wwPDB X-ray Structure Validation Summary Report (i)

Mar 7, 2026 – 04:04 AM UTC

PDB ID	:	6JLK / pdb_00006jlk
Title	:	XFEL structure of cyanobacterial photosystem II (1F state, dataset1)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2019-03-06
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:

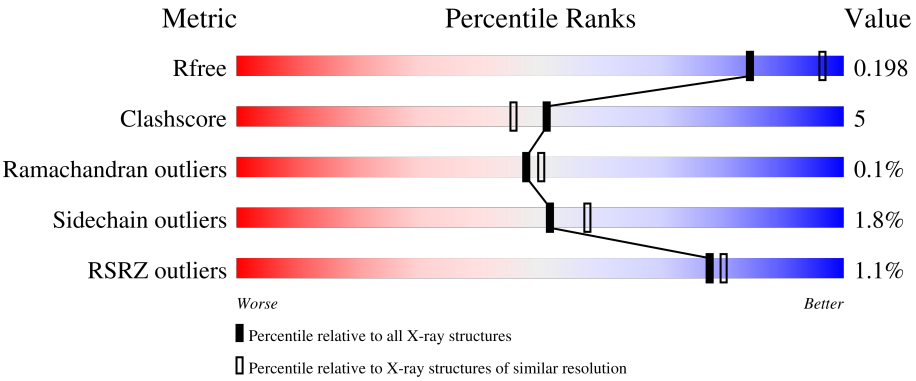
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	90% 7% ·
1	a	344	% 88% 8% · ·
2	B	505	91% 9%
2	b	505	% 90% 10%
3	C	455	89% 10% ·

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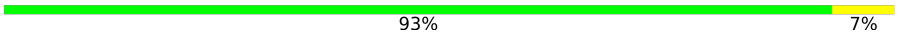
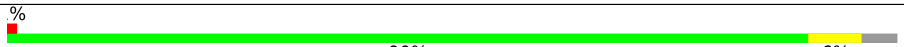
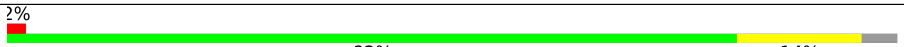
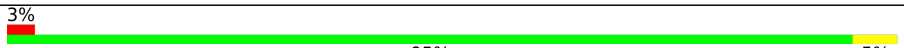
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	96%
16	v	137	92% 8%
17	Y	30	10% 73% 23%
17	y	30	10% 70% 23%
18	X	40	88% 10%
18	x	40	5% 90% 5% 5%
19	Z	62	6% 84% 16%
19	z	62	5% 77% 19%
20	R	34	35% 71% 12% 6% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	410	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	c	517	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 55631 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	53	0
			3019	1966	498	537	18			
1	a	334	Total	C	N	O	S	0	55	0
			3027	1973	498	538	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	7	0
			3518	2300	587	618	13			
3	c	455	Total	C	N	O	S	0	13	0
			3598	2356	599	629	14			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total 2	Fe 2	0	1
21	a	1	Total 2	Fe 2	0	1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 4	Cl 4	0	2
22	U	1	Total 1	Cl 1	0	0

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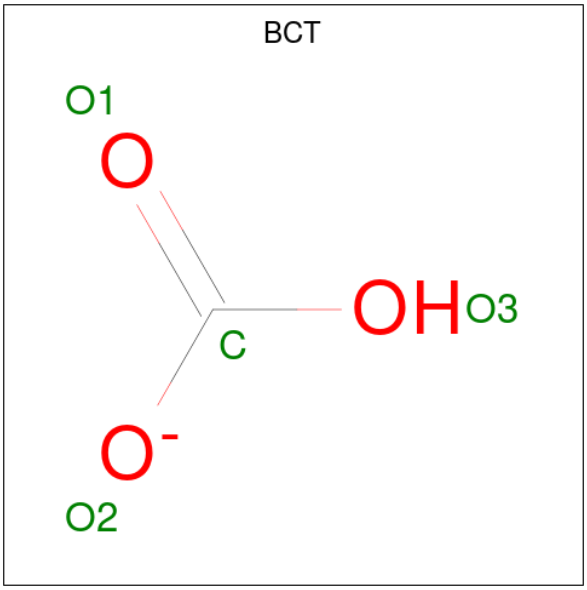
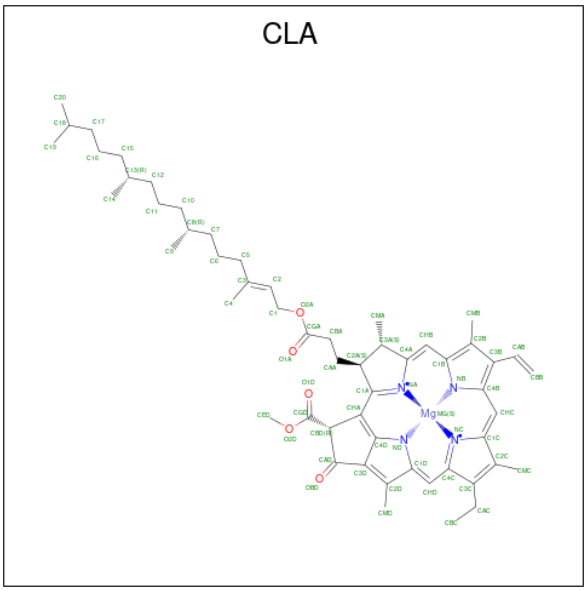
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2
22	v	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 8 2 6	0	1
23	a	1	Total C O 8 2 6	0	1

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



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

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

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

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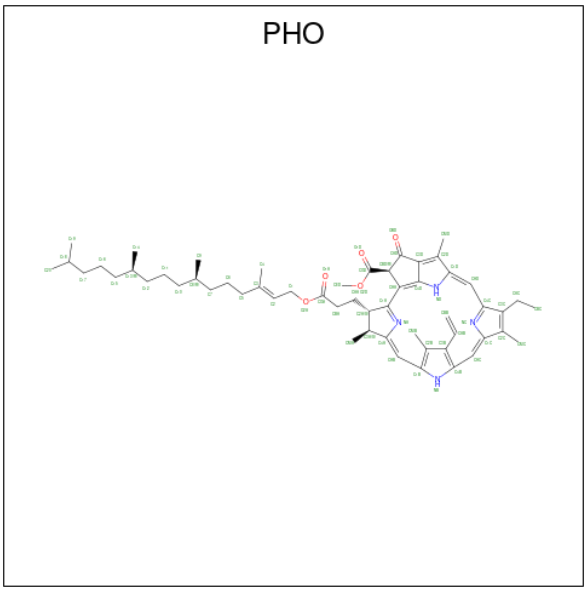
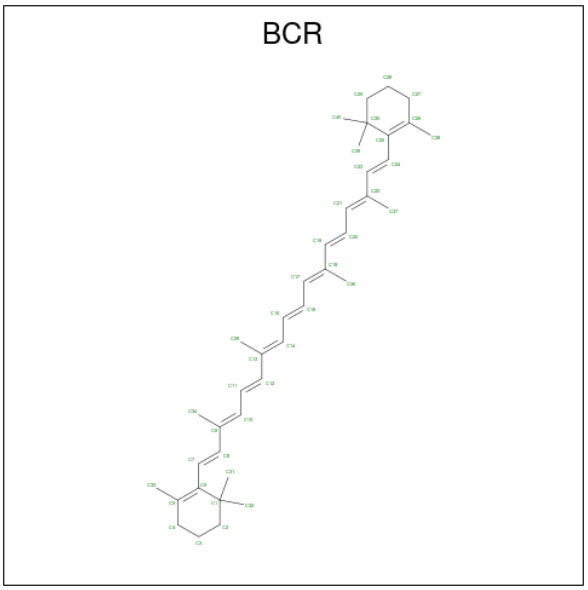
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



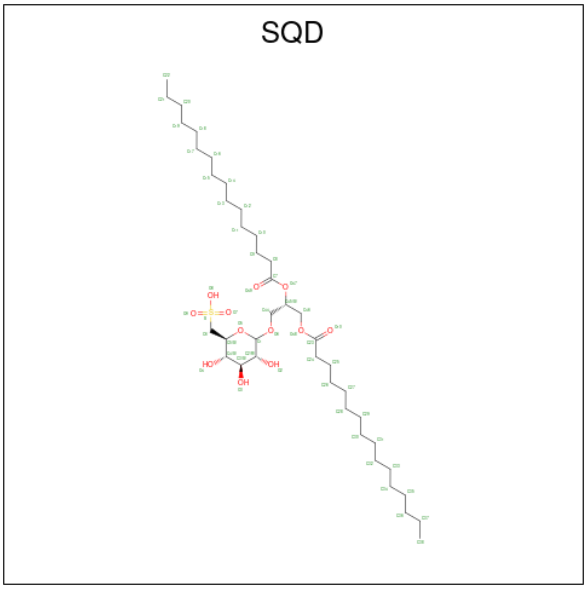
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C N O 64 55 4 5	0	0
25	A	1	Total C N O 128 110 8 10	0	1
25	a	1	Total C N O 64 55 4 5	0	0
25	a	1	Total C N O 128 110 8 10	0	1

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



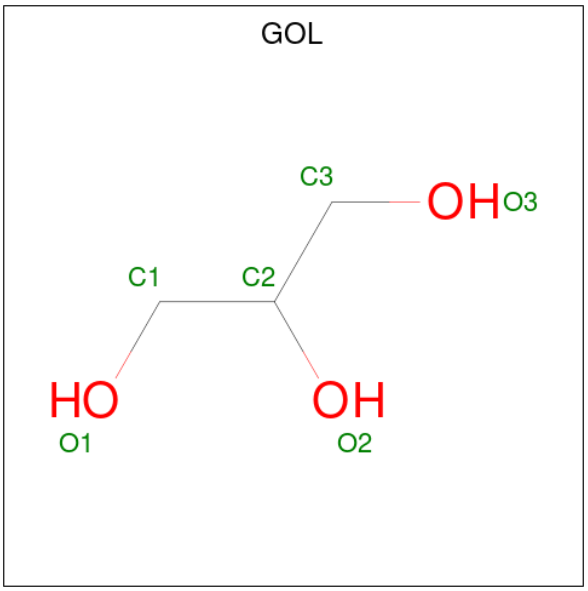
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



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

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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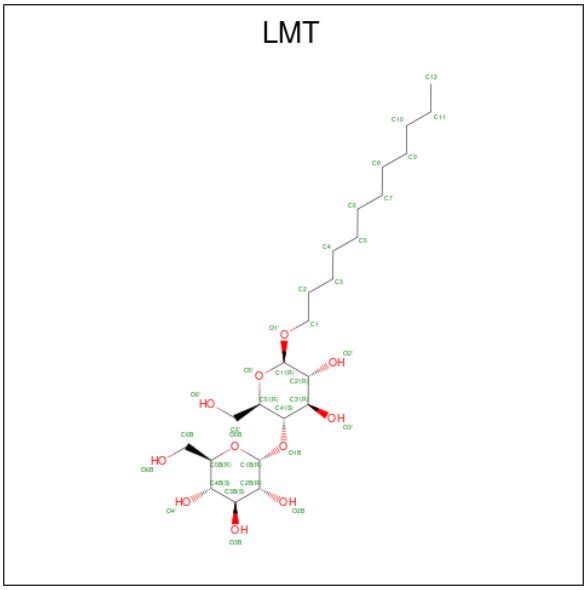
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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



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

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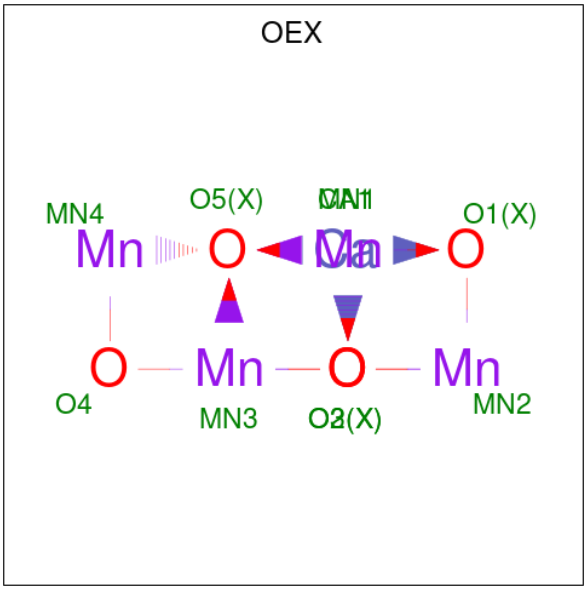
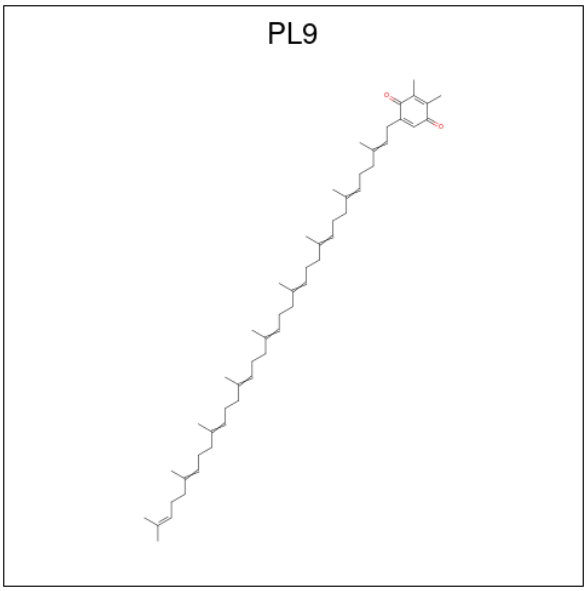
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
30	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

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



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

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

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

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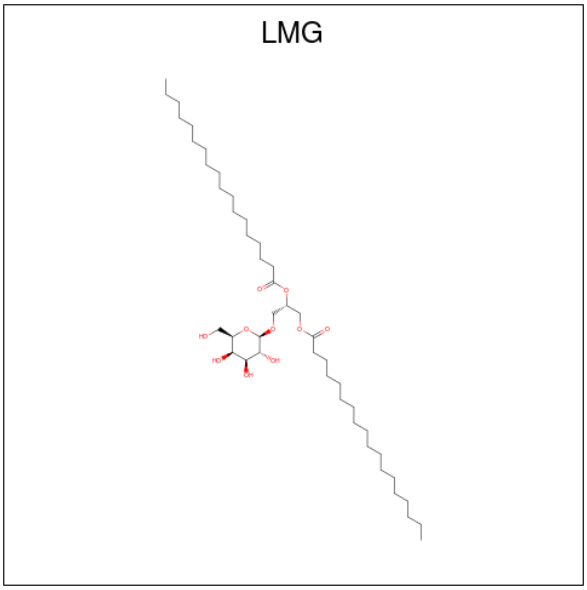
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 51 41 10	0	0
33	B	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0

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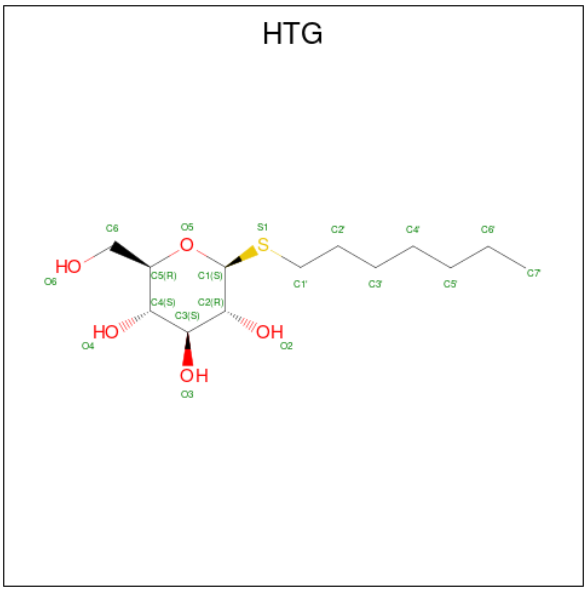
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 37 27 10	0	0
33	b	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	z	1	Total C O 39 29 10	0	0

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

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

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



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

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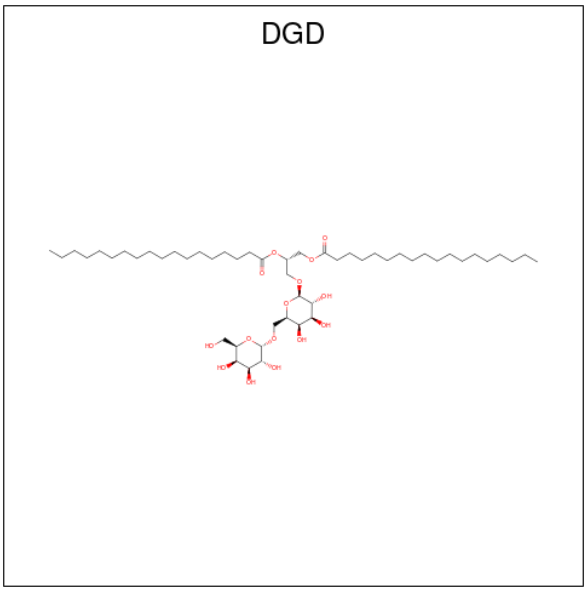
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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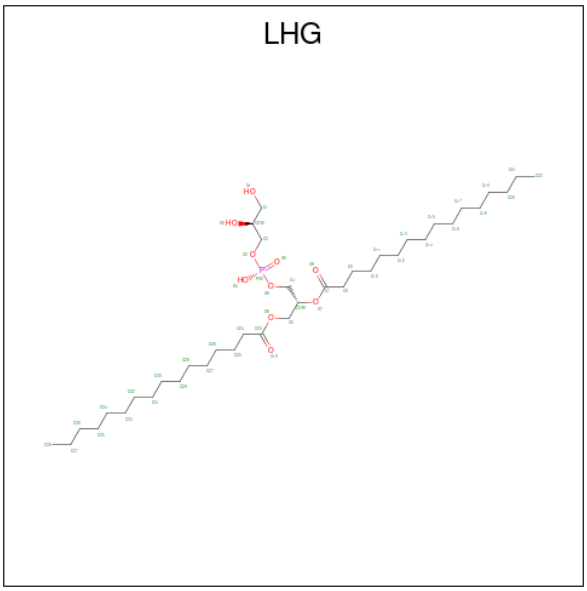
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	e	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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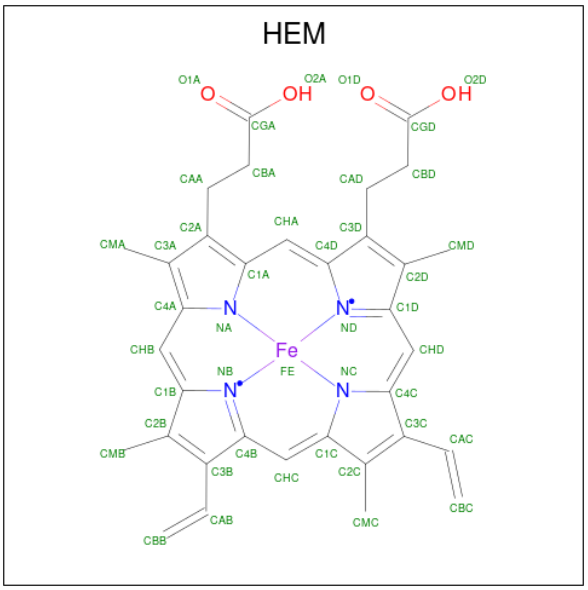
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	e	1	Total C O P 42 31 10 1	0	0

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

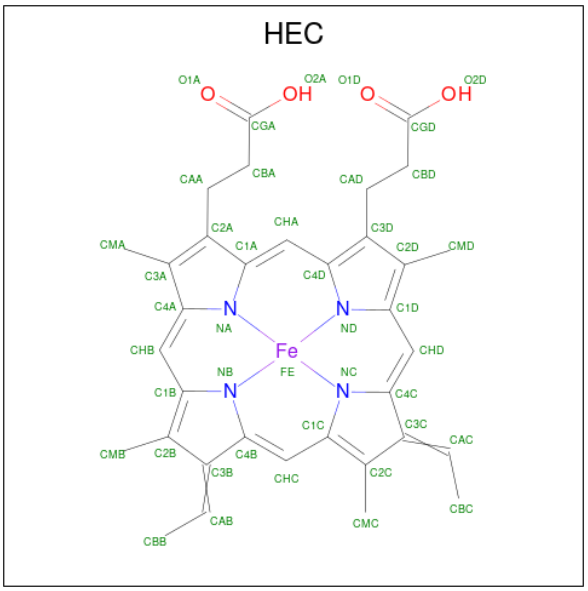


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	1	Total C Fe N O 43 34 1 4 4	0	0
38	e	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	166	Total	O	0	15
			179	179		
41	B	289	Total	O	0	4
			293	293		
41	C	229	Total	O	0	6
			233	233		
41	D	146	Total	O	0	5
			151	151		
41	E	32	Total	O	0	1
			33	33		
41	F	8	Total	O	0	0
			8	8		
41	H	44	Total	O	0	0
			44	44		
41	I	5	Total	O	0	0
			5	5		
41	J	12	Total	O	0	0
			12	12		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	18	Total O 19 19	0	1
41	M	19	Total O 19 19	0	0
41	O	175	Total O 177 177	0	2
41	T	16	Total O 17 17	0	1
41	U	82	Total O 82 82	0	0
41	V	113	Total O 115 115	0	2
41	Y	5	Total O 5 5	0	0
41	X	8	Total O 8 8	0	0
41	Z	1	Total O 1 1	0	0
41	a	155	Total O 167 167	0	14
41	b	259	Total O 262 262	0	3
41	c	202	Total O 207 207	0	7
41	d	134	Total O 137 137	0	3
41	e	16	Total O 16 16	0	0
41	f	7	Total O 7 7	0	0
41	h	42	Total O 42 42	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	7	Total O 7 7	0	0
41	l	9	Total O 9 9	0	0
41	m	16	Total O 16 16	0	0

Continued on next page...

Continued from previous page...

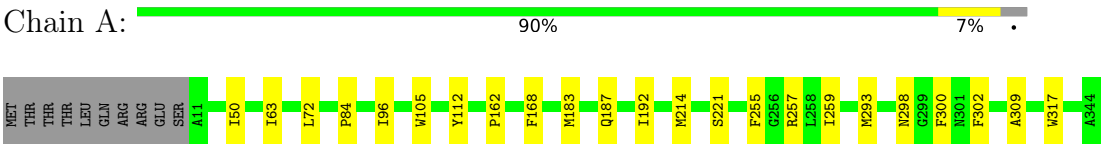
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	157	Total O 157 157	0	0
41	t	11	Total O 11 11	0	0
41	u	93	Total O 93 93	0	0
41	v	81	Total O 82 82	0	1
41	y	2	Total O 2 2	0	0
41	x	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

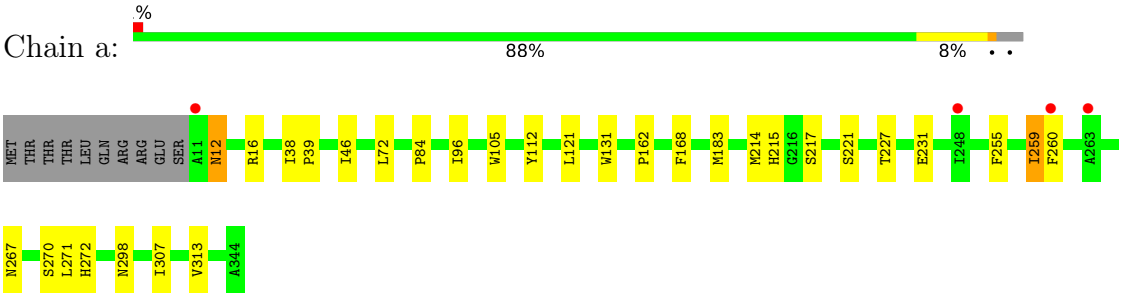
• Molecule 1: Photosystem II protein D1

Chain A:



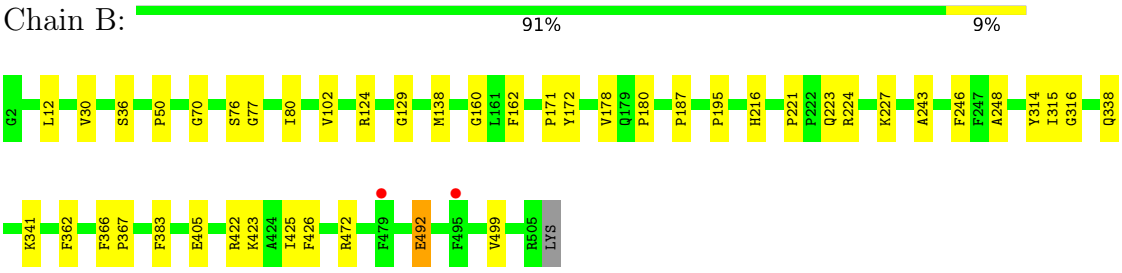
• Molecule 1: Photosystem II protein D1

Chain a:



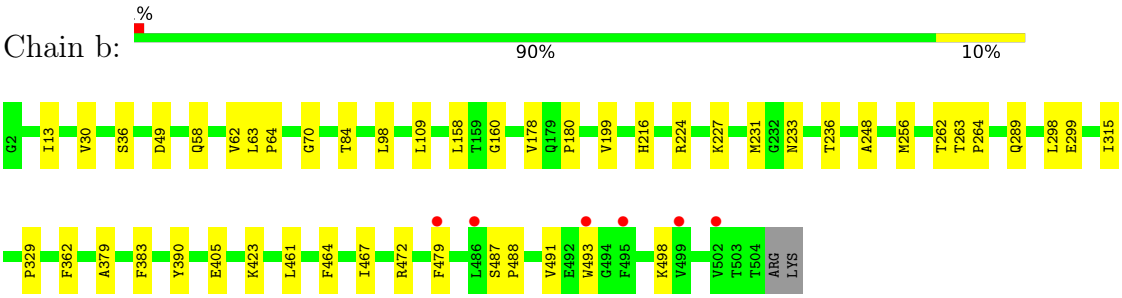
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



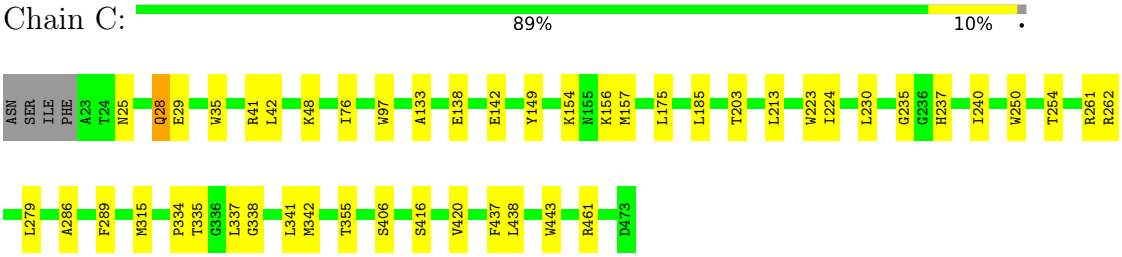
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



