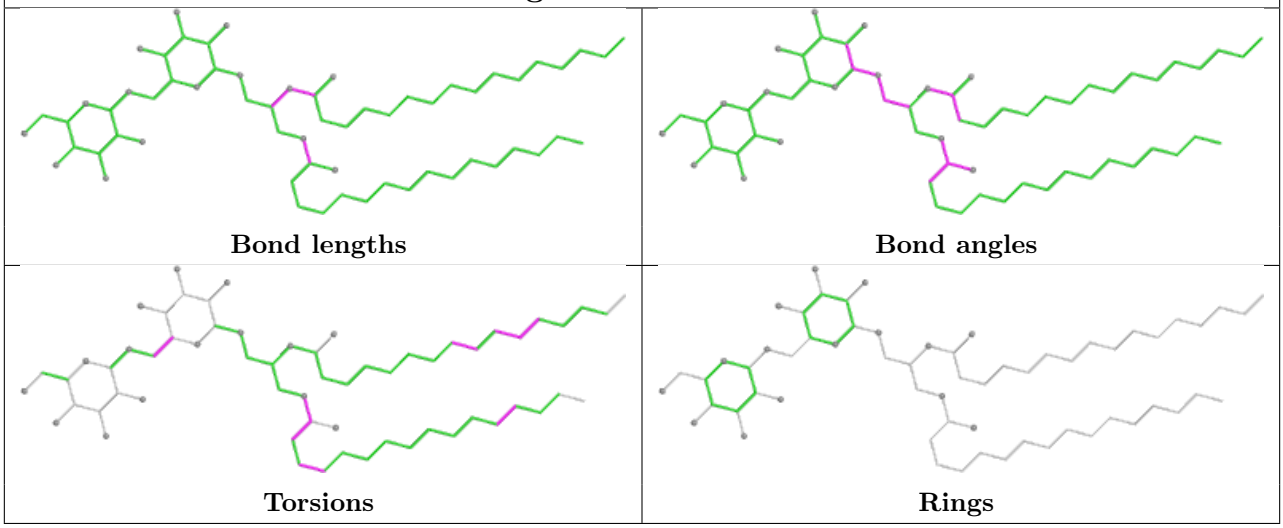
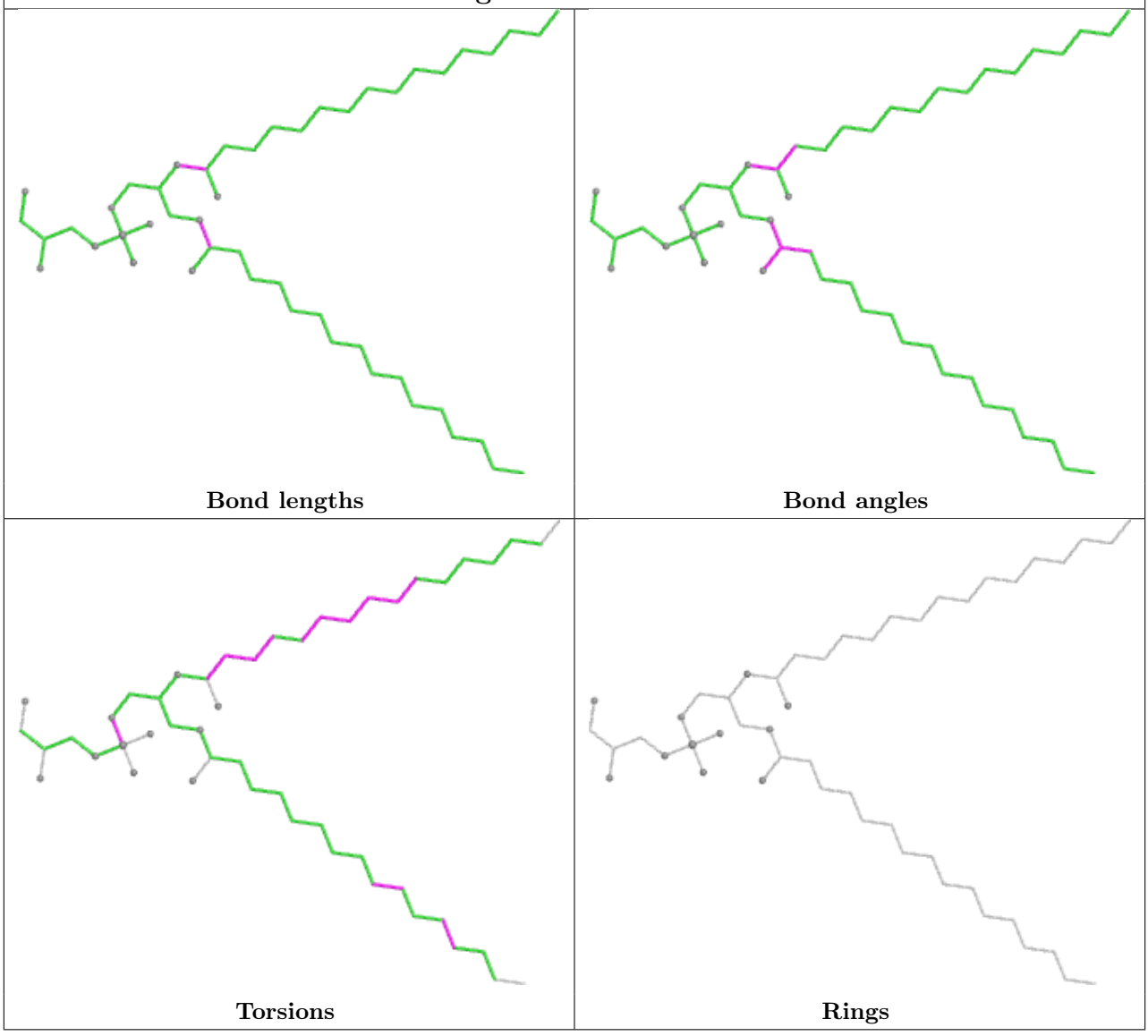


Rings

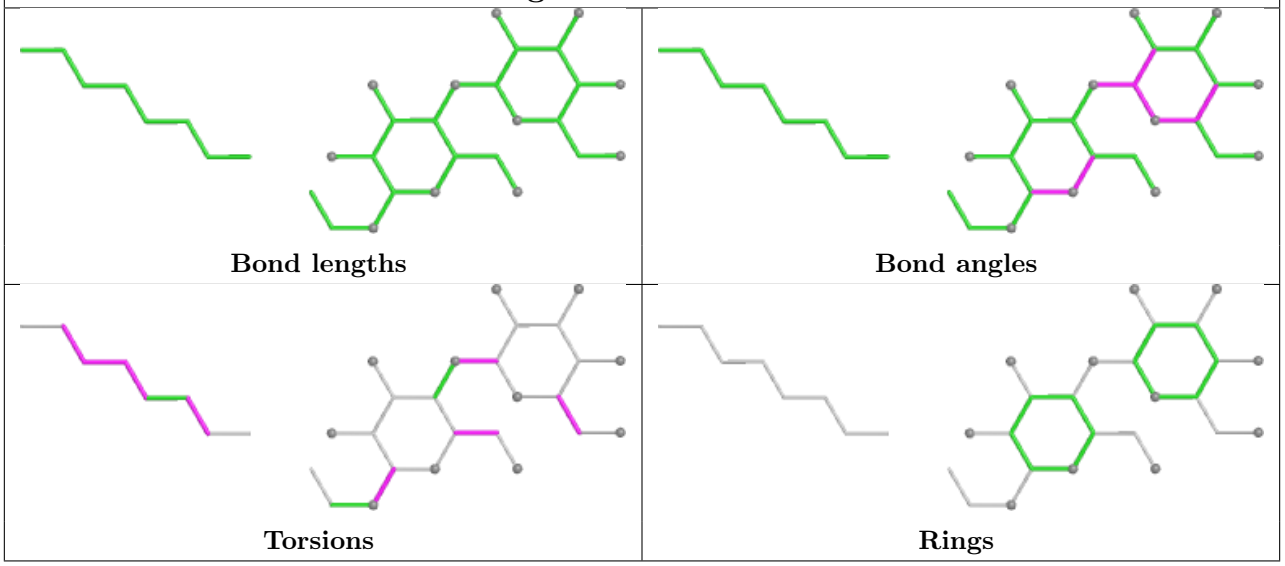
Ligand DGD c 520



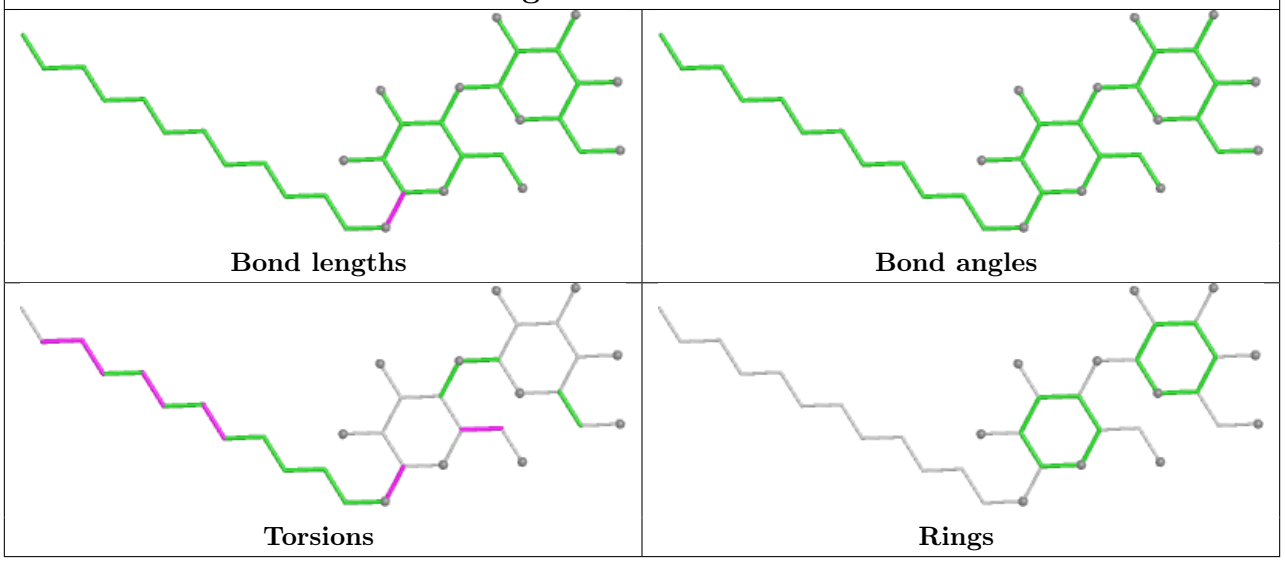
Ligand LHG l 103



Ligand LMT z 102



Ligand LMT B 634



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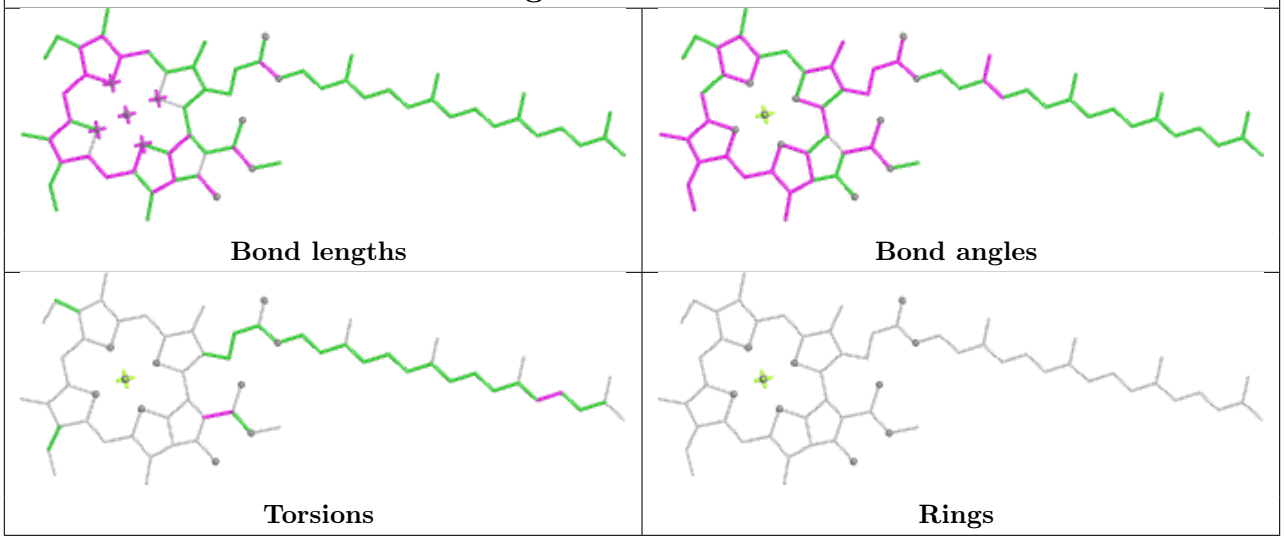

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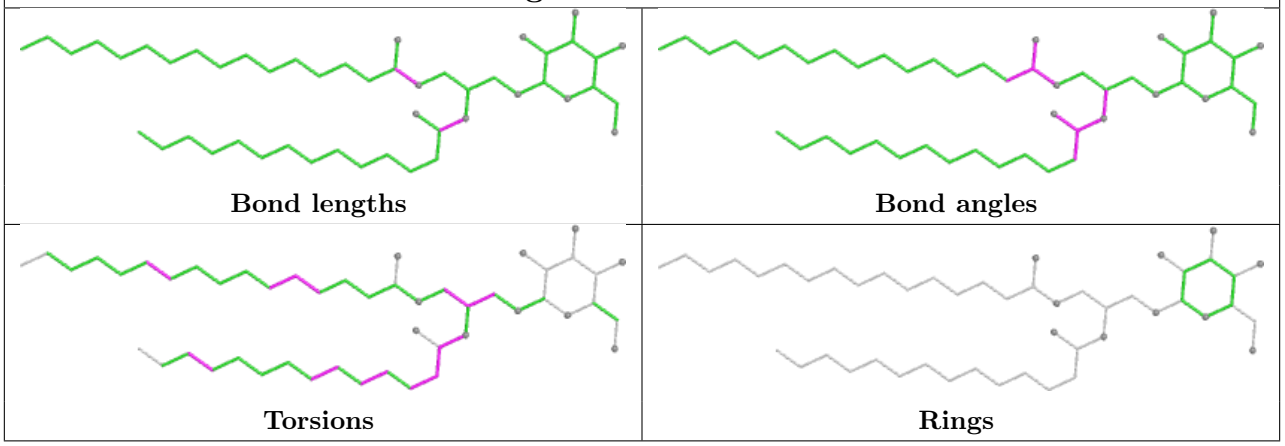

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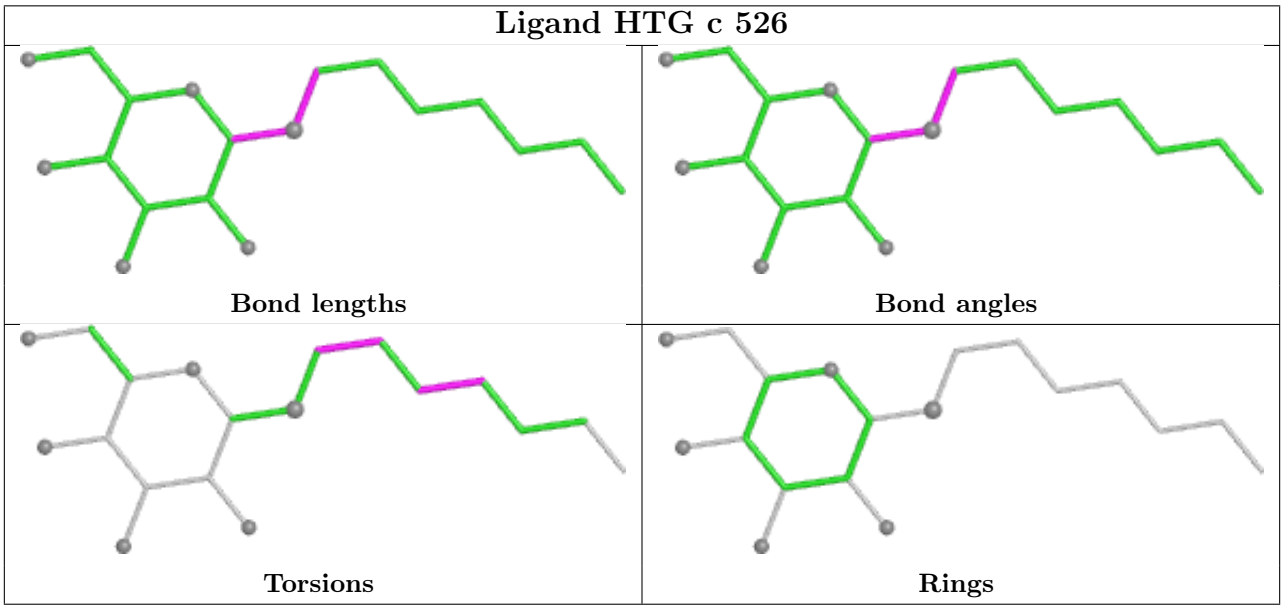
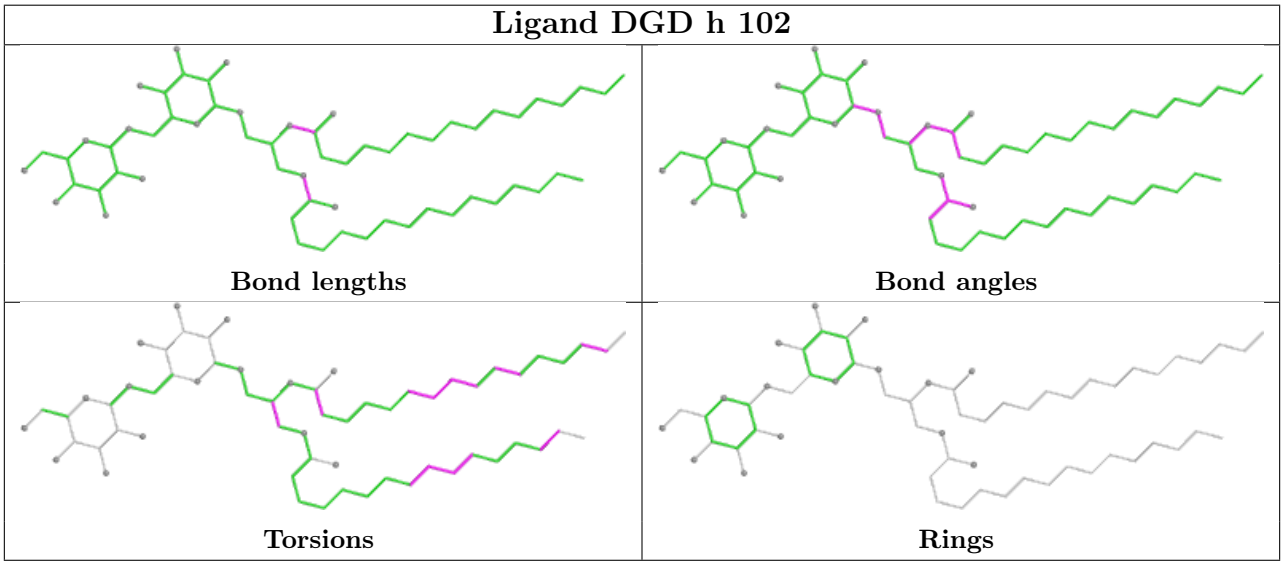


Ligand DGD h 102



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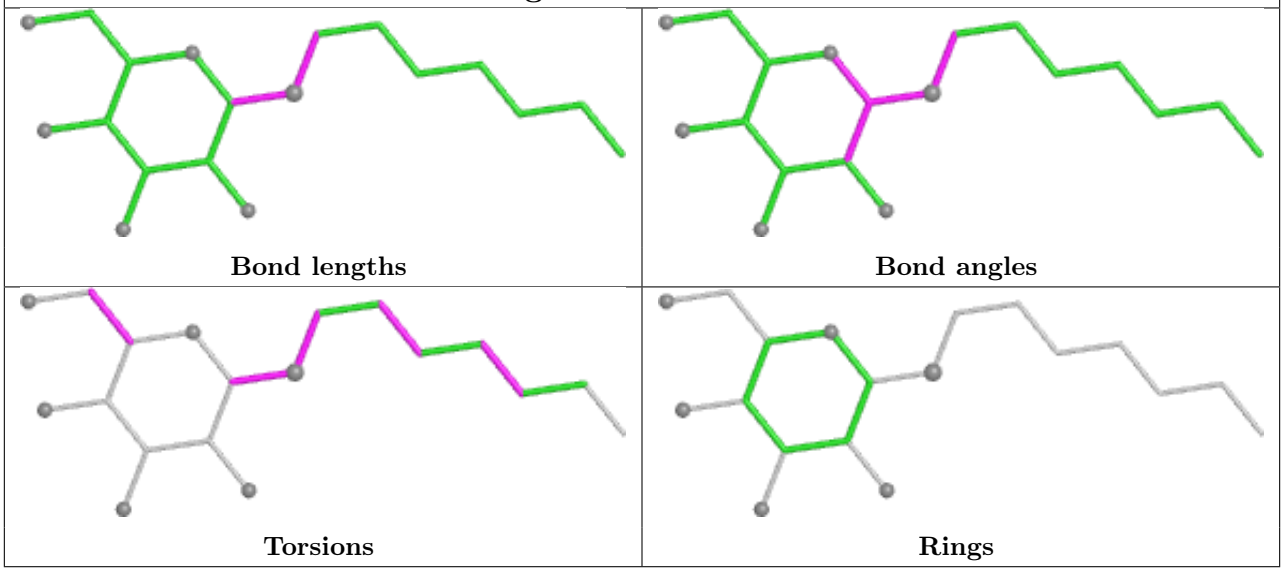
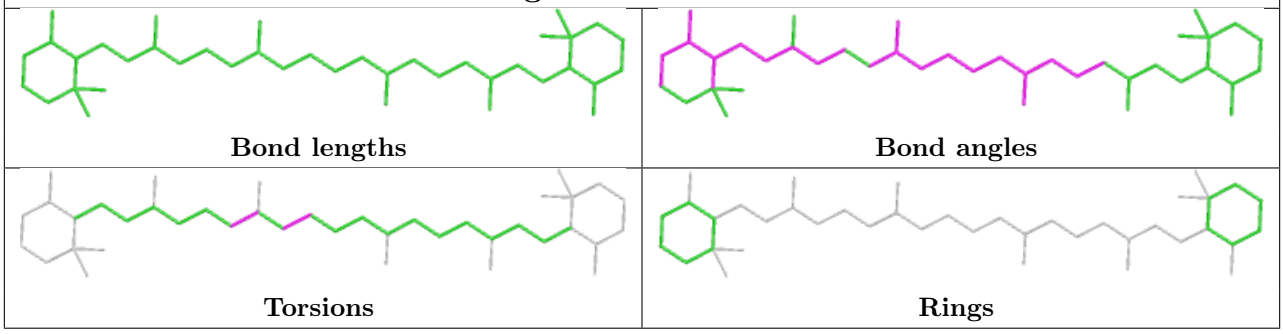
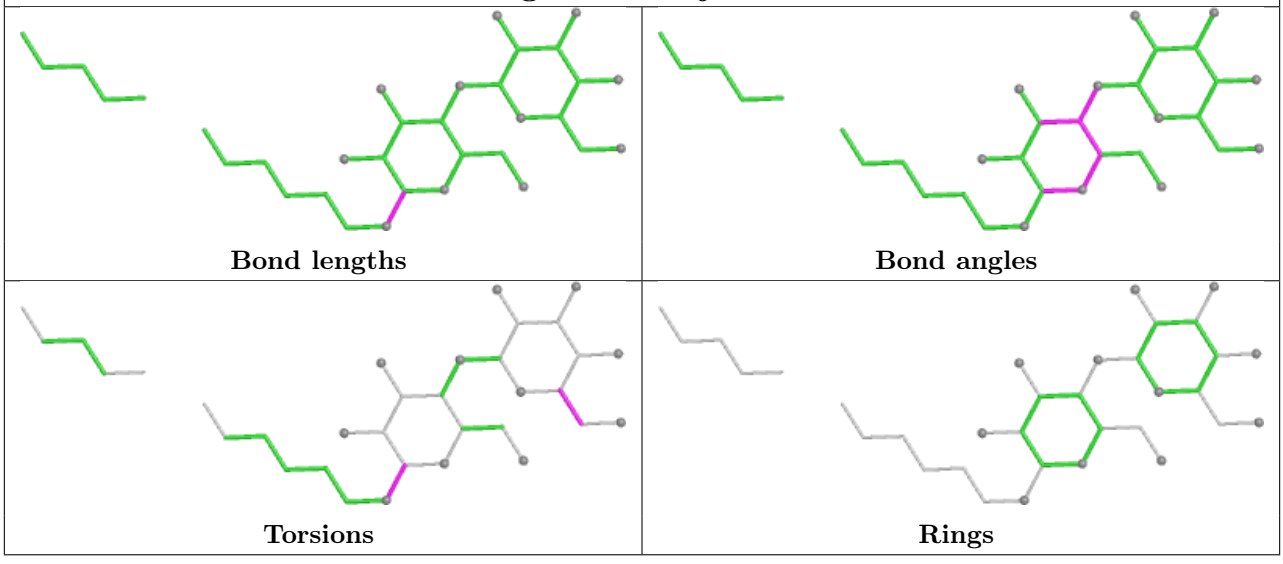


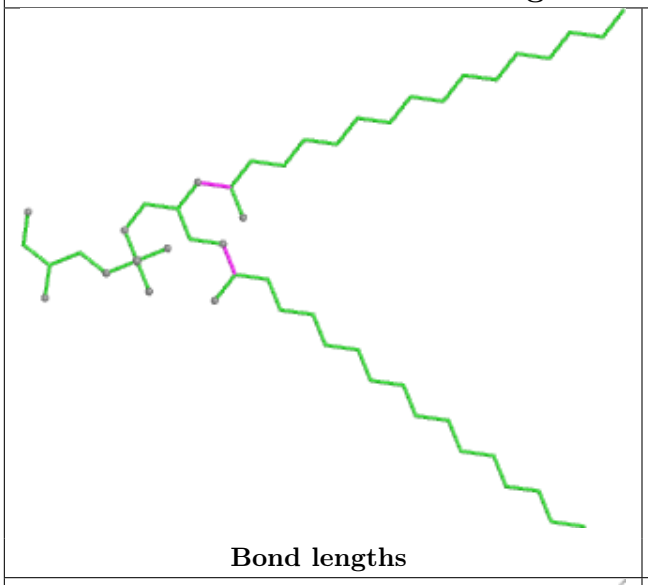
Ligand BCR T 102



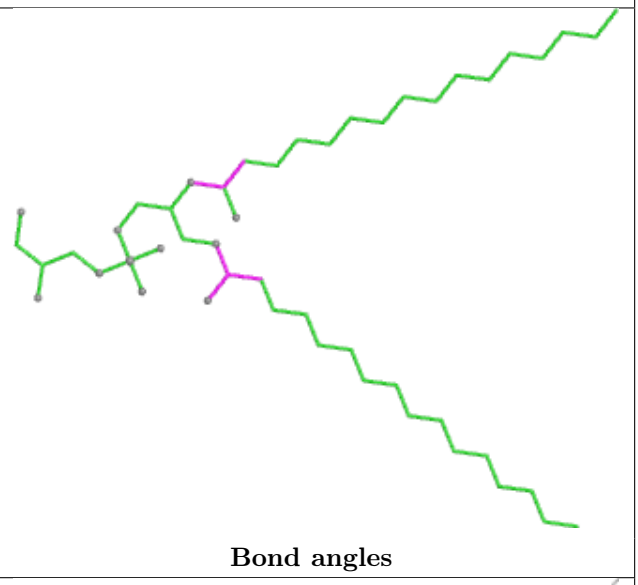
Ligand LMT j 2701



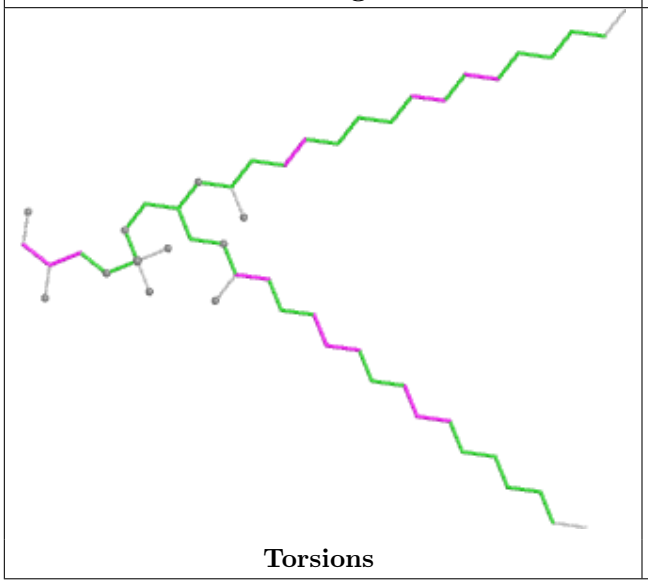
Ligand LHG d 412



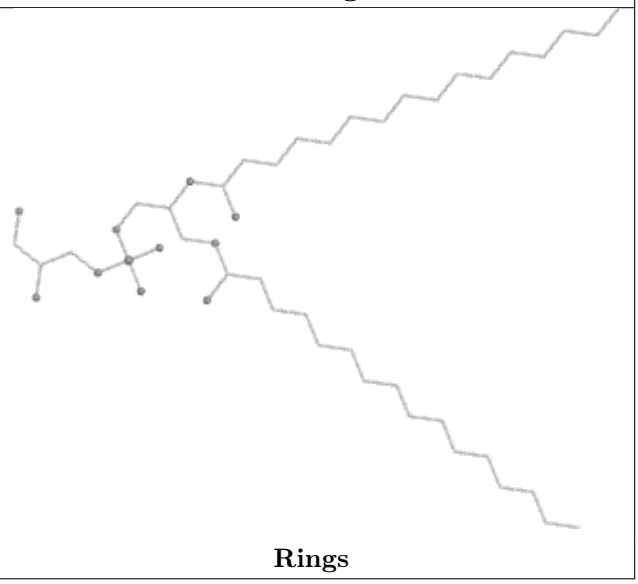
Bond lengths



Bond angles

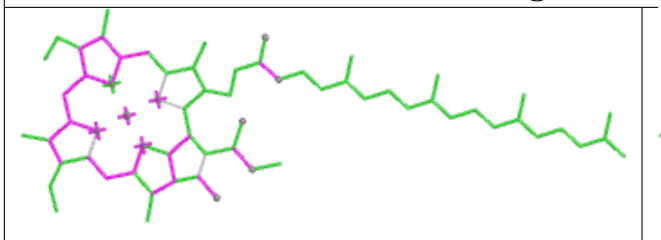


Torsions



Rings

Ligand CLA b 621



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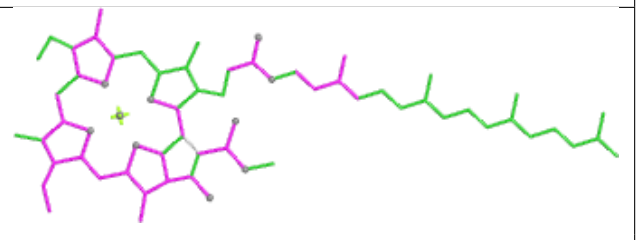
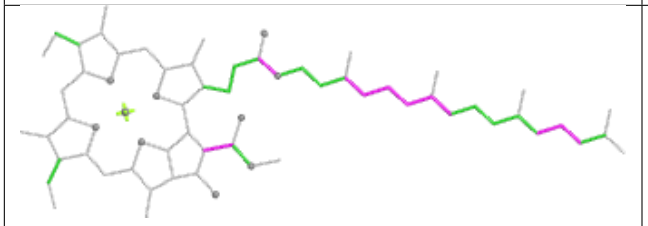


Bond angles



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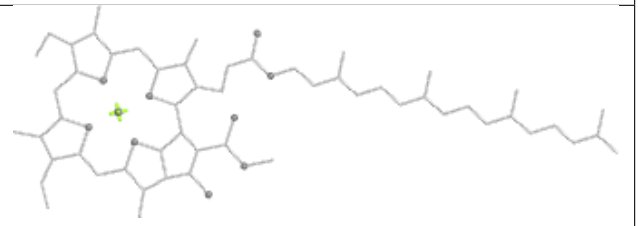
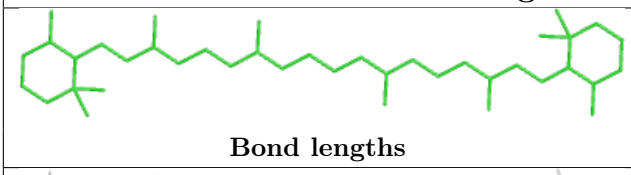


Rings

Ligand BCR a 2614



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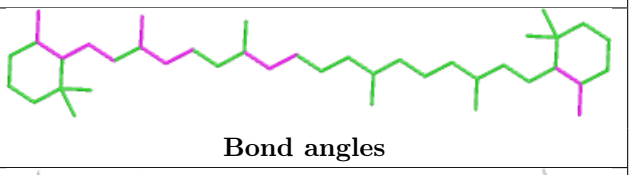
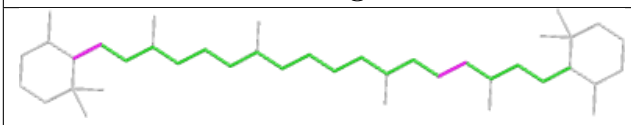


Bond angles



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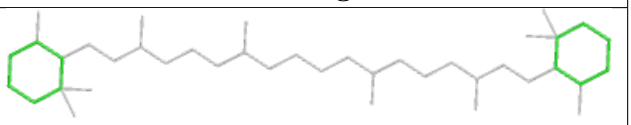
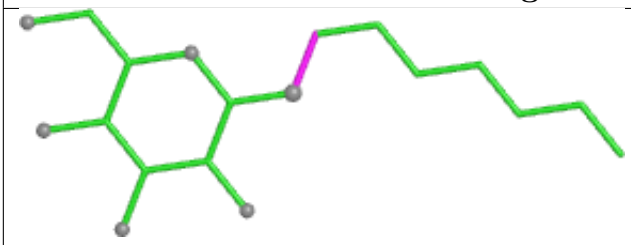
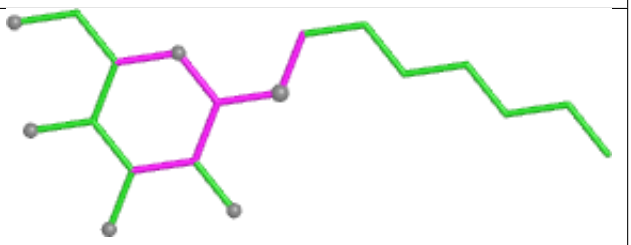


Rings

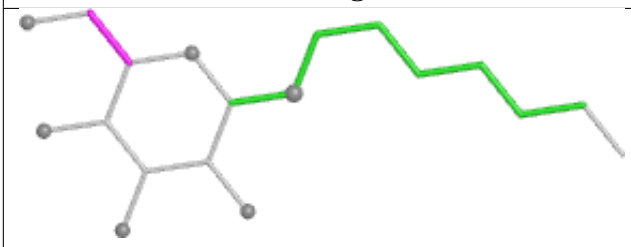
Ligand HTG B 625



Bond lengths



Bond angles



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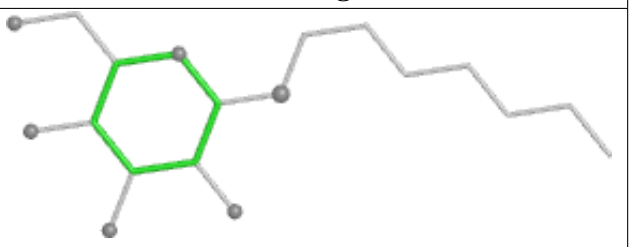
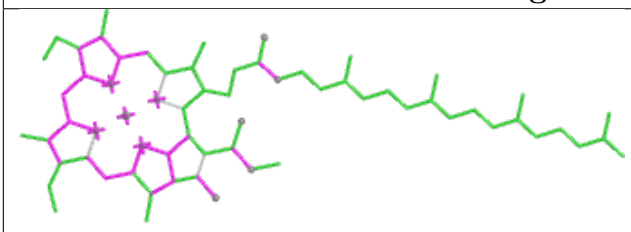
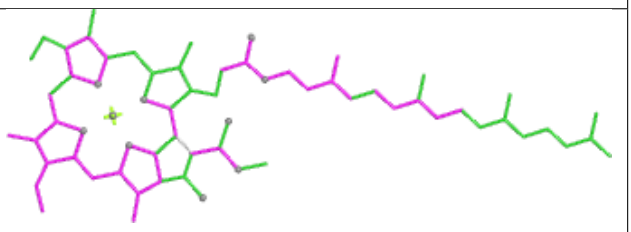


Rings

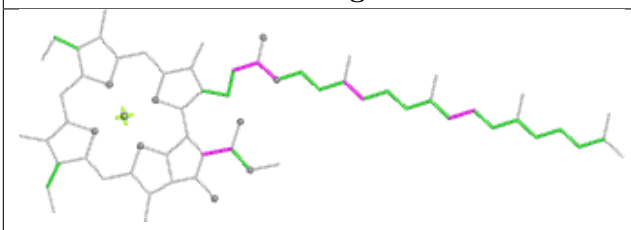
Ligand CLA c 513



Bond lengths



Bond angles



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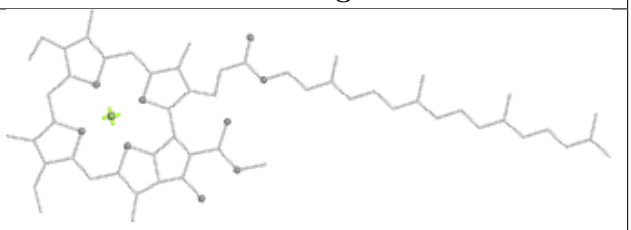
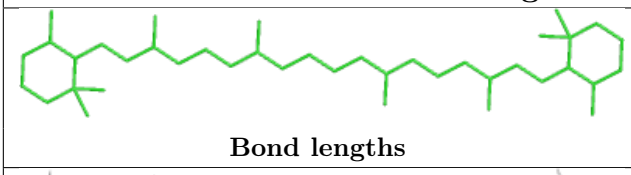
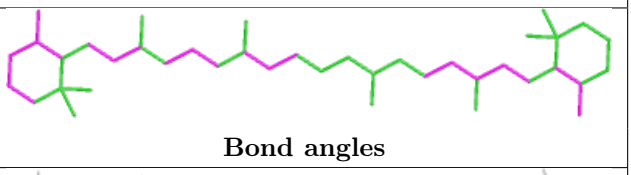
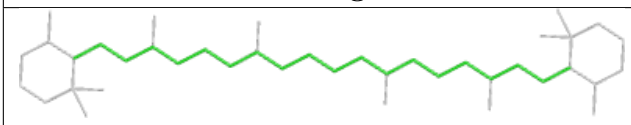


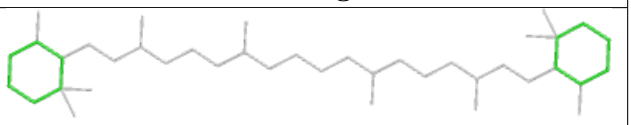
Rings

Ligand BCR K 101


Bond lengths


Bond angles


Torsions

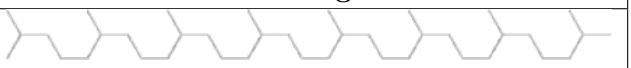

Rings

Ligand PL9 A 422

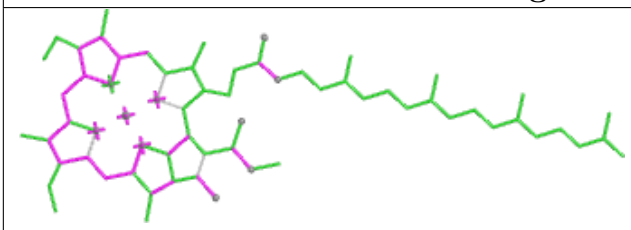

Bond lengths

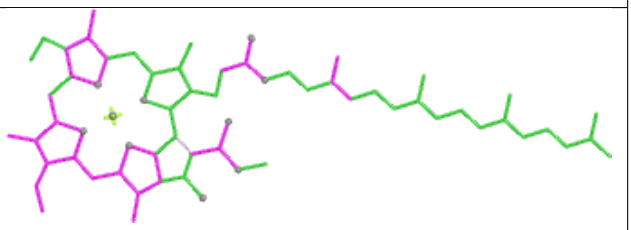

Bond angles

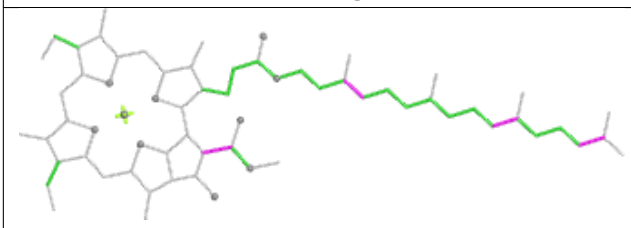

Torsions

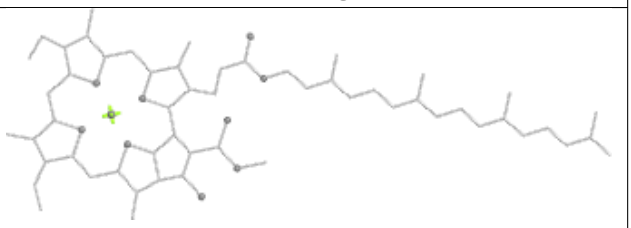

Rings

Ligand CLA c 507

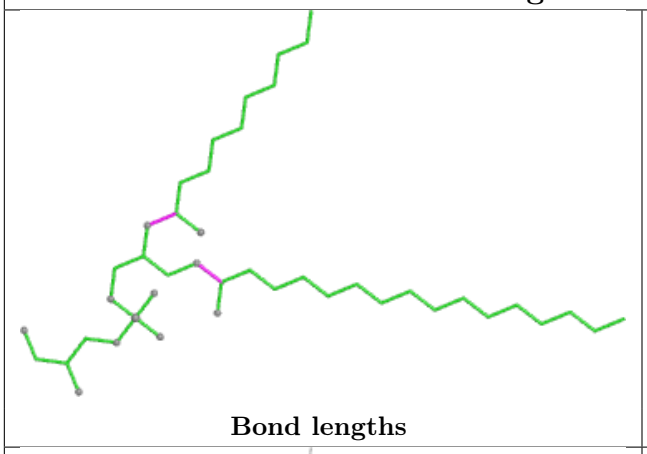

Bond lengths


Bond angles


Torsions


Rings

Ligand LHG d 403



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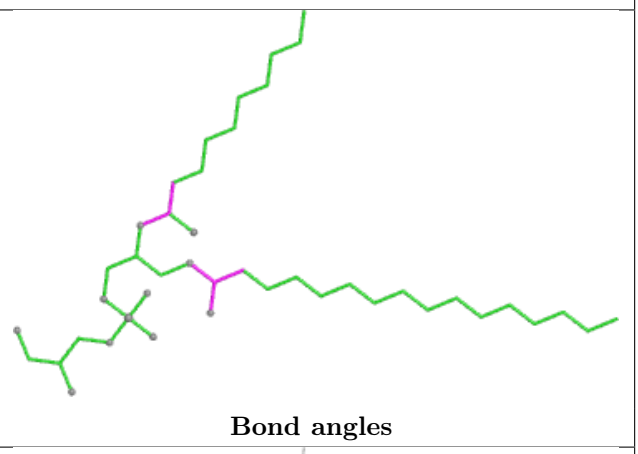
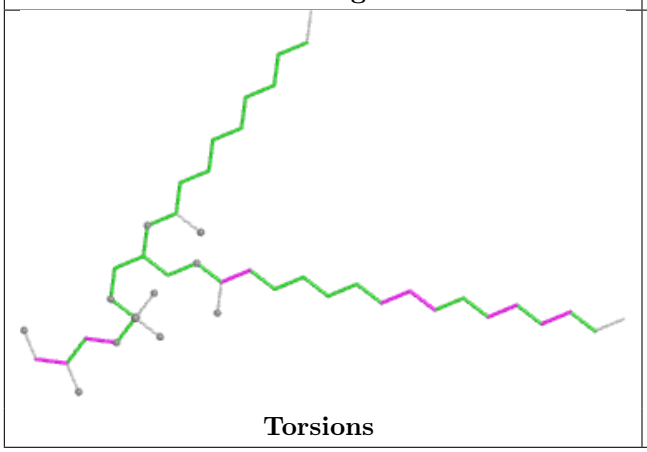


Bond angles



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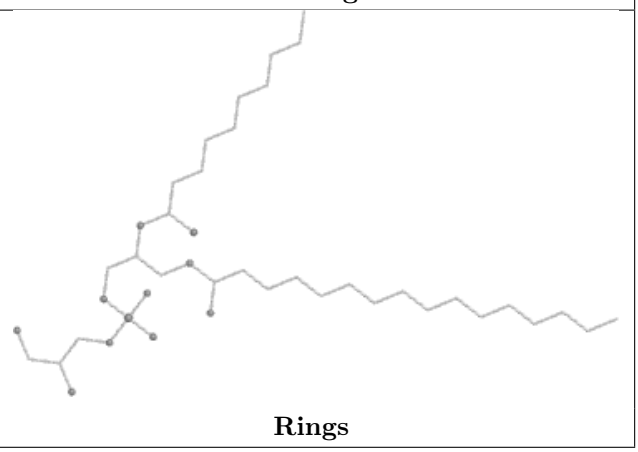
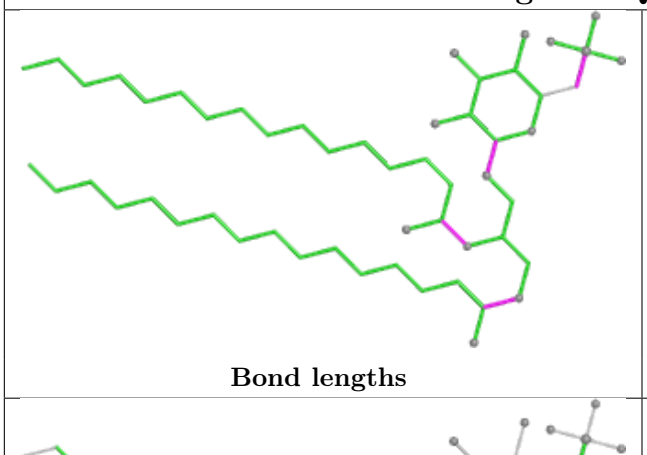


Rings

Ligand SQD D 2302



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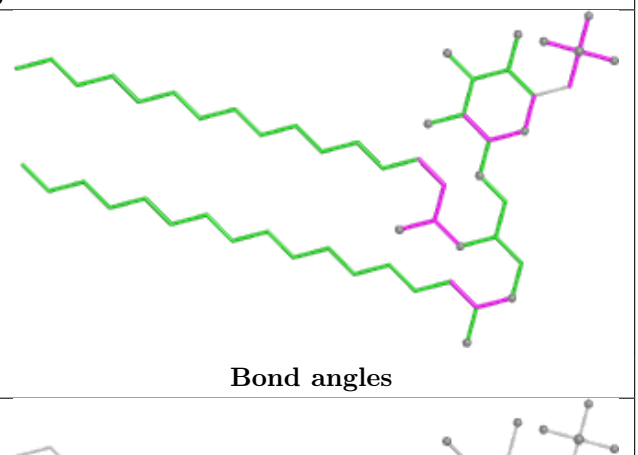
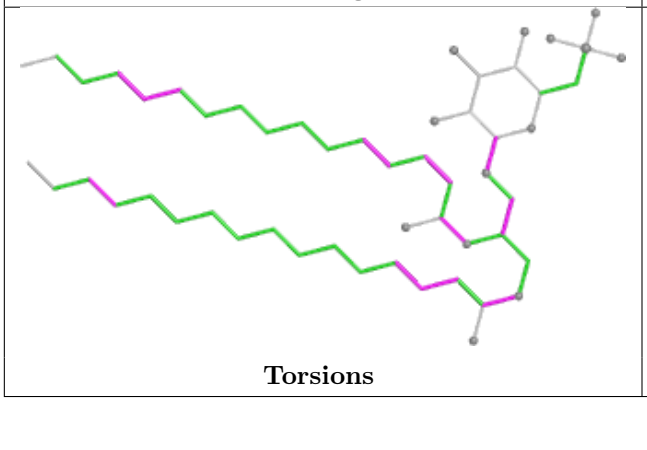


Bond angles



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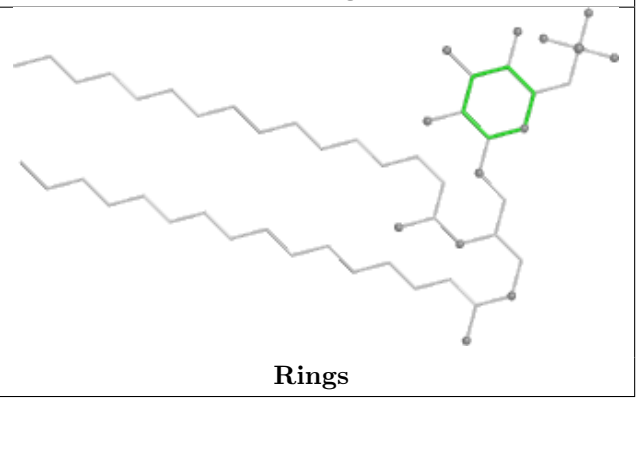
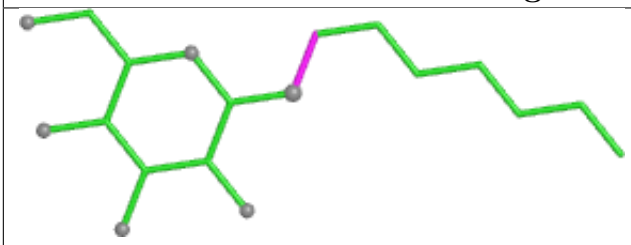


Rings

Ligand HTG b 602



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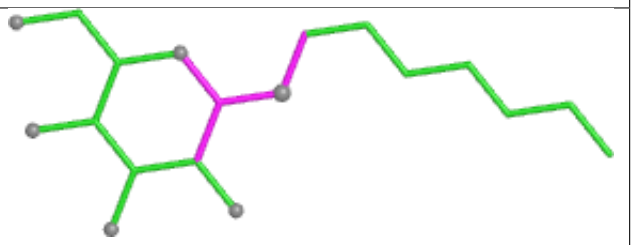
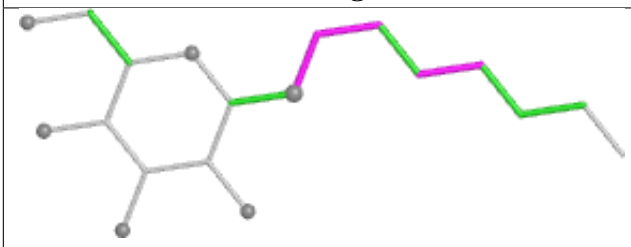


Bond angles



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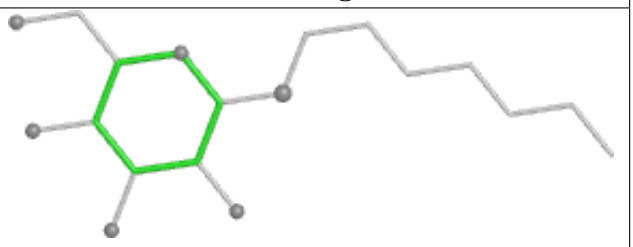
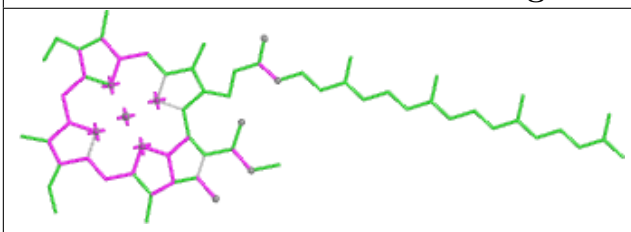


Rings

Ligand CLA b 608



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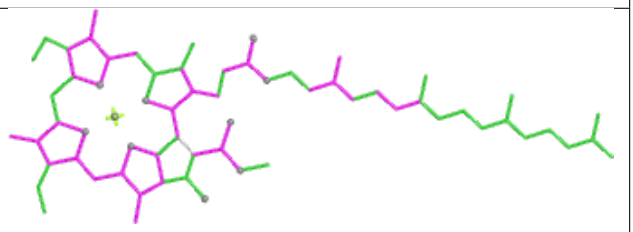
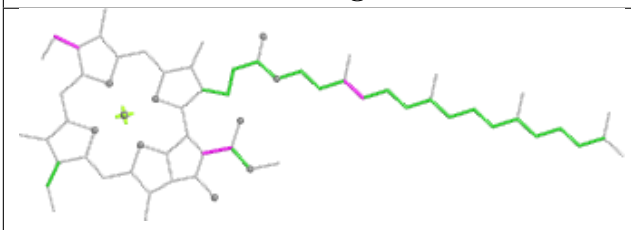


Bond angles



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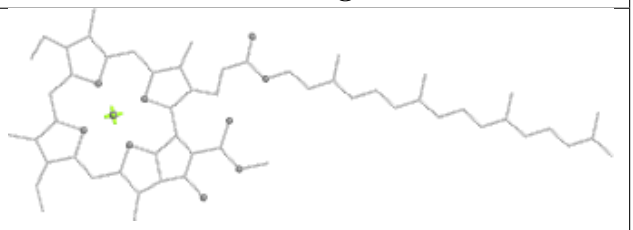
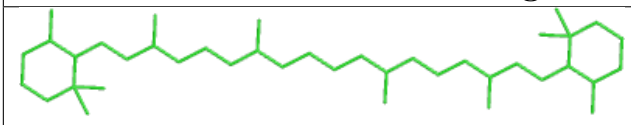


Rings

Ligand BCR Y 302



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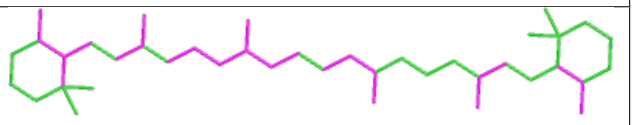
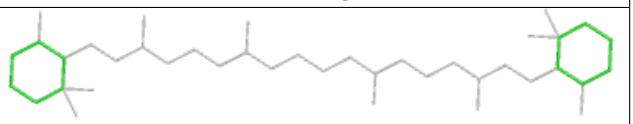


Bond angles

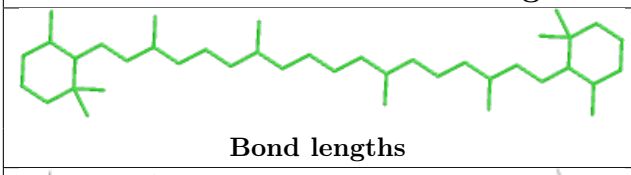


Torsions



Rings

Ligand BCR C 516



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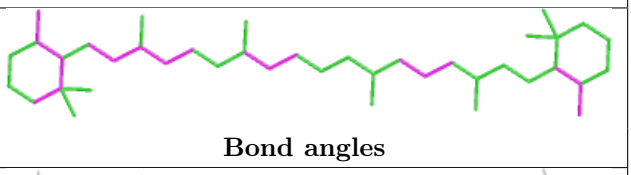
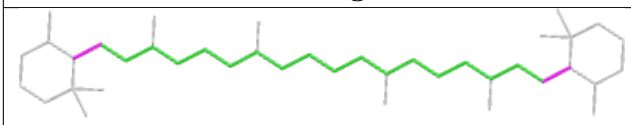


Bond angles



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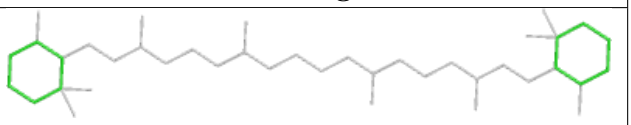
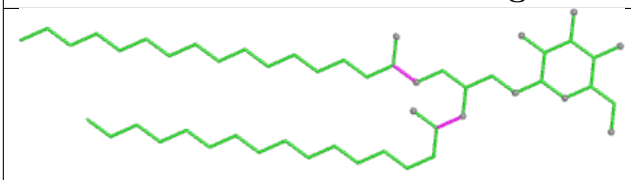


Rings

Ligand LMG m 2802



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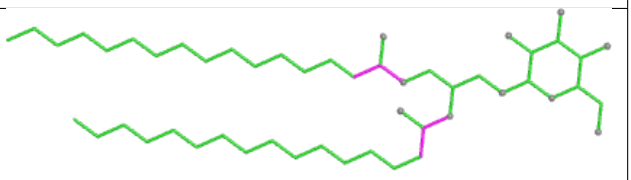
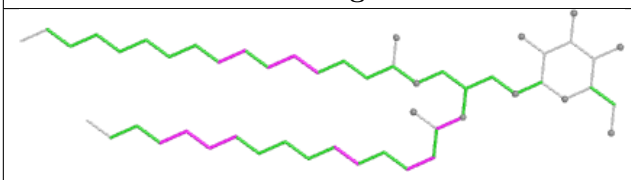


Bond angles



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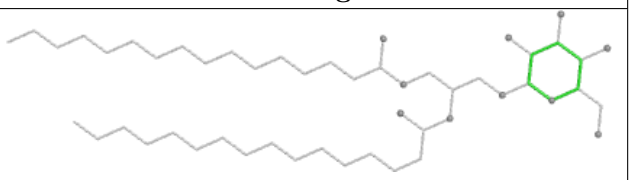
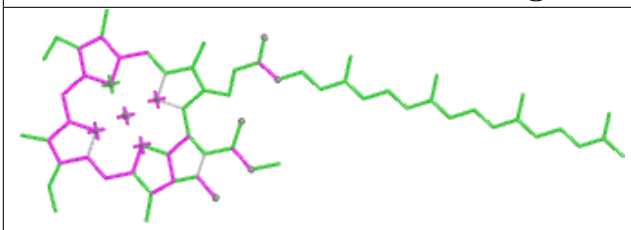


Rings

Ligand CLA b 618



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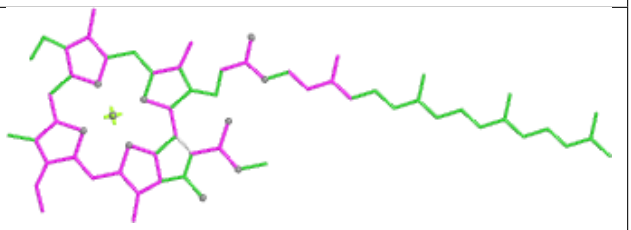
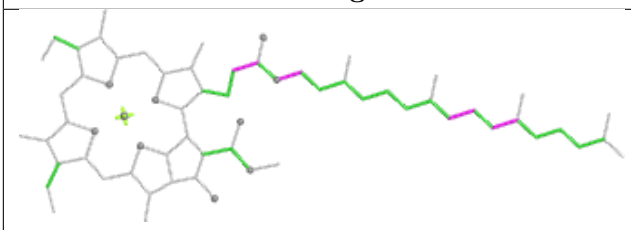


Bond angles



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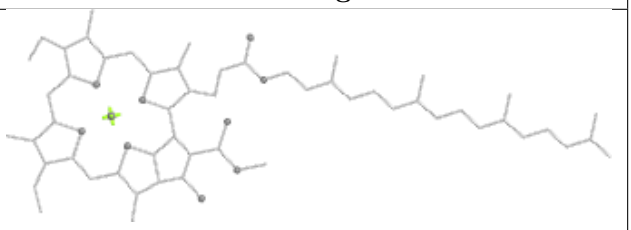
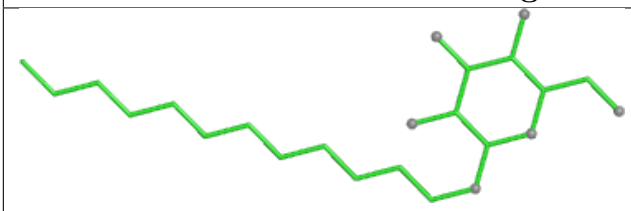
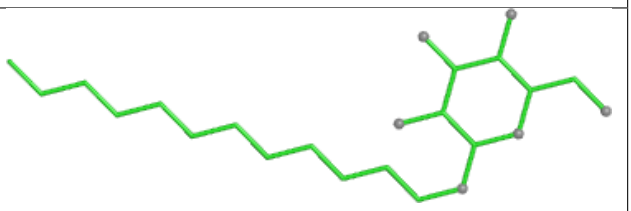
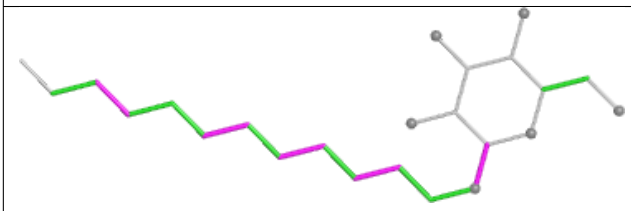


Rings

Ligand LMT A 420


Bond lengths


Bond angles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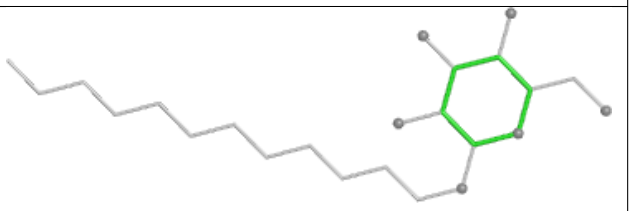
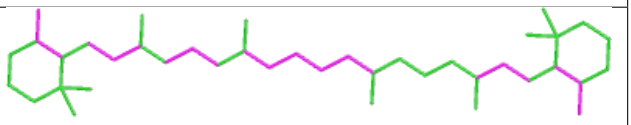
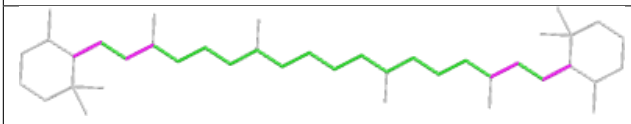

Rings

Ligand BCR D 2305


Bond lengths


Bond angles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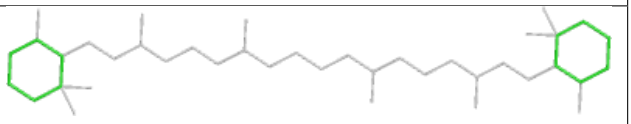
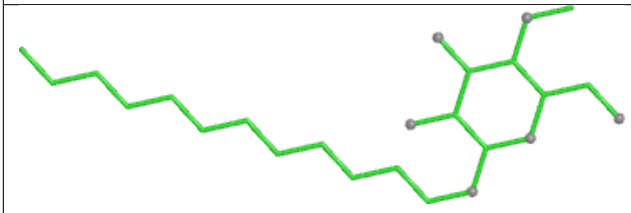

Rings

Ligand LMT d 404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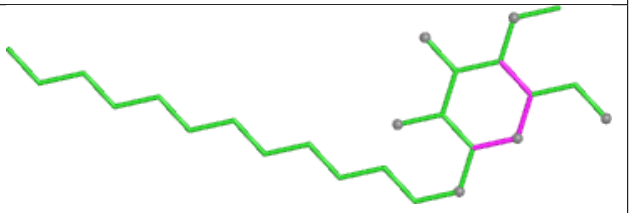
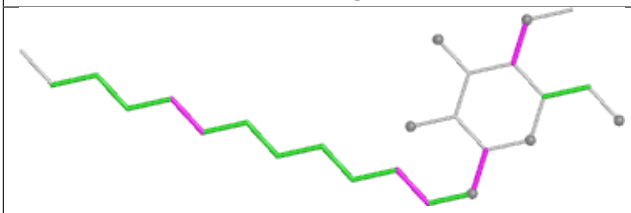

Bond angles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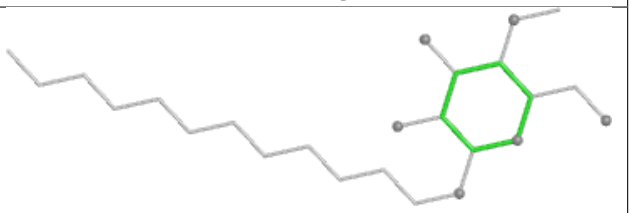
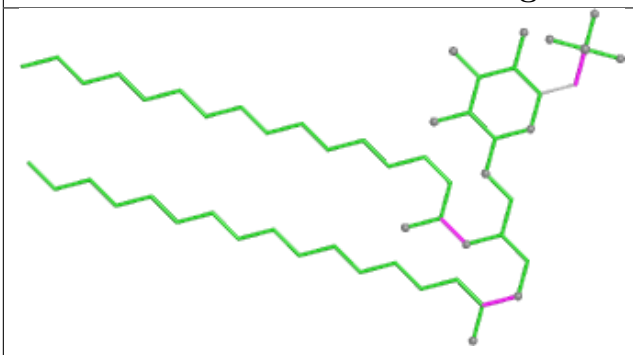

Rings

Ligand SQD a 2603



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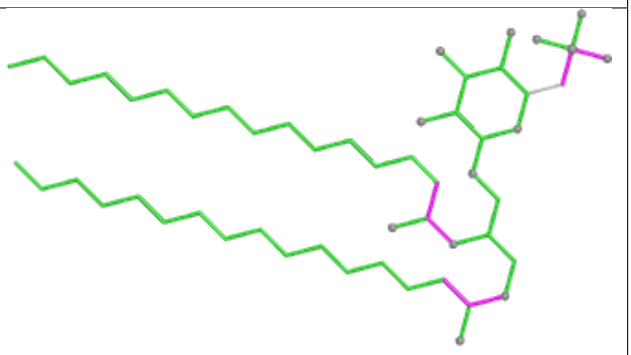
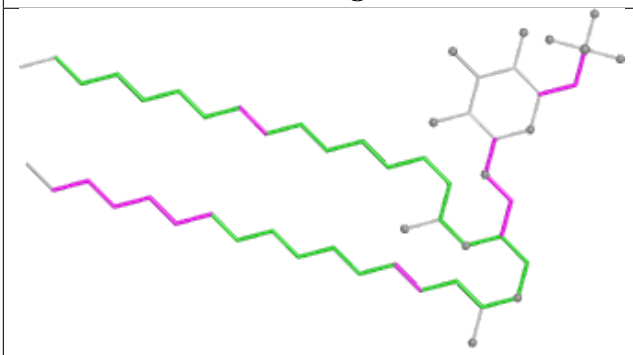


Bond angles



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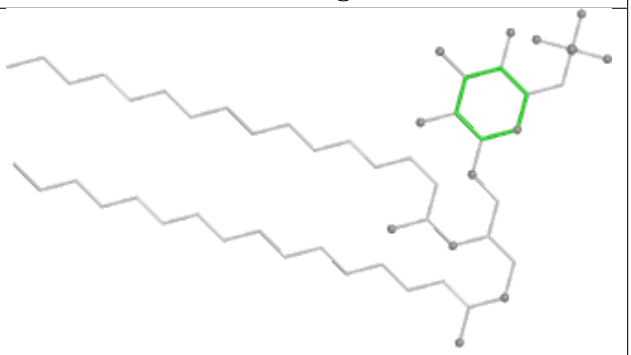
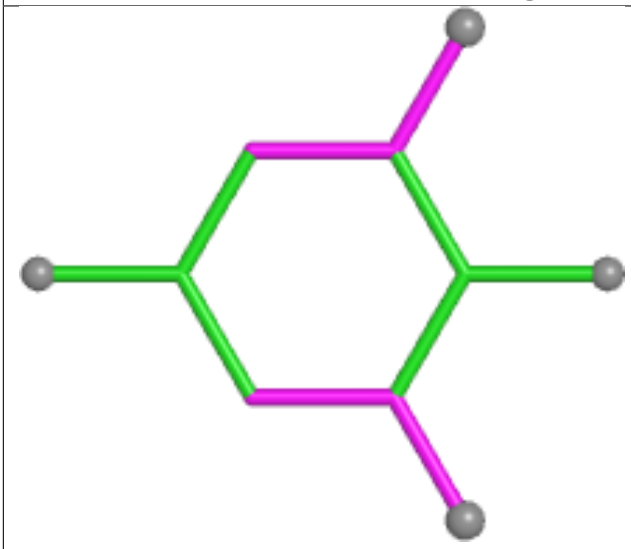


Rings

Ligand JOX a 2617



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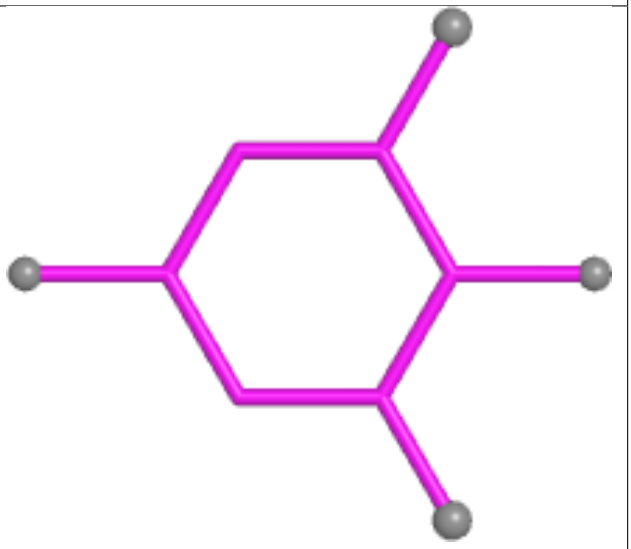
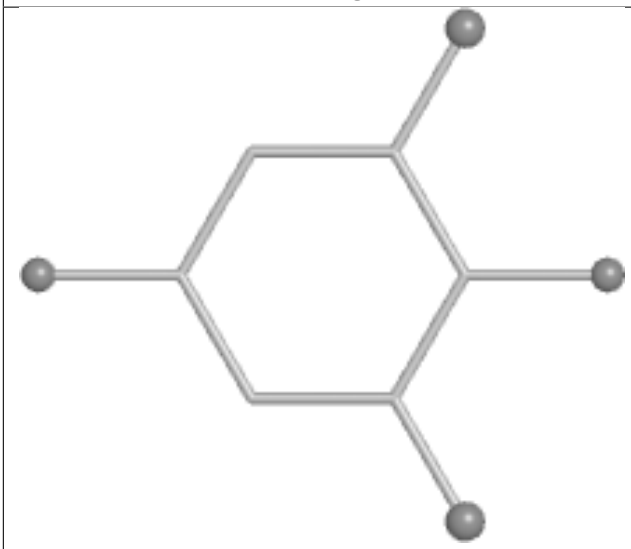


Bond angles



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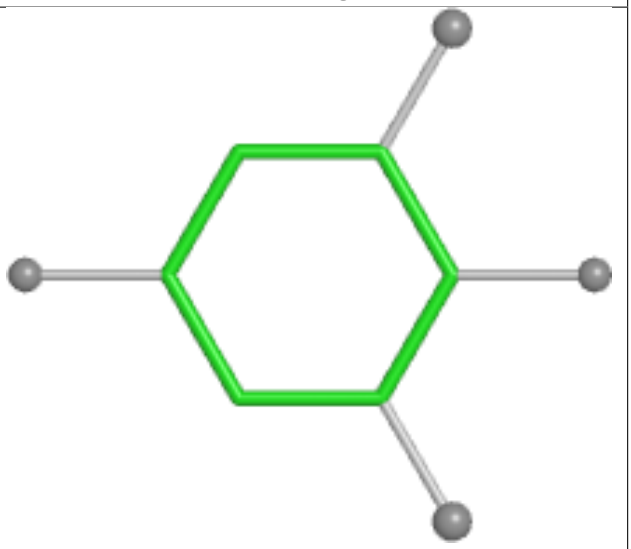
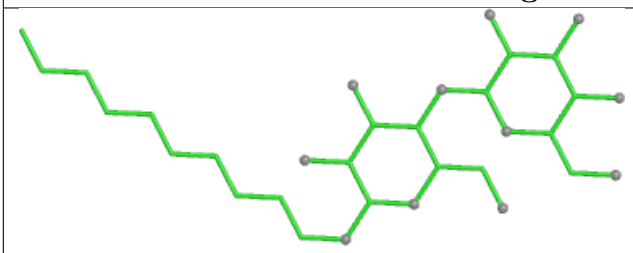


Rings

Ligand LMT A 414



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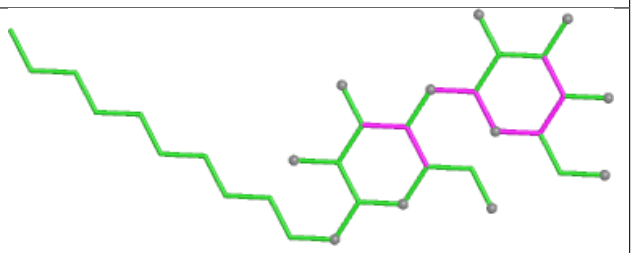
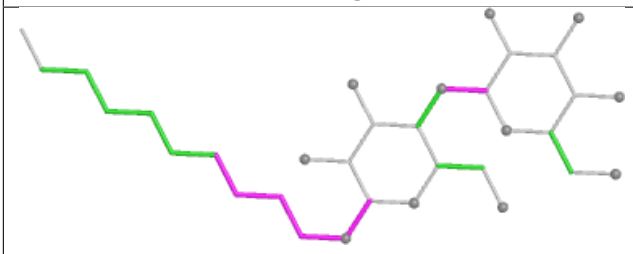


Bond angles



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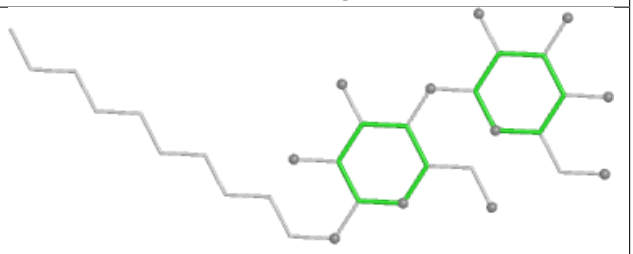
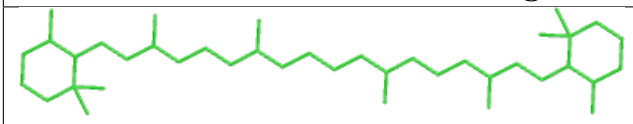
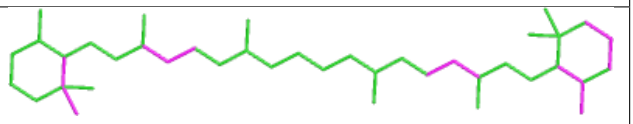


Rings

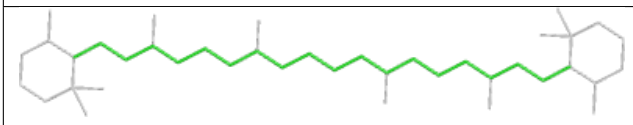
Ligand BCR B 619



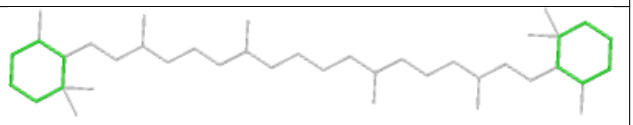
Bond lengths



Bond angles



Torsions

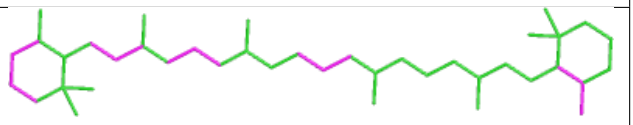


Rings

Ligand BCR B 620



Bond lengths



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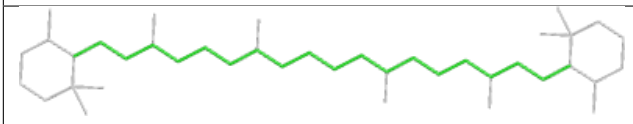

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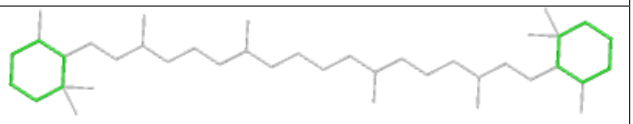
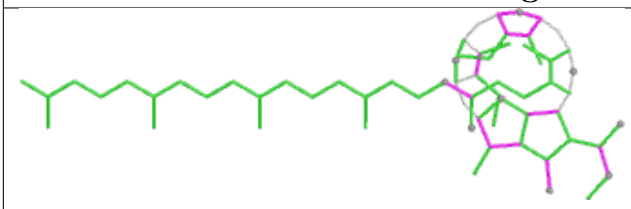


Rings

Ligand PHO A 408



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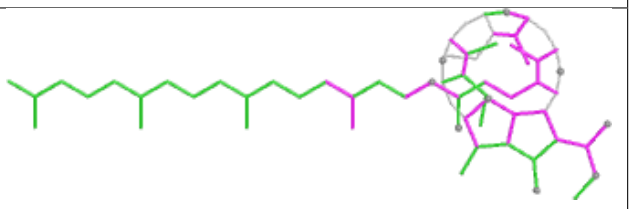
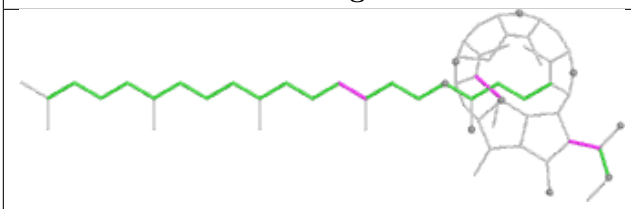


Bond angles



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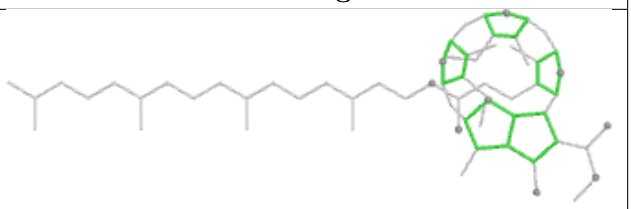
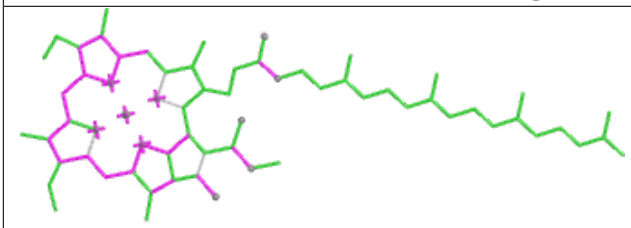