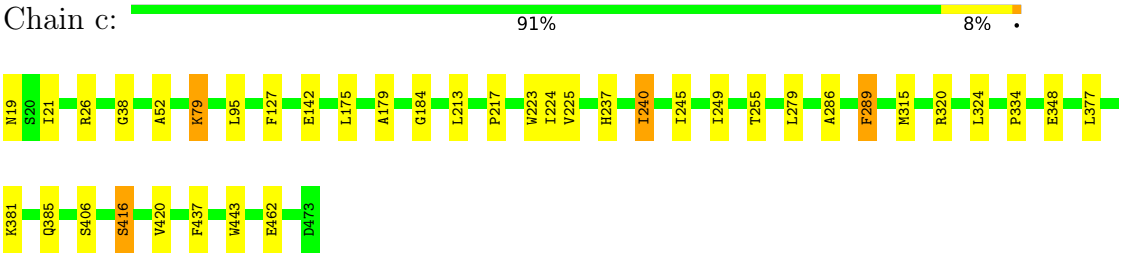
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



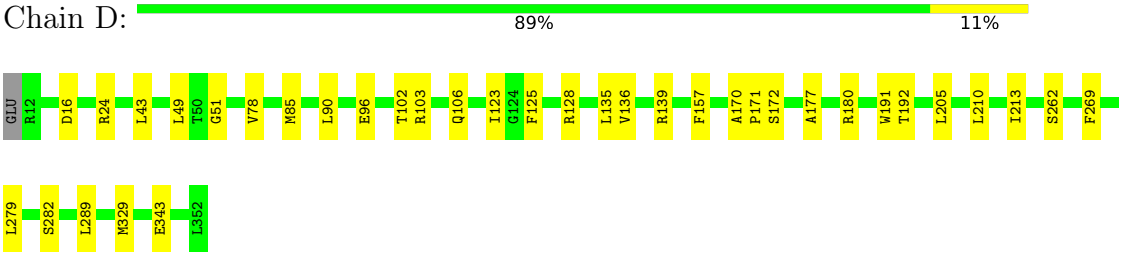
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



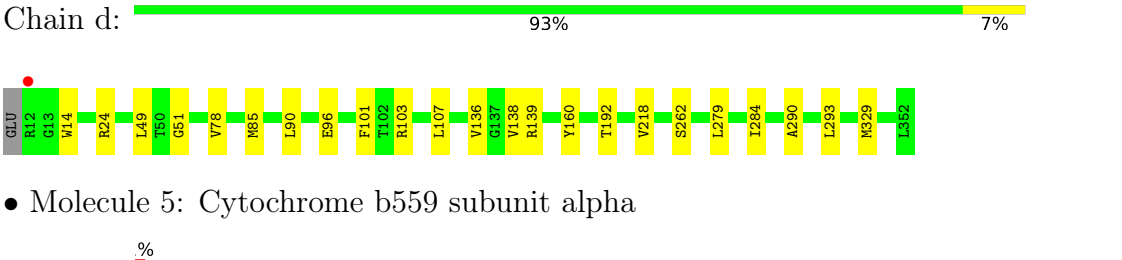
• Molecule 4: Photosystem II D2 protein

Chain D:



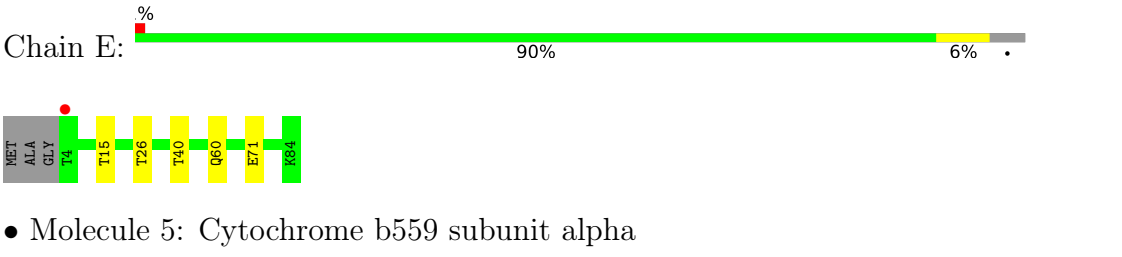
• Molecule 4: Photosystem II D2 protein

Chain d:



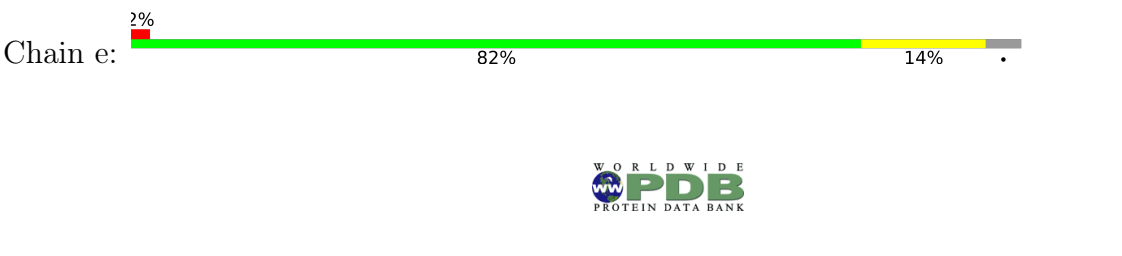
• Molecule 5: Cytochrome b559 subunit alpha

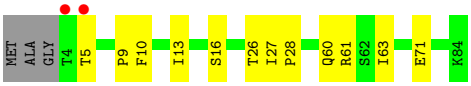
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

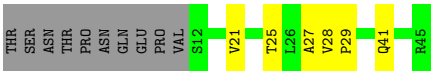
Chain e:





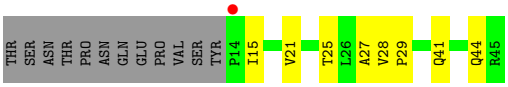
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



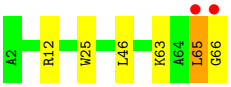
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



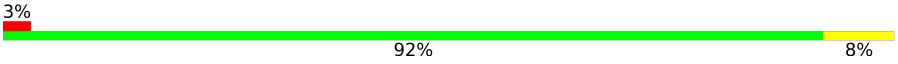
• Molecule 7: Photosystem II reaction center protein H

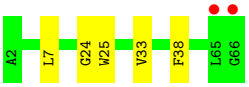
Chain H:



• Molecule 7: Photosystem II reaction center protein H

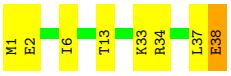
Chain h:





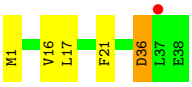
• Molecule 8: Photosystem II reaction center protein I

Chain I:



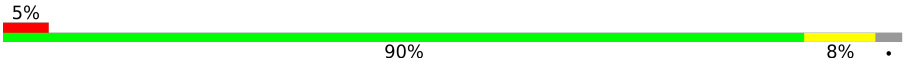
• Molecule 8: Photosystem II reaction center protein I

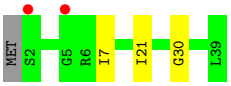
Chain i:



• Molecule 9: Photosystem II reaction center protein J

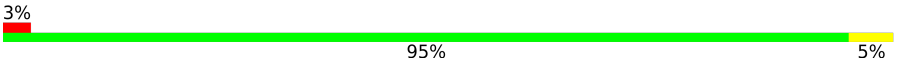
Chain J:





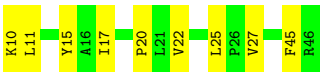
• Molecule 9: Photosystem II reaction center protein J

Chain j:



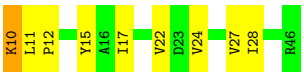
• Molecule 10: Photosystem II reaction center protein K

Chain K:



• Molecule 10: Photosystem II reaction center protein K

Chain k:

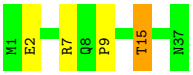


• Molecule 11: Photosystem II reaction center protein L

Chain L:

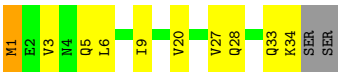
• Molecule 11: Photosystem II reaction center protein L

Chain l:



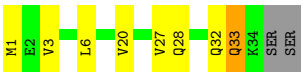
• Molecule 12: Photosystem II reaction center protein M

Chain M:



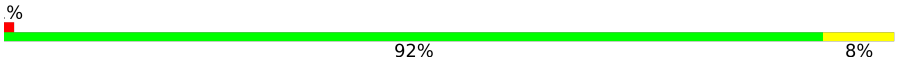
• Molecule 12: Photosystem II reaction center protein M

Chain m:



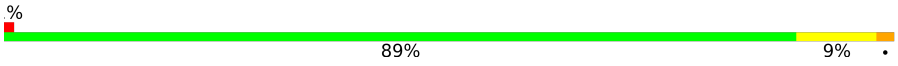
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

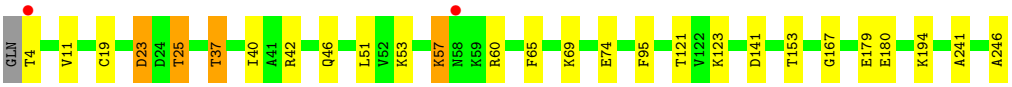
Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



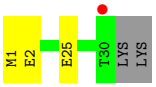


• Molecule 14: Photosystem II reaction center protein T

Chain T:

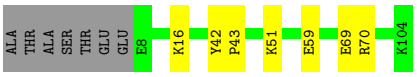
• Molecule 14: Photosystem II reaction center protein T

Chain t:



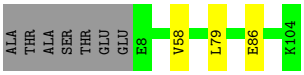
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



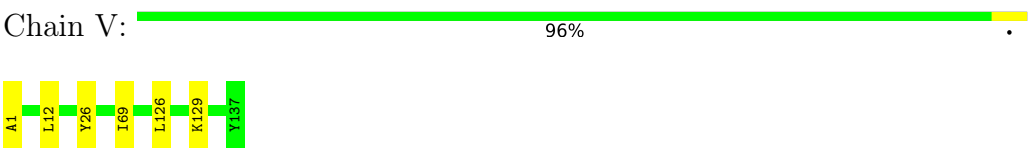
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



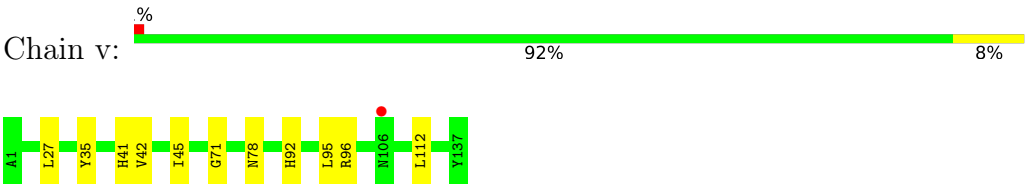
• Molecule 16: Cytochrome c-550

Chain V:



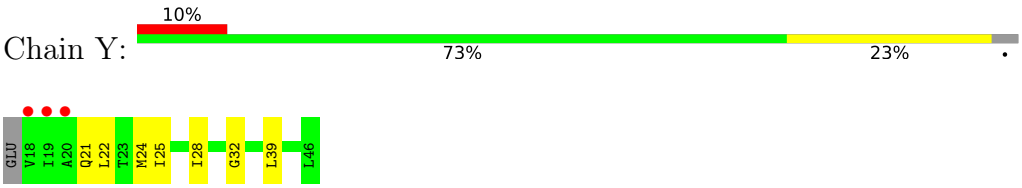
• Molecule 16: Cytochrome c-550

Chain v:



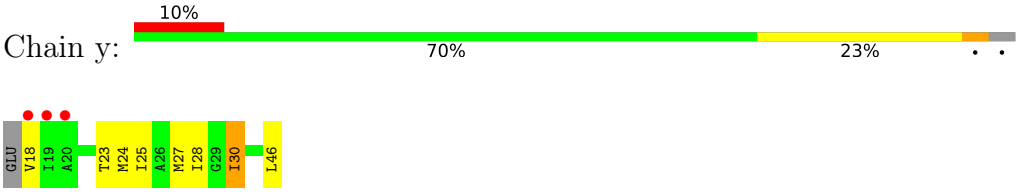
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



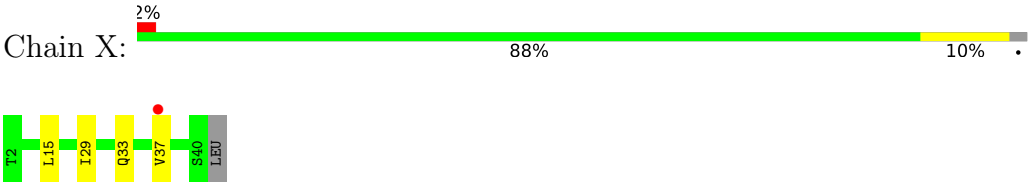
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



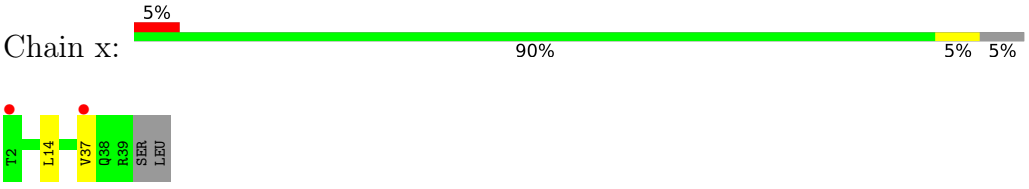
• Molecule 18: Photosystem II reaction center protein X

Chain X:



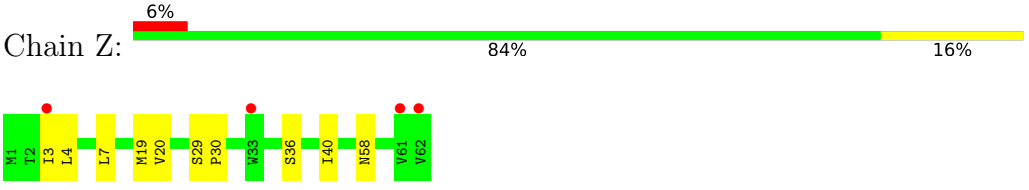
• Molecule 18: Photosystem II reaction center protein X

Chain x:



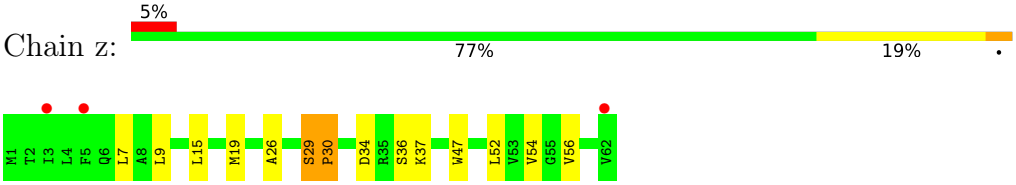
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



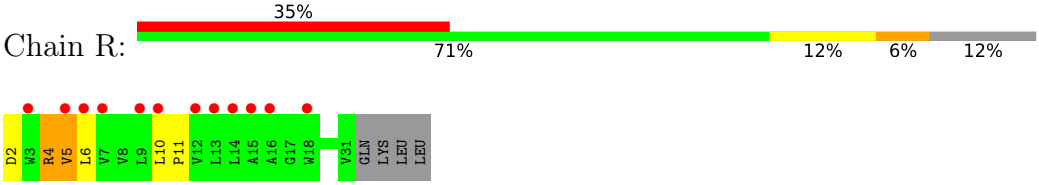
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.15) 99.8 (19.98-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.149 , 0.193 0.156 , 0.198	Depositor DCC
R_{free} test set	26831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 77.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55631	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: MG, LMT, OEX, HEC, PHO, BCT, HEM, GOL, DGD, CA, BCR, CL, PL9, UNL, FE2, FME, LMG, CLA, HTG, SQD, LHG

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	0.55	0/3121	0.82	0/4250
1	a	0.56	0/3135	0.79	0/4269
2	B	0.55	0/4191	0.81	1/5709 (0.0%)
2	b	0.53	0/4198	0.81	1/5720 (0.0%)
3	C	0.50	0/3643	0.80	4/4958 (0.1%)
3	c	0.48	0/3731	0.79	2/5076 (0.0%)
4	D	0.60	0/2952	0.80	3/4021 (0.1%)
4	d	0.56	0/2952	0.77	1/4021 (0.0%)
5	E	0.46	0/693	0.78	0/944
5	e	0.44	0/695	0.80	0/948
6	F	0.57	0/284	0.79	0/387
6	f	0.54	0/265	0.77	0/360
7	H	0.44	0/535	0.87	0/728
7	h	0.43	0/524	0.76	0/713
8	I	0.43	0/311	0.74	0/419
8	i	0.47	0/311	0.81	0/419
9	J	0.46	0/278	0.76	0/376
9	j	0.44	0/286	0.76	0/386
10	K	0.47	0/303	0.79	0/416
10	k	0.53	0/303	0.86	0/416
11	L	0.58	0/319	0.69	0/433
11	l	0.50	0/319	0.74	0/433
12	M	0.60	0/270	0.84	0/368
12	m	0.57	0/262	0.84	0/357
13	O	0.46	0/1958	0.78	0/2654
13	o	0.44	0/1937	0.79	0/2625
14	T	0.57	0/266	0.72	0/362
14	t	0.57	0/266	0.74	0/362
15	U	0.49	0/785	0.74	0/1064
15	u	0.47	0/785	0.70	0/1064
16	V	0.51	0/1109	0.75	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.46	0/1098	0.80	2/1488 (0.1%)
17	Y	0.49	0/216	0.85	0/289
17	y	0.42	0/216	0.75	0/289
18	X	0.41	0/290	0.79	0/392
18	x	0.41	0/284	0.75	0/384
19	Z	0.38	0/490	0.76	0/669
19	z	0.34	0/490	0.80	0/669
20	R	0.35	0/245	0.67	0/338
All	All	0.51	0/44316	0.79	14/60278 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	76	ILE	CA-C-N	6.94	127.52	119.47
3	C	76	ILE	C-N-CA	6.94	127.52	119.47
4	D	170	ALA	CA-C-N	-6.39	113.37	119.76
4	D	170	ALA	C-N-CA	-6.39	113.37	119.76
3	C	133	ALA	CA-C-N	-5.38	116.12	122.36

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	3019	0	2872	19	0
1	a	3027	0	2888	28	0
2	B	4021	0	3898	38	0
2	b	4022	0	3908	36	0
3	C	3518	0	3439	30	0
3	c	3598	0	3529	26	0
4	D	2849	0	2741	27	0
4	d	2849	0	2741	18	0
5	E	668	0	658	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	670	0	664	10	0
6	F	275	0	282	4	0
6	f	257	0	269	4	0
7	H	519	0	545	9	0
7	h	511	0	532	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	3	0
9	j	280	0	291	1	0
10	K	293	0	305	7	0
10	k	293	0	305	6	0
11	L	309	0	327	4	0
11	l	309	0	327	5	0
12	M	274	0	299	8	0
12	m	269	0	288	8	0
13	O	1903	0	1886	10	0
13	o	1891	0	1870	16	0
14	T	264	0	267	4	0
14	t	264	0	267	2	0
15	U	774	0	773	3	1
15	u	774	0	773	1	0
16	V	1085	0	1095	4	0
16	v	1077	0	1082	8	0
17	Y	215	0	246	5	0
17	y	215	0	246	5	0
18	X	287	0	317	3	0
18	x	281	0	312	2	0
19	Z	479	0	516	5	0
19	z	479	0	516	8	0
20	R	239	0	262	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	1	0
22	a	4	0	0	0	0
22	v	1	0	0	1	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	36	0
24	C	845	0	936	30	0
24	D	130	0	144	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	195	0	216	9	0
24	b	1040	0	1152	28	0
24	c	845	0	936	35	0
24	d	195	0	216	9	0
25	A	192	0	222	6	0
25	a	192	0	222	3	0
26	A	40	0	56	1	0
26	B	120	0	168	11	0
26	C	80	0	112	11	0
26	D	40	0	56	1	0
26	H	40	0	56	3	0
26	K	40	0	56	0	0
26	T	40	0	56	5	0
26	Y	40	0	56	4	0
26	a	40	0	56	1	0
26	b	120	0	168	10	0
26	c	80	0	112	5	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	1	0
26	t	40	0	56	5	0
26	y	40	0	56	2	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	53	2	0
27	L	54	0	78	3	0
27	a	108	0	156	3	0
27	f	43	0	53	1	1
28	A	24	0	32	1	0
28	B	42	0	56	1	0
28	C	12	0	16	0	0
28	O	6	0	8	0	0
28	T	12	0	16	3	0
28	V	24	0	32	0	0
28	a	18	0	23	2	0
28	b	30	0	40	0	0
28	c	12	0	16	2	0
28	o	6	0	8	0	0
28	t	6	0	8	1	0
28	v	18	0	24	1	0
29	A	35	0	46	2	0
29	B	25	0	35	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	35	0	46	1	0
29	D	35	0	46	1	0
29	F	35	0	46	0	0
29	M	70	0	92	4	0
29	T	25	0	35	0	0
29	a	70	0	92	2	0
29	b	25	0	35	3	0
29	f	35	0	46	1	0
29	m	70	0	92	3	0
30	A	20	0	0	0	0
30	a	20	0	0	0	0
31	A	110	0	160	9	0
31	D	110	0	160	1	0
31	a	110	0	160	14	0
31	d	110	0	160	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	C	34	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	A	51	0	72	4	0
33	B	51	0	72	1	0
33	C	102	0	144	7	0
33	D	51	0	72	1	0
33	Z	37	0	44	1	0
33	b	51	0	72	3	0
33	c	153	0	216	7	0
33	d	51	0	72	2	0
33	z	39	0	48	5	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	O	1	0	0	0	0
34	b	1	0	0	0	0
34	c	2	0	0	0	0
34	f	1	0	0	0	0
34	o	1	0	0	0	0
35	B	95	0	130	1	0
35	C	38	0	52	0	0
35	D	16	0	17	2	0
35	V	19	0	26	1	0
35	b	95	0	130	1	0
35	c	38	0	52	1	0
35	d	16	0	17	3	0
36	C	186	0	246	4	0
36	D	52	0	71	2	0
36	H	62	0	82	0	0
36	c	186	0	246	2	0
36	e	62	0	82	7	0
36	h	62	0	82	0	0
37	D	147	0	222	11	0
37	E	42	0	57	2	0
37	L	49	0	74	0	0
37	b	49	0	74	3	0
37	d	147	0	222	9	0
37	e	42	0	57	4	0
38	F	43	0	30	2	0
38	e	43	0	30	5	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	179	0	0	1	0
41	B	293	0	0	2	0
41	C	233	0	0	3	0
41	D	151	0	0	1	0
41	E	33	0	0	0	0
41	F	8	0	0	0	0
41	H	44	0	0	0	0
41	I	5	0	0	1	0
41	J	12	0	0	0	0
41	K	8	0	0	1	0
41	L	19	0	0	0	0
41	M	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	O	177	0	0	2	0
41	T	17	0	0	1	0
41	U	82	0	0	2	0
41	V	115	0	0	1	0
41	X	8	0	0	0	0
41	Y	5	0	0	0	0
41	Z	1	0	0	0	0
41	a	167	0	0	2	0
41	b	262	0	0	4	0
41	c	207	0	0	1	0
41	d	137	0	0	2	0
41	e	16	0	0	0	0
41	f	7	0	0	0	0
41	h	42	0	0	0	0
41	i	5	0	0	0	0
41	j	7	0	0	0	0
41	k	7	0	0	0	0
41	l	9	0	0	1	0
41	m	16	0	0	0	0
41	o	157	0	0	2	0
41	t	11	0	0	0	0
41	u	93	0	0	0	0
41	v	82	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	55631	0	54162	559	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 559 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[B]:MET:HG2	31:A:419[B]:PL9:H102	1.48	0.93
1:A:214[A]:MET:HG2	31:A:419[A]:PL9:H102	1.50	0.93
24:B:616:CLA:H71	24:B:617:CLA:H192	1.52	0.92
24:c:518:CLA:HHC	24:c:518:CLA:HBB1	1.56	0.87
24:c:506:CLA:H202	24:c:512:CLA:HBB1	1.61	0.82

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:69:GLU:OE1	27:f:101:SQD:O3[2_554]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/344 (112%)	375 (98%)	8 (2%)	1 (0%)	36	34
1	a	386/344 (112%)	377 (98%)	8 (2%)	1 (0%)	36	34
2	B	512/505 (101%)	509 (99%)	3 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	456/455 (100%)	448 (98%)	6 (1%)	2 (0%)	30	26
3	c	466/455 (102%)	454 (97%)	10 (2%)	2 (0%)	30	26
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	59 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	36 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5419/5384 (101%)	5300 (98%)	112 (2%)	7 (0%)	48	50

5 of 7 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	312/279 (112%)	312 (100%)	0	100 100
1	a	314/279 (112%)	313 (100%)	1 (0%)	86 91
2	B	412/403 (102%)	409 (99%)	3 (1%)	76 82
2	b	413/403 (102%)	407 (98%)	6 (2%)	57 64
3	C	357/356 (100%)	351 (98%)	6 (2%)	53 60
3	c	367/356 (103%)	355 (97%)	12 (3%)	33 34
4	D	290/277 (105%)	287 (99%)	3 (1%)	68 75
4	d	290/277 (105%)	287 (99%)	3 (1%)	68 75
5	E	74/73 (101%)	73 (99%)	1 (1%)	59 66
5	e	74/73 (101%)	72 (97%)	2 (3%)	39 41
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	24 (92%)	2 (8%)	12 7
7	H	55/54 (102%)	54 (98%)	1 (2%)	51 58
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37 39
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 39
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30 30
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 34
10	k	30/30 (100%)	28 (93%)	2 (7%)	15 10
11	L	36/35 (103%)	35 (97%)	1 (3%)	38 40
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 40
12	M	31/32 (97%)	29 (94%)	2 (6%)	15 11
12	m	30/32 (94%)	29 (97%)	1 (3%)	33 34
13	O	214/207 (103%)	209 (98%)	5 (2%)	44 49
13	o	211/207 (102%)	203 (96%)	8 (4%)	29 29
14	T	27/28 (96%)	25 (93%)	2 (7%)	13 8
14	t	27/28 (96%)	25 (93%)	2 (7%)	13 8
15	U	84/89 (94%)	82 (98%)	2 (2%)	43 47
15	u	84/89 (94%)	83 (99%)	1 (1%)	63 70
16	V	119/117 (102%)	119 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	v	118/117 (101%)	117 (99%)	1 (1%)	73 79
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24 22
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 1
18	X	32/33 (97%)	32 (100%)	0	100 100
18	x	31/33 (94%)	31 (100%)	0	100 100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 14
19	z	52/52 (100%)	49 (94%)	3 (6%)	18 14
20	R	25/29 (86%)	23 (92%)	2 (8%)	11 7
All	All	4500/4403 (102%)	4416 (98%)	84 (2%)	51 56

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	71	GLU
13	o	69	LYS
6	f	44	GLN
12	m	33	GLN
14	t	25[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	301	GLN
13	o	155	ASN
4	d	332	GLN
11	l	8	GLN
15	u	81	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.65	0	8,9,11	1.05	1 (12%)
12	FME	m	1	12	8,9,10	0.67	0	8,9,11	1.45	3 (37%)
14	FME	t	1	14	8,9,10	0.82	0	8,9,11	1.97	3 (37%)
14	FME	T	1	14	8,9,10	0.72	0	8,9,11	1.36	1 (12%)
12	FME	M	1	12	8,9,10	0.72	0	8,9,11	1.22	2 (25%)
8	FME	i	1	8	8,9,10	0.69	0	8,9,11	1.20	1 (12%)

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

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-3.45	117.52	122.82
14	t	1	FME	O-C-CA	-2.49	118.37	124.77
14	T	1	FME	O-C-CA	-2.49	118.38	124.77
14	t	1	FME	C-CA-N	2.44	114.20	109.50
12	m	1	FME	CA-N-CN	-2.29	119.30	122.82

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
12	m	1	FME	CB-CA-N-CN
8	I	1	FME	CB-CA-N-CN
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 267 ligands modelled in this entry, 25 are monoatomic and 18 are unknown - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	B	608	41	69,73,73	1.91	20 (28%)	82,113,113	2.64	34 (41%)
36	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.16	8 (10%)
36	DGD	c	522	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	5 (6%)
24	CLA	b	615	-	69,73,73	1.97	19 (27%)	82,113,113	2.73	30 (36%)
24	CLA	b	618	-	69,73,73	2.00	18 (26%)	82,113,113	2.67	31 (37%)
28	GOL	o	301	-	5,5,5	0.39	0	5,5,5	0.25	0
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.28	0
27	SQD	L	102	-	52,54,54	0.98	2 (3%)	62,65,65	1.54	10 (16%)
24	CLA	b	623	-	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
24	CLA	b	611	-	69,73,73	2.00	20 (28%)	82,113,113	2.76	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HTG	c	525	-	19,19,19	0.96	2 (10%)	23,24,24	1.38	1 (4%)
36	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.06	5 (6%)
24	CLA	b	624	-	69,73,73	1.98	20 (28%)	82,113,113	2.64	30 (36%)
40	HEC	V	205	16	46,50,50	1.75	9 (19%)	58,82,82	1.59	11 (18%)
24	CLA	A	410	-	69,73,73	2.03	20 (28%)	82,113,113	2.64	35 (42%)
35	HTG	b	632	-	19,19,19	1.03	2 (10%)	23,24,24	1.60	3 (13%)
27	SQD	A	412	-	52,54,54	0.92	2 (3%)	62,65,65	1.50	11 (17%)
24	CLA	C	509	-	69,73,73	2.09	20 (28%)	82,113,113	2.65	29 (35%)
28	GOL	a	420	34	5,5,5	0.34	0	5,5,5	0.44	0
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.00	4 (6%)
24	CLA	b	620	-	69,73,73	1.98	19 (27%)	82,113,113	2.67	31 (37%)
27	SQD	f	101	-	41,43,54	1.11	2 (4%)	51,54,65	1.44	8 (15%)
28	GOL	v	202	-	5,5,5	0.35	0	5,5,5	0.29	0
28	GOL	b	604	-	5,5,5	0.39	0	5,5,5	0.27	0
24	CLA	b	619	41	69,73,73	2.02	22 (31%)	82,113,113	2.68	31 (37%)
24	CLA	C	513	-	69,73,73	2.04	20 (28%)	82,113,113	2.62	31 (37%)
24	CLA	b	614	-	69,73,73	1.99	19 (27%)	82,113,113	2.80	32 (39%)
24	CLA	b	621	-	69,73,73	2.02	20 (28%)	82,113,113	2.63	32 (39%)
35	HTG	c	526	-	19,19,19	0.93	2 (10%)	23,24,24	1.34	2 (8%)
24	CLA	A	407	41	69,73,73	2.04	20 (28%)	82,113,113	2.73	33 (40%)
24	CLA	c	512	41	69,73,73	1.96	19 (27%)	82,113,113	2.69	29 (35%)
24	CLA	C	502	-	69,73,73	1.99	20 (28%)	82,113,113	2.63	30 (36%)
25	PHO	A	408	-	58,69,69	2.73	12 (20%)	55,99,99	2.89	13 (23%)
24	CLA	b	613	-	69,73,73	1.99	19 (27%)	82,113,113	2.60	29 (35%)
27	SQD	a	405	-	52,54,54	1.01	2 (3%)	62,65,65	1.17	5 (8%)
26	BCR	T	103	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	14 (25%)
26	BCR	Y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	10 (17%)
28	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.58	0
25	PHO	A	409[B]	-	58,69,69	2.78	15 (25%)	55,99,99	2.92	15 (27%)
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.31	7 (12%)
26	BCR	b	628	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
30	OEX	a	416[B]	41,3,1	0,15,15	-	-	-		
31	PL9	d	405[B]	-	55,55,55	0.67	2 (3%)	68,69,69	1.55	13 (19%)
31	PL9	D	405[A]	-	55,55,55	0.67	2 (3%)	68,69,69	1.74	22 (32%)
36	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.19	7 (9%)
24	CLA	C	507	41	69,73,73	2.02	20 (28%)	82,113,113	2.56	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DGD	c	521	-	63,63,67	0.88	2 (3%)	77,77,81	0.95	6 (7%)
24	CLA	C	511	3	69,73,73	2.04	19 (27%)	82,113,113	2.60	31 (37%)
31	PL9	A	419[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.79	21 (30%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.45	7 (12%)
28	GOL	V	203	-	5,5,5	0.39	0	5,5,5	0.30	0
28	GOL	c	503	-	5,5,5	0.40	0	5,5,5	0.64	0
24	CLA	c	513	-	69,73,73	2.05	20 (28%)	82,113,113	2.61	29 (35%)
24	CLA	c	516	3	69,73,73	1.99	19 (27%)	82,113,113	2.59	31 (37%)
28	GOL	V	204	-	5,5,5	0.36	0	5,5,5	0.36	0
28	GOL	C	525	-	5,5,5	0.35	0	5,5,5	0.51	0
35	HTG	b	631	-	19,19,19	0.75	1 (5%)	23,24,24	1.28	2 (8%)
29	LMT	M	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.98	3 (6%)
28	GOL	O	301	-	5,5,5	0.35	0	5,5,5	0.42	0
23	BCT	A	404[A]	21	3,3,3	0.47	0	2,3,3	1.28	0
35	HTG	B	624	-	19,19,19	0.72	1 (5%)	23,24,24	1.53	3 (13%)
37	LHG	d	406	-	48,48,48	0.91	3 (6%)	51,54,54	1.05	4 (7%)
24	CLA	B	613	-	69,73,73	1.96	18 (26%)	82,113,113	2.77	31 (37%)
24	CLA	B	615	-	69,73,73	2.01	19 (27%)	82,113,113	2.70	31 (37%)
37	LHG	D	407	-	48,48,48	0.85	2 (4%)	51,54,54	1.16	5 (9%)
29	LMT	a	419	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
33	LMG	b	629	-	51,51,55	0.90	2 (3%)	59,59,63	1.08	5 (8%)
26	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.97	1 (3%)
24	CLA	B	610	-	69,73,73	2.01	19 (27%)	82,113,113	2.62	31 (37%)
26	BCR	C	514	-	41,41,41	1.06	1 (2%)	56,56,56	1.51	9 (16%)
37	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.87	3 (5%)
35	HTG	B	625	-	19,19,19	0.97	1 (5%)	23,24,24	1.70	4 (17%)
24	CLA	B	605	-	69,73,73	1.96	20 (28%)	82,113,113	2.64	32 (39%)
24	CLA	c	518	-	69,73,73	2.05	19 (27%)	82,113,113	2.69	32 (39%)
29	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.66	0
38	HEM	F	102	6,5	50,50,50	1.57	6 (12%)	67,82,82	1.73	12 (17%)
28	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.30	0
27	SQD	a	414	-	52,54,54	0.91	2 (3%)	62,65,65	1.58	12 (19%)
35	HTG	B	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.08	1 (4%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	2 (3%)
25	PHO	a	418[B]	-	58,69,69	2.77	13 (22%)	55,99,99	3.03	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	4 (5%)
28	GOL	C	524	-	5,5,5	0.37	0	5,5,5	0.80	0
24	CLA	C	503	-	69,73,73	2.04	19 (27%)	82,113,113	2.58	28 (34%)
28	GOL	A	415	-	5,5,5	0.41	0	5,5,5	0.25	0
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
35	HTG	b	607	-	19,19,19	0.91	2 (10%)	23,24,24	1.11	1 (4%)
35	HTG	b	608	-	19,19,19	0.97	2 (10%)	23,24,24	1.19	3 (13%)
35	HTG	D	412	-	16,16,19	1.03	2 (12%)	20,21,24	1.32	1 (5%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.23	3 (6%)
30	OEX	A	418[B]	41,3,1	0,15,15	-	-	-		
33	LMG	c	524	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	7 (11%)
24	CLA	C	501	-	69,73,73	2.01	19 (27%)	82,113,113	2.70	30 (36%)
24	CLA	B	611	41	69,73,73	2.07	21 (30%)	82,113,113	2.66	34 (41%)
36	DGD	H	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	7 (9%)
23	BCT	a	417[A]	21	3,3,3	0.51	0	2,3,3	0.77	0
28	GOL	A	413	-	5,5,5	0.30	0	5,5,5	0.42	0
28	GOL	A	414	-	5,5,5	0.45	0	5,5,5	0.53	0
35	HTG	C	522	-	19,19,19	0.94	2 (10%)	23,24,24	1.41	2 (8%)
24	CLA	c	517	-	69,73,73	2.05	20 (28%)	82,113,113	2.76	33 (40%)
29	LMT	A	417	-	36,36,36	0.60	1 (2%)	47,47,47	1.27	4 (8%)
31	PL9	a	415[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.94	21 (30%)
24	CLA	c	510	-	69,73,73	1.99	20 (28%)	82,113,113	2.60	29 (35%)
25	PHO	a	411	-	58,69,69	2.81	13 (22%)	55,99,99	2.86	17 (30%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
24	CLA	B	607	-	69,73,73	1.99	20 (28%)	82,113,113	2.77	33 (40%)
24	CLA	b	617	-	69,73,73	2.06	20 (28%)	82,113,113	2.55	32 (39%)
24	CLA	b	612	-	69,73,73	2.03	20 (28%)	82,113,113	2.72	32 (39%)
24	CLA	B	614	-	69,73,73	2.01	18 (26%)	82,113,113	2.58	34 (41%)
26	BCR	A	411	-	41,41,41	1.00	1 (2%)	56,56,56	1.14	6 (10%)
30	OEX	a	416[A]	41,3,1	0,15,15	-	-	-		
25	PHO	A	409[A]	-	58,69,69	2.83	14 (24%)	55,99,99	2.86	13 (23%)
24	CLA	b	616	41	69,73,73	1.97	18 (26%)	82,113,113	2.69	30 (36%)
26	BCR	b	626	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	7 (12%)
37	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	5 (9%)
24	CLA	d	402	-	69,73,73	1.99	18 (26%)	82,113,113	2.68	32 (39%)
28	GOL	B	631	-	5,5,5	0.40	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	a	409	-	69,73,73	2.01	19 (27%)	82,113,113	2.64	31 (37%)
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.52	0
28	GOL	c	502	-	5,5,5	0.28	0	5,5,5	0.50	0
26	BCR	b	627	-	41,41,41	1.02	1 (2%)	56,56,56	1.26	4 (7%)
29	LMT	B	635	-	25,25,36	0.52	1 (4%)	30,30,47	0.84	1 (3%)
37	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.09	4 (9%)
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	15 (26%)
26	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.49	11 (19%)
24	CLA	c	514	-	69,73,73	2.07	19 (27%)	82,113,113	2.64	30 (36%)
24	CLA	d	401	41	69,73,73	2.04	19 (27%)	82,113,113	2.69	34 (41%)
24	CLA	B	609	-	69,73,73	2.00	20 (28%)	82,113,113	2.64	33 (40%)
24	CLA	c	509	41	69,73,73	2.01	19 (27%)	82,113,113	2.75	35 (42%)
27	SQD	B	621	-	52,54,54	0.97	2 (3%)	62,65,65	1.45	7 (11%)
35	HTG	d	411	-	16,16,19	1.05	2 (12%)	20,21,24	1.52	2 (10%)
28	GOL	B	629	-	5,5,5	0.33	0	5,5,5	0.40	0
33	LMG	B	622	-	51,51,55	0.93	2 (3%)	59,59,63	1.07	5 (8%)
24	CLA	C	512	-	69,73,73	2.00	20 (28%)	82,113,113	2.70	30 (36%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.98	4 (5%)
24	CLA	A	406	41	69,73,73	1.95	19 (27%)	82,113,113	2.76	34 (41%)
38	HEM	e	103	6,5	50,50,50	1.55	8 (16%)	67,82,82	1.65	15 (22%)
24	CLA	D	402	-	69,73,73	1.97	19 (27%)	82,113,113	2.74	31 (37%)
36	DGD	c	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	5 (6%)
28	GOL	v	203	-	5,5,5	0.40	0	5,5,5	0.24	0
24	CLA	B	612	-	69,73,73	1.98	18 (26%)	82,113,113	2.71	32 (39%)
24	CLA	C	510	-	69,73,73	2.05	20 (28%)	82,113,113	2.60	30 (36%)
23	BCT	A	404[B]	21	3,3,3	0.51	0	2,3,3	1.09	0
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	11 (19%)
28	GOL	V	201	-	5,5,5	0.40	0	5,5,5	0.34	0
24	CLA	a	410	41	69,73,73	1.98	20 (28%)	82,113,113	2.75	33 (40%)
33	LMG	c	523	-	51,51,55	0.90	2 (3%)	59,59,63	1.13	4 (6%)
37	LHG	e	102	-	41,41,48	1.03	2 (4%)	44,47,54	0.97	2 (4%)
28	GOL	v	201	-	5,5,5	0.33	0	5,5,5	0.24	0
35	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.68	4 (17%)
37	LHG	D	409	-	48,48,48	0.98	2 (4%)	51,54,54	1.04	3 (5%)
24	CLA	D	403	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	31 (37%)
28	GOL	b	605	-	5,5,5	0.36	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	1.06	1 (2%)
36	DGD	D	406	-	52,52,67	1.02	3 (5%)	60,60,81	1.18	5 (8%)
24	CLA	B	604	-	69,73,73	2.04	19 (27%)	82,113,113	2.72	32 (39%)
25	PHO	a	418[A]	-	58,69,69	2.77	13 (22%)	55,99,99	3.07	15 (27%)
28	GOL	T	101	-	5,5,5	0.46	0	5,5,5	0.16	0
28	GOL	V	202	-	5,5,5	0.40	0	5,5,5	0.39	0
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.91	0
29	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.92	1 (2%)
28	GOL	b	602	-	5,5,5	0.43	0	5,5,5	0.53	0
28	GOL	b	603	-	5,5,5	0.34	0	5,5,5	0.13	0
29	LMT	a	404	-	36,36,36	0.46	0	47,47,47	1.11	3 (6%)
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	1.01	3 (6%)
24	CLA	B	606	-	69,73,73	2.01	19 (27%)	82,113,113	2.77	30 (36%)
27	SQD	A	416	-	52,54,54	0.97	2 (3%)	62,65,65	1.12	3 (4%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.13	3 (5%)
30	OEX	A	418[A]	41,3,1	0,15,15	-	-	-		
26	BCR	D	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.71	10 (17%)
33	LMG	D	413	39	51,51,55	0.87	2 (3%)	59,59,63	1.00	5 (8%)
28	GOL	A	422	34	5,5,5	0.35	0	5,5,5	0.24	0
26	BCR	c	519	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	7 (12%)
26	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.45	6 (10%)
24	CLA	b	625	-	69,73,73	1.99	18 (26%)	82,113,113	2.72	32 (39%)
24	CLA	C	504	41	69,73,73	2.04	20 (28%)	82,113,113	2.69	29 (35%)
31	PL9	d	405[A]	-	55,55,55	0.71	2 (3%)	68,69,69	1.52	15 (22%)
37	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.01	4 (7%)
24	CLA	C	506	-	69,73,73	2.04	19 (27%)	82,113,113	2.55	31 (37%)
24	CLA	B	602	41	69,73,73	2.05	20 (28%)	82,113,113	2.69	29 (35%)
26	BCR	c	528	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	6 (10%)
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
24	CLA	c	507	-	69,73,73	2.03	21 (30%)	82,113,113	2.55	27 (32%)
31	PL9	a	415[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.93	20 (29%)
31	PL9	A	419[A]	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	22 (32%)
24	CLA	c	515	-	69,73,73	2.02	19 (27%)	82,113,113	2.63	31 (37%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.49	0
23	BCT	a	417[B]	21	3,3,3	0.53	0	2,3,3	0.85	0
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.29	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	PL9	D	405[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.67	19 (27%)
24	CLA	C	505	-	69,73,73	1.99	20 (28%)	82,113,113	2.57	28 (34%)
24	CLA	b	622	-	69,73,73	2.02	20 (28%)	82,113,113	2.56	29 (35%)
24	CLA	B	616	-	69,73,73	1.97	18 (26%)	82,113,113	2.67	29 (35%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
27	SQD	F	103	-	41,43,54	1.09	2 (4%)	51,54,65	1.56	11 (21%)
24	CLA	B	603	-	69,73,73	2.04	20 (28%)	82,113,113	2.72	32 (39%)
24	CLA	a	412	-	69,73,73	2.01	19 (27%)	82,113,113	2.71	32 (39%)
24	CLA	c	508	-	69,73,73	2.04	19 (27%)	82,113,113	2.69	28 (34%)
33	LMG	A	421	-	51,51,55	0.94	2 (3%)	59,59,63	1.11	4 (6%)
37	LHG	b	634	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	4 (7%)
24	CLA	A	405	-	69,73,73	2.02	20 (28%)	82,113,113	2.61	30 (36%)
26	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.50	8 (14%)
35	HTG	V	206	-	19,19,19	0.93	2 (10%)	23,24,24	1.23	3 (13%)
28	GOL	a	401	-	5,5,5	0.45	0	5,5,5	0.52	0
28	GOL	B	626	-	5,5,5	0.44	0	5,5,5	0.40	0
24	CLA	B	617	-	69,73,73	2.01	19 (27%)	82,113,113	2.69	29 (35%)
33	LMG	c	501	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
26	BCR	a	413	-	41,41,41	1.04	1 (2%)	56,56,56	1.13	6 (10%)
28	GOL	t	102	-	5,5,5	0.49	0	5,5,5	0.11	0
33	LMG	d	413	39	51,51,55	0.93	2 (3%)	59,59,63	0.94	3 (5%)
26	BCR	d	404	-	41,41,41	1.13	1 (2%)	56,56,56	1.71	12 (21%)
35	HTG	b	601	-	19,19,19	0.90	1 (5%)	23,24,24	1.02	2 (8%)
24	CLA	b	610	41	69,73,73	2.05	20 (28%)	82,113,113	2.66	29 (35%)
24	CLA	C	508	-	69,73,73	2.06	20 (28%)	82,113,113	2.63	26 (31%)
24	CLA	c	506	-	69,73,73	1.98	19 (27%)	82,113,113	2.62	29 (35%)
29	LMT	m	102	-	36,36,36	0.47	0	47,47,47	0.85	1 (2%)
24	CLA	c	511	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	32 (39%)
35	HTG	B	633	-	19,19,19	0.92	1 (5%)	23,24,24	1.28	1 (4%)
40	HEC	v	205	16	46,50,50	1.71	10 (21%)	58,82,82	1.63	12 (20%)
28	GOL	B	630	-	5,5,5	0.41	0	5,5,5	0.27	0
29	LMT	F	101	-	36,36,36	0.47	0	47,47,47	0.95	1 (2%)
24	CLA	d	403	-	69,73,73	2.01	21 (30%)	82,113,113	2.72	32 (39%)
26	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.42	9 (16%)

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
24	CLA	B	608	41	1/1/15/20	5/39/115/115	-
36	DGD	C	516	-	-	13/51/91/95	0/2/2/2
36	DGD	c	522	-	-	14/51/91/95	0/2/2/2
24	CLA	b	615	-	1/1/15/20	7/39/115/115	-
24	CLA	b	618	-	1/1/15/20	5/39/115/115	-
28	GOL	o	301	-	-	4/4/4/4	-
28	GOL	a	402	-	-	2/4/4/4	-
27	SQD	L	102	-	-	23/49/69/69	0/1/1/1
24	CLA	b	623	-	1/1/15/20	20/39/115/115	-
24	CLA	b	611	-	1/1/15/20	5/39/115/115	-
35	HTG	c	525	-	-	3/10/30/30	0/1/1/1
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	b	624	-	1/1/15/20	3/39/115/115	-
40	HEC	V	205	16	-	6/14/54/54	-
24	CLA	A	410	-	1/1/15/20	10/39/115/115	-
35	HTG	b	632	-	-	6/10/30/30	0/1/1/1
27	SQD	A	412	-	-	12/49/69/69	0/1/1/1
24	CLA	C	509	-	1/1/15/20	13/39/115/115	-
28	GOL	a	420	34	-	3/4/4/4	-
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
24	CLA	b	620	-	1/1/15/20	3/39/115/115	-
27	SQD	f	101	-	-	13/38/58/69	0/1/1/1
28	GOL	v	202	-	-	2/4/4/4	-
28	GOL	b	604	-	-	2/4/4/4	-
24	CLA	b	619	41	1/1/15/20	5/39/115/115	-
24	CLA	C	513	-	1/1/15/20	6/39/115/115	-
24	CLA	b	614	-	1/1/15/20	5/39/115/115	-
24	CLA	b	621	-	1/1/15/20	2/39/115/115	-
35	HTG	c	526	-	-	0/10/30/30	0/1/1/1
24	CLA	A	407	41	-	3/39/115/115	-
24	CLA	c	512	41	1/1/15/20	7/39/115/115	-
24	CLA	C	502	-	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	A	408	-	-	3/37/103/103	0/5/6/6
24	CLA	b	613	-	1/1/15/20	3/39/115/115	-
27	SQD	a	405	-	-	15/49/69/69	0/1/1/1
26	BCR	T	103	-	-	1/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
25	PHO	A	409[B]	-	-	0/37/103/103	0/5/6/6
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	b	628	-	-	0/29/63/63	0/2/2/2
31	PL9	d	405[B]	-	-	8/53/73/73	0/1/1/1
31	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1
36	DGD	e	101	-	-	27/51/91/95	0/2/2/2
24	CLA	C	507	41	1/1/15/20	8/39/115/115	-
36	DGD	c	521	-	-	15/51/91/95	0/2/2/2
24	CLA	C	511	3	1/1/15/20	3/39/115/115	-
31	PL9	A	419[B]	-	-	10/53/73/73	0/1/1/1
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	203	-	-	1/4/4/4	-
28	GOL	c	503	-	-	1/4/4/4	-
24	CLA	c	513	-	1/1/15/20	3/39/115/115	-
24	CLA	c	516	3	1/1/15/20	5/39/115/115	-
28	GOL	V	204	-	-	0/4/4/4	-
28	GOL	C	525	-	-	0/4/4/4	-
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
28	GOL	O	301	-	-	2/4/4/4	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
37	LHG	d	406	-	-	11/53/53/53	-
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	CLA	B	615	-	1/1/15/20	12/39/115/115	-
37	LHG	D	407	-	-	11/53/53/53	-
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
33	LMG	b	629	-	-	11/46/66/70	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
24	CLA	B	610	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
37	LHG	D	408	-	-	7/53/53/53	-
35	HTG	B	625	-	-	4/10/30/30	0/1/1/1
24	CLA	B	605	-	1/1/15/20	4/39/115/115	-
24	CLA	c	518	-	-	5/39/115/115	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
38	HEM	F	102	6,5	-	8/14/54/54	-
28	GOL	b	606	-	-	1/4/4/4	-
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
37	LHG	d	408	-	-	10/53/53/53	-
25	PHO	a	418[B]	-	-	1/37/103/103	0/5/6/6
36	DGD	C	518	-	-	10/51/91/95	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	C	503	-	1/1/15/20	1/39/115/115	-
28	GOL	A	415	-	-	2/4/4/4	-
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
35	HTG	b	607	-	-	1/10/30/30	0/1/1/1
35	HTG	b	608	-	-	0/10/30/30	0/1/1/1
35	HTG	D	412	-	-	0/7/27/30	0/1/1/1
29	LMT	C	521	-	-	9/21/61/61	0/2/2/2
33	LMG	c	524	-	-	4/46/66/70	0/1/1/1
24	CLA	C	501	-	1/1/15/20	4/39/115/115	-
24	CLA	B	611	41	1/1/15/20	3/39/115/115	-
36	DGD	H	102	-	-	12/51/91/95	0/2/2/2
28	GOL	A	413	-	-	0/4/4/4	-
28	GOL	A	414	-	-	2/4/4/4	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	CLA	c	517	-	1/1/15/20	11/39/115/115	-
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
31	PL9	a	415[B]	-	-	14/53/73/73	0/1/1/1
24	CLA	c	510	-	1/1/15/20	1/39/115/115	-
25	PHO	a	411	-	-	3/37/103/103	0/5/6/6
28	GOL	T	102	-	-	2/4/4/4	-
24	CLA	B	607	-	1/1/15/20	2/39/115/115	-
24	CLA	b	617	-	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	612	-	1/1/15/20	3/39/115/115	-
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
25	PHO	A	409[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	b	616	41	1/1/15/20	2/39/115/115	-
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
37	LHG	L	101	-	-	14/53/53/53	-
24	CLA	d	402	-	1/1/15/20	4/39/115/115	-
28	GOL	B	631	-	-	0/4/4/4	-
24	CLA	a	409	-	1/1/15/20	4/39/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
28	GOL	c	502	-	-	0/4/4/4	-
26	BCR	b	627	-	-	0/29/63/63	0/2/2/2
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
37	LHG	E	101	-	-	23/46/46/53	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	c	514	-	1/1/15/20	15/39/115/115	-
24	CLA	d	401	41	1/1/15/20	4/39/115/115	-
24	CLA	c	509	41	1/1/15/20	4/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
35	HTG	d	411	-	-	1/7/27/30	0/1/1/1
28	GOL	B	629	-	-	2/4/4/4	-
33	LMG	B	622	-	-	6/46/66/70	0/1/1/1
24	CLA	C	512	-	1/1/15/20	9/39/115/115	-
36	DGD	h	102	-	-	12/51/91/95	0/2/2/2
24	CLA	A	406	41	1/1/15/20	2/39/115/115	-
38	HEM	e	103	6,5	-	10/14/54/54	-
24	CLA	D	402	-	1/1/15/20	0/39/115/115	-
36	DGD	c	520	-	-	14/51/91/95	0/2/2/2
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	B	612	-	1/1/15/20	3/39/115/115	-
24	CLA	C	510	-	1/1/15/20	7/39/115/115	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
28	GOL	V	201	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	410	41	-	6/39/115/115	-
33	LMG	c	523	-	-	13/46/66/70	0/1/1/1
37	LHG	e	102	-	-	16/46/46/53	-
28	GOL	v	201	-	-	2/4/4/4	-
35	HTG	C	523	-	-	2/10/30/30	0/1/1/1
37	LHG	D	409	-	-	10/53/53/53	-
24	CLA	D	403	-	1/1/15/20	4/39/115/115	-
28	GOL	b	605	-	-	2/4/4/4	-
29	LMT	D	401	-	-	9/21/61/61	0/2/2/2
36	DGD	D	406	-	-	23/47/67/95	0/1/1/2
24	CLA	B	604	-	1/1/15/20	1/39/115/115	-
25	PHO	a	418[A]	-	-	0/37/103/103	0/5/6/6
28	GOL	T	101	-	-	0/4/4/4	-
28	GOL	V	202	-	-	2/4/4/4	-
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
29	LMT	f	102	-	-	10/21/61/61	0/2/2/2
28	GOL	b	602	-	-	0/4/4/4	-
28	GOL	b	603	-	-	0/4/4/4	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
29	LMT	m	103	-	-	7/21/61/61	0/2/2/2
24	CLA	B	606	-	1/1/15/20	4/39/115/115	-
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
33	LMG	D	413	39	-	8/46/66/70	0/1/1/1
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
28	GOL	A	422	34	-	2/4/4/4	-
26	BCR	c	519	-	-	1/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	b	625	-	1/1/15/20	8/39/115/115	-
24	CLA	C	504	41	1/1/15/20	3/39/115/115	-
31	PL9	d	405[A]	-	-	5/53/73/73	0/1/1/1
37	LHG	d	407	-	-	7/53/53/53	-
24	CLA	C	506	-	1/1/15/20	6/39/115/115	-
24	CLA	B	602	41	1/1/15/20	13/39/115/115	-
26	BCR	c	528	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	14/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	507	-	1/1/15/20	6/39/115/115	-
31	PL9	a	415[A]	-	-	17/53/73/73	0/1/1/1
31	PL9	A	419[A]	-	-	14/53/73/73	0/1/1/1
24	CLA	c	515	-	1/1/15/20	8/39/115/115	-
28	GOL	B	636	-	-	0/4/4/4	-
35	HTG	B	632	-	-	3/10/30/30	0/1/1/1
31	PL9	D	405[B]	-	-	7/53/73/73	0/1/1/1
24	CLA	C	505	-	1/1/15/20	6/39/115/115	-
24	CLA	b	622	-	1/1/15/20	2/39/115/115	-
24	CLA	B	616	-	1/1/15/20	13/39/115/115	-
33	LMG	z	101	-	-	15/34/54/70	0/1/1/1
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
24	CLA	B	603	-	1/1/15/20	2/39/115/115	-
24	CLA	a	412	-	1/1/15/20	11/39/115/115	-
24	CLA	c	508	-	-	1/39/115/115	-
33	LMG	A	421	-	-	19/46/66/70	0/1/1/1
37	LHG	b	634	-	-	15/53/53/53	-
24	CLA	A	405	-	1/1/15/20	4/39/115/115	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
35	HTG	V	206	-	-	2/10/30/30	0/1/1/1
28	GOL	a	401	-	-	1/4/4/4	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	B	617	-	1/1/15/20	6/39/115/115	-
33	LMG	c	501	-	-	16/46/66/70	0/1/1/1
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
28	GOL	t	102	-	-	0/4/4/4	-
33	LMG	d	413	39	-	11/46/66/70	0/1/1/1
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	b	610	41	1/1/15/20	17/39/115/115	-
24	CLA	C	508	-	1/1/15/20	2/39/115/115	-
24	CLA	c	506	-	1/1/15/20	3/39/115/115	-
29	LMT	m	102	-	-	8/21/61/61	0/2/2/2
24	CLA	c	511	-	1/1/15/20	11/39/115/115	-
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	v	205	16	-	6/14/54/54	-
28	GOL	B	630	-	-	4/4/4/4	-
29	LMT	F	101	-	-	5/21/61/61	0/2/2/2
24	CLA	d	403	-	1/1/15/20	5/39/115/115	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2