Rings

Ligand CLA b 620



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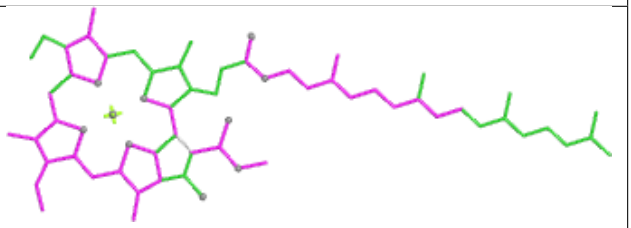
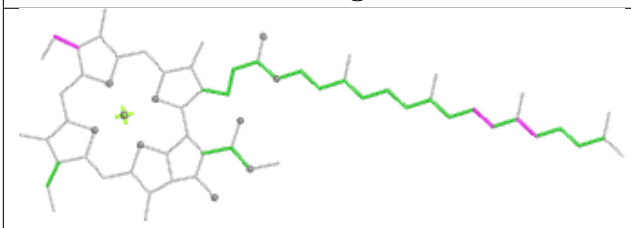


Bond angles



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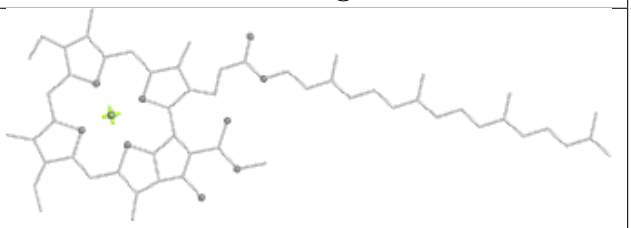
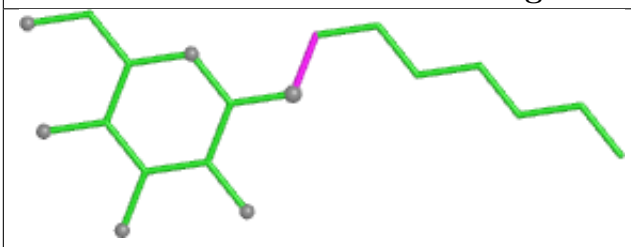


Rings

Ligand HTG o 301



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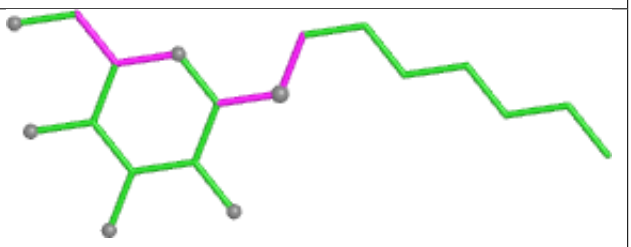
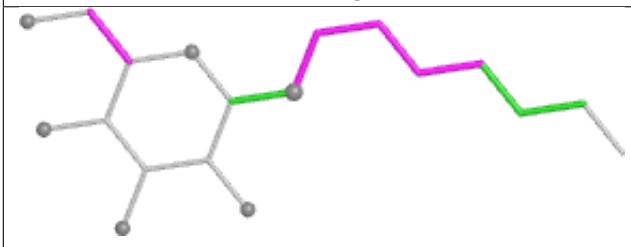


Bond angles



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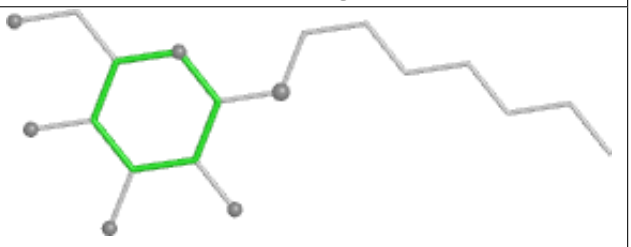
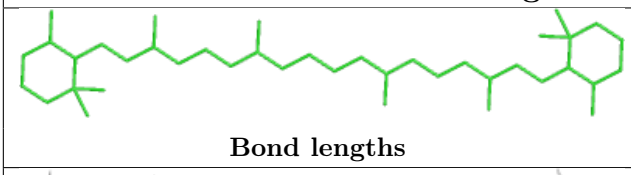


Rings

Ligand BCR B 618



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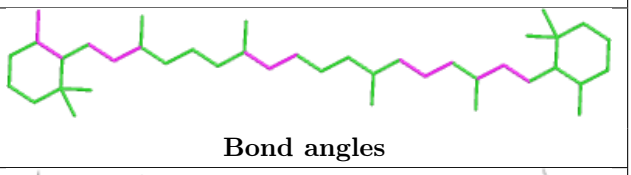
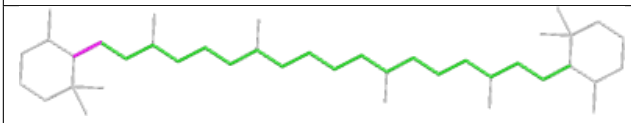


Bond angles



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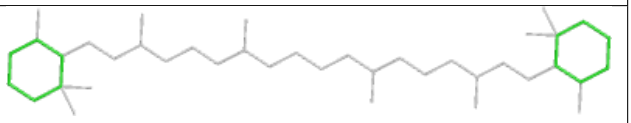
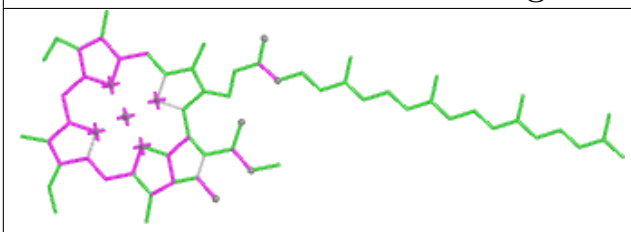


Rings

Ligand CLA b 613



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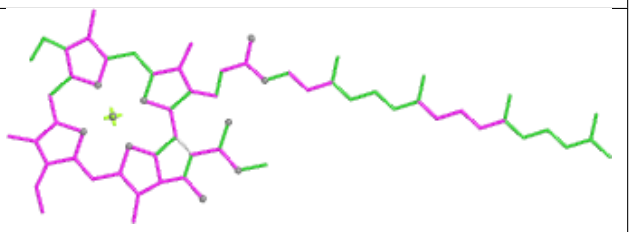
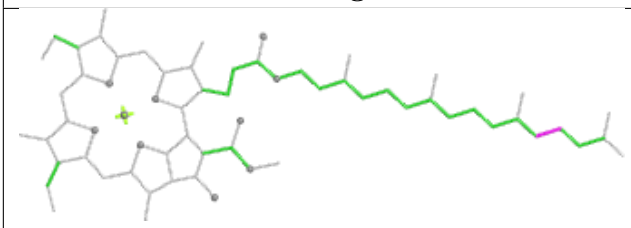


Bond angles



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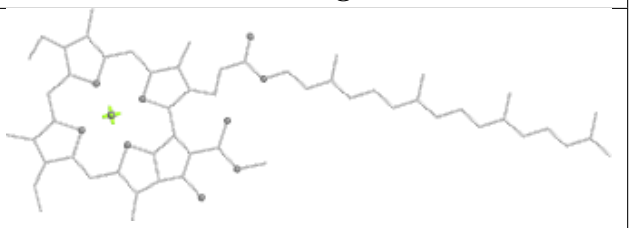
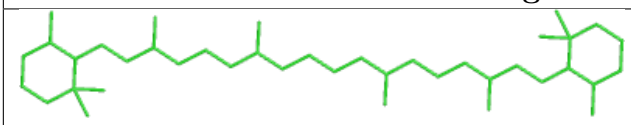


Rings

Ligand BCR B 633



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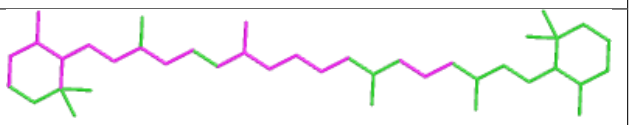
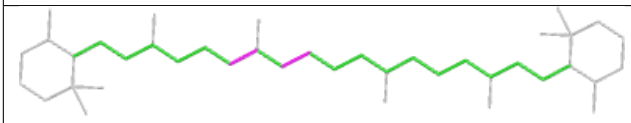


Bond angles



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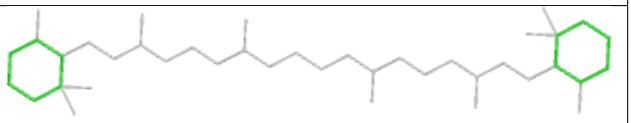
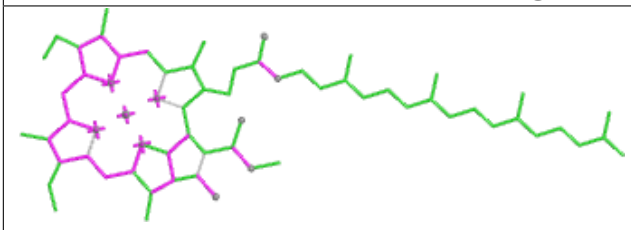


Rings

Ligand CLA c 515



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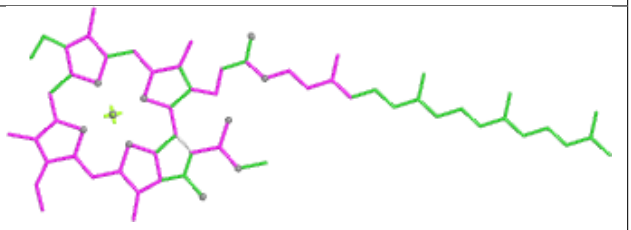
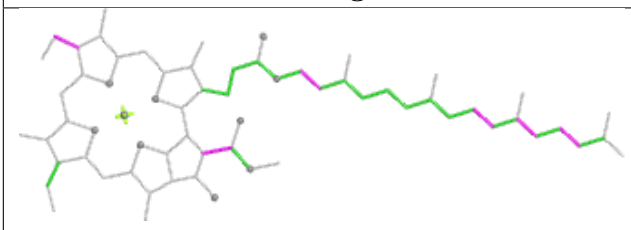


Bond angles



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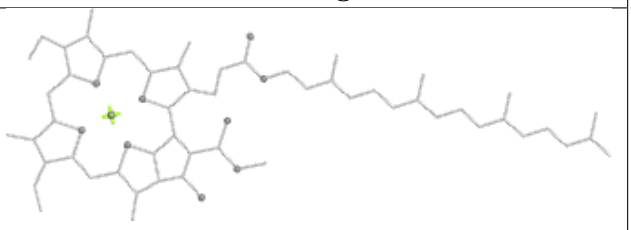
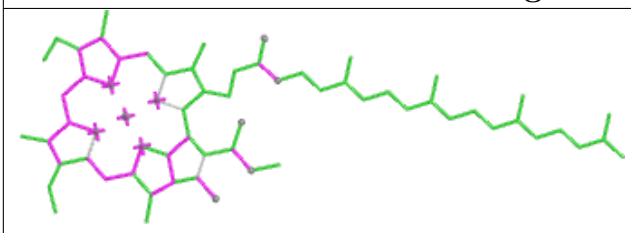


Rings

Ligand CLA B 609



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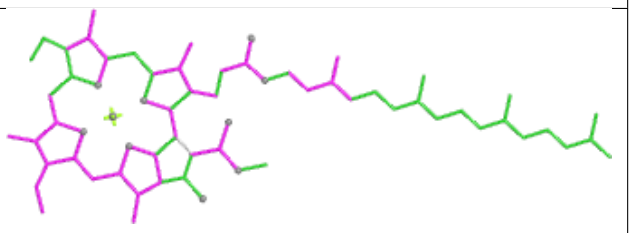
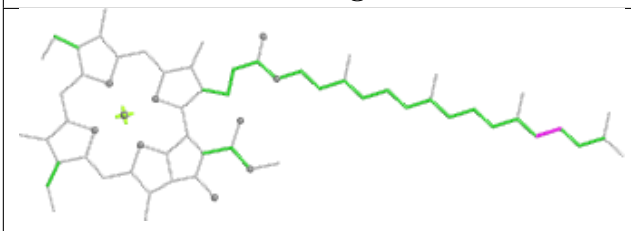


Bond angles



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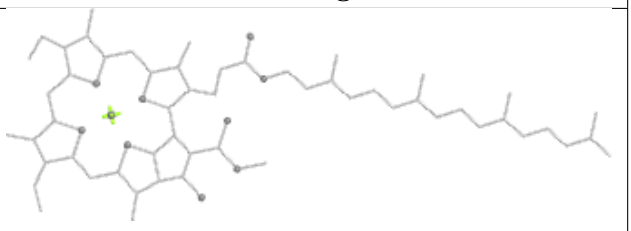
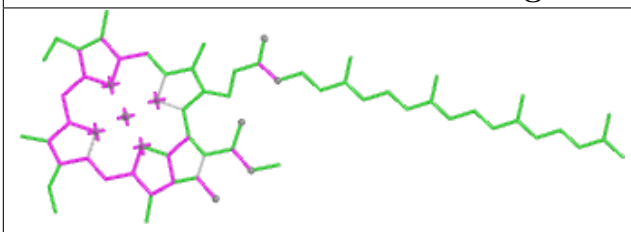


Rings

Ligand CLA B 611



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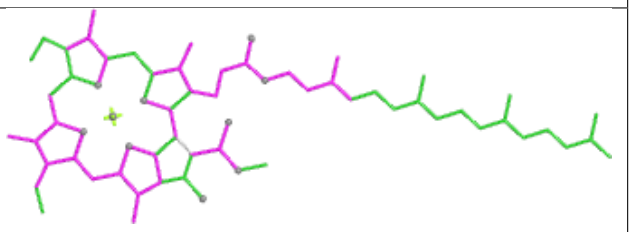
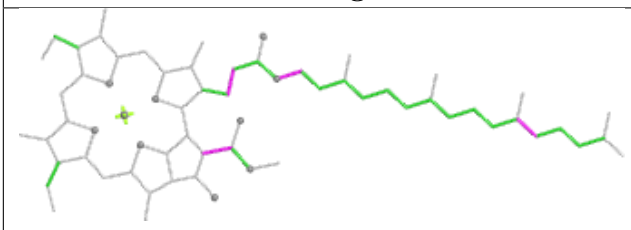


Bond angles



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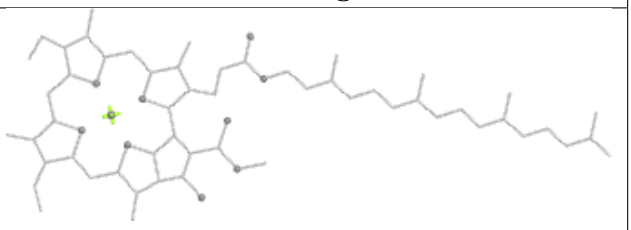
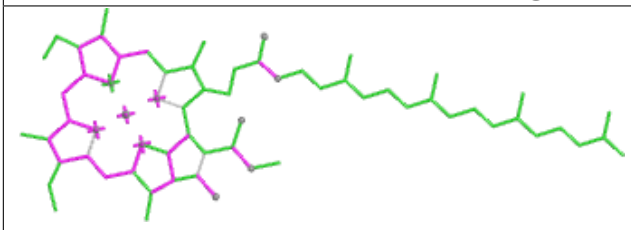


Rings

Ligand CLA d 408



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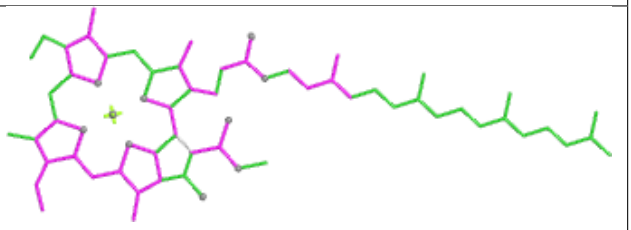
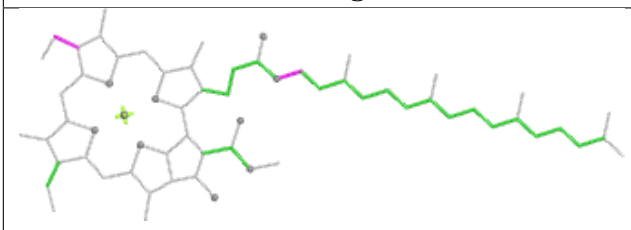


Bond angles



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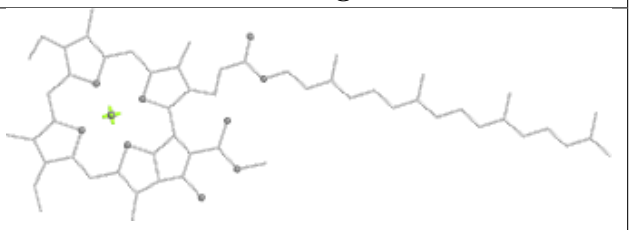
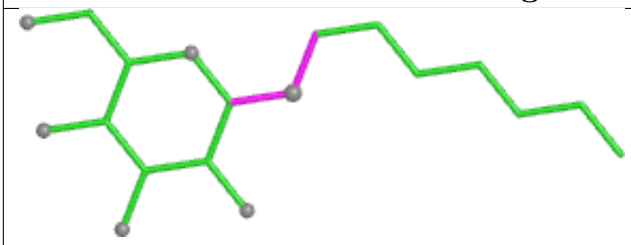


Rings

Ligand HTG C 521



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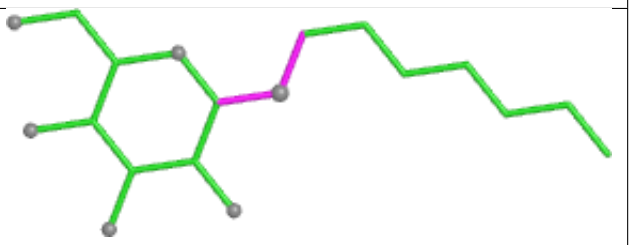
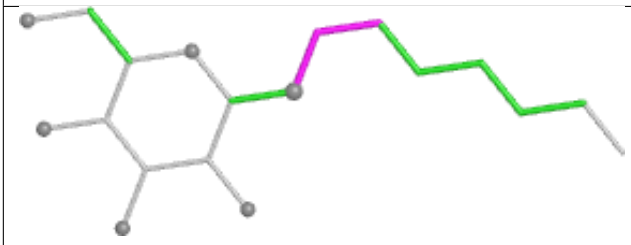


Bond angles



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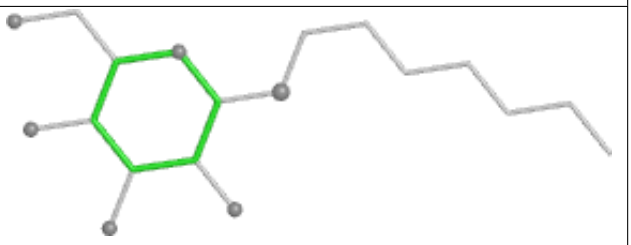
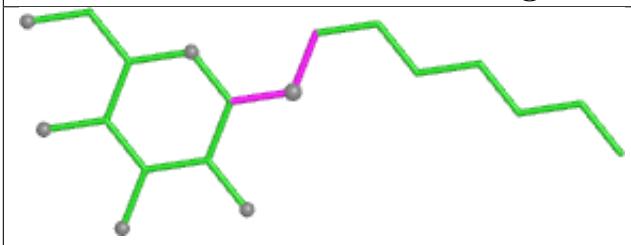
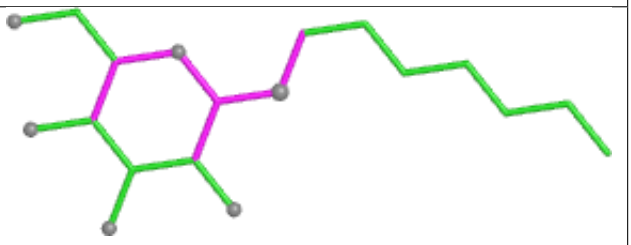


Rings

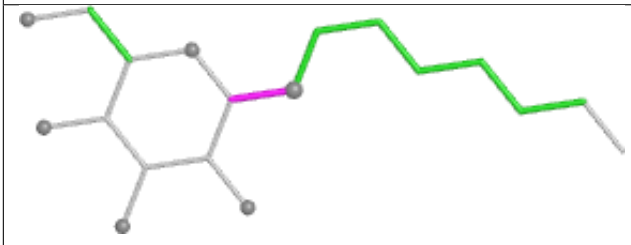
Ligand HTG C 522



Bond lengths



Bond angles



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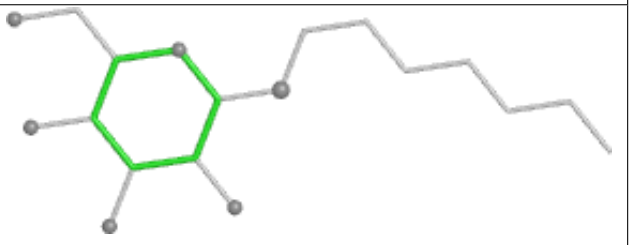
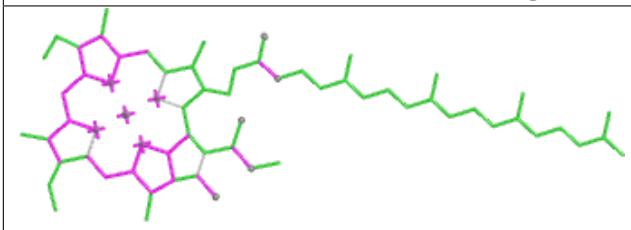
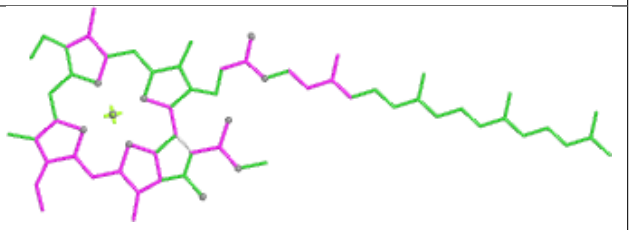


Rings

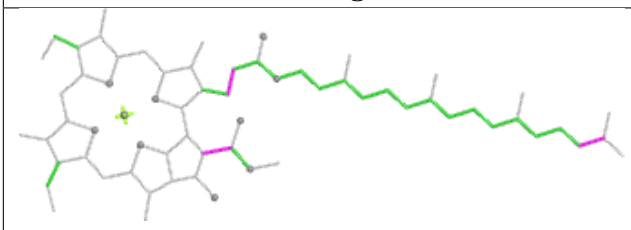
Ligand CLA C 502



Bond lengths



Bond angles



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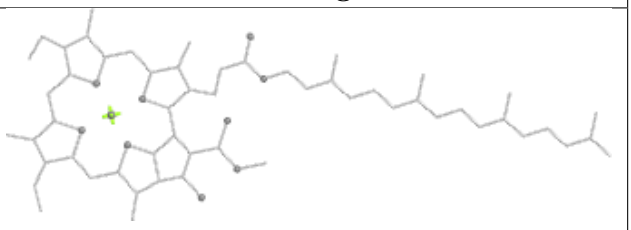
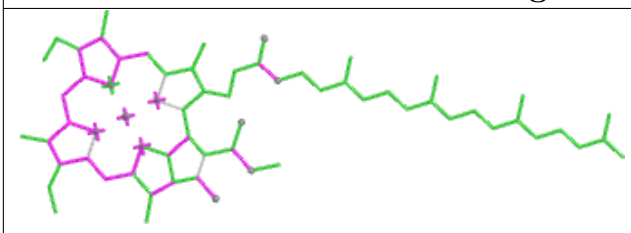


Rings

Ligand CLA c 504



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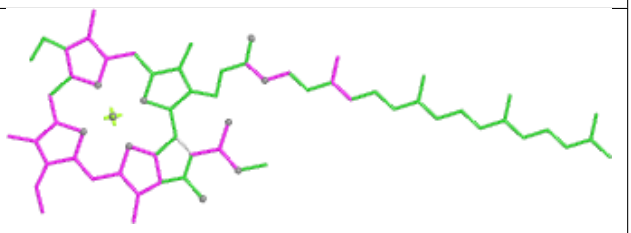

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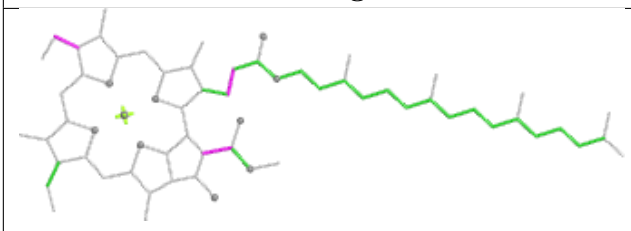
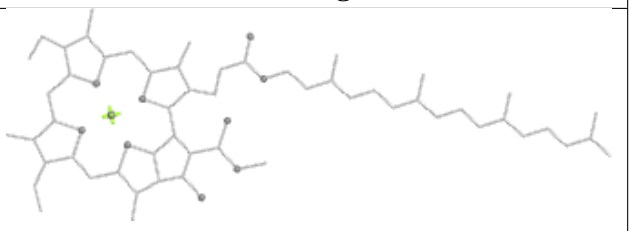
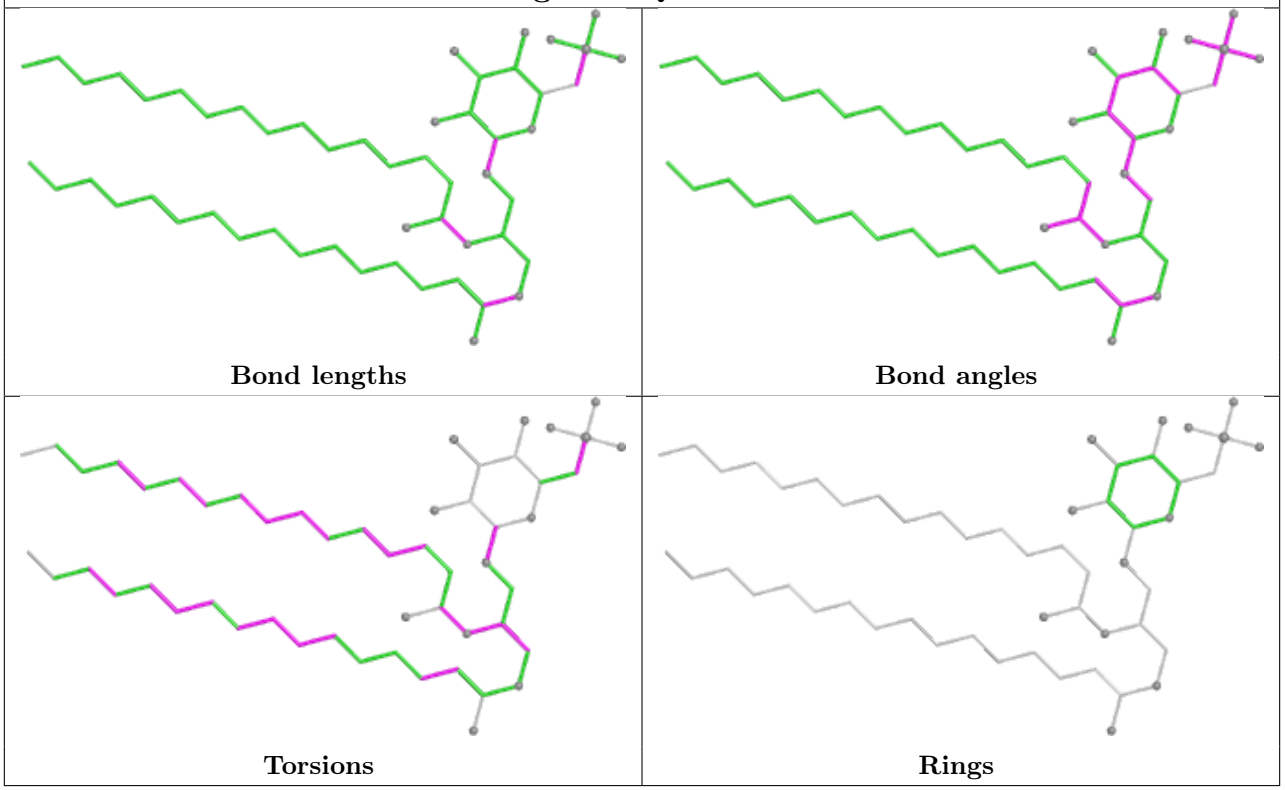


Torsions

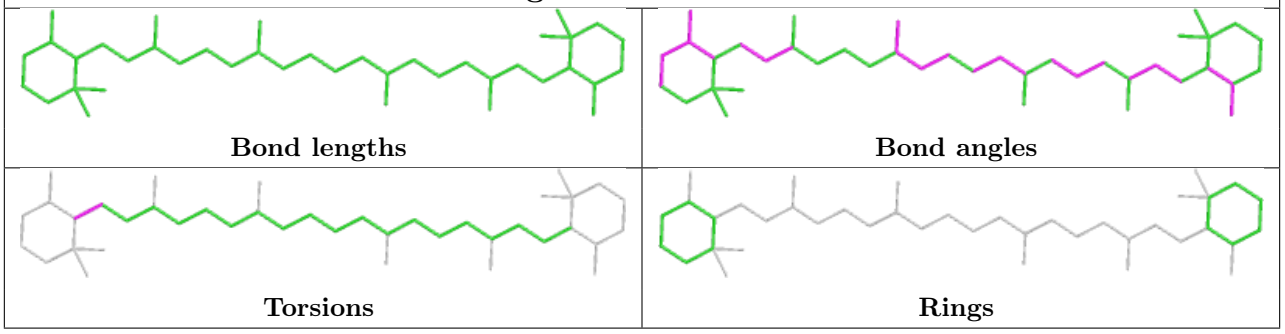


Rings

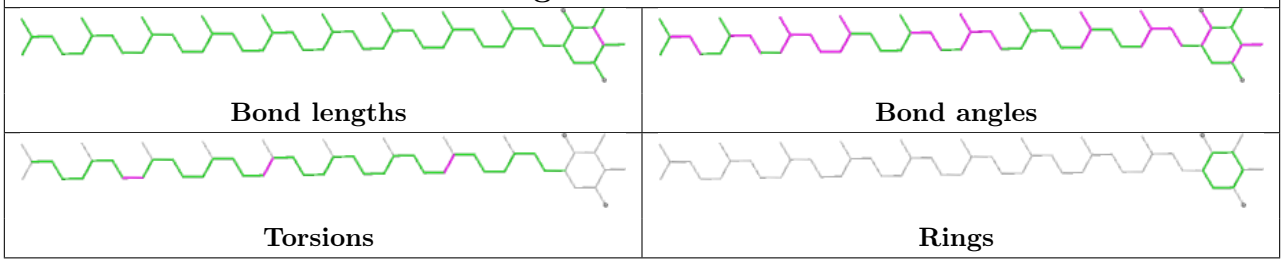
Ligand SQD l 101



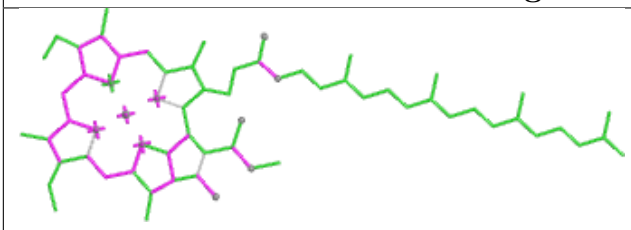
Ligand BCR b 622



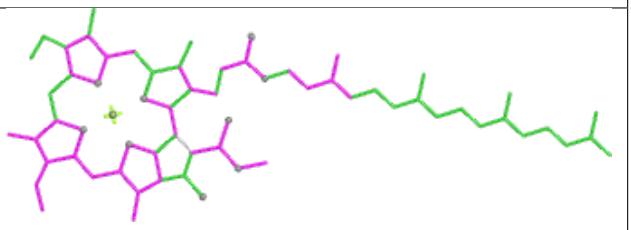
Ligand PL9 d 411



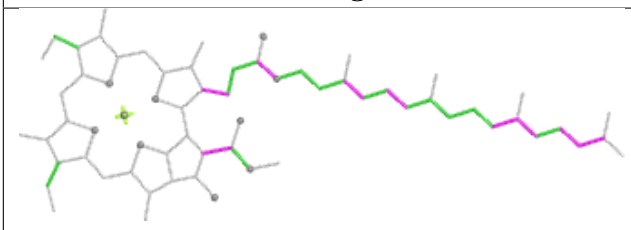
Ligand CLA C 507



Bond lengths



Bond angles



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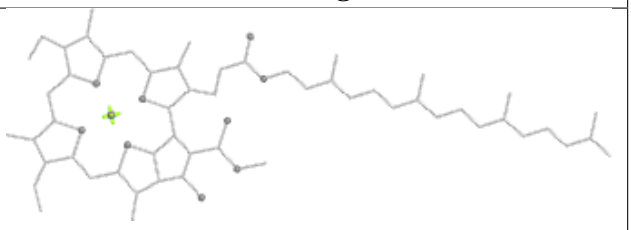
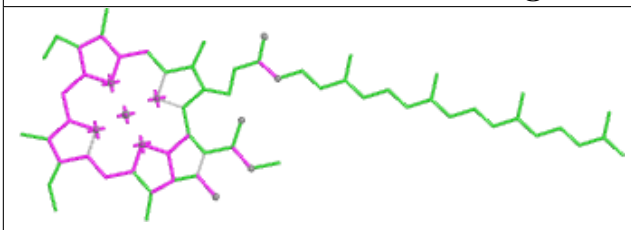


Rings

Ligand CLA C 510



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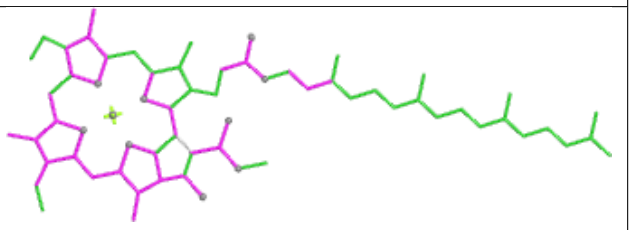

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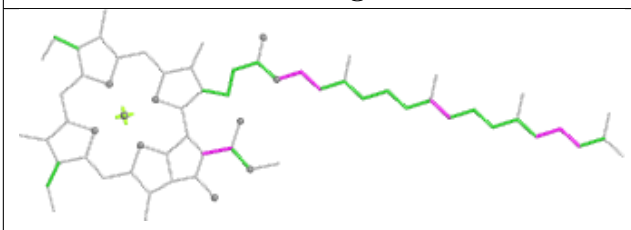

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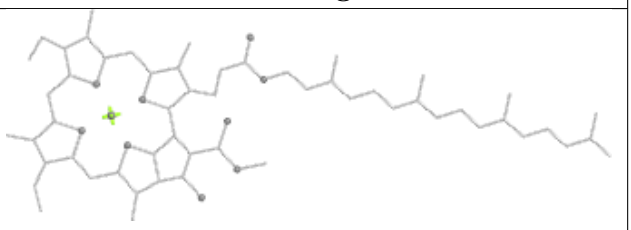
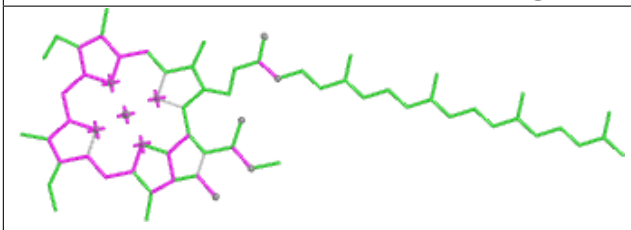


Rings

Ligand CLA c 505



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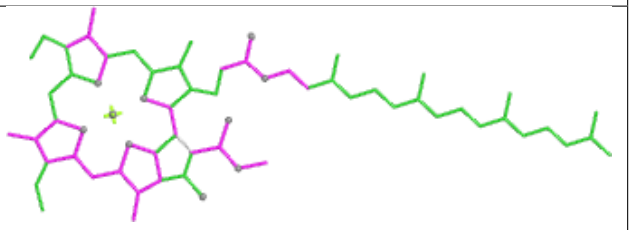

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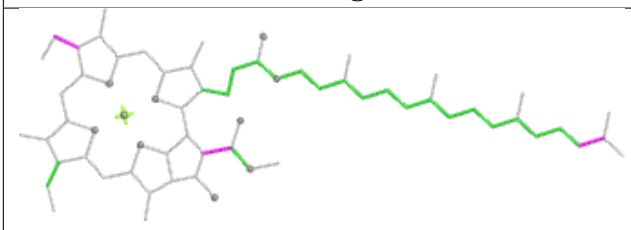

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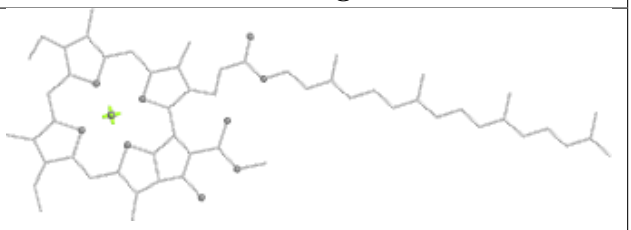
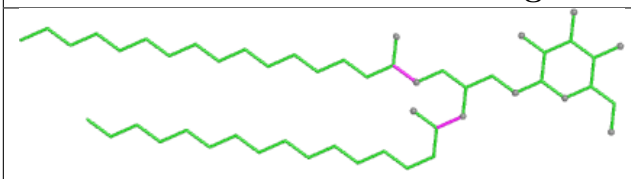


Rings

Ligand LMG c 501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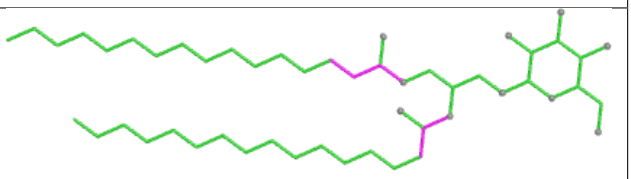
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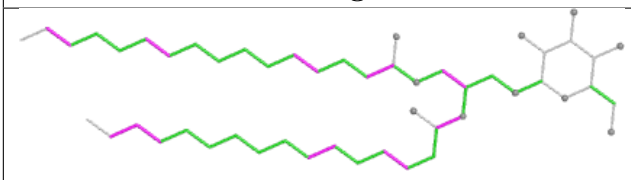
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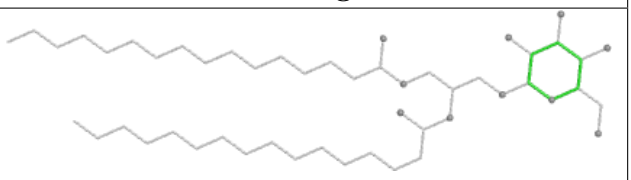
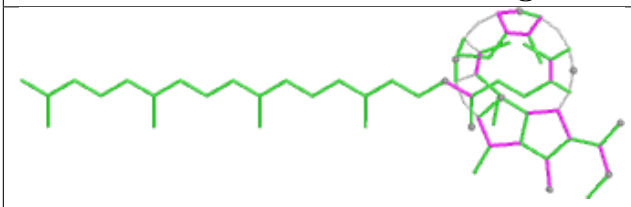

Rings

Ligand PHO a 2612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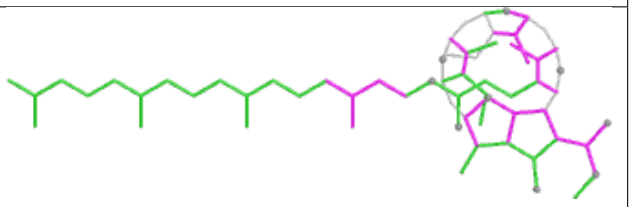
Bond angles


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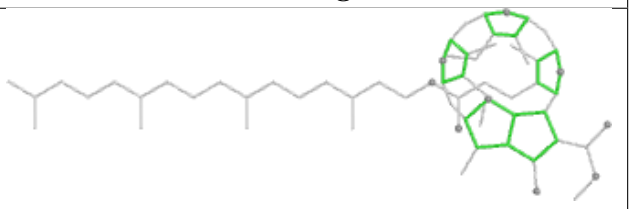
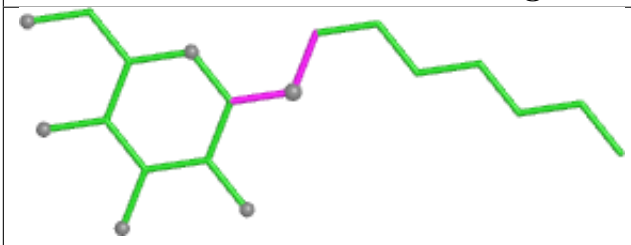

Rings

Ligand HTG b 603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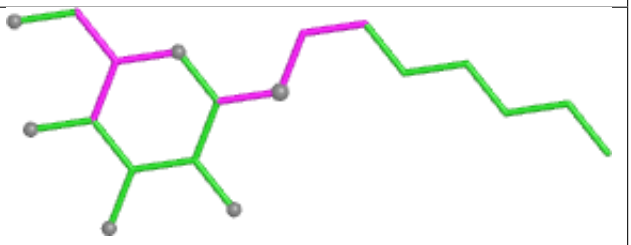
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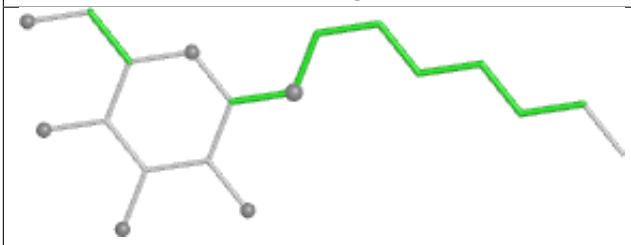
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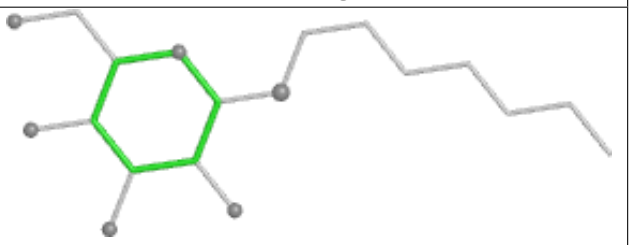
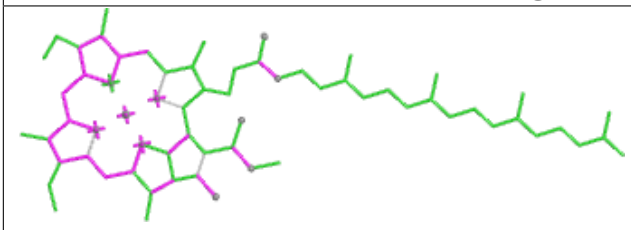

Rings

Ligand CLA c 514



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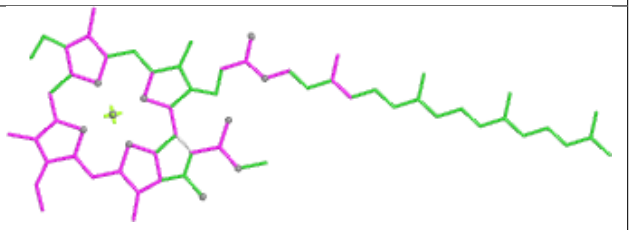

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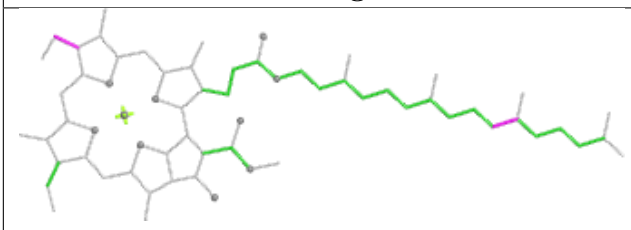

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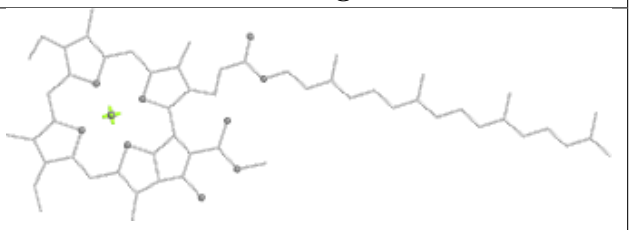
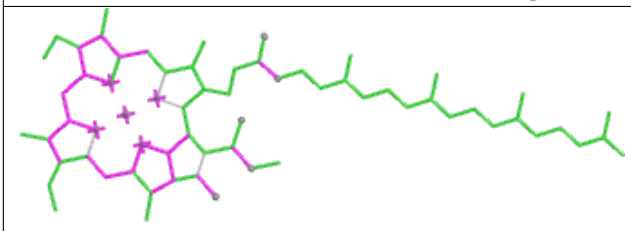


Rings

Ligand CLA C 508



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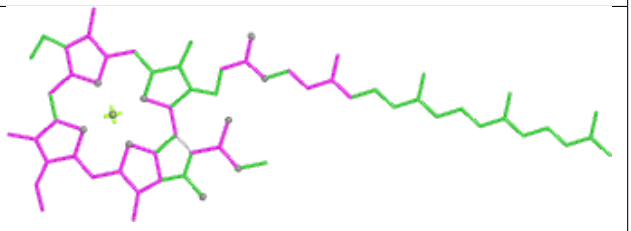

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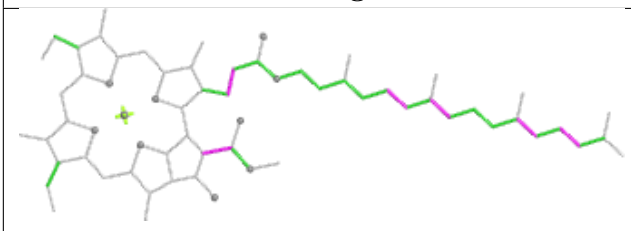

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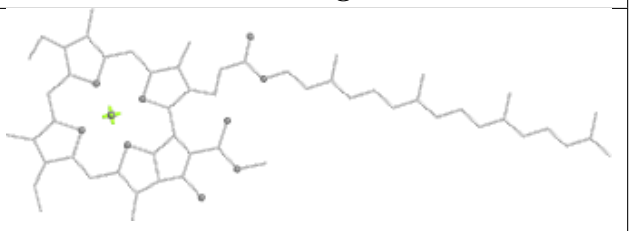
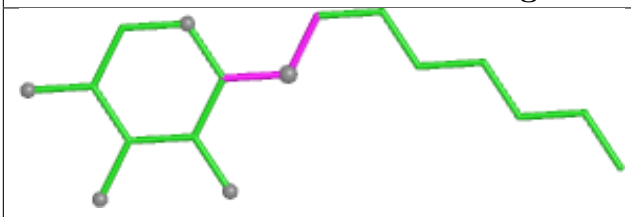


Rings

Ligand HTG H 101



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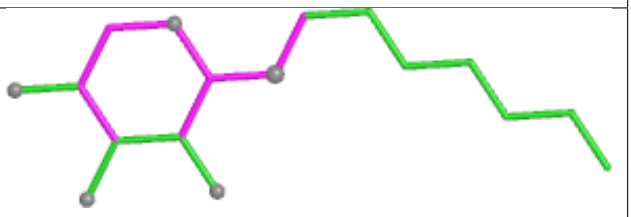

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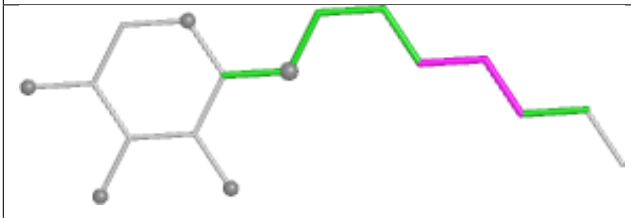

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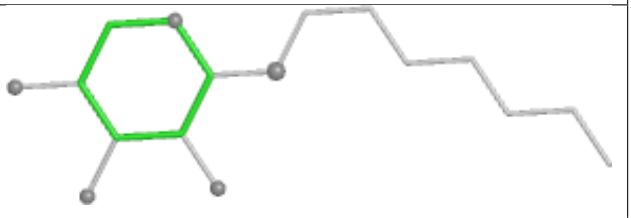
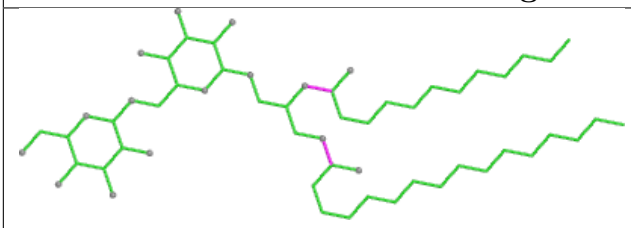


Rings

Ligand DGD C 519



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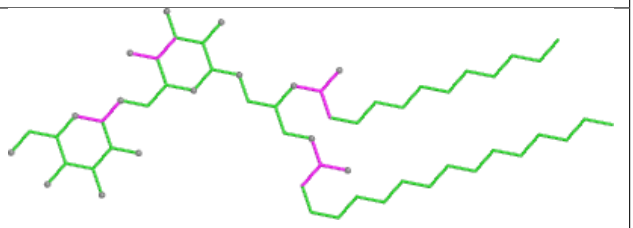

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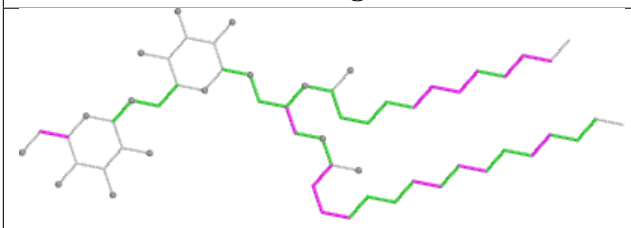

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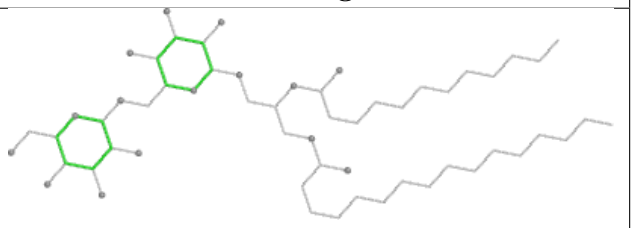
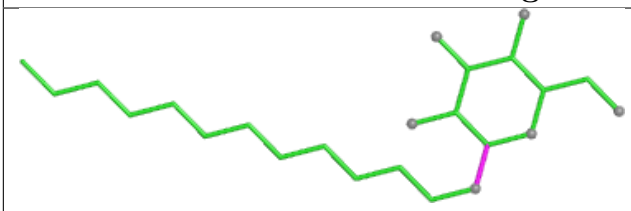


Rings

Ligand LMT T 103



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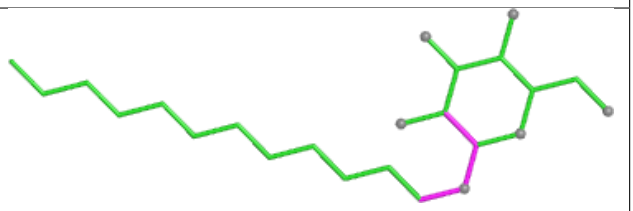
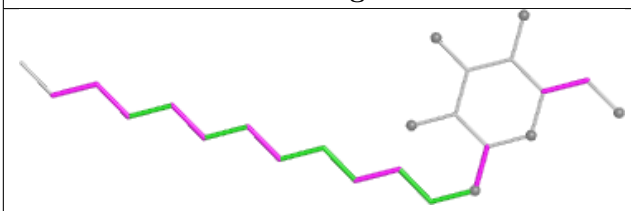


Bond angles



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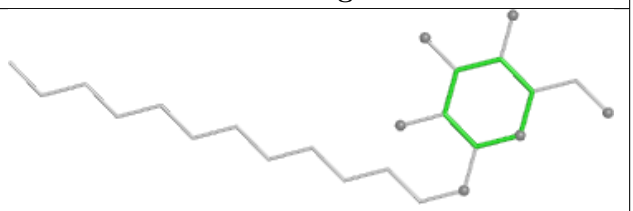
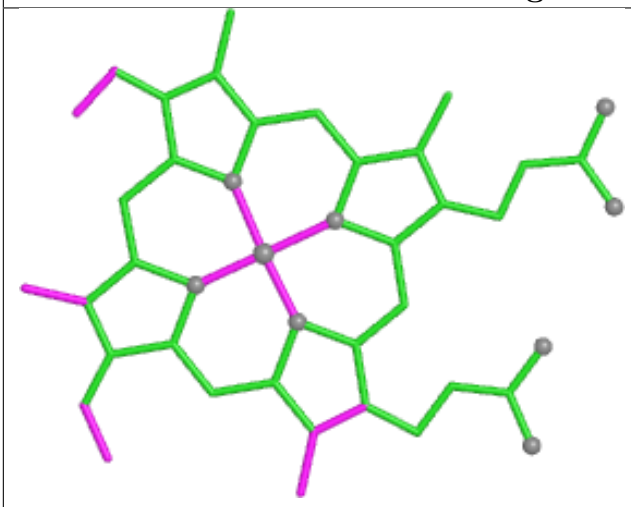


Rings

Ligand HEC v 201



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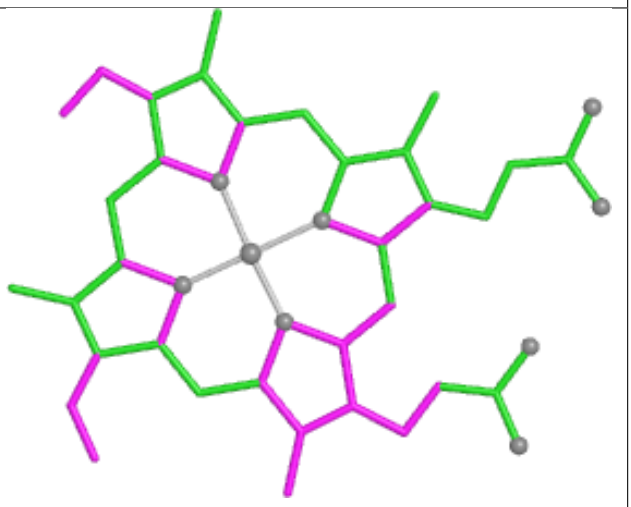
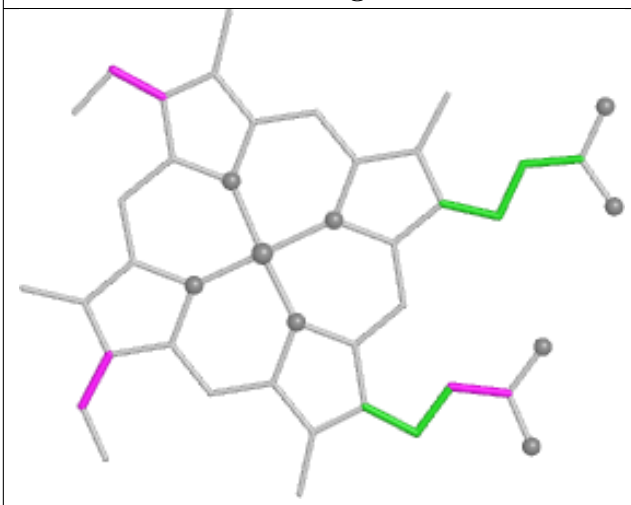


Bond angles



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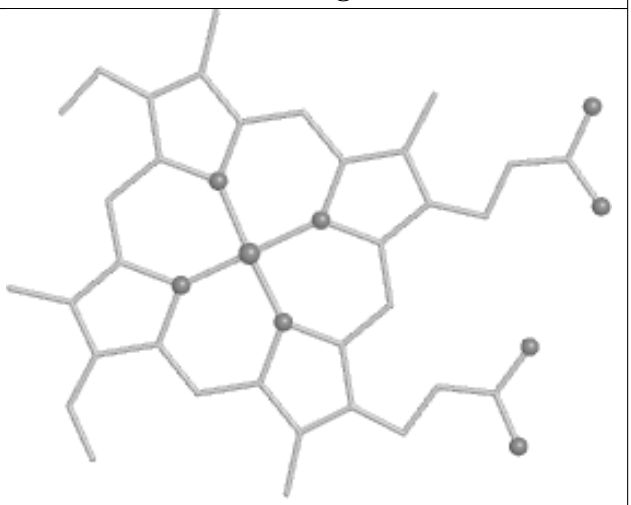
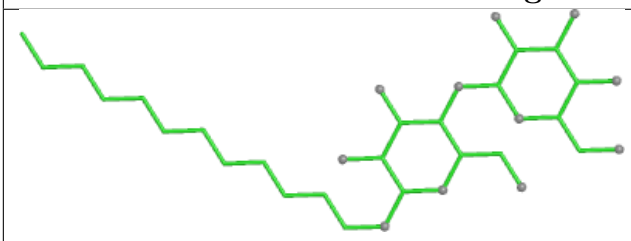


Rings

Ligand LMT d 401



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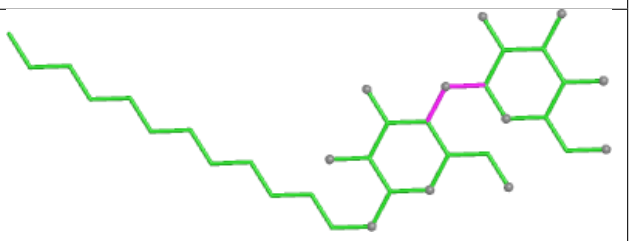
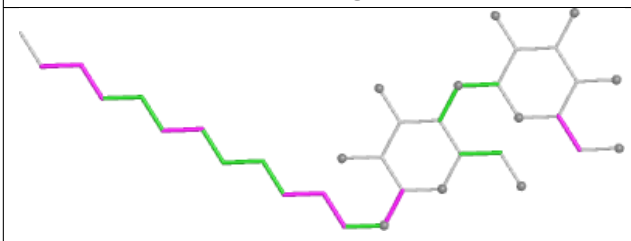


Bond angles



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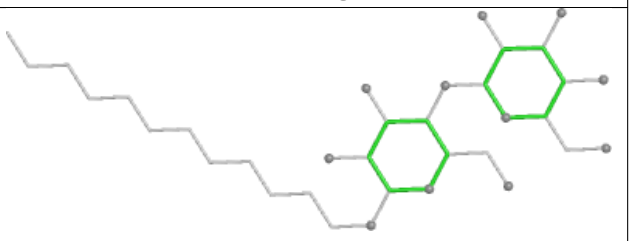
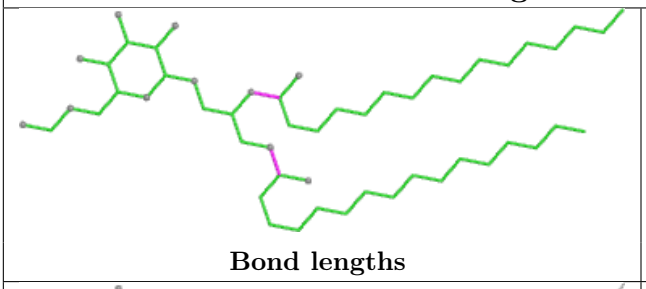
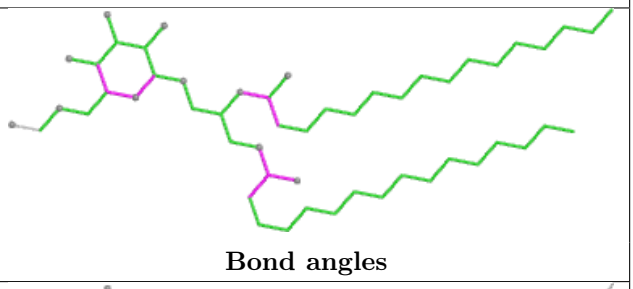


Rings

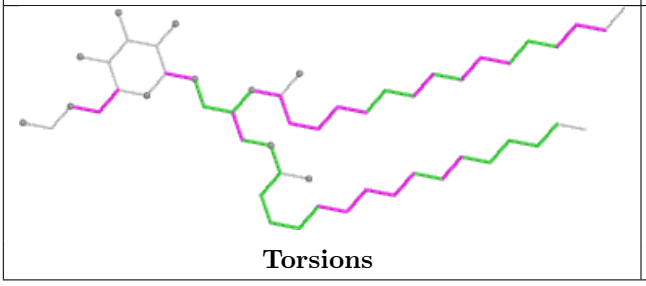
Ligand DGD D 2307



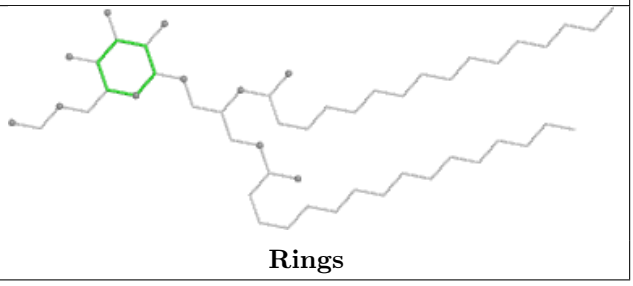
Bond lengths



Bond angles

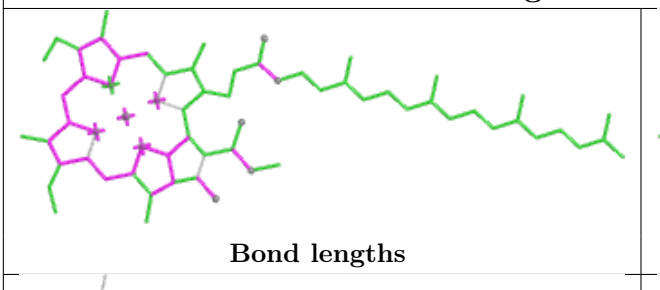


Torsions



Rings

Ligand CLA C 506



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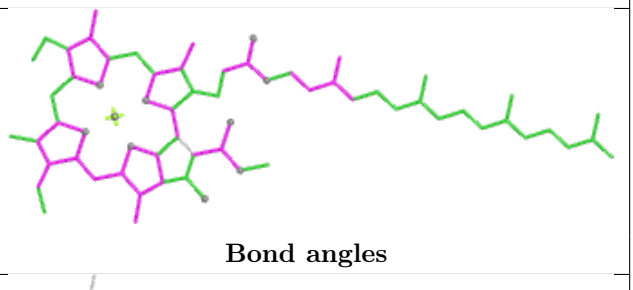

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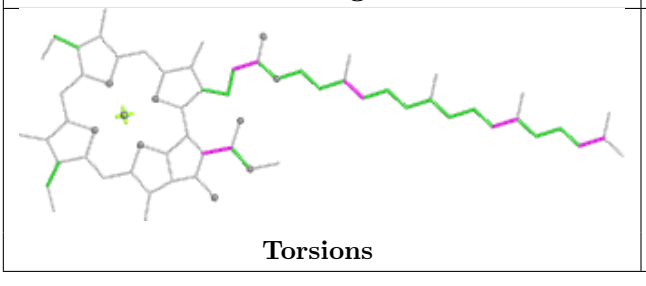

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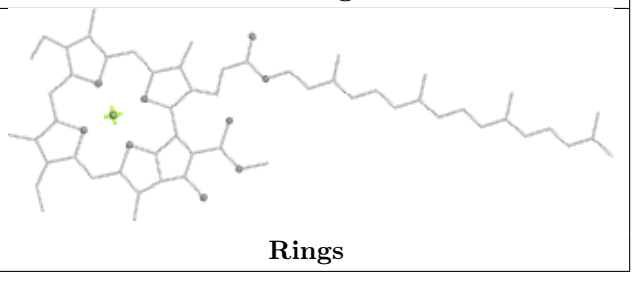
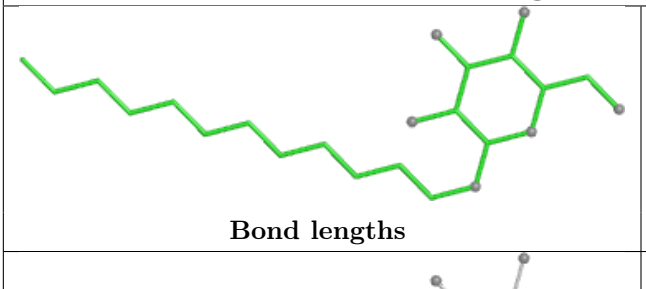


Rings

Ligand LMT f 101



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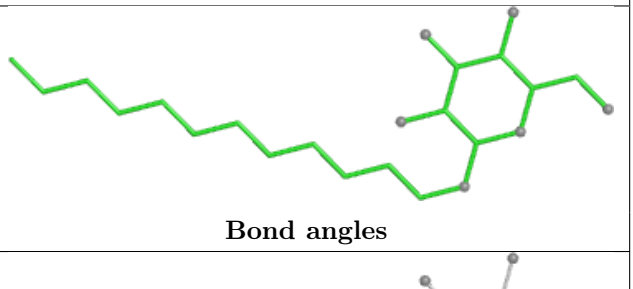
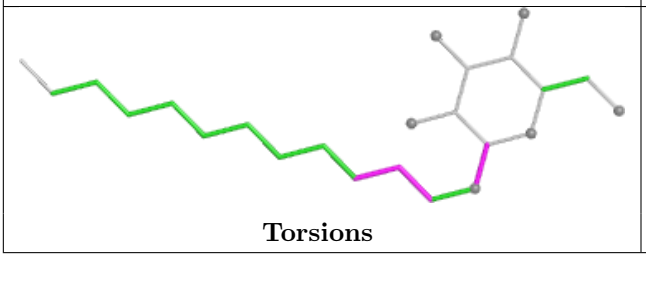


Bond angles



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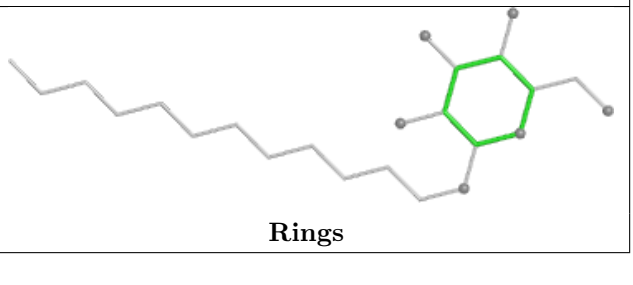
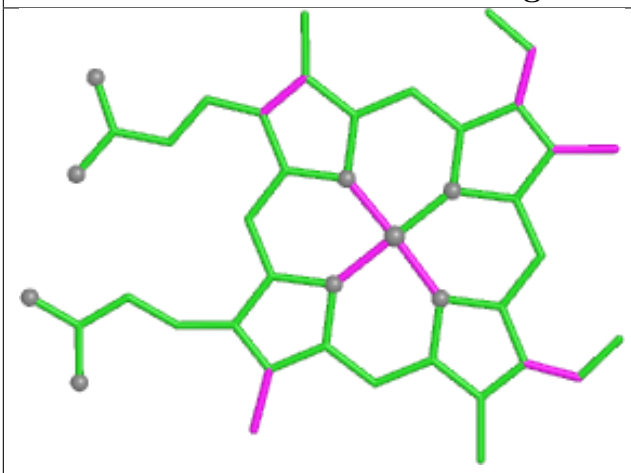


Rings

Ligand HEM e 103



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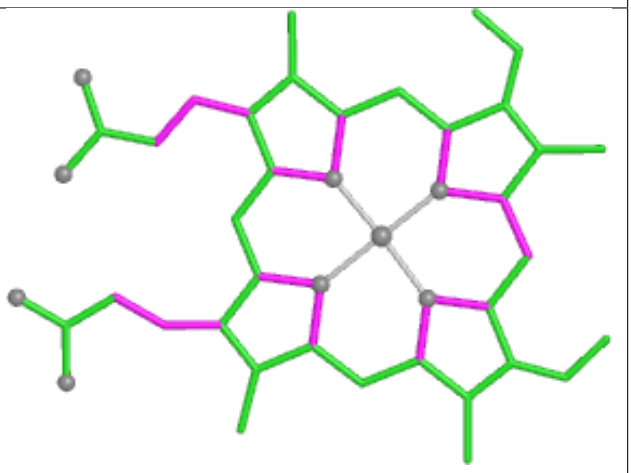
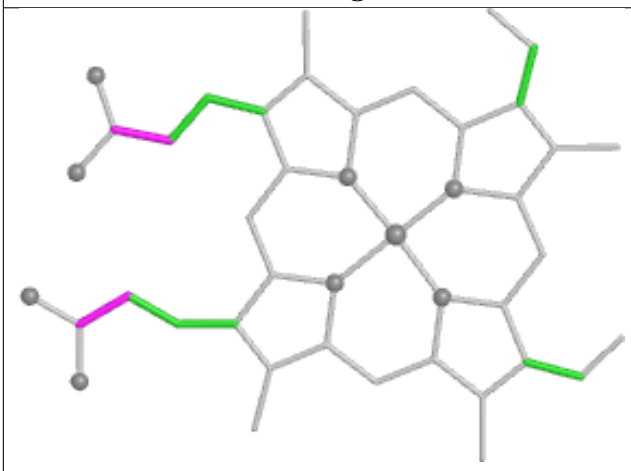


Bond angles



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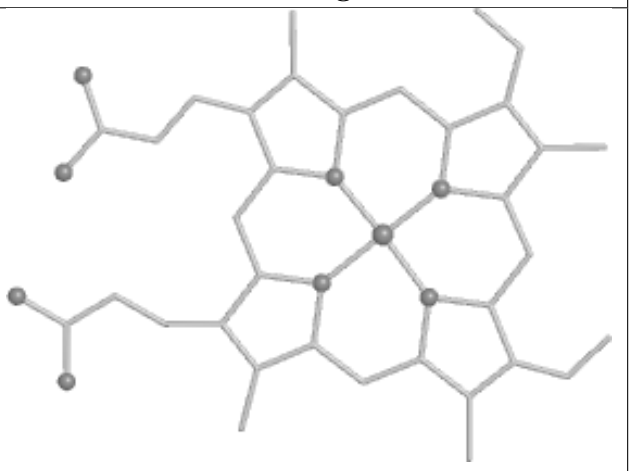
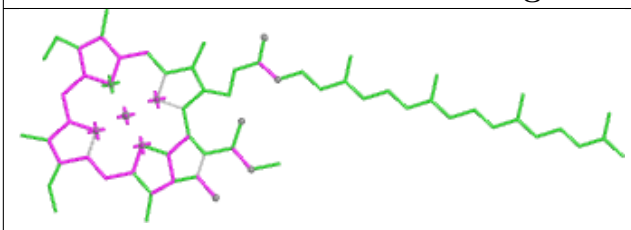
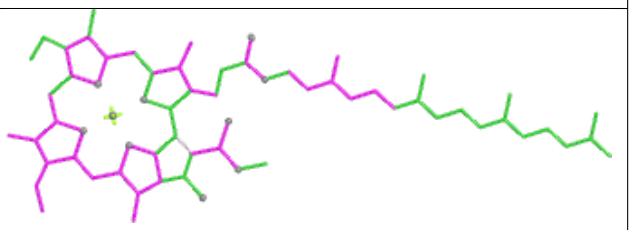


Rings

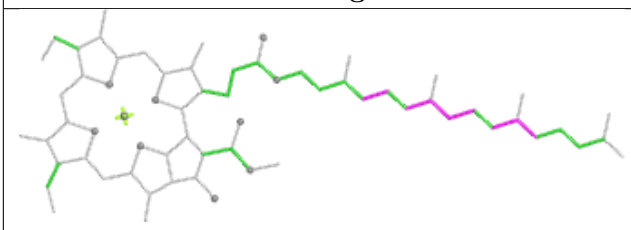
Ligand CLA A 410



Bond lengths



Bond angles



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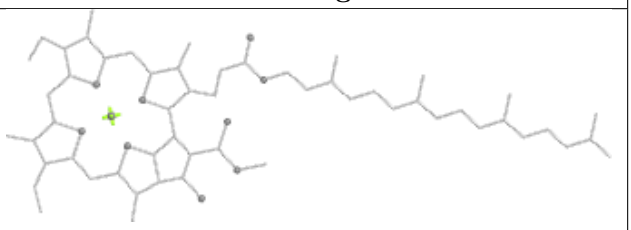
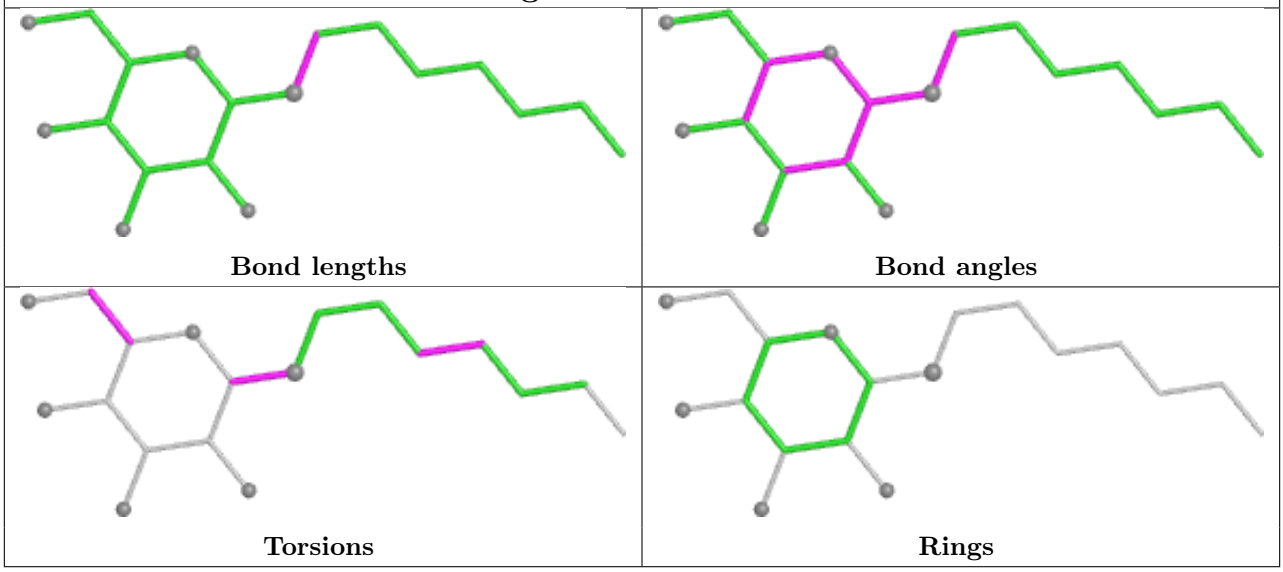
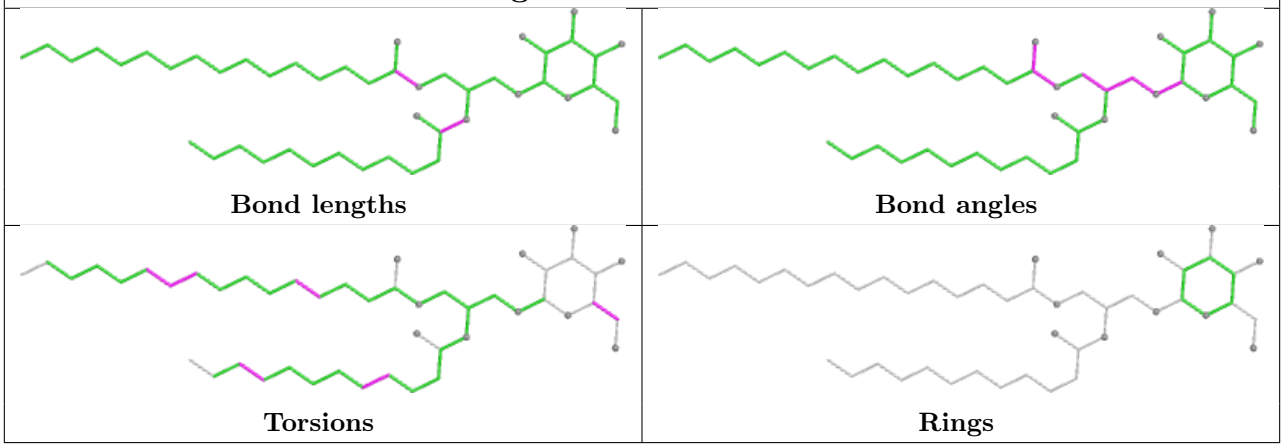


Rings

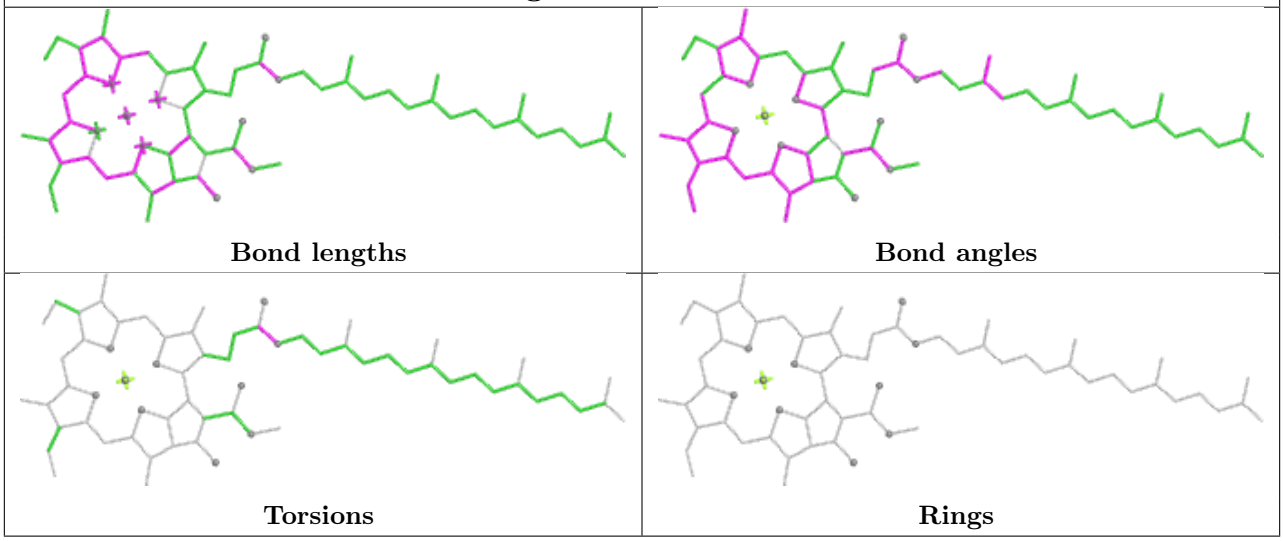
Ligand HTG V 204



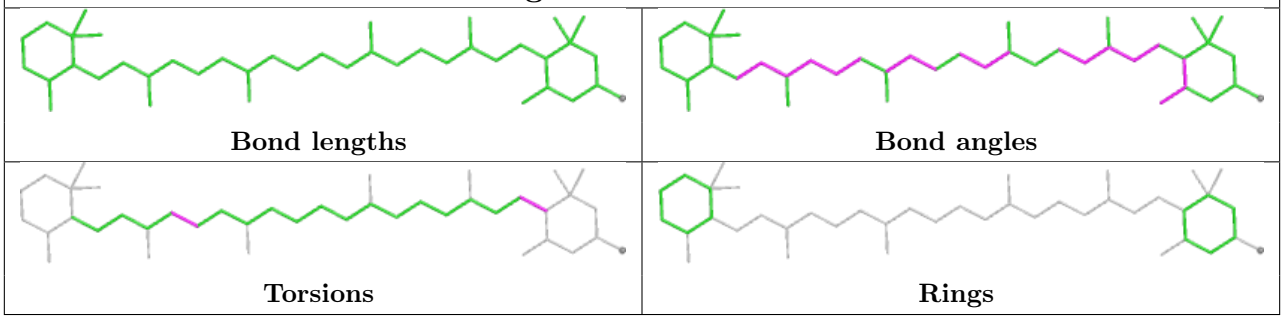
Ligand LMG D 2312



Ligand CLA C 512



Ligand RRX h 101



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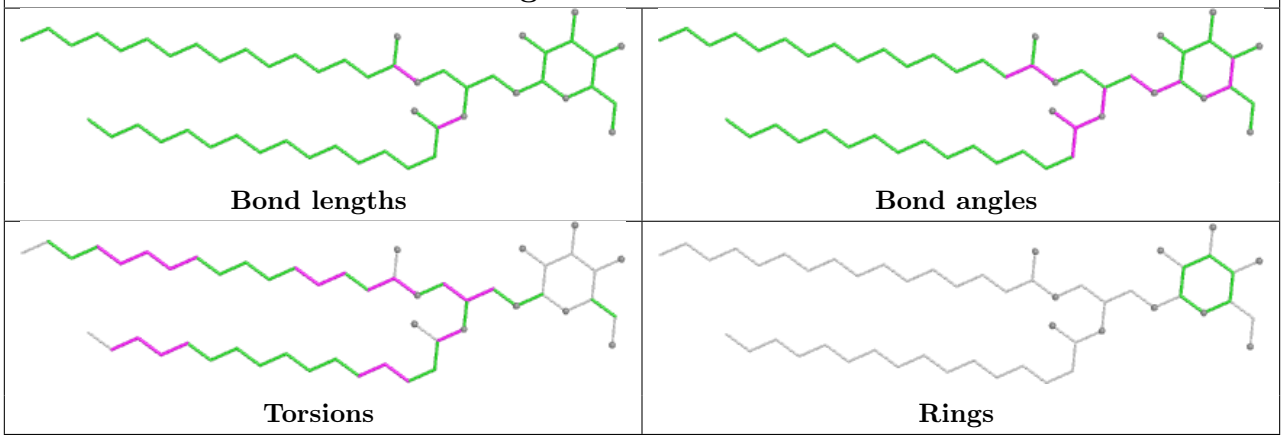