The worst 5 of 1627 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	418[A]	PHO	C1B-C2B	9.33	1.49	1.39
25	A	408	PHO	C1D-C2D	9.28	1.49	1.39
25	A	408	PHO	C1B-C2B	9.22	1.49	1.39
25	a	411	PHO	C1D-C2D	9.13	1.49	1.39
25	A	409[A]	PHO	C1D-C2D	9.13	1.49	1.39

The worst 5 of 2921 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409[B]	PHO	C2D-C1D-ND	11.23	117.55	109.43
25	A	409[A]	PHO	C2D-C1D-ND	11.13	117.47	109.43
25	A	408	PHO	C2D-C1D-ND	11.01	117.39	109.43
25	a	418[A]	PHO	C2D-C1D-ND	10.87	117.29	109.43
24	B	613	CLA	C1D-ND-C4D	-10.81	98.72	106.31

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	410	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 1262 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	C14-C13-C15-C16
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

159 monomers are involved in 345 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	608	CLA	1	0
36	C	516	DGD	1	0
24	b	618	CLA	1	0
28	a	402	GOL	1	0
27	L	102	SQD	3	0
24	b	623	CLA	1	0
35	c	525	HTG	1	0
36	C	517	DGD	2	0
24	b	624	CLA	5	0
24	A	410	CLA	4	0
27	A	412	SQD	6	0
24	C	509	CLA	3	0
28	a	420	GOL	1	0
33	C	519	LMG	4	0
24	b	620	CLA	3	0
27	f	101	SQD	1	1
24	b	619	CLA	4	0
24	C	513	CLA	6	0
24	b	614	CLA	6	0
24	b	621	CLA	2	0
24	A	407	CLA	1	0
24	c	512	CLA	3	0
24	C	502	CLA	3	0
25	A	408	PHO	1	0
24	b	613	CLA	2	0
27	a	405	SQD	1	0
26	T	103	BCR	5	0
26	Y	101	BCR	4	0
25	A	409[B]	PHO	2	0
26	B	618	BCR	3	0
26	b	628	BCR	3	0
36	e	101	DGD	7	0
24	C	507	CLA	3	0
36	c	521	DGD	1	0
24	C	511	CLA	2	0
31	A	419[B]	PL9	4	0
26	h	101	BCR	4	0
28	c	503	GOL	2	0
24	c	513	CLA	6	0
24	c	516	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	M	103	LMT	1	0
37	d	406	LHG	2	0
24	B	613	CLA	1	0
24	B	615	CLA	4	0
37	D	407	LHG	1	0
29	a	419	LMT	1	0
33	b	629	LMG	3	0
26	B	619	BCR	3	0
24	B	610	CLA	3	0
26	C	514	BCR	6	0
37	D	408	LHG	1	0
24	c	518	CLA	5	0
29	b	630	LMT	3	0
38	F	102	HEM	2	0
27	a	414	SQD	2	0
35	B	623	HTG	1	0
37	d	408	LHG	6	0
25	a	418[B]	PHO	1	0
36	C	518	DGD	1	0
24	C	503	CLA	3	0
26	H	101	BCR	3	0
35	D	412	HTG	2	0
29	C	521	LMT	1	0
33	c	524	LMG	2	0
24	C	501	CLA	1	0
24	B	611	CLA	1	0
28	A	414	GOL	1	0
24	c	517	CLA	2	0
29	A	417	LMT	2	0
31	a	415[B]	PL9	7	0
24	c	510	CLA	7	0
28	T	102	GOL	2	0
24	B	607	CLA	4	0
24	b	612	CLA	2	0
24	B	614	CLA	3	0
26	A	411	BCR	1	0
25	A	409[A]	PHO	3	0
26	b	626	BCR	4	0
24	d	402	CLA	3	0
24	a	409	CLA	4	0
26	b	627	BCR	3	0
37	E	101	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	t	101	BCR	5	0
26	C	515	BCR	5	0
24	c	514	CLA	3	0
24	d	401	CLA	4	0
24	B	609	CLA	1	0
24	c	509	CLA	1	0
27	B	621	SQD	3	0
35	d	411	HTG	3	0
33	B	622	LMG	1	0
24	C	512	CLA	4	0
24	A	406	CLA	3	0
38	e	103	HEM	5	0
24	D	402	CLA	3	0
36	c	520	DGD	1	0
24	B	612	CLA	1	0
24	C	510	CLA	3	0
24	a	410	CLA	3	0
33	c	523	LMG	3	0
37	e	102	LHG	4	0
28	v	201	GOL	1	0
37	D	409	LHG	9	0
24	D	403	CLA	1	0
29	D	401	LMT	1	0
36	D	406	DGD	2	0
24	B	604	CLA	2	0
25	a	418[A]	PHO	2	0
28	T	101	GOL	1	0
29	M	101	LMT	3	0
29	f	102	LMT	1	0
29	a	404	LMT	1	0
29	m	103	LMT	2	0
24	B	606	CLA	2	0
27	A	416	SQD	1	0
33	C	520	LMG	3	0
26	D	404	BCR	1	0
33	D	413	LMG	1	0
26	c	519	BCR	3	0
26	B	620	BCR	5	0
24	b	625	CLA	2	0
37	d	407	LHG	1	0
24	C	506	CLA	2	0
24	B	602	CLA	2	0

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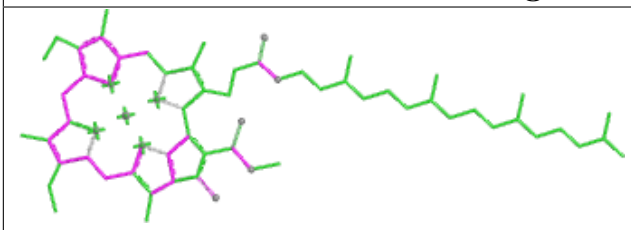
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	528	BCR	2	0
33	Z	101	LMG	1	0
24	c	507	CLA	4	0
31	a	415[A]	PL9	7	0
31	A	419[A]	PL9	5	0
24	c	515	CLA	2	0
31	D	405[B]	PL9	1	0
24	C	505	CLA	5	0
24	b	622	CLA	3	0
24	B	616	CLA	6	0
33	z	101	LMG	5	0
27	F	103	SQD	2	0
24	B	603	CLA	2	0
24	a	412	CLA	2	0
24	c	508	CLA	2	0
33	A	421	LMG	4	0
37	b	634	LHG	3	0
24	A	405	CLA	4	0
26	y	101	BCR	2	0
35	V	206	HTG	1	0
24	B	617	CLA	6	0
33	c	501	LMG	2	0
26	a	413	BCR	1	0
28	t	102	GOL	1	0
33	d	413	LMG	2	0
26	d	404	BCR	3	0
35	b	601	HTG	1	0
24	b	610	CLA	2	0
24	C	508	CLA	3	0
24	c	506	CLA	3	0
29	m	102	LMT	1	0
24	c	511	CLA	2	0
28	B	630	GOL	1	0
24	d	403	CLA	2	0
26	k	101	BCR	1	0

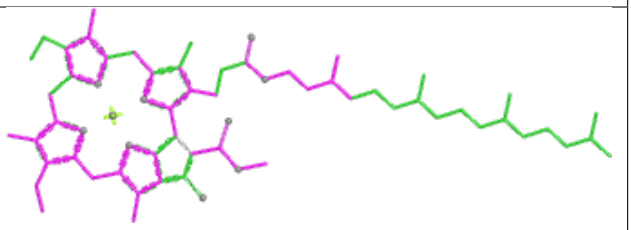
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

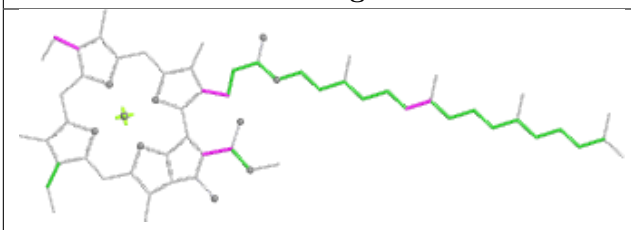
Ligand CLA B 608



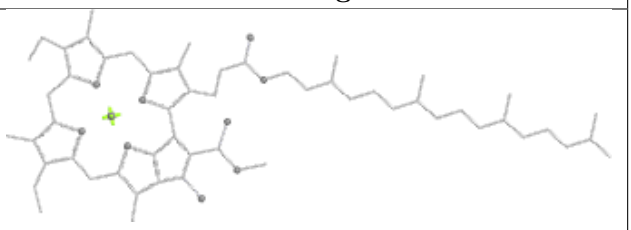
Bond lengths



Bond angles

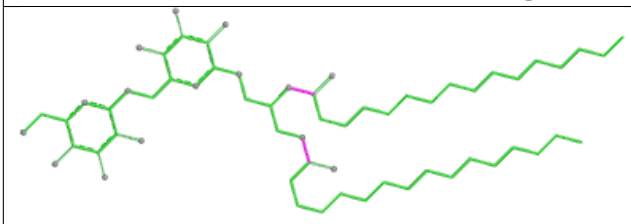


Torsions

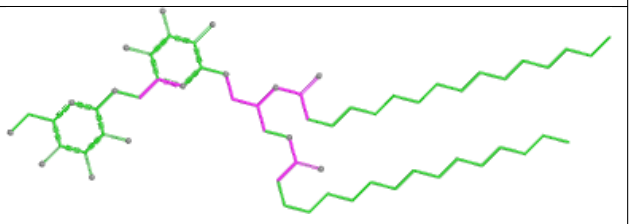


Rings

Ligand DGD C 516



Bond lengths



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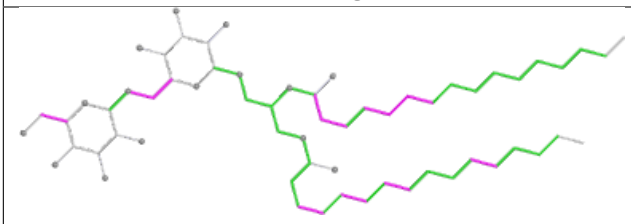

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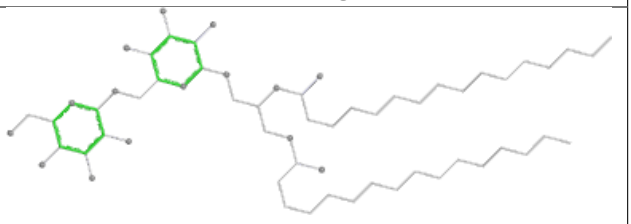
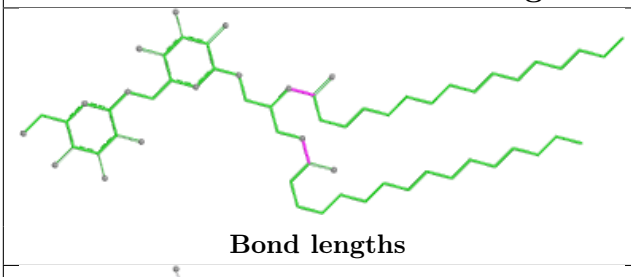
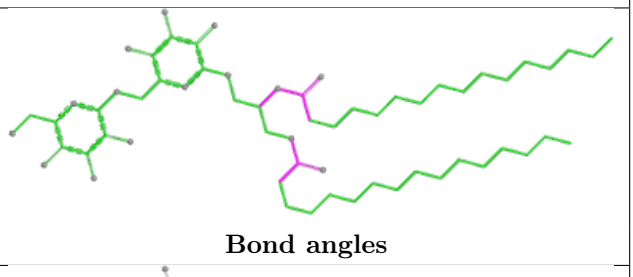


Rings

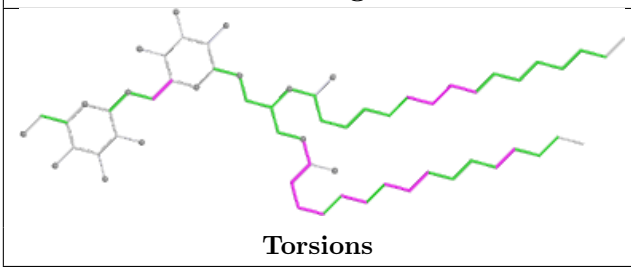
Ligand DGD c 522



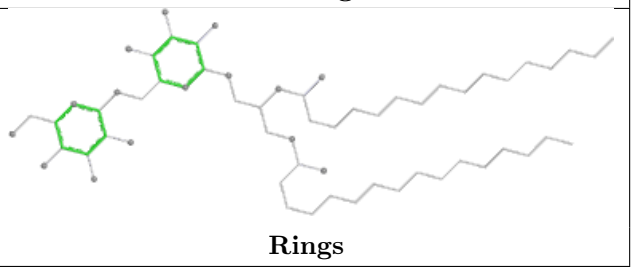
Bond lengths



Bond angles

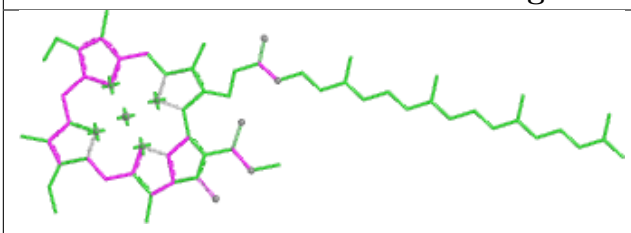


Torsions



Rings

Ligand CLA b 615



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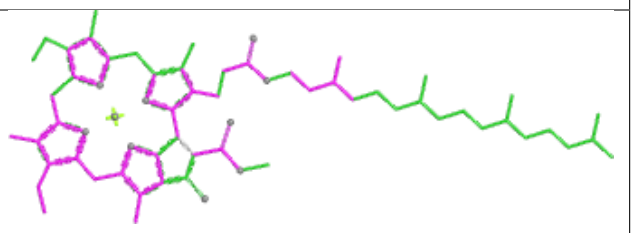

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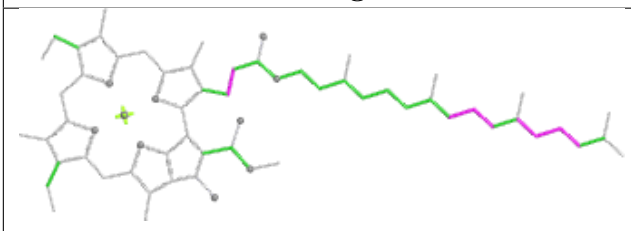
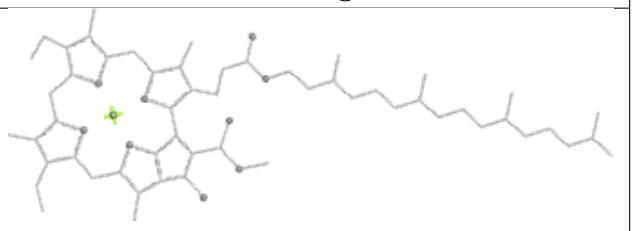
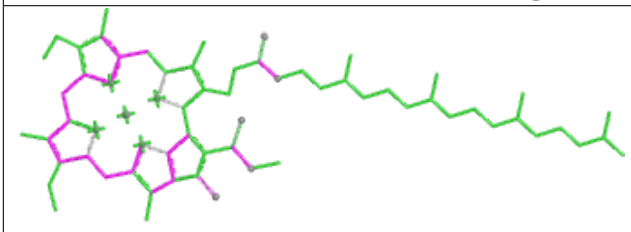


Torsions



Rings

Ligand CLA b 618



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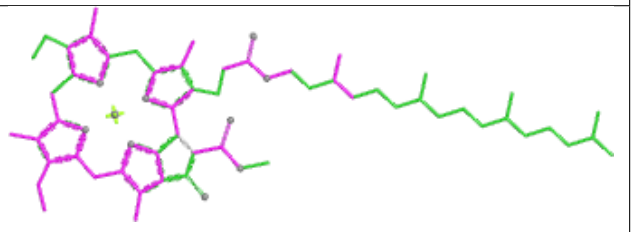
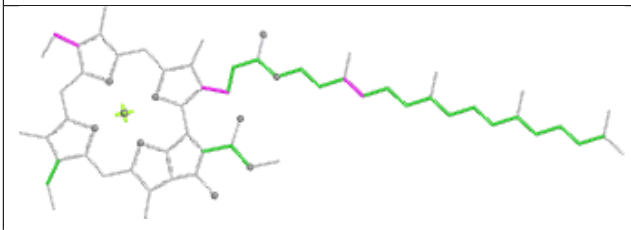


Bond angles



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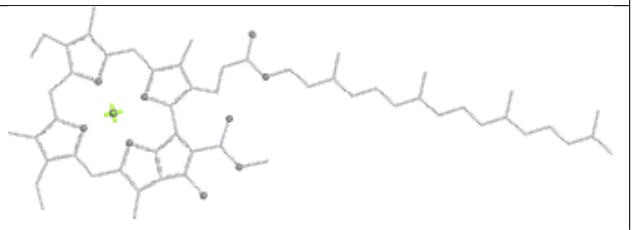
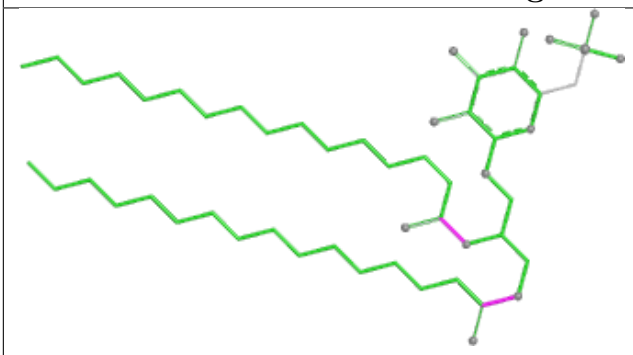


Rings

Ligand SQD L 102



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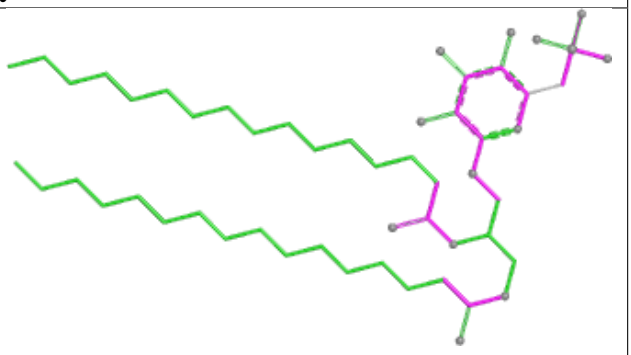

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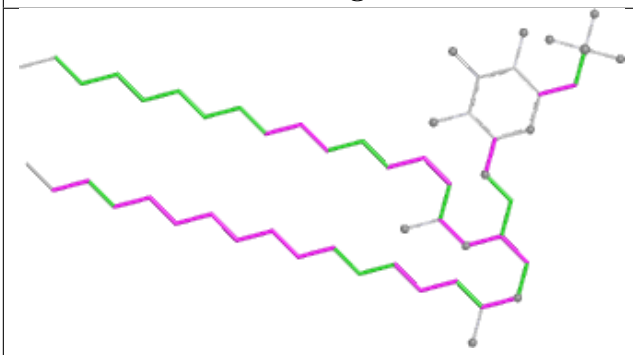

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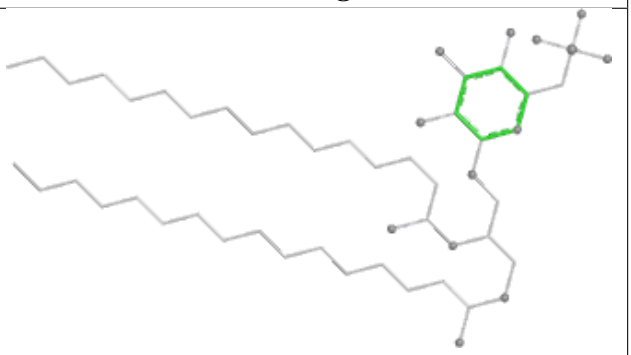
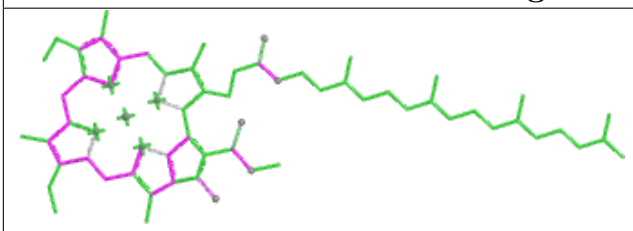


Rings

Ligand CLA b 623



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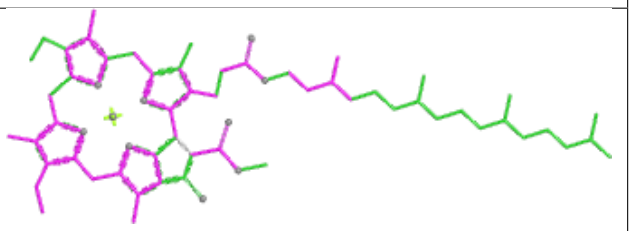
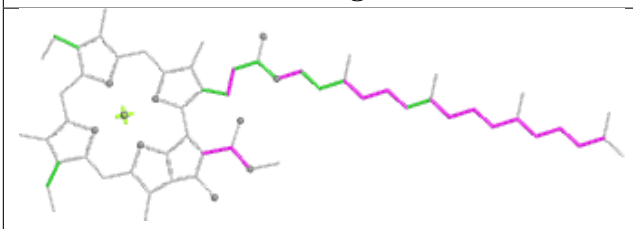


Bond angles



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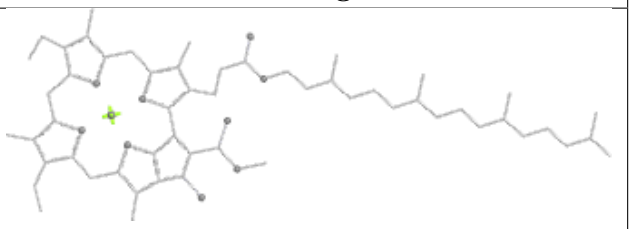
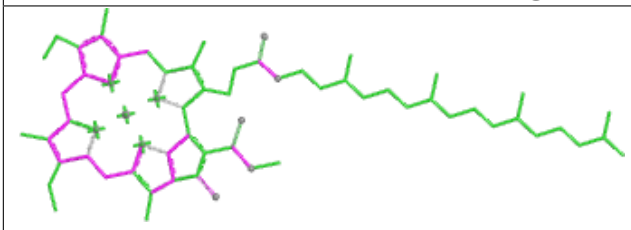


Rings

Ligand CLA b 611



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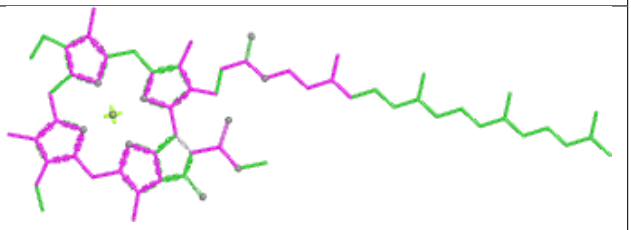
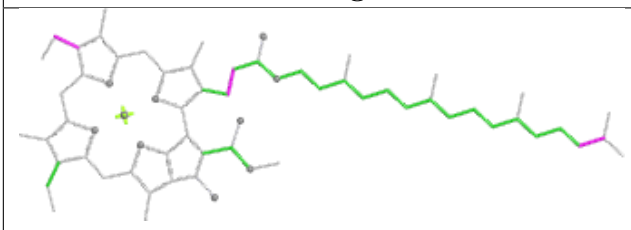


Bond angles



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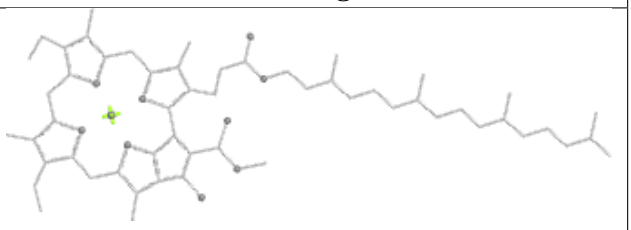
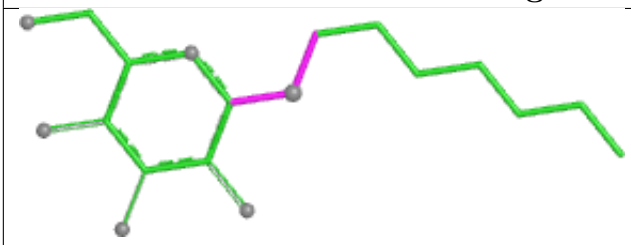
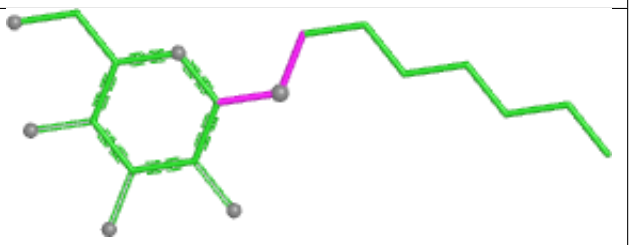


Rings

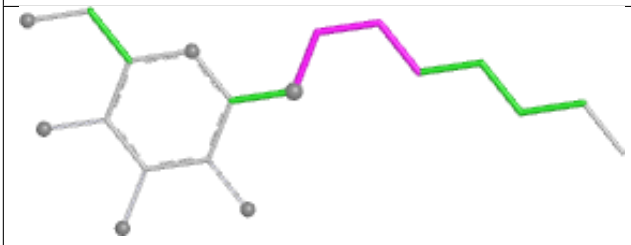
Ligand HTG c 525



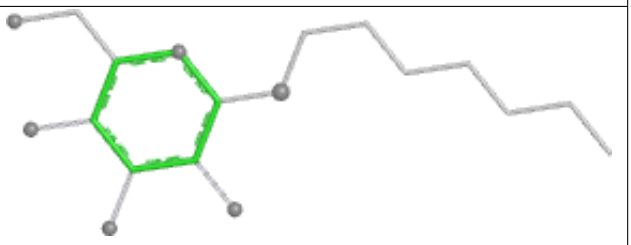
Bond lengths



Bond angles

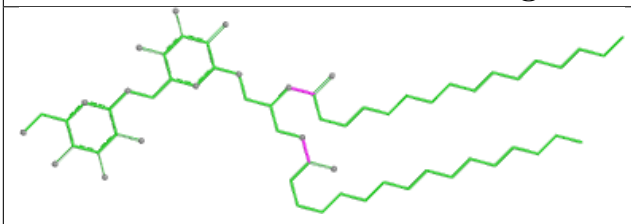


Torsions

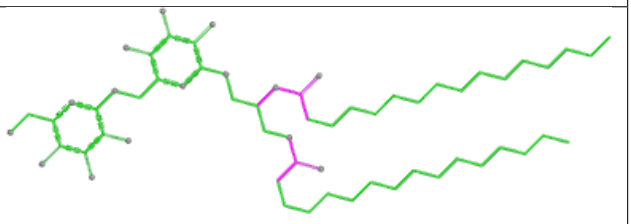


Rings

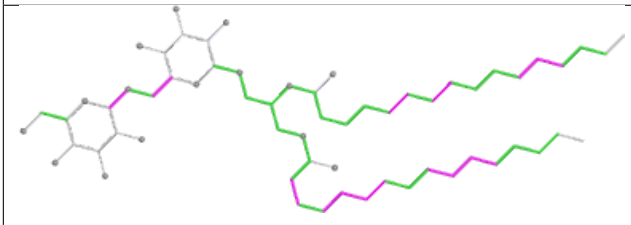
Ligand DGD C 517



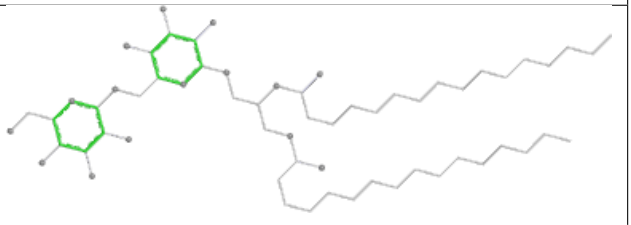
Bond lengths



Bond angles

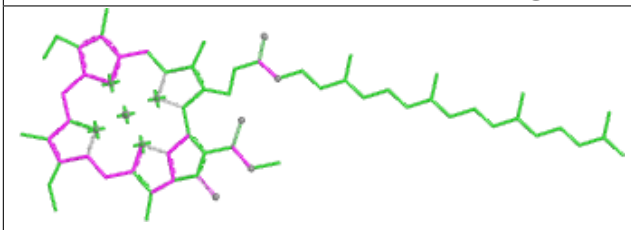


Torsions

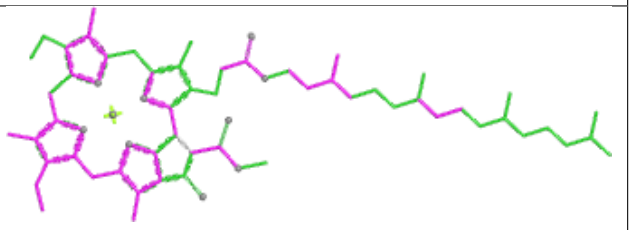


Rings

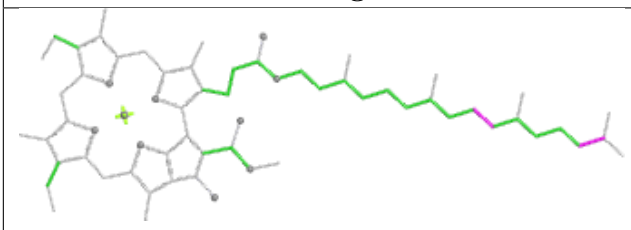
Ligand CLA b 624



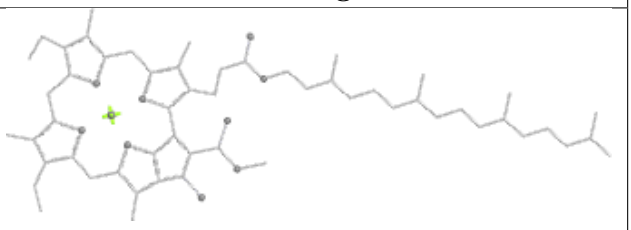
Bond lengths



Bond angles

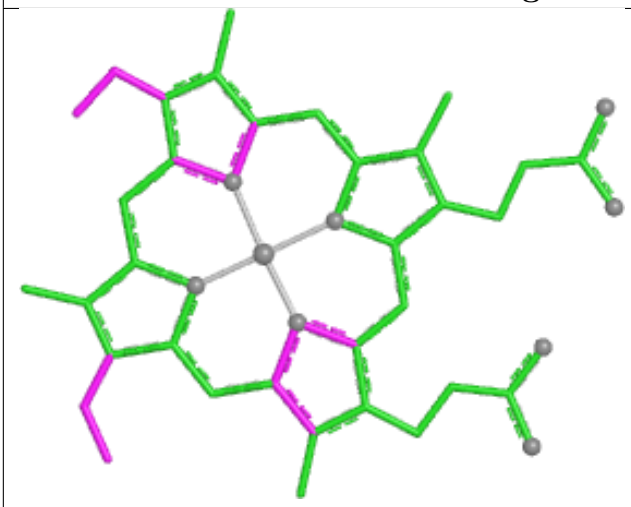


Torsions



Rings

Ligand HEC V 205



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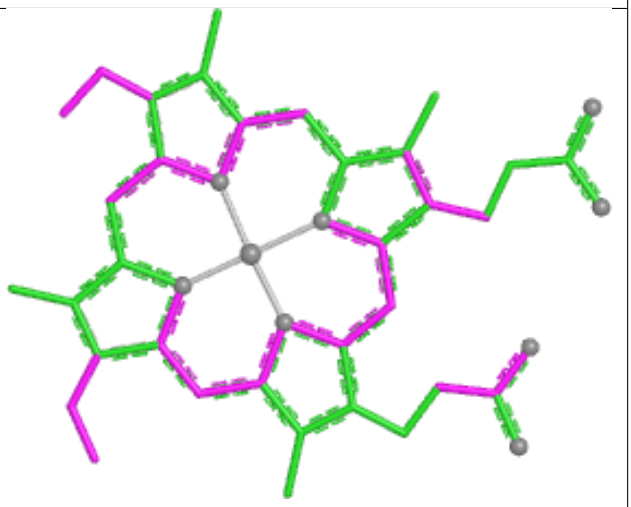
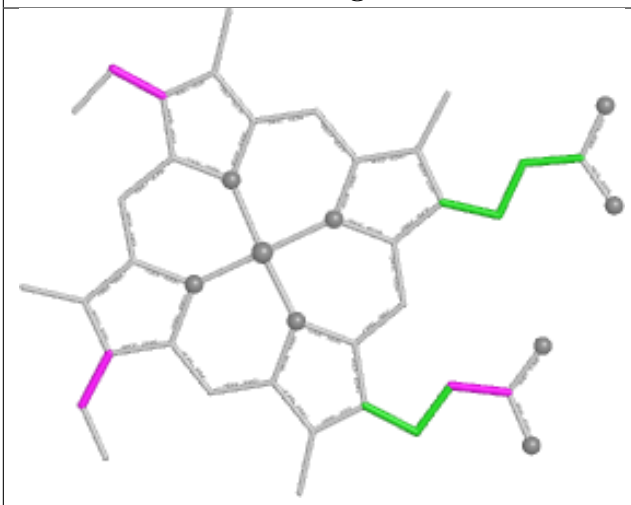
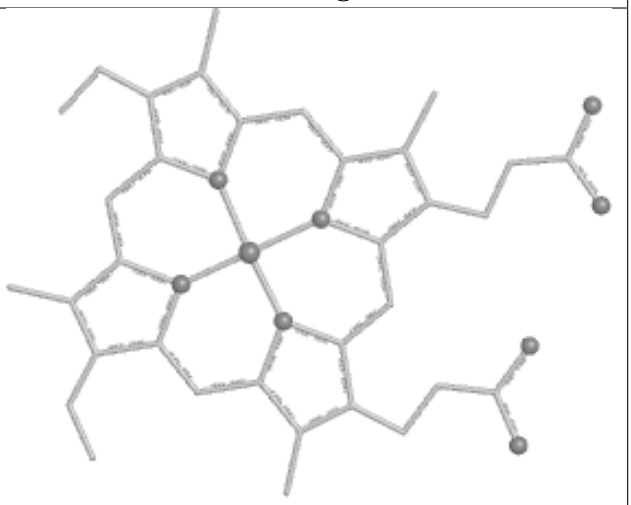


Bond angles

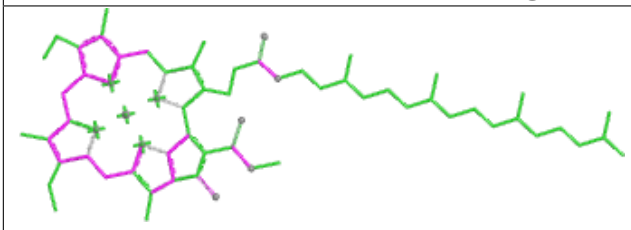


Torsions



Rings

Ligand CLA A 410



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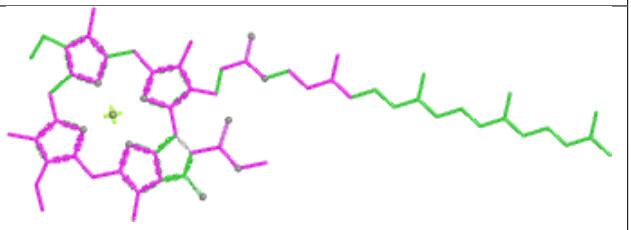
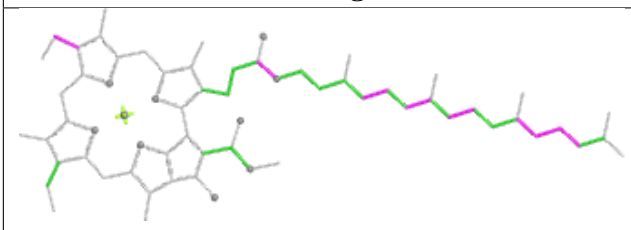
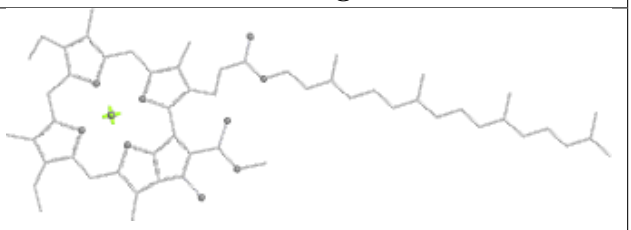


Bond angles

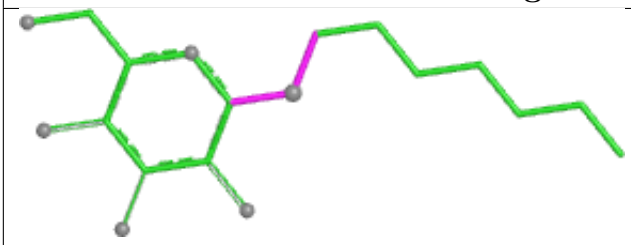


Torsions



Rings

Ligand HTG b 632



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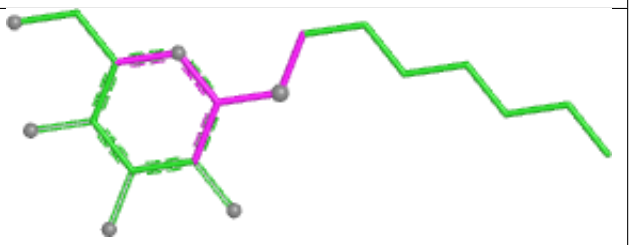
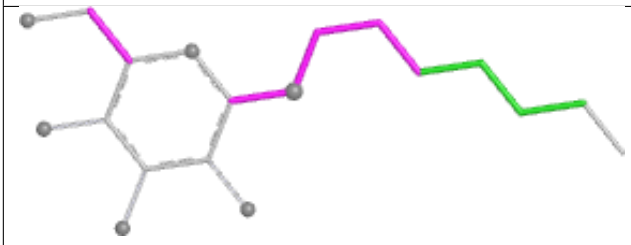


Bond angles



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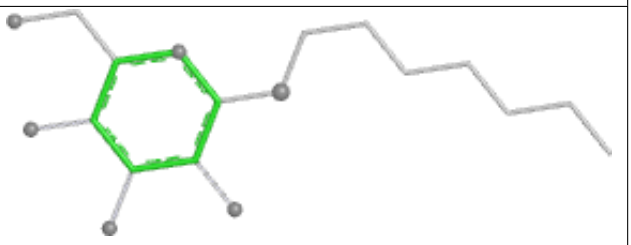
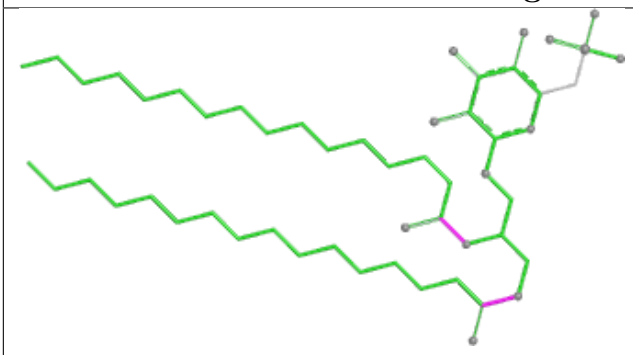
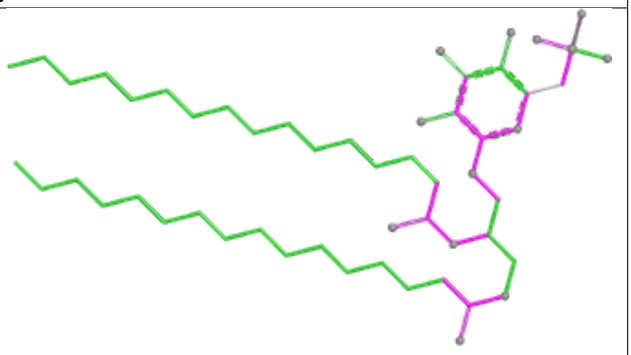


Rings

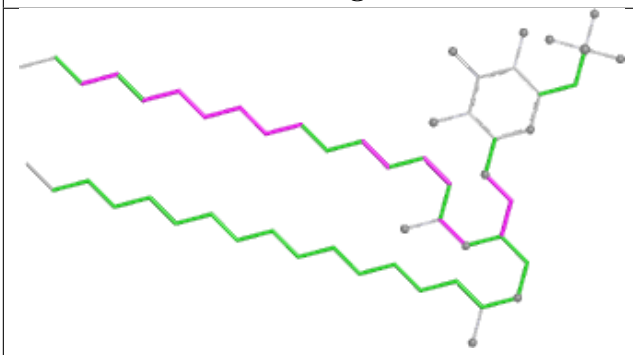
Ligand SQD A 412



Bond lengths



Bond angles



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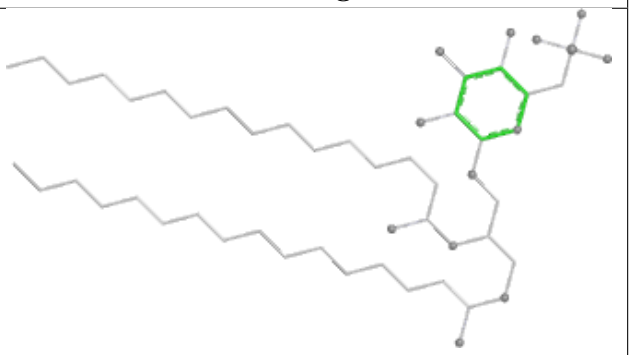
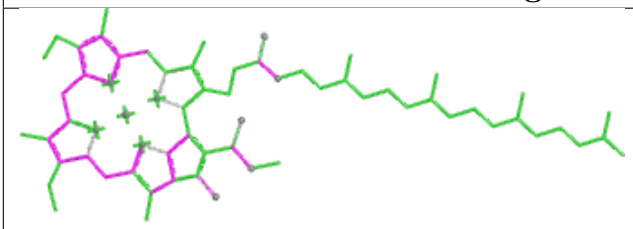


Rings

Ligand CLA C 509



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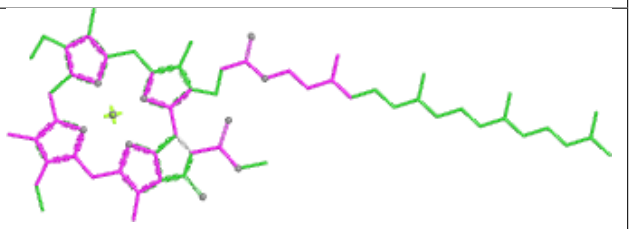
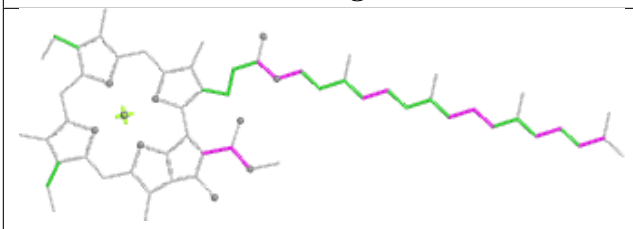
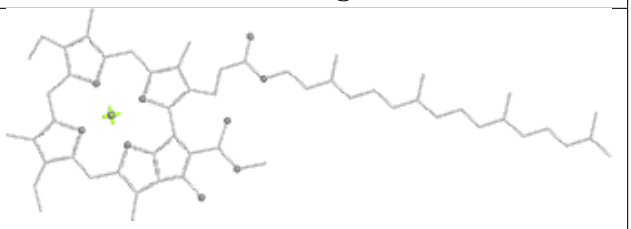


Bond angles

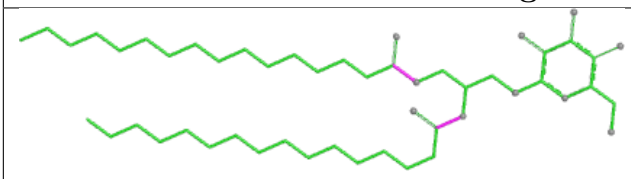


Torsions

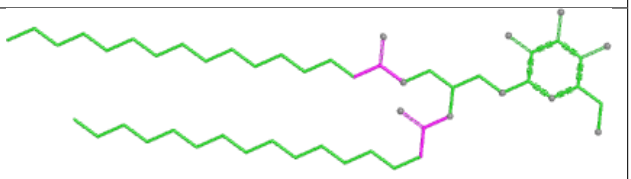


Rings

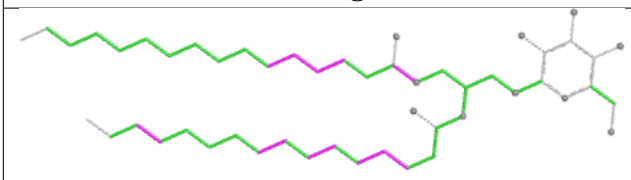
Ligand LMG C 519



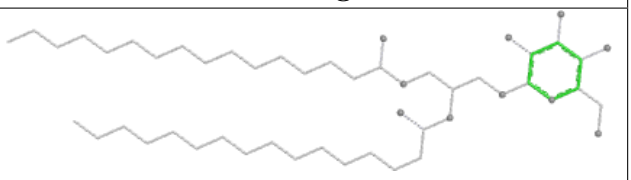
Bond lengths



Bond angles

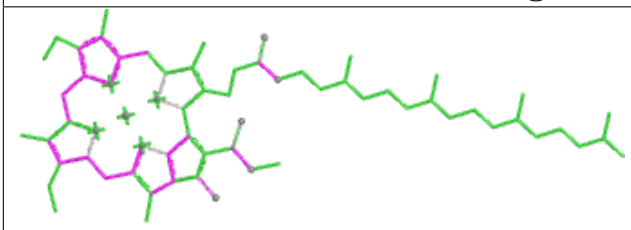


Torsions

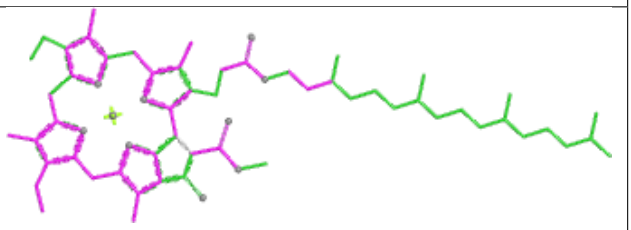


Rings

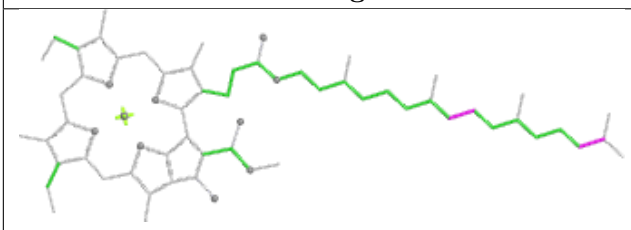
Ligand CLA b 620



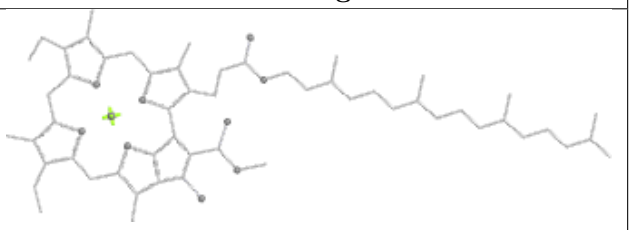
Bond lengths



Bond angles

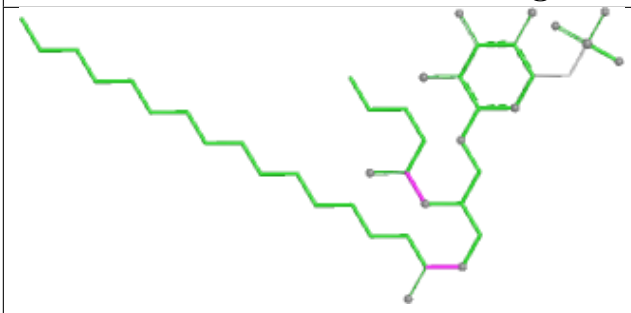


Torsions

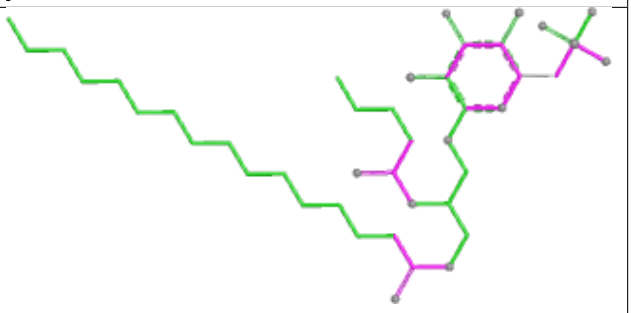


Rings

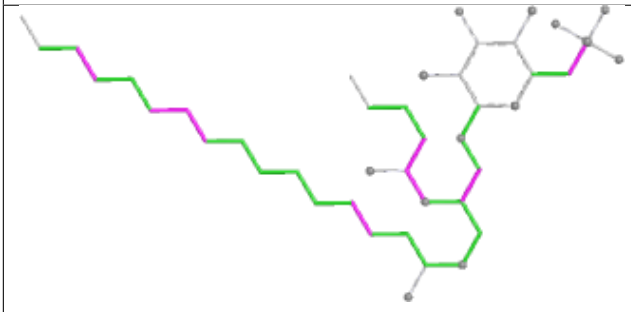
Ligand SQD f 101



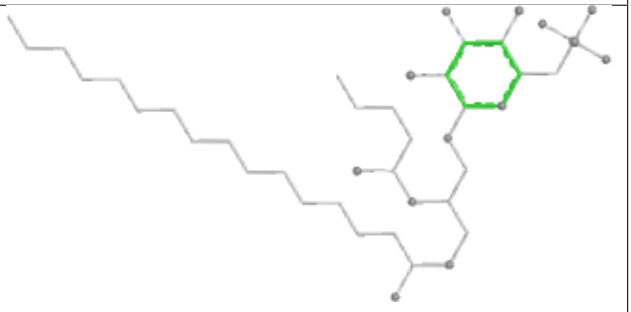
Bond lengths



Bond angles

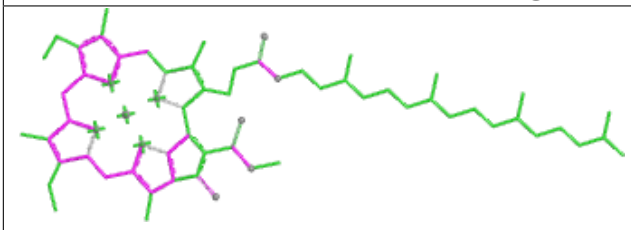


Torsions



Rings

Ligand CLA b 619



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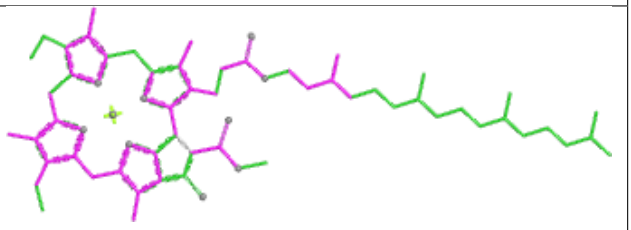
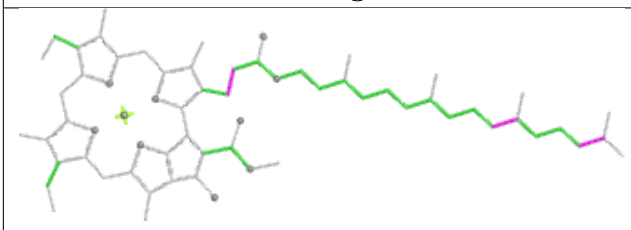
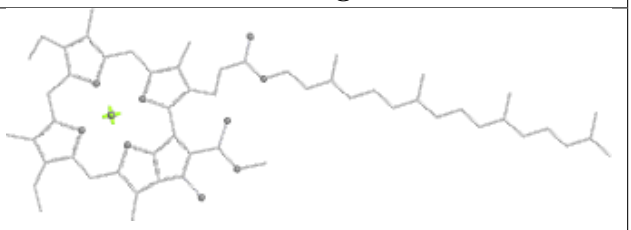