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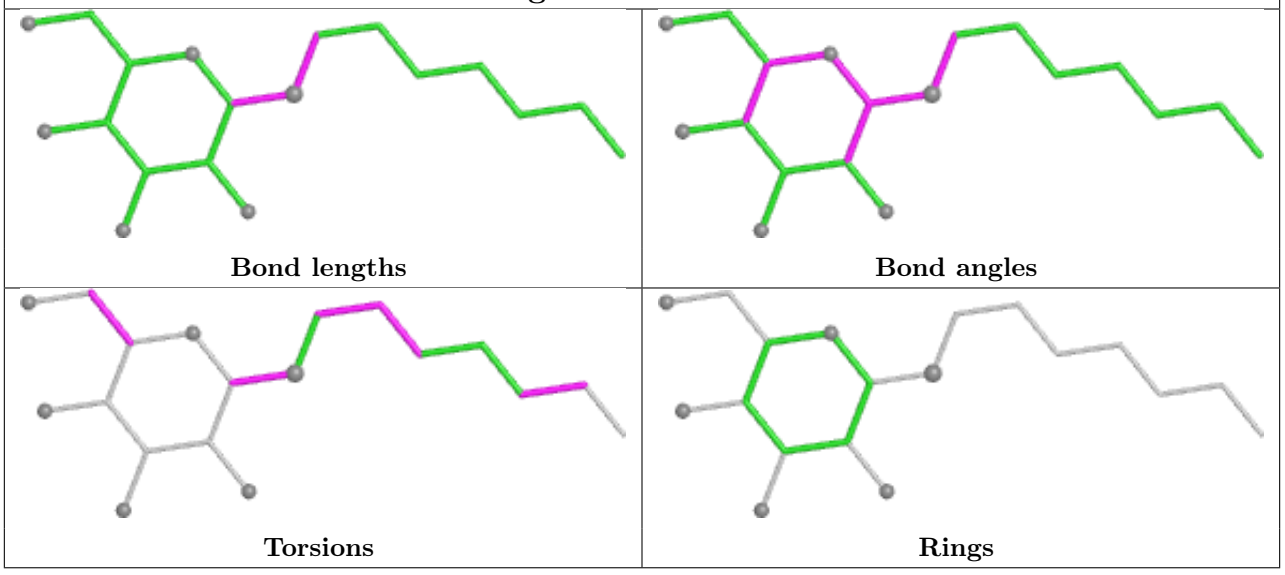
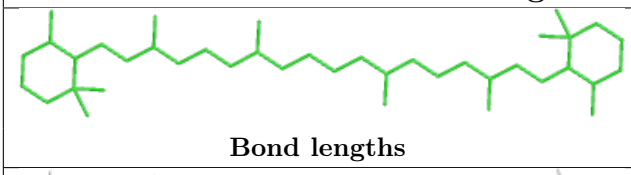
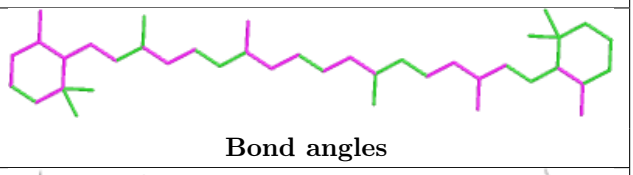


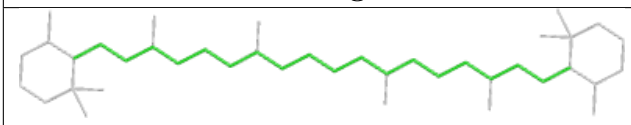
Ligand BCR z 101



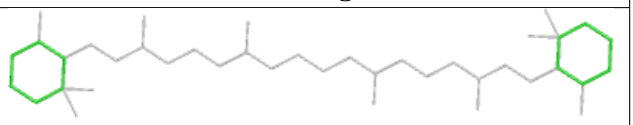
Bond lengths



Bond angles

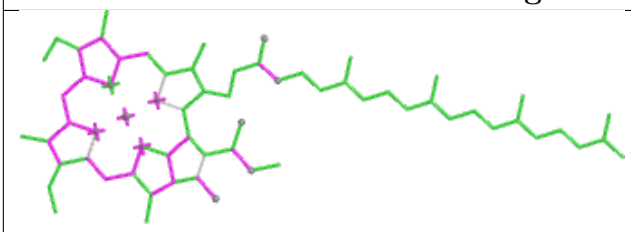


Torsions



Rings

Ligand CLA B 613



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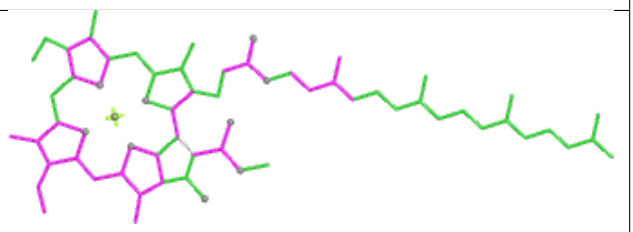
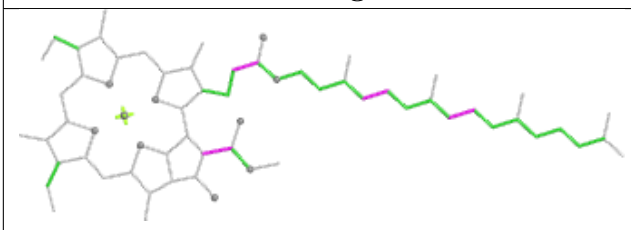


Bond angles



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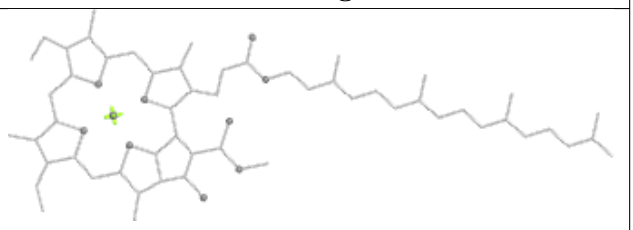
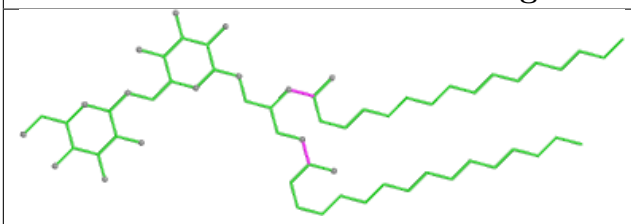
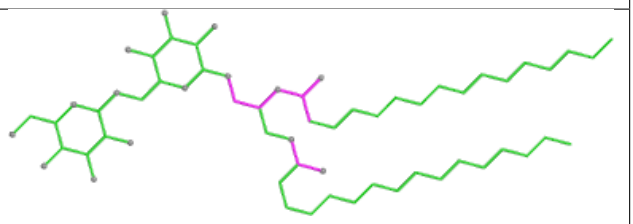


Rings

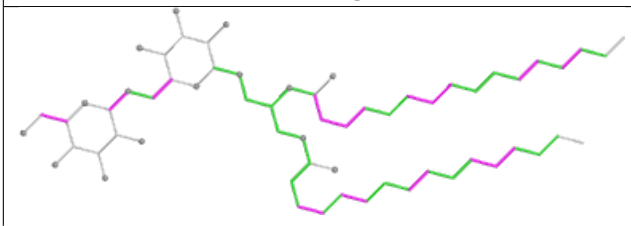
Ligand DGD C 517



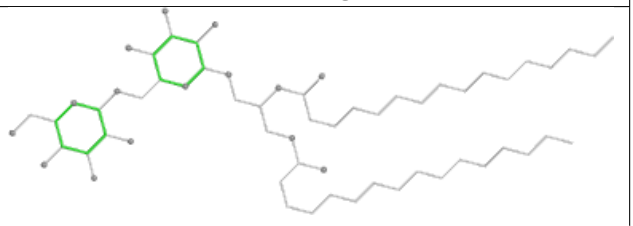
Bond lengths



Bond angles

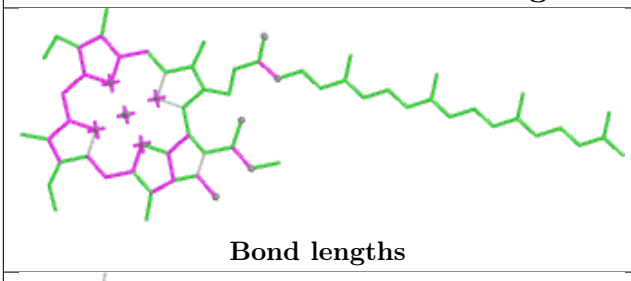


Torsions



Rings

Ligand CLA c 511



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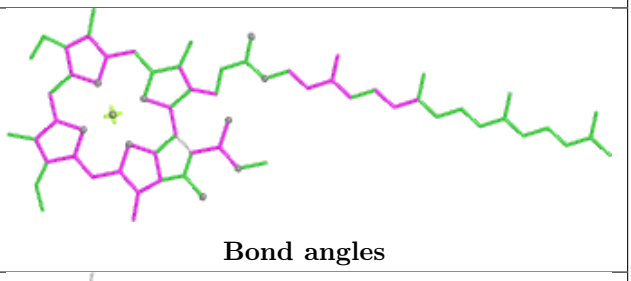
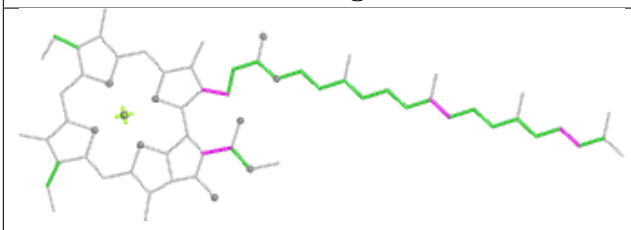


Bond angles



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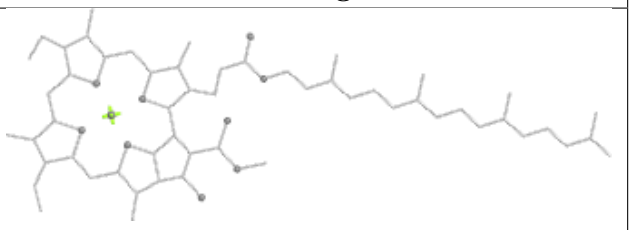
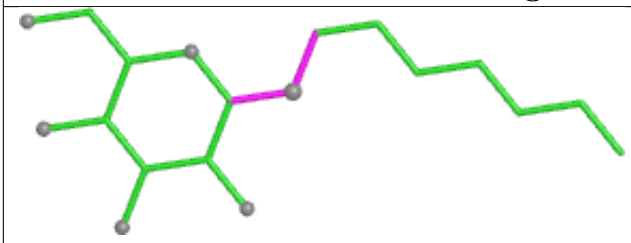


Rings

Ligand HTG d 407



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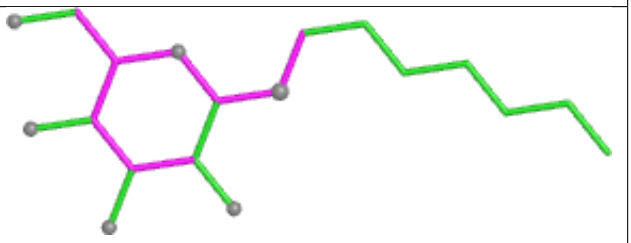
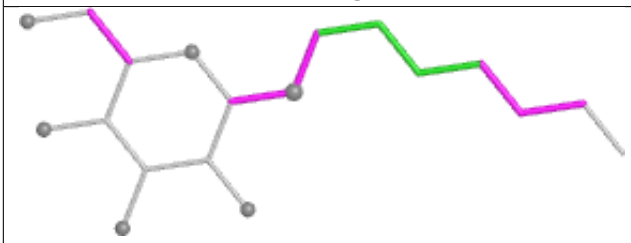


Bond angles



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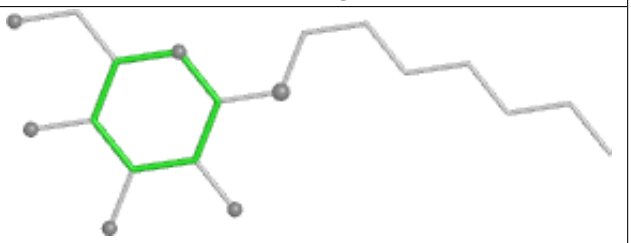
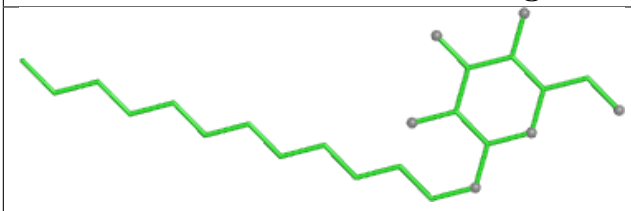


Rings

Ligand LMT F 102



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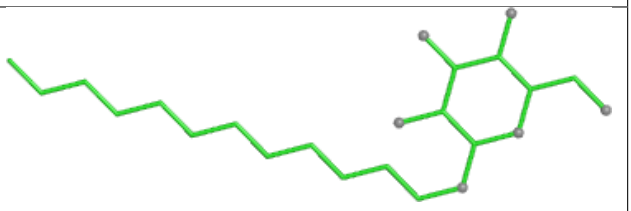
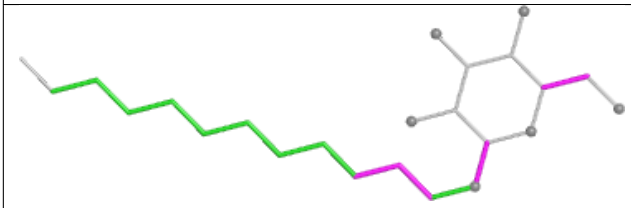


Bond angles



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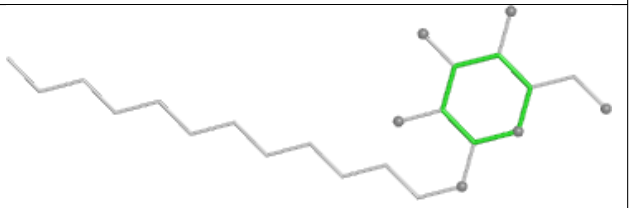
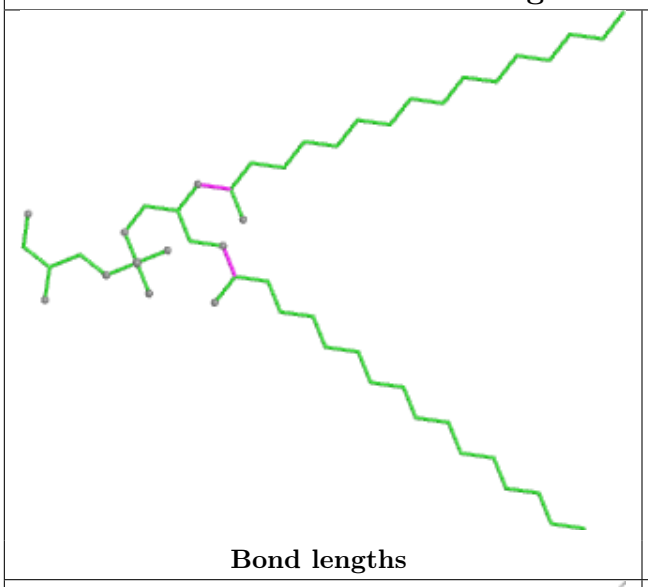
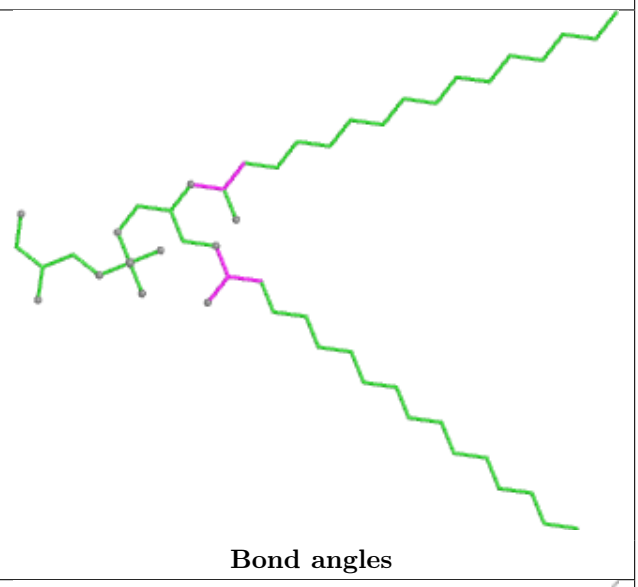


Rings

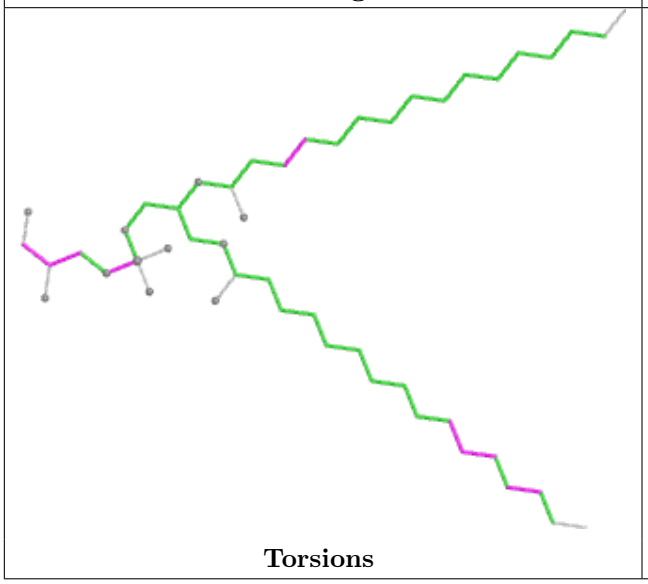
Ligand LHG d 413



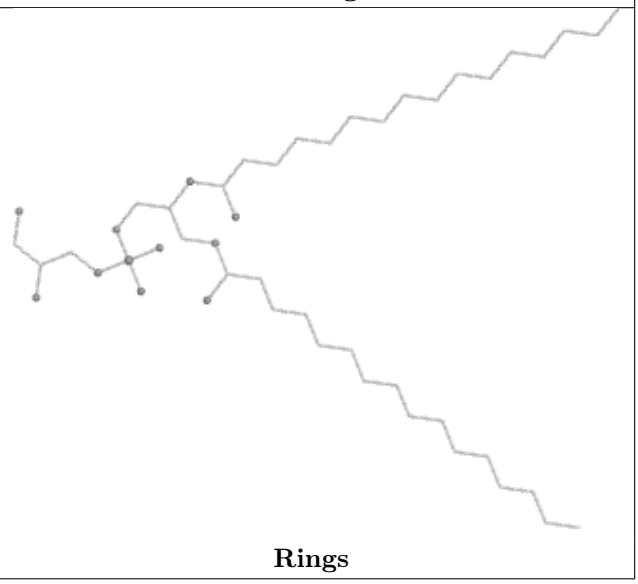
Bond lengths



Bond angles

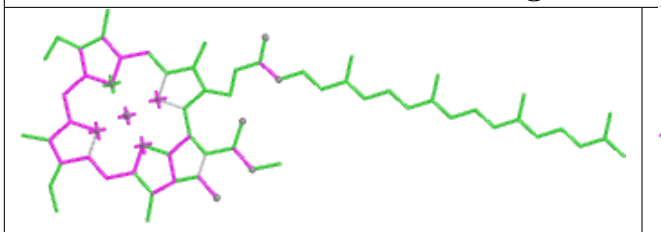


Torsions

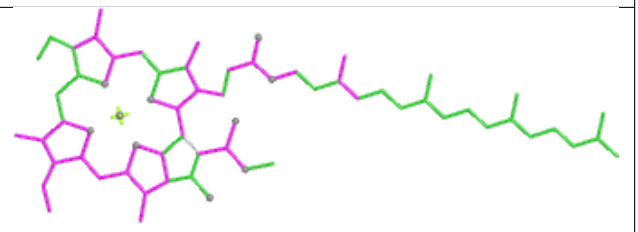


Rings

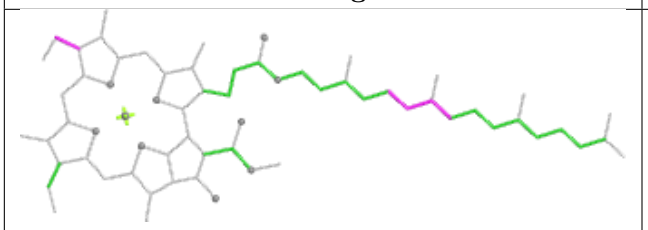
Ligand CLA B 604



Bond lengths



Bond angles



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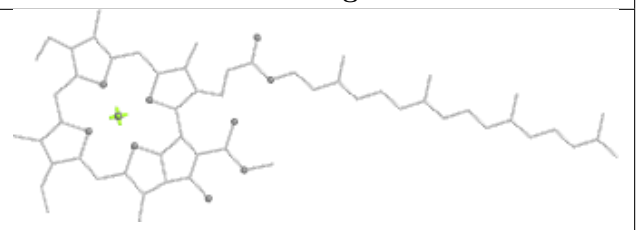
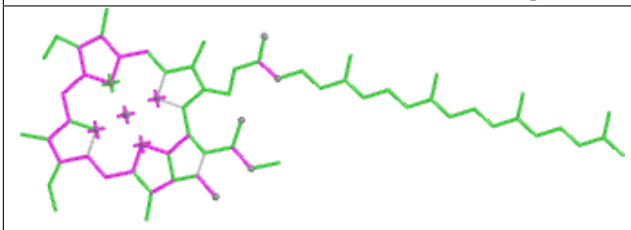
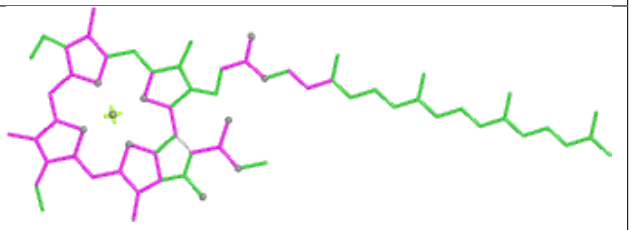


Rings

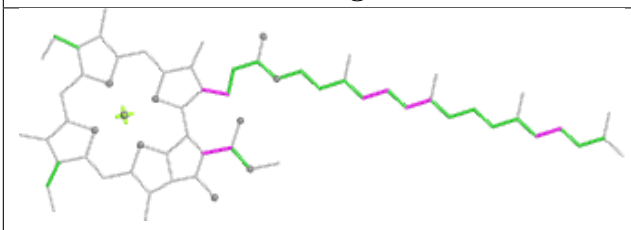
Ligand CLA B 605



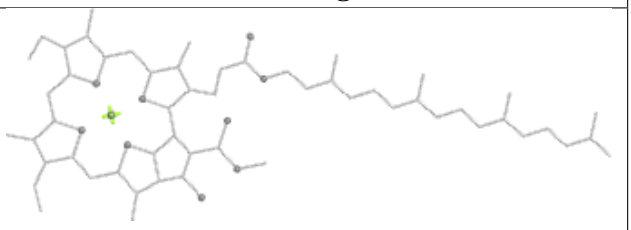
Bond lengths



Bond angles

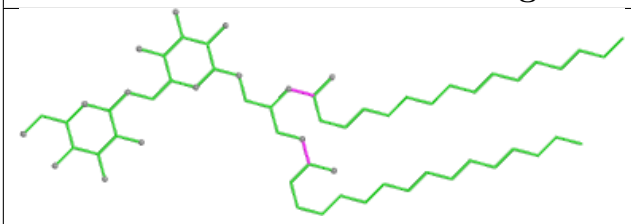


Torsions



Rings

Ligand DGD H 103



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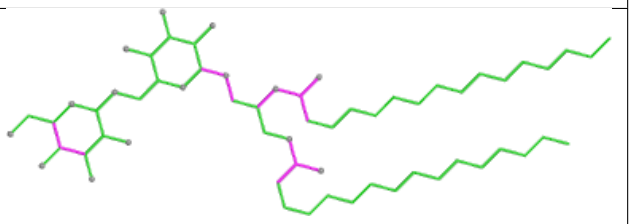
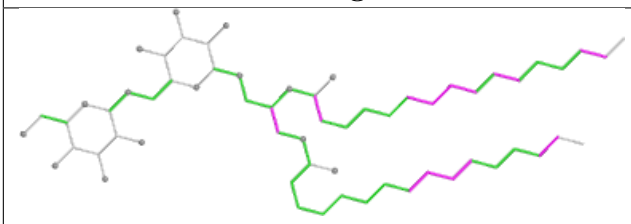


Bond angles



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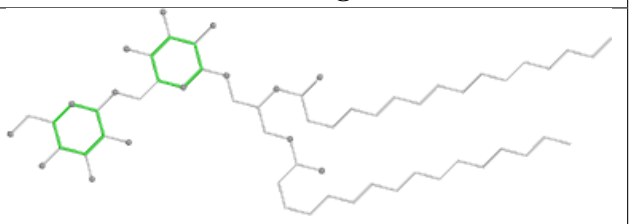
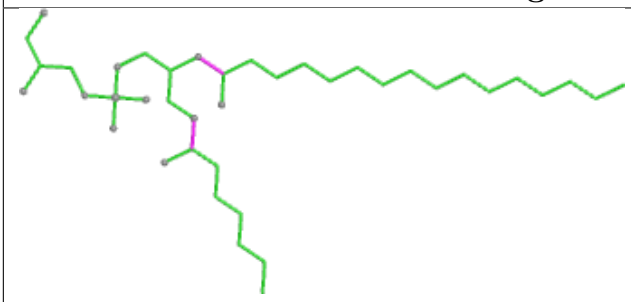


Rings

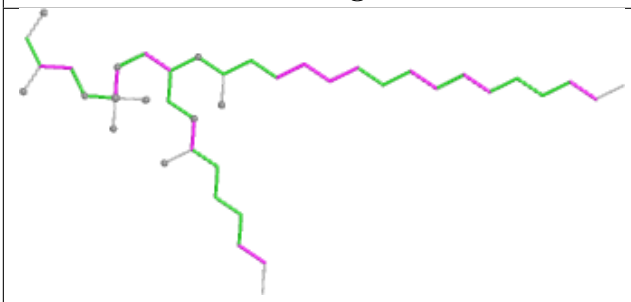
Ligand LHG e 101



Bond lengths



Bond angles



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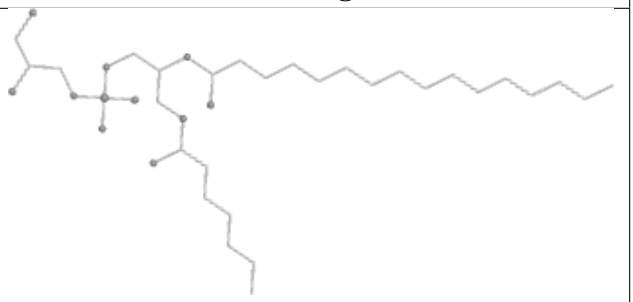
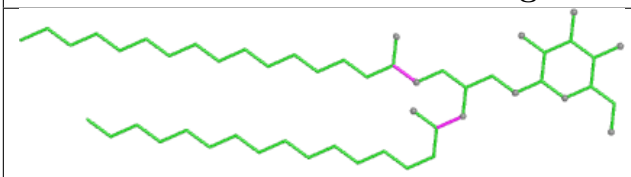
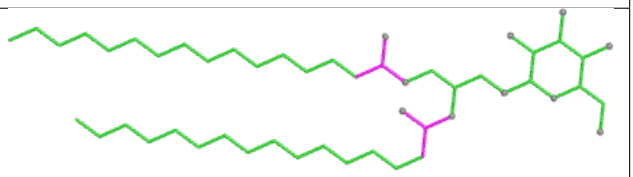


Rings

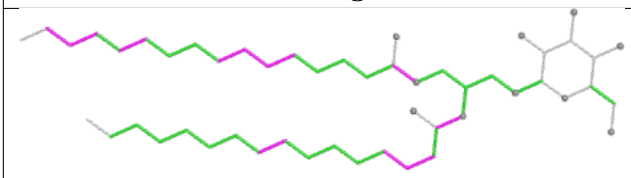
Ligand LMG C 520



Bond lengths



Bond angles



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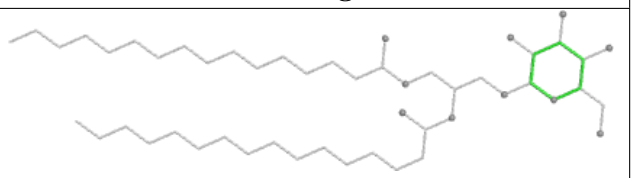
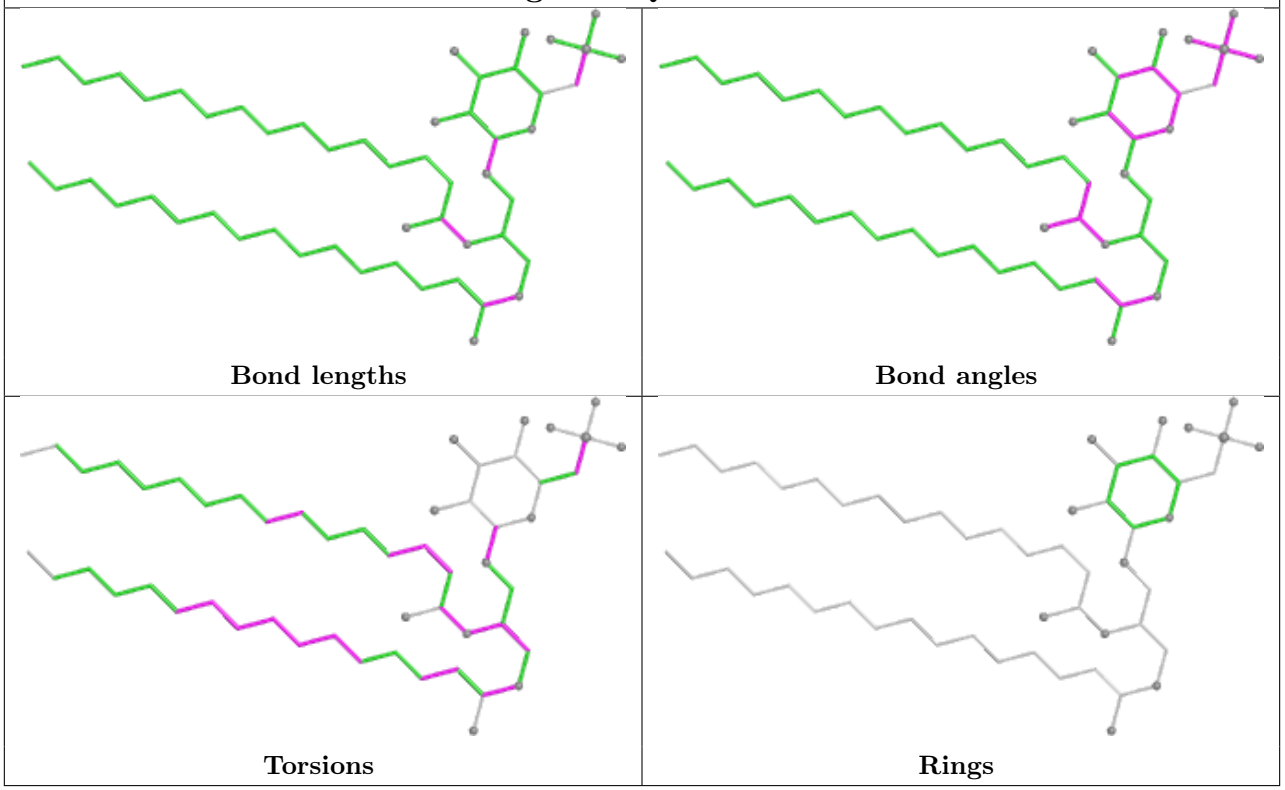
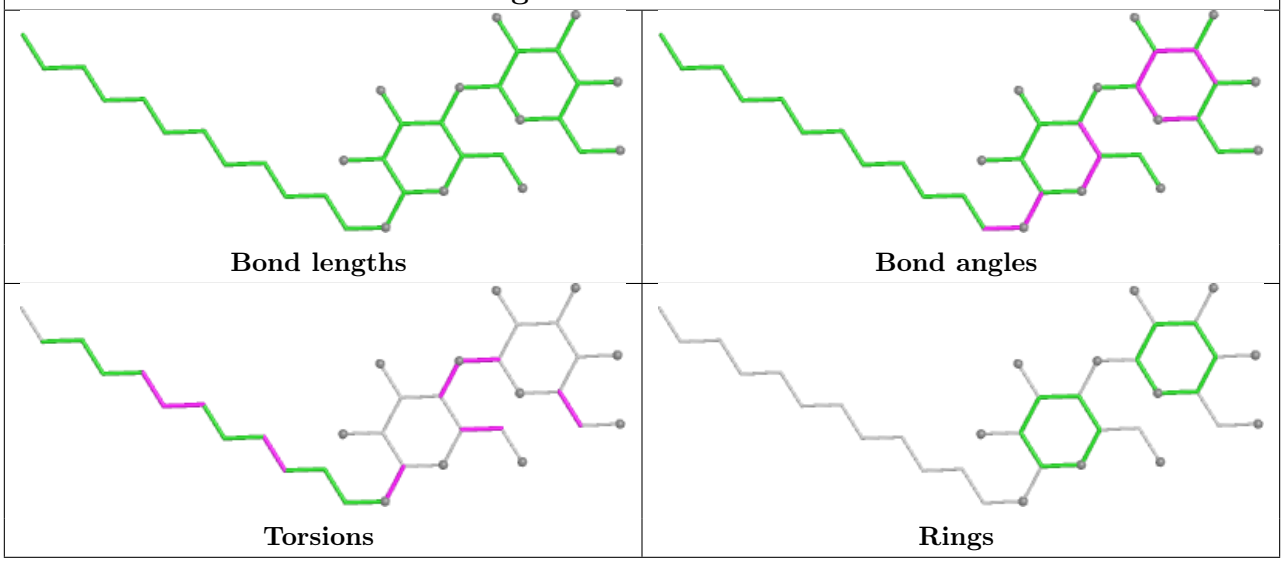


Rings

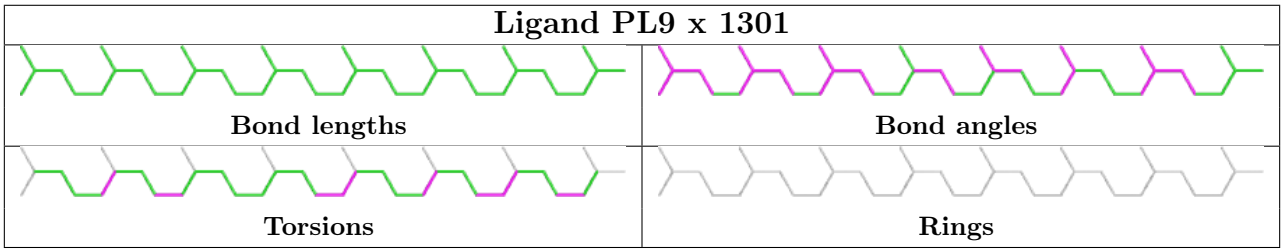
Ligand SQD B 621



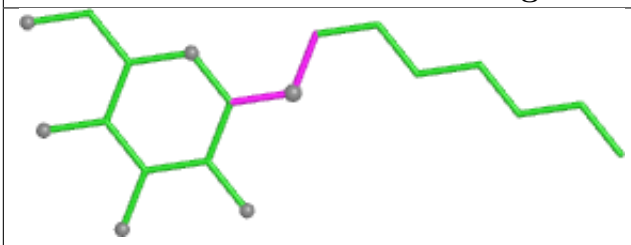
Ligand LMT m 2804



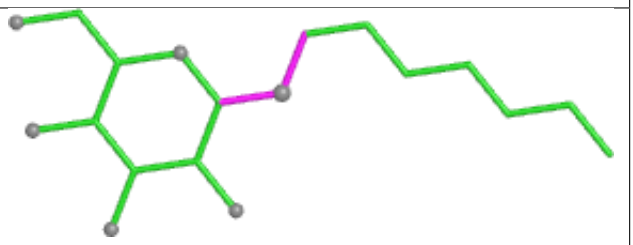
Ligand PL9 x 1301



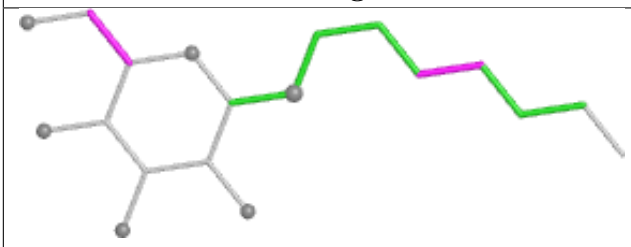
Ligand HTG B 626



Bond lengths



Bond angles



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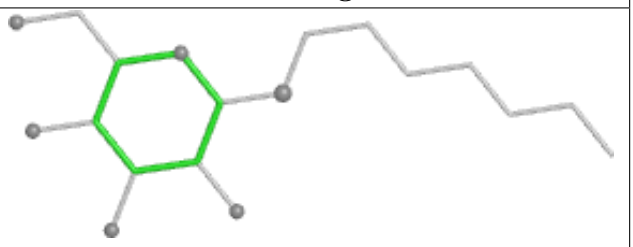
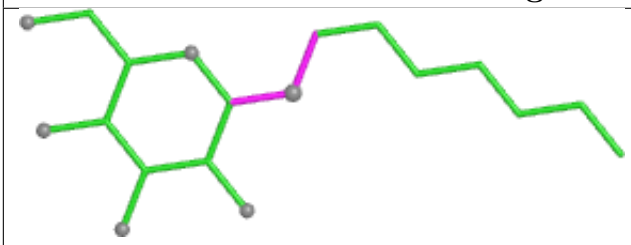


Rings

Ligand HTG c 523



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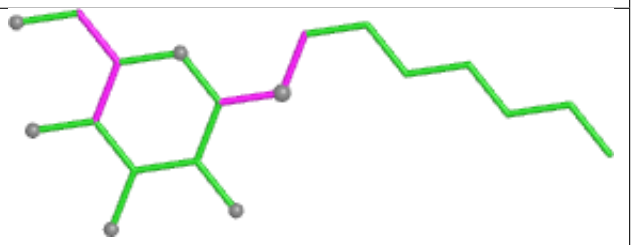
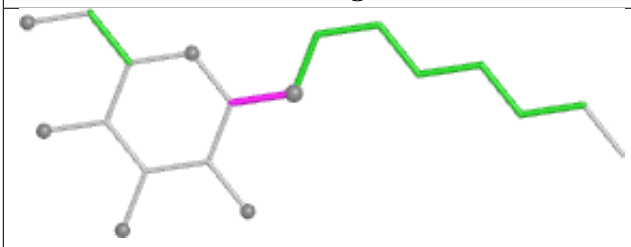


Bond angles



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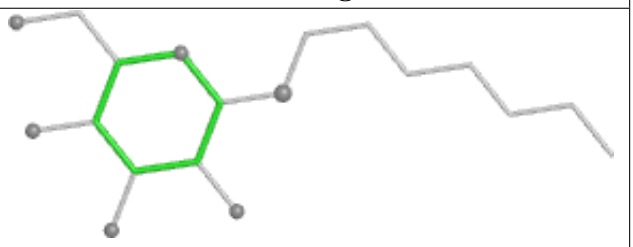
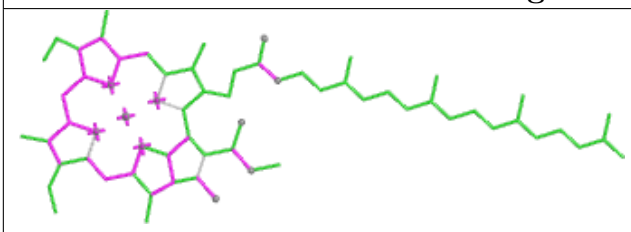


Rings

Ligand CLA b 612



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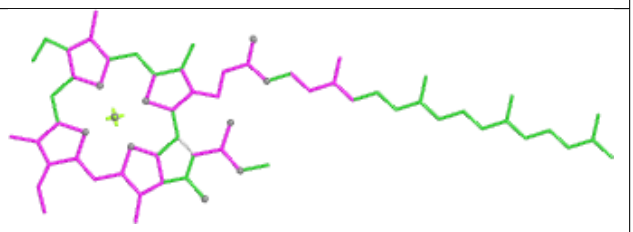
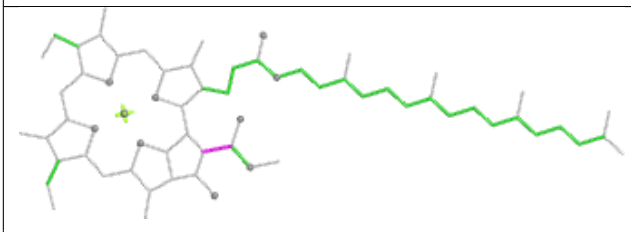


Bond angles



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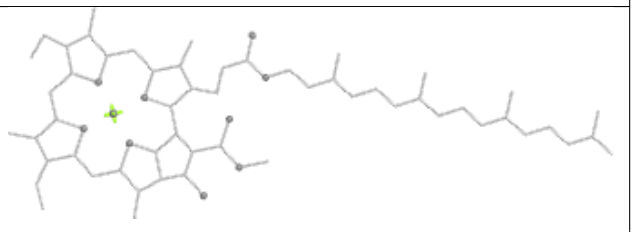
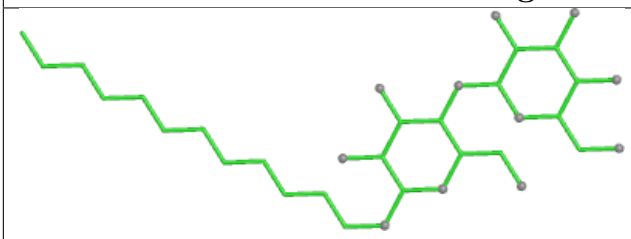


Rings

Ligand LMT M 102



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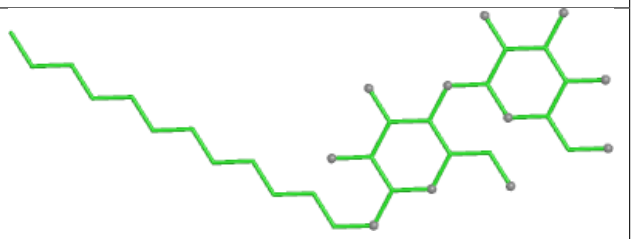
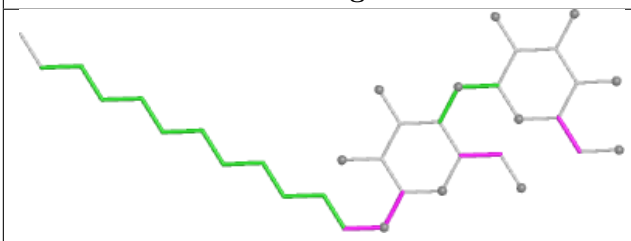


Bond angles



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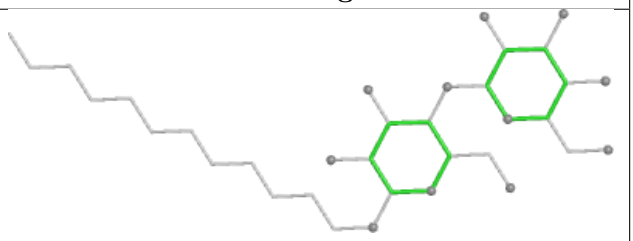
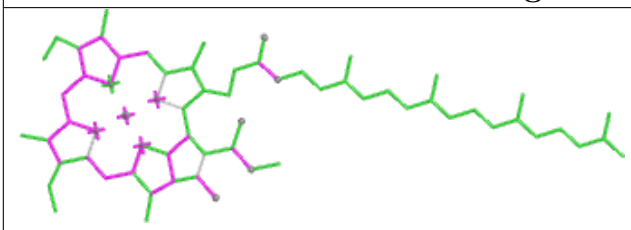


Rings

Ligand CLA B 606



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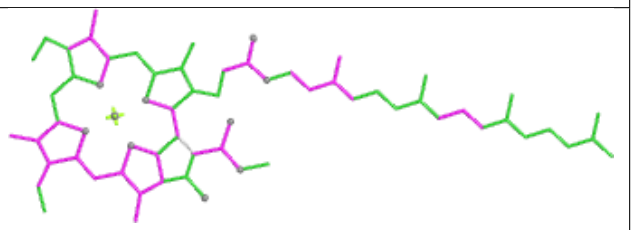
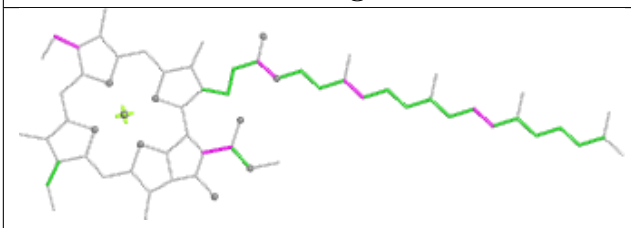


Bond angles



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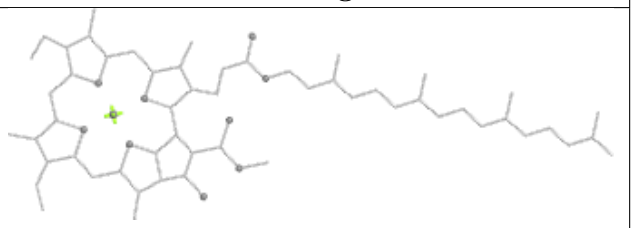
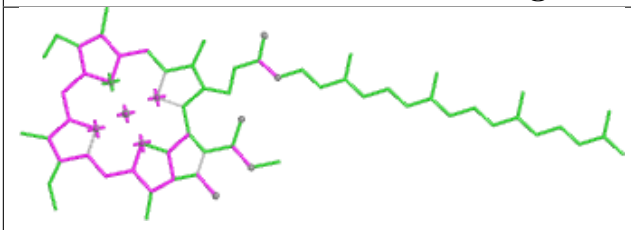


Rings

Ligand CLA c 509



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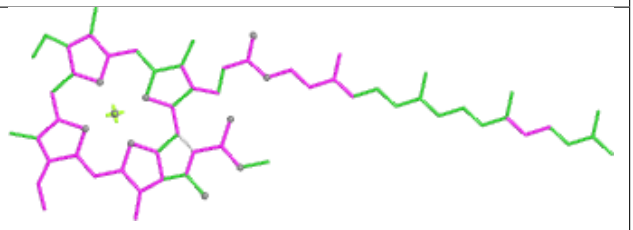
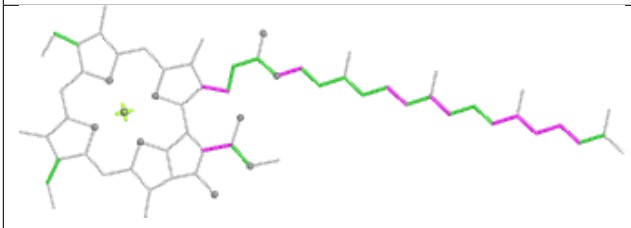


Bond angles



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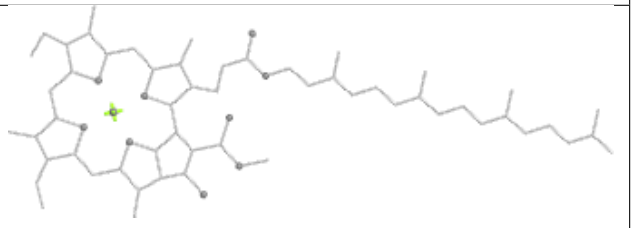
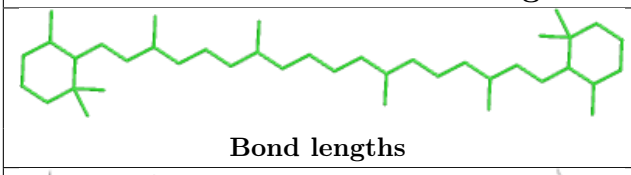


Rings

Ligand BCR C 515



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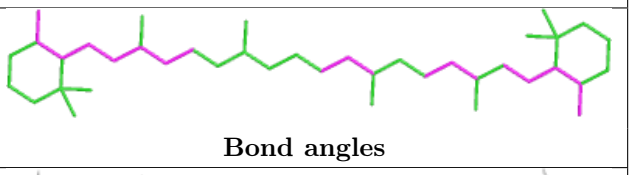
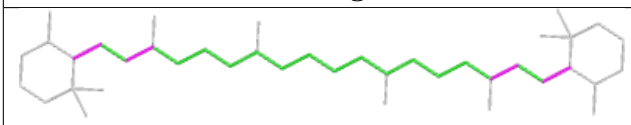


Bond angles



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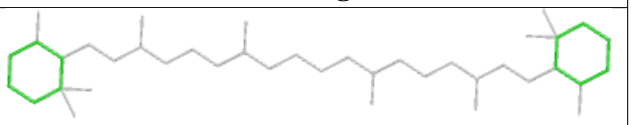
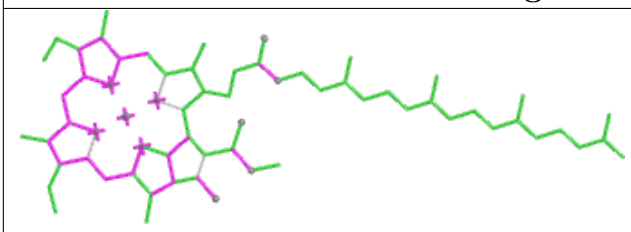


Rings

Ligand CLA C 505



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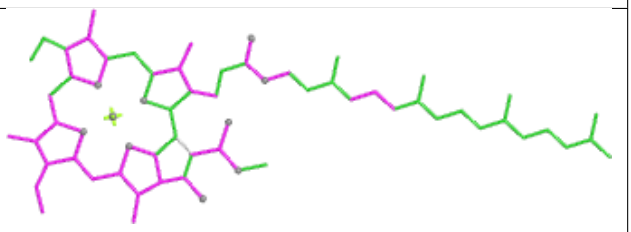
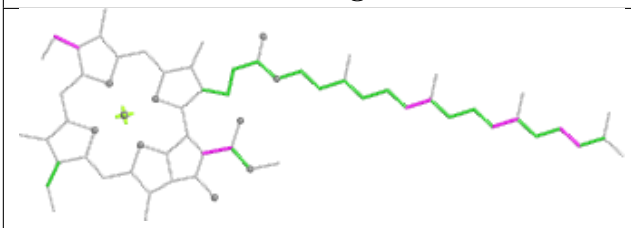


Bond angles



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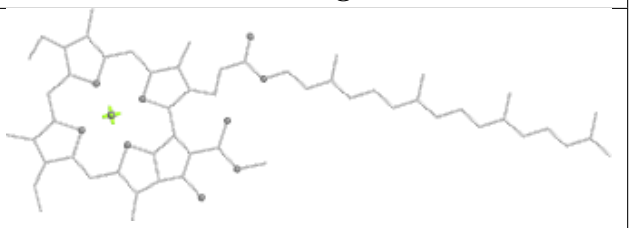
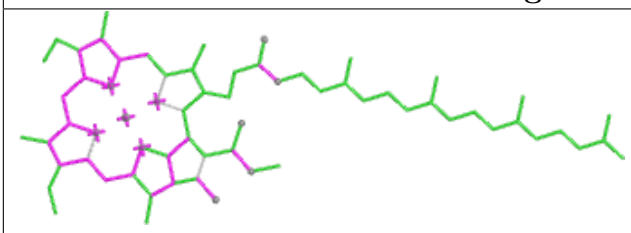
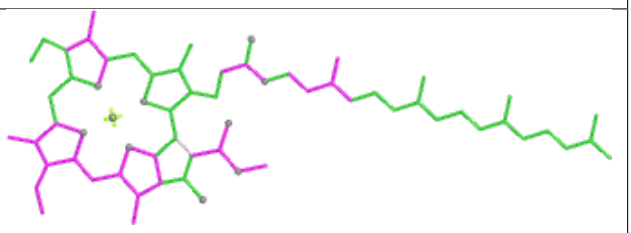


Rings

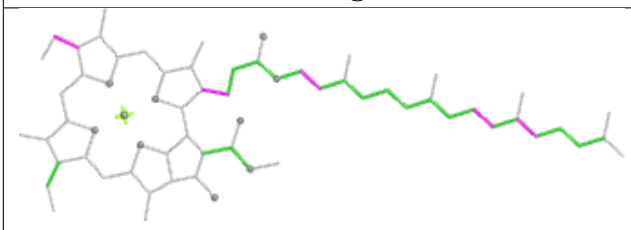
Ligand CLA C 514



Bond lengths



Bond angles



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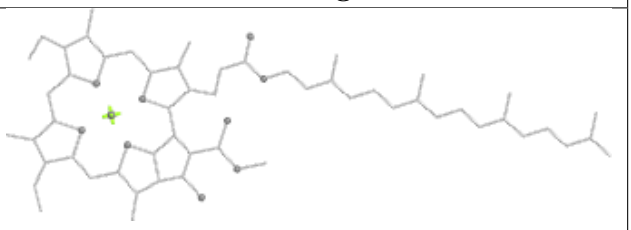
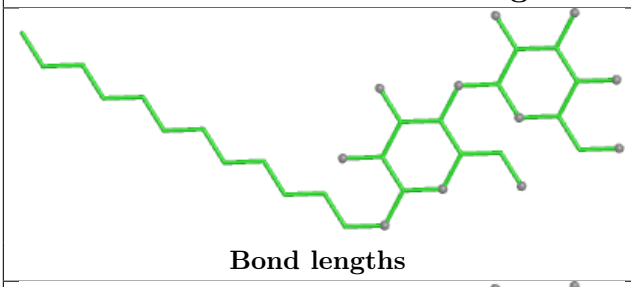
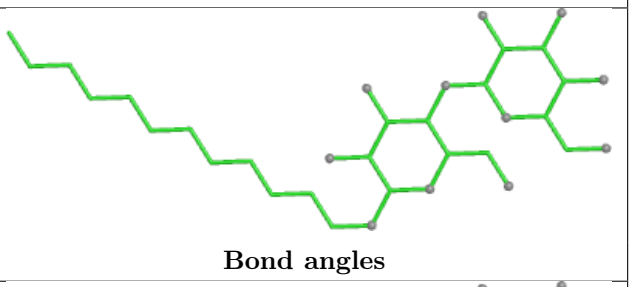
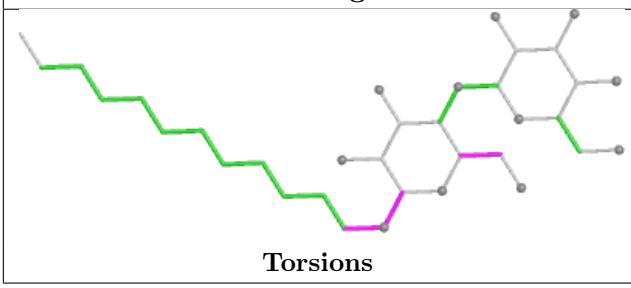


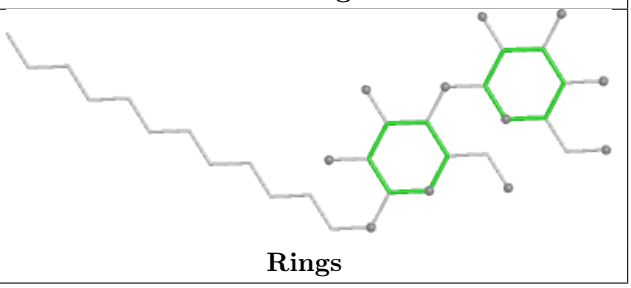
Rings

Ligand LMT m 2803

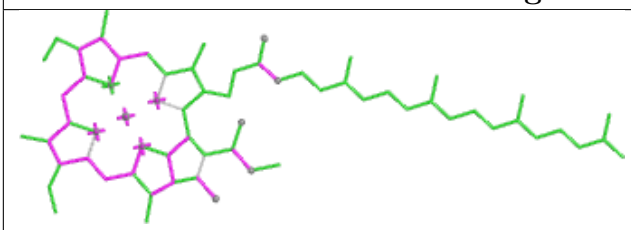

Bond lengths

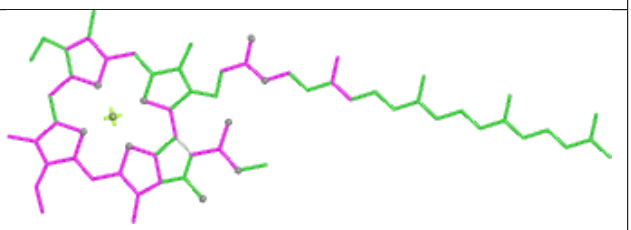

Bond angles

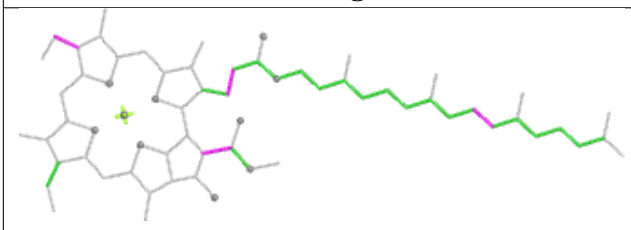

Torsions

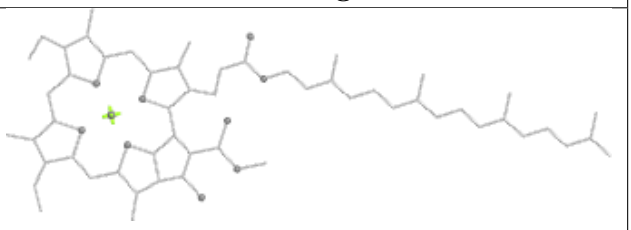

Rings

Ligand CLA B 607

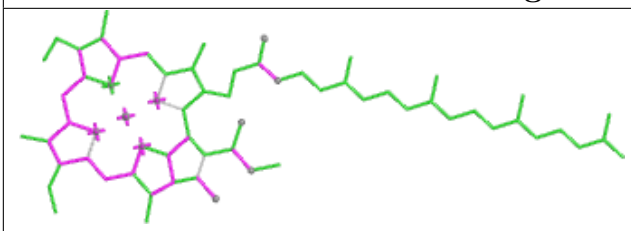

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA B 610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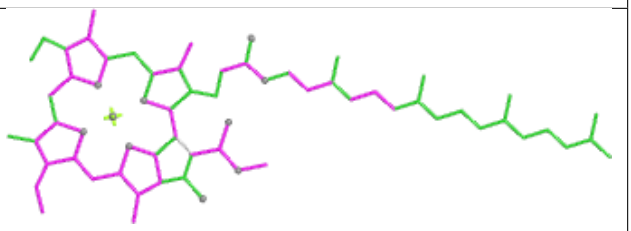
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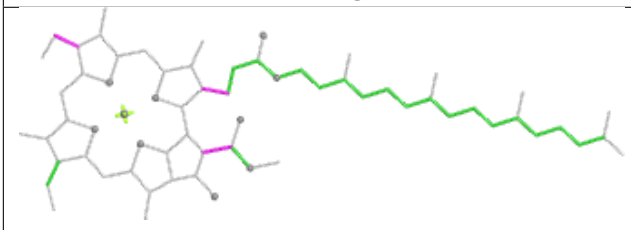
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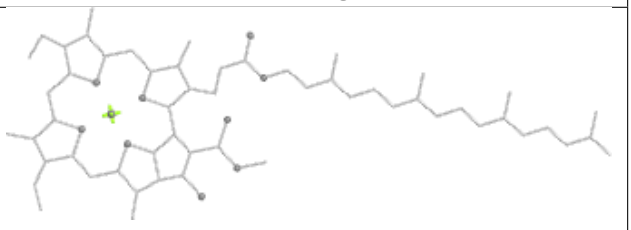
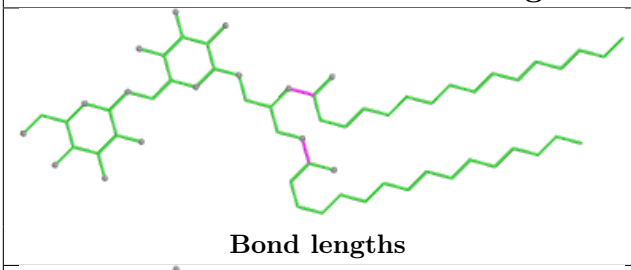

Rings

Ligand DGD c 518



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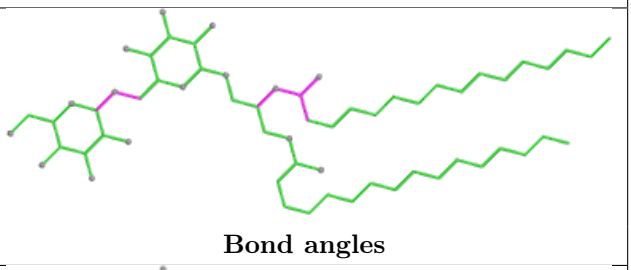

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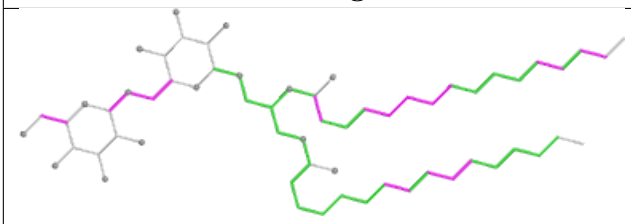

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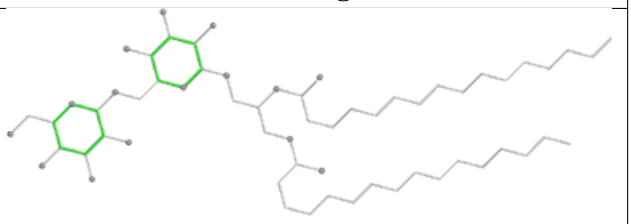
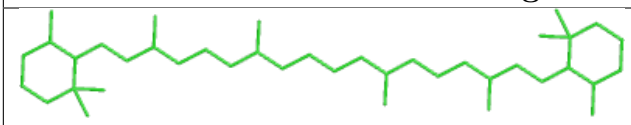


Rings

Ligand BCR A 411



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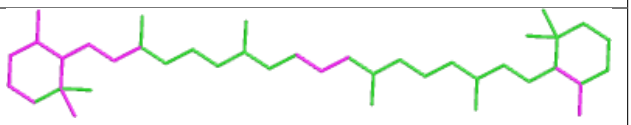
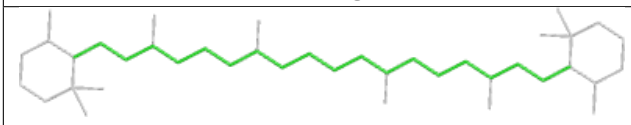


Bond angles



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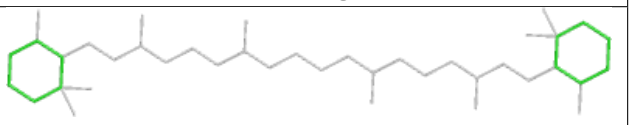
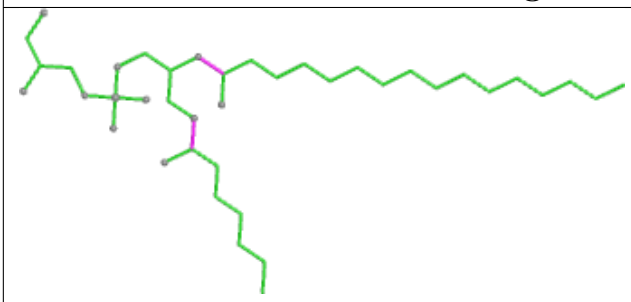


Rings

Ligand LHG E 101



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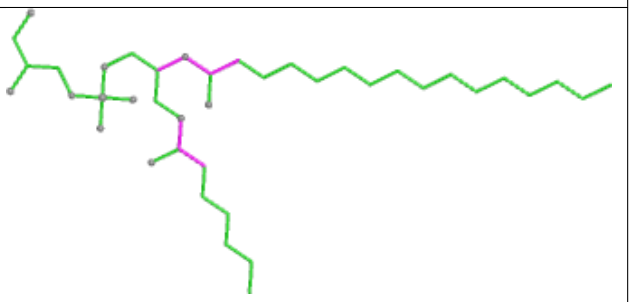

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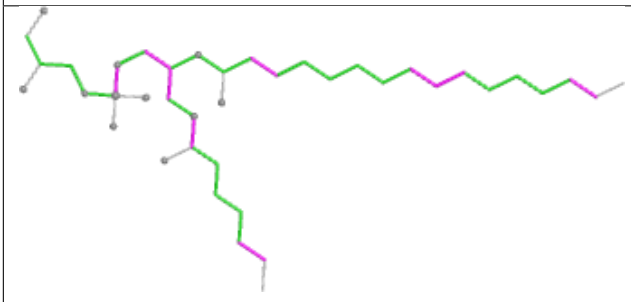

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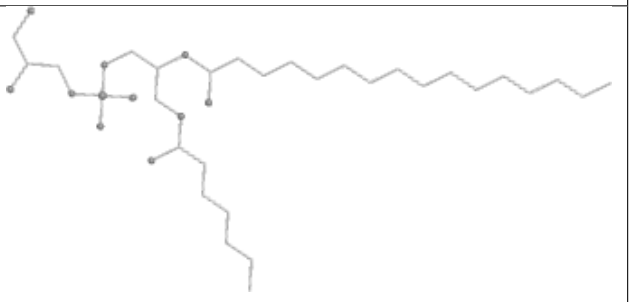
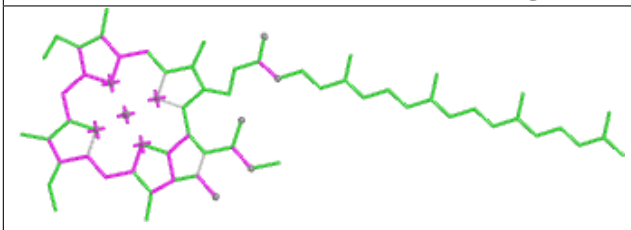


Rings

Ligand CLA B 615



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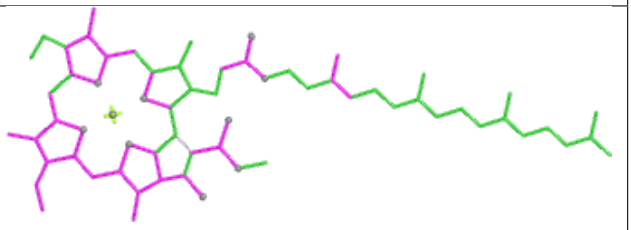
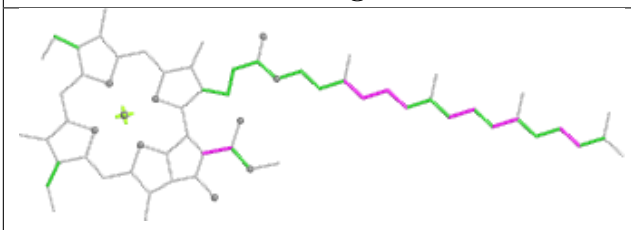


Bond angles



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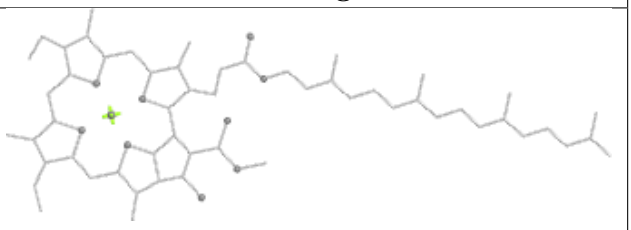

Rings

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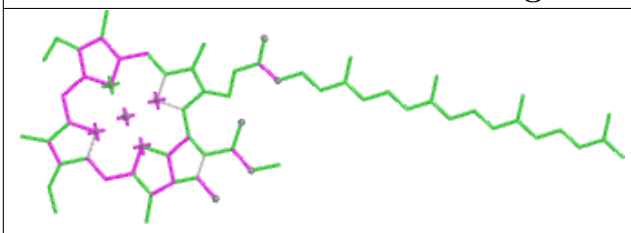

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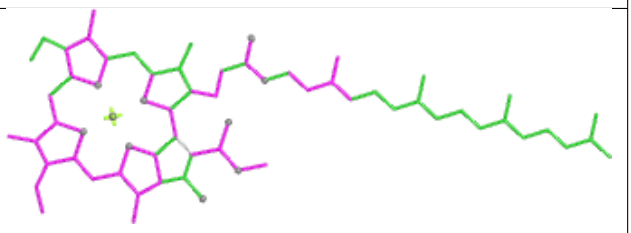
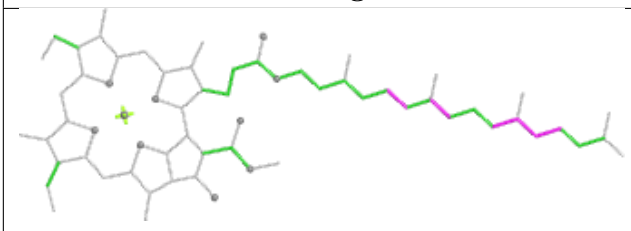


Bond angles



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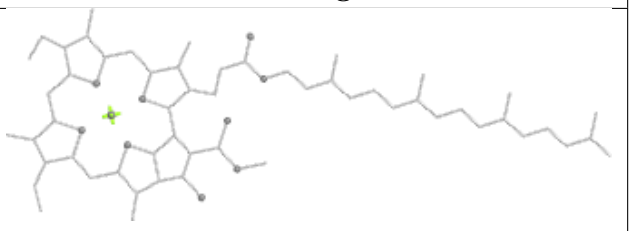
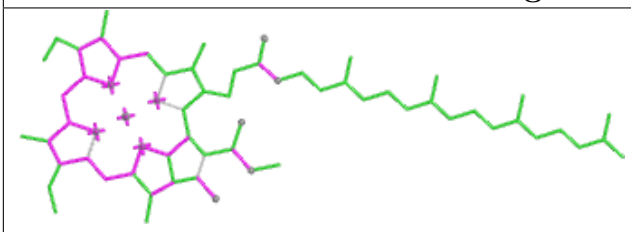


Rings

Ligand CLA C 503



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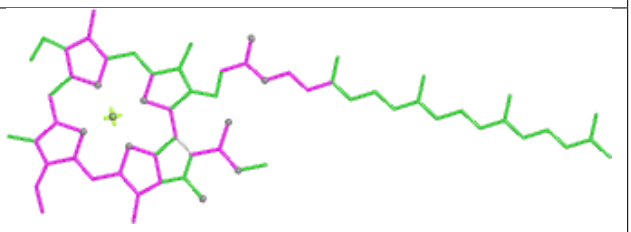
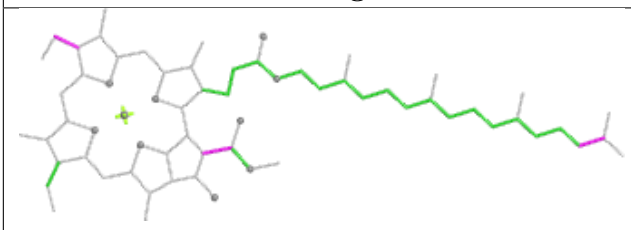


Bond angles



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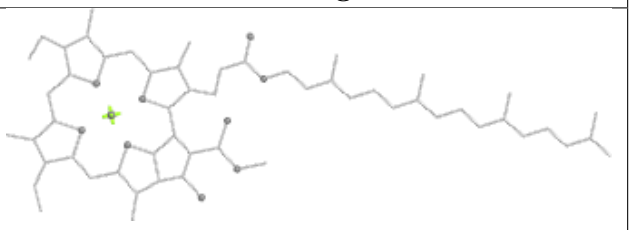
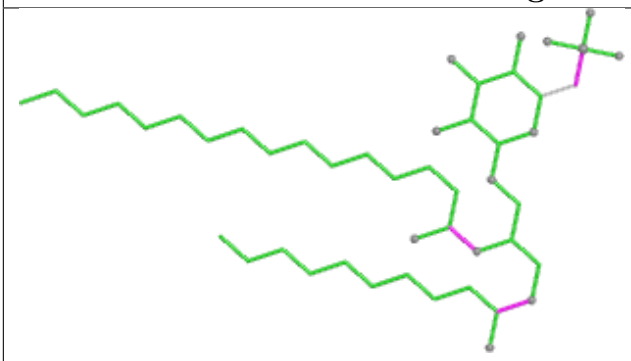


Rings

Ligand SQD b 601



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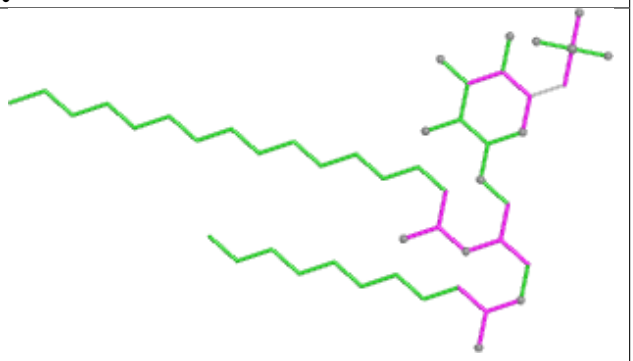
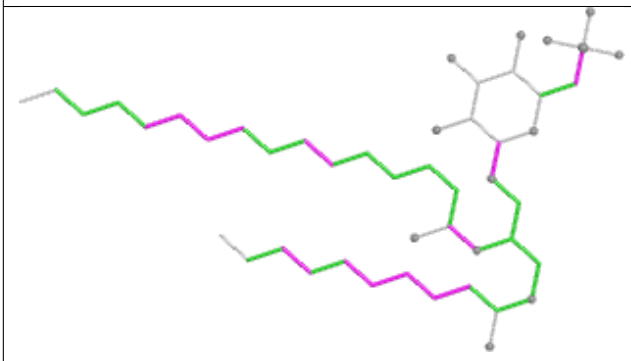


Bond angles



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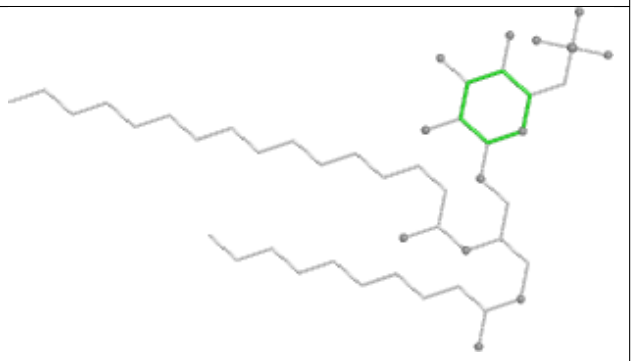
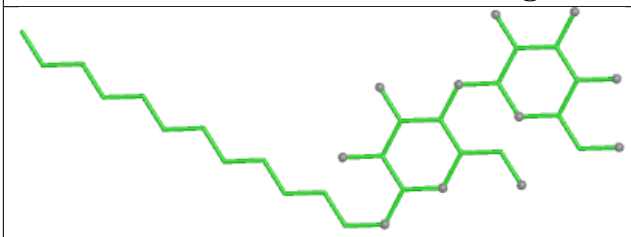


Rings

Ligand LMT B 623



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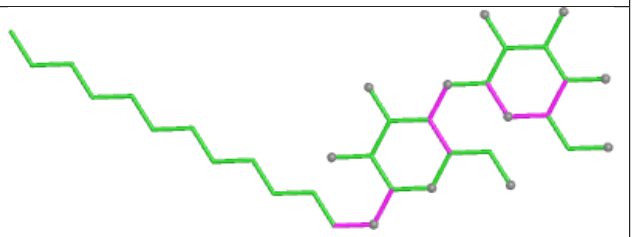
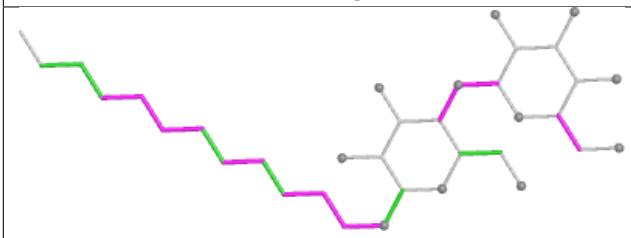


Bond angles



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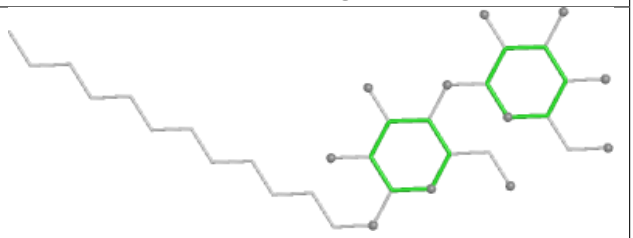
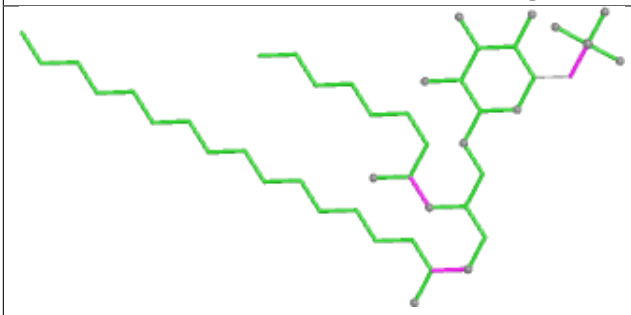