Bond angles

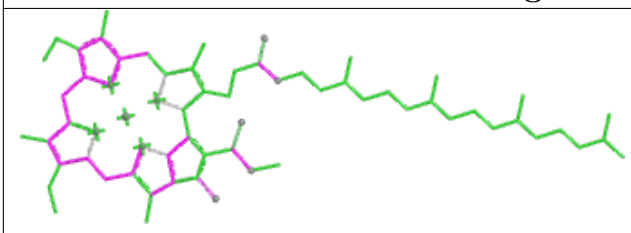


Torsions

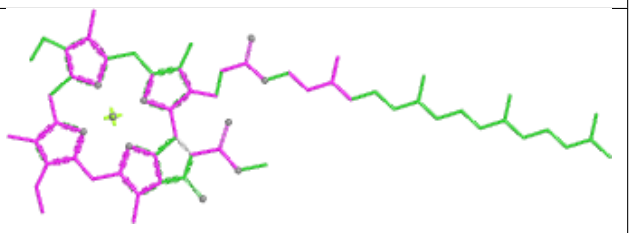


Rings

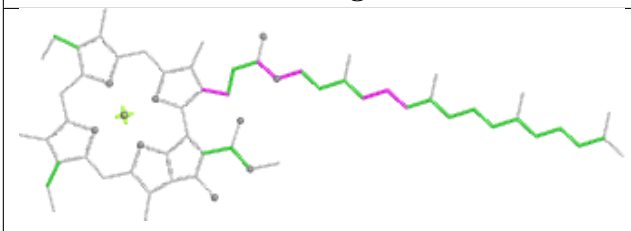
Ligand CLA C 513



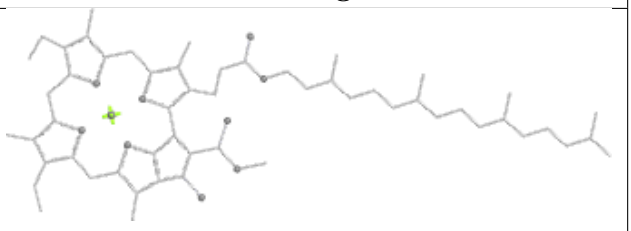
Bond lengths



Bond angles

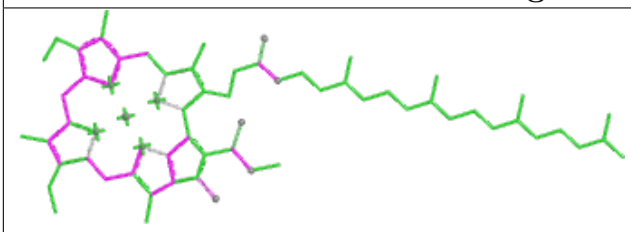


Torsions

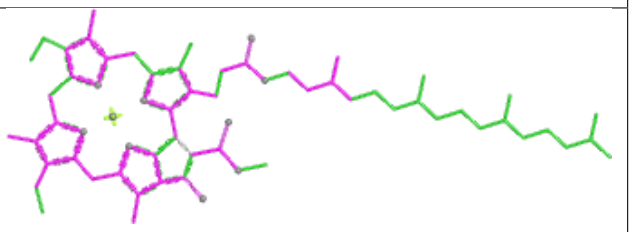


Rings

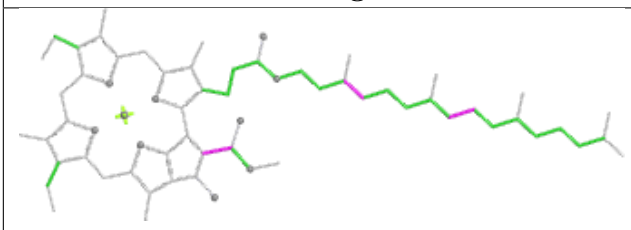
Ligand CLA b 614



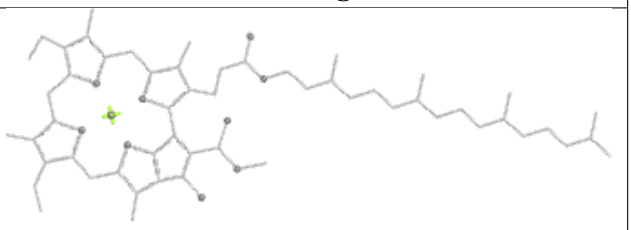
Bond lengths



Bond angles

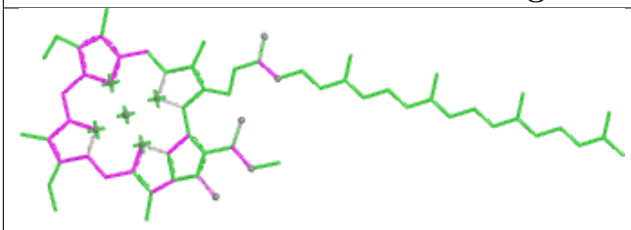


Torsions

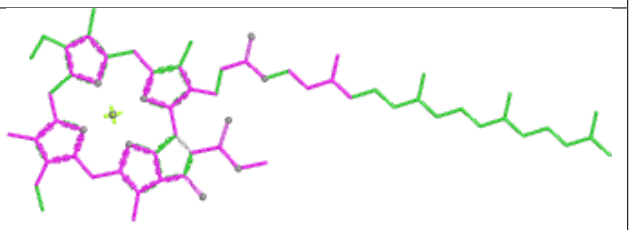


Rings

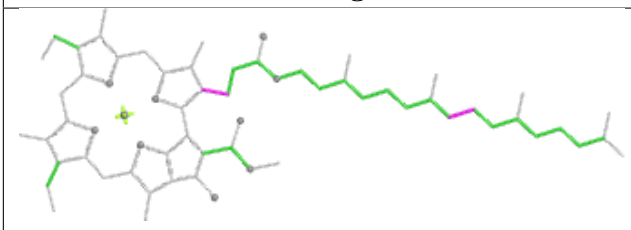
Ligand CLA b 621



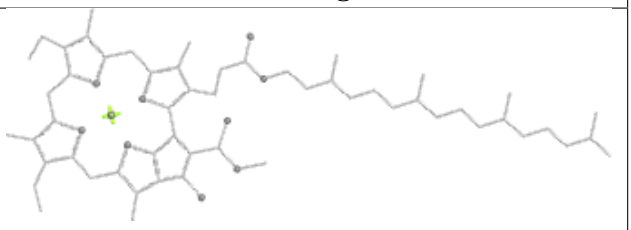
Bond lengths



Bond angles

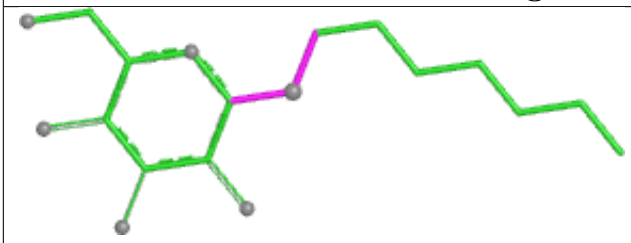


Torsions

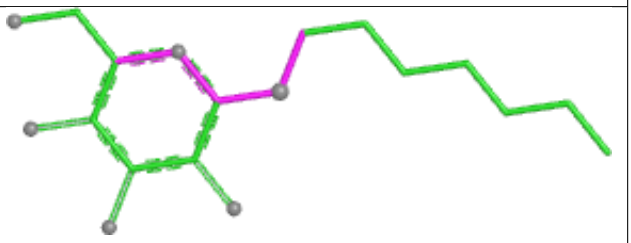


Rings

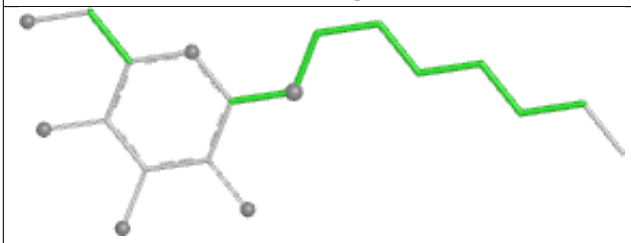
Ligand HTG c 526



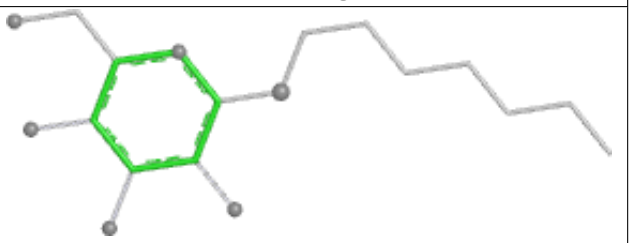
Bond lengths



Bond angles

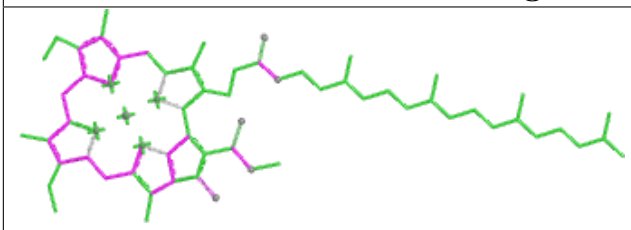


Torsions

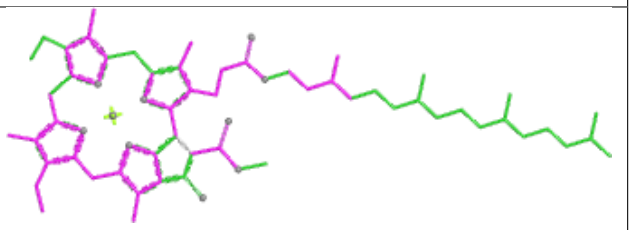


Rings

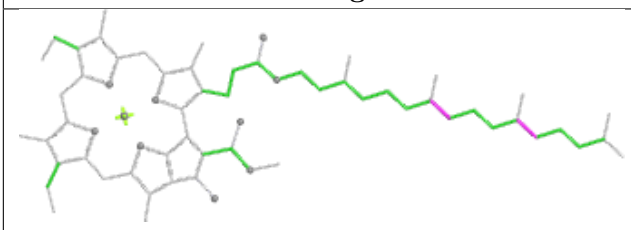
Ligand CLA A 407



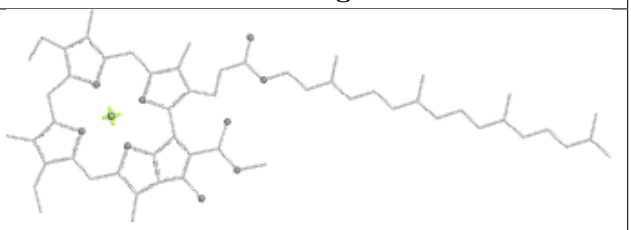
Bond lengths



Bond angles

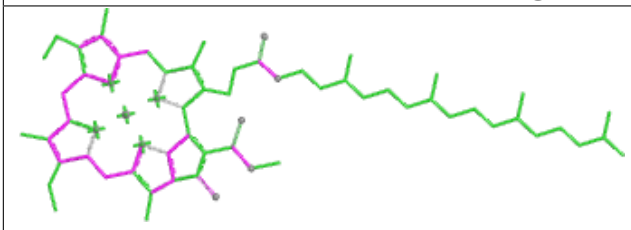


Torsions

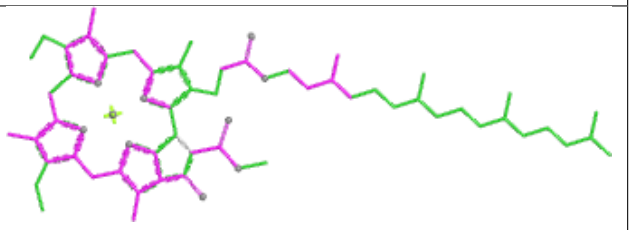


Rings

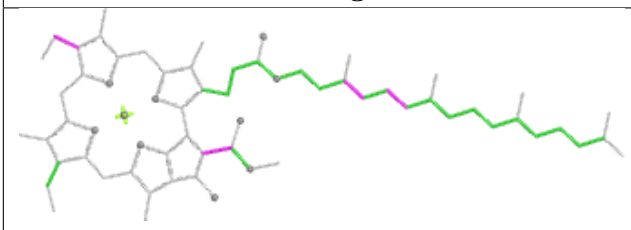
Ligand CLA c 512



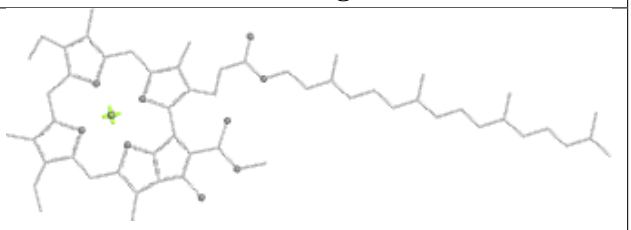
Bond lengths



Bond angles

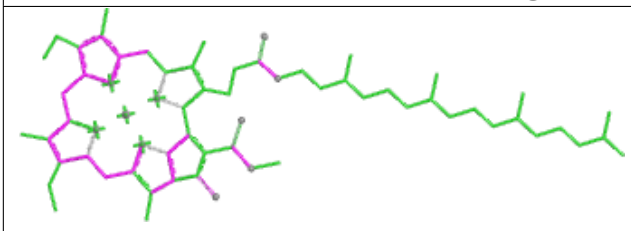


Torsions

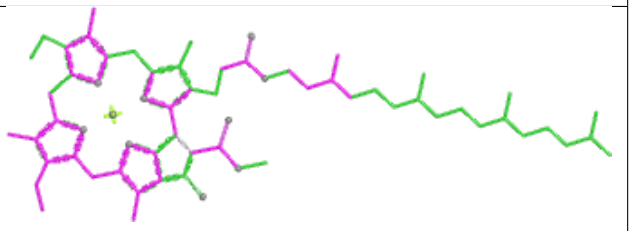


Rings

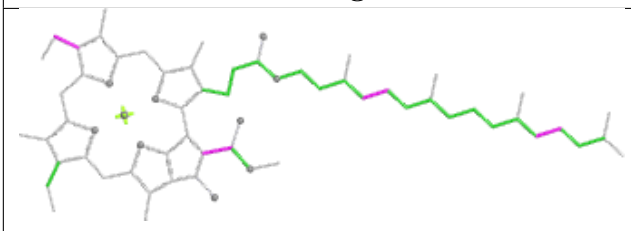
Ligand CLA C 502



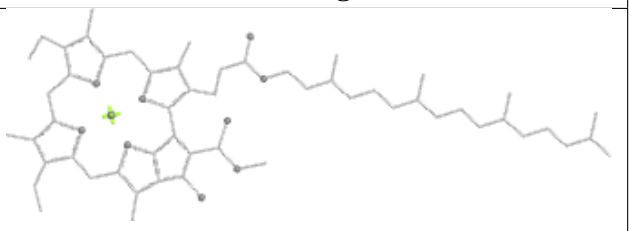
Bond lengths



Bond angles

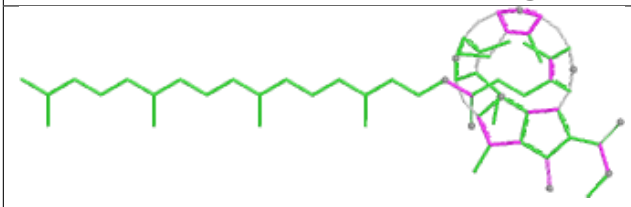


Torsions



Rings

Ligand PHO A 408



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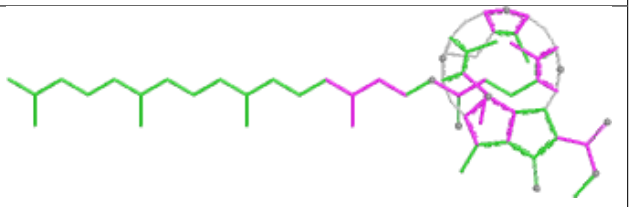
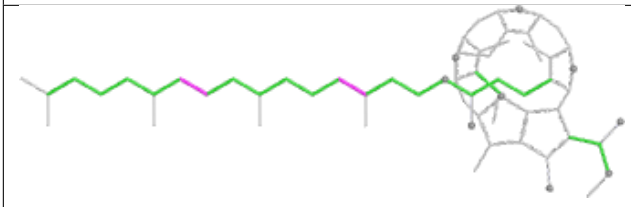
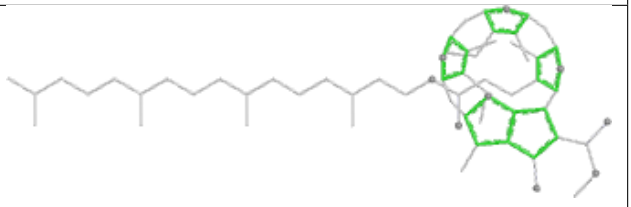


Bond angles

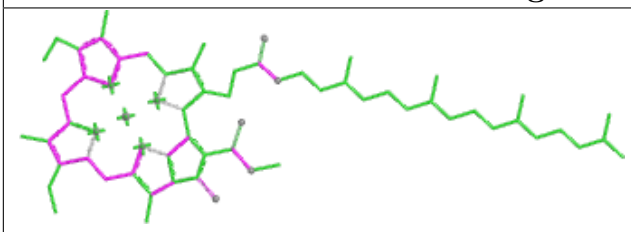


Torsions

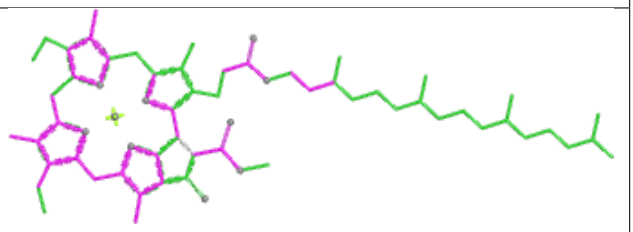


Rings

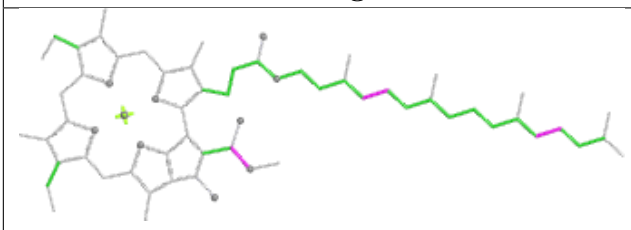
Ligand CLA b 613



Bond lengths



Bond angles



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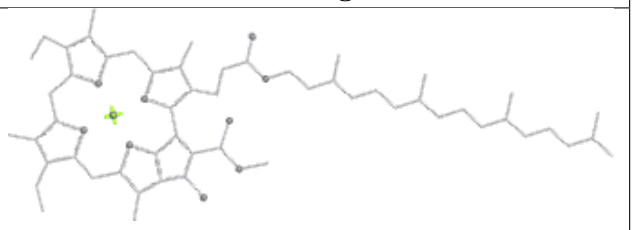
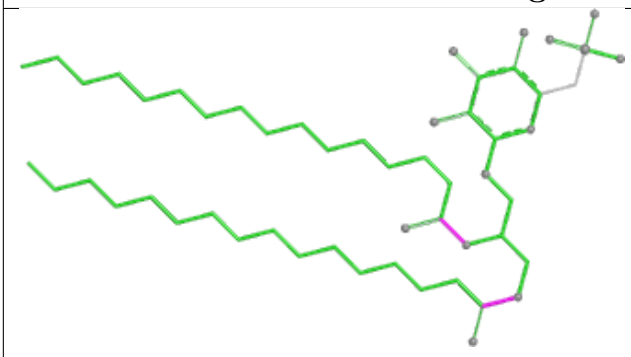


Rings

Ligand SQD a 405



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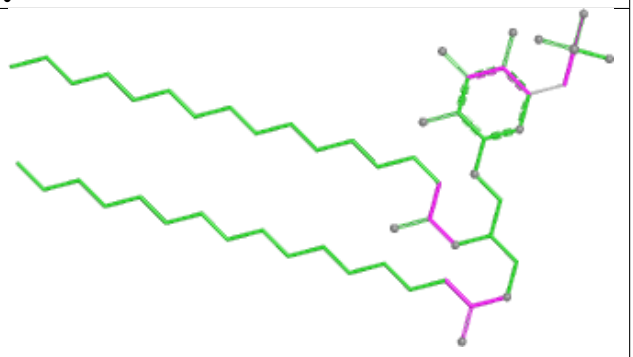
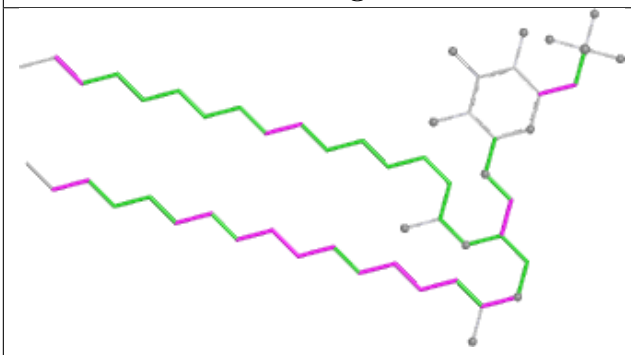
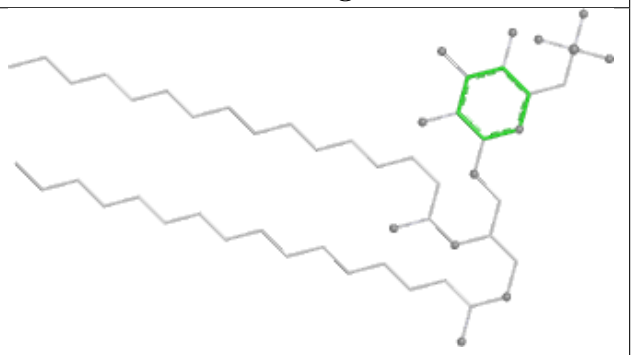


Bond angles

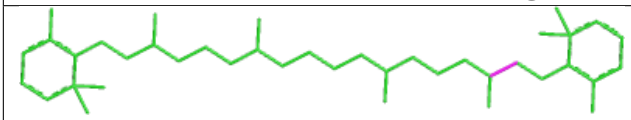


Torsions

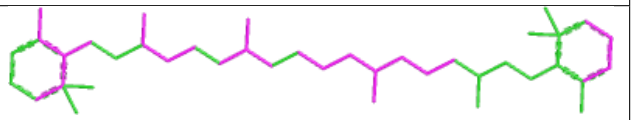


Rings

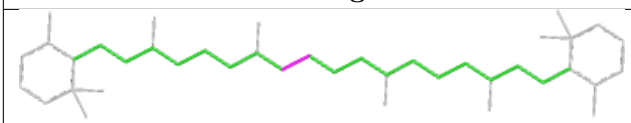
Ligand BCR T 103



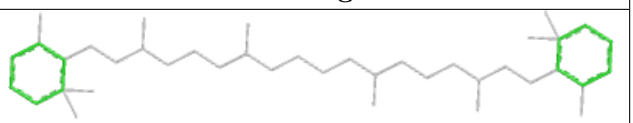
Bond lengths



Bond angles

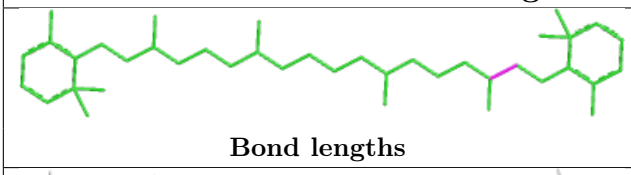


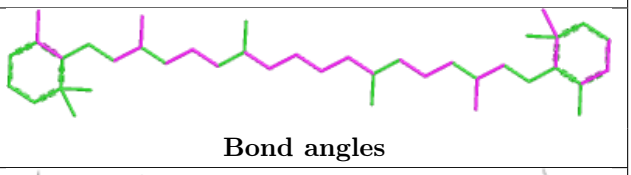
Torsions

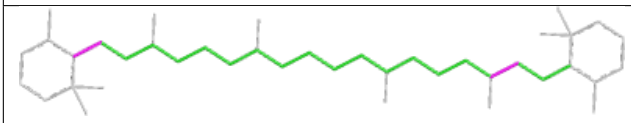


Rings

Ligand BCR Y 101


Bond lengths


Bond angles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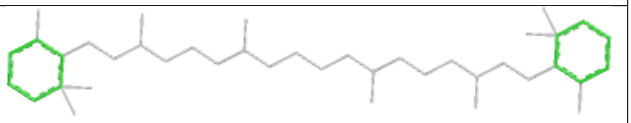
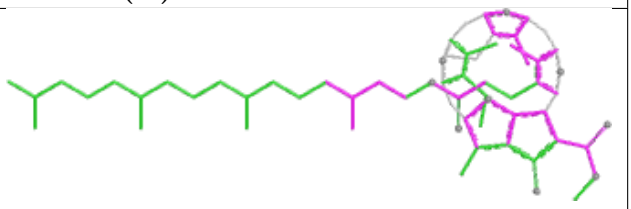
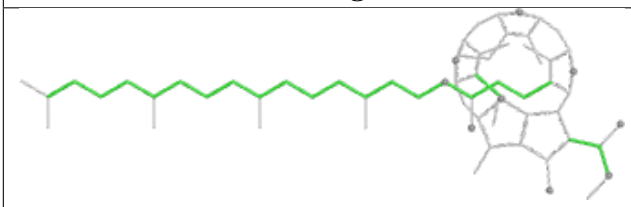

Rings

Ligand PHO A 409 (B)