Rings

Ligand SQD A 412



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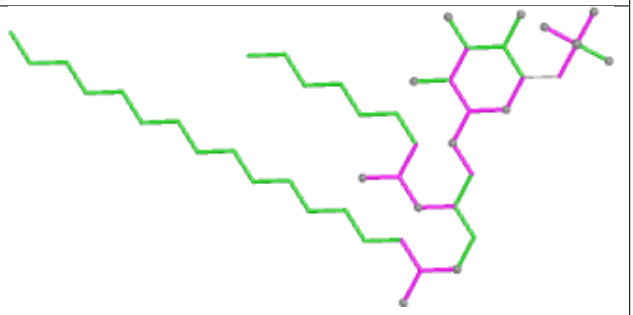
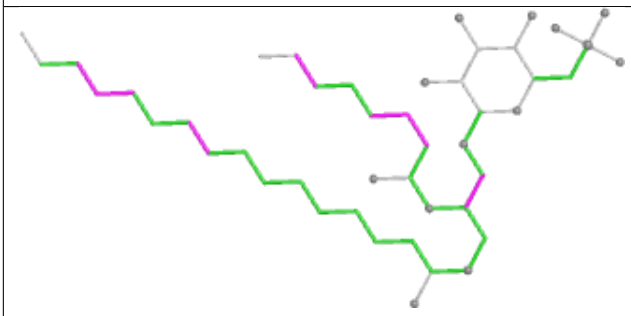


Bond angles



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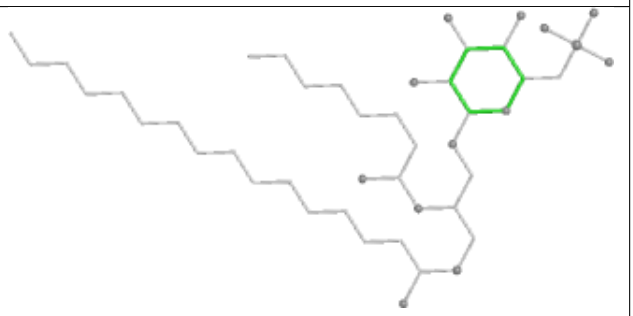
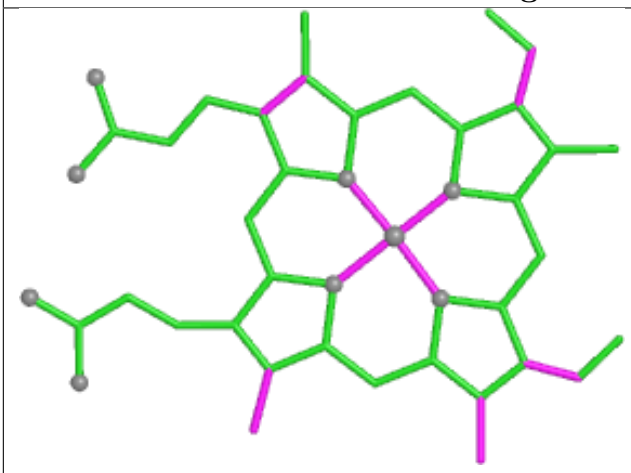


Rings

Ligand HEM F 101



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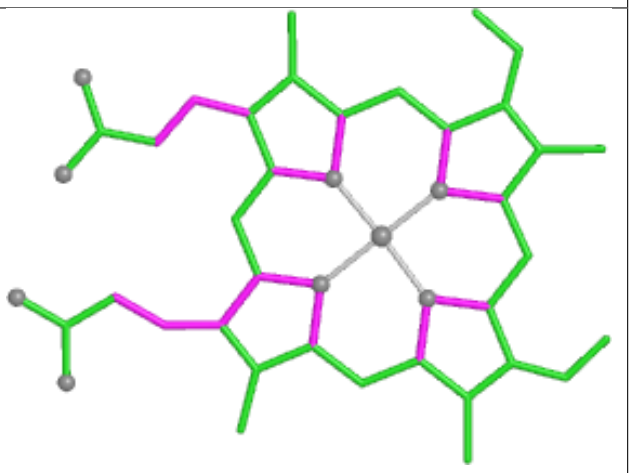
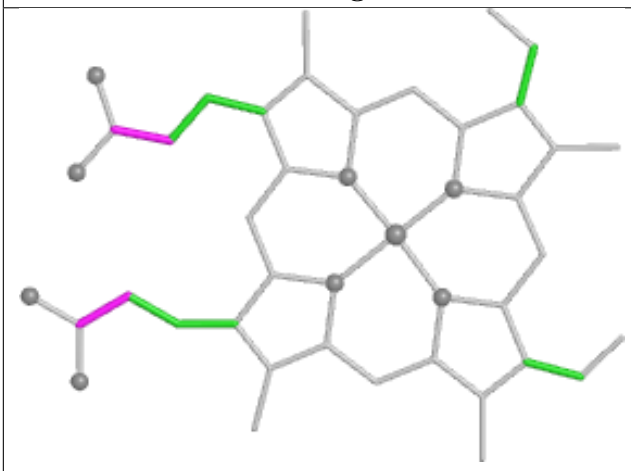


Bond angles



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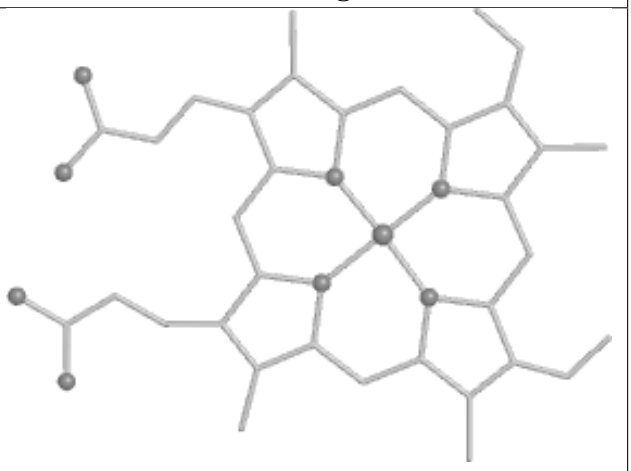
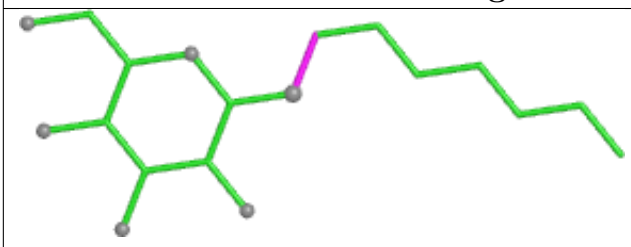


Rings

Ligand HTG B 624 (B)



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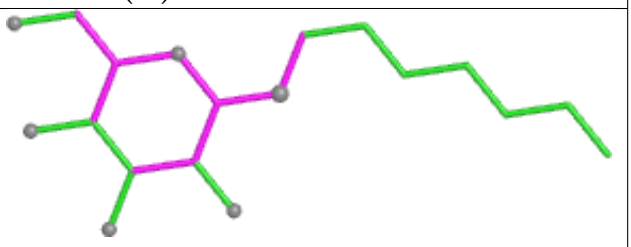
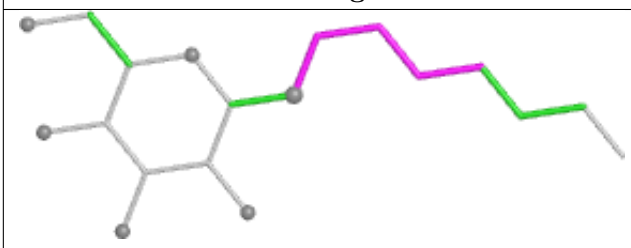


Bond angles



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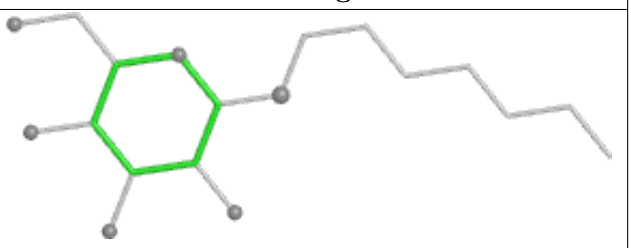
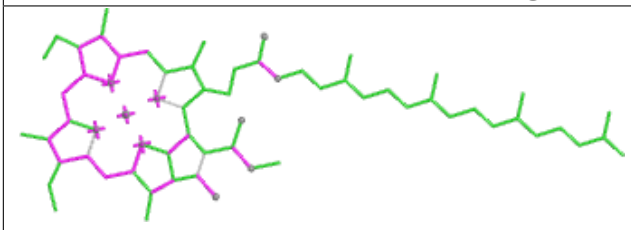


Rings

Ligand CLA C 509



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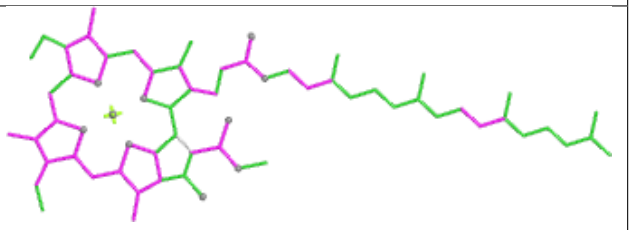
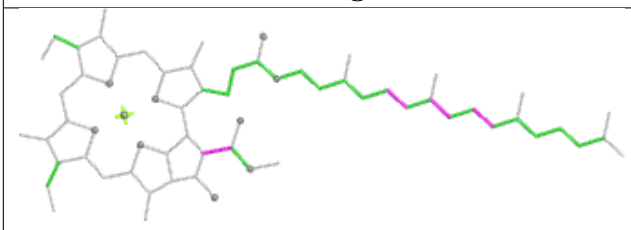


Bond angles



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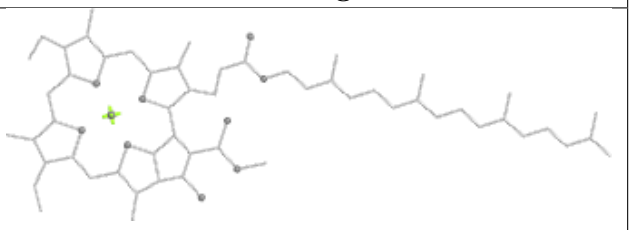
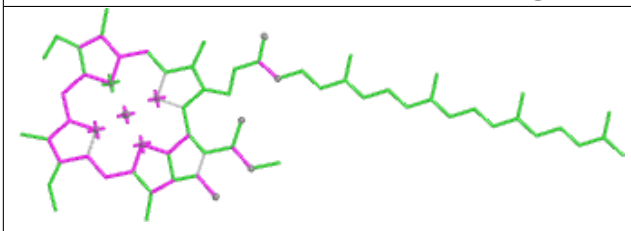
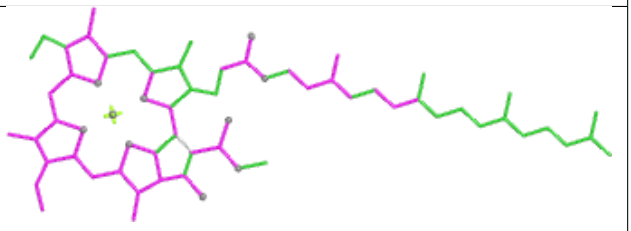


Rings

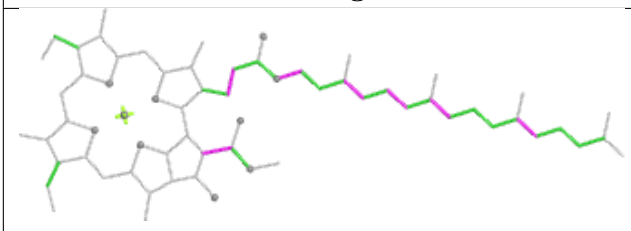
Ligand CLA c 510



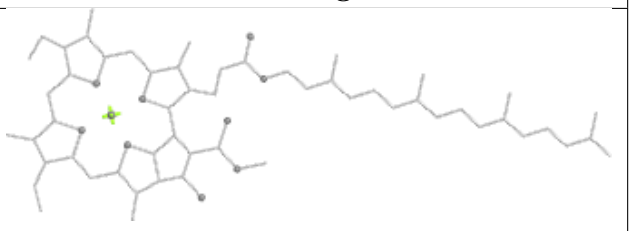
Bond lengths



Bond angles

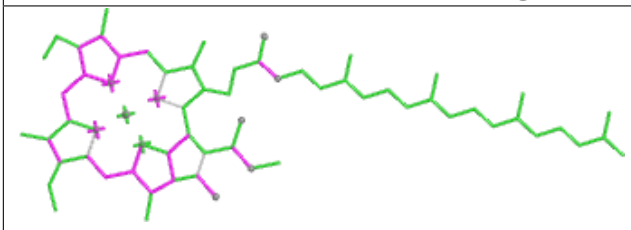


Torsions

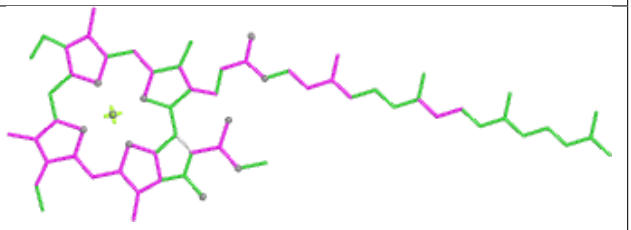


Rings

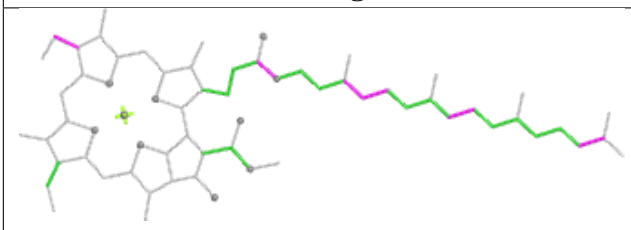
Ligand CLA D 2304



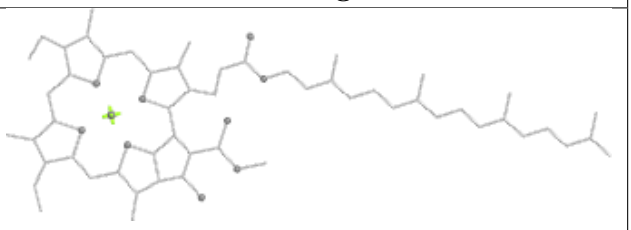
Bond lengths



Bond angles

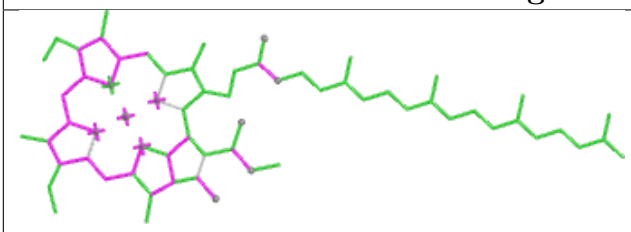


Torsions

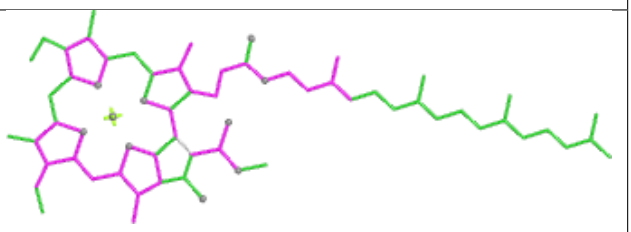


Rings

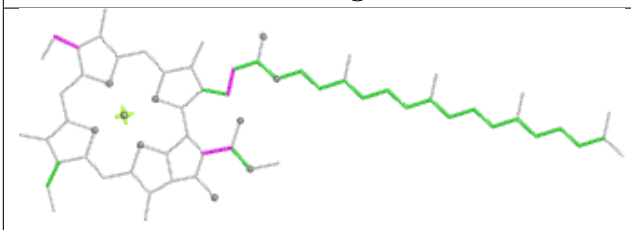
Ligand CLA b 607



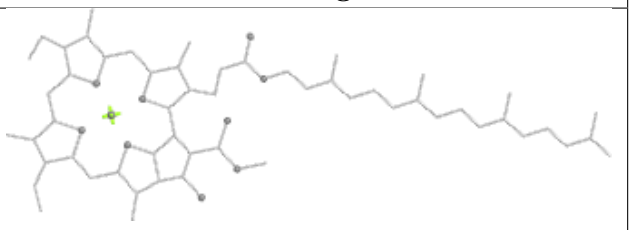
Bond lengths



Bond angles

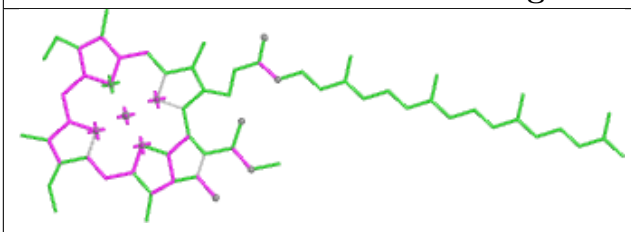


Torsions

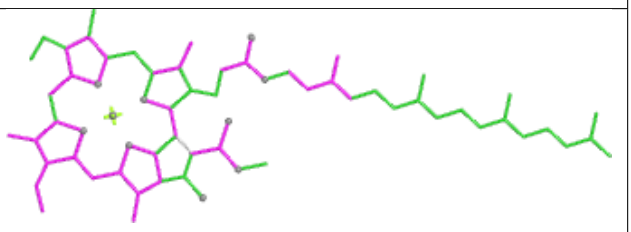


Rings

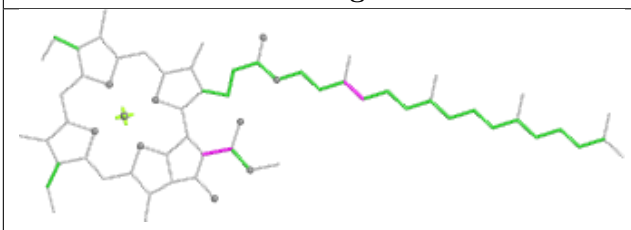
Ligand CLA b 610



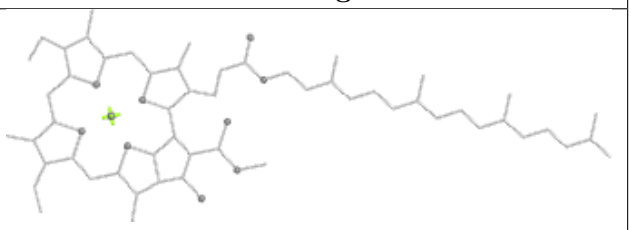
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.28	5 (1%)	72	76	30, 46, 86, 139	3 (0%)
1	a	334/344 (97%)	-0.24	9 (2%)	56	60	27, 47, 87, 143	5 (1%)
2	B	505/505 (100%)	-0.26	8 (1%)	70	74	28, 52, 92, 138	7 (1%)
2	b	483/505 (95%)	-0.21	4 (0%)	82	84	33, 53, 83, 143	9 (1%)
3	C	451/455 (99%)	-0.18	4 (0%)	81	83	39, 59, 83, 164	2 (0%)
3	c	455/455 (100%)	-0.16	2 (0%)	88	90	45, 61, 81, 136	0
4	D	340/342 (99%)	-0.35	2 (0%)	85	87	24, 49, 75, 113	1 (0%)
4	d	341/342 (99%)	-0.32	1 (0%)	90	91	26, 50, 77, 138	2 (0%)
5	E	80/83 (96%)	0.31	7 (8%)	15	17	50, 76, 128, 144	1 (1%)
5	e	79/83 (95%)	0.39	5 (6%)	26	29	46, 78, 124, 137	1 (1%)
6	F	34/44 (77%)	-0.12	2 (5%)	28	32	52, 64, 114, 124	0
6	f	32/44 (72%)	0.22	4 (12%)	8	8	53, 66, 119, 132	0
7	H	63/63 (100%)	0.12	3 (4%)	35	40	53, 69, 85, 111	0
7	h	63/63 (100%)	0.41	1 (1%)	70	74	48, 72, 89, 117	1 (1%)
8	I	31/38 (81%)	0.75	6 (19%)	3	4	53, 71, 146, 152	0
8	i	31/38 (81%)	0.51	4 (12%)	7	8	51, 67, 129, 137	0
9	J	36/40 (90%)	-0.07	1 (2%)	55	59	48, 67, 111, 135	0
9	j	39/40 (97%)	0.05	1 (2%)	57	61	55, 68, 131, 162	0
10	K	37/37 (100%)	-0.24	0	100	100	43, 67, 84, 92	1 (2%)
10	k	37/37 (100%)	0.03	0	100	100	58, 69, 95, 114	0
11	L	37/37 (100%)	-0.24	1 (2%)	56	60	24, 45, 88, 153	1 (2%)
11	l	36/37 (97%)	-0.31	0	100	100	25, 45, 102, 158	2 (5%)
12	M	32/36 (88%)	-0.41	0	100	100	27, 47, 66, 106	2 (6%)
12	m	33/36 (91%)	-0.21	1 (3%)	52	56	27, 49, 100, 129	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.15	2 (0%)	82	84	33, 60, 104, 154	3 (1%)
13	o	243/244 (99%)	-0.12	1 (0%)	88	90	31, 60, 108, 162	4 (1%)
14	T	29/32 (90%)	-0.25	1 (3%)	48	52	39, 46, 82, 150	0
14	t	29/32 (90%)	-0.22	1 (3%)	48	52	40, 46, 80, 129	0
15	U	97/104 (93%)	-0.23	2 (2%)	63	67	43, 55, 86, 105	1 (1%)
15	u	97/104 (93%)	-0.19	0	100	100	49, 58, 80, 136	0
16	V	137/137 (100%)	-0.26	0	100	100	36, 54, 80, 100	1 (0%)
16	v	137/137 (100%)	-0.17	1 (0%)	84	85	40, 66, 91, 110	1 (0%)
17	Y	30/30 (100%)	0.33	1 (3%)	49	53	70, 83, 113, 124	0
17	y	30/30 (100%)	0.34	1 (3%)	49	53	75, 88, 105, 136	0
18	X	38/40 (95%)	0.22	1 (2%)	57	61	66, 79, 111, 122	0
18	x	35/40 (87%)	0.20	2 (5%)	29	33	44, 80, 122, 134	1 (2%)
19	Z	61/62 (98%)	0.18	2 (3%)	49	53	66, 81, 124, 140	0
19	z	60/62 (96%)	0.49	4 (6%)	24	27	75, 88, 132, 159	0
All	All	5210/5346 (97%)	-0.16	90 (1%)	69	73	24, 56, 97, 164	50 (0%)

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	61	VAL	4.2
2	B	479	PHE	4.1
8	I	28	PRO	4.1
8	i	28	PRO	4.0
5	e	6	GLY	4.0

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	0.11	114,129,141,143	0
19	FME	Z	1	10/11	0.90	0.12	96,112,117,118	0
14	FME	T	1	10/11	0.94	0.09	48,54,84,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HSK	D	336[A]	10/12	0.96	0.08	49,51,51,51	7
4	HSK	D	336[B]	11/12	0.96	0.08	50,51,51,51	8
14	FME	t	1	10/11	0.96	0.08	46,51,77,79	0
12	FME	M	1	10/11	0.96	0.09	48,56,80,81	0
4	HSK	d	336[B]	11/12	0.97	0.08	51,56,59,62	8
8	FME	i	1	10/11	0.97	0.06	52,60,62,64	0
12	FME	m	1	10/11	0.97	0.08	43,57,81,84	0
8	FME	I	1	10/11	0.97	0.07	49,59,63,64	0
4	HSK	d	336[A]	10/12	0.97	0.08	51,56,59,60	7

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
29	GOL	E	104	6/6	0.56	0.13	124,126,128,129	0
34	DMS	X	101	4/4	0.56	0.17	172,174,175,175	0
34	DMS	A	425	4/4	0.58	0.25	152,153,153,155	0
34	DMS	O	308	4/4	0.61	0.21	124,127,127,132	0
34	DMS	U	504	4/4	0.62	0.22	119,124,127,129	0
34	DMS	C	534	4/4	0.63	0.25	141,141,143,143	0
34	DMS	v	210	4/4	0.64	0.22	137,140,140,143	0
34	DMS	c	542	4/4	0.65	0.27	148,149,150,151	0
34	DMS	o	309	4/4	0.65	0.27	131,139,139,141	0
34	DMS	B	645	4/4	0.65	0.17	124,125,125,127	0
34	DMS	o	310	4/4	0.66	0.22	144,147,149,149	0
34	DMS	c	546	4/4	0.67	0.23	151,153,154,154	0
34	DMS	a	2624	4/4	0.67	0.25	79,105,106,109	0
34	DMS	B	642	4/4	0.68	0.24	95,106,108,114	0
34	DMS	c	541	4/4	0.68	0.29	121,128,129,132	0
34	DMS	c	549	4/4	0.68	0.20	124,126,128,128	0
34	DMS	H	104	4/4	0.69	0.17	129,131,133,133	0
30	UNL	j	2702	16/-	0.69	0.23	89,96,108,111	0
30	UNL	a	2616	27/-	0.70	0.19	86,103,140,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	GOL	v	202	6/6	0.70	0.12	113,114,116,118	0
34	DMS	O	311	4/4	0.72	0.33	130,135,136,138	0
34	DMS	C	537	4/4	0.72	0.19	143,143,144,146	0
34	DMS	d	420	4/4	0.72	0.16	121,122,123,124	0
38	LHG	e	101	40/49	0.72	0.18	93,156,201,202	0
29	GOL	O	304	6/6	0.73	0.17	86,101,103,106	0
34	DMS	C	535	4/4	0.73	0.22	109,109,110,112	0
29	GOL	b	631	6/6	0.74	0.15	84,100,106,106	0
34	DMS	l	104	4/4	0.74	0.18	134,136,139,140	0
37	DGD	D	2307	53/66	0.74	0.21	96,121,171,177	0
30	UNL	A	416	28/-	0.74	0.18	93,104,133,143	0
34	DMS	b	640	4/4	0.75	0.20	110,112,115,117	0
30	UNL	E	103	9/-	0.75	0.21	75,83,107,110	0
30	UNL	i	101	19/-	0.76	0.14	88,112,144,146	0
34	DMS	B	640	4/4	0.76	0.35	154,155,156,157	0
30	UNL	c	527	12/-	0.76	0.33	104,113,125,126	0
34	DMS	V	211	4/4	0.76	0.19	109,112,114,114	0
30	UNL	k	301	16/-	0.76	0.27	89,109,125,126	0
34	DMS	v	212	4/4	0.76	0.19	133,135,138,138	0
34	DMS	c	547	4/4	0.76	0.23	132,138,140,141	0
34	DMS	a	2620	4/4	0.76	0.19	142,146,149,151	0
34	DMS	c	548	4/4	0.77	0.17	123,130,130,130	0
30	UNL	b	627	15/-	0.77	0.21	90,97,113,114	0
30	UNL	b	629	8/-	0.77	0.22	72,94,106,108	0
28	LMT	j	2701	34/35	0.77	0.15	79,145,158,159	0
34	DMS	V	213	4/4	0.77	0.23	115,118,119,120	0
34	DMS	B	646	4/4	0.78	0.17	94,96,102,107	0
34	DMS	O	319	4/4	0.78	0.18	131,134,135,136	0
34	DMS	v	214	4/4	0.78	0.17	131,135,135,136	0
36	HTG	B	624[A]	19/19	0.78	0.19	56,72,85,87	19
36	HTG	B	624[B]	19/19	0.78	0.19	57,72,86,88	19
36	HTG	C	522	19/19	0.78	0.16	88,124,137,140	0
36	HTG	i	102	19/19	0.78	0.13	68,143,157,158	0
34	DMS	d	422	4/4	0.78	0.19	118,121,124,128	0
34	DMS	o	316	4/4	0.78	0.22	85,101,104,108	0
34	DMS	B	637	4/4	0.79	0.19	121,124,125,126	0
34	DMS	O	307	4/4	0.79	0.21	98,107,107,110	0
30	UNL	B	629	15/-	0.79	0.24	90,105,111,112	0
28	LMT	F	102	24/35	0.79	0.17	114,127,159,161	0
36	HTG	d	407	19/19	0.79	0.15	102,133,146,148	0
34	DMS	O	317	4/4	0.79	0.25	114,115,117,120	0
34	DMS	O	318	4/4	0.79	0.28	115,117,119,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	A	427	4/4	0.79	0.21	103,106,107,108	0
34	DMS	O	314	4/4	0.80	0.17	117,121,126,133	0
34	DMS	B	643	4/4	0.80	0.18	99,101,107,111	0
36	HTG	B	627	19/19	0.80	0.16	67,130,145,148	0
34	DMS	c	537	4/4	0.80	0.20	116,122,123,125	0
36	HTG	V	204	19/19	0.80	0.16	71,95,125,126	0
34	DMS	O	309	4/4	0.80	0.19	117,118,118,120	0
34	DMS	v	211	4/4	0.80	0.17	120,122,123,123	0
29	GOL	V	203	6/6	0.80	0.13	98,111,118,123	0
34	DMS	T	104	4/4	0.80	0.25	156,160,160,161	0
30	UNL	b	632	10/-	0.81	0.15	83,93,104,105	0
34	DMS	C	536	4/4	0.81	0.17	134,137,138,140	0
34	DMS	c	543	4/4	0.81	0.15	116,121,122,123	0
28	LMT	m	2804	35/35	0.81	0.18	79,146,162,166	0
34	DMS	o	311	4/4	0.81	0.19	86,101,102,104	0
34	DMS	o	315	4/4	0.81	0.32	135,137,138,138	0
30	UNL	D	2313	12/-	0.81	0.22	93,112,114,115	0
34	DMS	A	429	4/4	0.81	0.25	128,129,130,132	0
34	DMS	B	635	4/4	0.81	0.23	130,132,133,133	0
29	GOL	O	305	6/6	0.81	0.17	70,91,97,105	0
30	UNL	c	525	6/-	0.82	0.26	95,97,98,101	0
30	UNL	C	501	40/-	0.82	0.19	102,120,136,139	0
29	GOL	c	529	6/6	0.82	0.11	124,131,132,133	0
29	GOL	c	530	6/6	0.82	0.11	79,107,118,124	0
29	GOL	d	416	6/6	0.82	0.13	129,131,132,133	0
28	LMT	A	414	33/35	0.82	0.17	72,117,128,135	0
29	GOL	J	301	6/6	0.82	0.14	100,103,110,111	0
34	DMS	O	313	4/4	0.82	0.20	103,110,110,111	0
34	DMS	A	428	4/4	0.82	0.24	118,118,118,120	0
34	DMS	O	316	4/4	0.82	0.16	107,108,109,110	0
36	HTG	H	101	17/19	0.82	0.17	109,127,151,151	0
34	DMS	o	305	4/4	0.82	0.18	117,117,119,120	0
36	HTG	b	625	19/19	0.82	0.17	58,83,106,108	0
29	GOL	D	2301	6/6	0.82	0.14	87,93,100,104	0
34	DMS	c	538	4/4	0.82	0.16	136,137,139,141	0
34	DMS	c	539	4/4	0.82	0.19	110,112,114,119	0
34	DMS	o	313	4/4	0.82	0.19	100,102,103,111	0
41	MG	K	102	1/1	0.82	0.15	85,85,85,85	0
34	DMS	C	528	4/4	0.83	0.20	110,114,115,117	0
30	UNL	b	628	10/-	0.83	0.23	94,111,114,116	0
34	DMS	o	306	4/4	0.83	0.28	118,119,124,125	0
26	SQD	D	2308	45/54	0.83	0.14	92,119,145,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	JOX	A	418	10/10	0.83	0.14	65,87,88,94	0
36	HTG	C	525	19/19	0.83	0.12	91,137,156,156	0
34	DMS	O	315	4/4	0.83	0.13	107,114,115,121	0
28	LMT	d	401	35/35	0.83	0.18	63,106,125,130	0
34	DMS	o	314	4/4	0.83	0.18	112,113,117,118	0
30	UNL	I	102	40/-	0.83	0.15	101,119,151,152	0
34	DMS	b	637	4/4	0.83	0.15	89,107,109,112	0
29	GOL	c	531	6/6	0.83	0.11	116,118,119,120	0
38	LHG	E	101	40/49	0.83	0.15	94,137,163,165	0
34	DMS	b	642	4/4	0.83	0.15	153,154,156,159	0
28	LMT	d	404	25/35	0.83	0.19	91,129,162,164	0
28	LMT	f	101	24/35	0.84	0.13	102,124,156,160	0
30	UNL	C	523	10/-	0.84	0.21	99,101,107,112	0
36	HTG	B	625	19/19	0.84	0.15	77,130,138,140	19
29	GOL	u	501	6/6	0.84	0.16	84,92,98,102	0
34	DMS	c	540	4/4	0.84	0.18	111,115,116,117	0
28	LMT	J	303	24/35	0.84	0.16	80,95,144,147	0
29	GOL	v	204	6/6	0.84	0.15	92,115,115,123	0
34	DMS	A	430	4/4	0.84	0.20	115,127,127,130	0
30	UNL	e	102	15/-	0.84	0.17	74,93,101,101	0
36	HTG	c	523	19/19	0.84	0.12	99,121,130,133	0
30	UNL	a	2601	15/-	0.84	0.20	79,86,93,96	0
29	GOL	U	501	6/6	0.84	0.15	105,111,113,115	0
28	LMT	T	103	24/35	0.84	0.17	58,91,129,132	0
34	DMS	b	643	4/4	0.84	0.18	125,131,133,136	0
34	DMS	c	532	4/4	0.84	0.20	87,89,96,102	0
34	DMS	d	423	4/4	0.84	0.16	133,137,137,140	0
41	MG	k	303	1/1	0.84	0.15	91,91,91,91	0
29	GOL	B	632	6/6	0.85	0.17	87,96,98,101	0
30	UNL	b	630	21/-	0.85	0.14	56,79,122,124	0
23	CLA	B	602	65/65	0.85	0.12	58,83,121,131	0
34	DMS	V	208	4/4	0.85	0.15	99,108,109,113	0
27	LMG	c	522	51/55	0.85	0.14	65,117,127,130	0
34	DMS	o	308	4/4	0.85	0.14	127,131,133,135	0
34	DMS	V	212	4/4	0.85	0.16	98,111,112,115	0
34	DMS	B	647	4/4	0.85	0.20	105,106,112,112	0
26	SQD	D	2302	54/54	0.85	0.17	75,106,174,176	0
29	GOL	O	302	6/6	0.85	0.11	78,82,87,91	0
34	DMS	c	544	4/4	0.85	0.13	105,110,113,115	0
36	HTG	c	524	19/19	0.85	0.14	62,108,119,121	19
36	HTG	c	526	19/19	0.85	0.14	120,165,175,175	0
30	UNL	B	628	18/-	0.85	0.17	85,96,116,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	b	636	4/4	0.85	0.16	101,102,104,106	0
34	DMS	t	102	4/4	0.85	0.21	129,132,137,137	0
34	DMS	v	208	4/4	0.85	0.17	125,126,127,129	0
29	GOL	O	303	6/6	0.85	0.13	96,106,114,114	0
28	LMT	B	634	35/35	0.85	0.16	55,133,160,162	0
34	DMS	D	2320	4/4	0.85	0.17	144,144,144,147	0
34	DMS	V	207	4/4	0.86	0.17	137,139,141,141	0
30	UNL	B	631	32/-	0.86	0.15	66,97,116,117	0
34	DMS	o	307	4/4	0.86	0.22	104,107,109,111	0
30	UNL	Y	301	12/-	0.86	0.20	114,116,120,121	0
34	DMS	B	641	4/4	0.86	0.12	93,102,102,104	0
30	UNL	c	502	36/-	0.86	0.18	91,115,128,130	0
34	DMS	D	2319	4/4	0.86	0.15	104,105,107,118	0
29	GOL	B	630	6/6	0.86	0.14	94,104,109,117	0
28	LMT	m	2803	35/35	0.86	0.14	61,101,118,121	0
36	HTG	b	626	19/19	0.86	0.14	98,151,158,158	0
34	DMS	b	635	4/4	0.86	0.21	98,102,105,109	0
28	LMT	z	102	33/35	0.86	0.15	80,141,156,157	0
30	UNL	E	102	6/-	0.86	0.16	83,87,87,89	0
34	DMS	b	638	4/4	0.86	0.24	159,163,163,165	0
34	DMS	v	209	4/4	0.86	0.16	82,93,96,102	0
34	DMS	T	105	4/4	0.86	0.20	124,129,130,130	0
29	GOL	v	203	6/6	0.86	0.14	81,87,91,92	0
34	DMS	U	505	4/4	0.86	0.18	66,72,89,105	0
34	DMS	v	213	4/4	0.86	0.14	119,119,119,123	0
34	DMS	V	206	4/4	0.86	0.14	81,98,100,101	0
25	BCR	T	102	40/40	0.87	0.11	44,56,82,85	0
29	GOL	a	2618	6/6	0.87	0.13	107,112,115,116	0
26	SQD	d	417	33/54	0.87	0.14	100,120,146,151	0
36	HTG	I	101	19/19	0.87	0.11	83,126,141,145	0
34	DMS	u	502	4/4	0.87	0.24	127,129,129,131	0
36	HTG	b	604	19/19	0.87	0.13	79,131,144,147	0
34	DMS	u	504	4/4	0.87	0.16	74,90,95,98	0
26	SQD	l	101	54/54	0.87	0.15	59,88,126,130	0
27	LMG	C	520	51/55	0.87	0.17	59,91,107,114	0
34	DMS	D	2317	4/4	0.87	0.19	99,105,106,109	0
30	UNL	A	423	9/-	0.87	0.20	84,89,93,94	0
31	JOX	A	419	10/10	0.87	0.13	60,69,76,78	0
33	PL9	A	422	39/55	0.87	0.21	88,101,124,127	0
34	DMS	O	306	4/4	0.87	0.25	146,150,150,153	0
27	LMG	C	527	51/55	0.87	0.15	71,123,148,152	0
30	UNL	T	101	13/-	0.87	0.23	93,100,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	LMT	M	101	35/35	0.87	0.16	84,157,181,181	0
34	DMS	b	641	4/4	0.87	0.16	75,76,78,84	4
28	LMT	Z	101	35/35	0.88	0.14	68,142,184,187	0
30	UNL	J	304	5/-	0.88	0.23	97,98,103,104	0
26	SQD	b	601	48/54	0.88	0.14	66,96,152,156	0
34	DMS	C	531	4/4	0.88	0.17	98,102,103,107	0
28	LMT	M	102	35/35	0.88	0.12	59,106,136,139	0
26	SQD	a	2603	54/54	0.88	0.15	55,89,136,138	0
34	DMS	U	503	4/4	0.88	0.23	118,119,119,120	0
36	HTG	d	415	19/19	0.88	0.18	80,117,124,125	19
34	DMS	O	310	4/4	0.88	0.17	103,103,103,108	0
33	PL9	x	1301	39/55	0.88	0.20	94,113,131,132	0
34	DMS	v	207	4/4	0.88	0.17	107,110,111,114	0
29	GOL	U	502	6/6	0.88	0.14	73,82,89,97	0
28	LMT	i	103	24/35	0.88	0.15	67,119,153,155	0
29	GOL	o	303	6/6	0.88	0.14	71,83,104,109	0
29	GOL	b	644	6/6	0.89	0.21	75,97,105,105	0
28	LMT	B	623	35/35	0.89	0.12	89,122,148,149	0
30	UNL	m	2801	15/-	0.89	0.18	68,85,119,123	0
23	CLA	b	606	65/65	0.89	0.13	66,88,129,133	0
29	GOL	a	2602	6/6	0.89	0.19	64,79,91,91	0
30	UNL	d	405	37/-	0.89	0.18	74,101,137,137	0
26	SQD	B	621	54/54	0.89	0.14	60,92,128,131	0
29	GOL	C	524	6/6	0.89	0.11	101,110,113,118	0
34	DMS	d	419	4/4	0.90	0.17	92,94,98,106	0
29	GOL	A	415	6/6	0.90	0.19	72,80,92,93	0
30	UNL	l	102	16/-	0.90	0.17	67,90,115,121	0
25	BCR	B	633	40/40	0.90	0.11	46,62,78,79	0
34	DMS	A	426	4/4	0.90	0.18	94,103,103,114	0
34	DMS	C	530	4/4	0.90	0.19	115,117,118,123	0
30	UNL	t	101	8/-	0.90	0.20	75,84,103,103	0
34	DMS	v	206	4/4	0.90	0.16	84,102,103,104	0
27	LMG	c	501	51/55	0.90	0.15	67,90,101,105	0
30	UNL	c	528	5/-	0.90	0.17	87,89,97,97	0
34	DMS	a	2622	4/4	0.90	0.15	105,107,110,115	0
34	DMS	c	534	4/4	0.90	0.20	142,143,143,144	0
34	DMS	V	202	4/4	0.90	0.20	115,124,124,124	0
30	UNL	D	2314	18/-	0.91	0.13	67,79,113,117	0
34	DMS	d	418	4/4	0.91	0.24	98,99,100,111	0
23	CLA	C	507	65/65	0.91	0.11	57,81,109,112	0
34	DMS	c	535	4/4	0.91	0.20	108,108,110,114	0
34	DMS	u	503	4/4	0.91	0.18	81,101,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	x	1302	18/-	0.91	0.13	76,86,120,124	0
29	GOL	A	417	6/6	0.91	0.13	110,113,118,126	0
34	DMS	O	312	4/4	0.91	0.14	108,109,110,113	0
40	RRX	h	101	41/41	0.91	0.13	56,81,103,119	0
28	LMT	A	420	24/35	0.91	0.14	63,104,142,148	0
36	HTG	B	626	19/19	0.91	0.13	64,93,111,116	0
27	LMG	A	413	51/55	0.92	0.13	64,82,106,110	0
27	LMG	m	2802	51/55	0.92	0.14	56,81,98,107	0
23	CLA	B	617	65/65	0.92	0.12	49,59,122,126	0
34	DMS	a	2621	4/4	0.92	0.18	115,115,116,118	0
36	HTG	C	521	19/19	0.92	0.11	108,112,121,121	0
34	DMS	a	2623	4/4	0.93	0.13	100,107,108,111	0
34	DMS	o	312	4/4	0.93	0.13	95,98,101,105	0
34	DMS	V	210	4/4	0.93	0.13	101,105,108,111	0
25	BCR	b	623	40/40	0.93	0.09	43,57,74,79	0
34	DMS	c	545	4/4	0.93	0.12	123,124,125,127	0
27	LMG	B	622	51/55	0.93	0.12	57,81,98,100	0
27	LMG	c	521	49/55	0.93	0.13	60,94,118,121	0
37	DGD	h	102	62/66	0.93	0.13	52,71,117,119	0
38	LHG	D	2309	49/49	0.93	0.12	50,63,78,81	0
23	CLA	b	619	65/65	0.93	0.12	41,49,109,113	0
38	LHG	d	412	49/49	0.93	0.12	55,66,79,85	0
36	HTG	b	603	19/19	0.93	0.12	70,89,107,110	0
34	DMS	B	644	4/4	0.93	0.12	82,82,86,88	0
31	JOX	a	2617	10/10	0.93	0.09	64,69,89,91	0
34	DMS	V	209	4/4	0.93	0.13	81,89,95,100	0
23	CLA	a	2613	65/65	0.94	0.11	39,48,130,137	0
25	BCR	C	516	40/40	0.94	0.10	54,66,87,91	0
34	DMS	d	421	4/4	0.94	0.13	75,89,94,98	0
26	SQD	a	2615	48/54	0.94	0.12	66,86,112,114	0
30	UNL	D	2315	18/-	0.94	0.15	65,90,111,113	0
25	BCR	D	2305	40/40	0.94	0.10	50,60,85,86	0
23	CLA	B	615	65/65	0.94	0.11	40,49,105,113	0
37	DGD	C	518	62/66	0.94	0.10	48,63,101,111	0
23	CLA	C	514	65/65	0.94	0.10	66,78,111,115	0
37	DGD	c	518	62/66	0.94	0.12	43,57,106,110	0
25	BCR	d	410	40/40	0.94	0.09	54,61,83,86	0
25	BCR	z	101	40/40	0.94	0.11	68,78,93,97	0
32	BCT	a	2608	4/4	0.94	0.14	56,61,66,74	0
26	SQD	A	412	46/54	0.94	0.11	76,88,106,108	0
36	HTG	b	602	19/19	0.94	0.11	56,64,79,79	0
40	RRX	H	102	41/41	0.94	0.10	48,75,95,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	d	406	18/-	0.94	0.17	70,93,104,106	0
23	CLA	c	509	65/65	0.94	0.11	57,76,111,115	0
23	CLA	c	516	65/65	0.94	0.09	61,79,103,108	0
31	JOX	a	2619	10/10	0.95	0.12	46,49,54,56	10
25	BCR	C	515	40/40	0.95	0.09	55,78,88,89	0
34	DMS	C	529	4/4	0.95	0.16	94,101,101,102	0
23	CLA	B	610	65/65	0.95	0.08	47,58,69,73	0
23	CLA	b	621	65/65	0.95	0.09	48,61,128,132	0
23	CLA	B	607	65/65	0.95	0.08	40,52,83,91	0
25	BCR	Y	302	40/40	0.95	0.08	55,64,70,71	0
25	BCR	a	2614	40/40	0.95	0.07	38,48,55,57	0
34	DMS	b	639	4/4	0.95	0.13	93,96,97,98	0
29	GOL	B	648	6/6	0.95	0.12	54,74,84,89	0
34	DMS	D	2316	4/4	0.95	0.11	65,77,86,90	0
23	CLA	c	515	65/65	0.95	0.10	60,71,101,105	0
36	HTG	o	301	19/19	0.95	0.11	62,70,85,87	0
29	GOL	C	526	6/6	0.95	0.12	65,81,89,93	0
25	BCR	c	517	40/40	0.95	0.09	52,66,87,89	0
37	DGD	H	103	62/66	0.95	0.12	51,69,100,104	0
23	CLA	C	513	65/65	0.95	0.09	62,75,115,122	0
37	DGD	c	519	62/66	0.95	0.11	52,65,112,125	0
34	DMS	B	639	4/4	0.95	0.14	84,84,91,92	0
34	DMS	c	536	4/4	0.95	0.13	64,74,76,78	0
38	LHG	D	2310	49/49	0.95	0.10	45,52,69,85	0
25	BCR	y	101	40/40	0.95	0.08	53,65,71,74	0
38	LHG	d	403	43/49	0.95	0.11	46,59,91,96	0
27	LMG	D	2312	47/55	0.95	0.09	48,59,97,100	0
23	CLA	d	409	65/65	0.95	0.09	54,61,126,133	0
38	LHG	l	103	49/49	0.95	0.10	46,57,79,86	0
25	BCR	B	618	40/40	0.95	0.08	43,51,57,60	0
25	BCR	B	619	40/40	0.95	0.08	45,55,76,79	0
27	LMG	d	414	51/55	0.95	0.10	54,69,105,109	0
23	CLA	b	611	65/65	0.95	0.09	47,53,90,96	0
23	CLA	D	2304	65/65	0.96	0.08	49,58,128,136	0
23	CLA	C	504	65/65	0.96	0.07	47,58,66,80	0
25	BCR	B	620	40/40	0.96	0.08	50,56,67,71	0
23	CLA	C	505	65/65	0.96	0.09	45,54,89,93	0
23	CLA	B	611	65/65	0.96	0.09	47,55,67,72	0
23	CLA	b	612	65/65	0.96	0.07	34,44,63,67	0
23	CLA	b	614	65/65	0.96	0.09	52,63,74,86	0
25	BCR	K	101	40/40	0.96	0.09	57,64,69,70	0
23	CLA	b	615	65/65	0.96	0.08	49,56,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	616	65/65	0.96	0.07	40,47,68,73	0
23	CLA	C	508	65/65	0.96	0.09	51,64,83,84	0
25	BCR	b	622	40/40	0.96	0.08	44,54,66,68	0
23	CLA	b	620	65/65	0.96	0.08	47,57,88,90	0
25	BCR	b	624	40/40	0.96	0.08	48,61,76,76	0
23	CLA	C	509	65/65	0.96	0.09	46,56,115,132	0
37	DGD	C	517	62/66	0.96	0.11	42,55,109,112	0
34	DMS	C	532	4/4	0.96	0.10	67,68,73,74	0
37	DGD	C	519	58/66	0.96	0.09	43,53,79,93	0
23	CLA	c	505	65/65	0.96	0.08	45,54,70,78	0
23	CLA	c	506	65/65	0.96	0.08	47,60,66,82	0
23	CLA	C	510	65/65	0.96	0.09	53,63,84,88	0
23	CLA	c	510	65/65	0.96	0.09	48,62,75,83	0
37	DGD	c	520	62/66	0.96	0.10	47,59,86,95	0
23	CLA	c	511	65/65	0.96	0.09	46,56,114,137	0
33	PL9	D	2306	55/55	0.96	0.07	38,47,55,64	0
34	DMS	D	2318	4/4	0.96	0.12	82,85,90,92	0
38	LHG	D	2311	39/49	0.96	0.09	51,59,92,97	0
33	PL9	d	411	55/55	0.96	0.08	37,46,56,65	0
23	CLA	c	513	65/65	0.96	0.08	46,57,68,79	0
23	CLA	c	514	65/65	0.96	0.08	55,65,73,75	0
23	CLA	C	511	65/65	0.96	0.07	47,56,68,78	0
23	CLA	A	410	65/65	0.96	0.10	41,50,123,127	0
39	HEM	e	103	43/43	0.96	0.09	65,76,109,133	0
23	CLA	A	407	65/65	0.96	0.09	36,47,109,115	0
34	DMS	b	634	4/4	0.96	0.14	81,86,88,92	0
24	PHO	A	408	64/64	0.96	0.07	35,43,49,52	0
24	PHO	A	409	64/64	0.96	0.07	41,49,58,61	0
23	CLA	B	603	65/65	0.97	0.07	41,54,70,76	0
23	CLA	C	512	65/65	0.97	0.07	55,63,74,81	0
23	CLA	c	504	65/65	0.97	0.08	45,59,72,83	0
23	CLA	B	616	65/65	0.97	0.08	43,55,83,95	0
34	DMS	c	533	4/4	0.97	0.11	59,63,63,65	0
23	CLA	B	608	65/65	0.97	0.07	34,44,61,73	0
23	CLA	c	507	65/65	0.97	0.08	46,56,91,95	0
23	CLA	c	508	65/65	0.97	0.07	49,57,80,86	0
23	CLA	C	502	65/65	0.97	0.07	48,58,75,83	0
23	CLA	a	2610	65/65	0.97	0.10	38,46,116,121	0
34	DMS	V	205	4/4	0.97	0.12	67,74,74,77	0
23	CLA	C	503	65/65	0.97	0.06	41,53,70,76	0
34	DMS	v	205	4/4	0.97	0.10	75,77,83,86	0
32	BCT	A	421	4/4	0.97	0.06	59,60,65,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	512	65/65	0.97	0.08	51,59,89,100	0
25	BCR	k	302	40/40	0.97	0.08	53,64,78,79	0
23	CLA	B	609	65/65	0.97	0.07	45,54,73,79	0
23	CLA	b	607	65/65	0.97	0.09	48,57,69,76	0
23	CLA	b	609	65/65	0.97	0.07	37,46,85,92	0
23	CLA	b	610	65/65	0.97	0.07	39,49,60,63	0
23	CLA	d	402	65/65	0.97	0.06	35,41,50,62	0
23	CLA	B	604	65/65	0.97	0.07	42,51,66,72	0
35	CA	b	605	1/1	0.97	0.05	72,72,72,72	0
23	CLA	C	506	65/65	0.97	0.08	51,59,80,81	0
23	CLA	b	613	65/65	0.97	0.07	41,53,72,77	0
38	LHG	L	101	49/49	0.97	0.08	46,57,73,76	0
24	PHO	a	2611	64/64	0.97	0.06	38,42,49,57	0
24	PHO	a	2612	64/64	0.97	0.06	39,49,59,65	0
38	LHG	d	413	49/49	0.97	0.07	40,49,71,73	0
25	BCR	A	411	40/40	0.97	0.06	38,48,58,62	0
34	DMS	B	638	4/4	0.97	0.09	61,68,73,82	0
23	CLA	B	606	65/65	0.97	0.07	37,47,62,64	0
23	CLA	B	612	65/65	0.97	0.06	39,47,66,70	0
23	CLA	B	613	65/65	0.97	0.07	39,46,56,61	0
23	CLA	b	618	65/65	0.97	0.07	40,46,93,96	0
23	CLA	B	614	65/65	0.97	0.07	37,45,91,99	0
34	DMS	A	424	4/4	0.98	0.09	48,50,52,59	0
23	CLA	A	406	65/65	0.98	0.06	34,41,51,63	0
23	CLA	D	2303	65/65	0.98	0.06	33,42,62,72	0
23	CLA	A	405	65/65	0.98	0.06	33,41,55,77	0
23	CLA	b	608	65/65	0.98	0.07	40,52,71,75	0
34	DMS	C	533	4/4	0.98	0.07	61,64,65,66	0
23	CLA	d	408	65/65	0.98	0.06	31,42,60,71	0
39	HEM	F	101	43/43	0.98	0.06	61,71,100,119	0
23	CLA	a	2609	65/65	0.98	0.06	35,41,55,69	0
23	CLA	B	605	65/65	0.98	0.07	37,44,85,94	0
34	DMS	o	304	4/4	0.98	0.07	43,53,55,59	0
34	DMS	B	636	4/4	0.98	0.09	43,47,47,59	0
41	MG	j	2703	1/1	0.98	0.10	60,60,60,60	0
23	CLA	b	617	65/65	0.98	0.06	41,49,56,58	0
42	HEC	v	201	43/43	0.98	0.06	49,56,62,69	0
22	CL	A	403	1/1	0.99	0.05	46,46,46,46	0
35	CA	B	601	1/1	0.99	0.05	68,68,68,68	0
35	CA	O	301	1/1	0.99	0.06	77,77,77,77	0
22	CL	a	2606	1/1	0.99	0.08	48,48,48,48	0
41	MG	J	302	1/1	0.99	0.09	58,58,58,58	0

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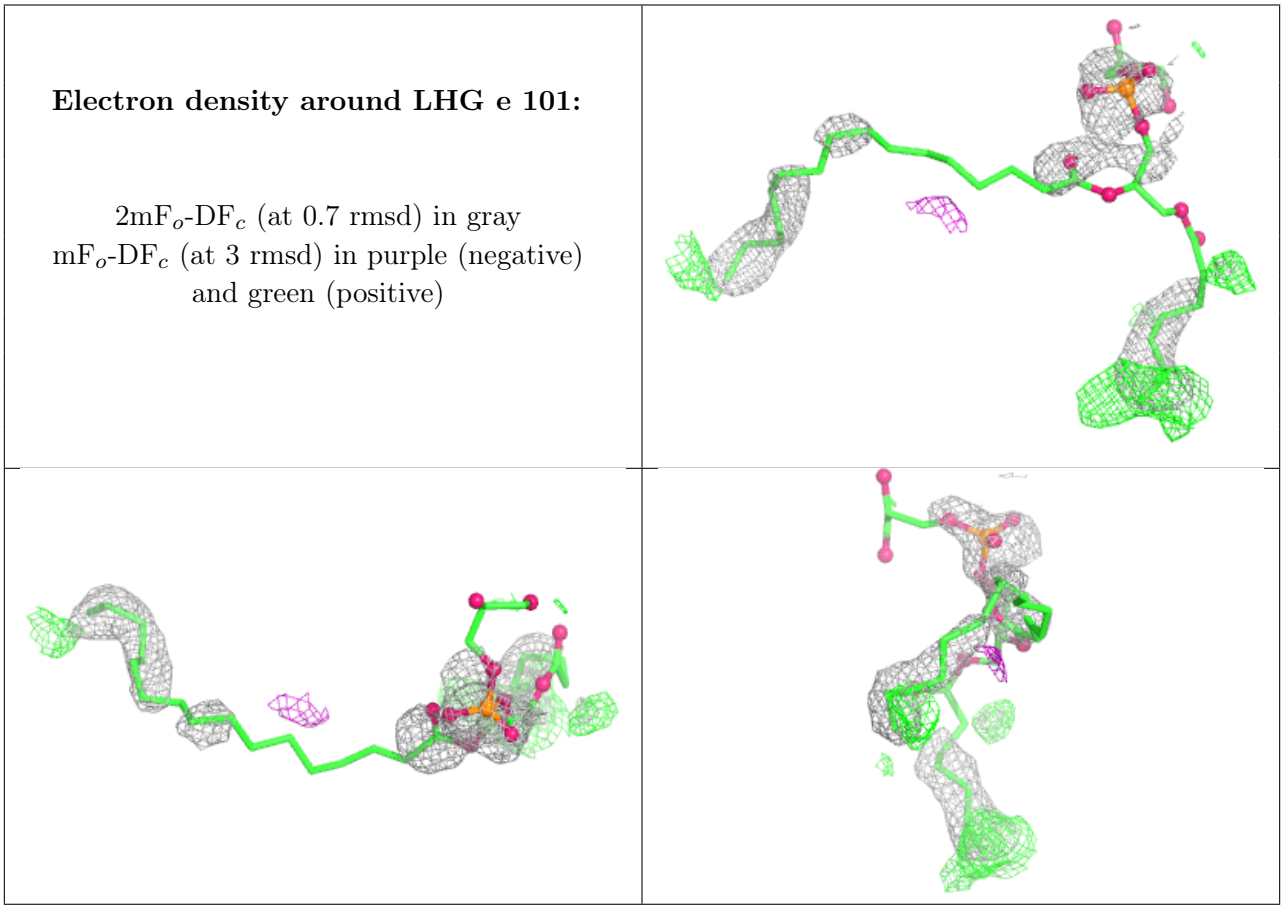
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CA	c	503	1/1	0.99	0.03	73,73,73,73	0
35	CA	o	302	1/1	0.99	0.03	74,74,74,74	0
34	DMS	b	633	4/4	0.99	0.06	45,50,52,61	0
42	HEC	V	201	43/43	0.99	0.06	41,46,52,56	0
20	OEX	A	401	10/10	0.99	0.03	41,46,50,52	0
22	CL	a	2607	1/1	1.00	0.03	46,46,46,46	0
21	FE2	a	2605	1/1	1.00	0.01	52,52,52,52	0
20	OEX	a	2604	10/10	1.00	0.02	41,46,51,52	0
22	CL	A	404	1/1	1.00	0.06	43,43,43,43	0
21	FE2	A	402	1/1	1.00	0.01	54,54,54,54	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.

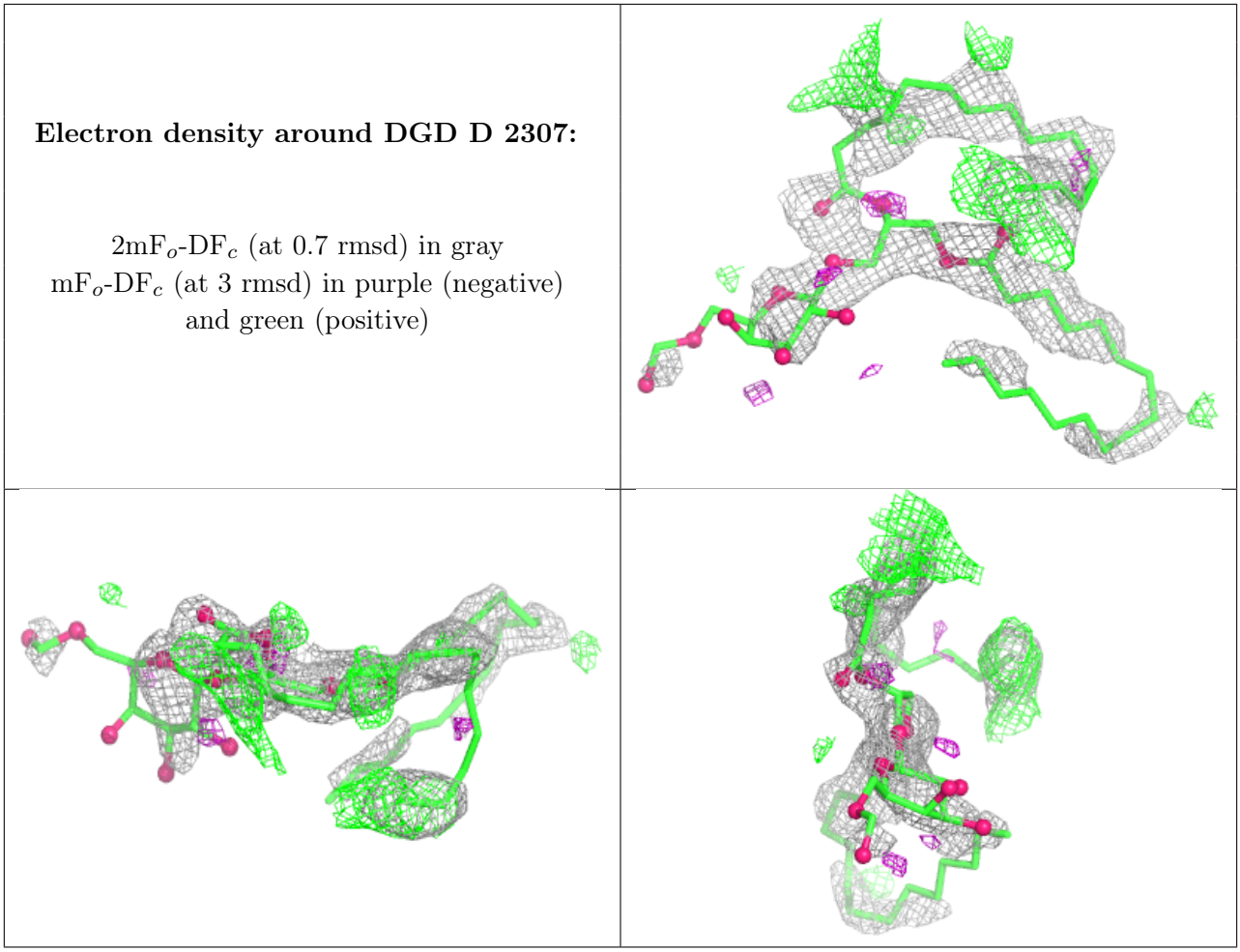
Electron density around LHG e 101:

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



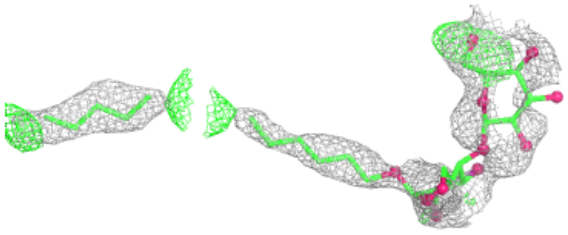
Electron density around DGD D 2307:

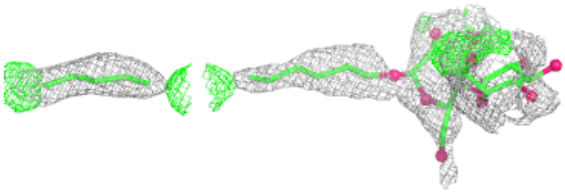
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

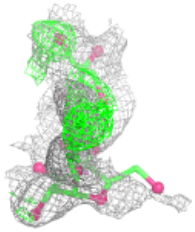


Electron density around LMT j 2701:

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

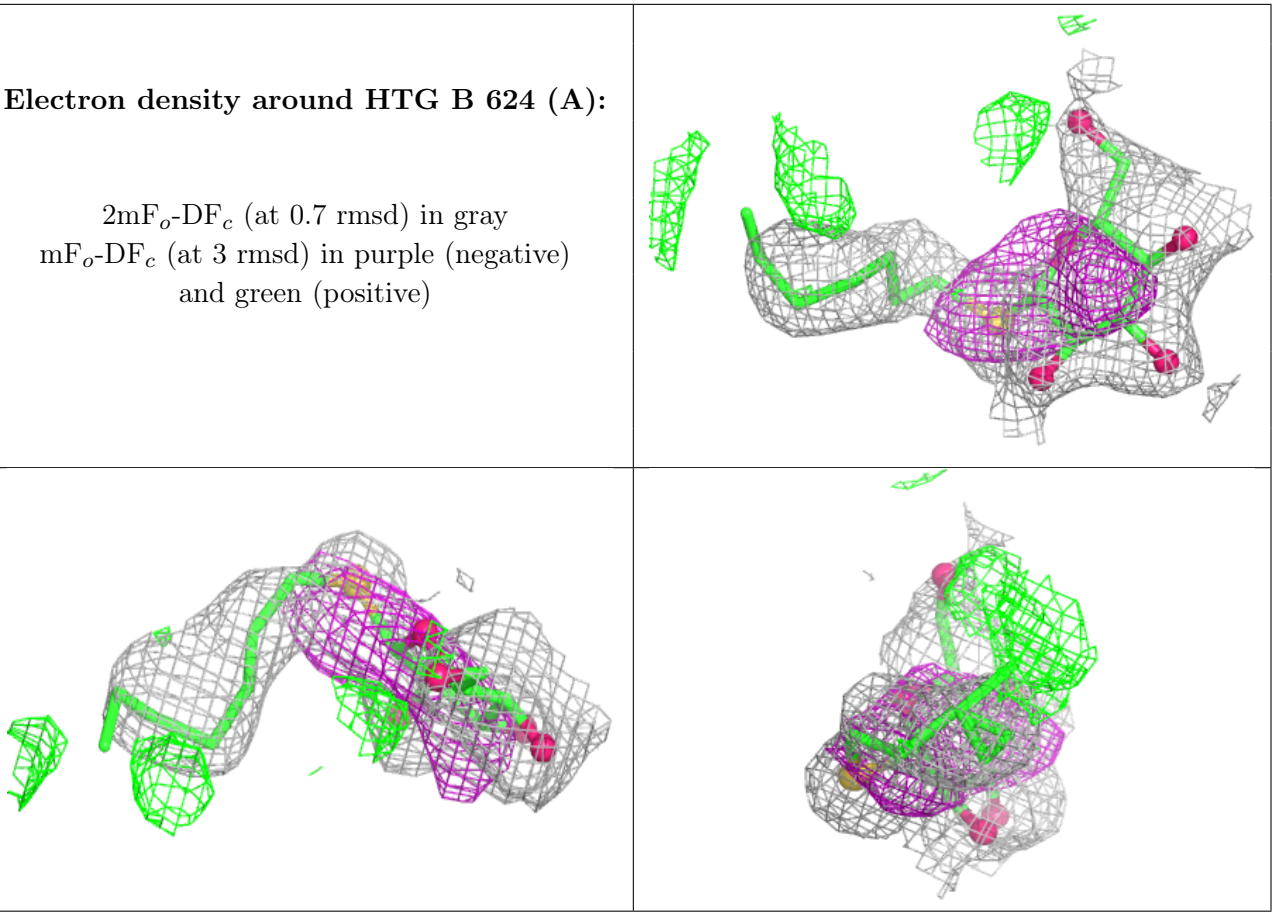






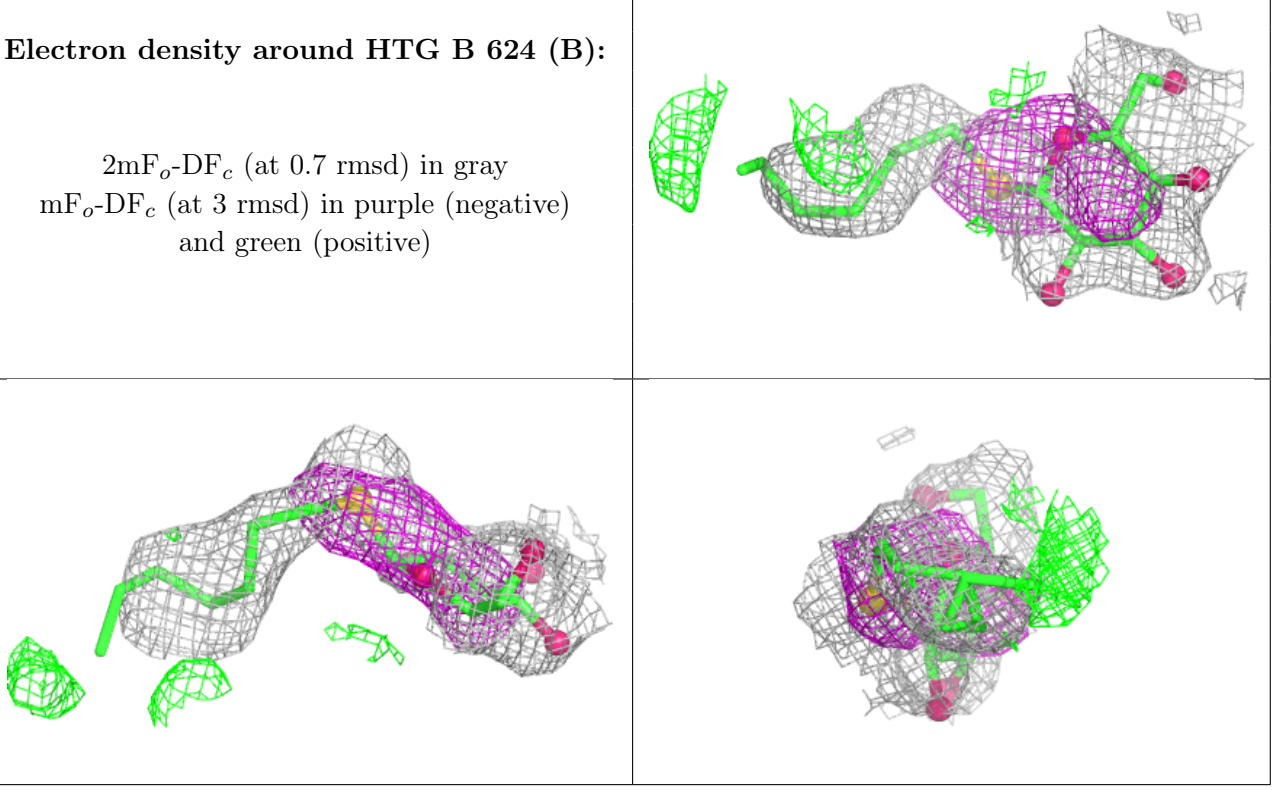
Electron density around HTG B 624 (A):

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



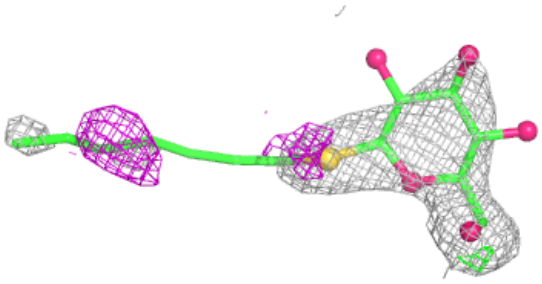
Electron density around HTG B 624 (B):

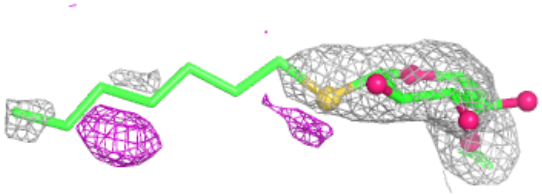
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

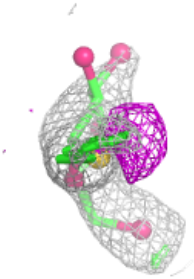


Electron density around HTG C 522:

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

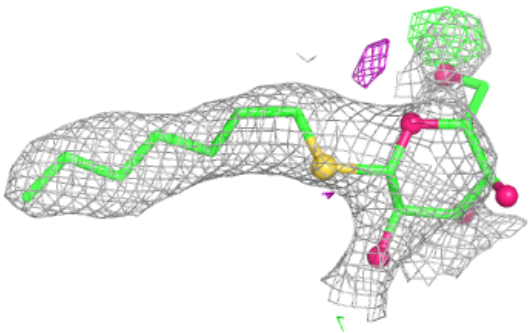


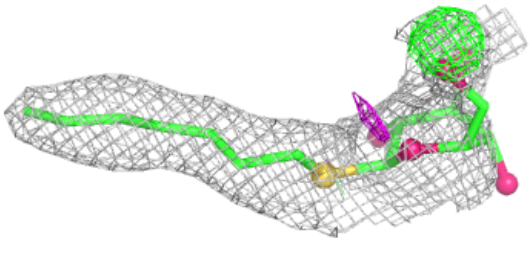


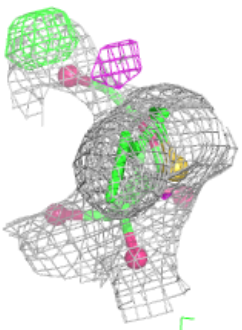


Electron density around HTG i 102:

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

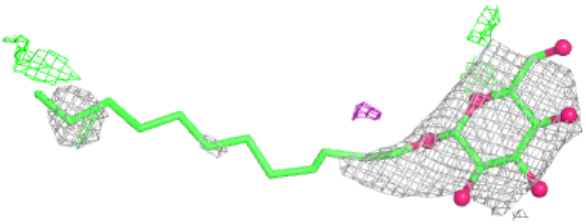


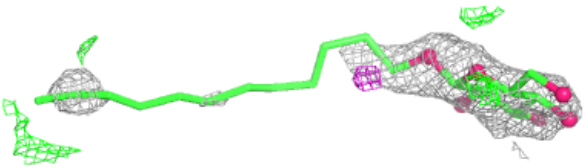


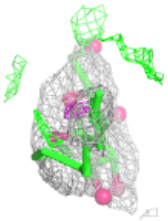


Electron density around LMT F 102:

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

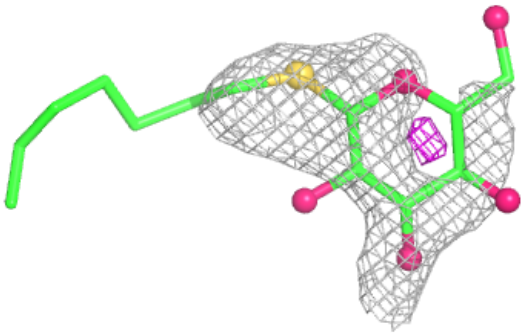


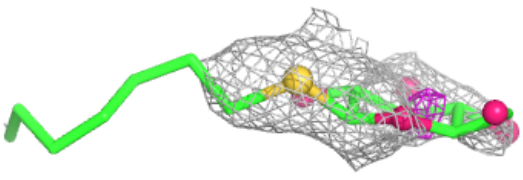


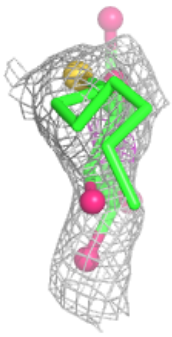


Electron density around HTG d 407:

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

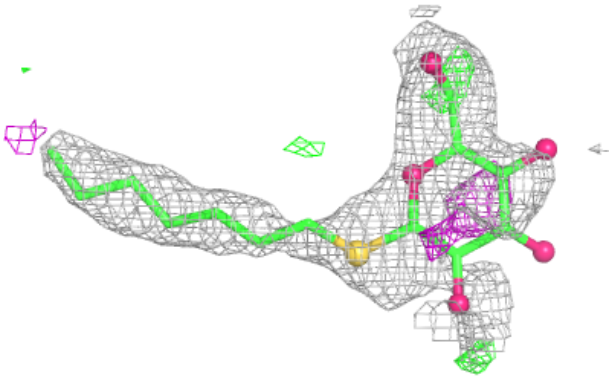


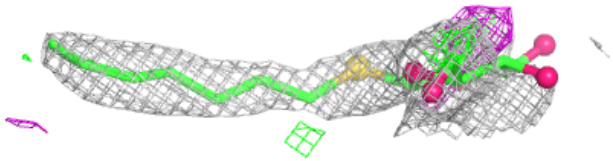


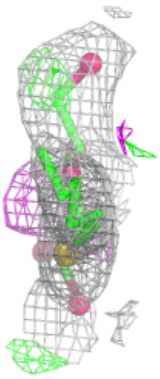


Electron density around HTG B 627:

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

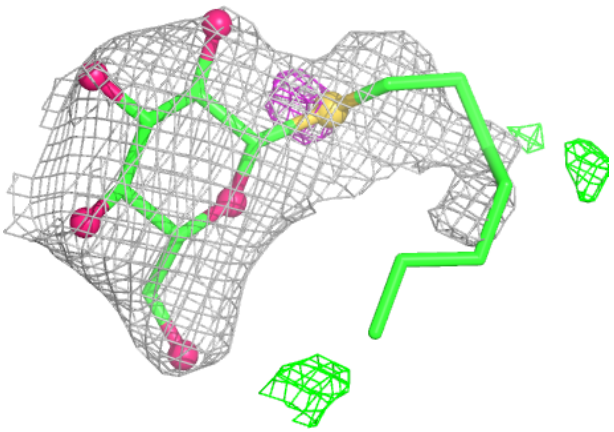


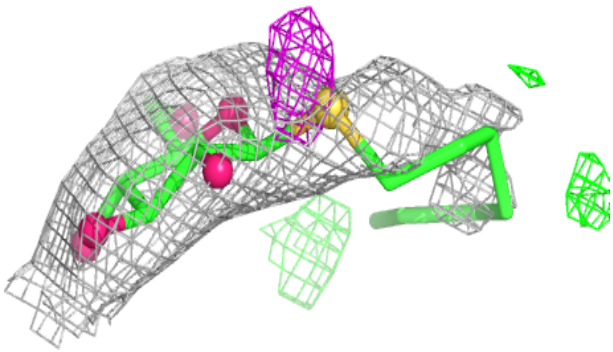


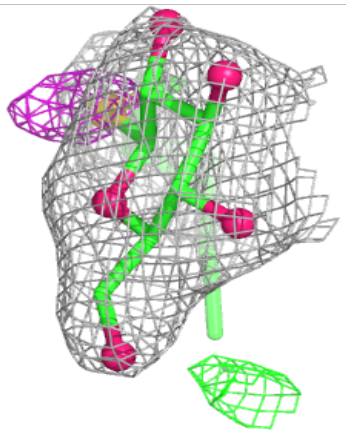


Electron density around HTG V 204:

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

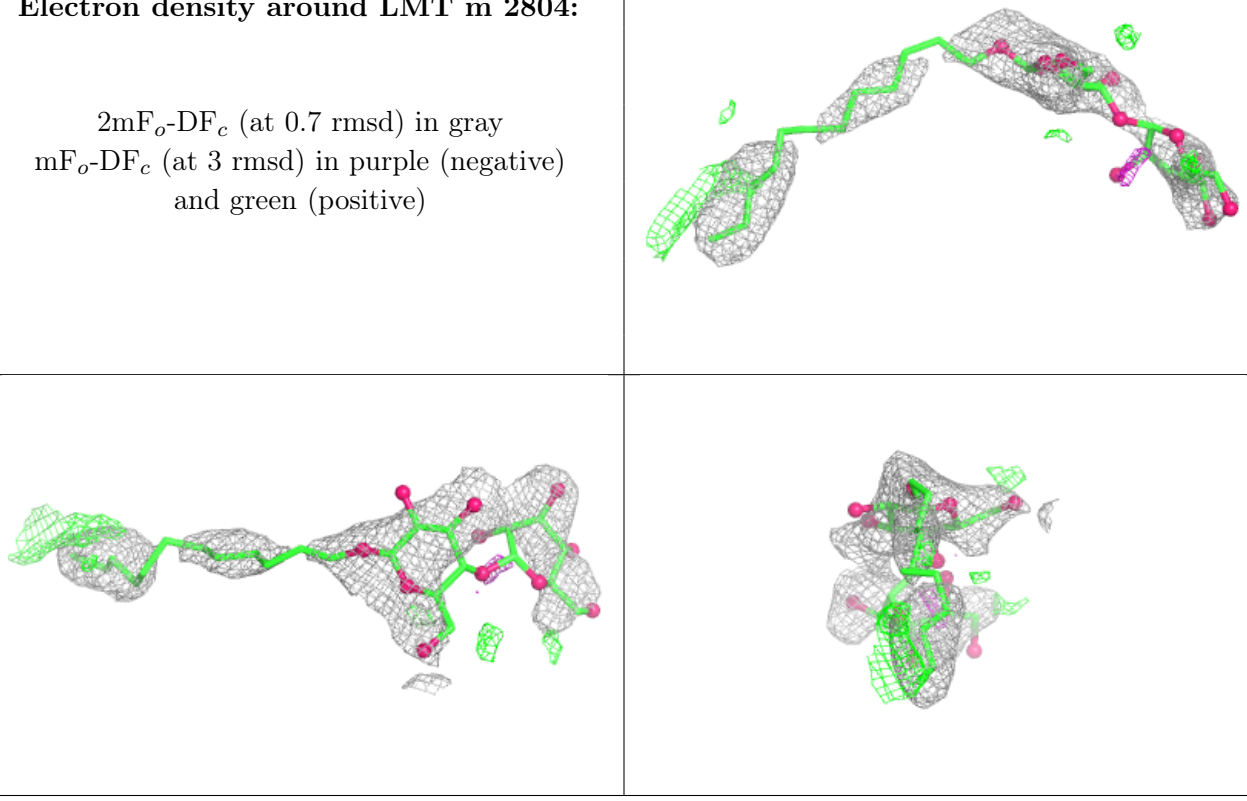






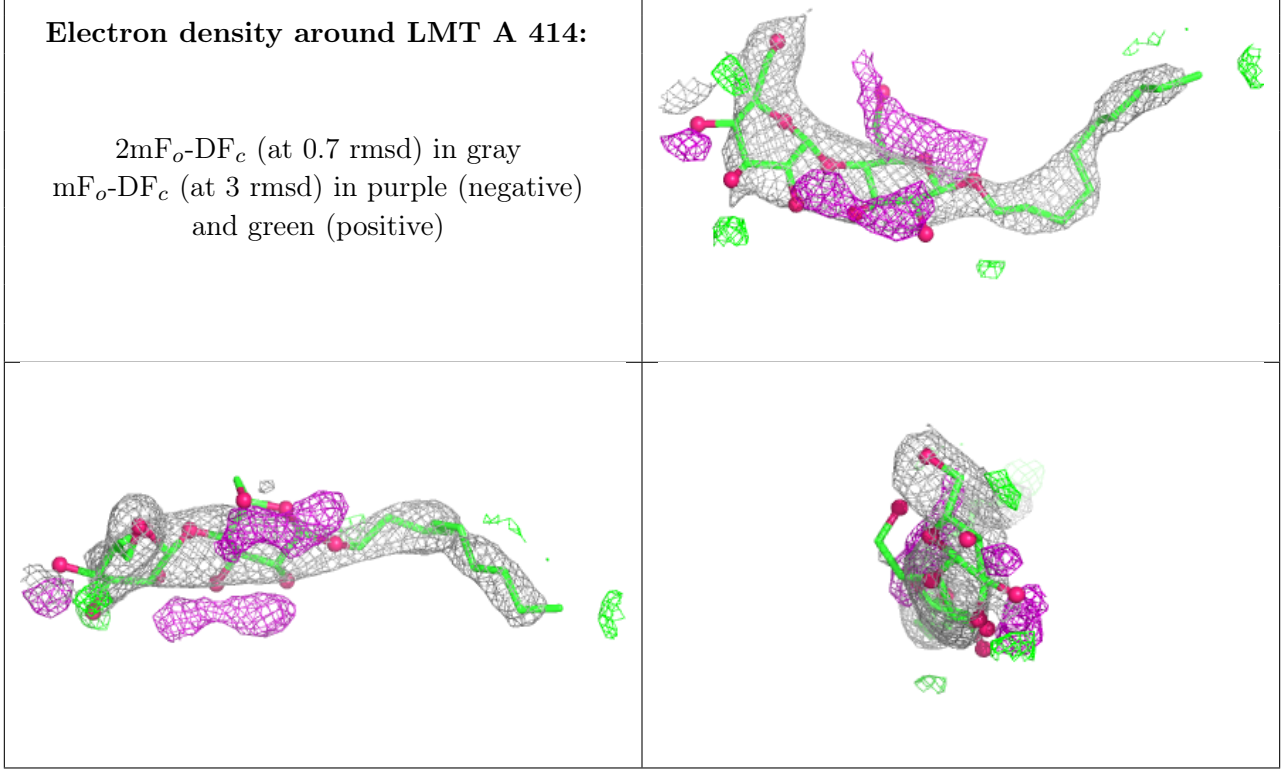
Electron density around LMT m 2804:

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



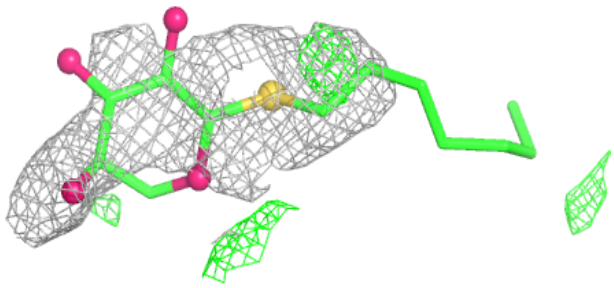
Electron density around LMT A 414:

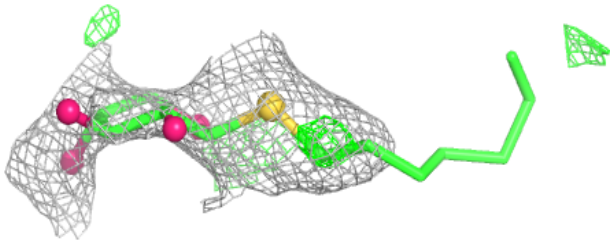
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

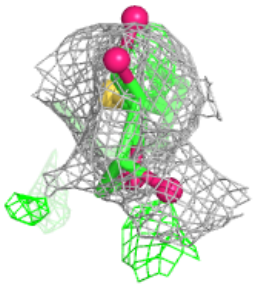


Electron density around HTG H 101:

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

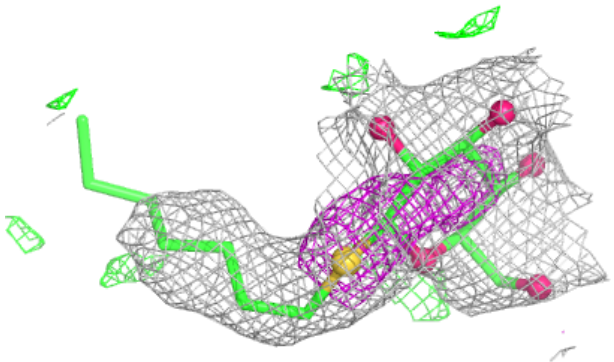


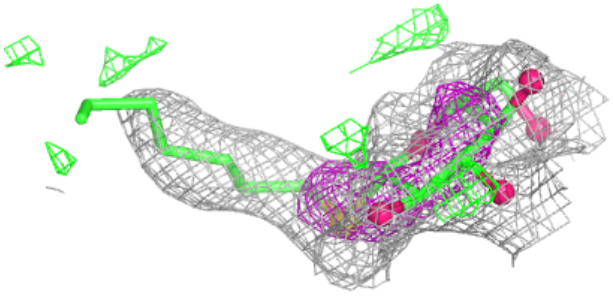


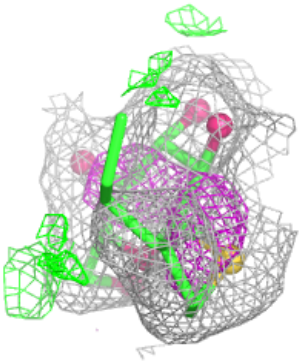


Electron density around HTG b 625:

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

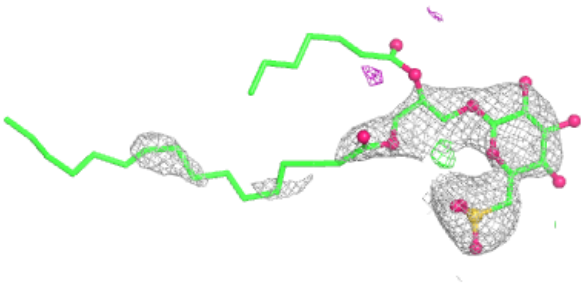


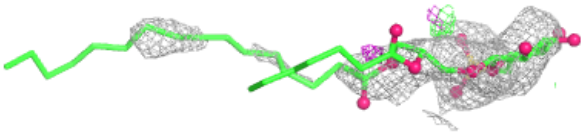


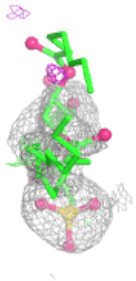


Electron density around SQD D 2308:

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

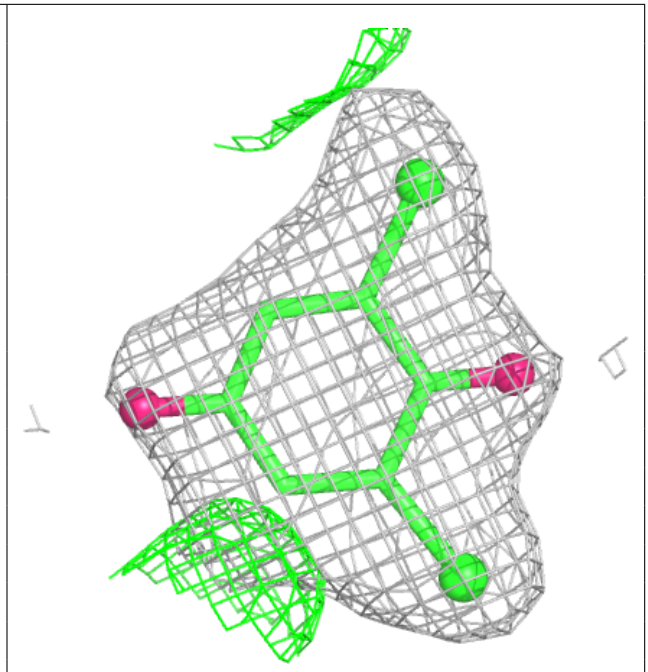


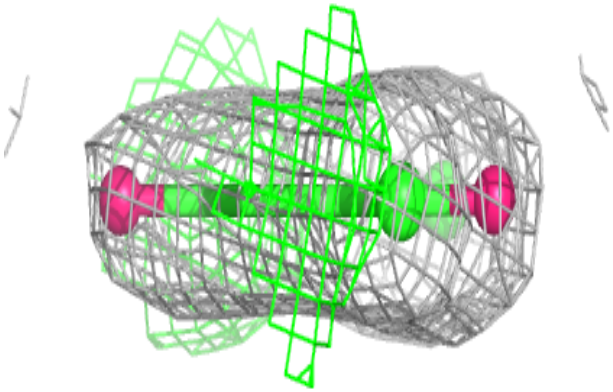


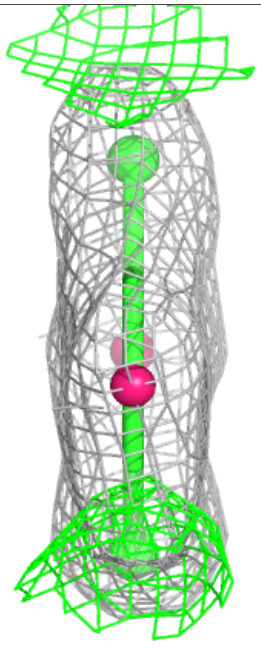


Electron density around JOX A 418:

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

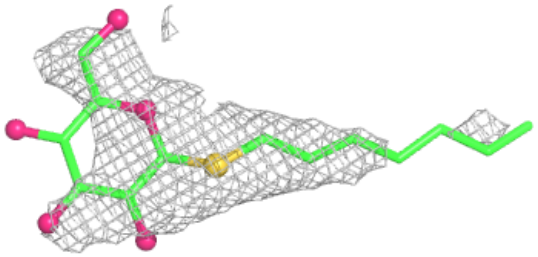


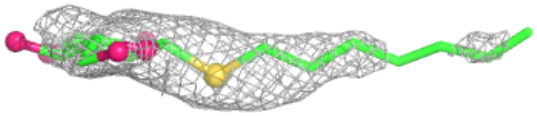


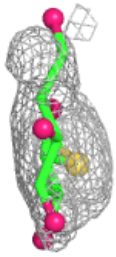


Electron density around HTG C 525:

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

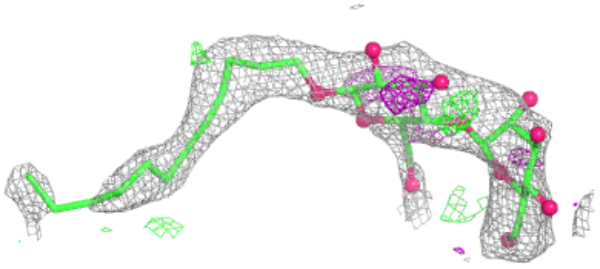


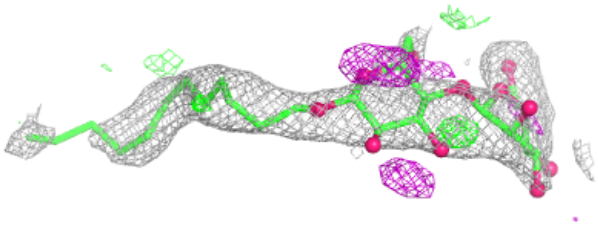


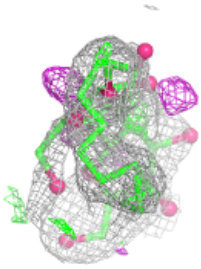


Electron density around LMT d 401:

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

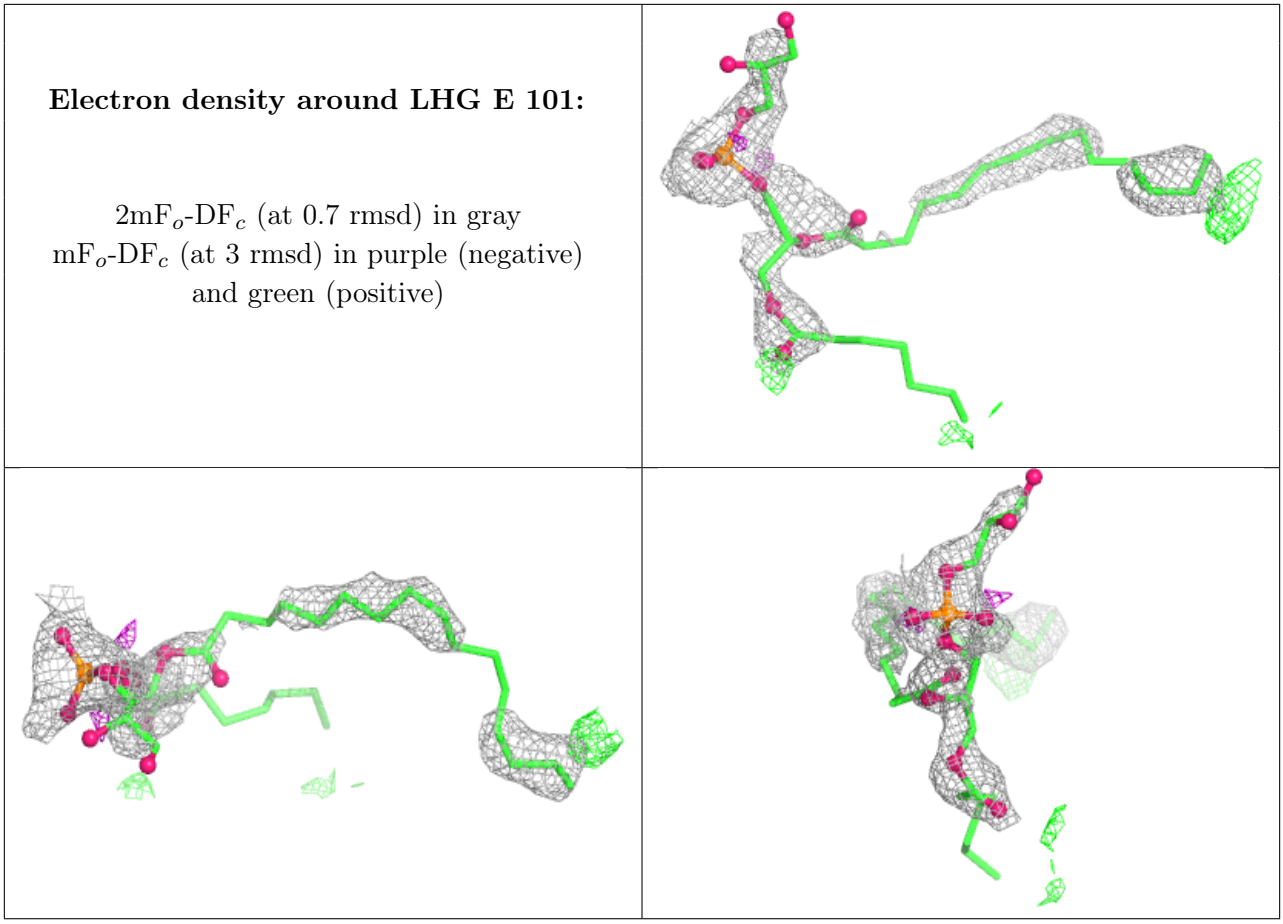






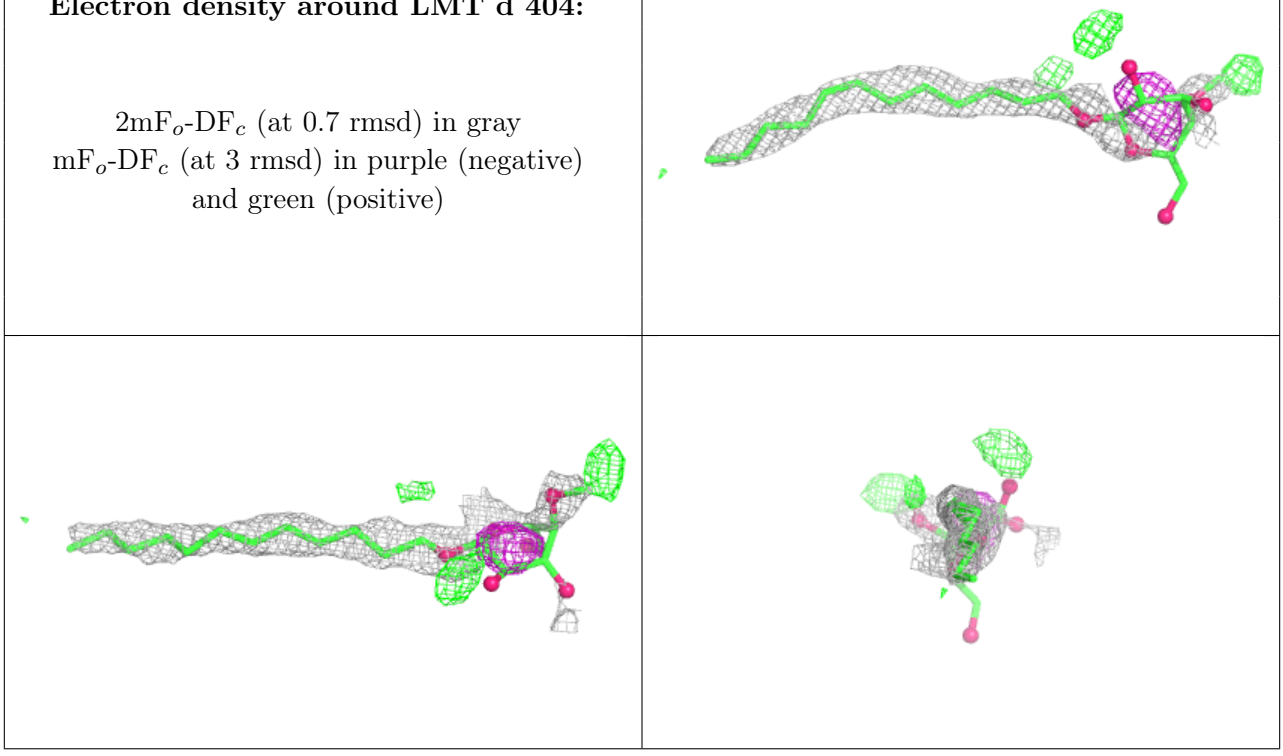
Electron density around LHG E 101:

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



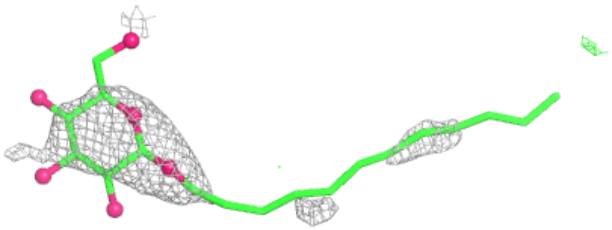
Electron density around LMT d 404:

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

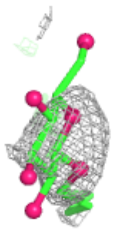


Electron density around LMT f 101:

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

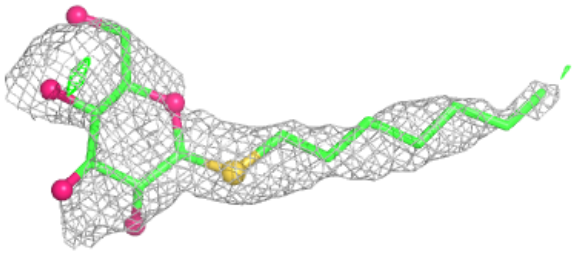


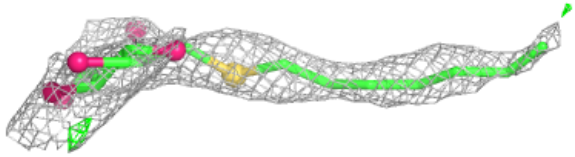


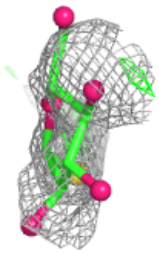


Electron density around HTG B 625:

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

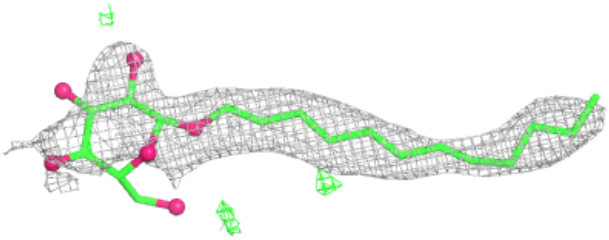


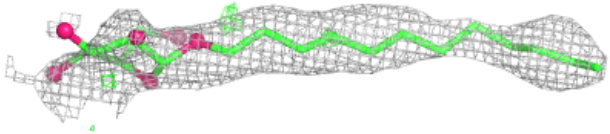


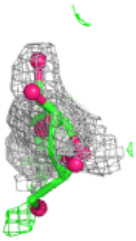


Electron density around LMT J 303:

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

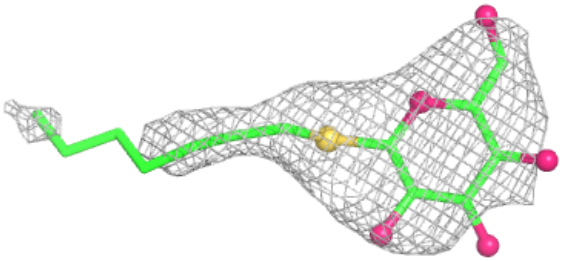


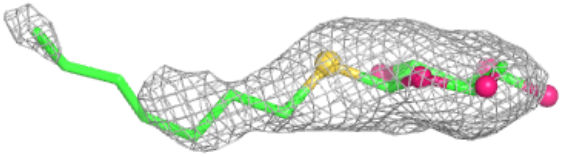


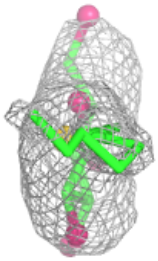


Electron density around HTG c 523:

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

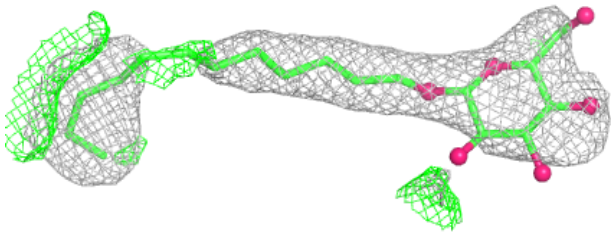


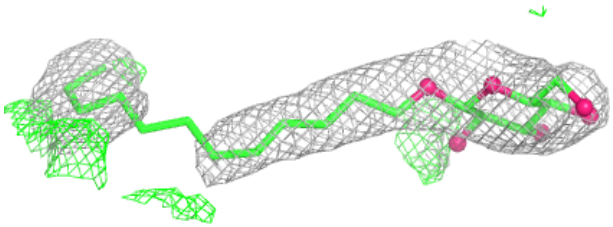


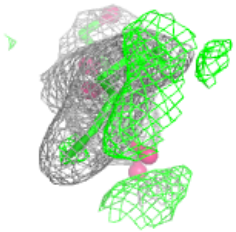


Electron density around LMT T 103:

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

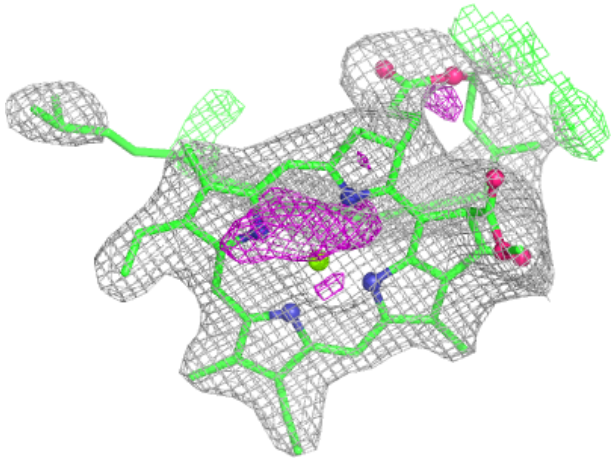


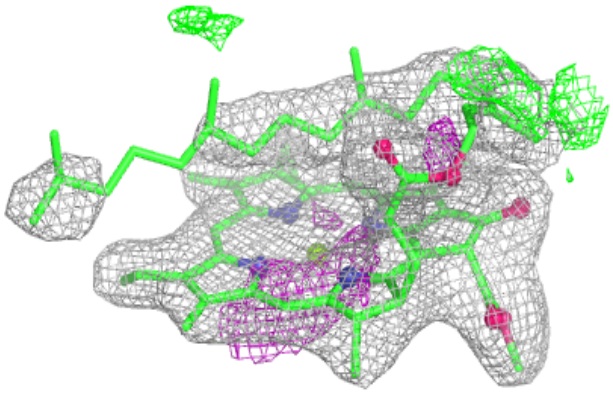


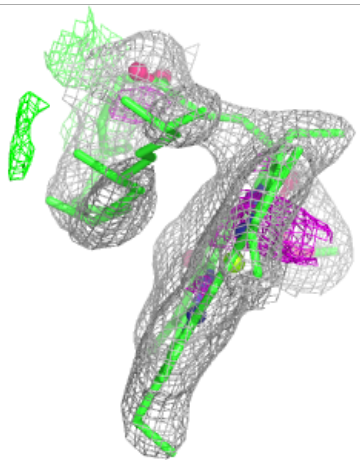


Electron density around CLA B 602:

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

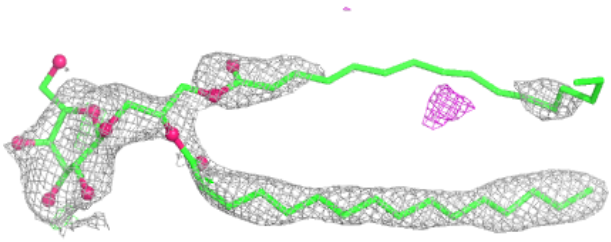


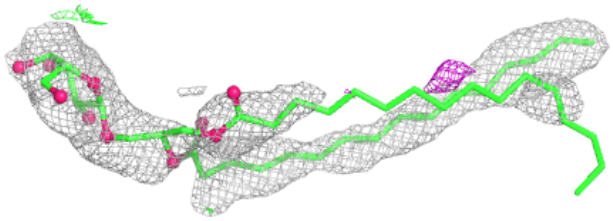


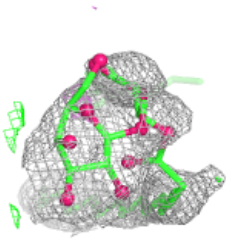


Electron density around LMG c 522:

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

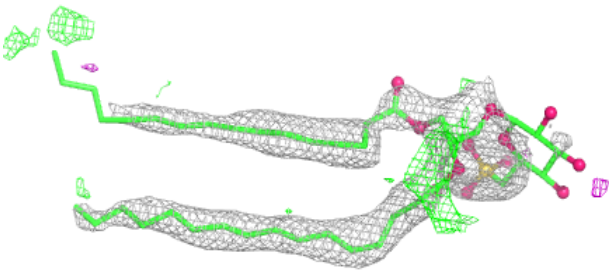


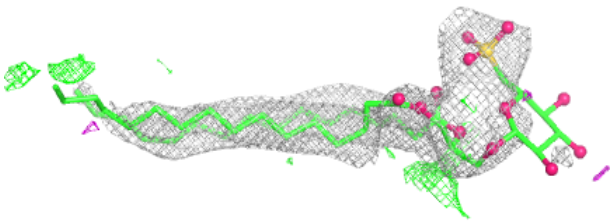


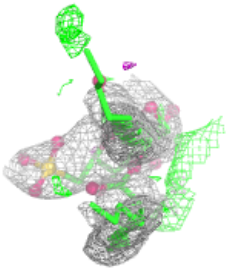


Electron density around SQD D 2302:

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

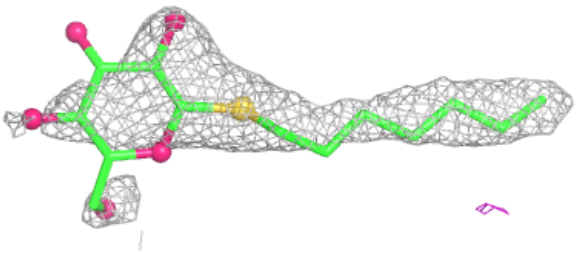


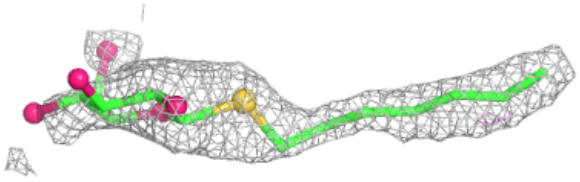


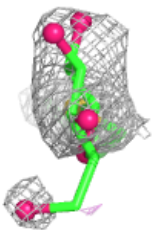


Electron density around HTG c 524:

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

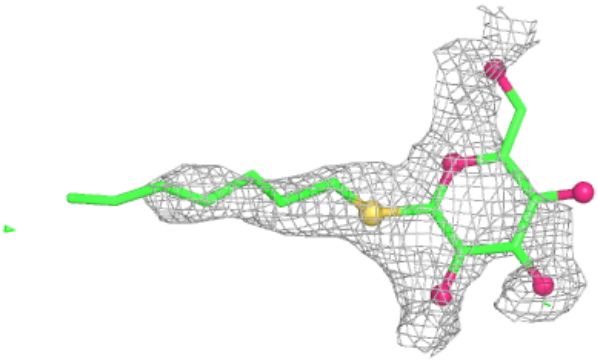


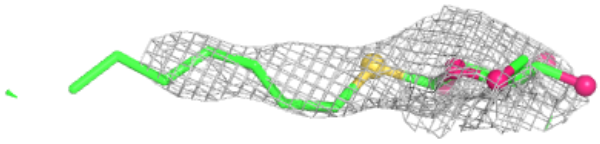


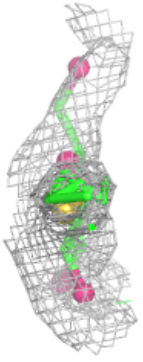


Electron density around HTG c 526:

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

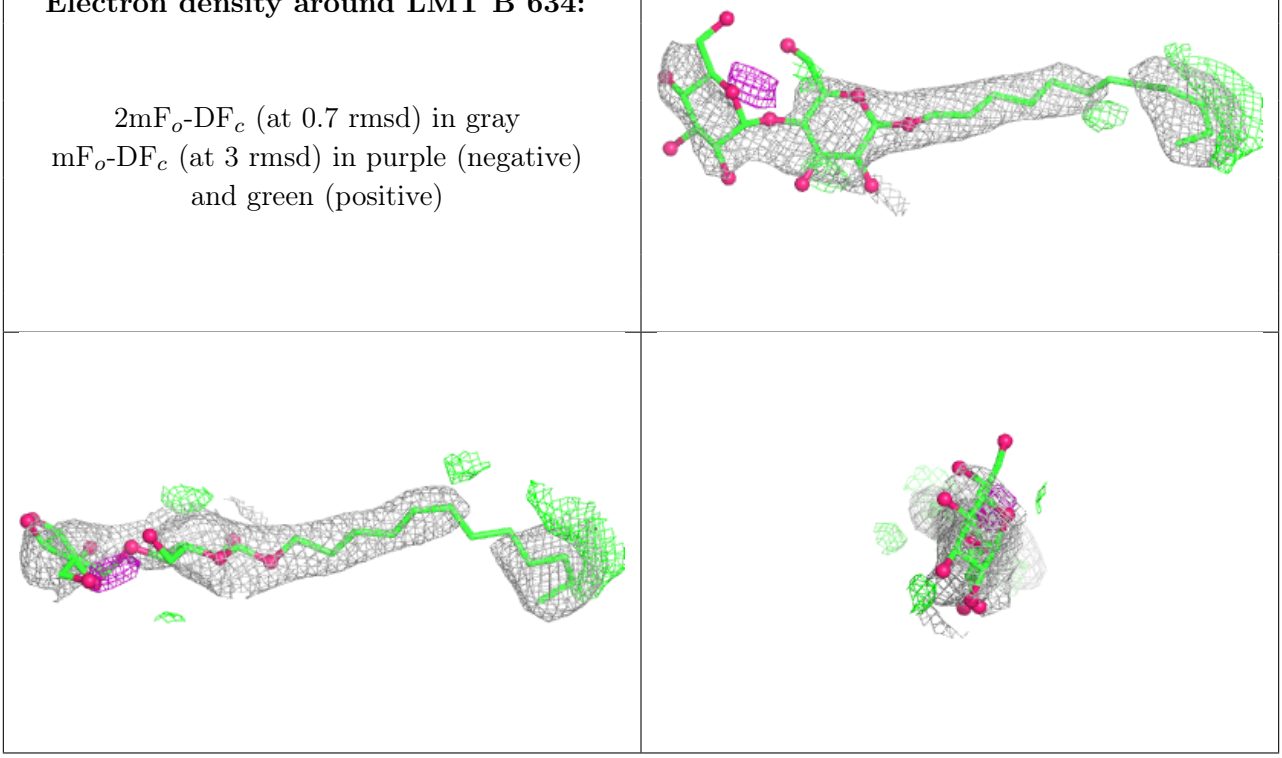






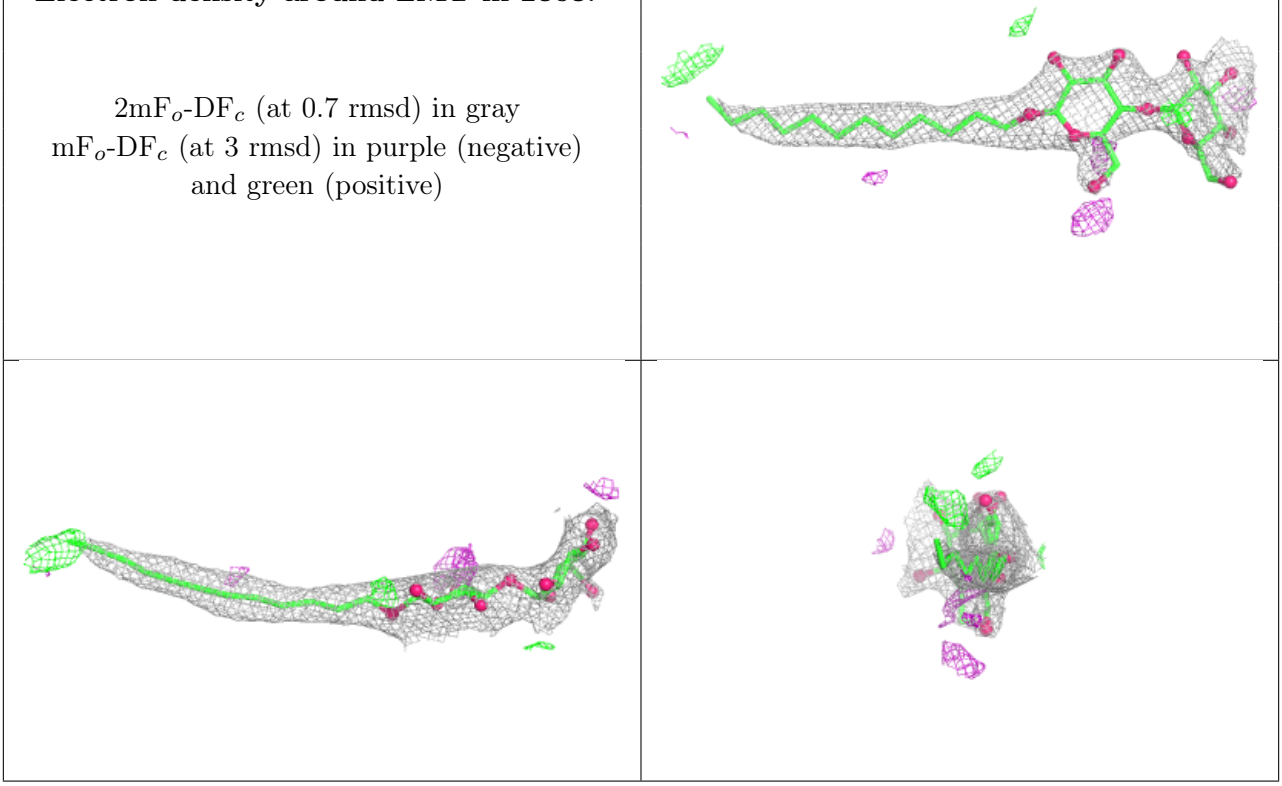
Electron density around LMT B 634:

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



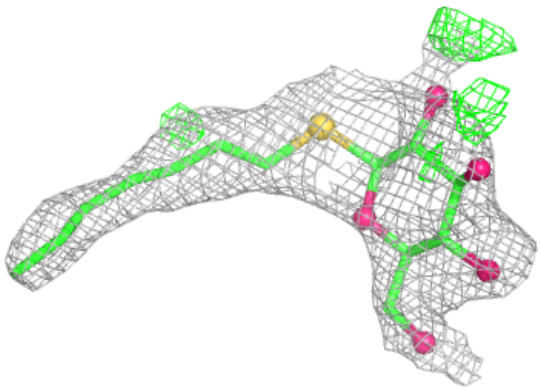
Electron density around LMT m 2803:

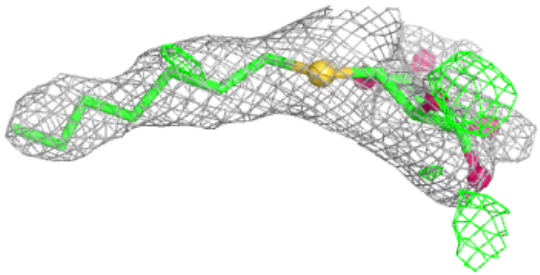
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

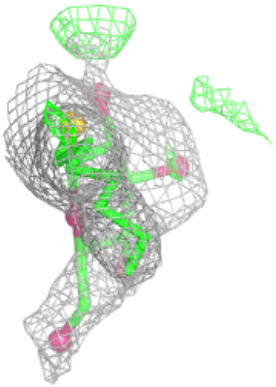


Electron density around HTG b 626:

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

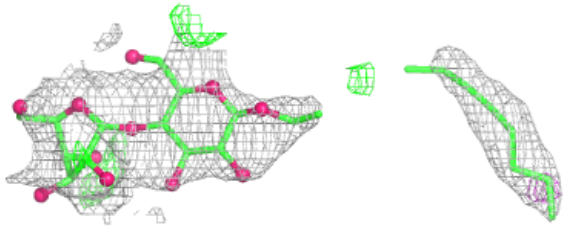


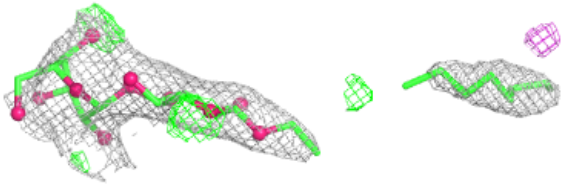


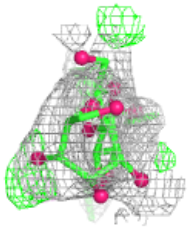


Electron density around LMT z 102:

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

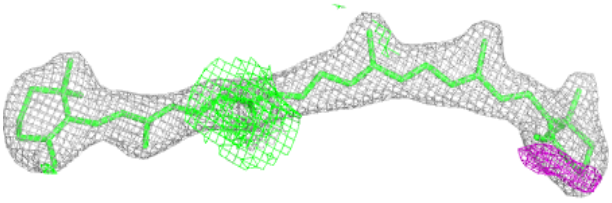


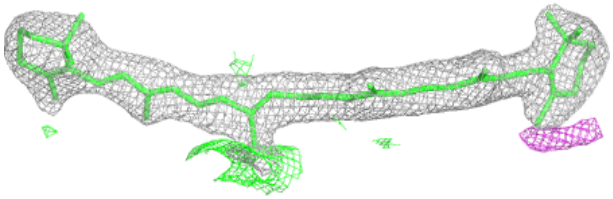


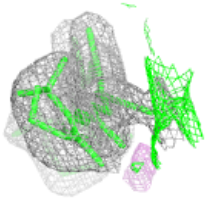


Electron density around BCR T 102:

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

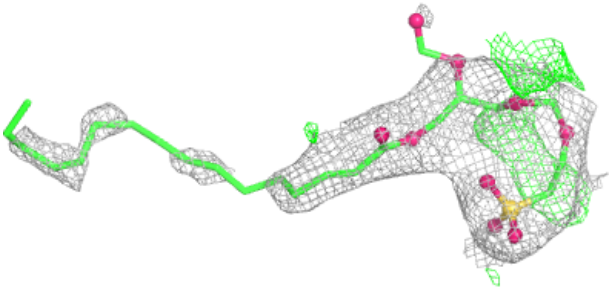


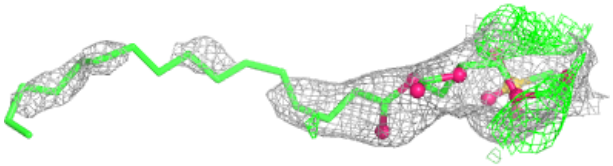


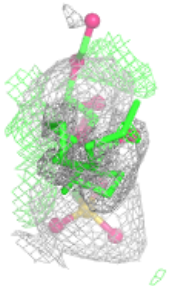


Electron density around SQD d 417:

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

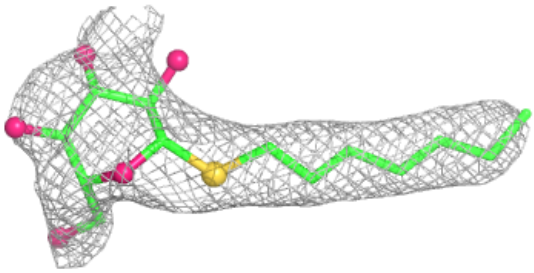


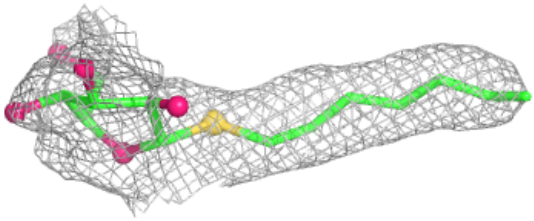


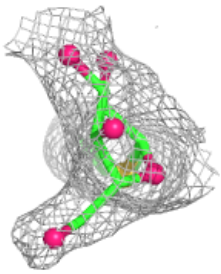


Electron density around HTG I 101:

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

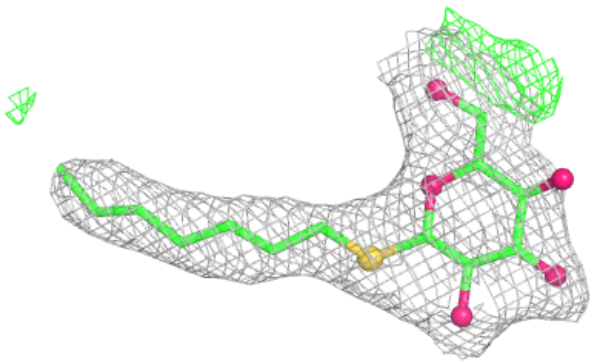


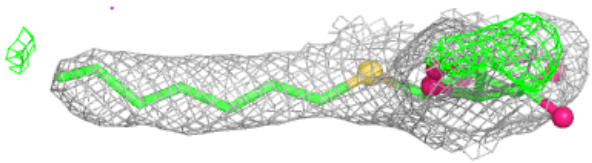


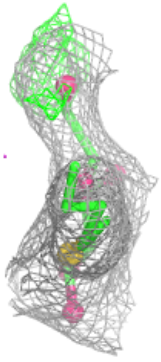


Electron density around HTG b 604:

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

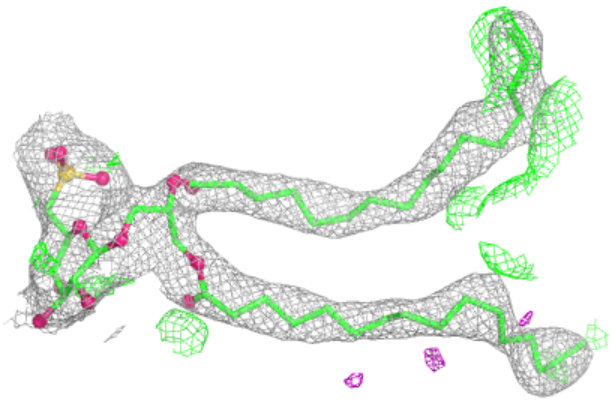


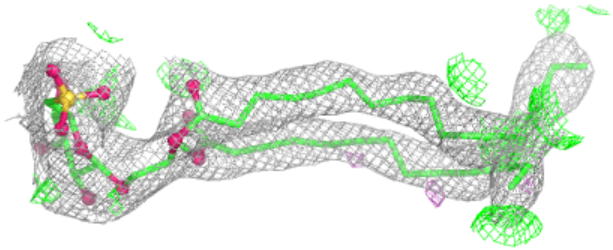


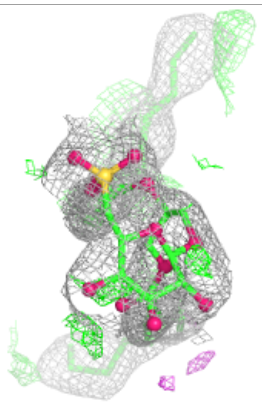


Electron density around SQD l 101:

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

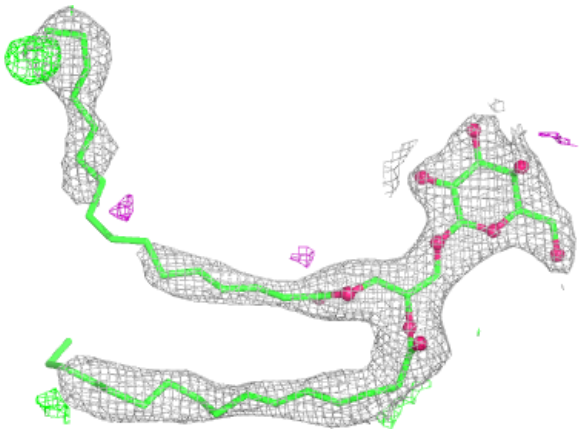


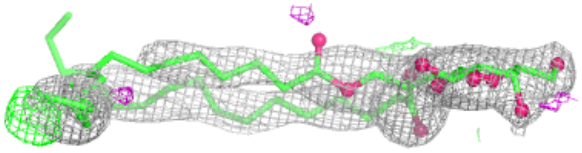


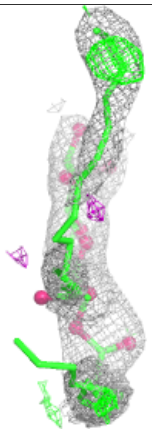


Electron density around LMG C 520:

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

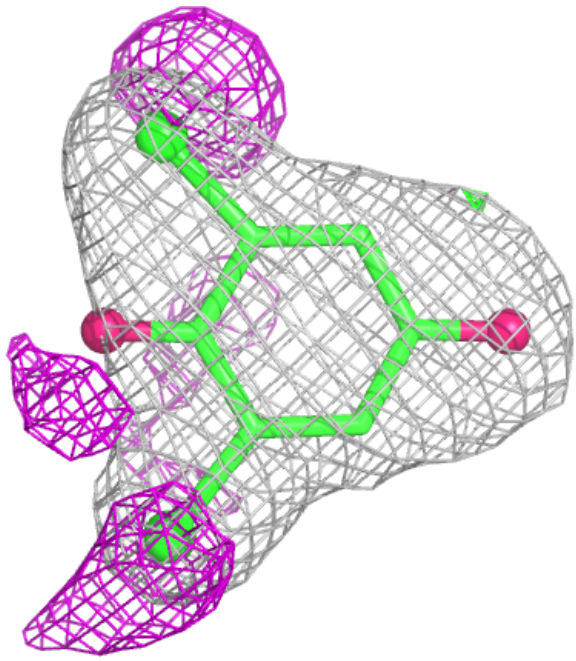


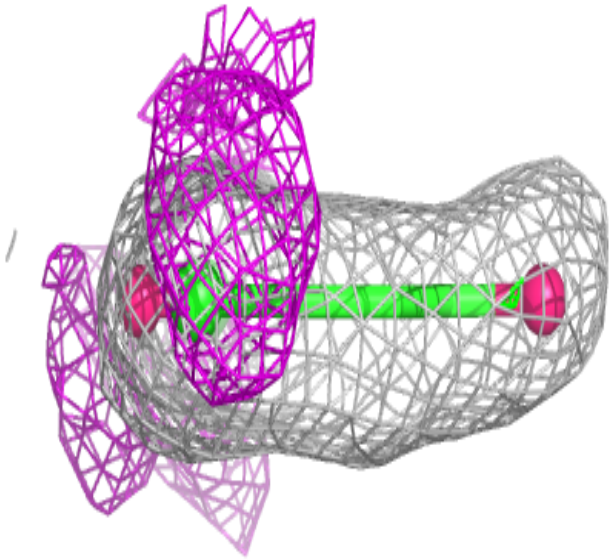


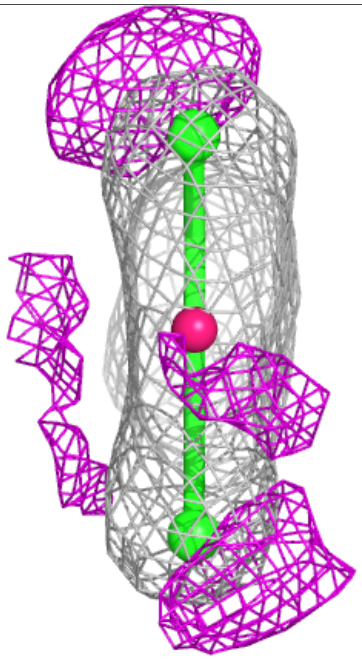


Electron density around JOX A 419:

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

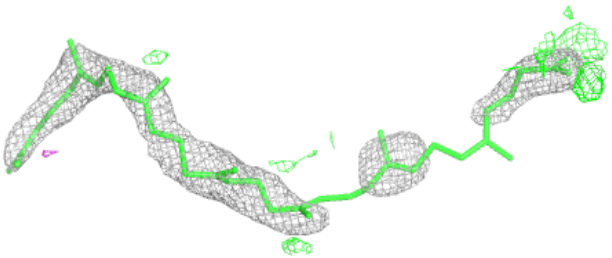


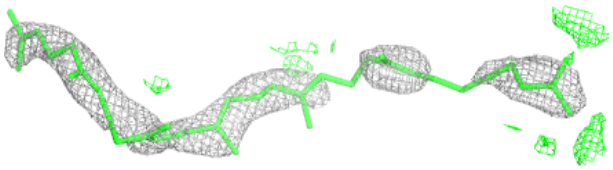


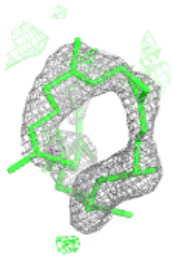


Electron density around PL9 A 422:

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

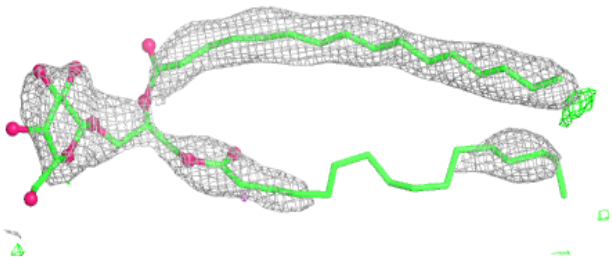


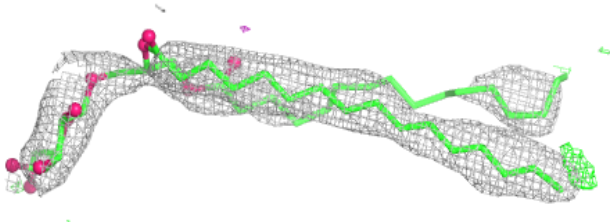


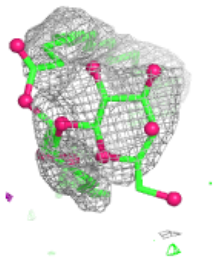


Electron density around LMG C 527:

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

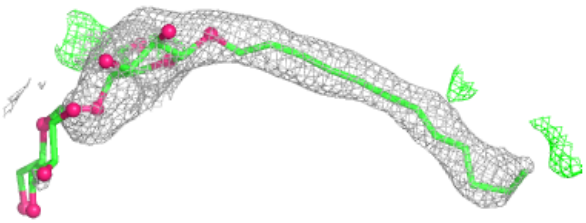


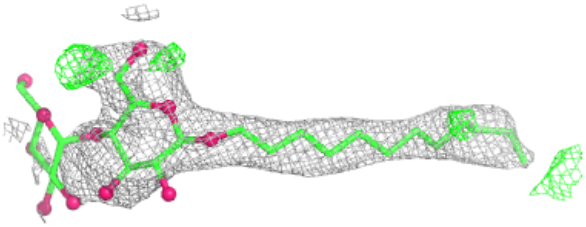


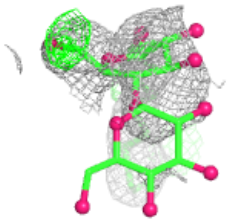


Electron density around LMT M 101:

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

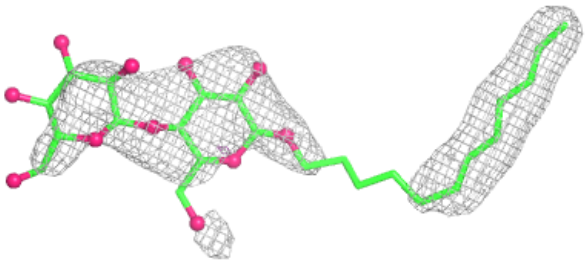


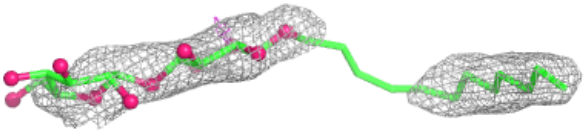


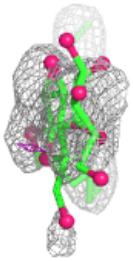


Electron density around LMT Z 101:

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

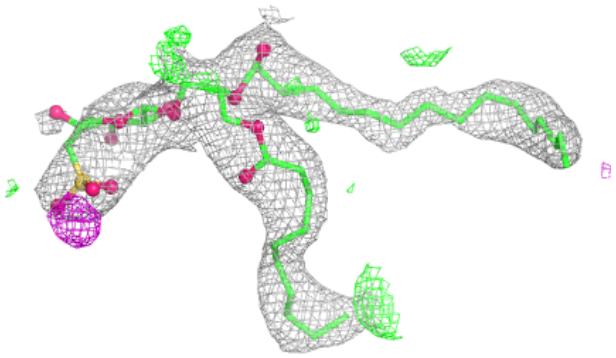


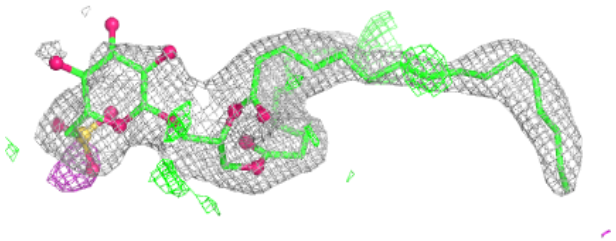


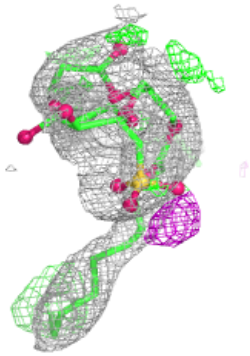


Electron density around SQD b 601:

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

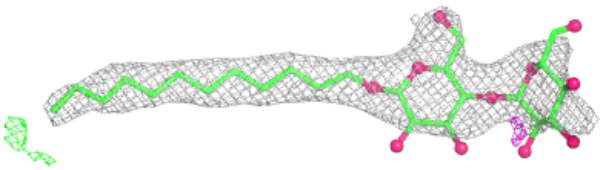


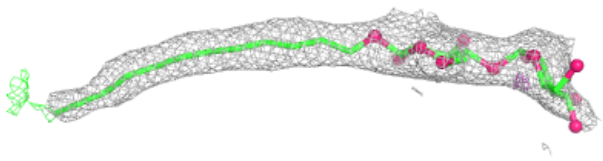


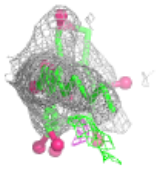


Electron density around LMT M 102:

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

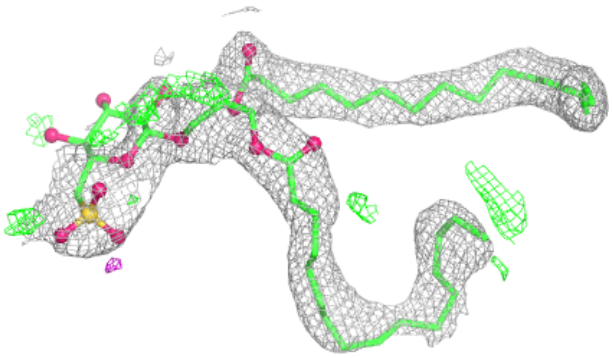


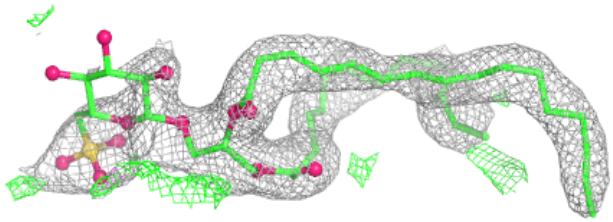


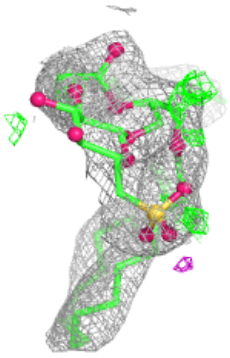


Electron density around SQD a 2603:

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

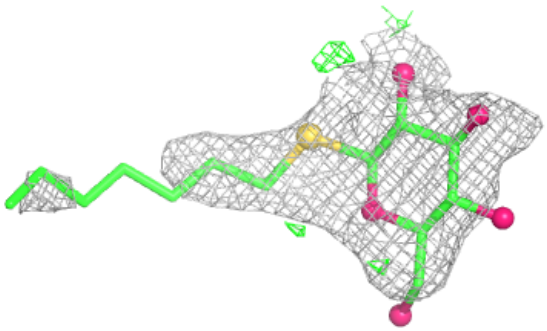


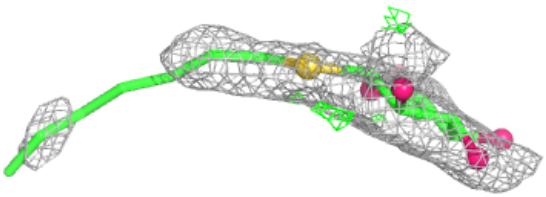


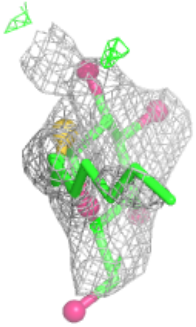


Electron density around HTG d 415:

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

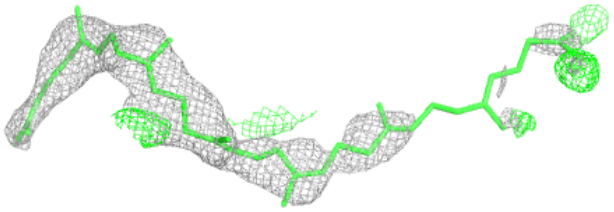


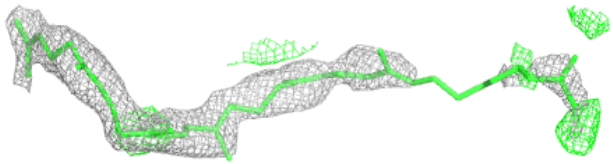


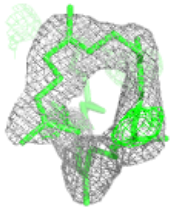


Electron density around PL9 x 1301:

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

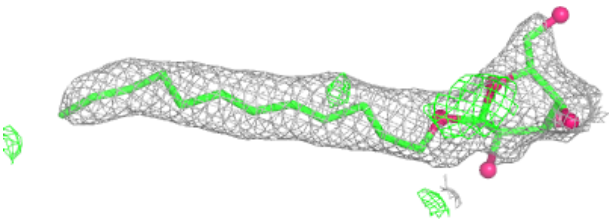


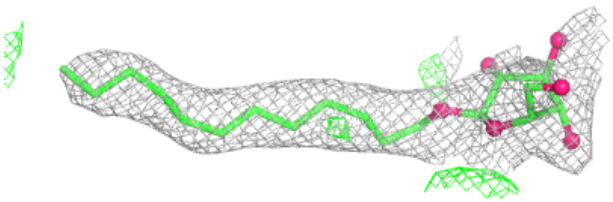


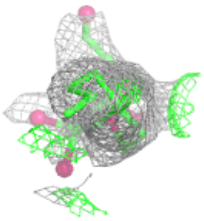


Electron density around LMT i 103:

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

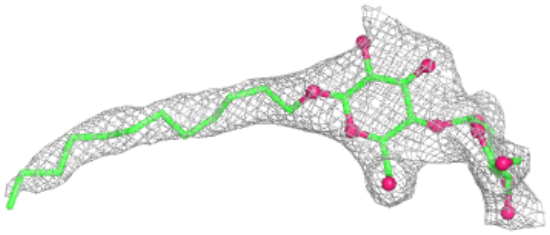


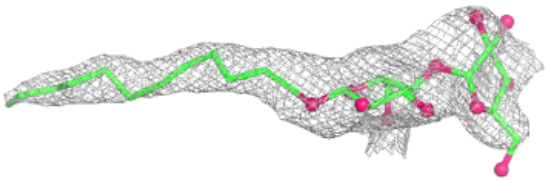


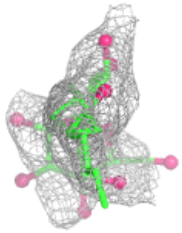


Electron density around LMT B 623:

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

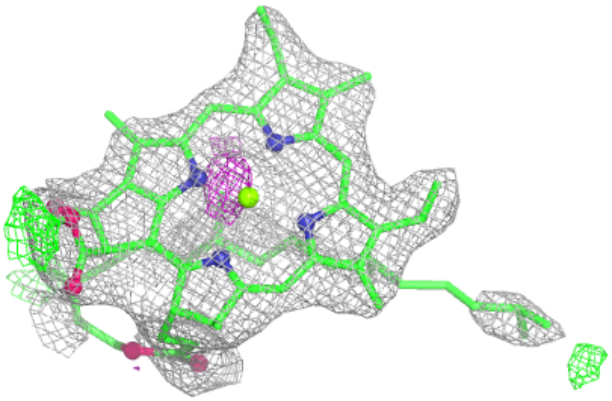


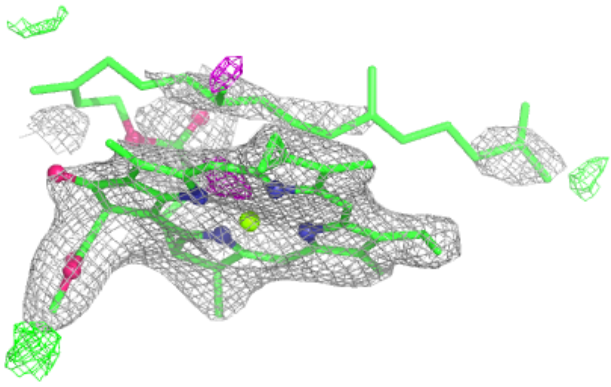


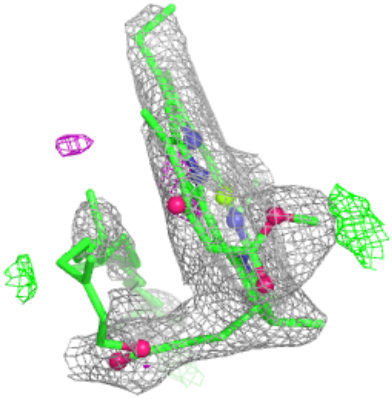


Electron density around CLA b 606:

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

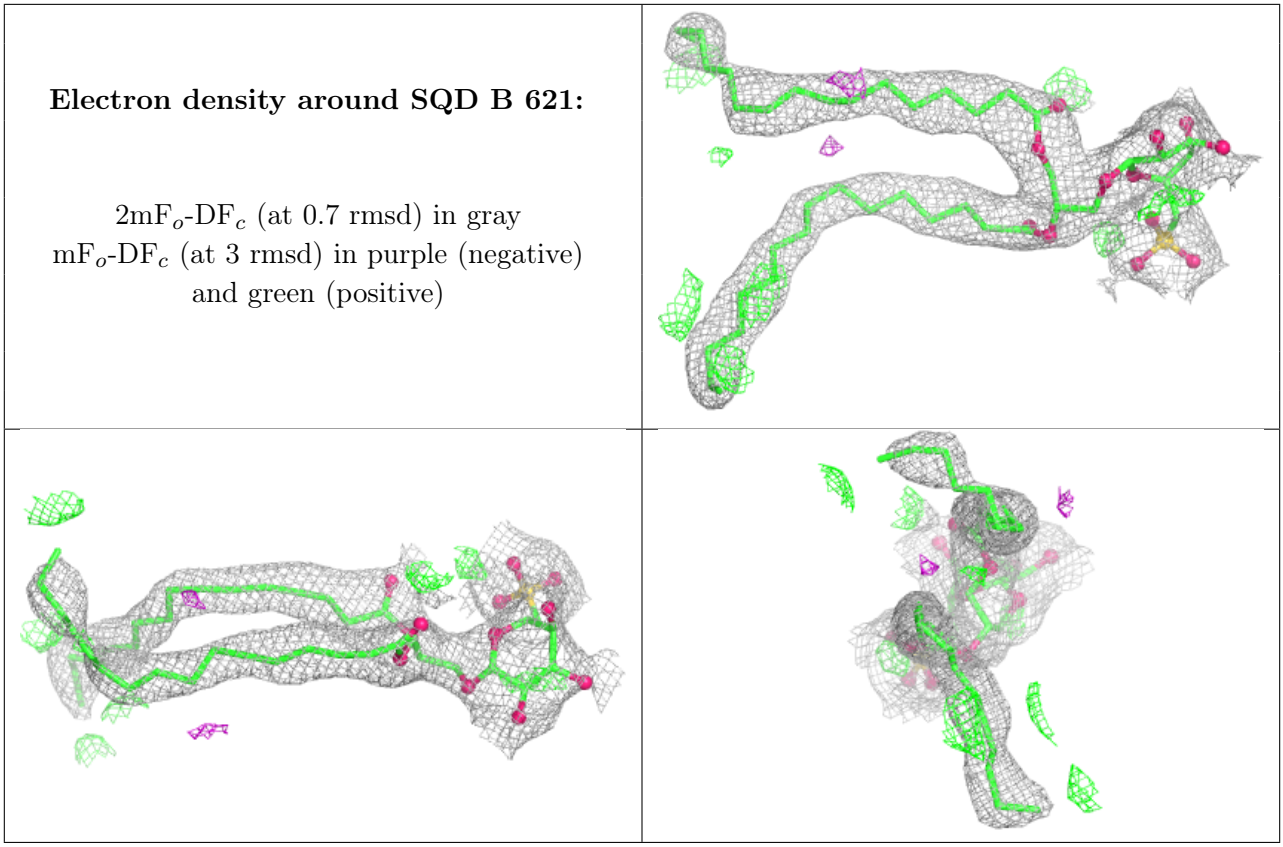






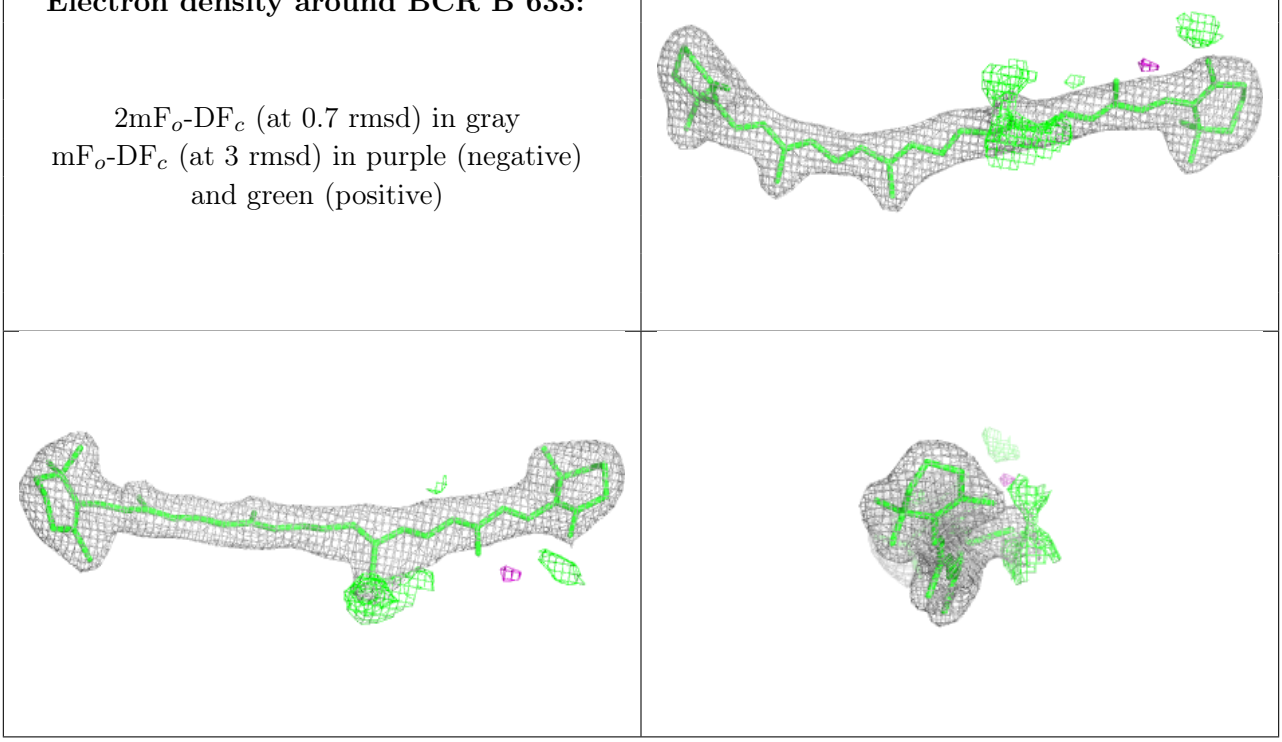
Electron density around SQD B 621:

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



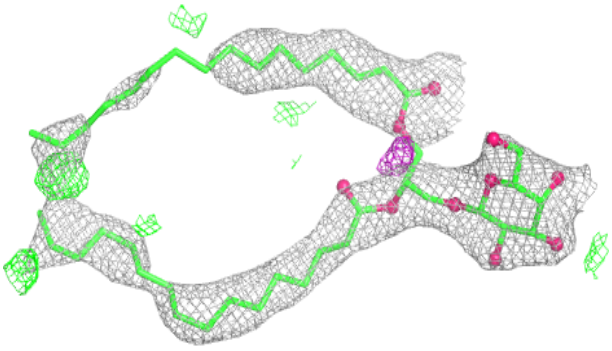
Electron density around BCR B 633:

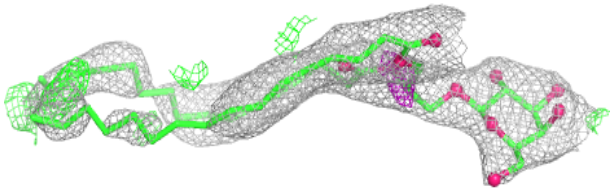
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

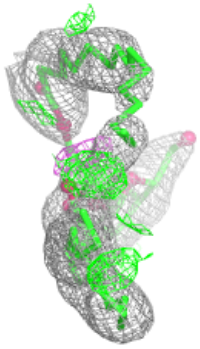


Electron density around LMG c 501:

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

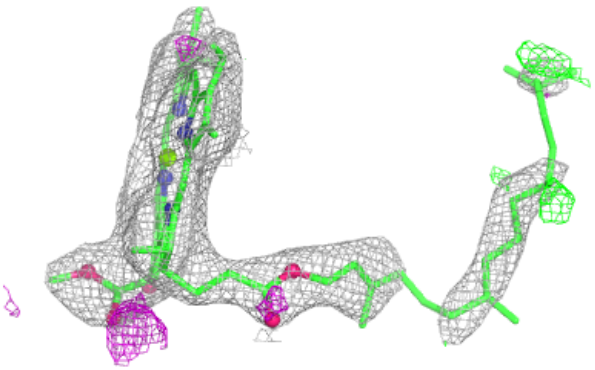


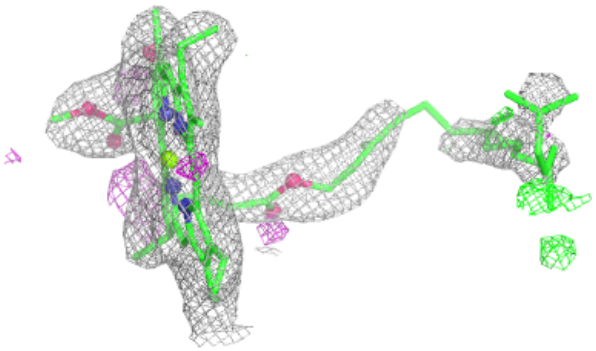


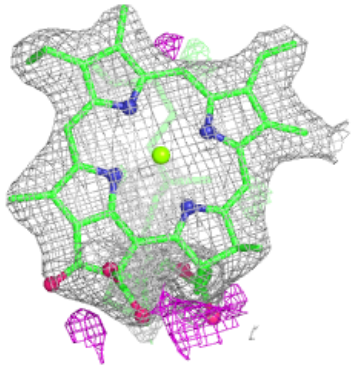


Electron density around CLA C 507:

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

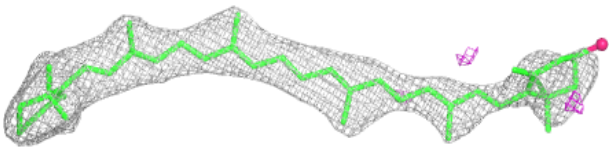


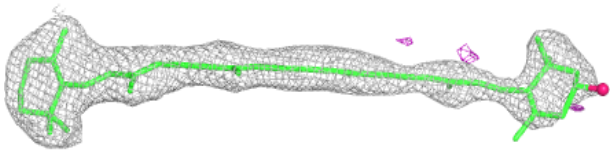


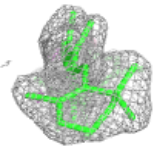


Electron density around RRX h 101:

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

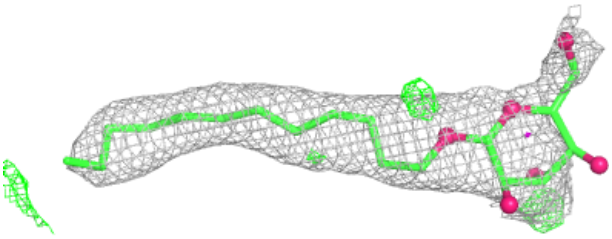


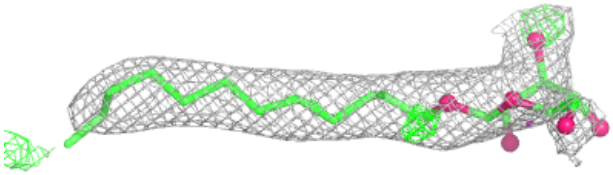


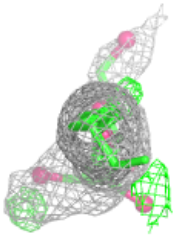


Electron density around LMT A 420:

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

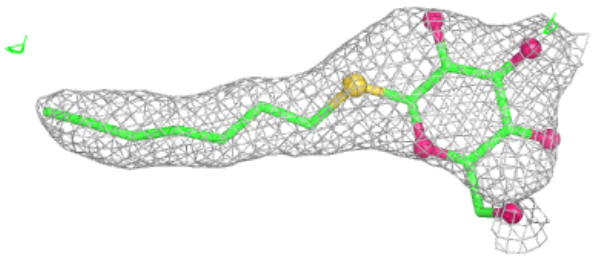


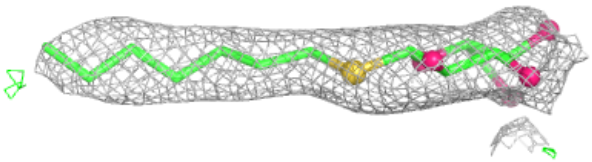


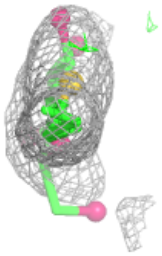


Electron density around HTG B 626:

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

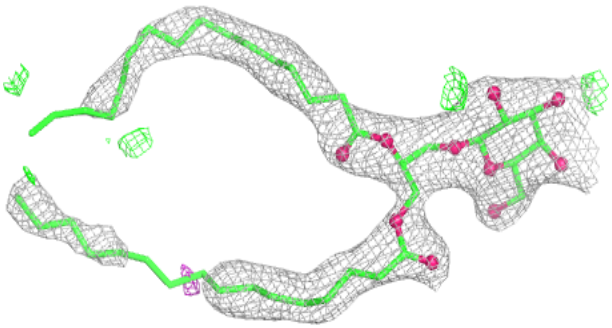


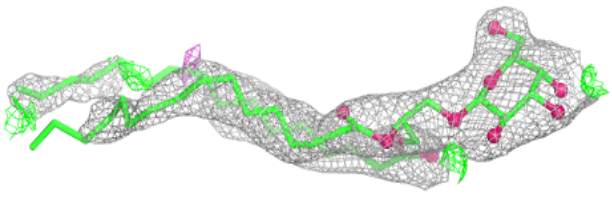


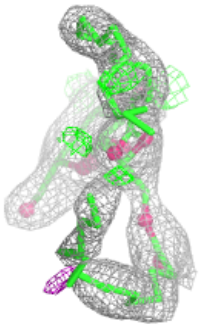


Electron density around LMG A 413:

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

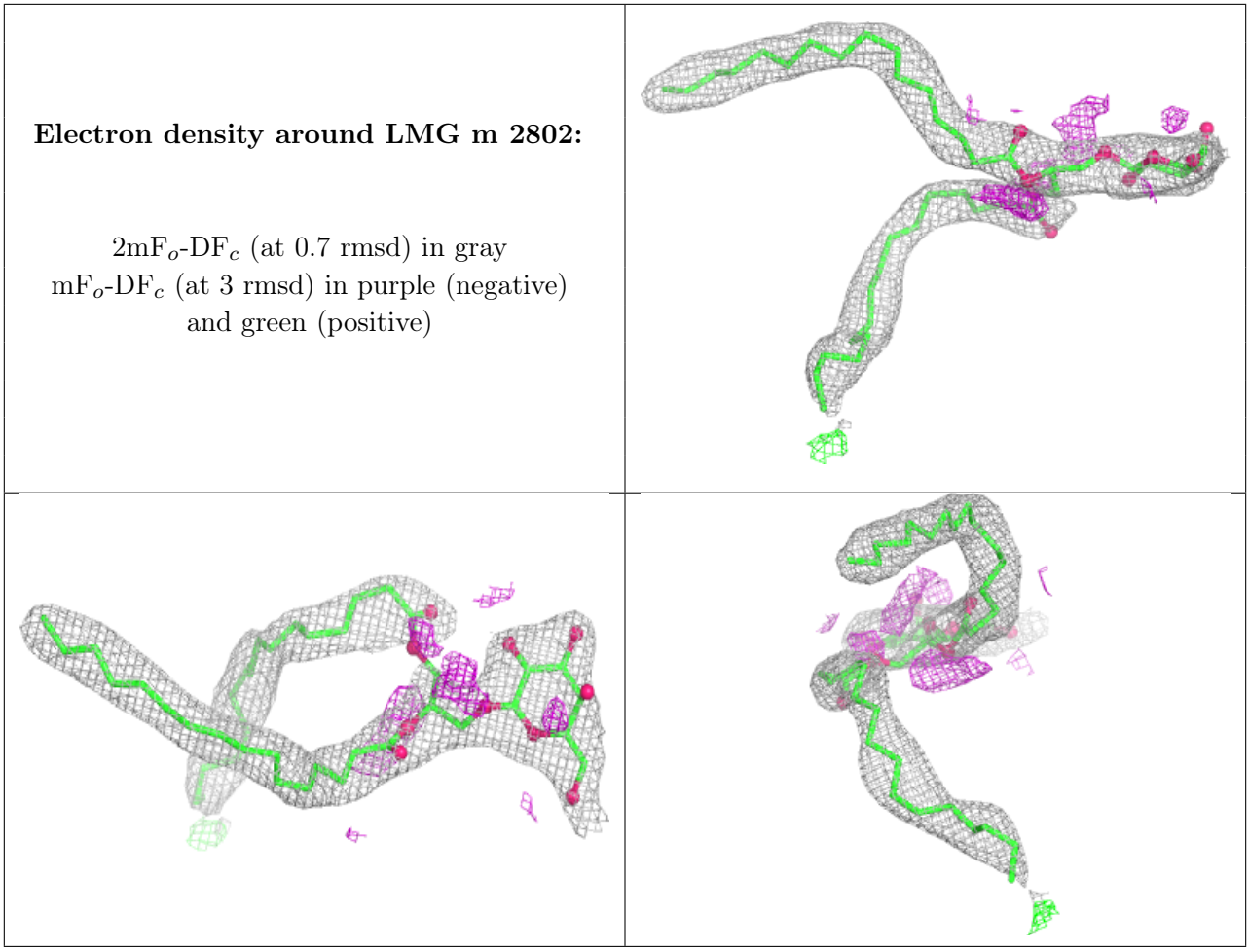






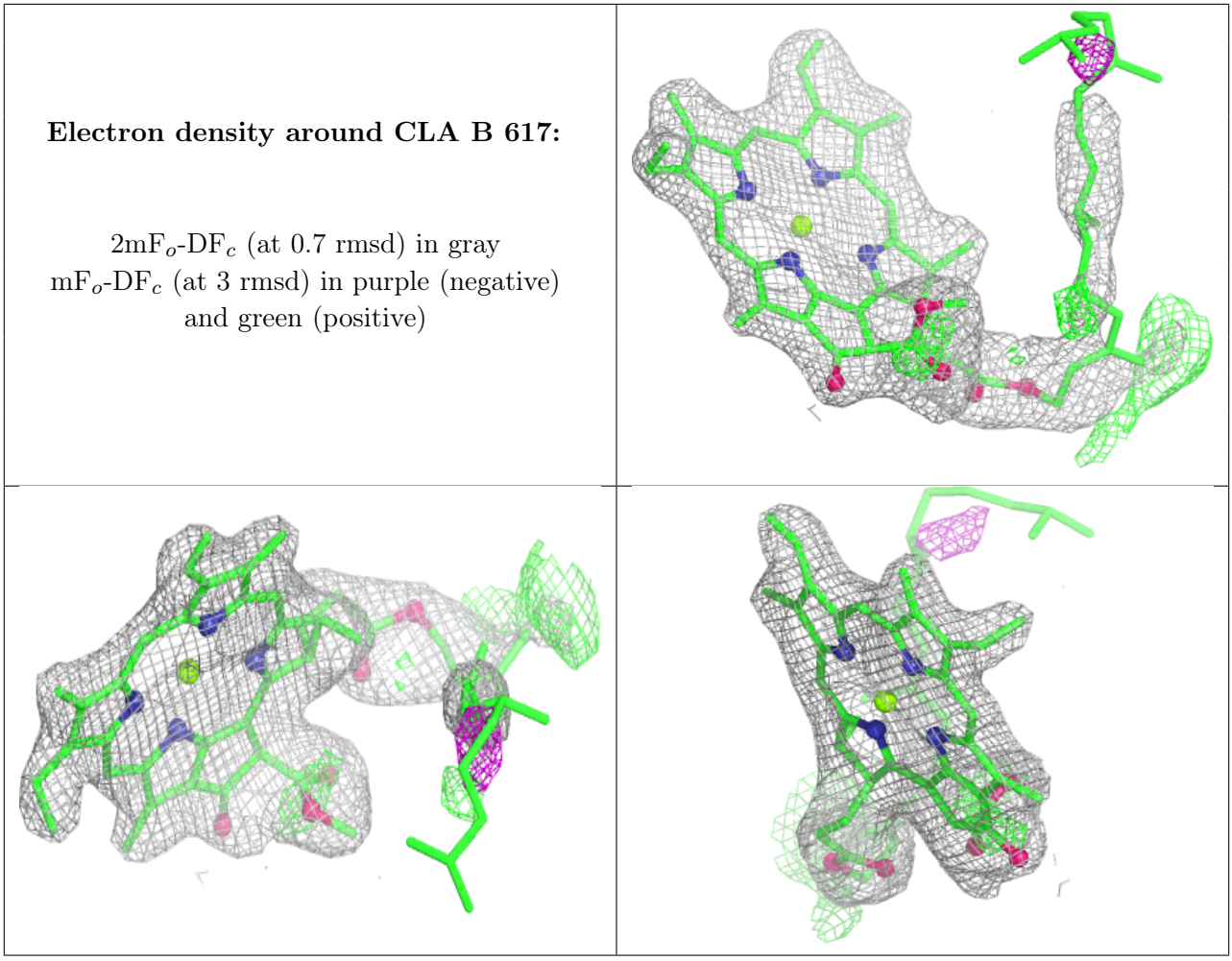
Electron density around LMG m 2802:

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



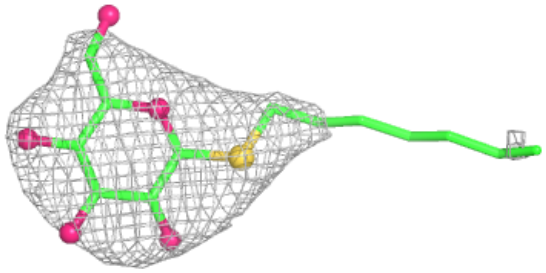
Electron density around CLA B 617:

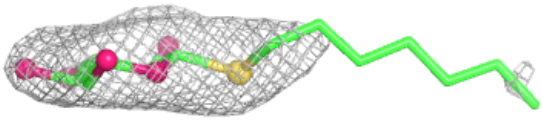
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

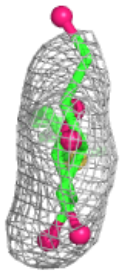


Electron density around HTG C 521:

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

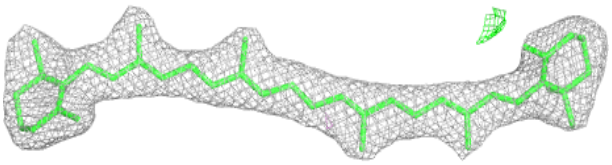


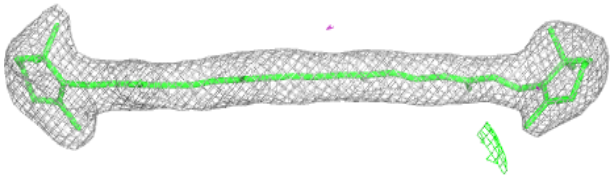


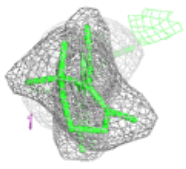


Electron density around BCR b 623:

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

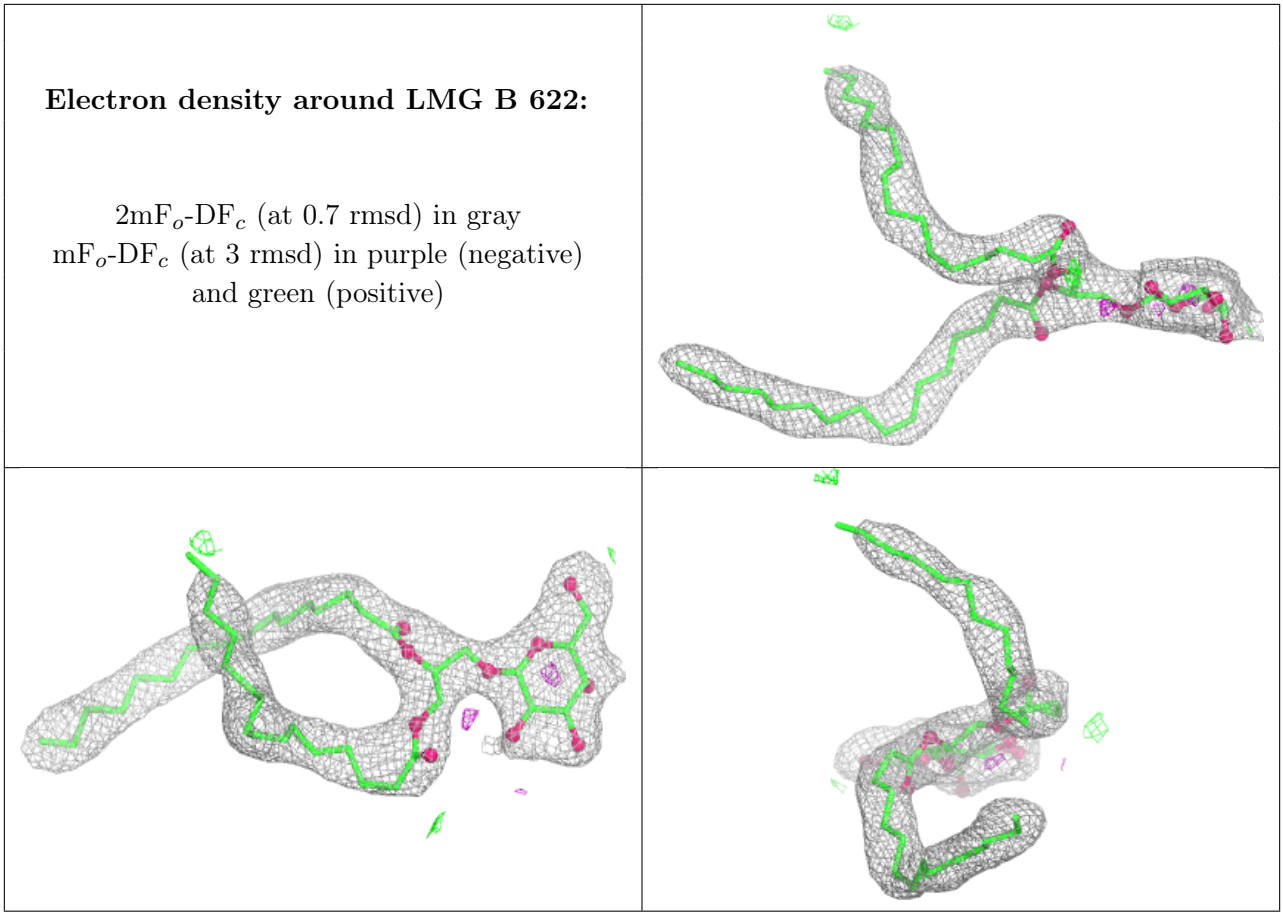






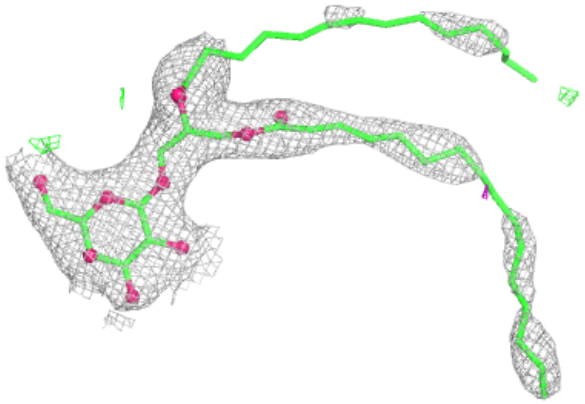
Electron density around LMG B 622:

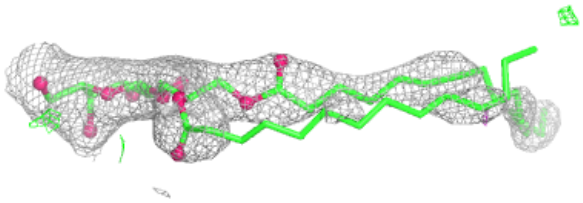
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

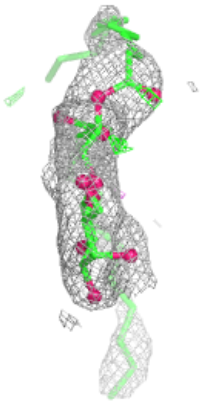


Electron density around LMG c 521:

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

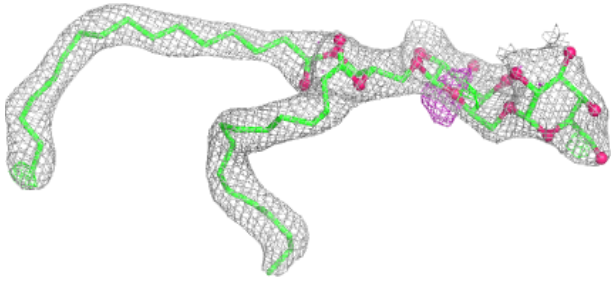


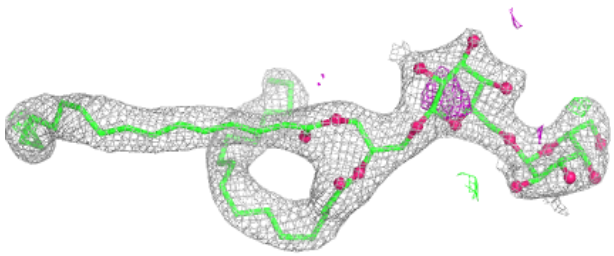




Electron density around DGD h 102:

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

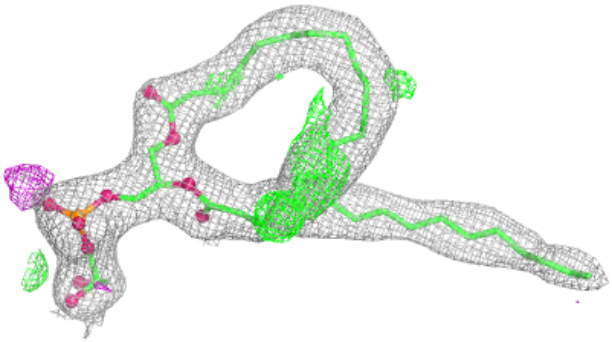


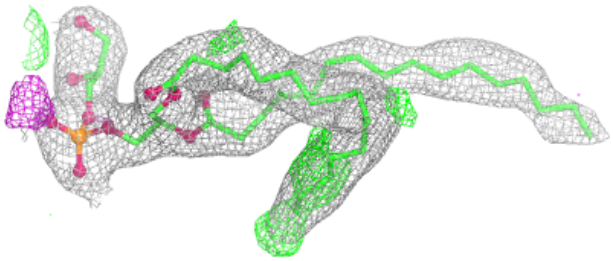




Electron density around LHG D 2309:

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

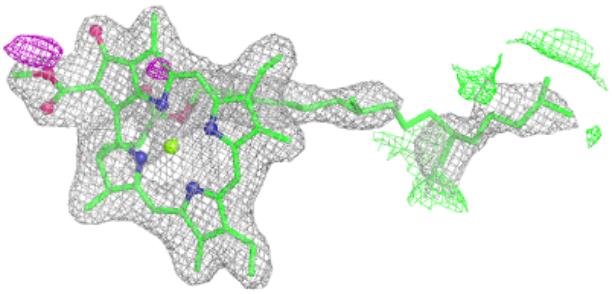


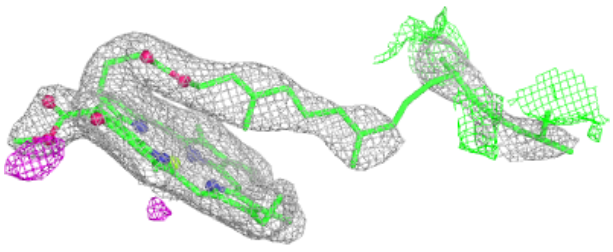


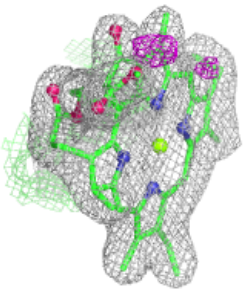


Electron density around CLA b 619:

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

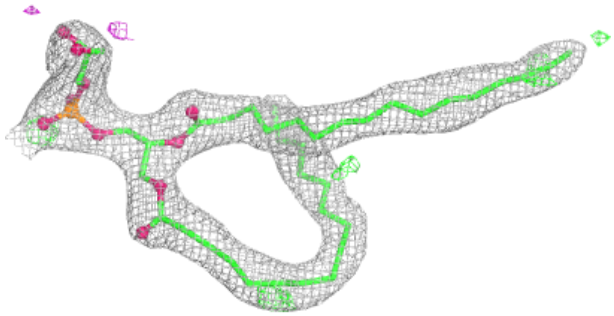


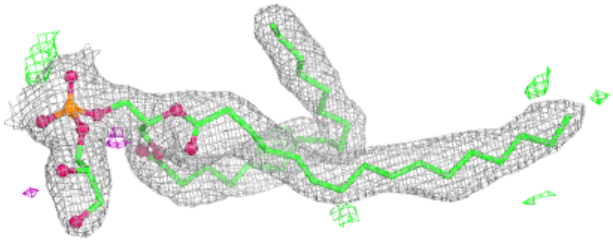


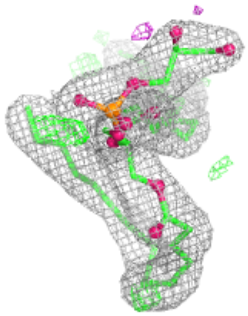


Electron density around LHG d 412:

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

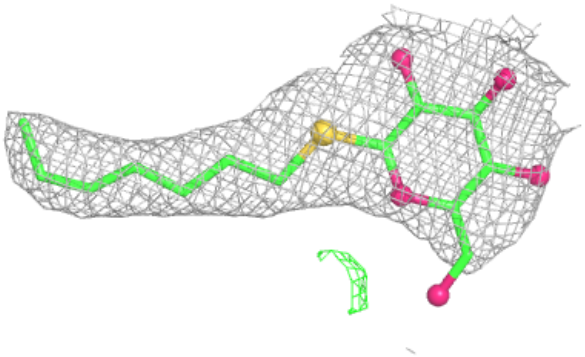


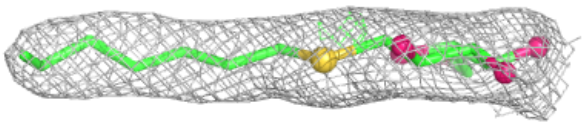


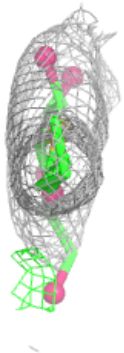


Electron density around HTG b 603:

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

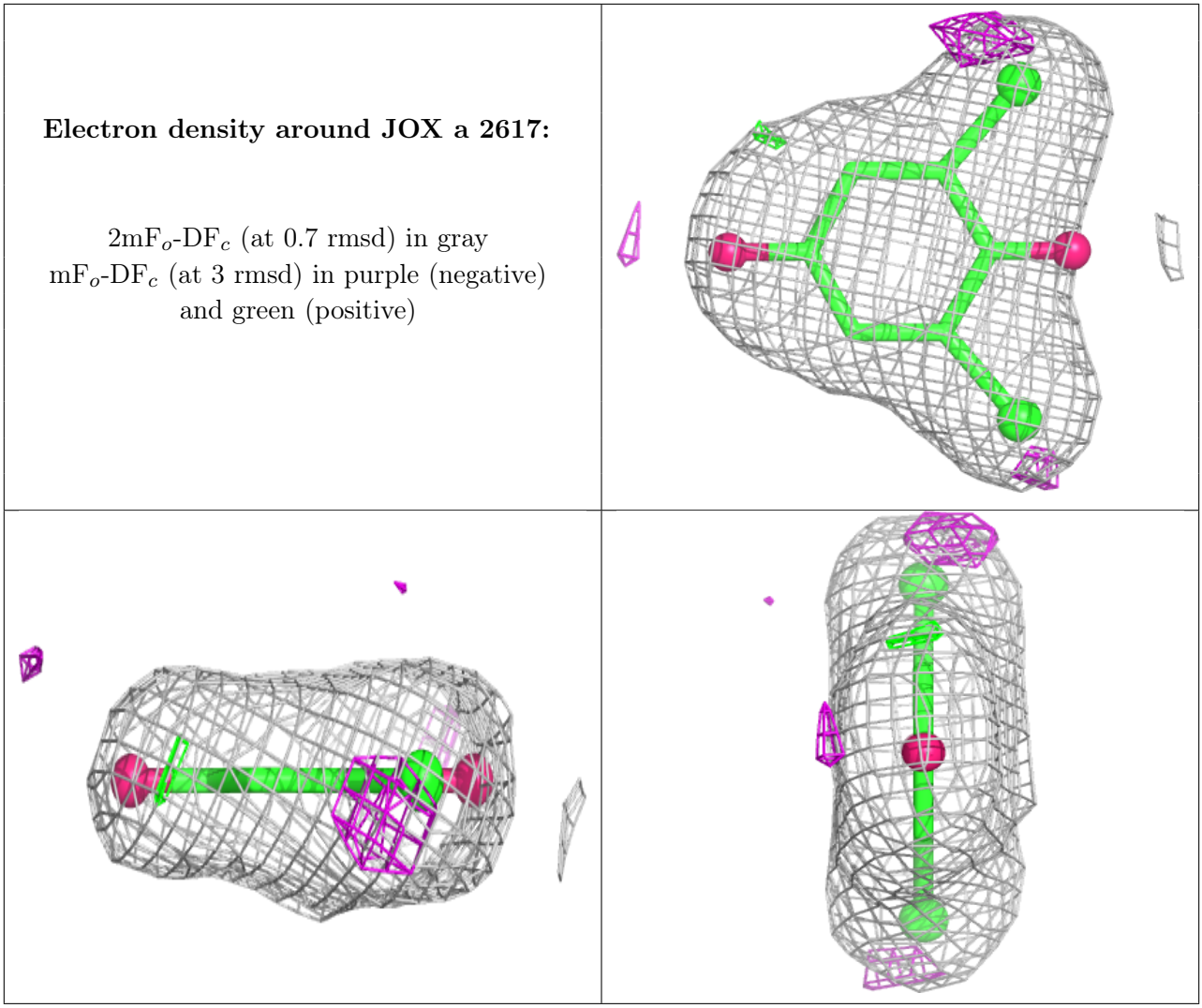






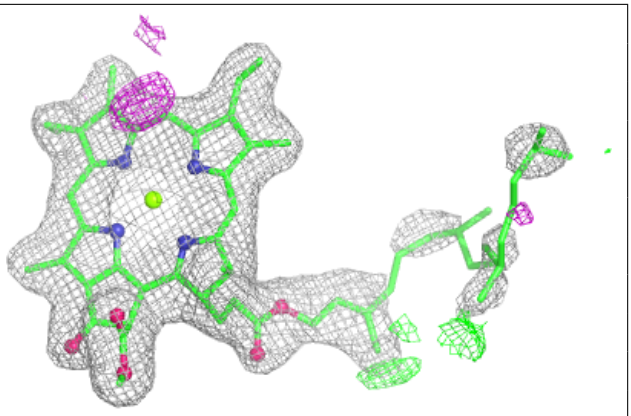
Electron density around JOX a 2617:

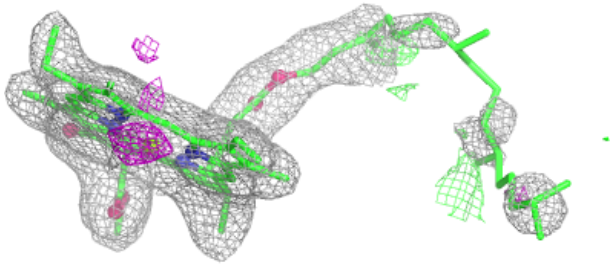
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA a 2613:

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

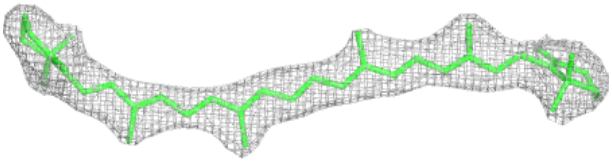


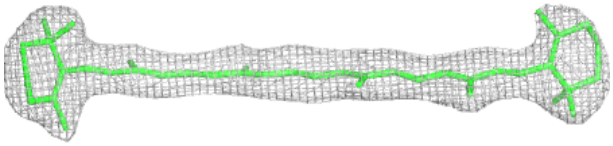




Electron density around BCR C 516:

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

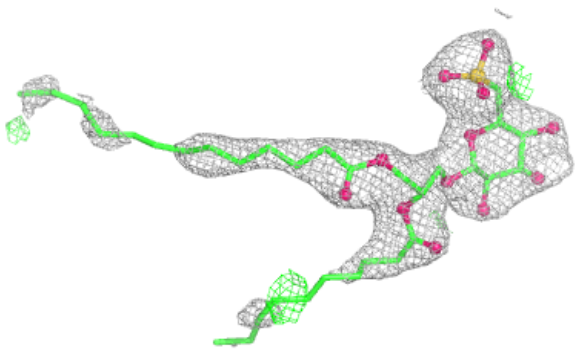


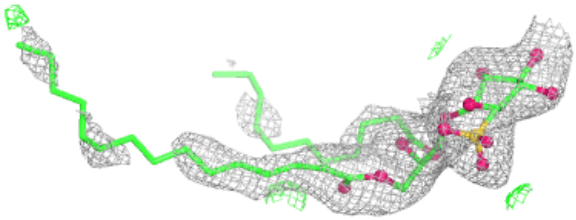


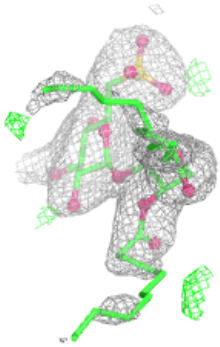


Electron density around SQD a 2615:

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

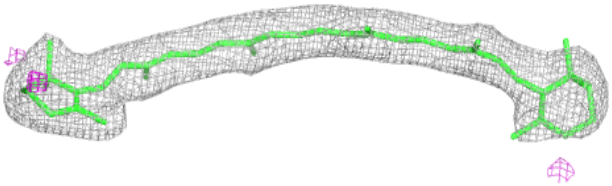


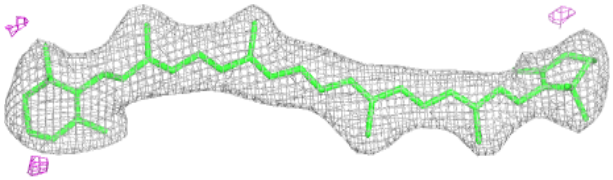


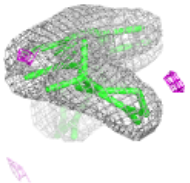


Electron density around BCR D 2305:

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

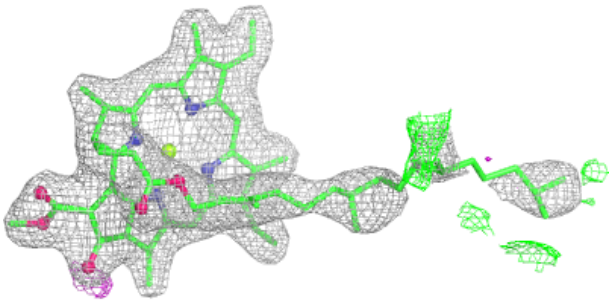


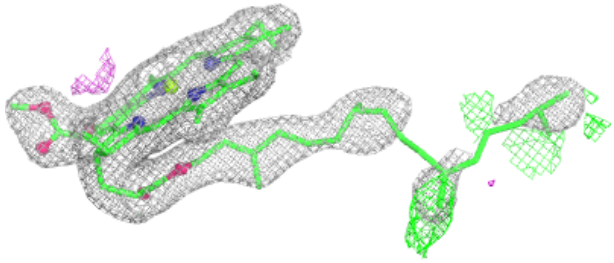


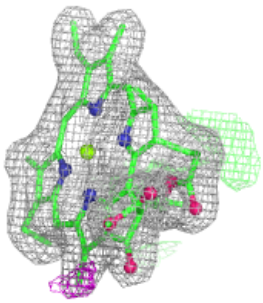


Electron density around CLA B 615:

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

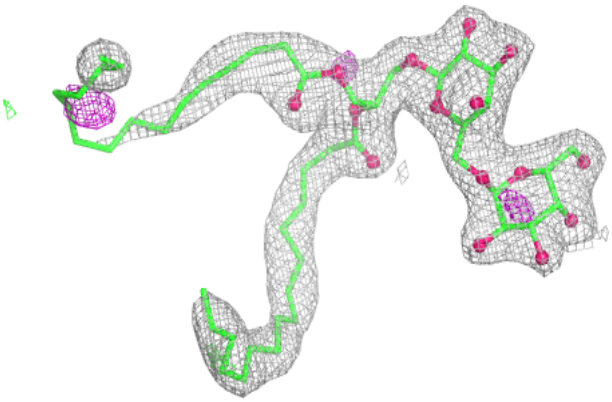


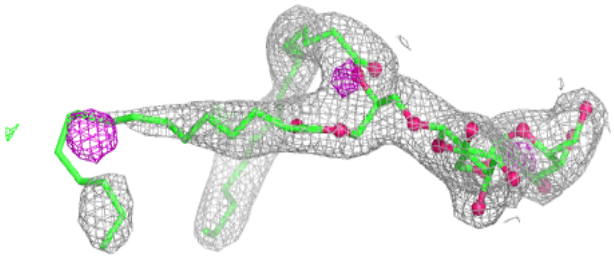


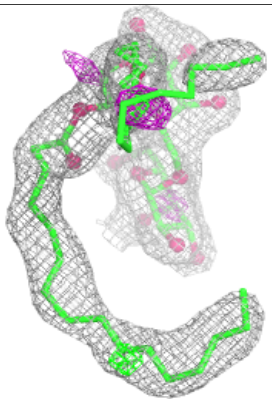


Electron density around DGD C 518:

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

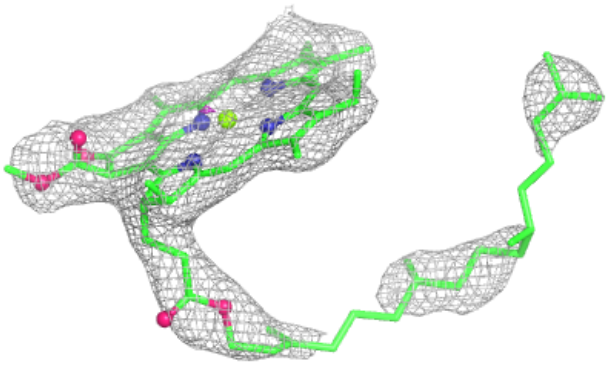


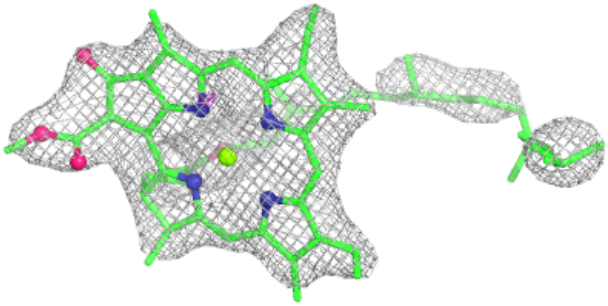


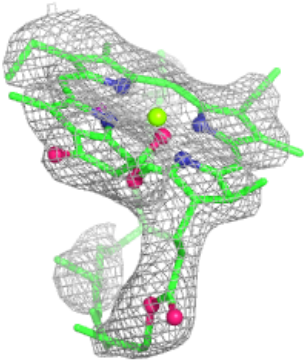


Electron density around CLA C 514:

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

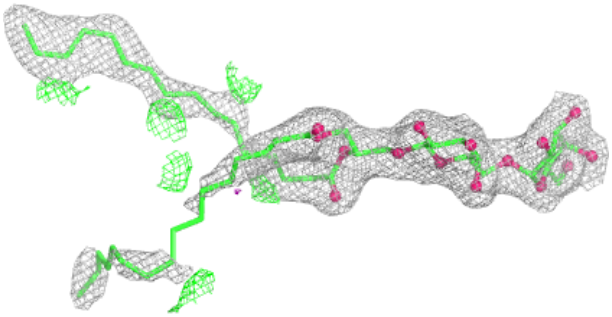


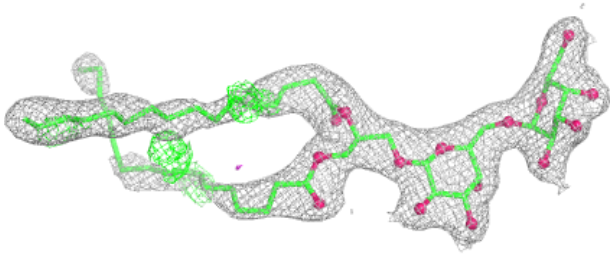


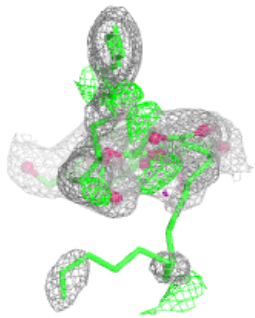


Electron density around DGD c 518:

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

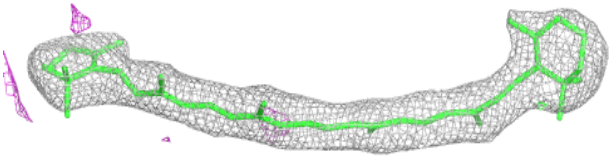


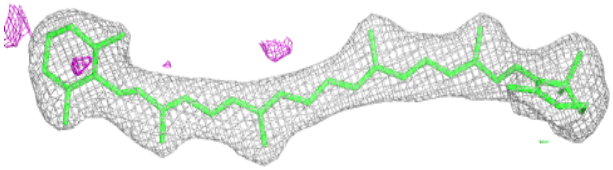


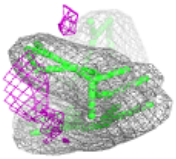


Electron density around BCR d 410:

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

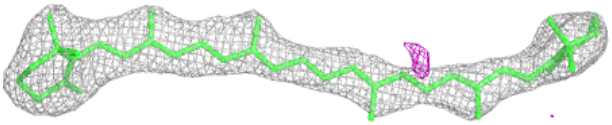


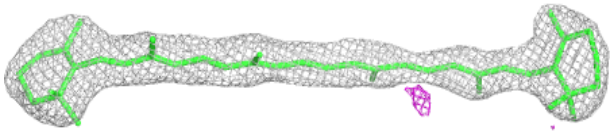


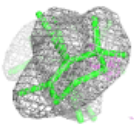


Electron density around BCR z 101:

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

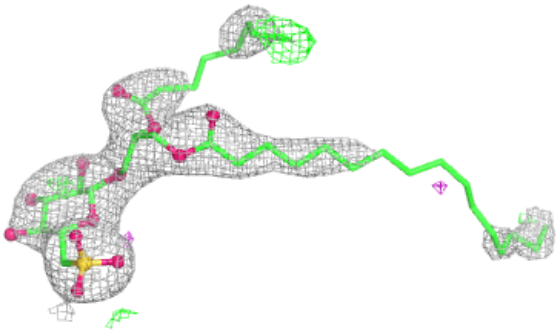


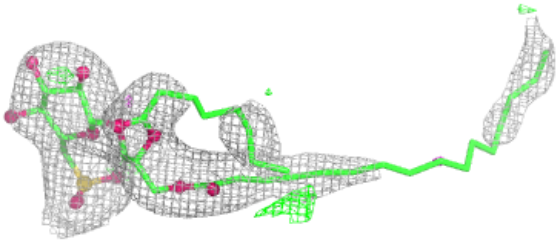


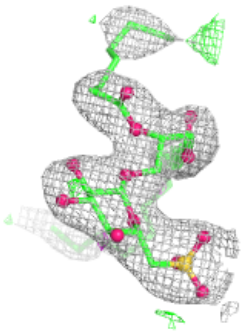


Electron density around SQD A 412:

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

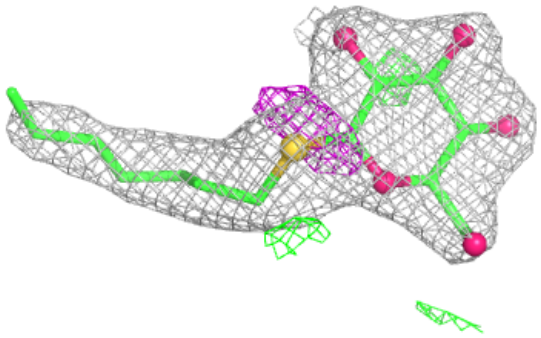


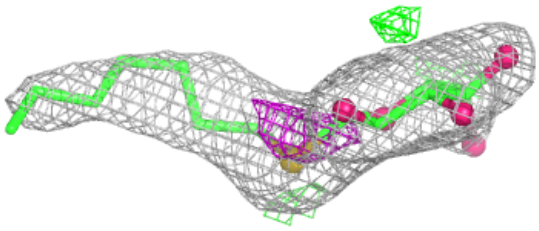


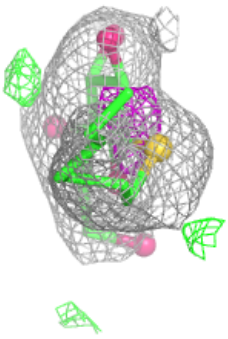


Electron density around HTG b 602:

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

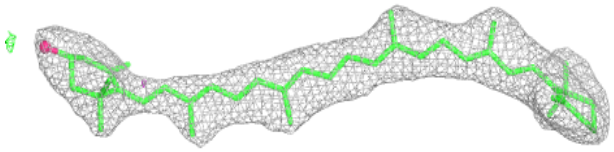


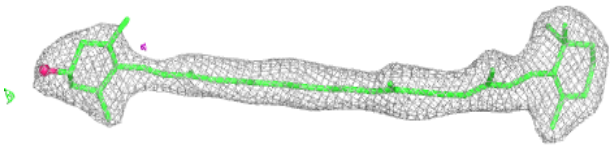


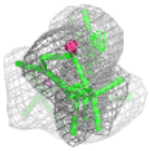


Electron density around RRX H 102:

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

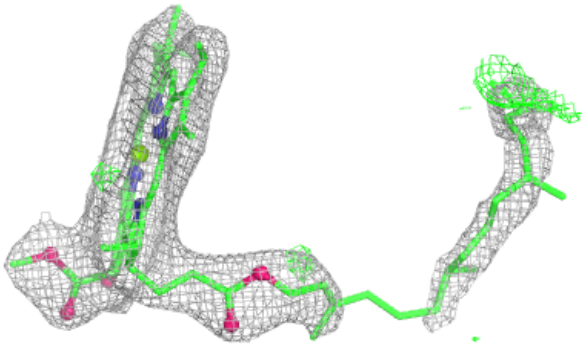


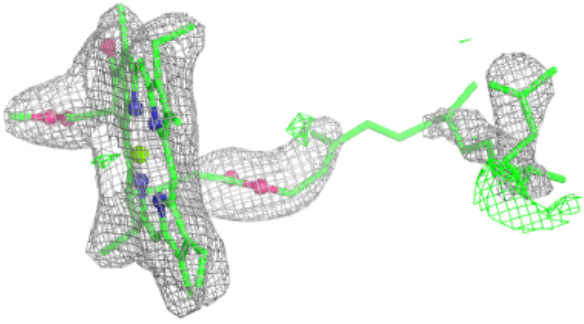


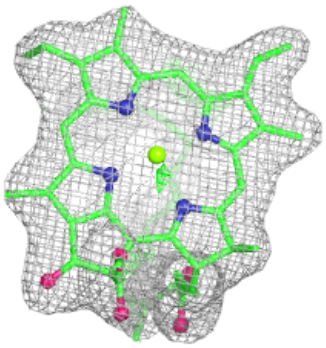


Electron density around CLA c 509:

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

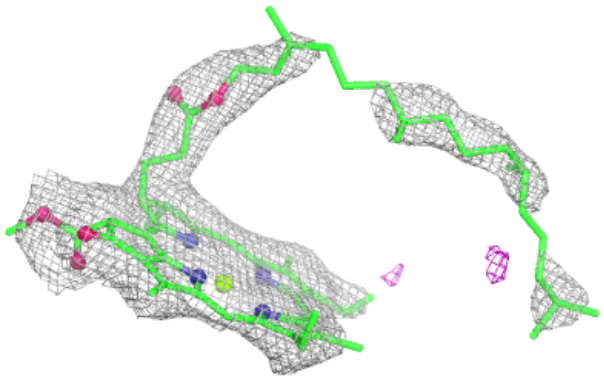


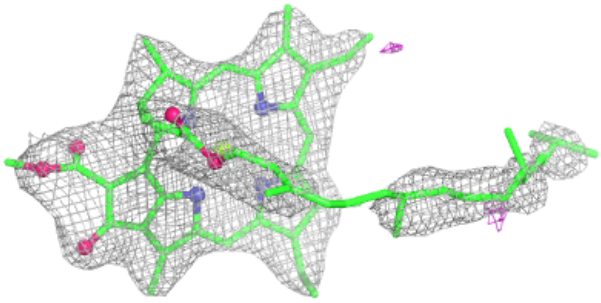


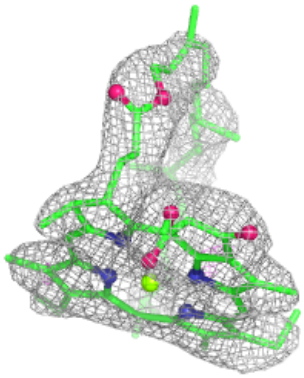


Electron density around CLA c 516:

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

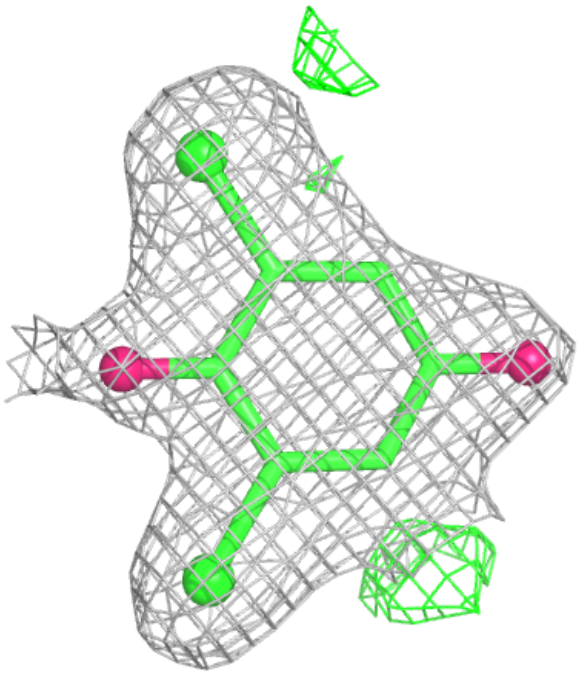


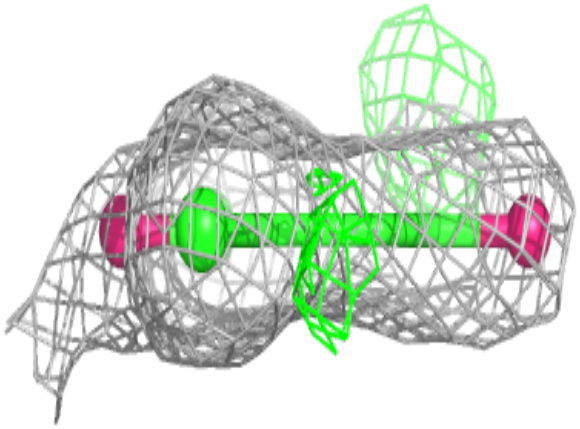


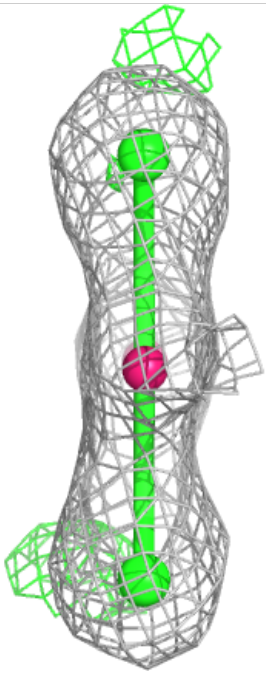


Electron density around JOX a 2619:

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

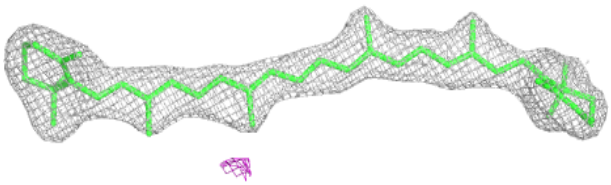


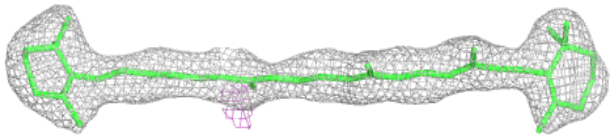


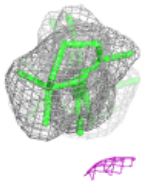


Electron density around BCR C 515:

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

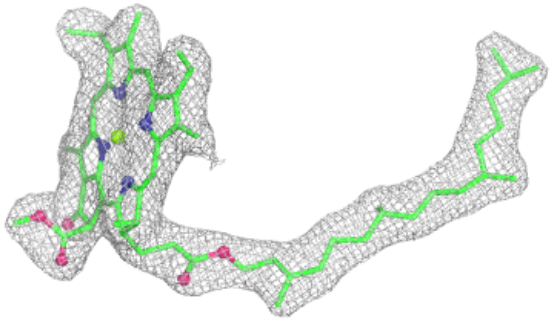


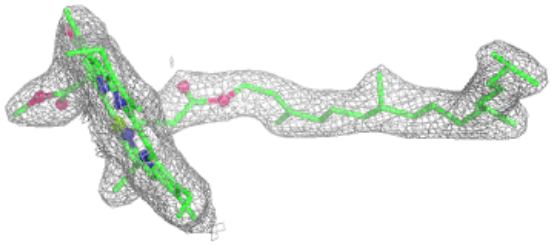


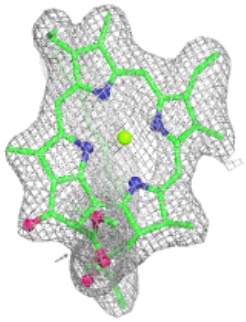


Electron density around CLA B 610:

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

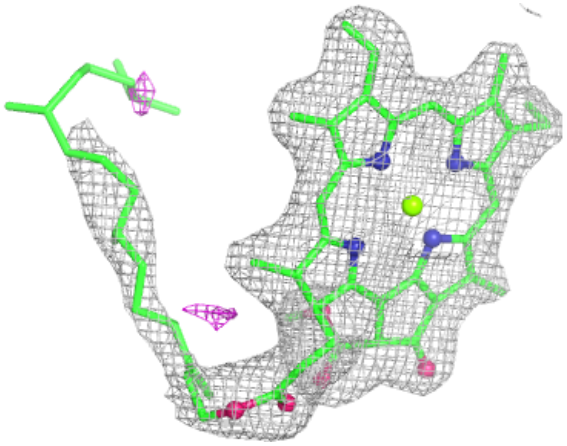


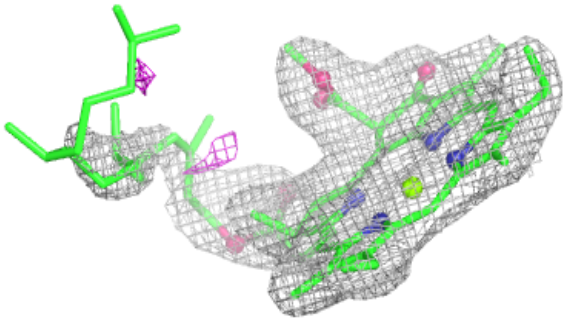


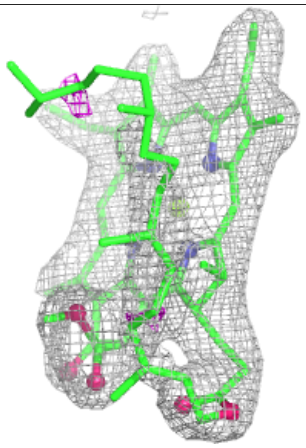


Electron density around CLA b 621:

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

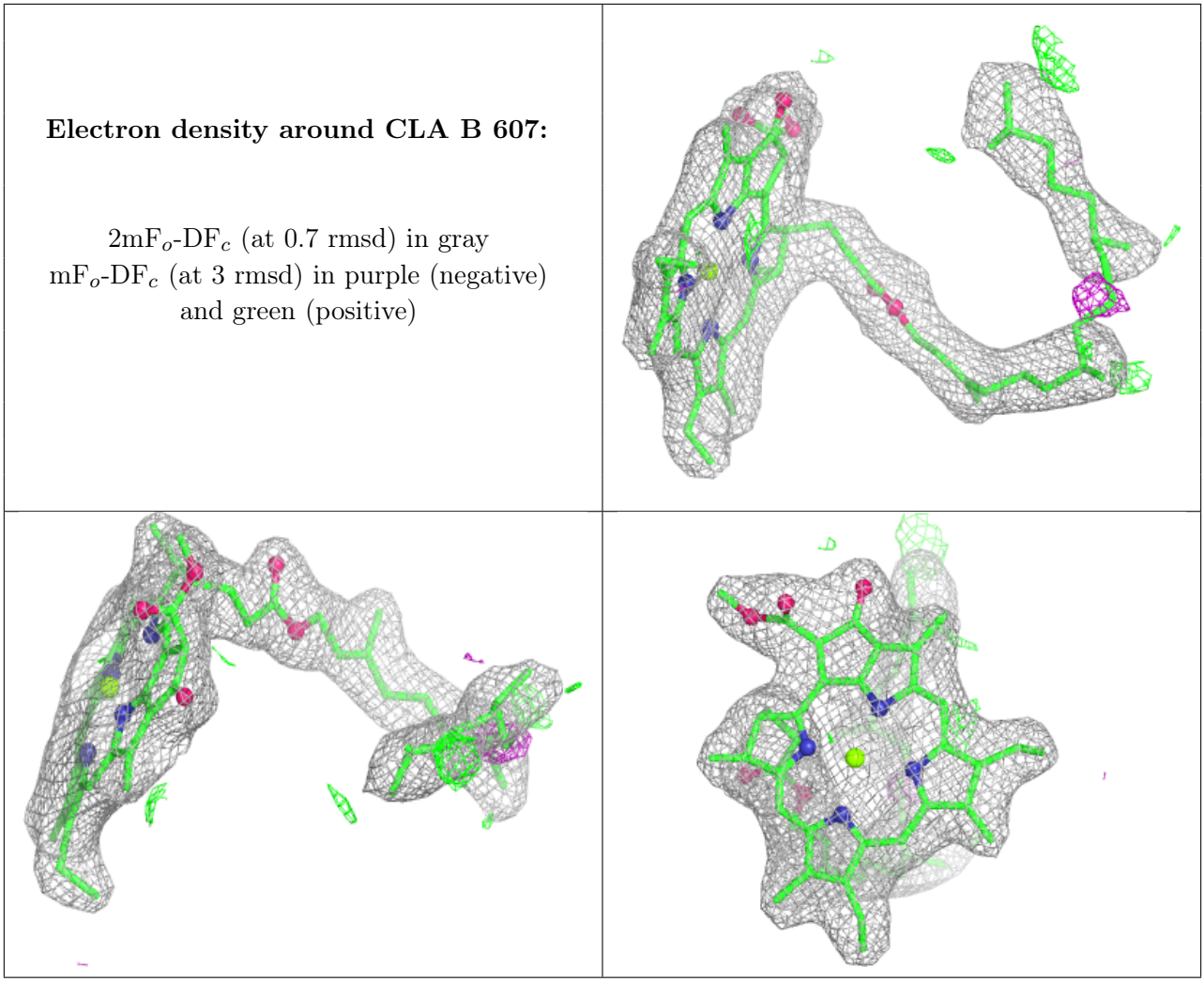






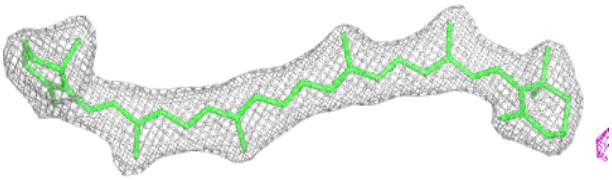
Electron density around CLA B 607:

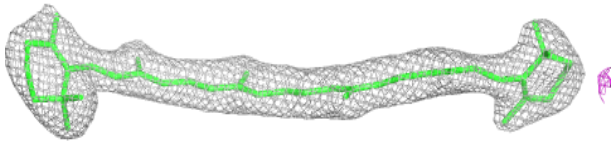
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

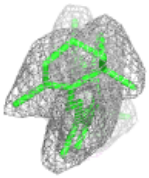


Electron density around BCR Y 302:

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

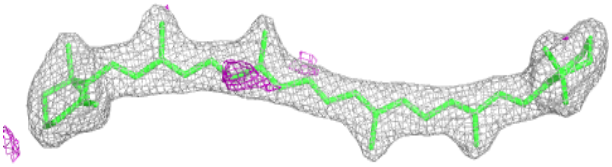


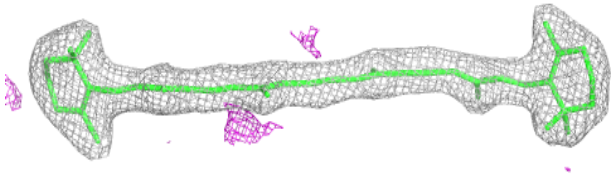


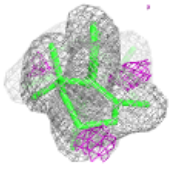


Electron density around BCR a 2614:

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

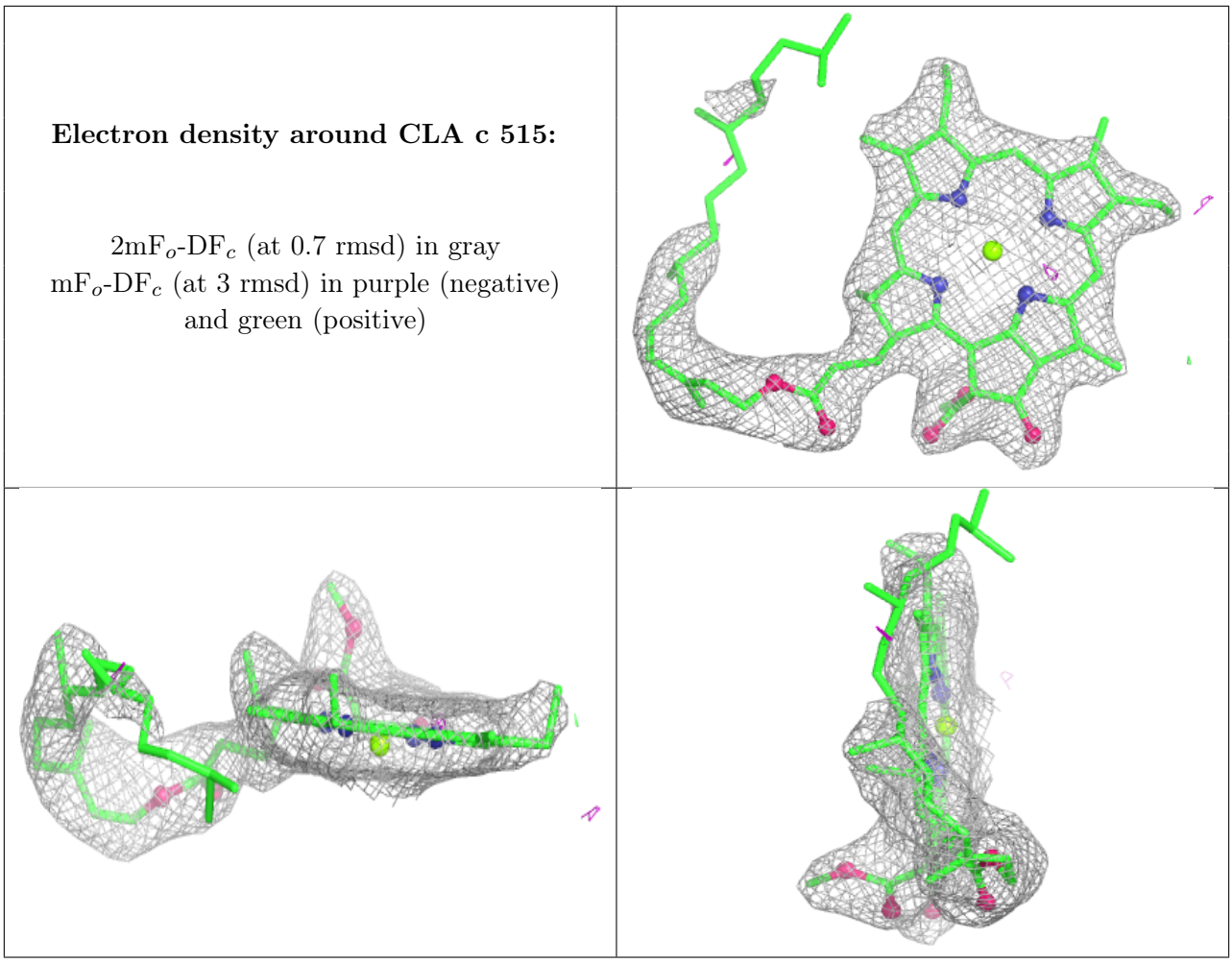






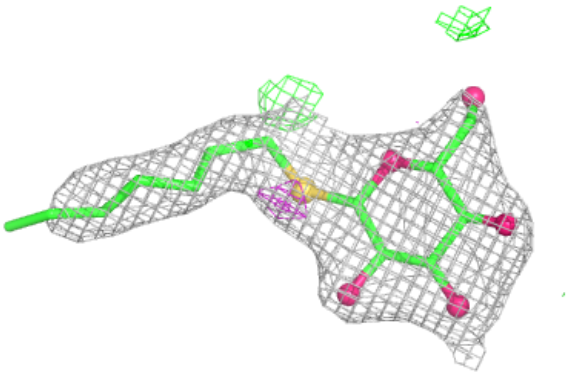
Electron density around CLA c 515:

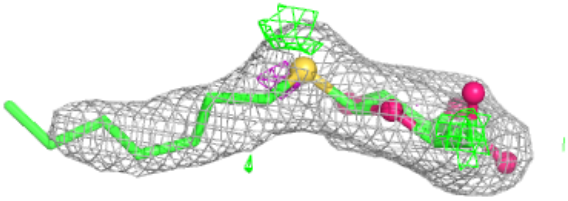
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

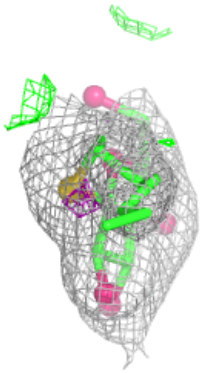


Electron density around HTG o 301:

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

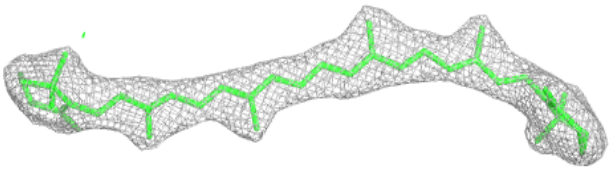


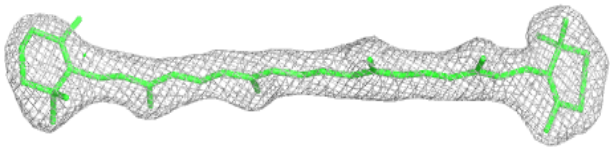


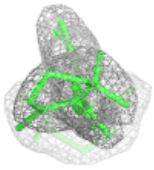


Electron density around BCR c 517:

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

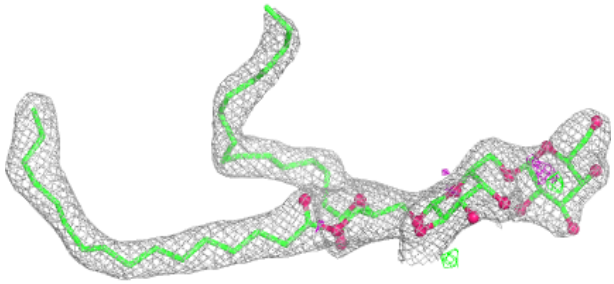


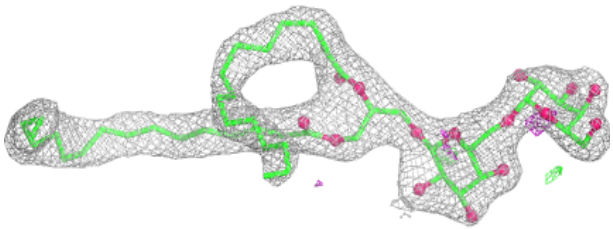


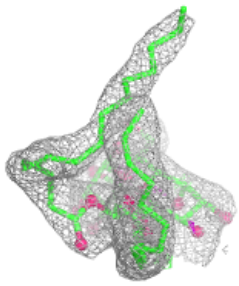


Electron density around DGD H 103:

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

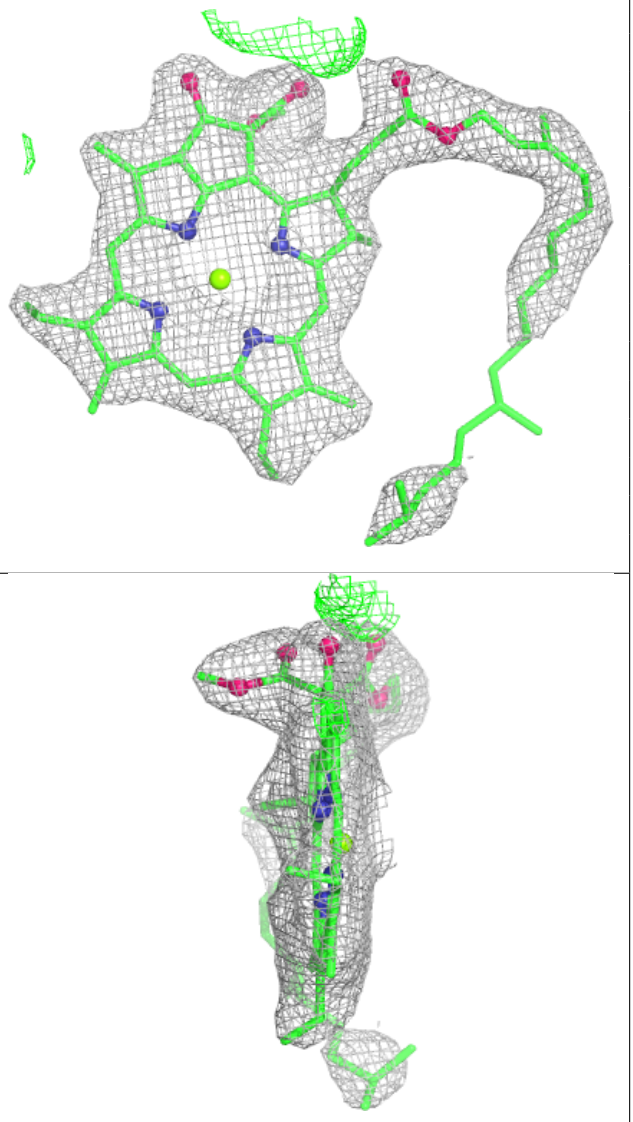






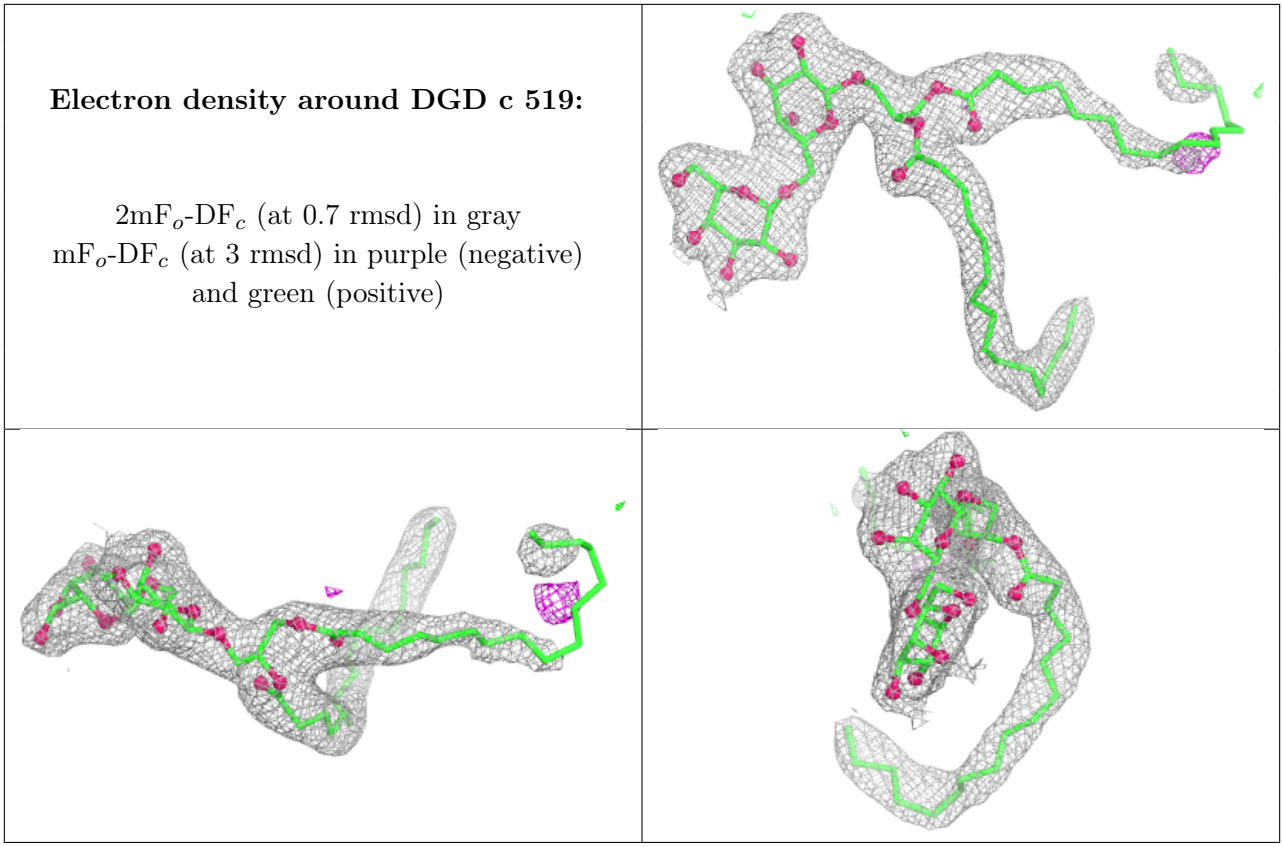
Electron density around CLA C 513:

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



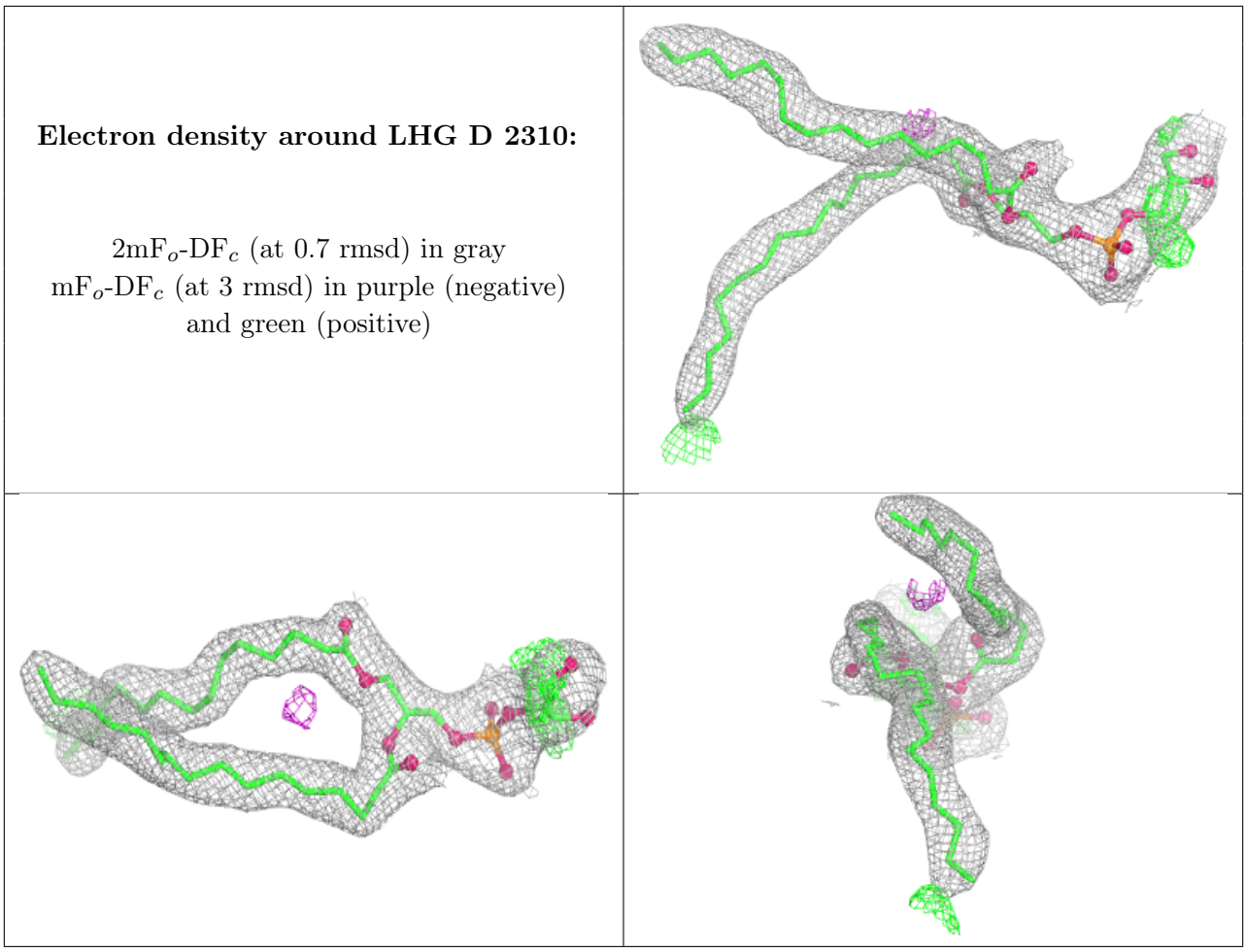
Electron density around DGD c 519:

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



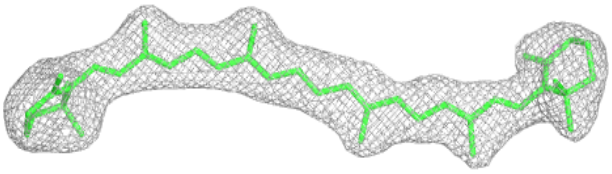
Electron density around LHG D 2310:

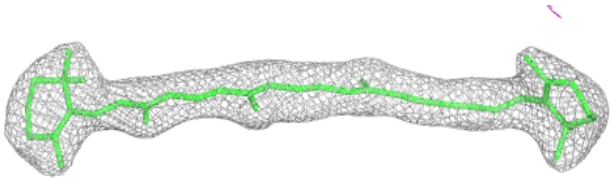
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

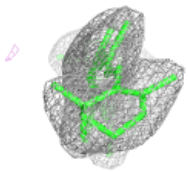


Electron density around BCR y 101:

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

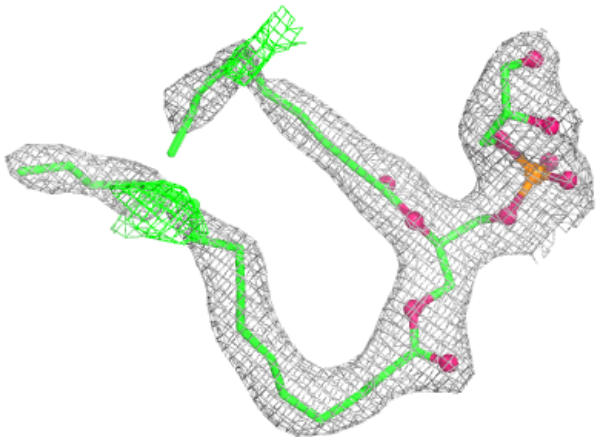


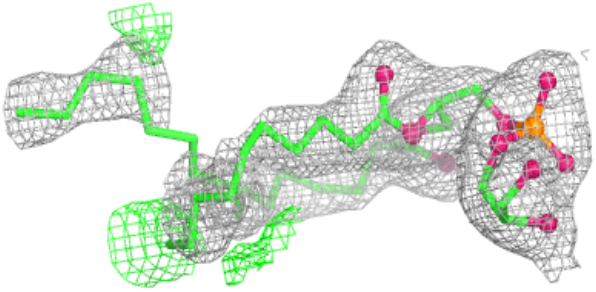


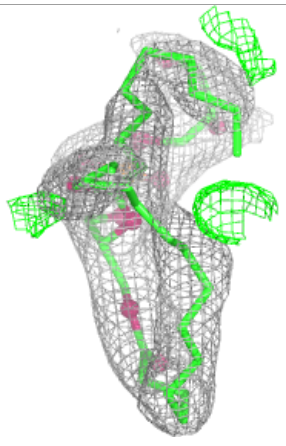


Electron density around LHG d 403:

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

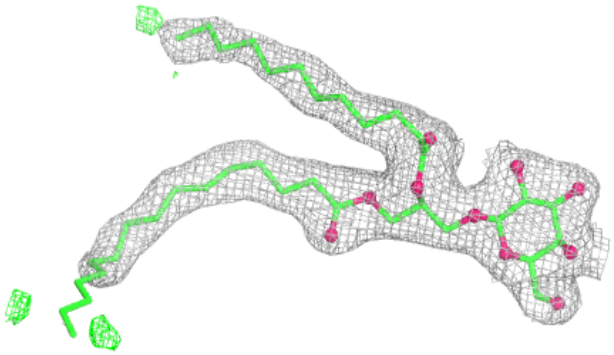


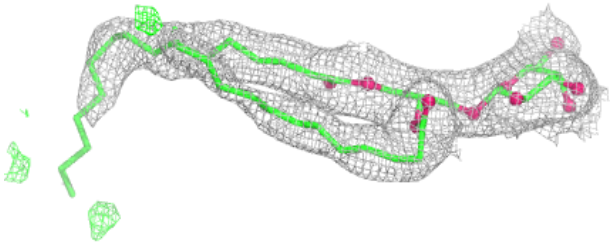


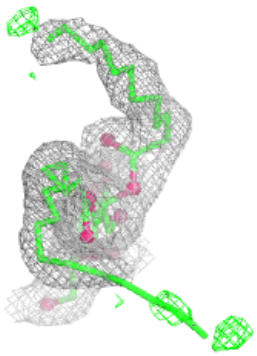


Electron density around LMG D 2312:

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

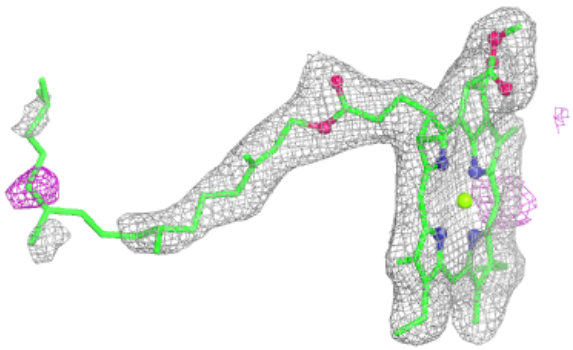


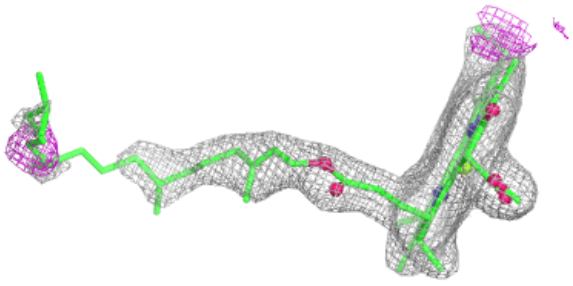


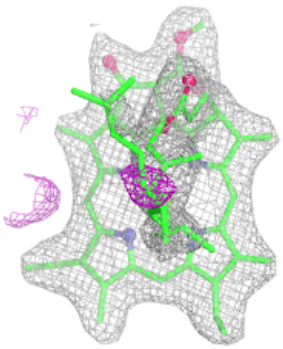


Electron density around CLA d 409:

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

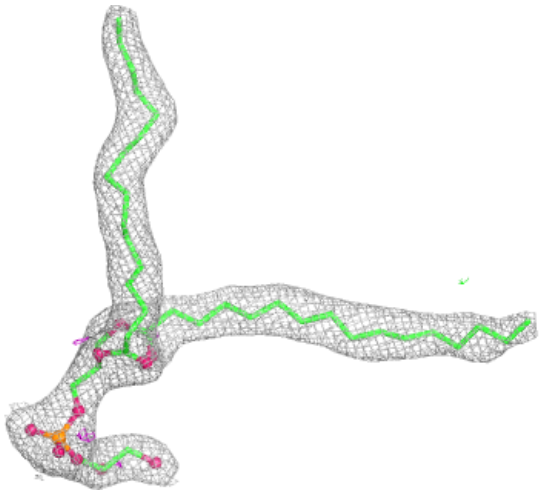


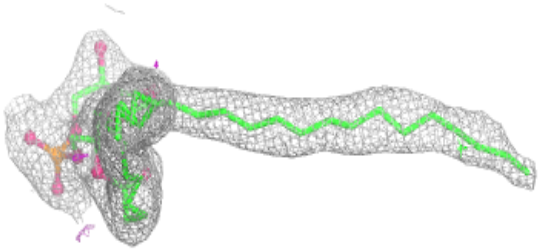


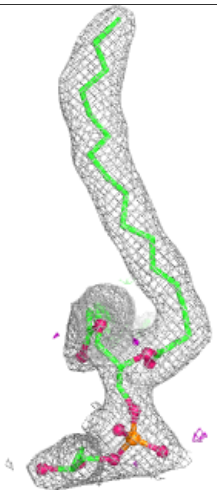


Electron density around LHG l 103:

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

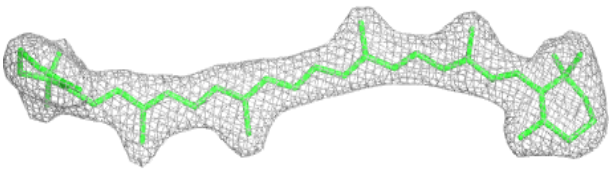


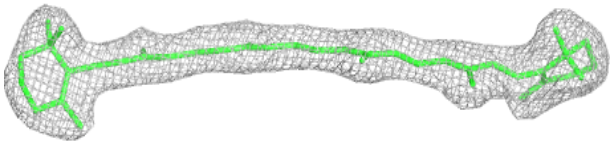


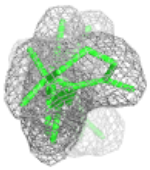


Electron density around BCR B 618:

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

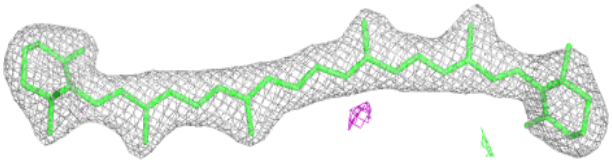


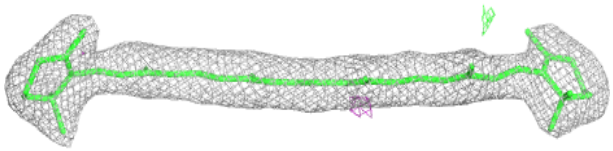


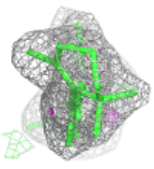


Electron density around BCR B 619:

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

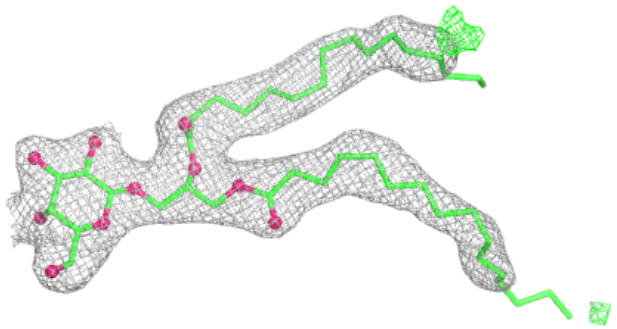


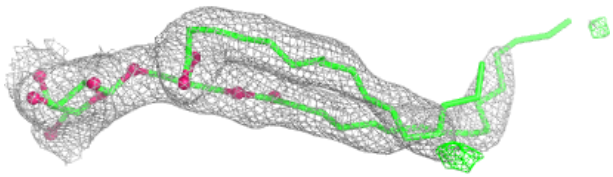




Electron density around LMG d 414:

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

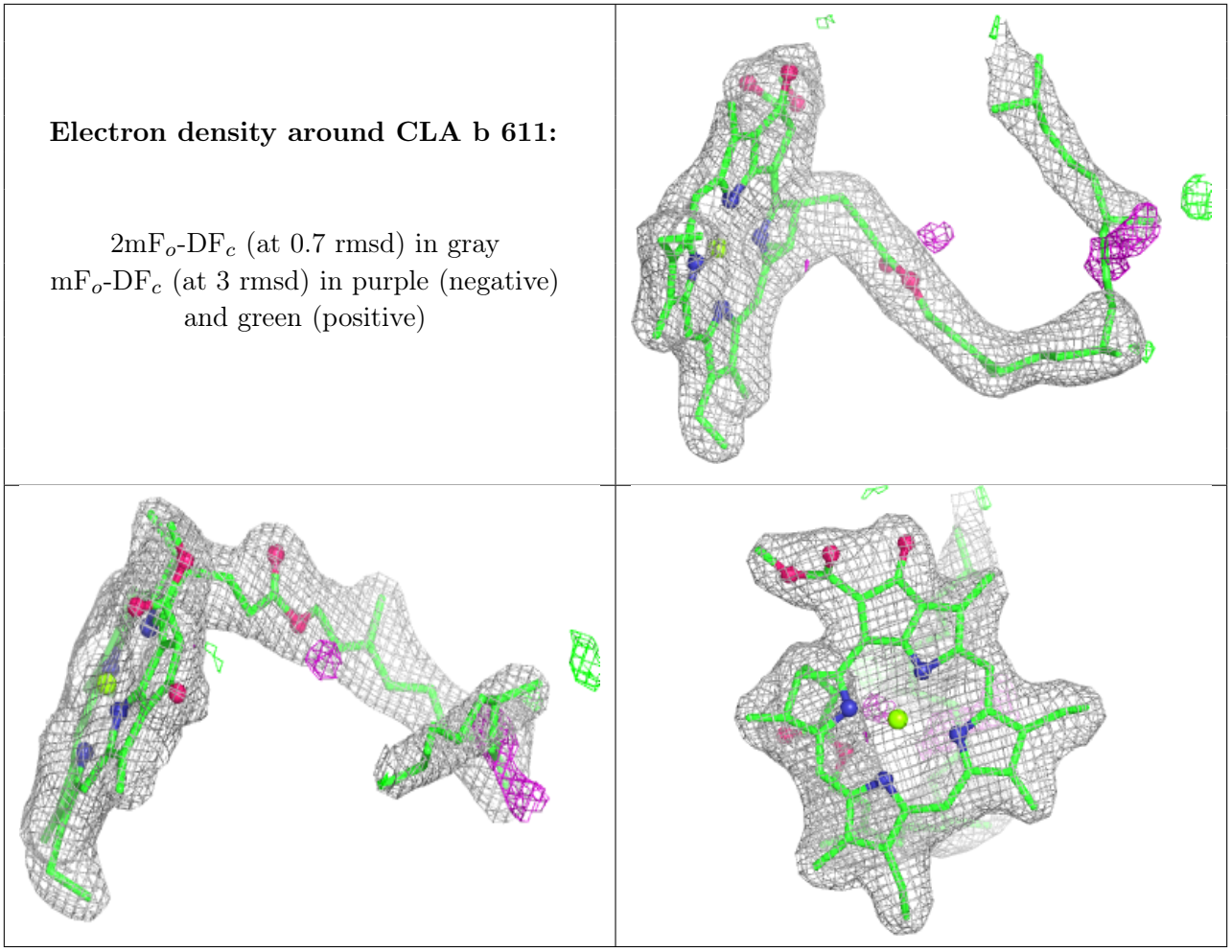






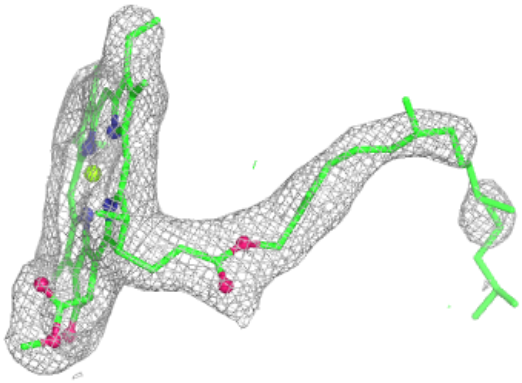
Electron density around CLA b 611:

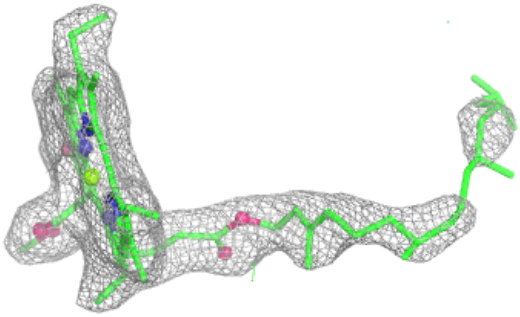
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

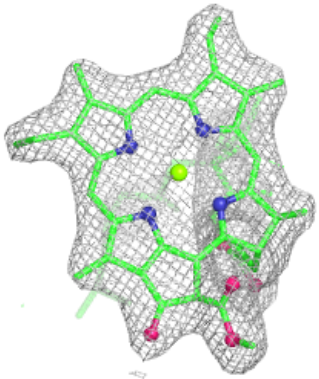


Electron density around CLA D 2304:

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

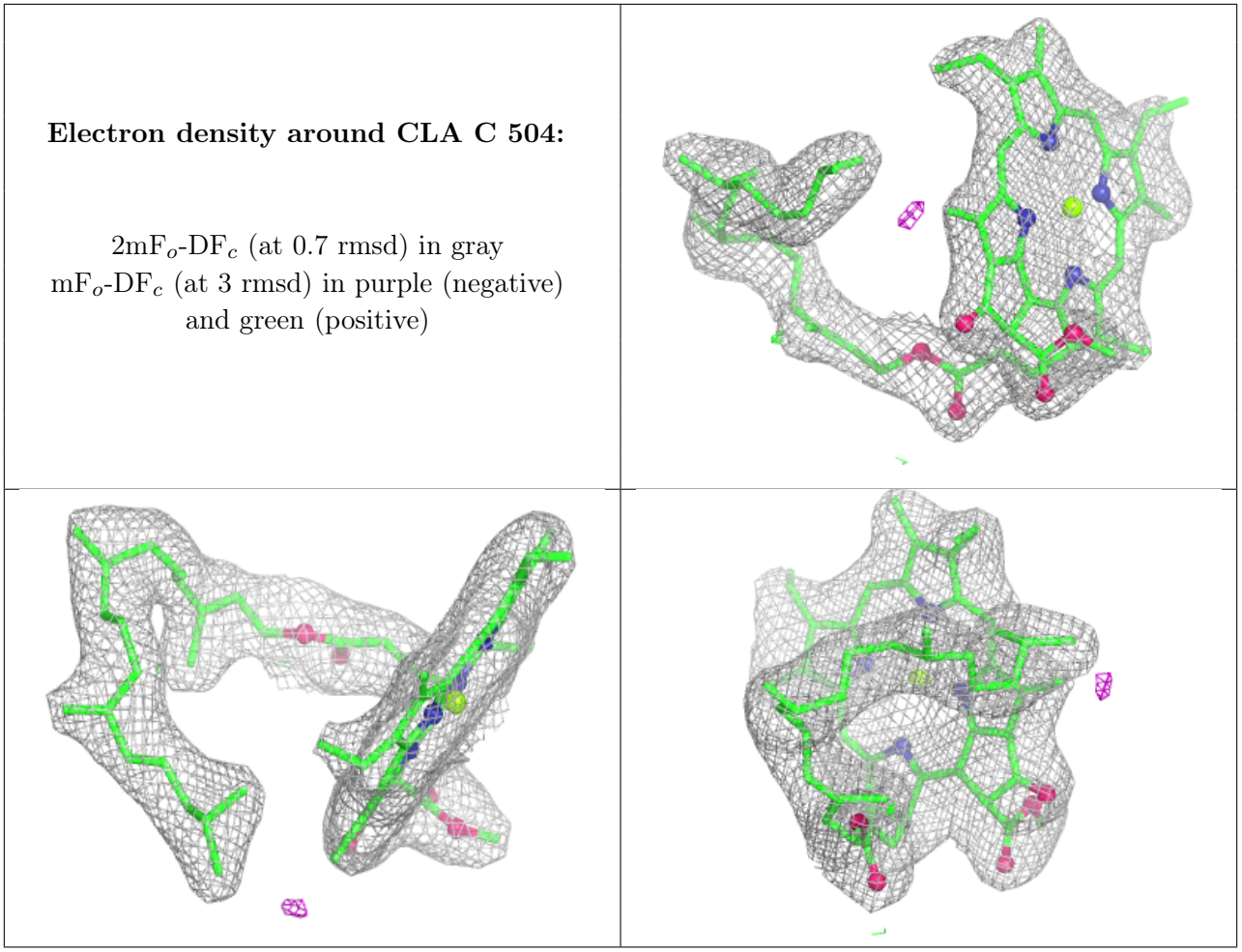






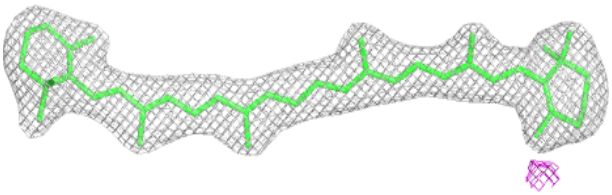
Electron density around CLA C 504:

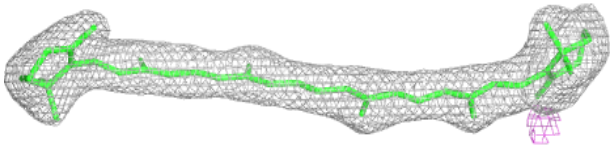
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

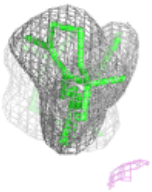


Electron density around BCR B 620:

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

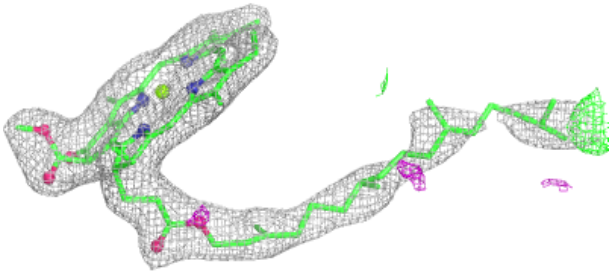


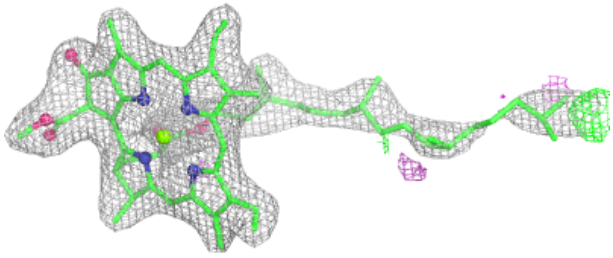


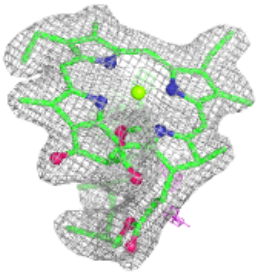


Electron density around CLA C 505:

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

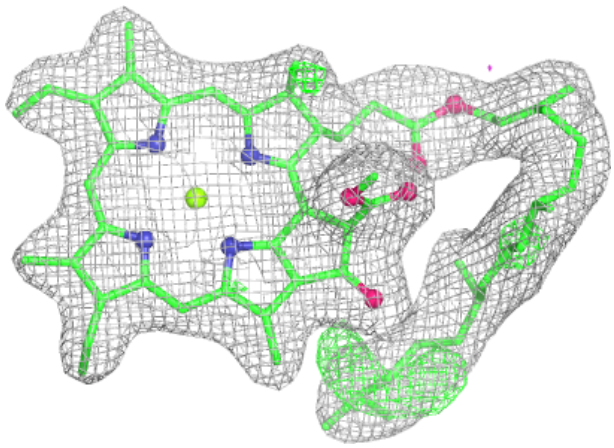


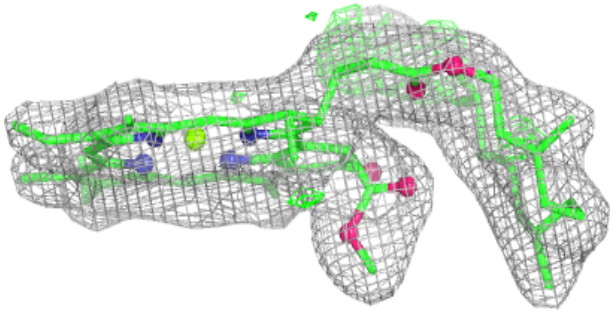


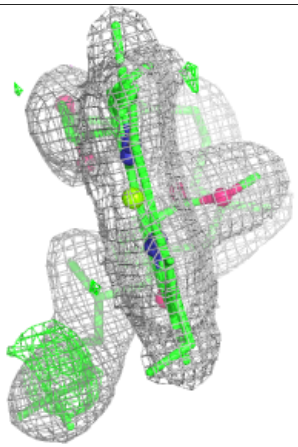


Electron density around CLA B 611:

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

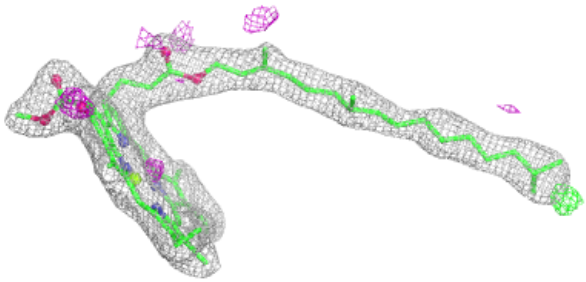


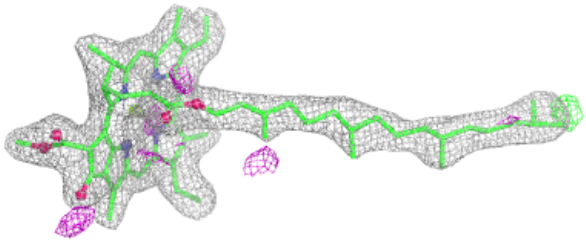


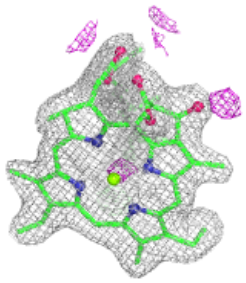


Electron density around CLA b 612:

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

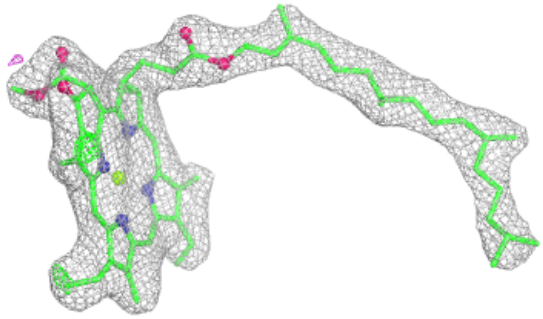


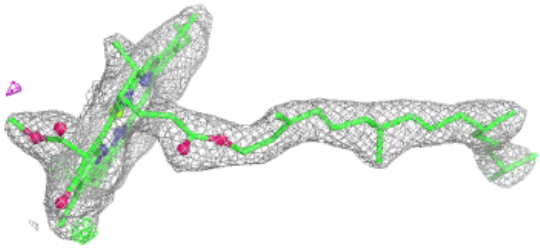


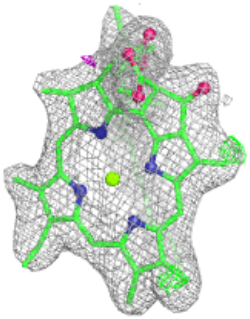


Electron density around CLA b 614:

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

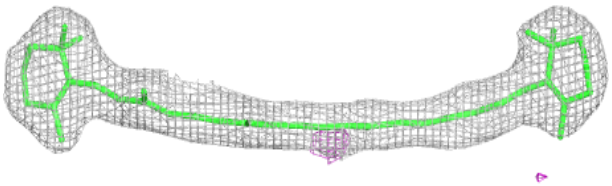


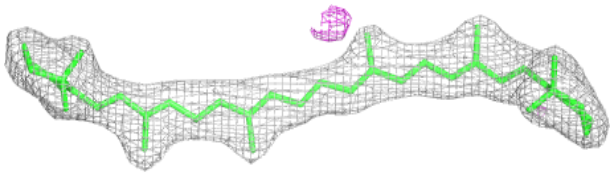


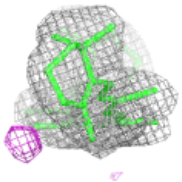


Electron density around BCR K 101:

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

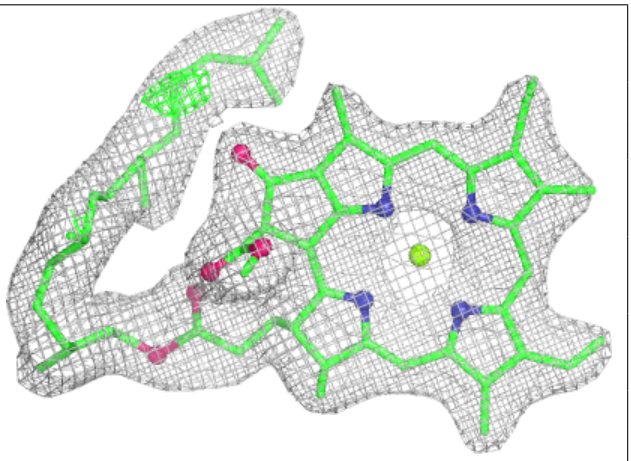


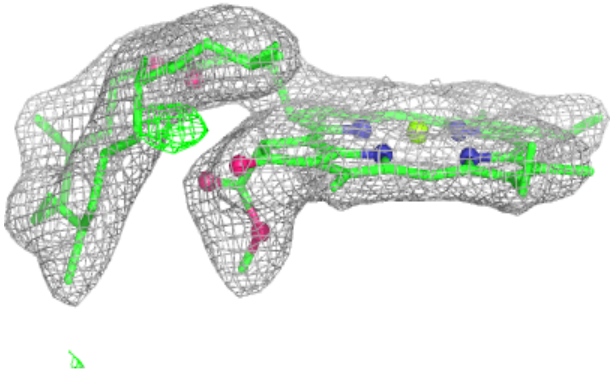


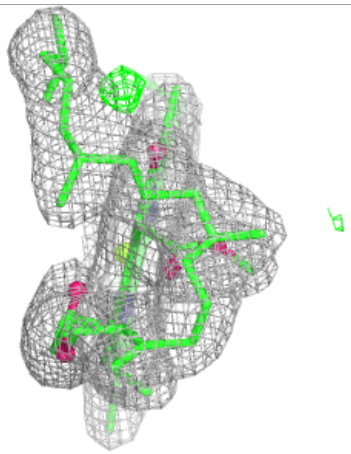


Electron density around CLA b 615:

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

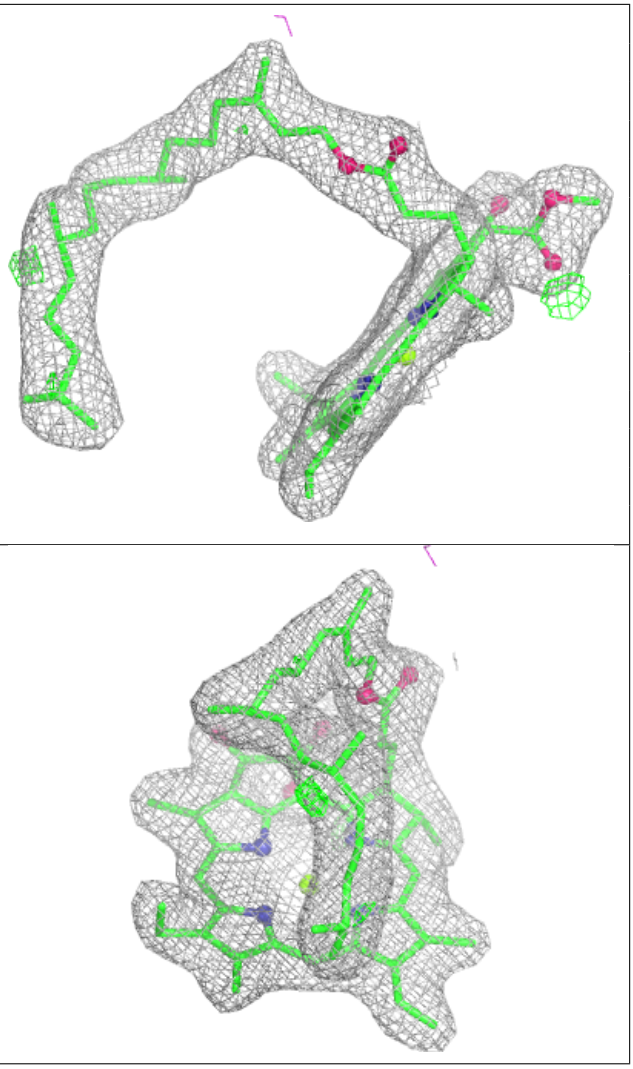






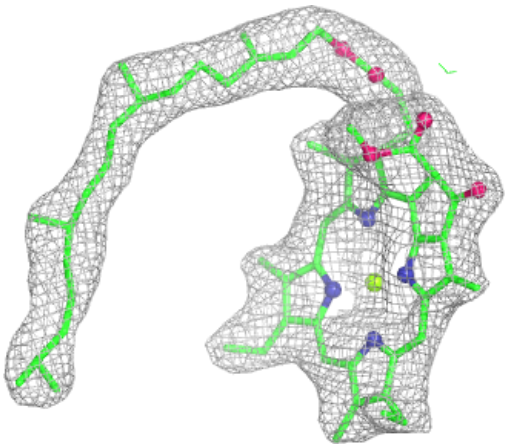
Electron density around CLA b 616:

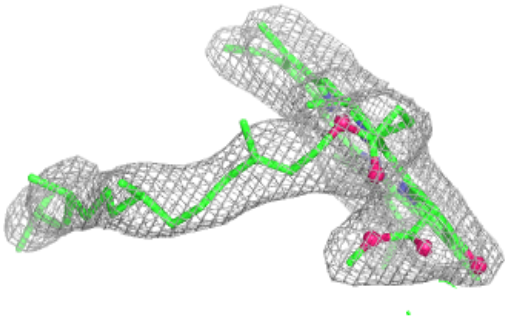
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

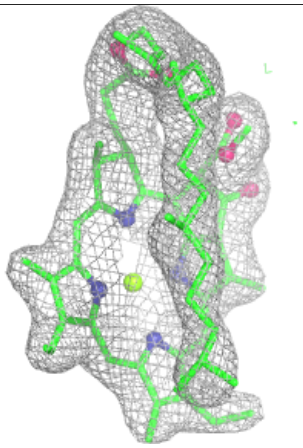


Electron density around CLA C 508:

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

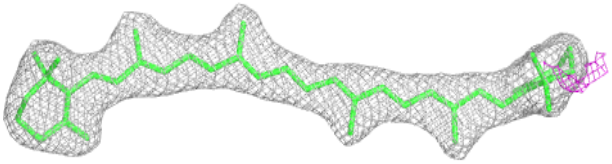


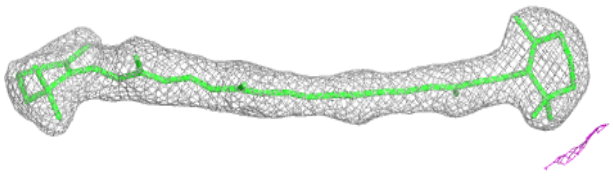


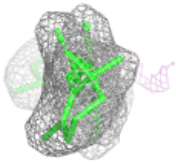


Electron density around BCR b 622:

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

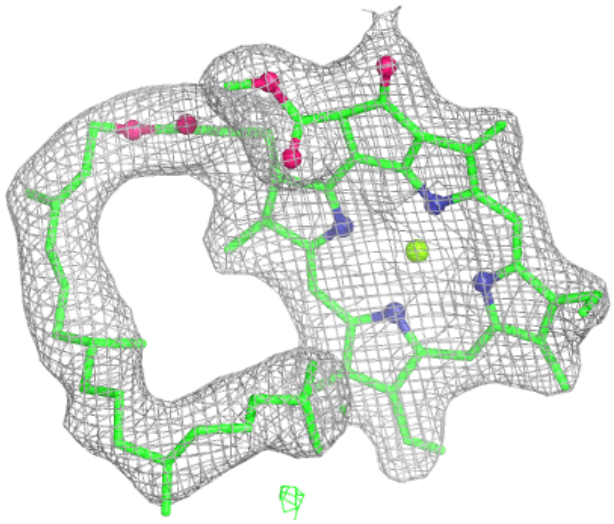


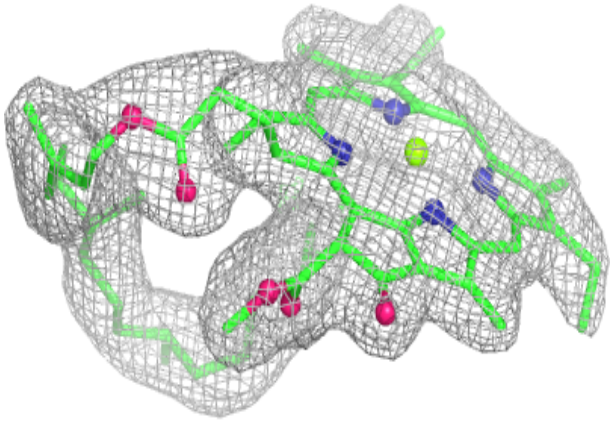


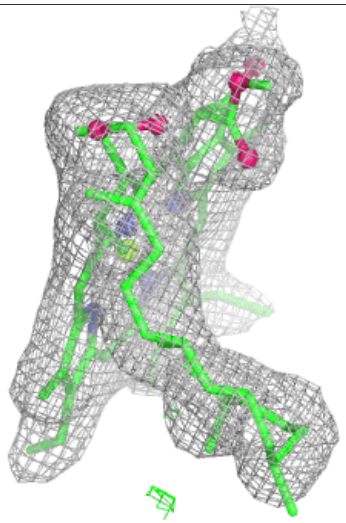


Electron density around CLA b 620:

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

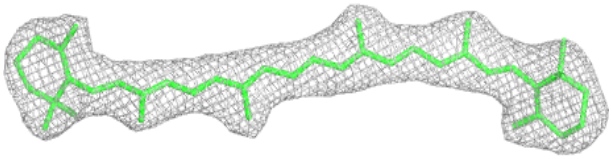


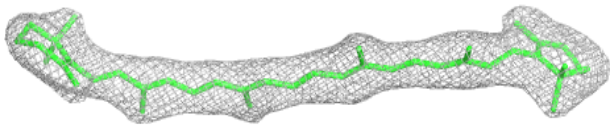


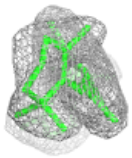


Electron density around BCR b 624:

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

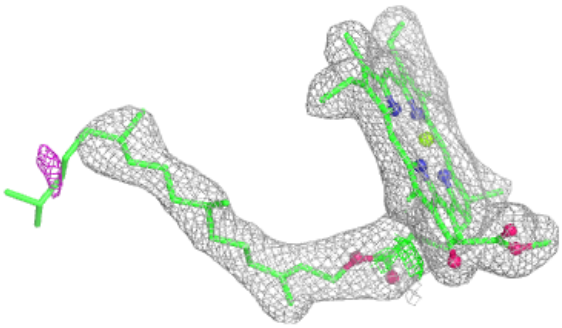


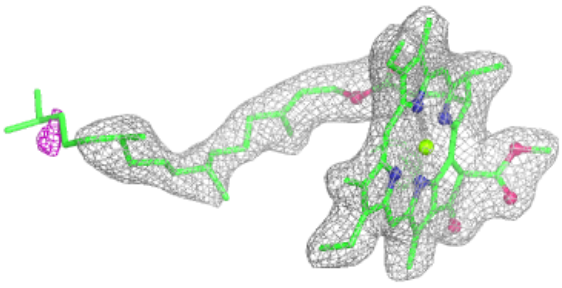


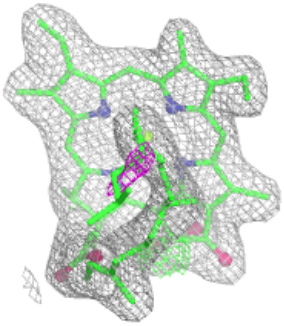


Electron density around CLA C 509:

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

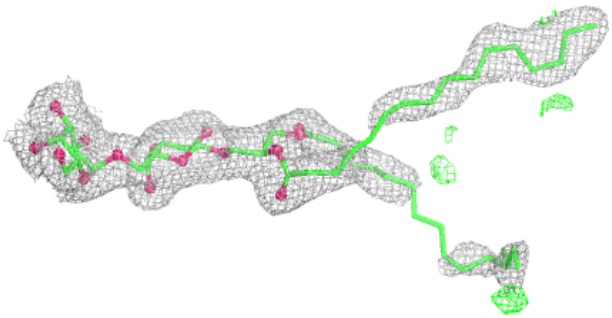


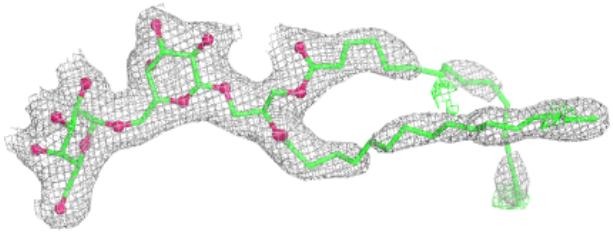


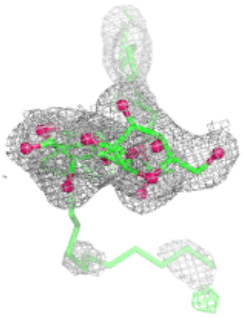


Electron density around DGD C 517:

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

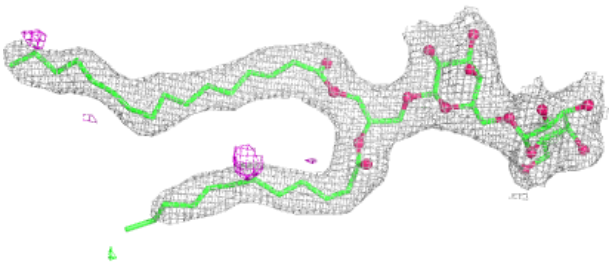


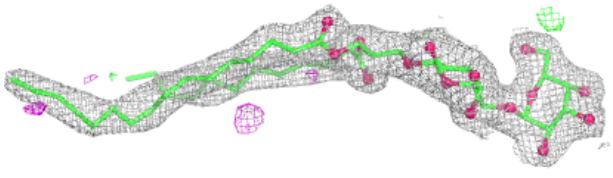


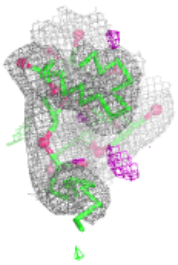


Electron density around DGD C 519:

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

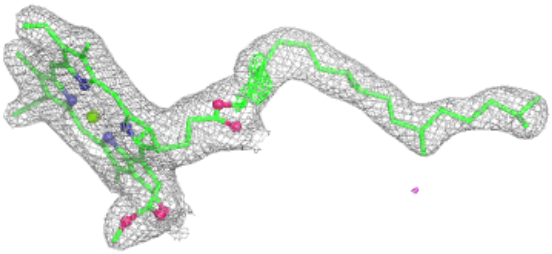


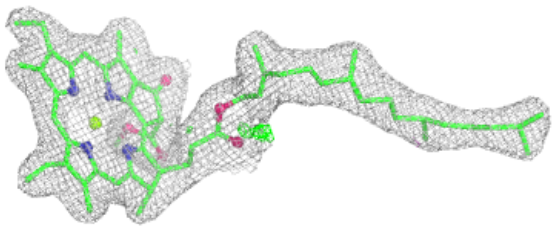


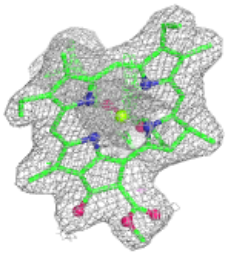


Electron density around CLA c 505:

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

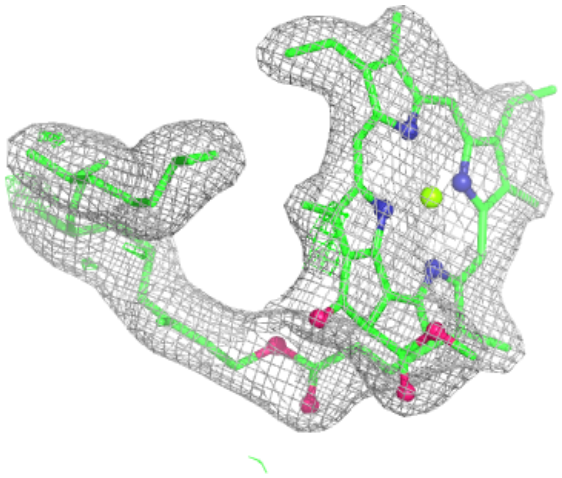


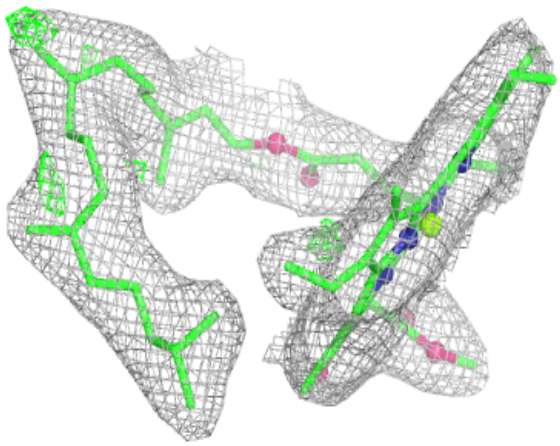


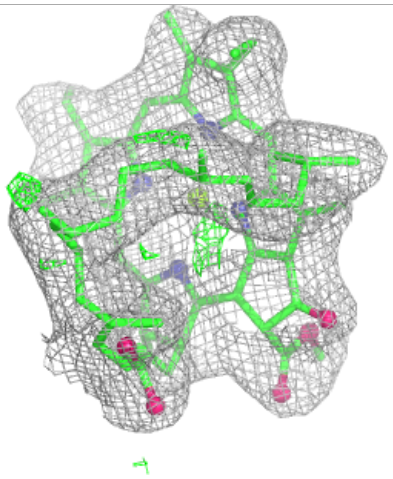


Electron density around CLA c 506:

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

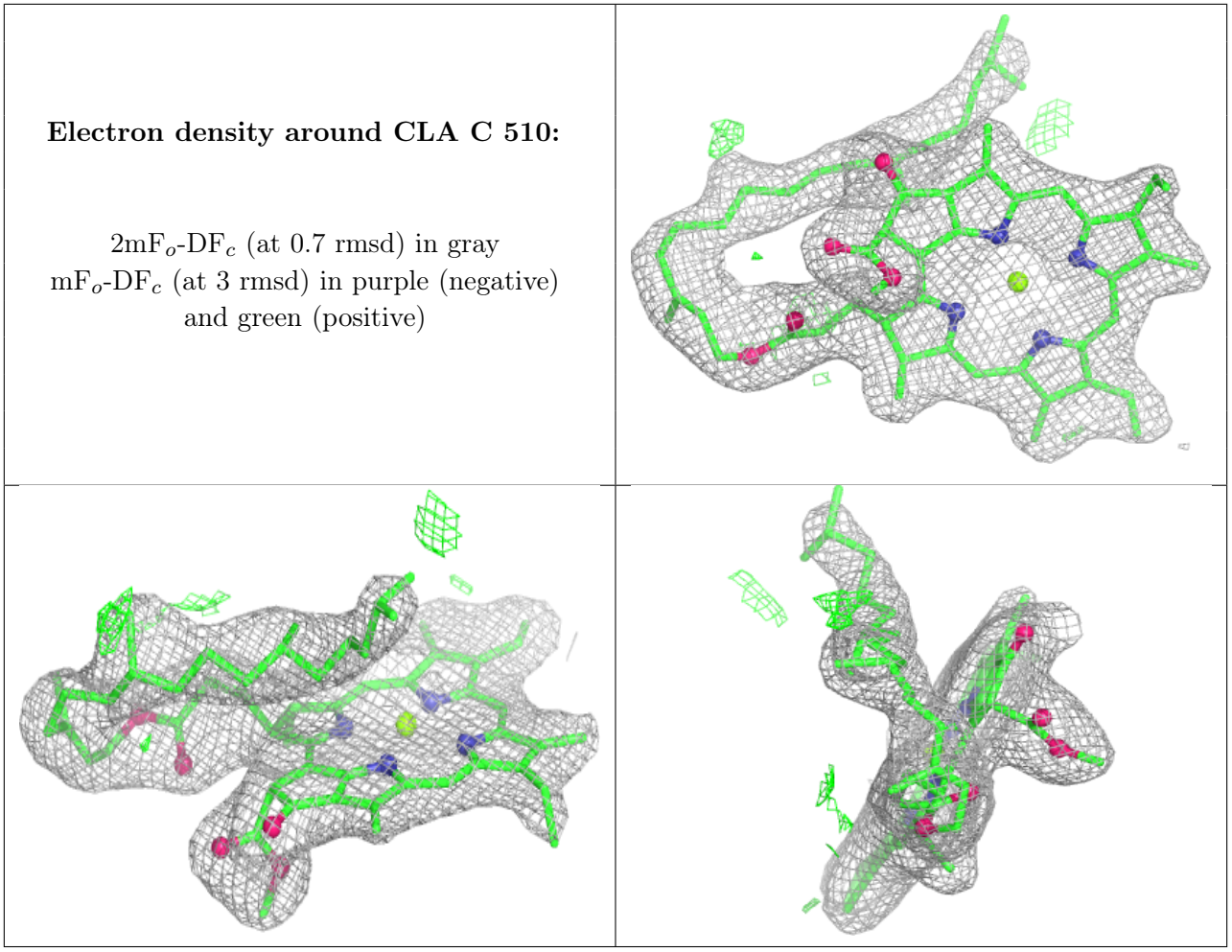






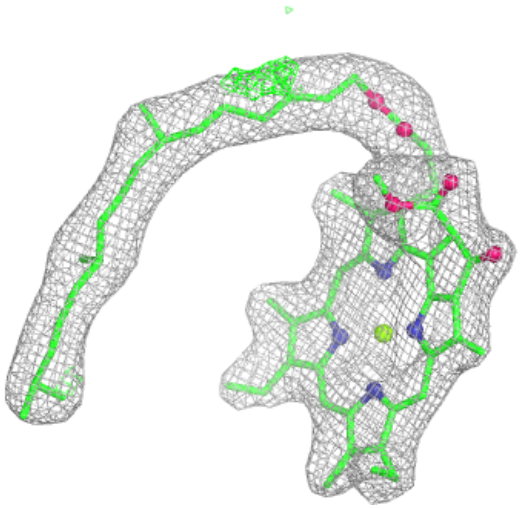
Electron density around CLA C 510:

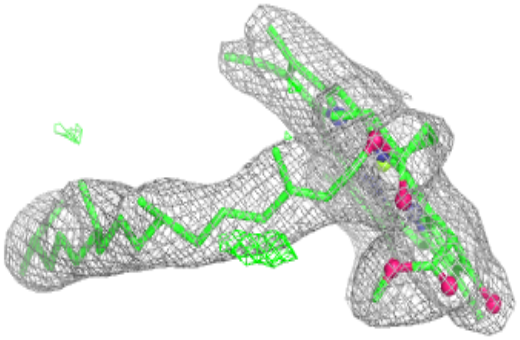
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

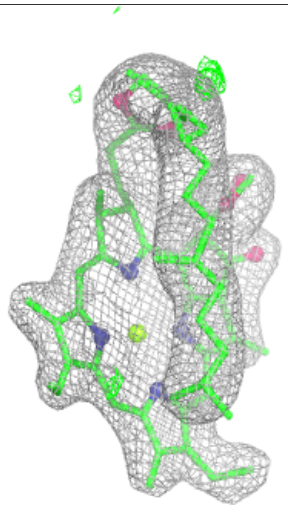


Electron density around CLA c 510:

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

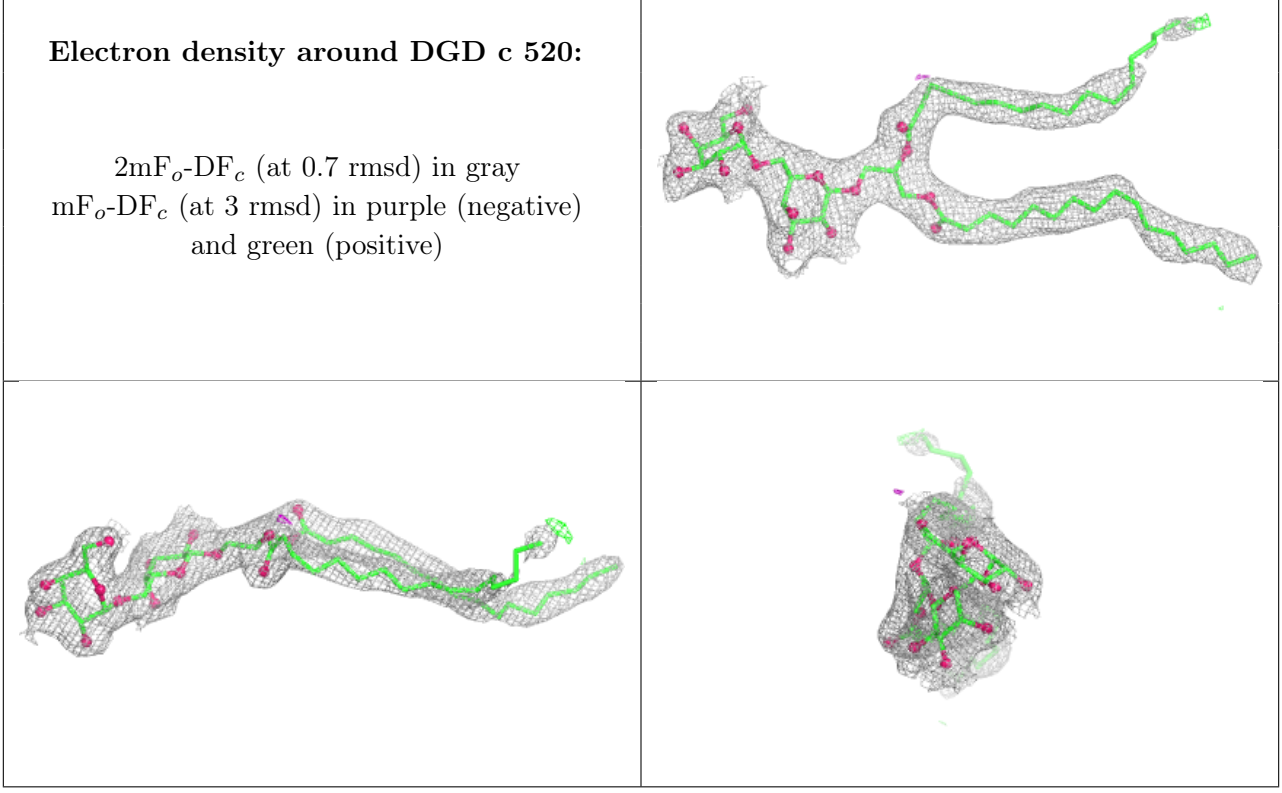






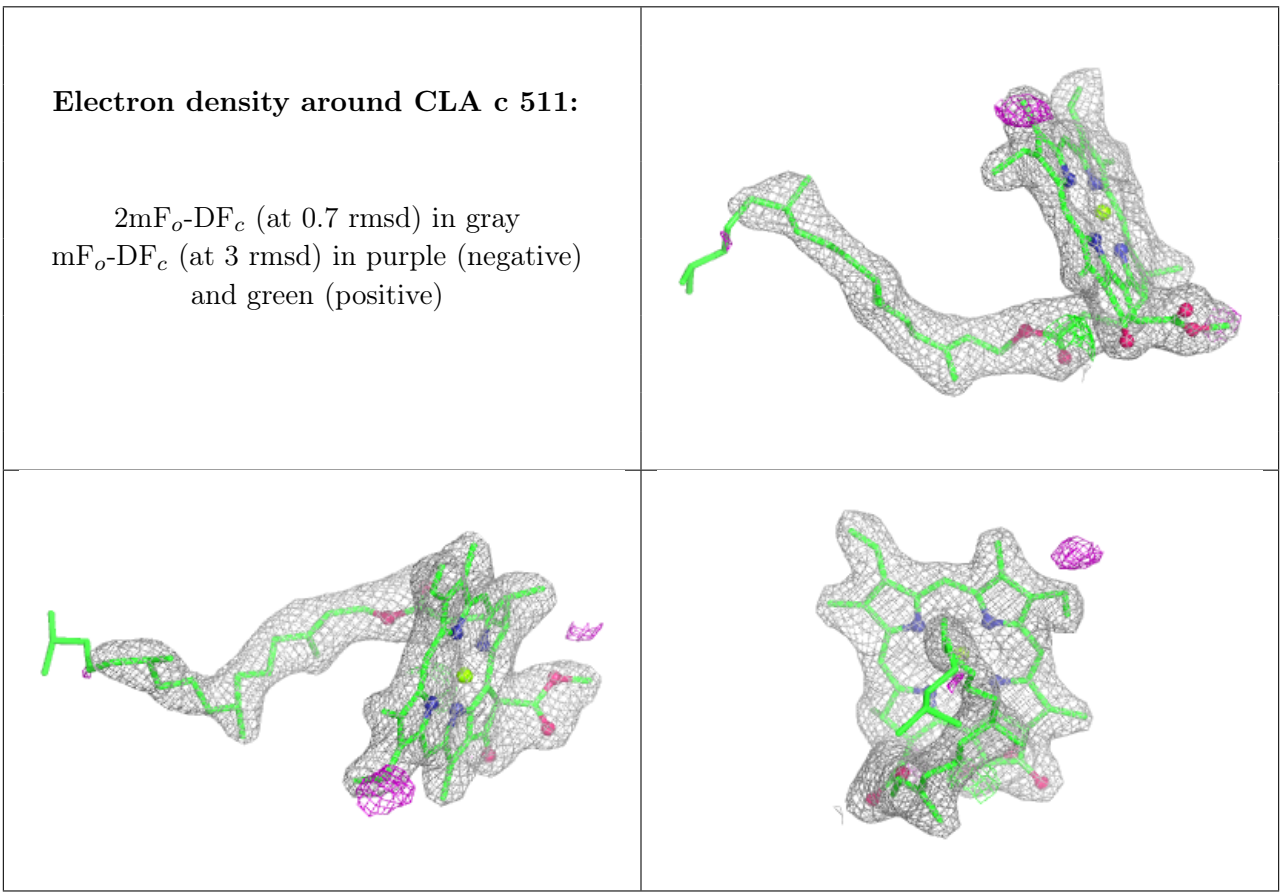
Electron density around DGD c 520:

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



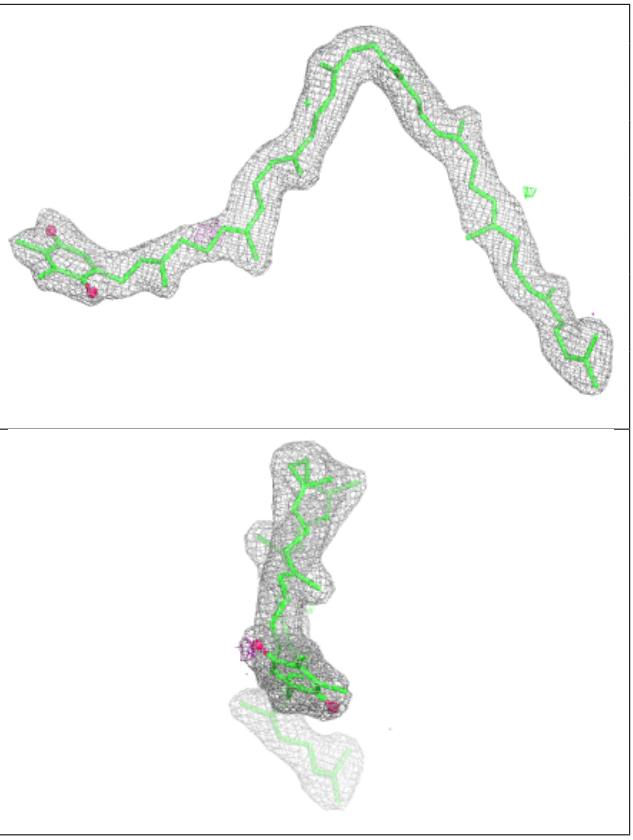
Electron density around CLA c 511:

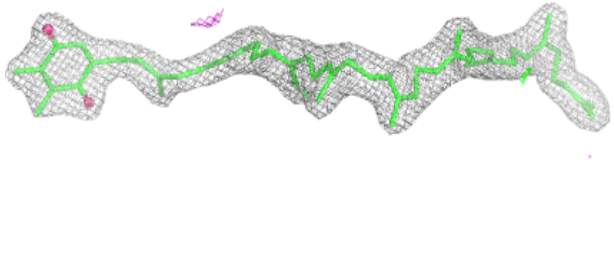
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PL9 D 2306:

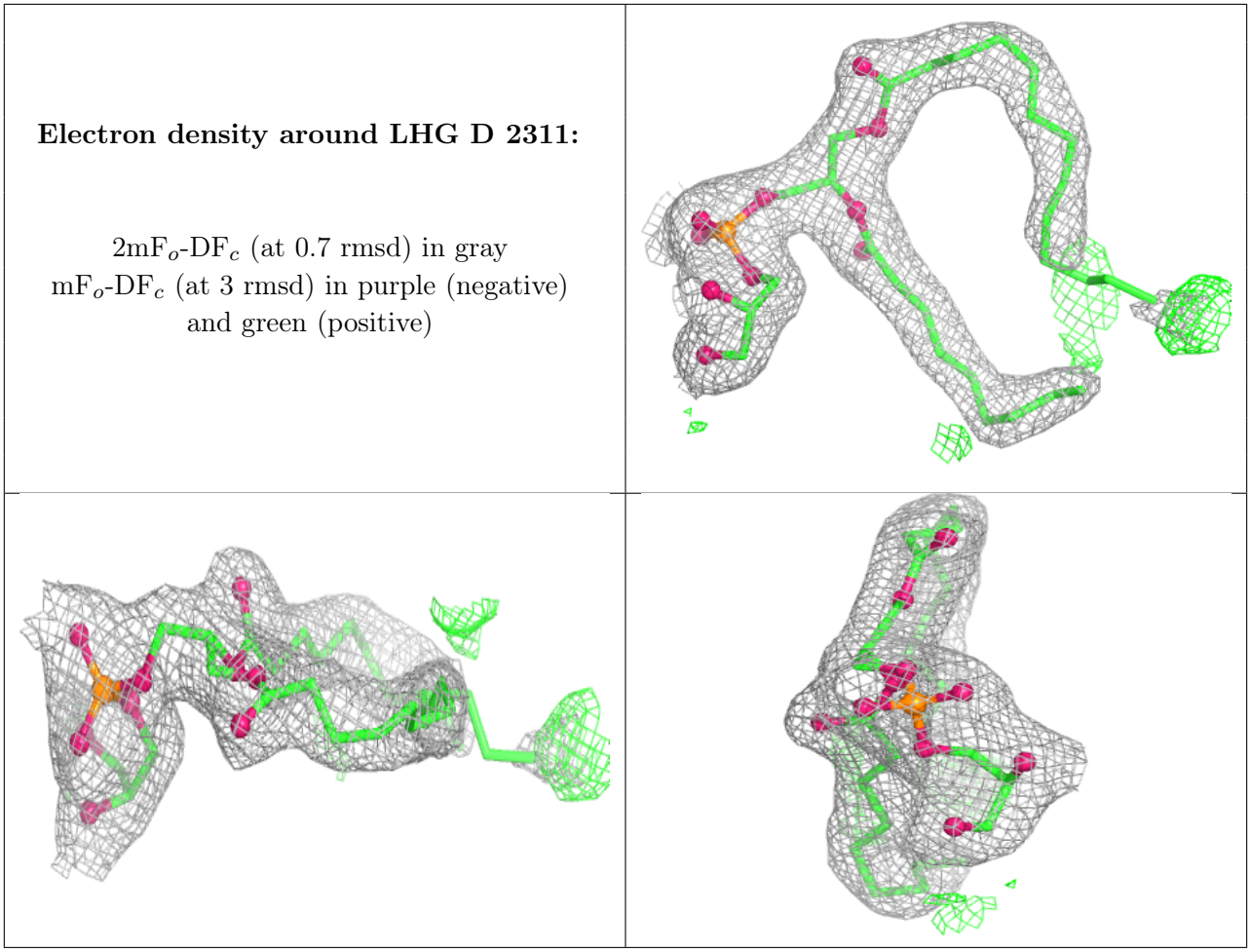
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





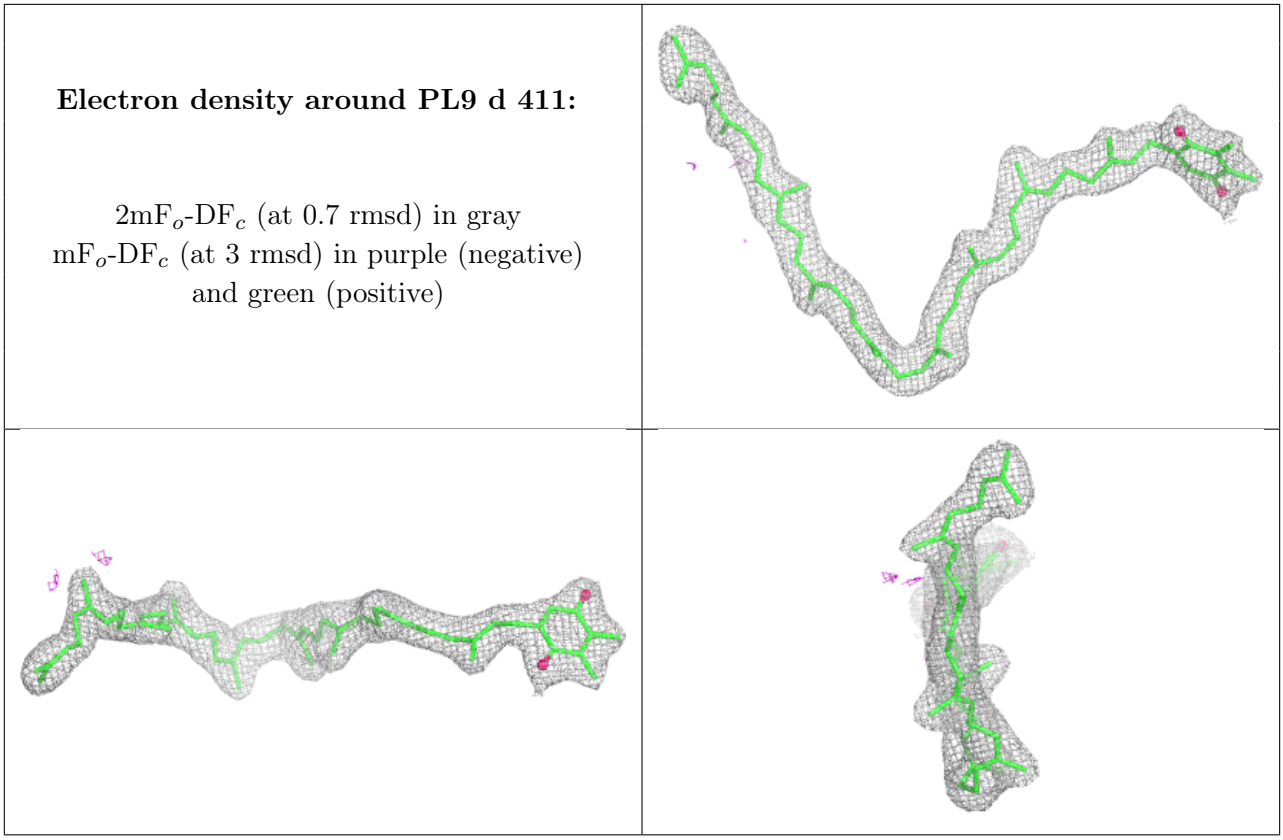
Electron density around LHG D 2311:

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



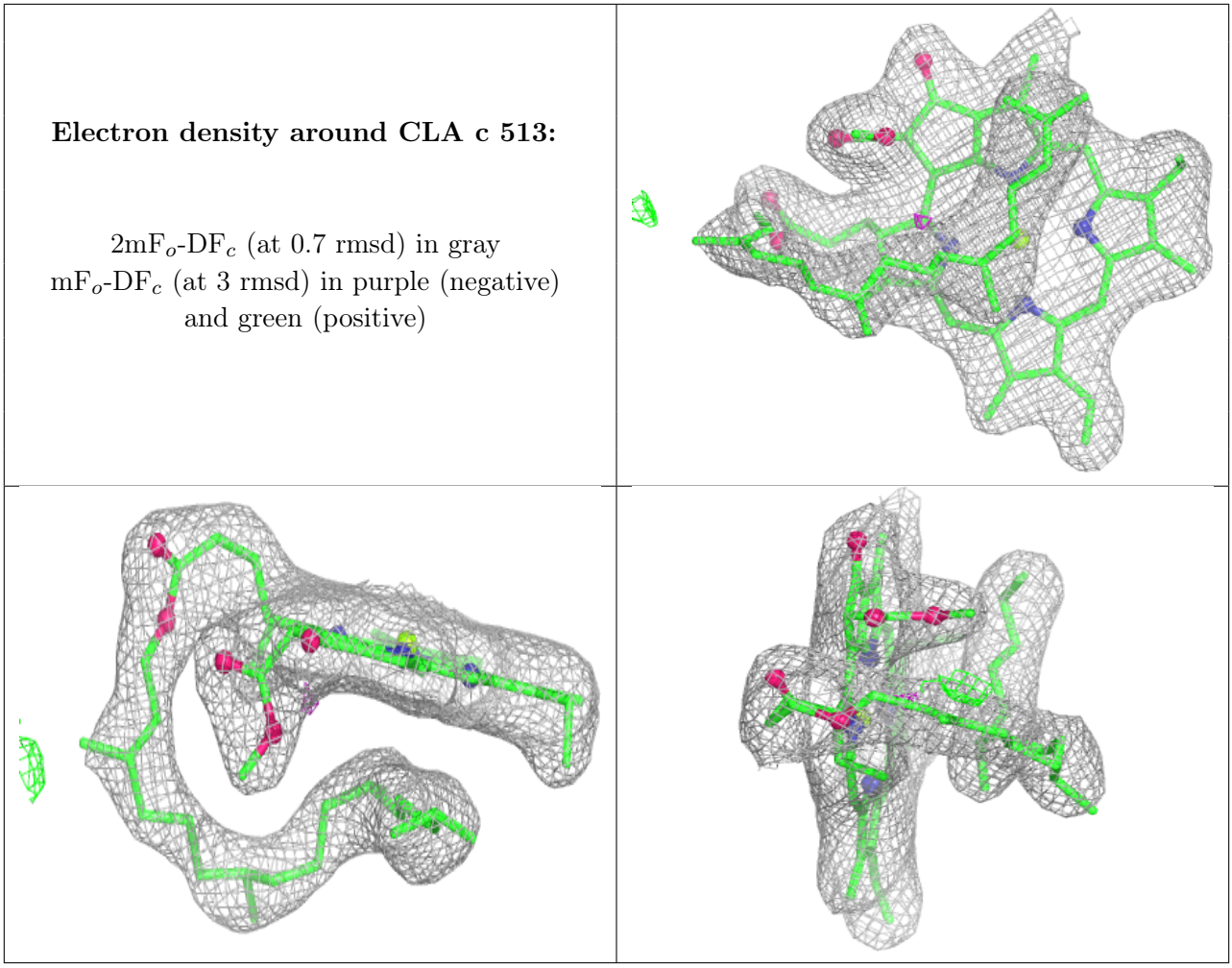
Electron density around PL9 d 411:

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



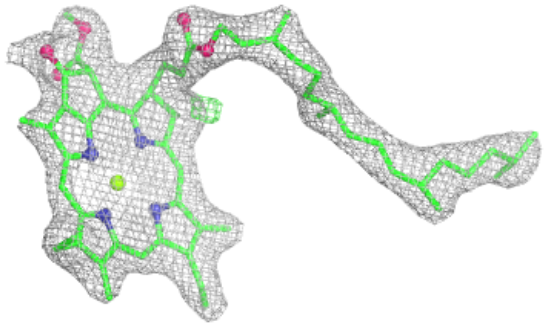
Electron density around CLA c 513:

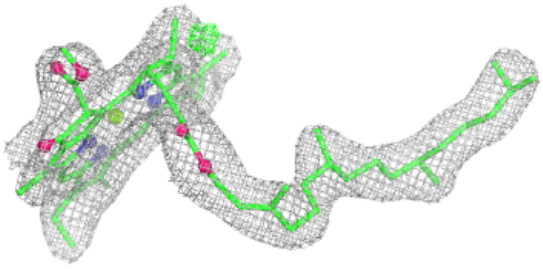
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

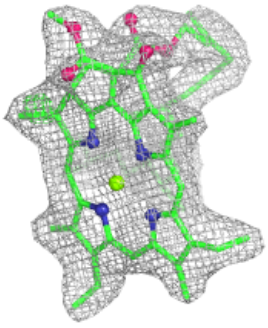


Electron density around CLA c 514:

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

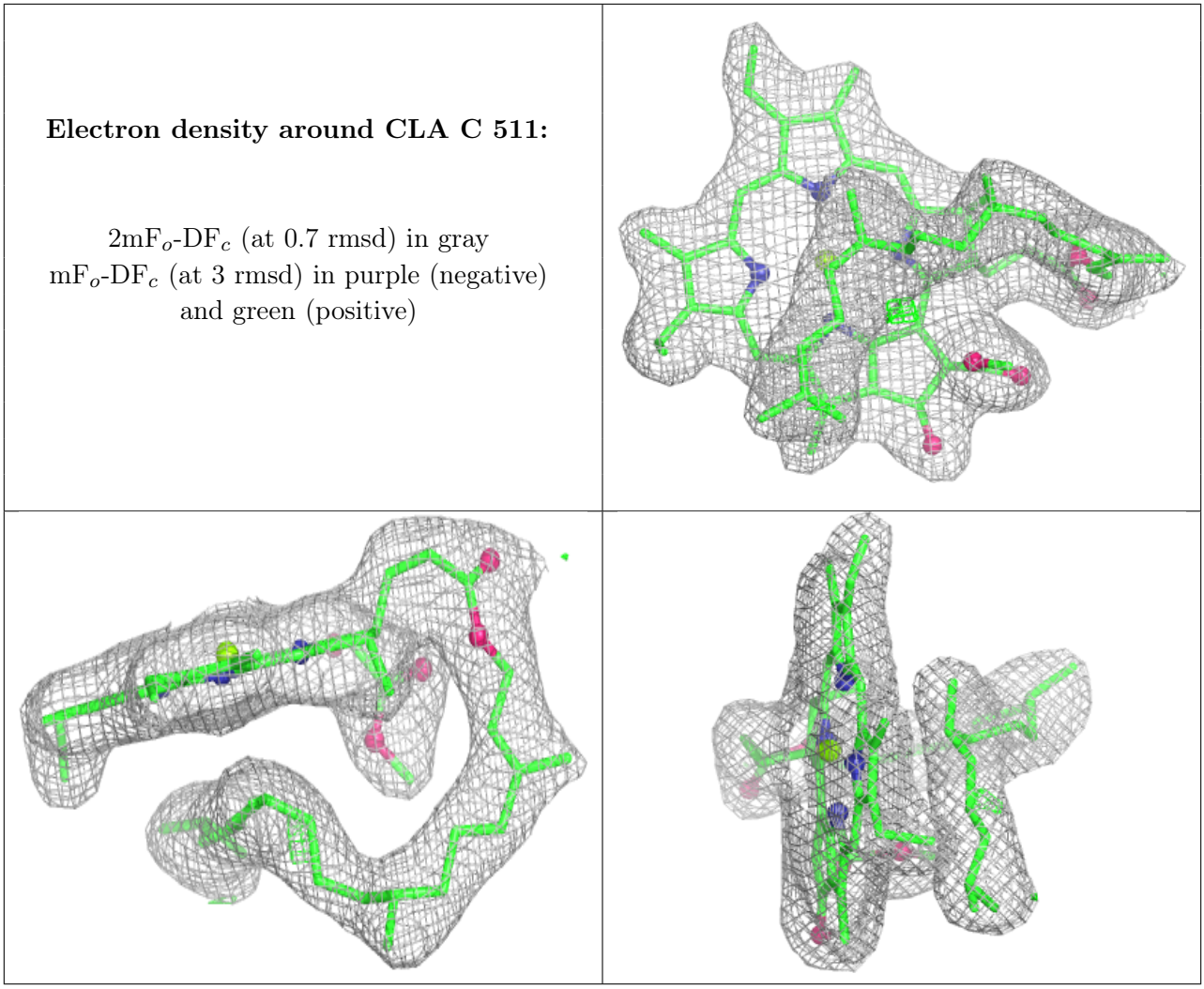






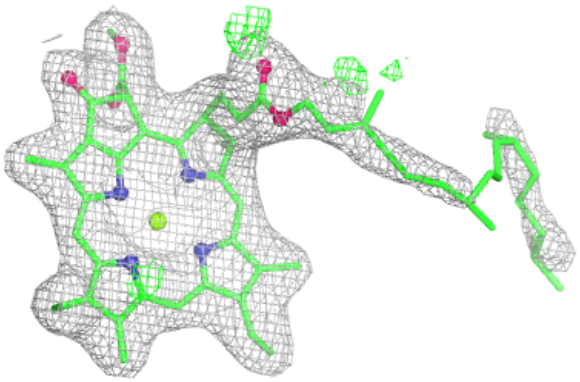
Electron density around CLA C 511:

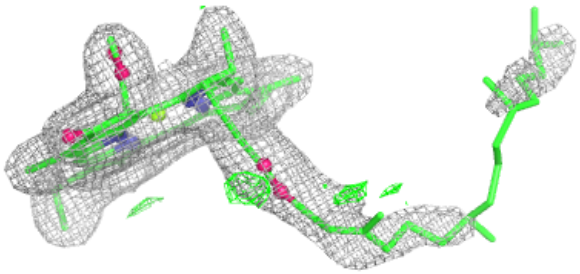
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

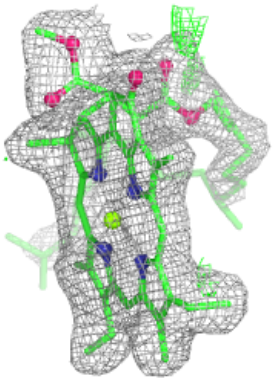


Electron density around CLA A 410:

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

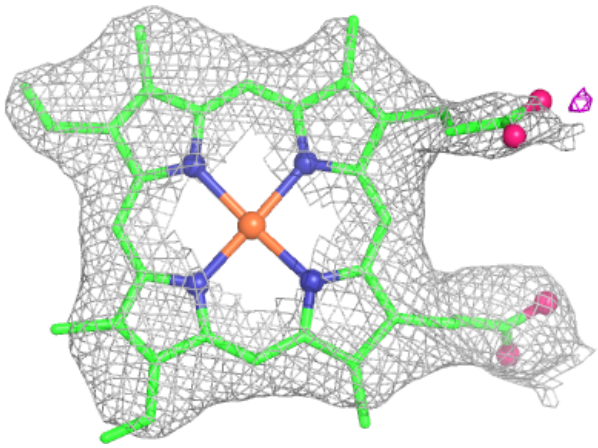


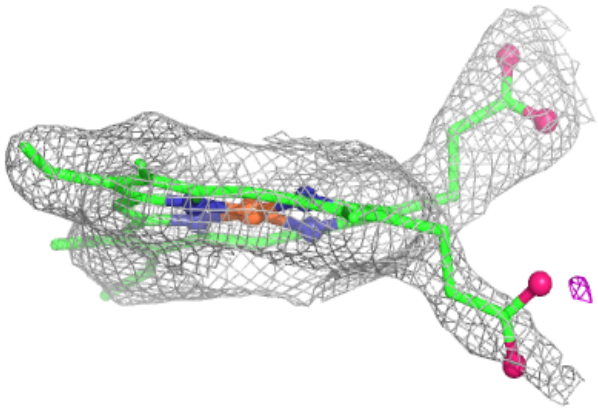


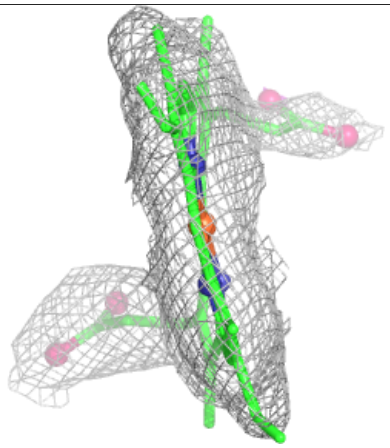


Electron density around HEM e 103:

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

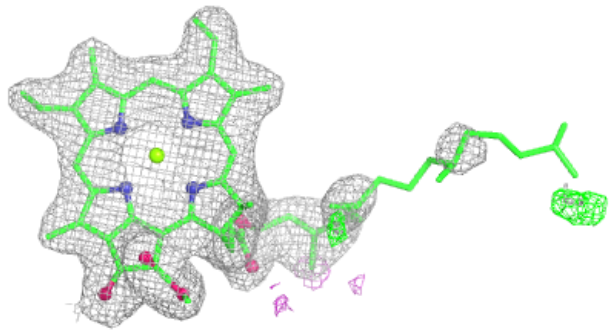


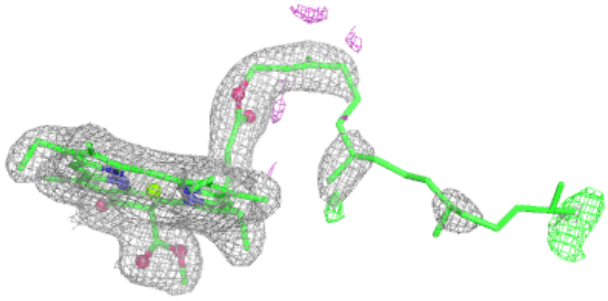


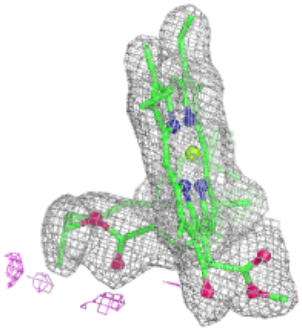


Electron density around CLA A 407:

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

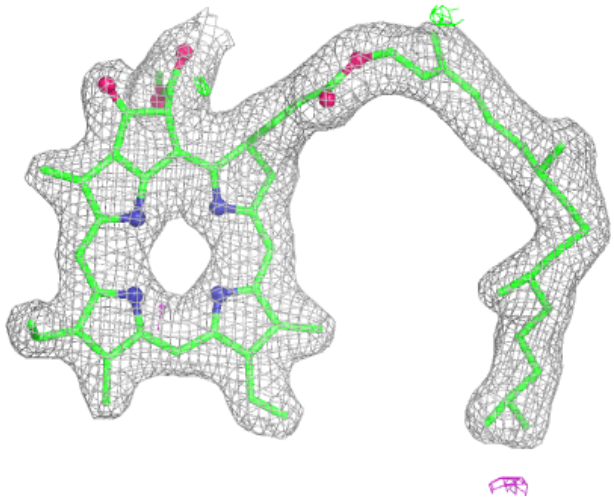


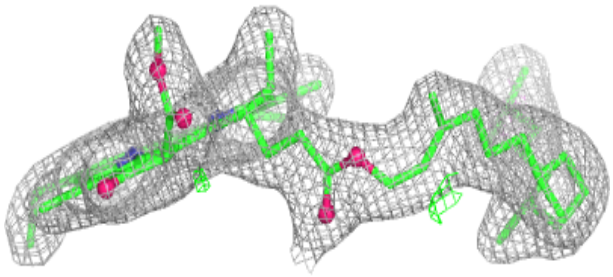


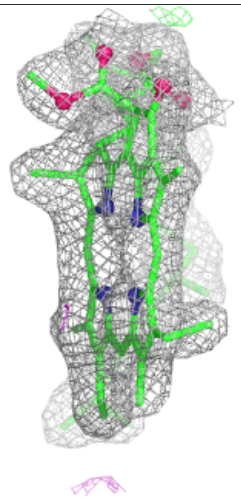


Electron density around PHO A 408:

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

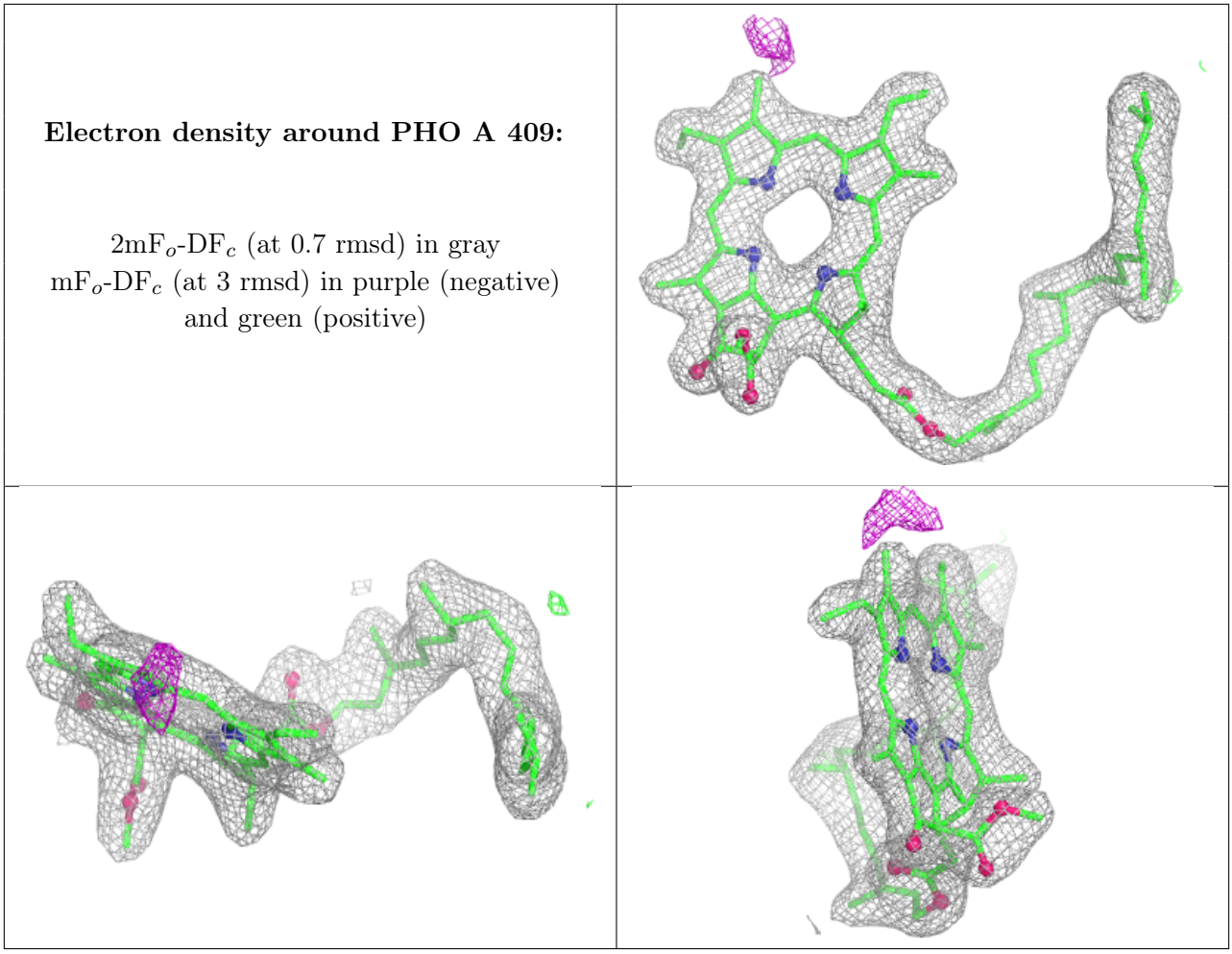






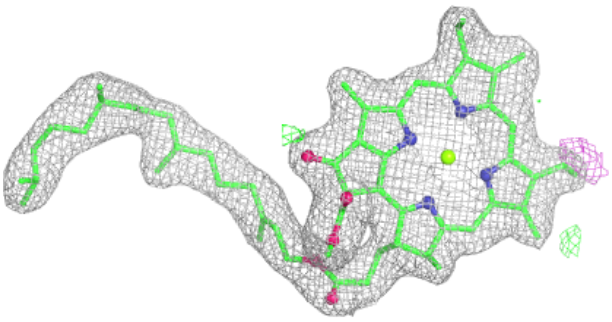
Electron density around PHO A 409:

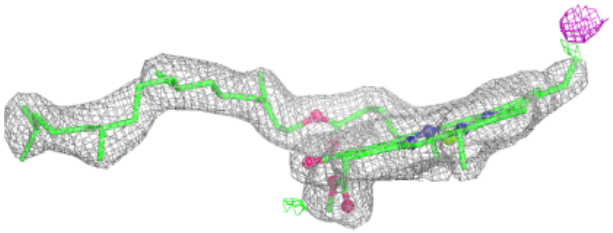
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

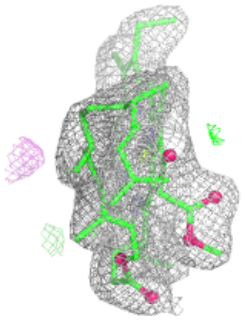


Electron density around CLA B 603:

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

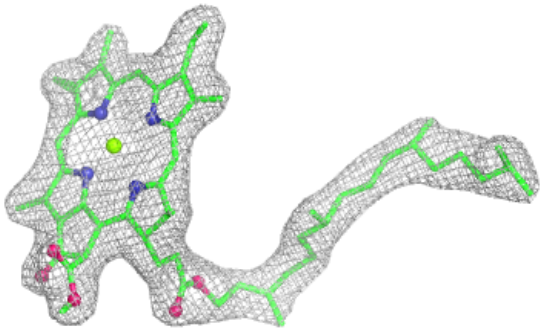


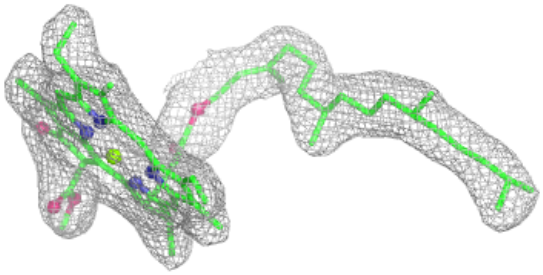


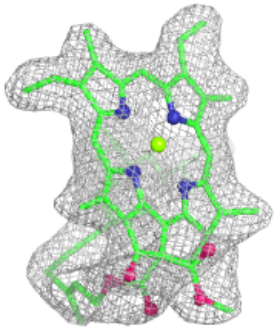


Electron density around CLA C 512:

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

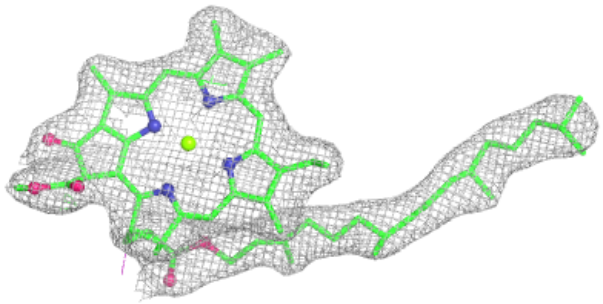


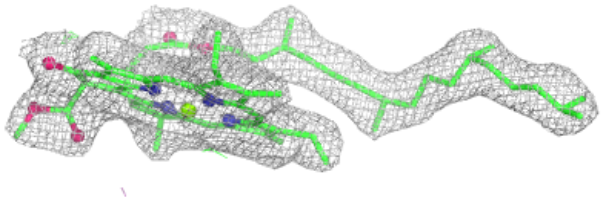


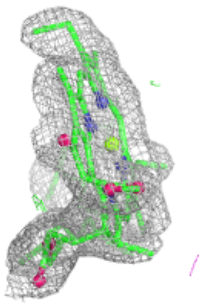


Electron density around CLA c 504:

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

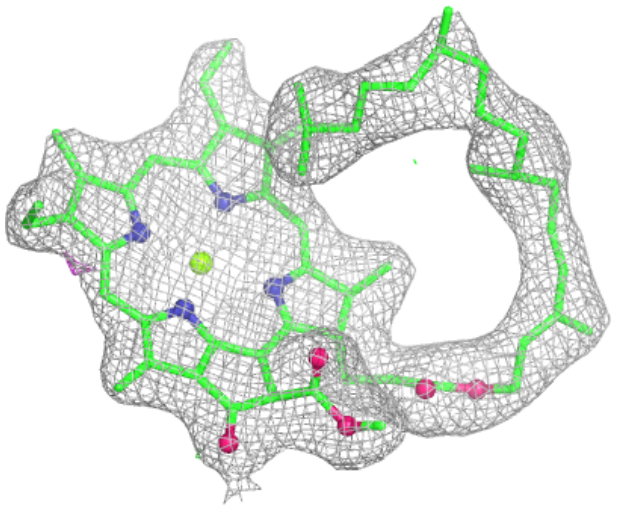


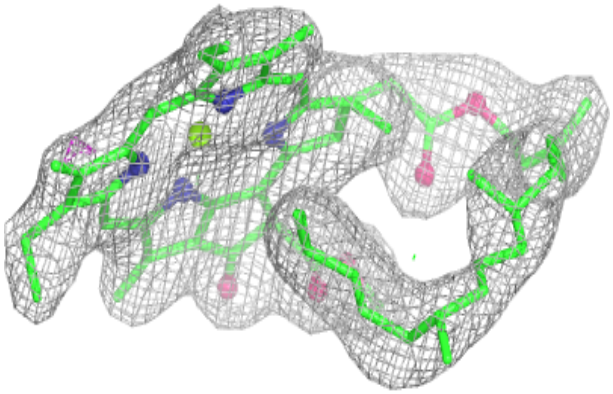


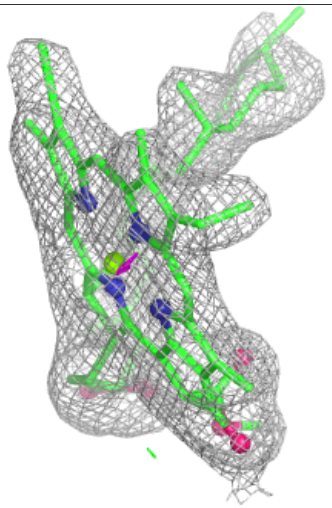


Electron density around CLA B 616:

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

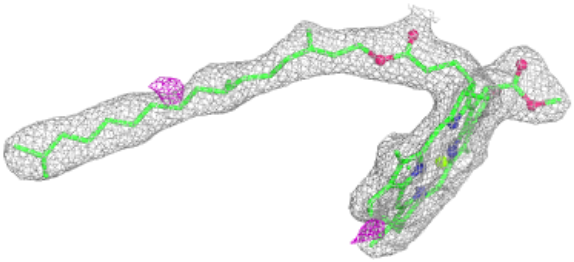


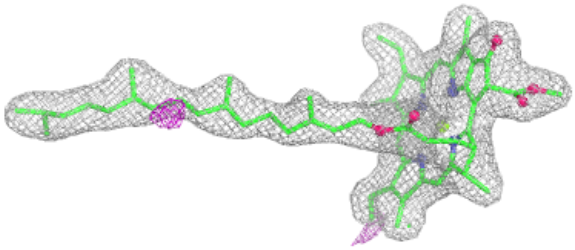


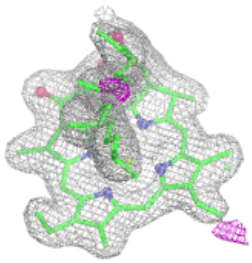


Electron density around CLA B 608:

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

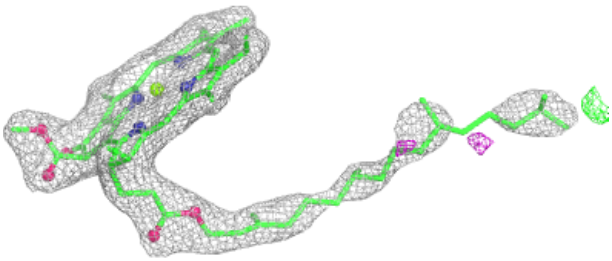


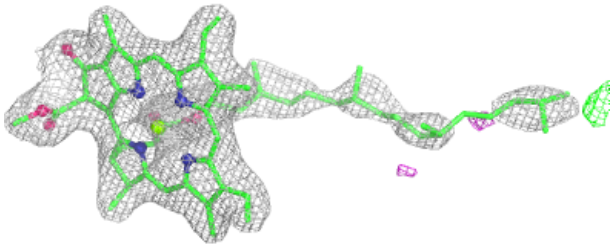


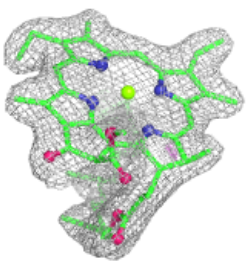


Electron density around CLA c 507:

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

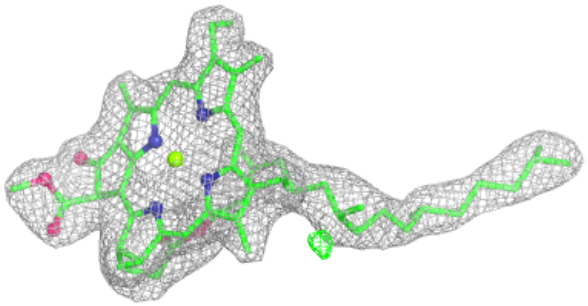


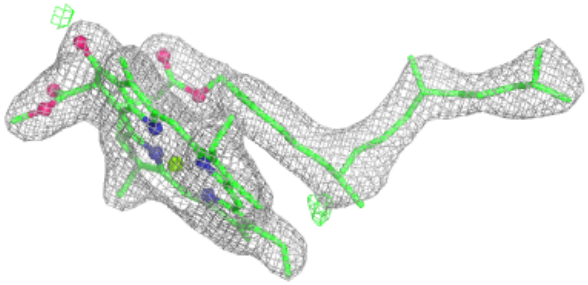


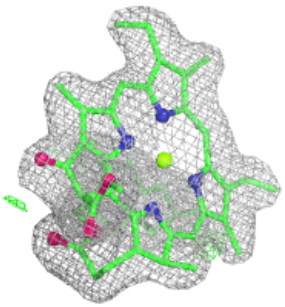


Electron density around CLA c 508:

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

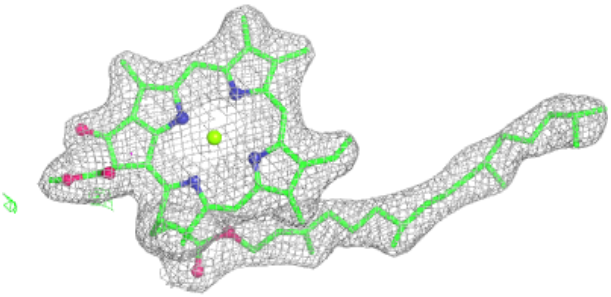


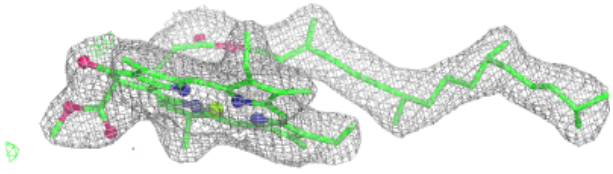


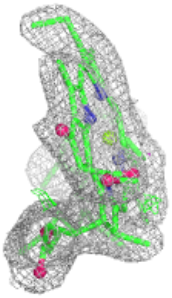


Electron density around CLA C 502:

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

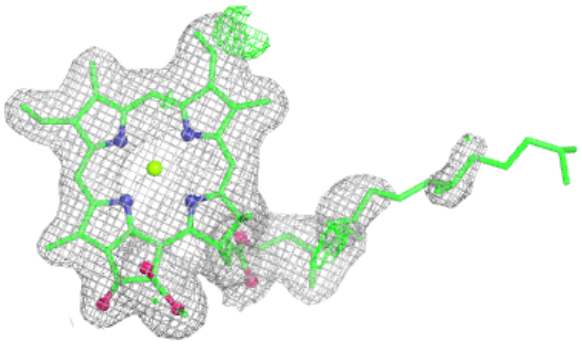


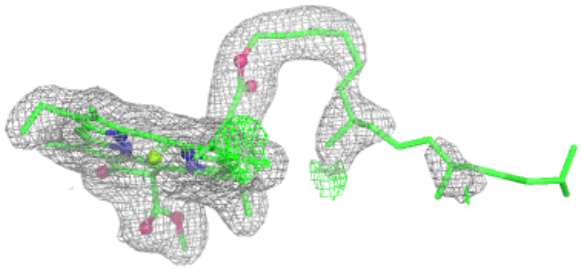


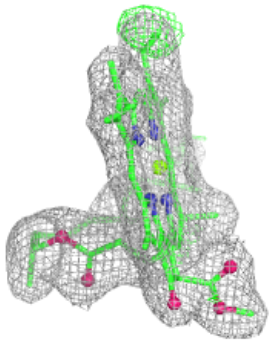


Electron density around CLA a 2610:

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

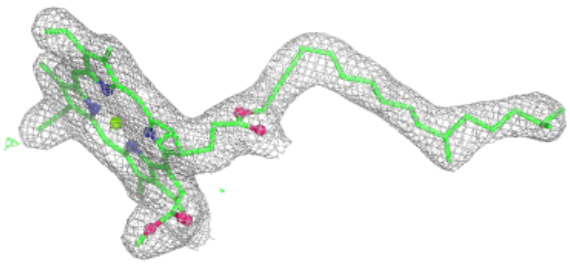


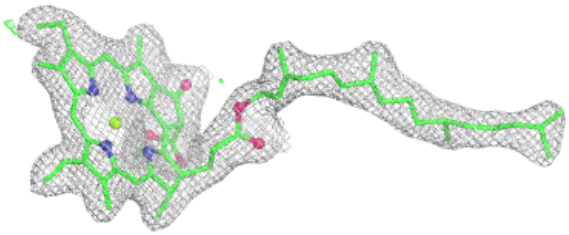


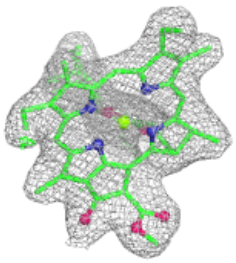


Electron density around CLA C 503:

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

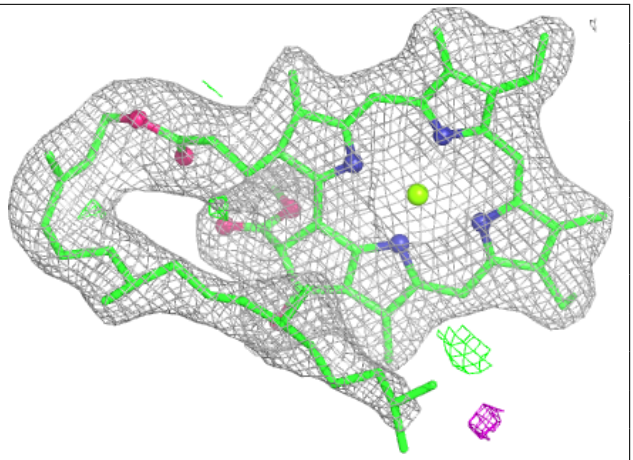


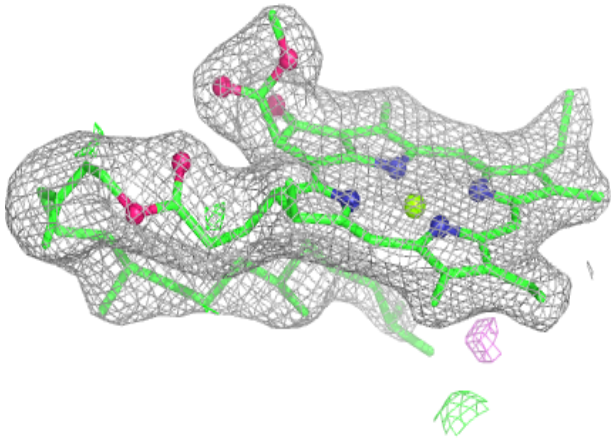


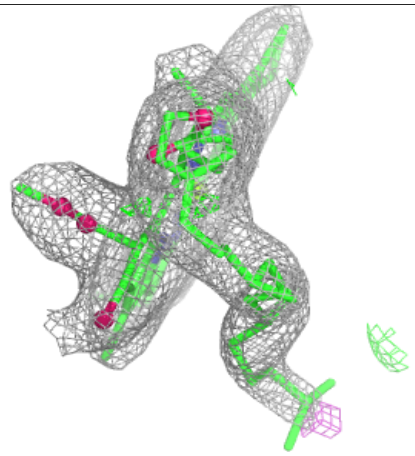


Electron density around CLA c 512:

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

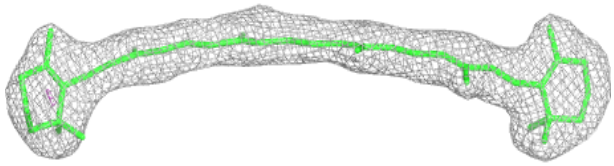


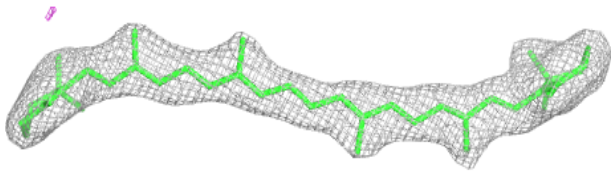


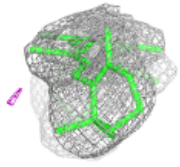


Electron density around BCR k 302:

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

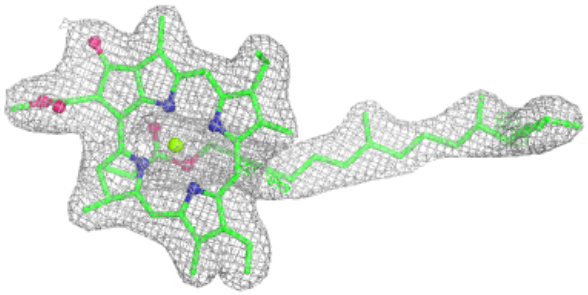


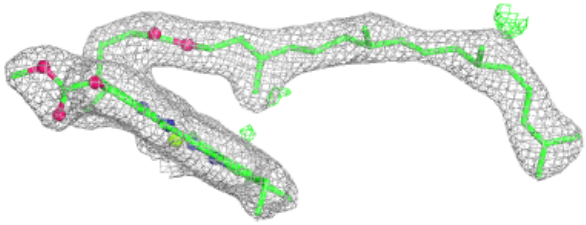


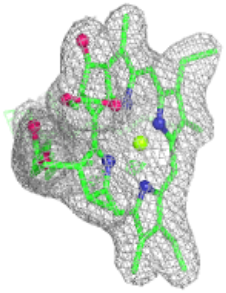


Electron density around CLA B 609:

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

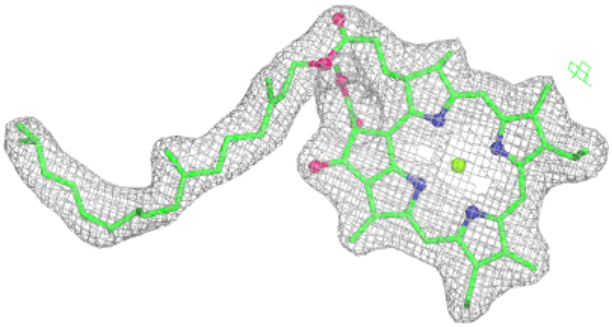


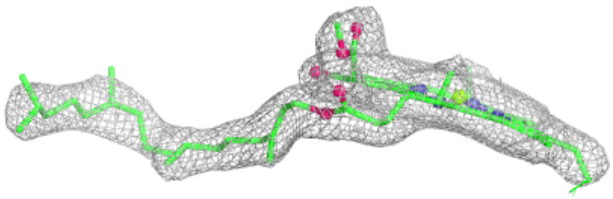




Electron density around CLA b 607:

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

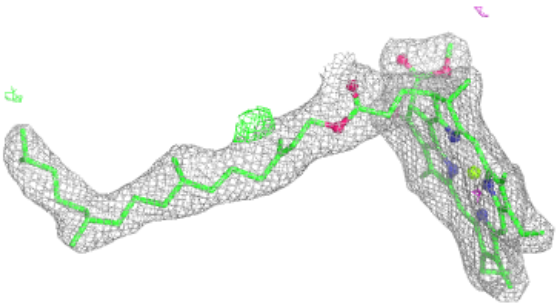


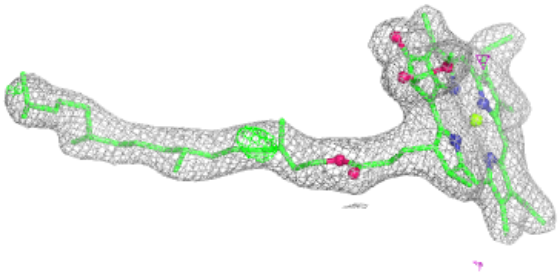


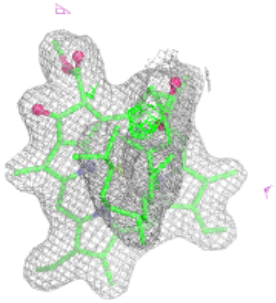


Electron density around CLA b 609:

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

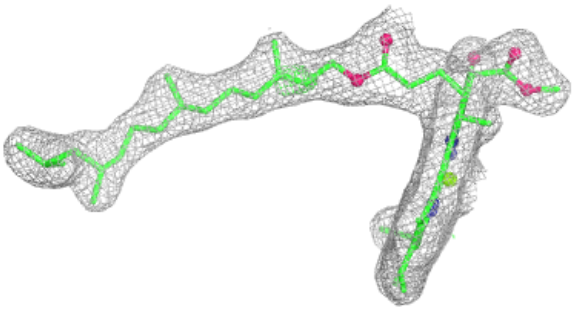


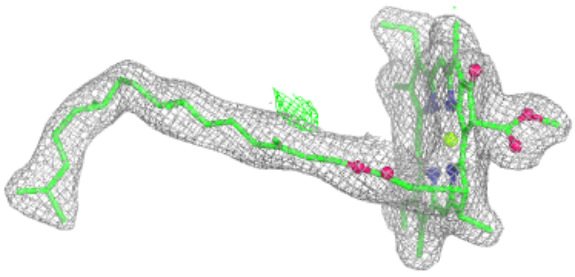


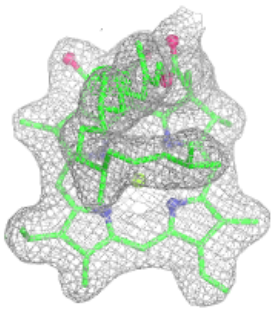


Electron density around CLA b 610:

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

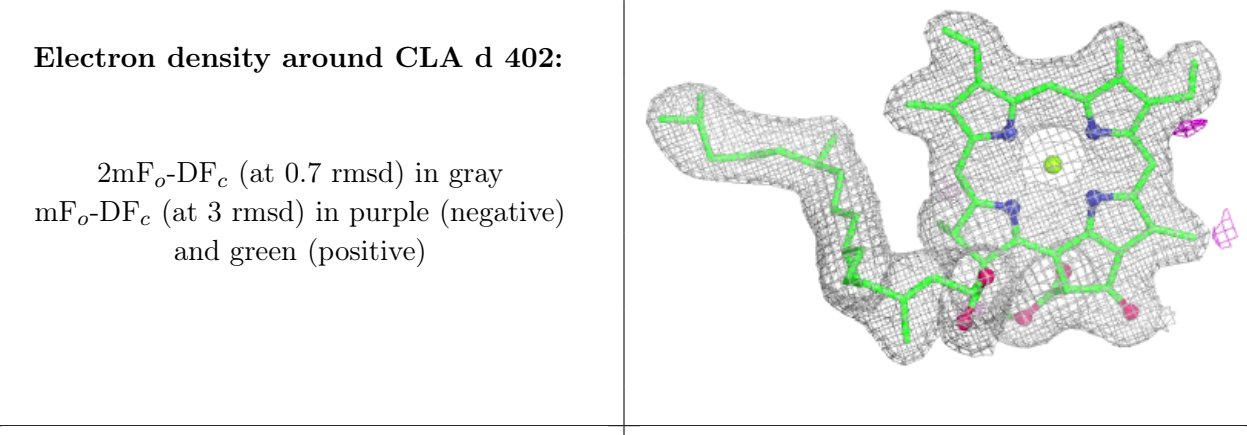






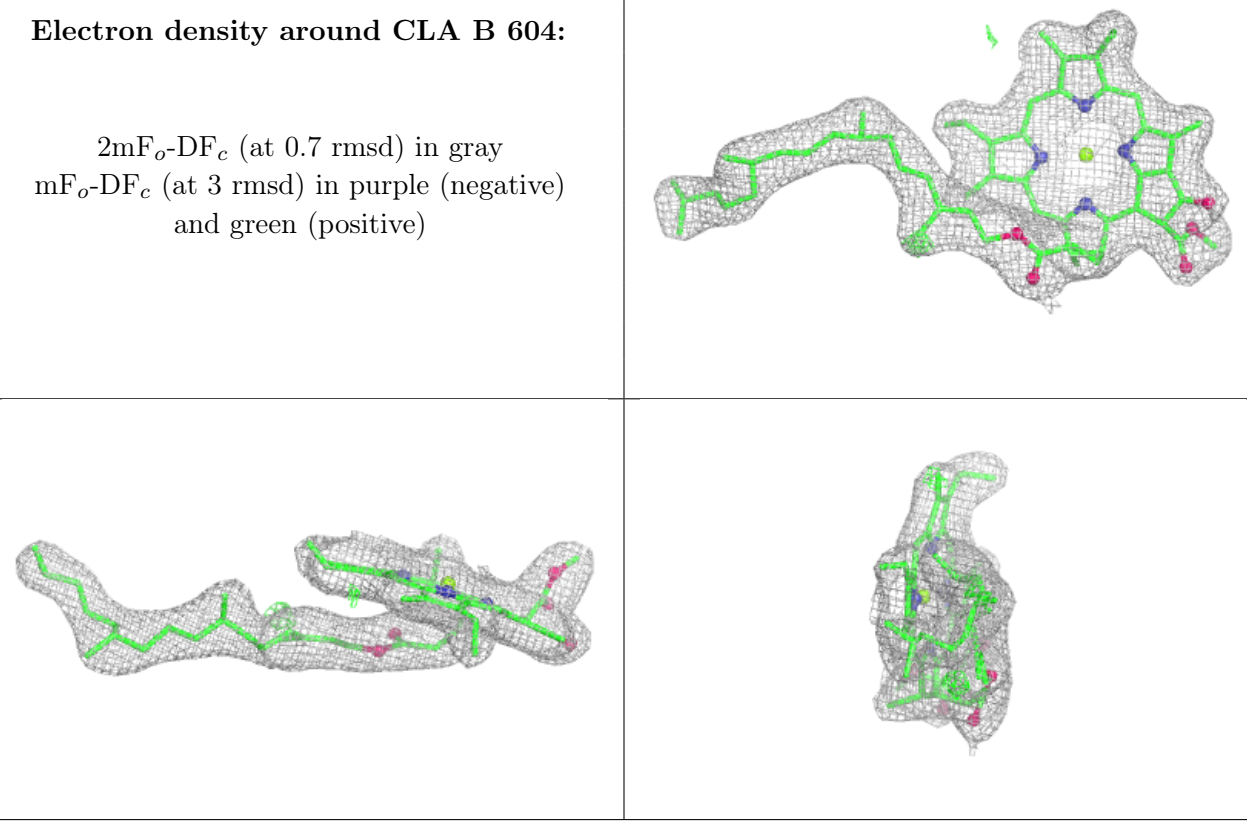
Electron density around CLA d 402:

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



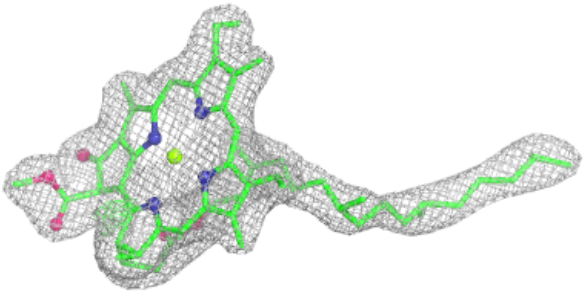
Electron density around CLA B 604:

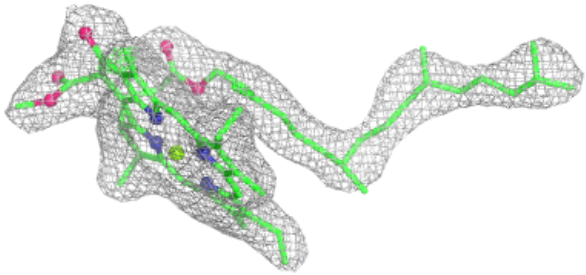
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

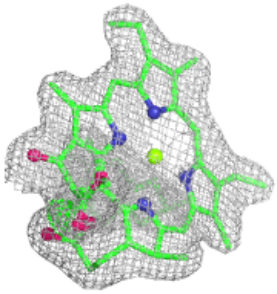


Electron density around CLA C 506:

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

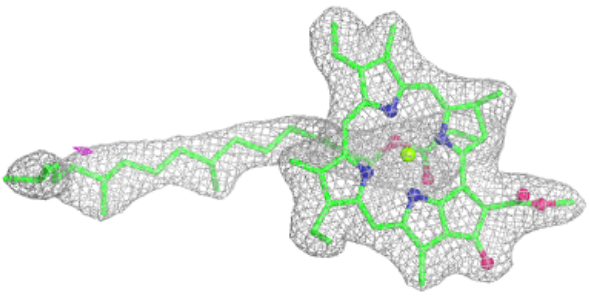


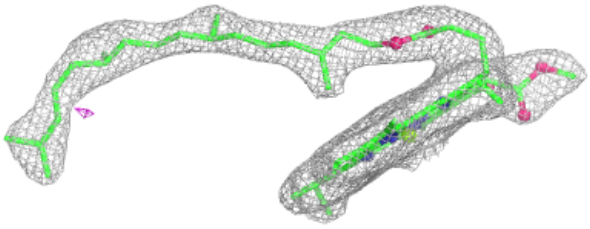


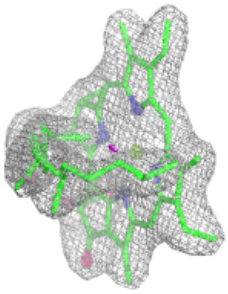


Electron density around CLA b 613:

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

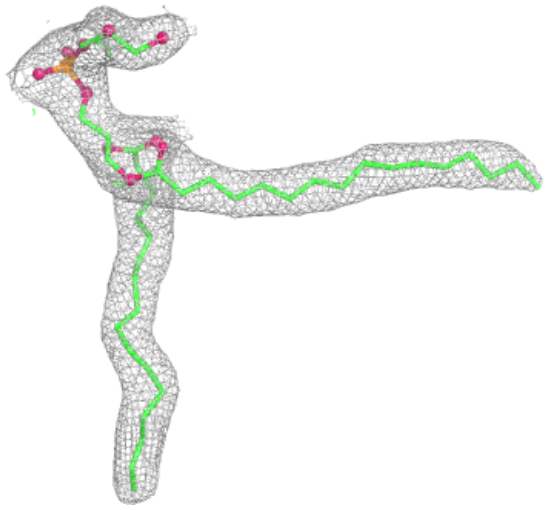


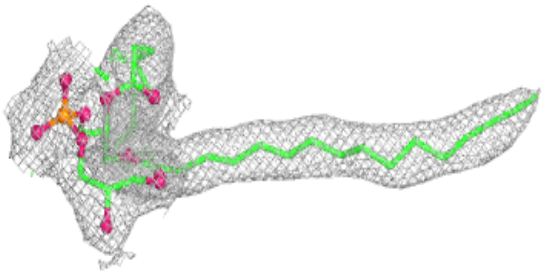


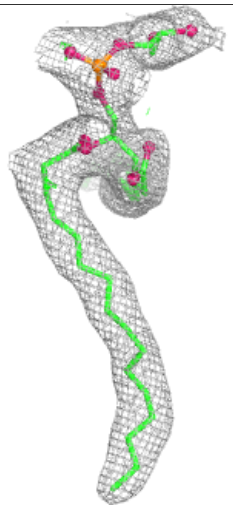


Electron density around LHG L 101:

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

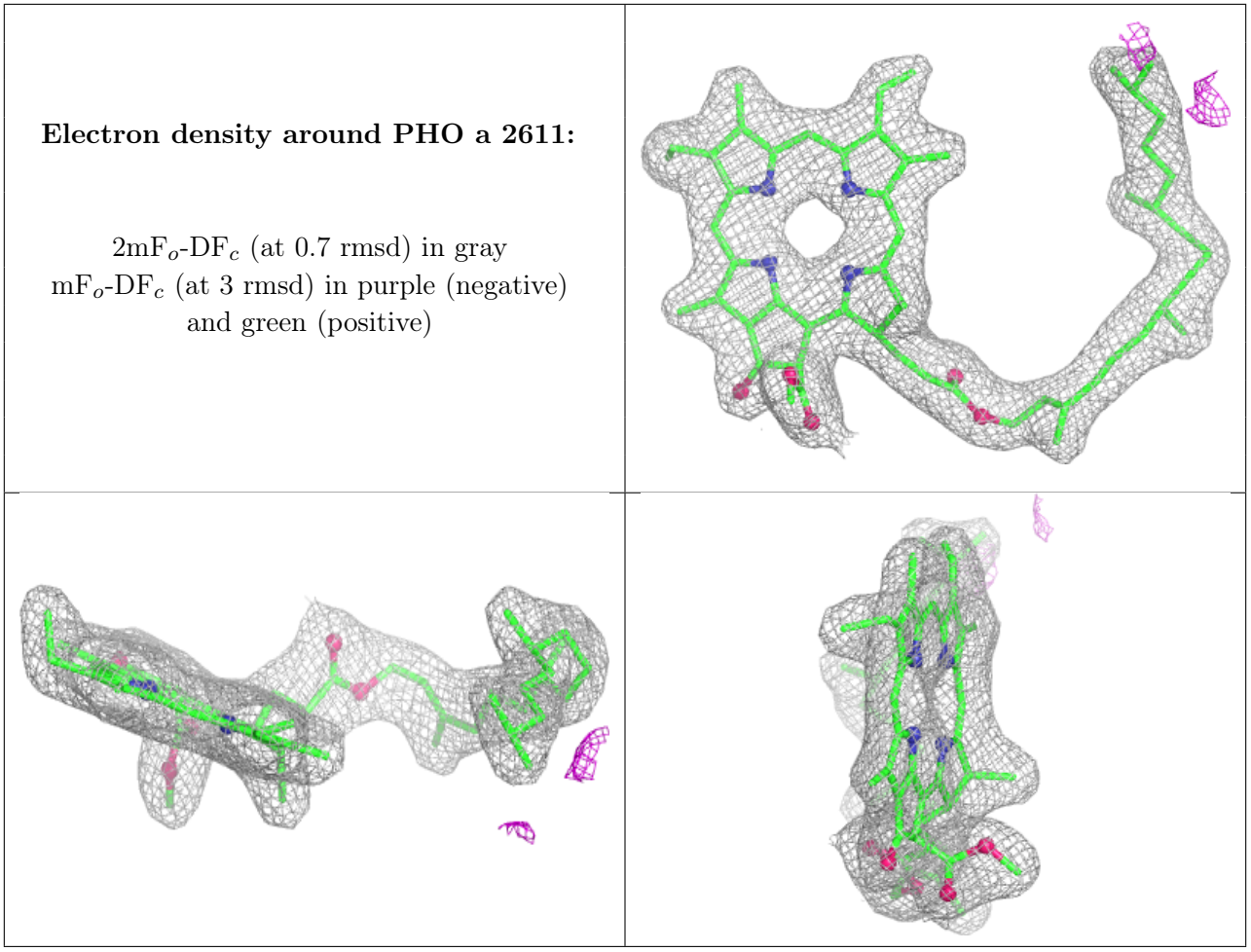






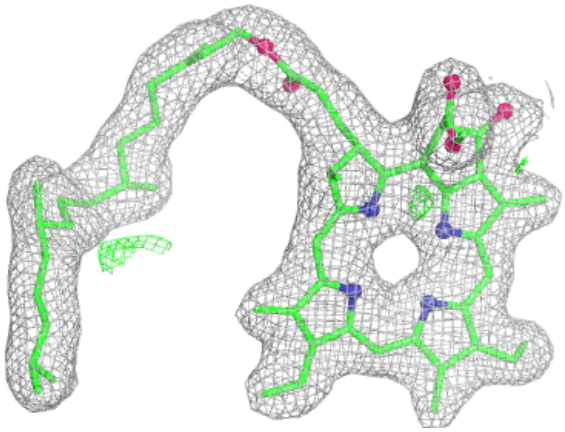
Electron density around PHO a 2611:

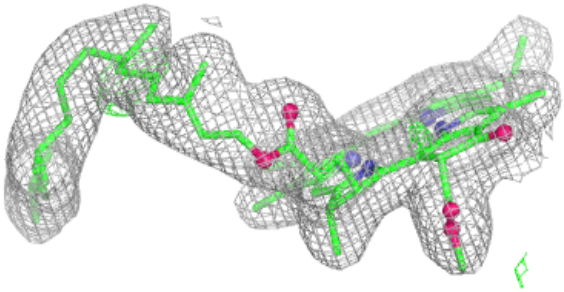
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO a 2612:

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

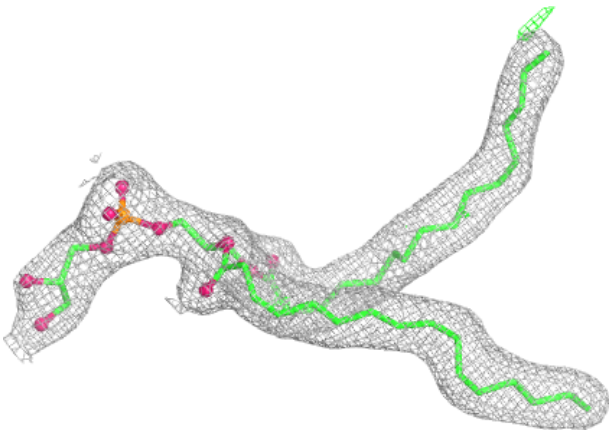


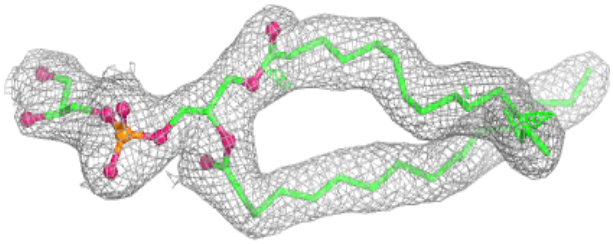


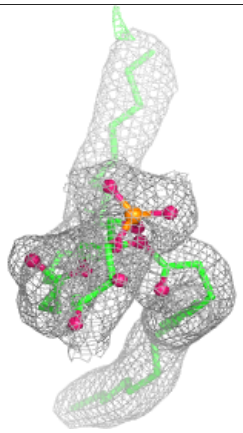


Electron density around LHG d 413:

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

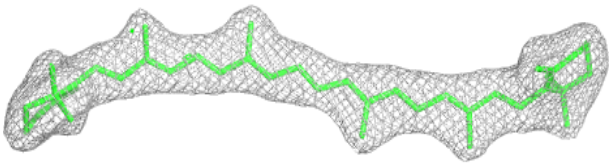


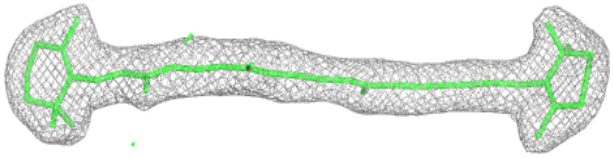


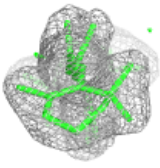


Electron density around BCR A 411:

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

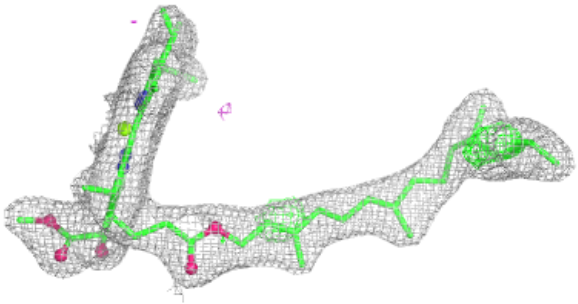


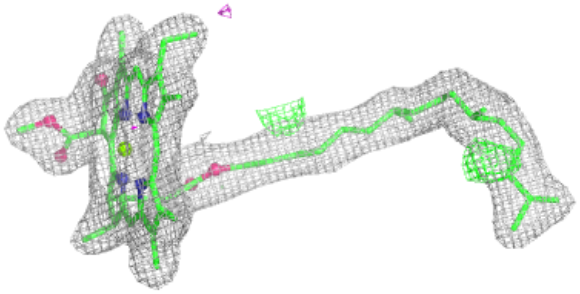


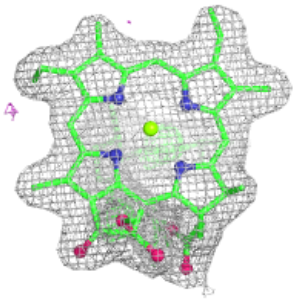


Electron density around CLA B 606:

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

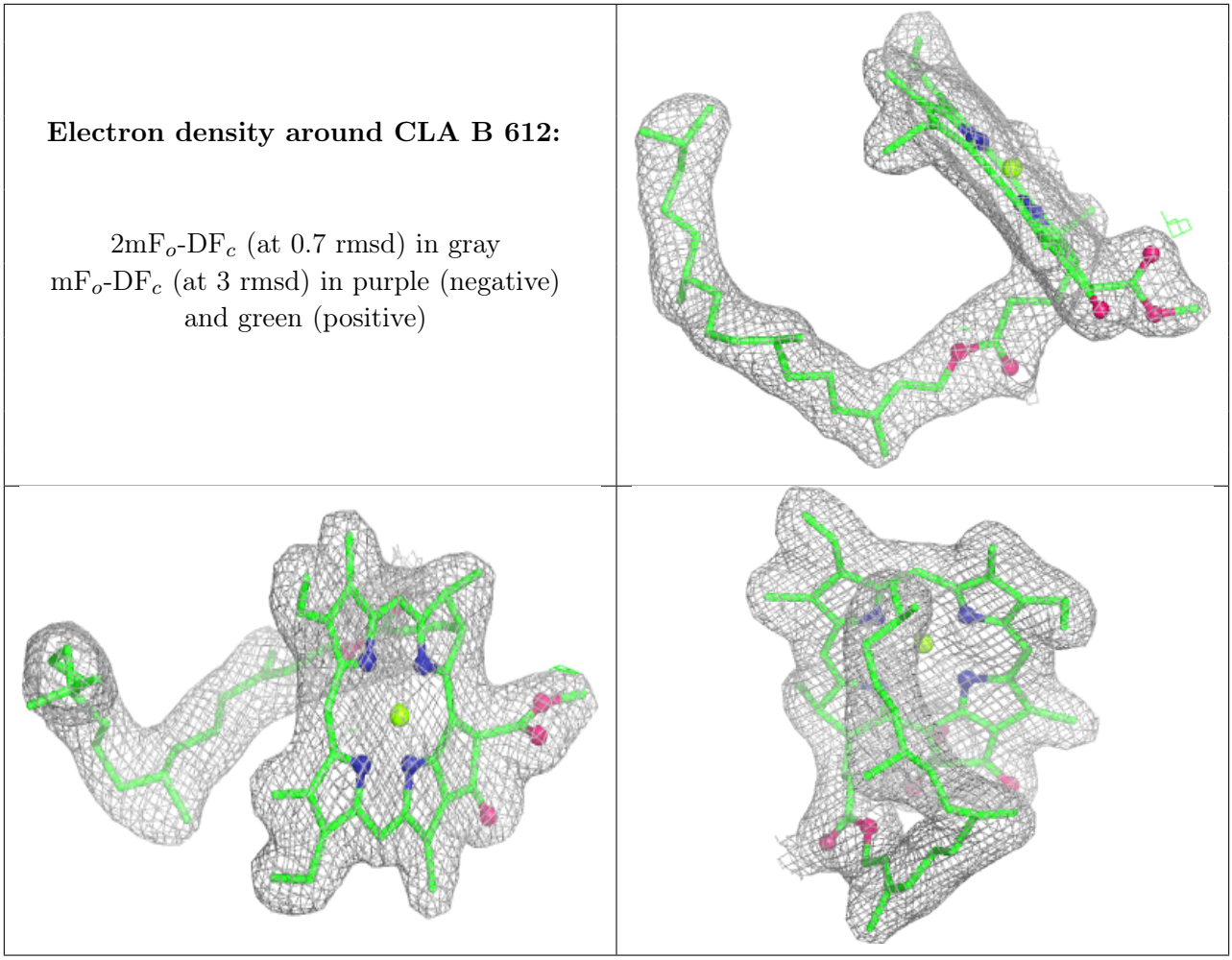






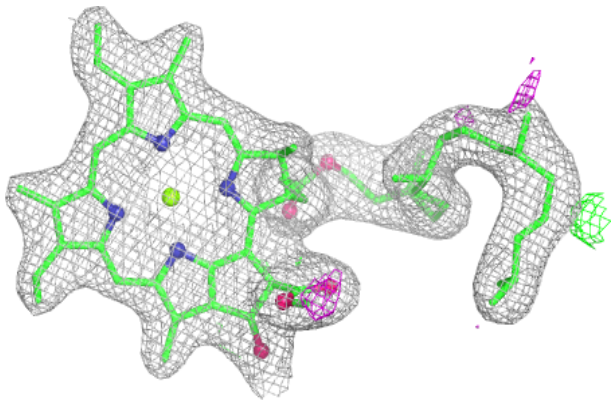
Electron density around CLA B 612:

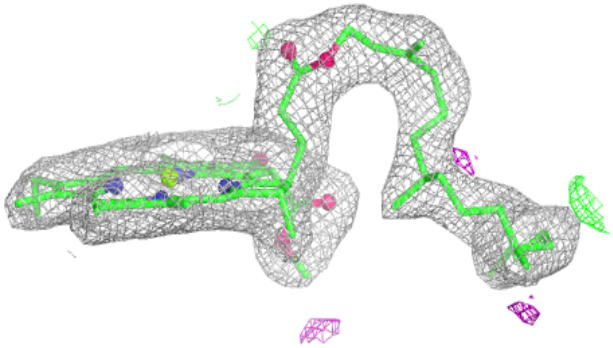
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

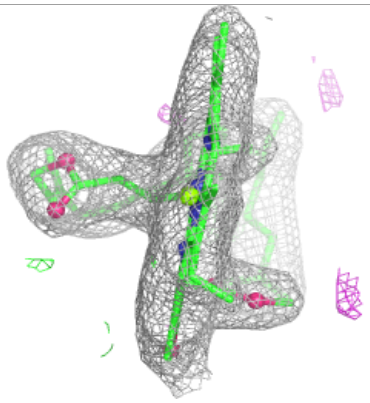


Electron density around CLA B 613:

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

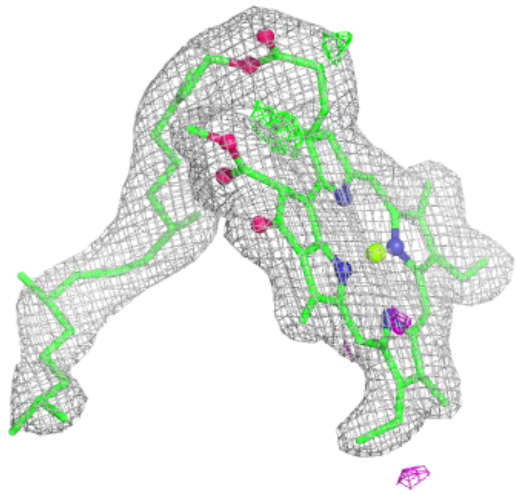


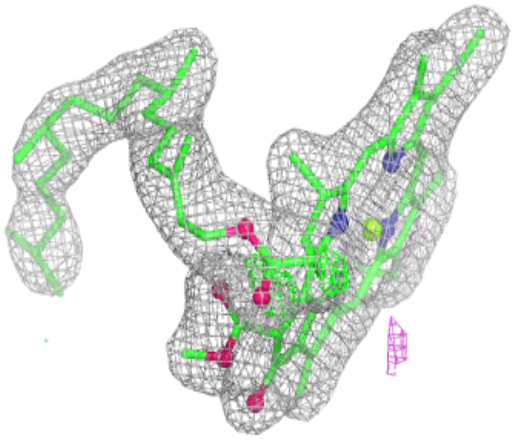


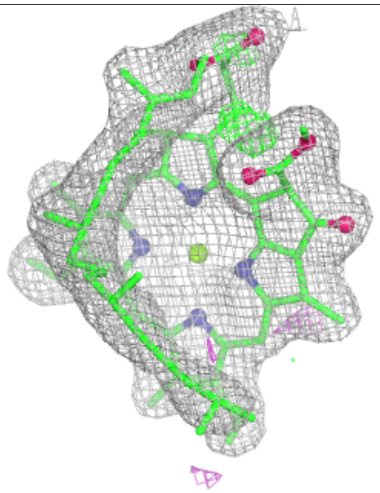


Electron density around CLA b 618:

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

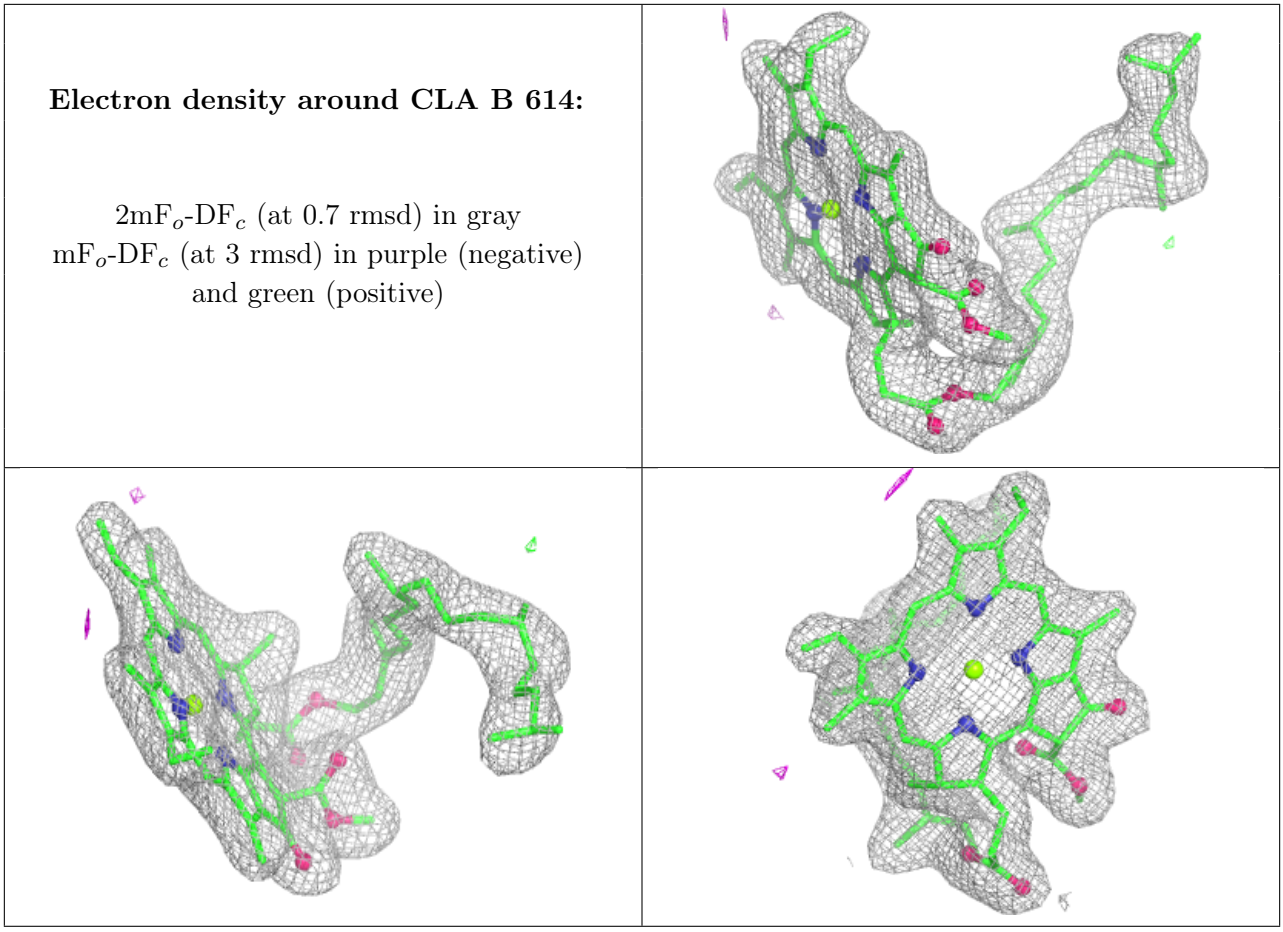






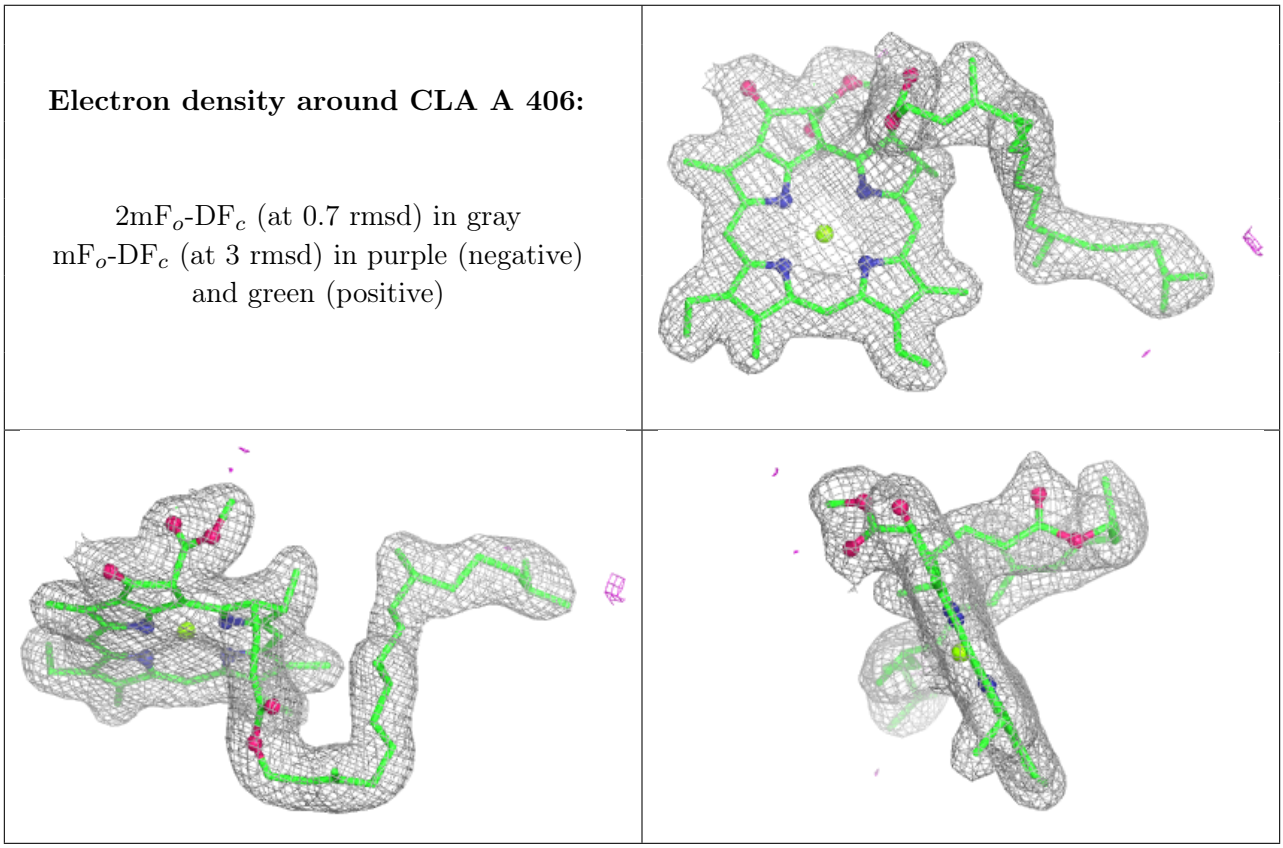
Electron density around CLA B 614:

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



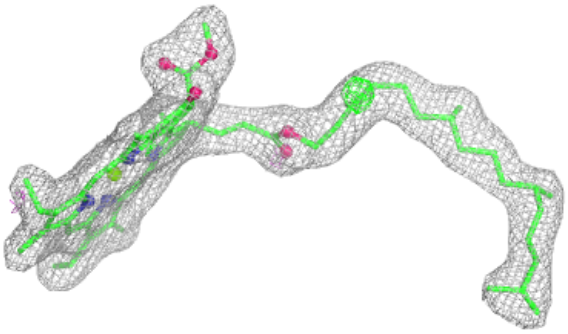
Electron density around CLA A 406:

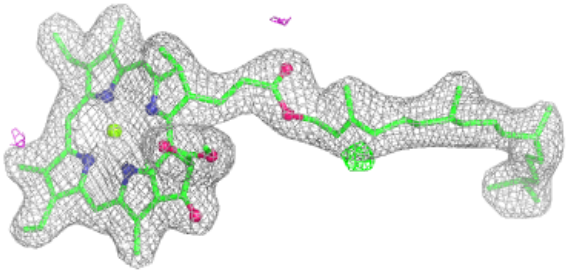
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

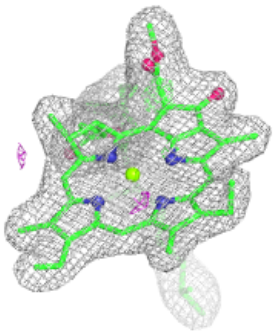


Electron density around CLA D 2303:

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

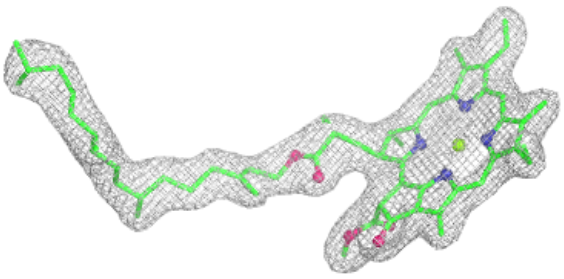


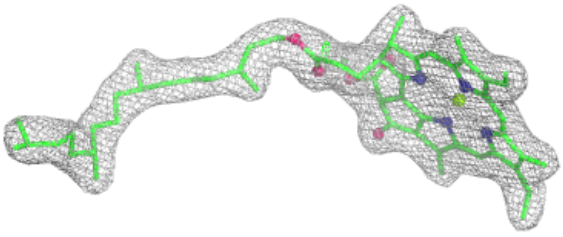


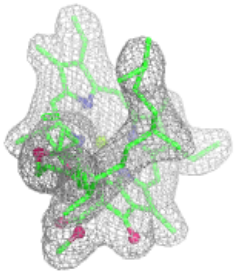


Electron density around CLA A 405:

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

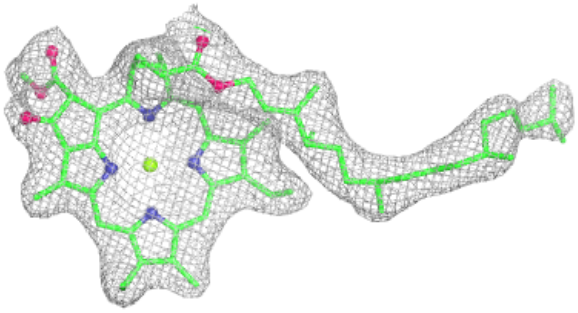


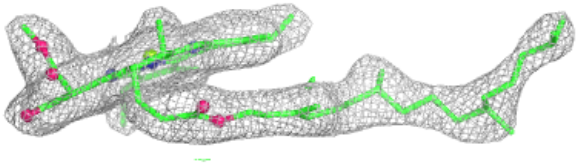


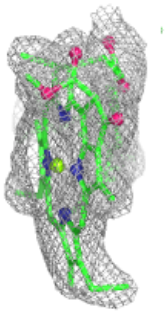


Electron density around CLA b 608:

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

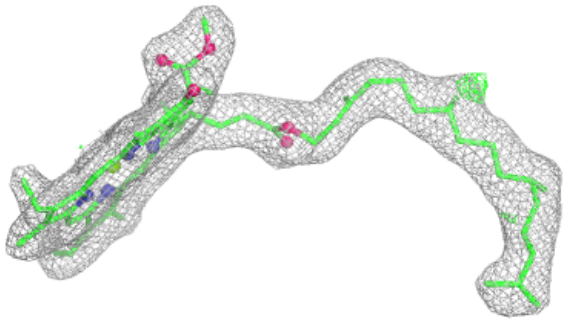


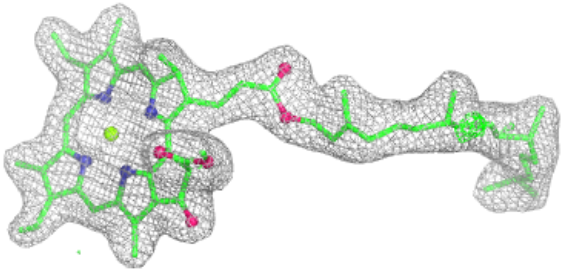


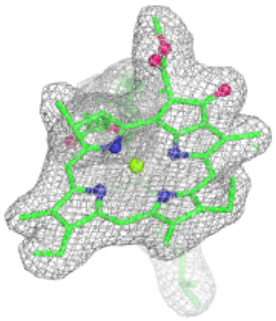


Electron density around CLA d 408:

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

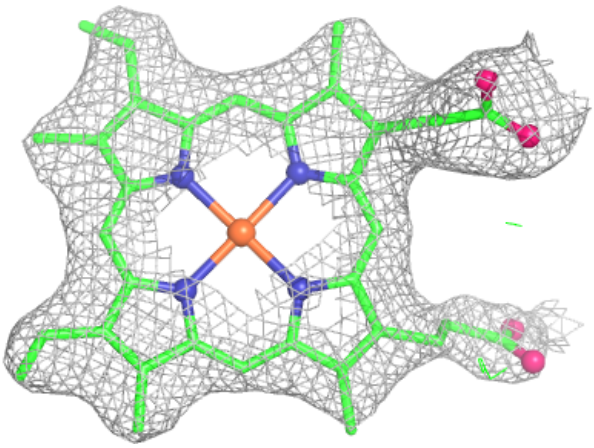


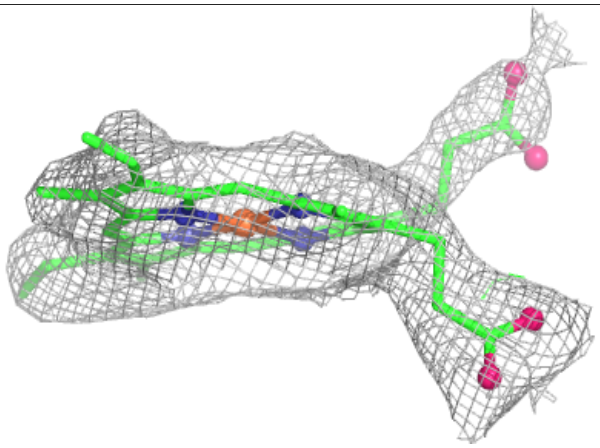


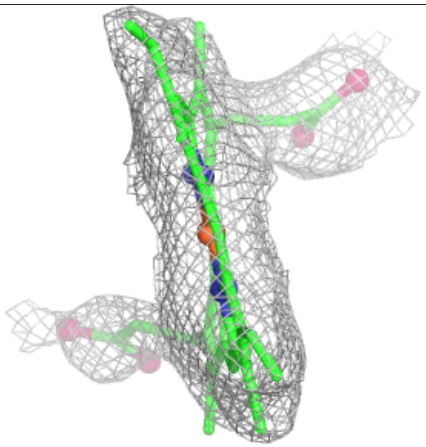


Electron density around HEM F 101:

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

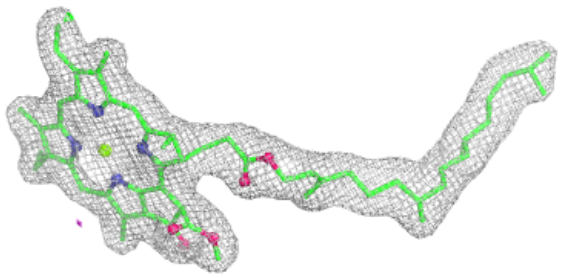


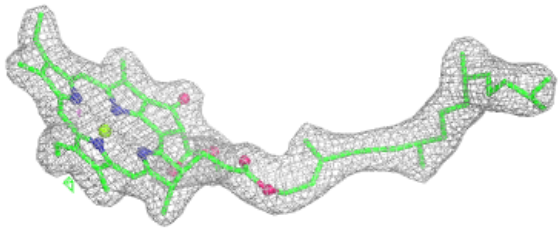




Electron density around CLA a 2609:

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

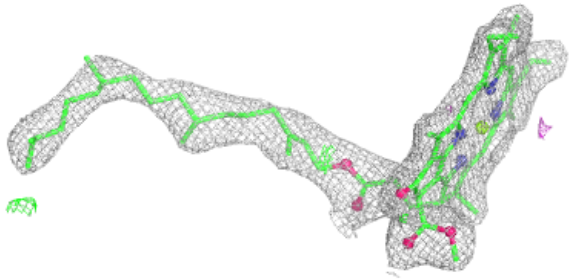


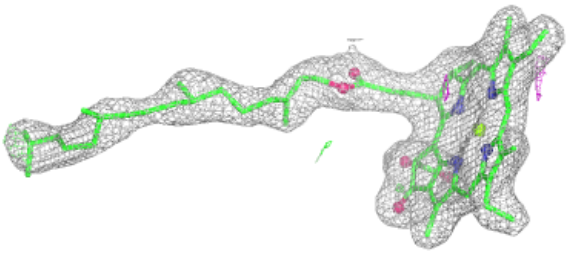


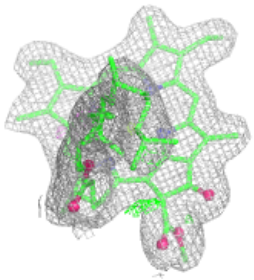


Electron density around CLA B 605:

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

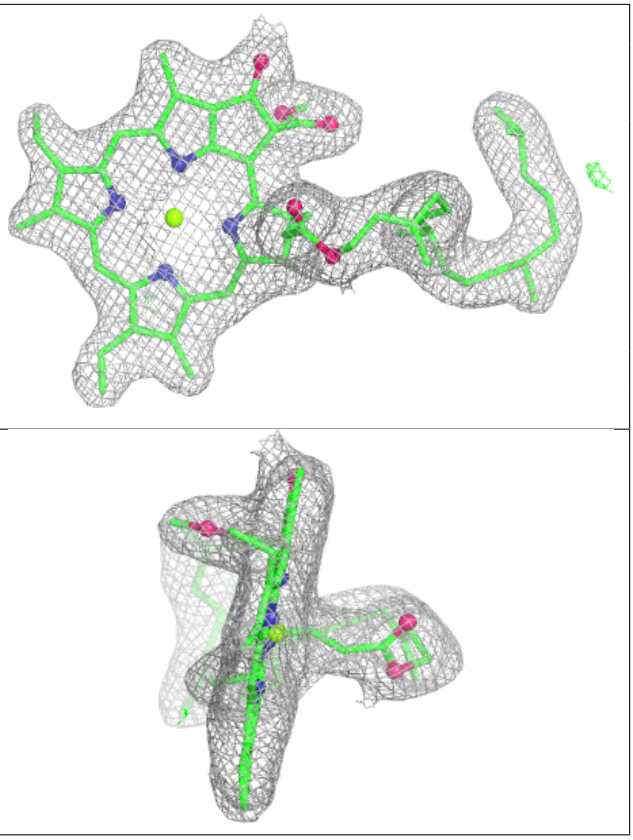


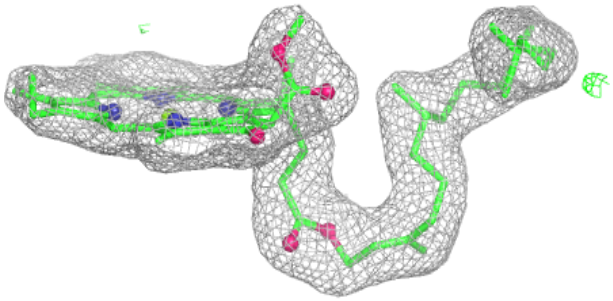




Electron density around CLA b 617:

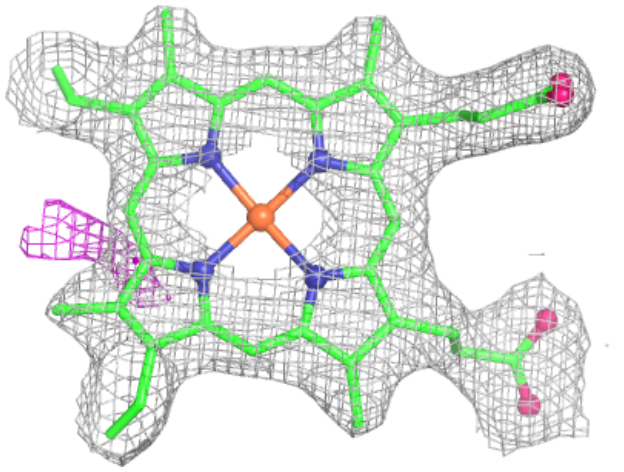
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

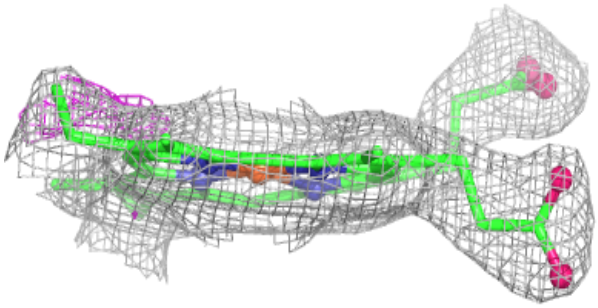




Electron density around HEC v 201:

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

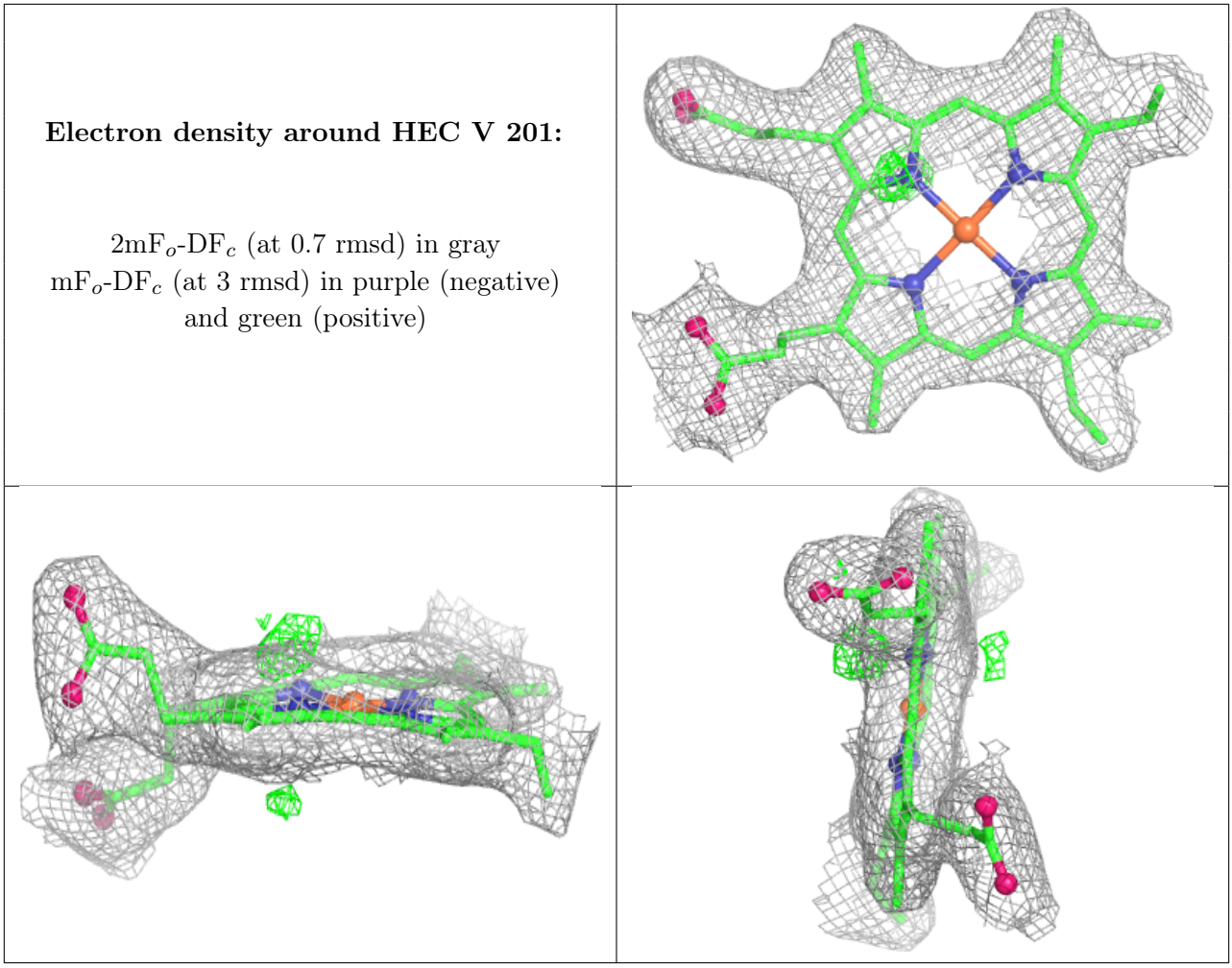






Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.