Bond lengths


Bond angles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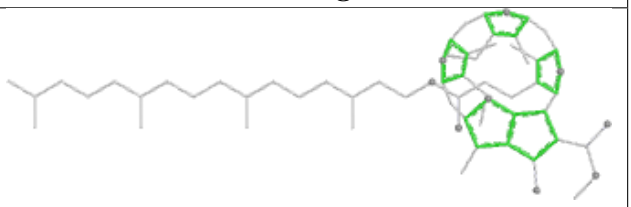
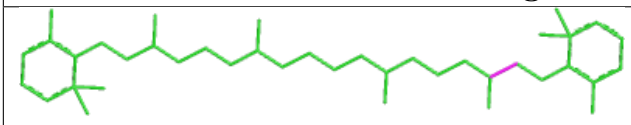
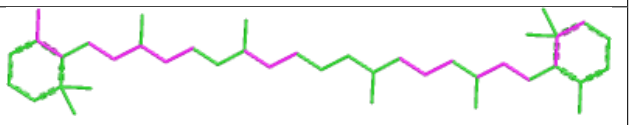
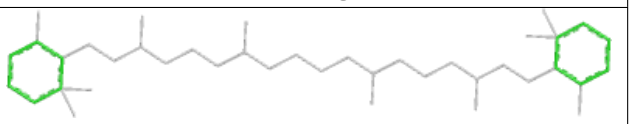

Rings

Ligand BCR B 618


Bond lengths

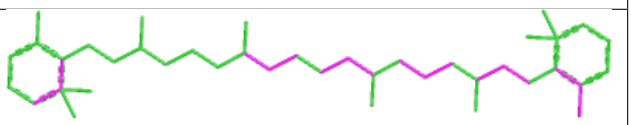

Bond angles

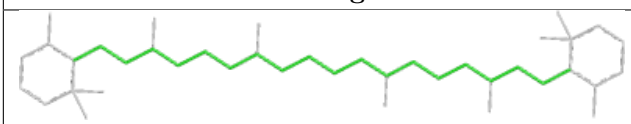
Torsions

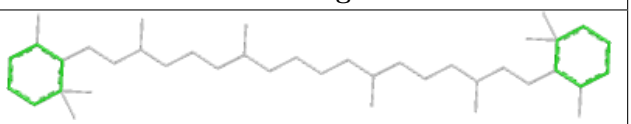

Rings

Ligand BCR b 628

Bond lengths


Bond angles

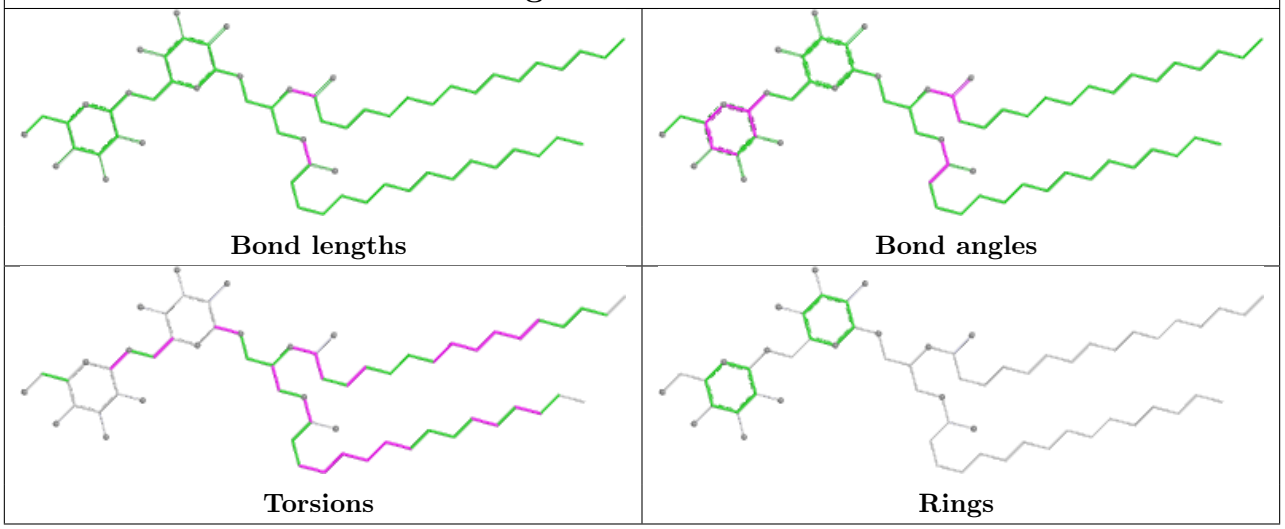

Torsions


Rings

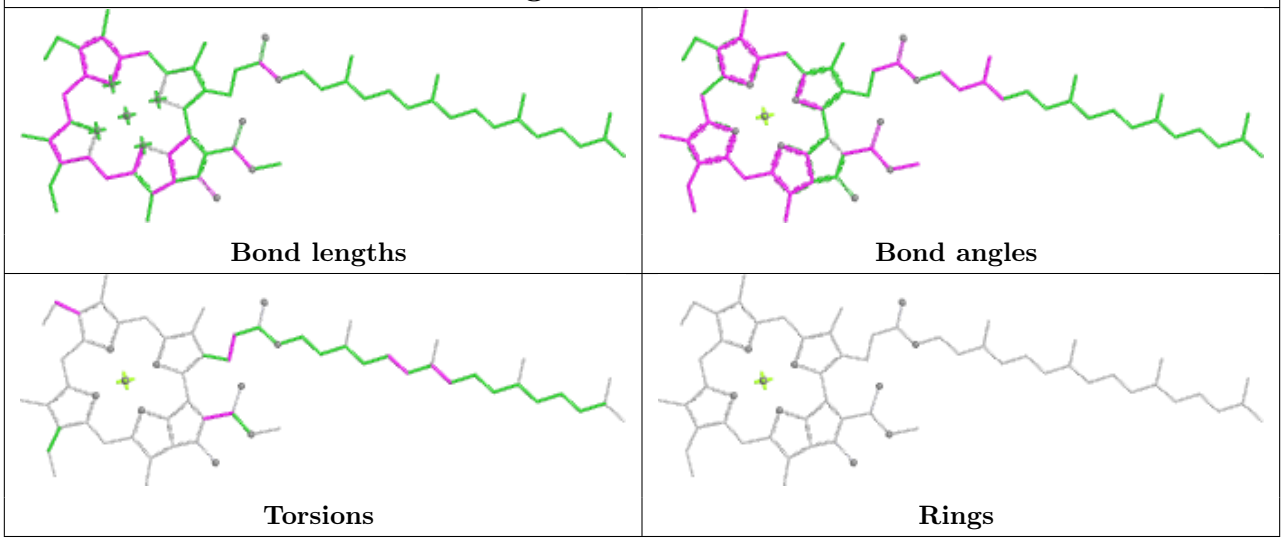
Ligand PL9 d 405 (B)

Ligand PL9 D 405 (A)

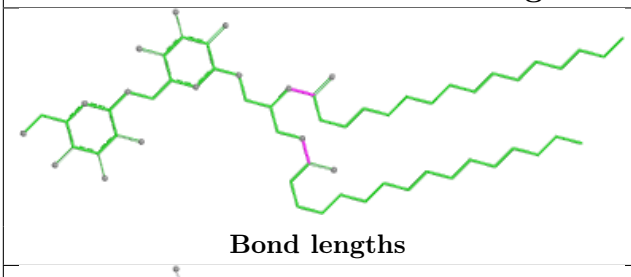
Ligand DGD e 101



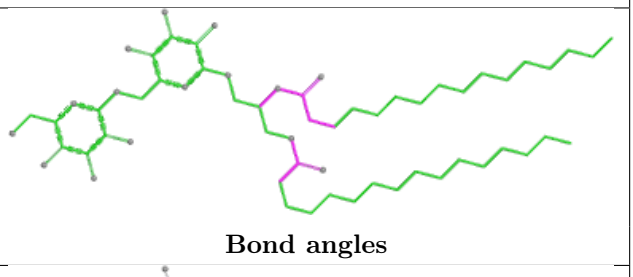
Ligand CLA C 507



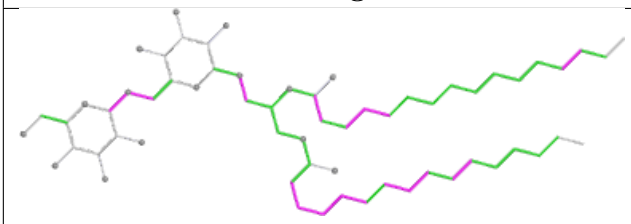
Ligand DGD c 521



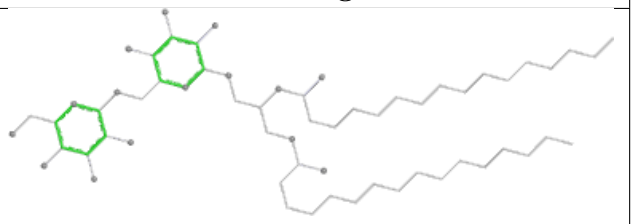
Bond lengths



Bond angles

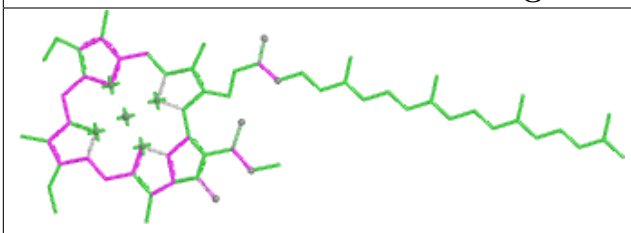


Torsions

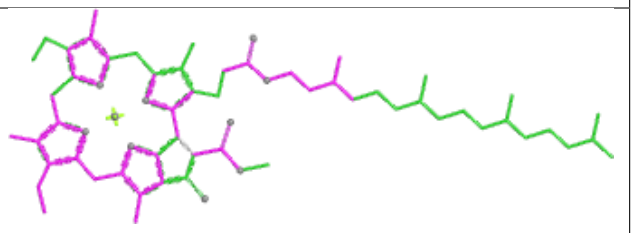


Rings

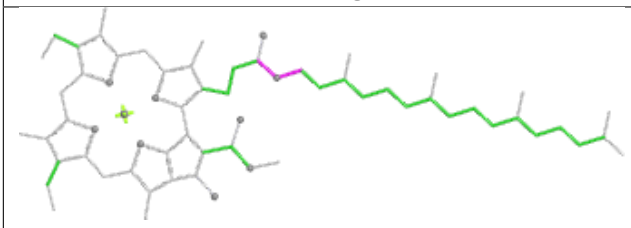
Ligand CLA C 511



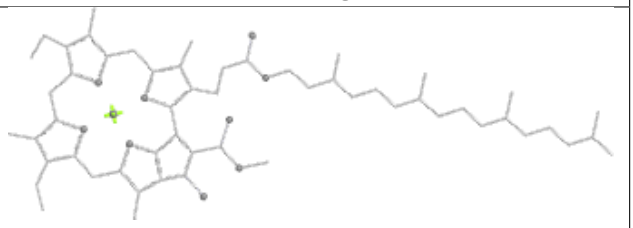
Bond lengths



Bond angles

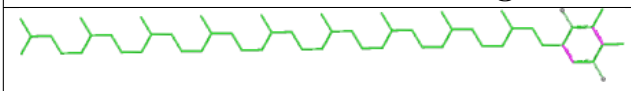


Torsions

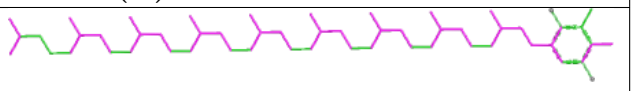


Rings

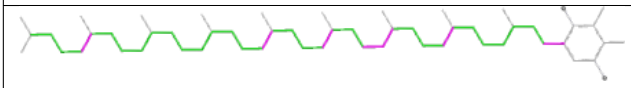
Ligand PL9 A 419 (B)



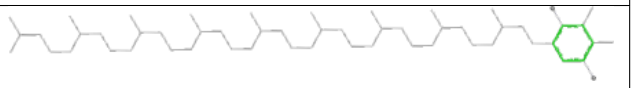
Bond lengths



Bond angles

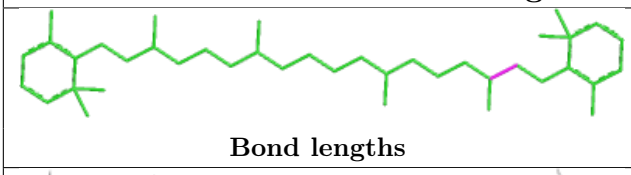


Torsions

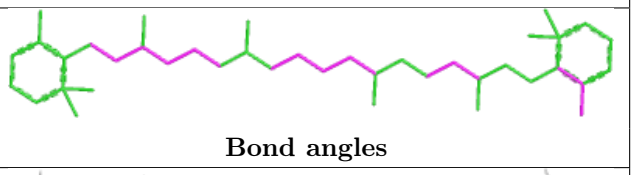


Rings

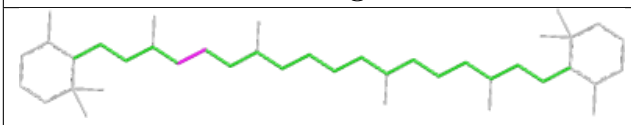
Ligand BCR h 101



Bond lengths



Bond angles



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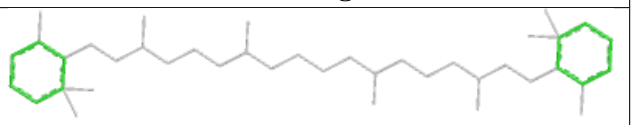
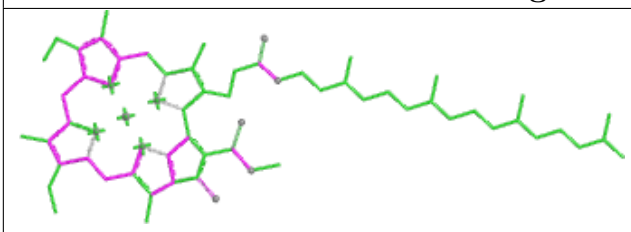


Rings

Ligand CLA c 513



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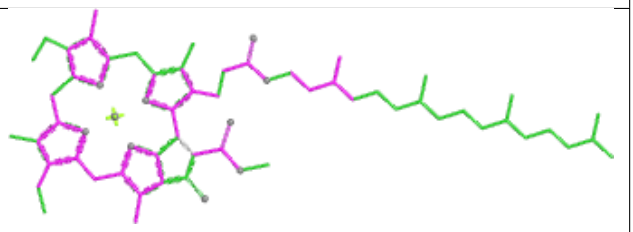
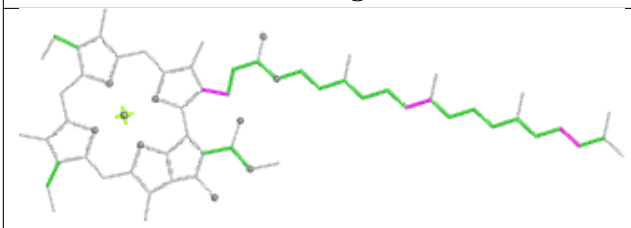


Bond angles



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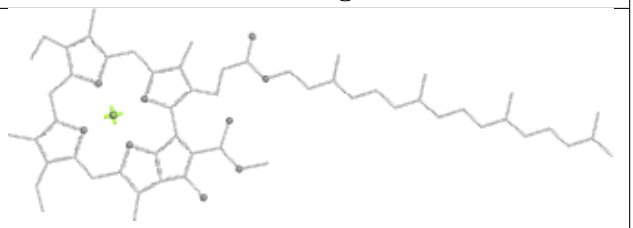
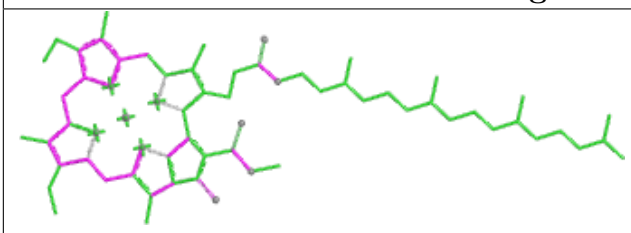
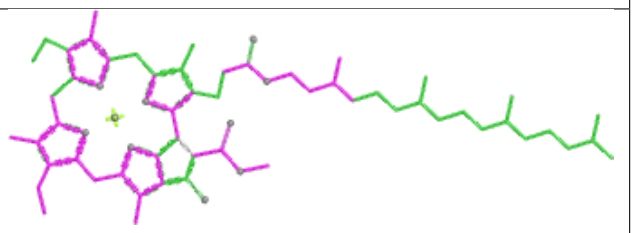


Rings

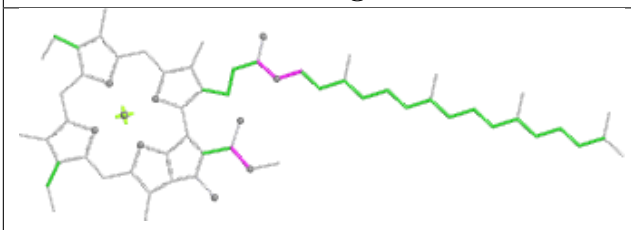
Ligand CLA c 516



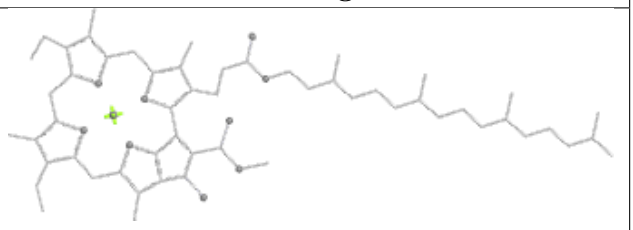
Bond lengths



Bond angles

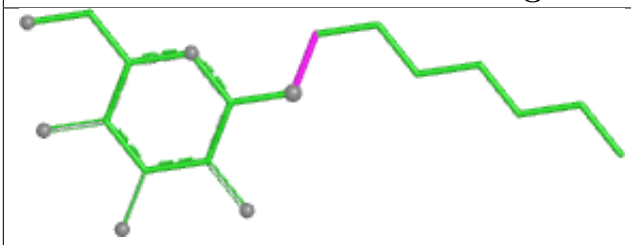


Torsions



Rings

Ligand HTG b 631



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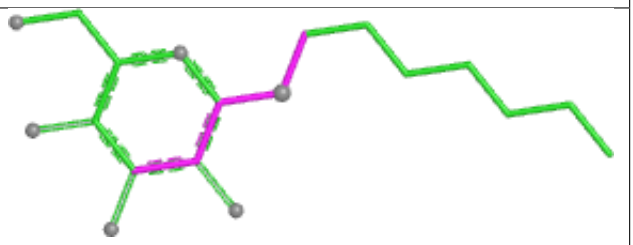
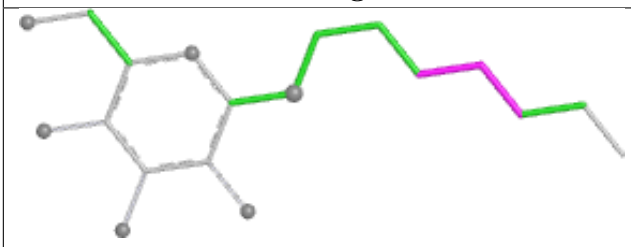
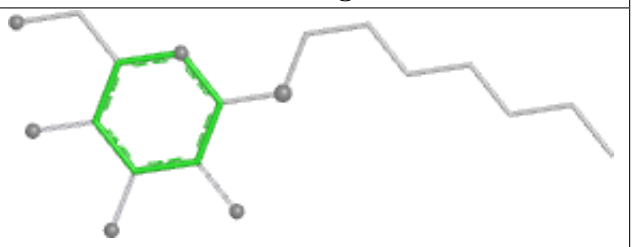


Bond angles

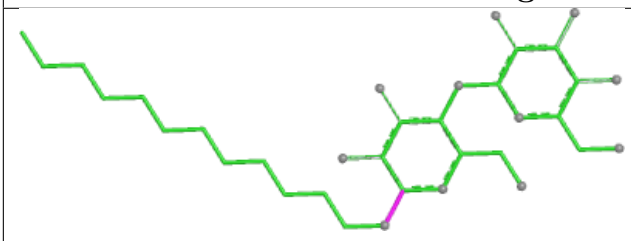


Torsions



Rings

Ligand LMT M 103



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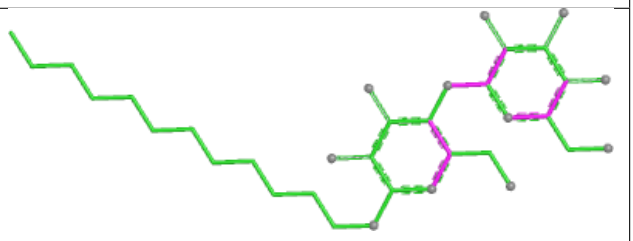
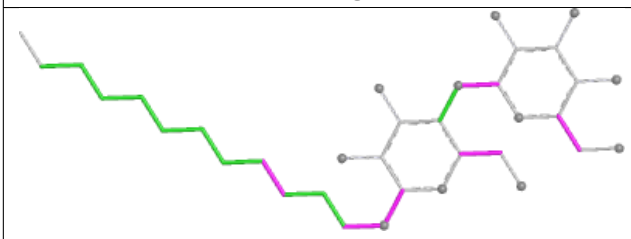


Bond angles



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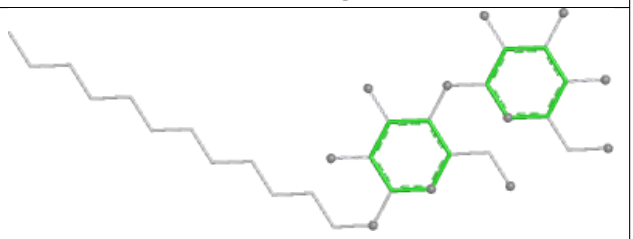
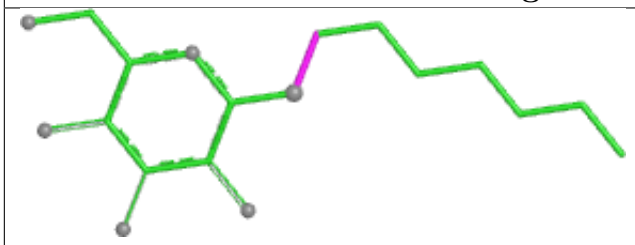


Rings

Ligand HTG B 624



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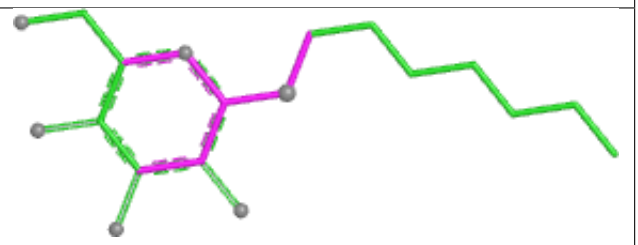
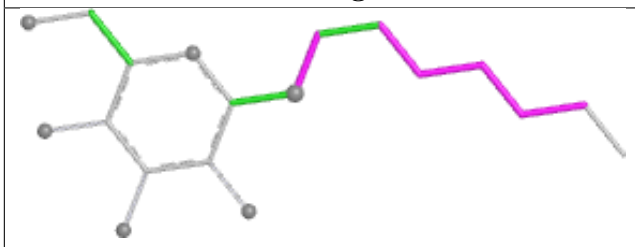


Bond angles



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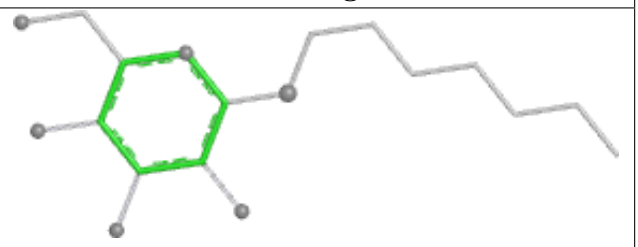
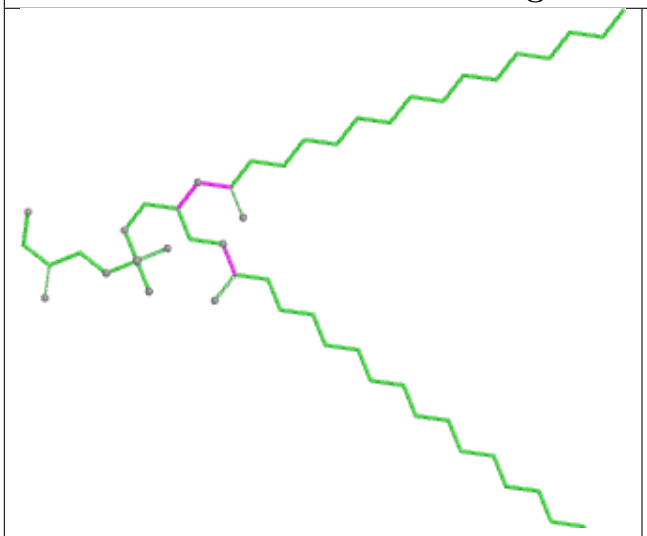
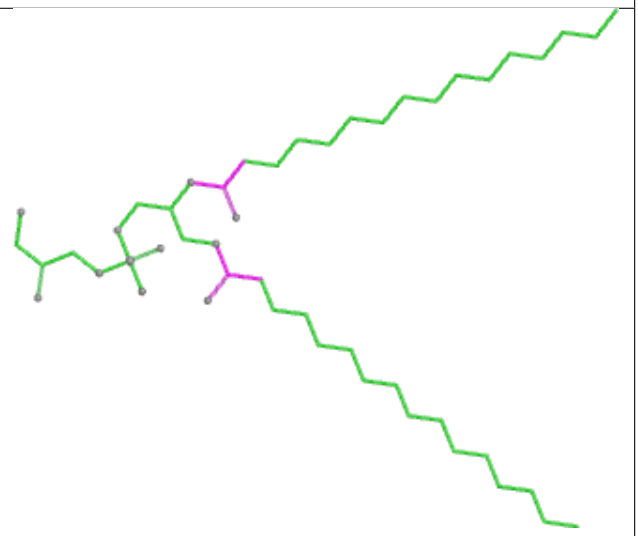


Rings

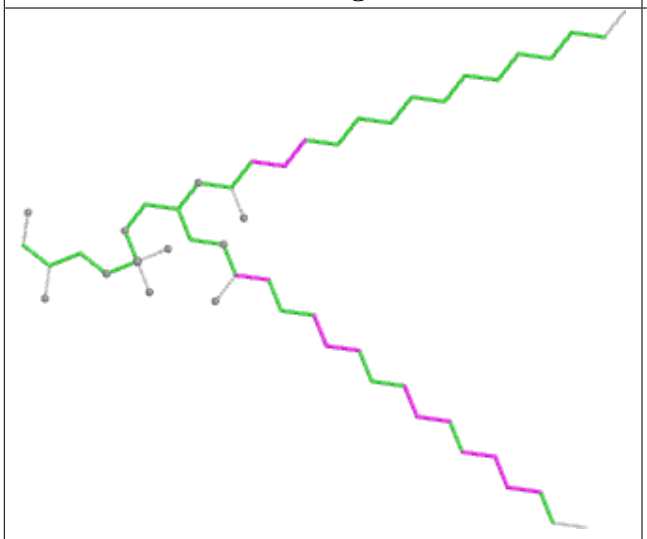
Ligand LHG d 406



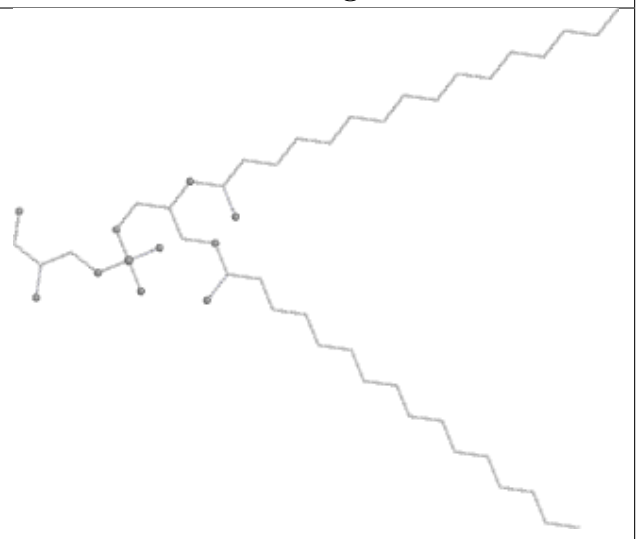
Bond lengths



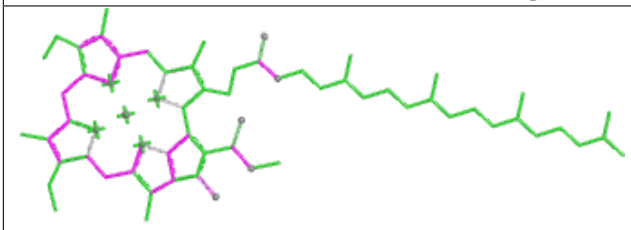
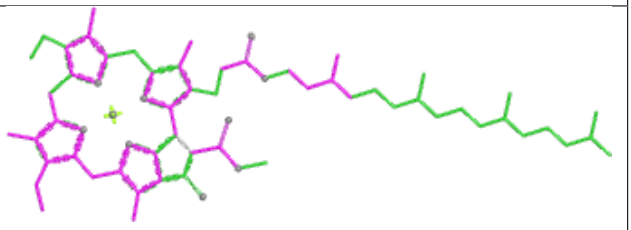
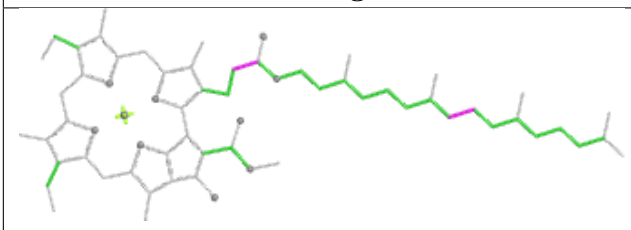
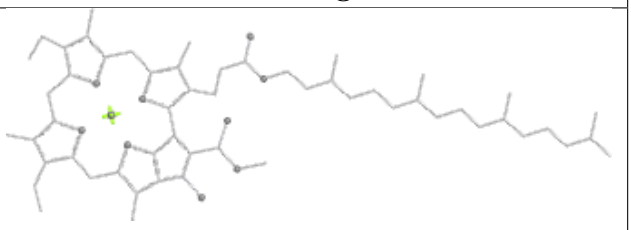
Bond angles

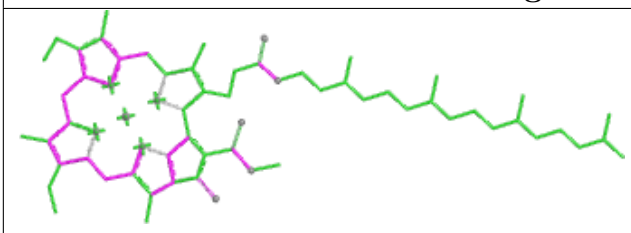
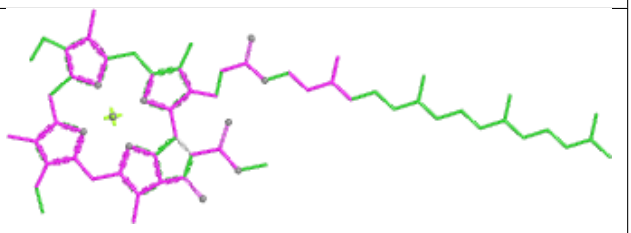
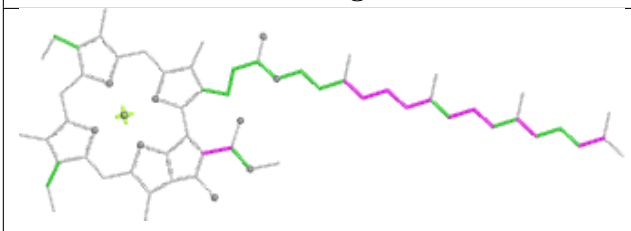
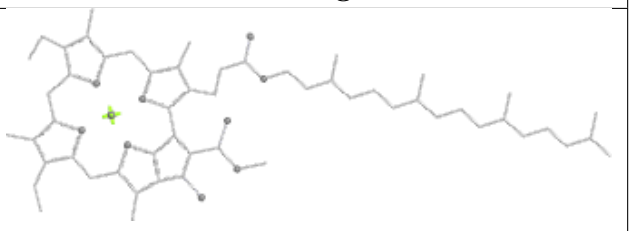


Torsions

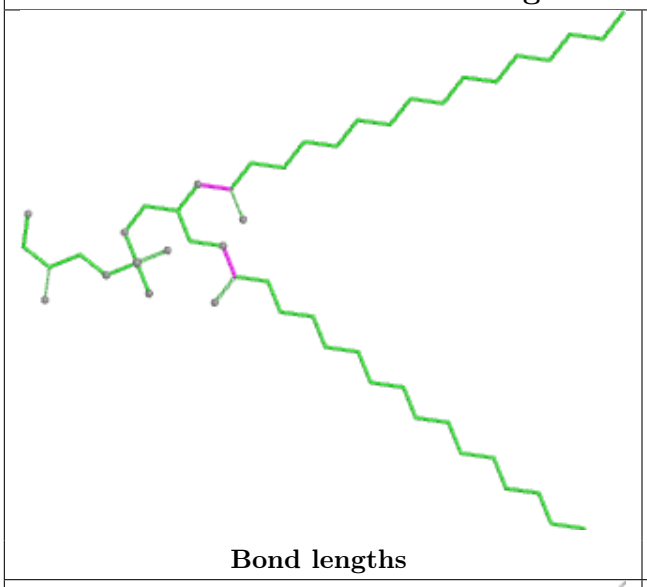


Rings

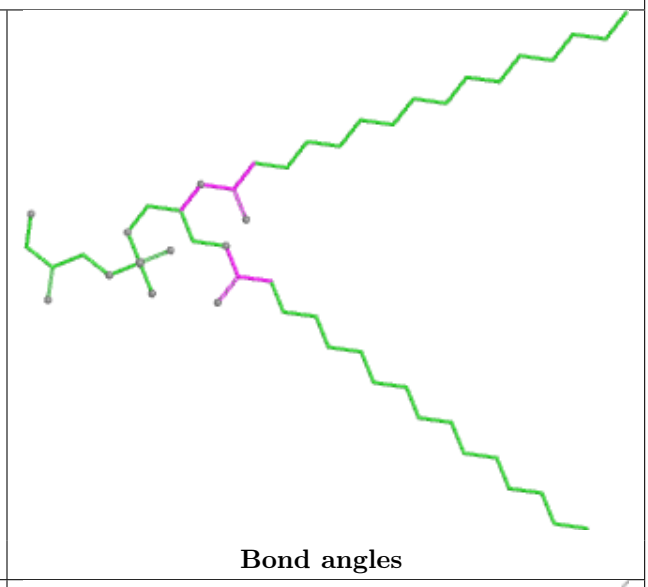
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

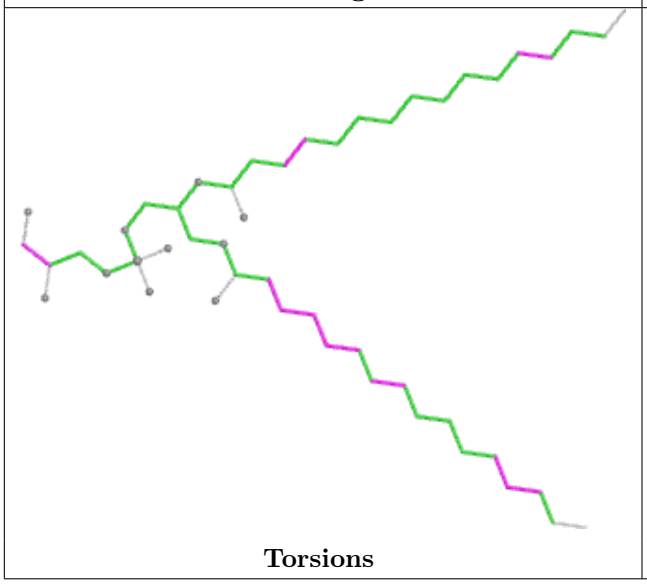
Ligand LHG D 407



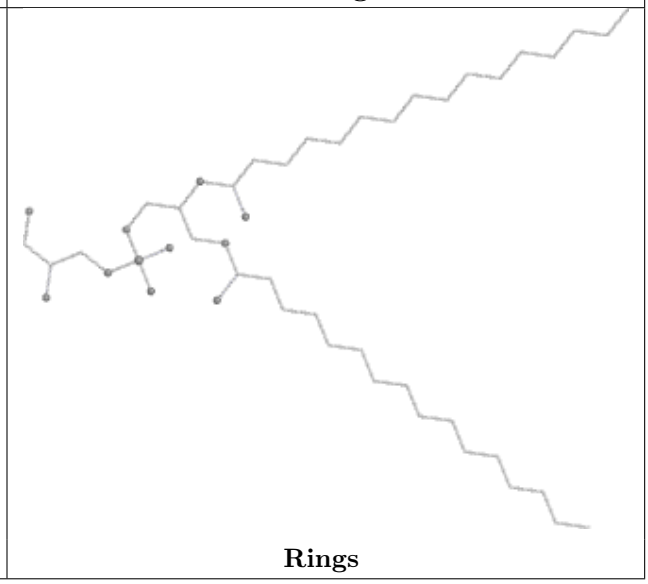
Bond lengths



Bond angles

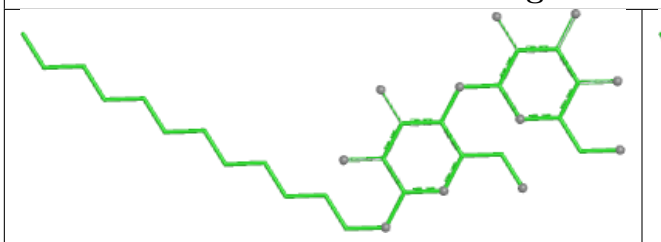


Torsions

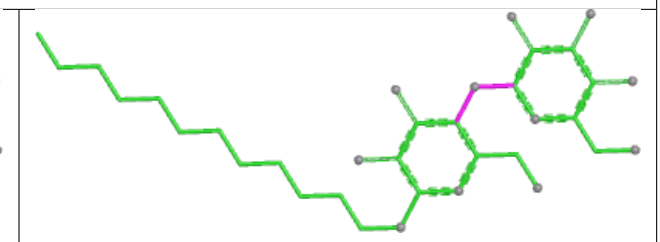


Rings

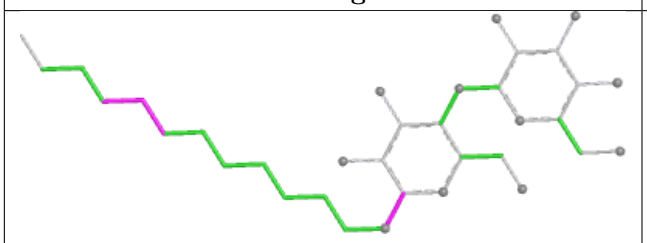
Ligand LMT a 419



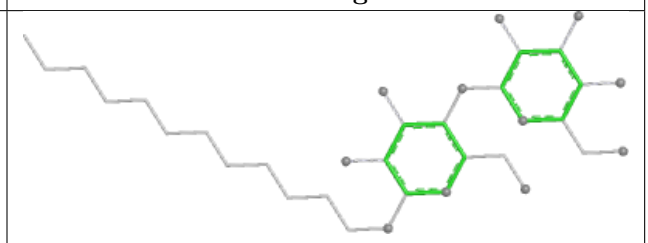
Bond lengths



Bond angles

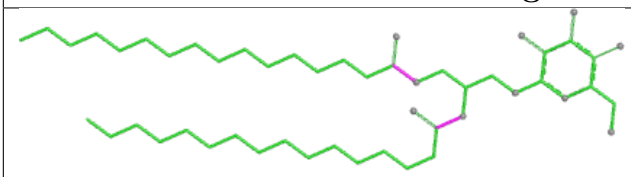


Torsions

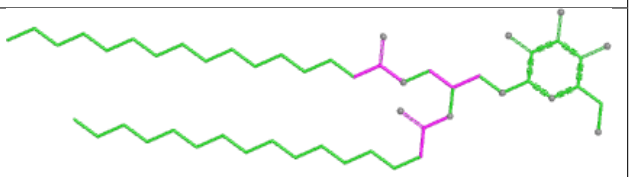


Rings

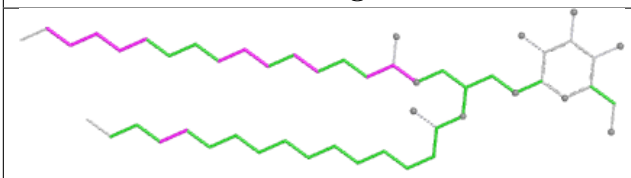
Ligand LMG b 629



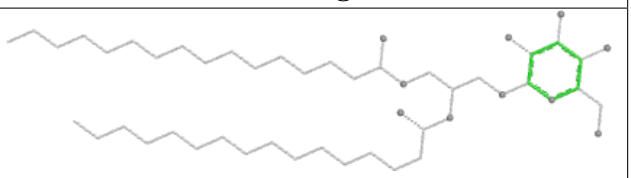
Bond lengths



Bond angles

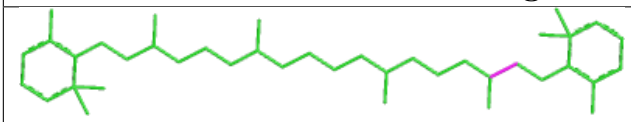


Torsions

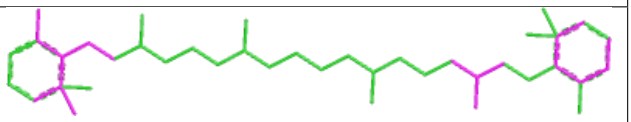


Rings

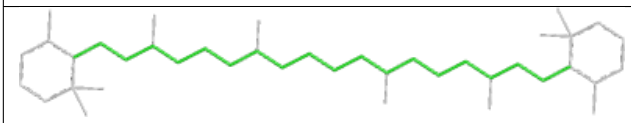
Ligand BCR B 619



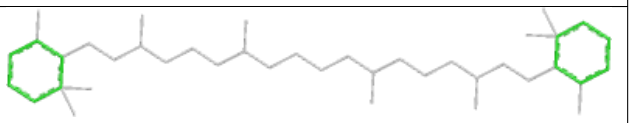
Bond lengths



Bond angles



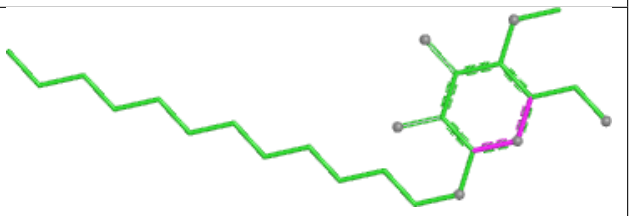
Torsions



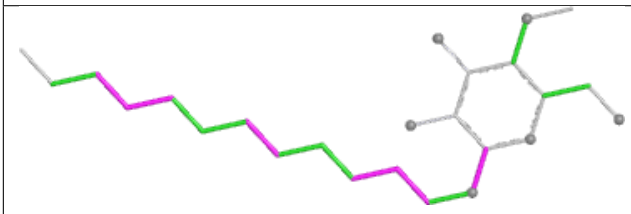
Rings

Ligand LMT T 104

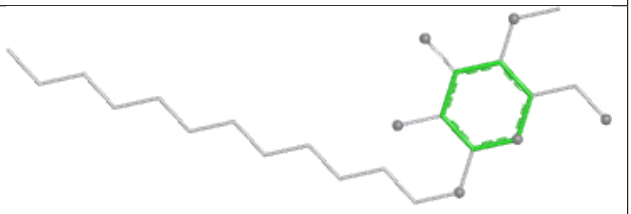
Bond lengths



Bond angles

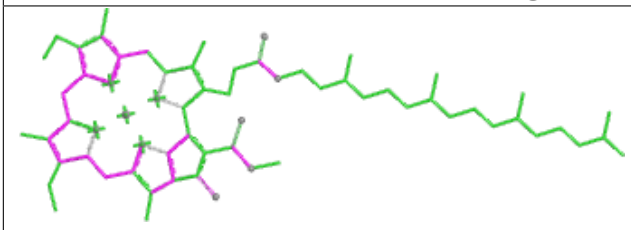


Torsions



Rings

Ligand CLA B 610



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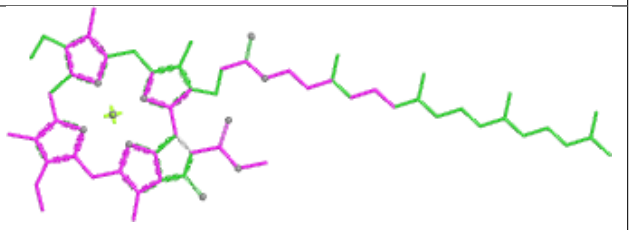
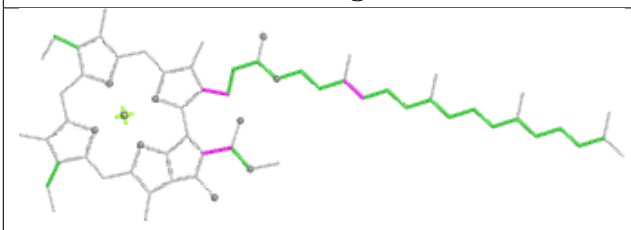


Bond angles



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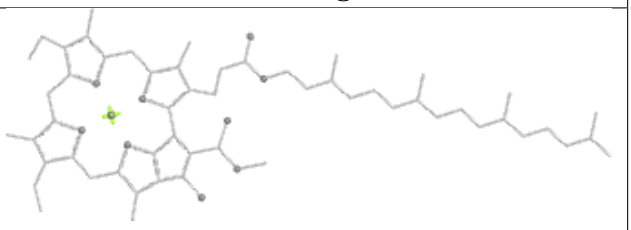
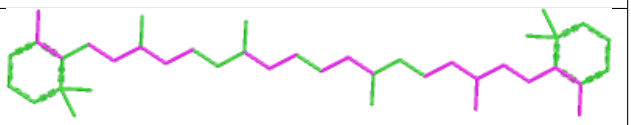


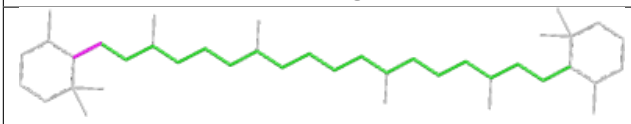
Rings

Ligand BCR C 514

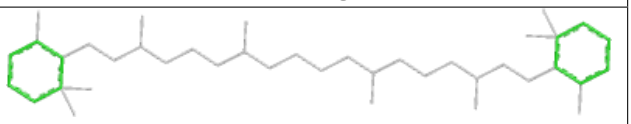
Bond lengths



Bond angles

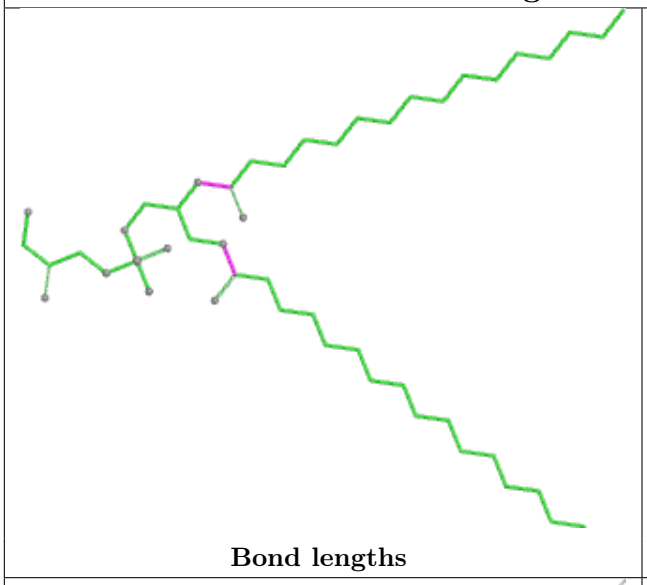


Torsions



Rings

Ligand LHG D 408



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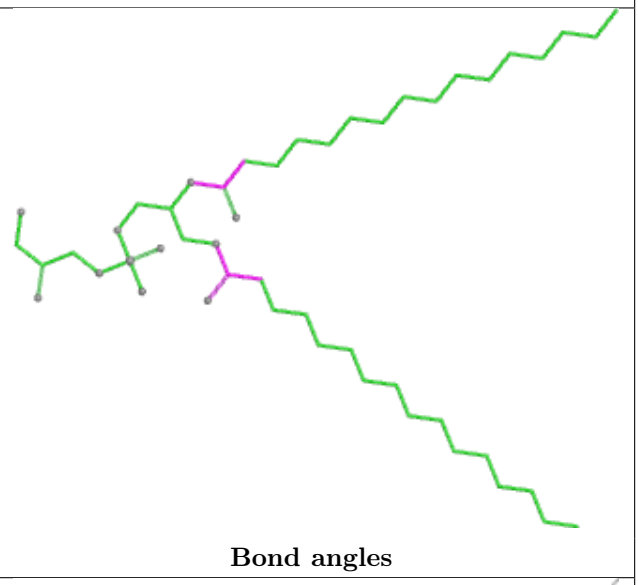
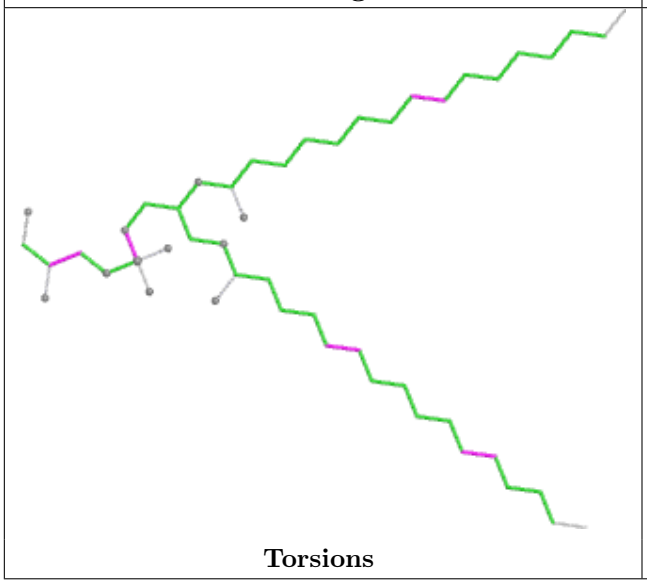
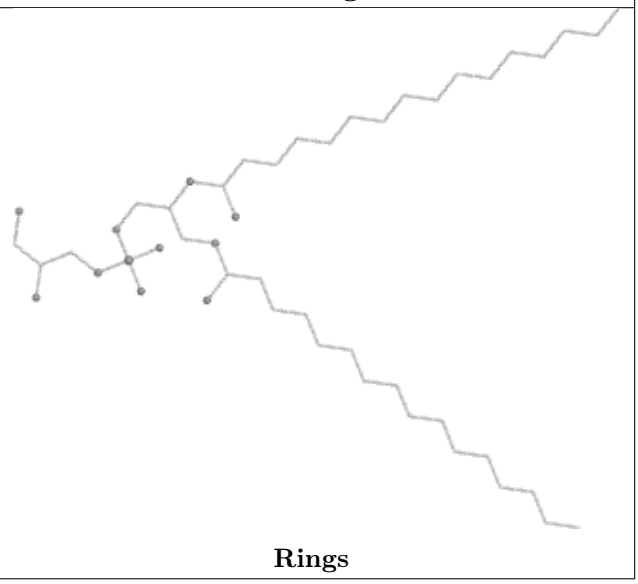


Bond angles

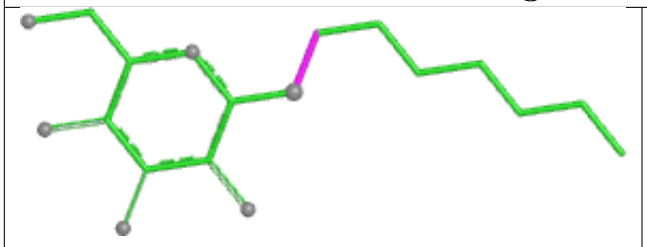


Torsions

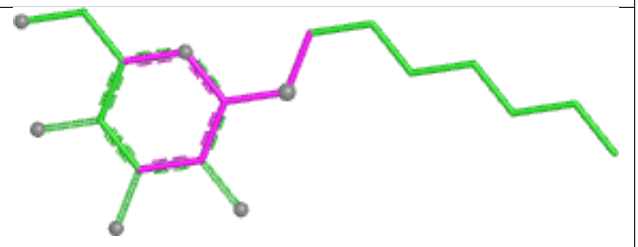


Rings

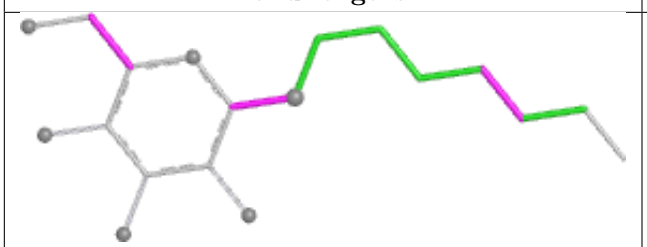
Ligand HTG B 625



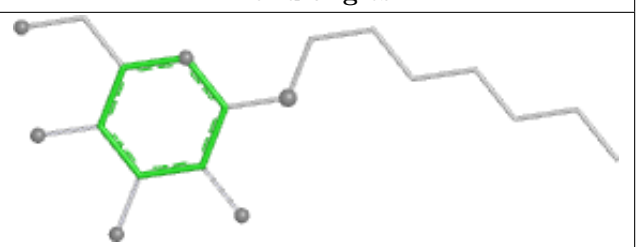
Bond lengths



Bond angles

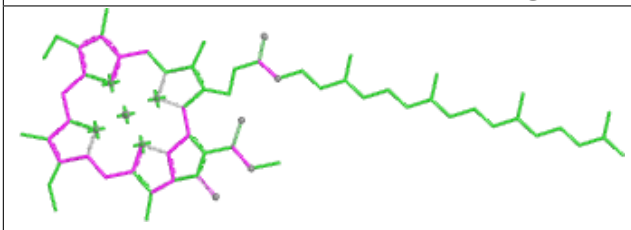


Torsions

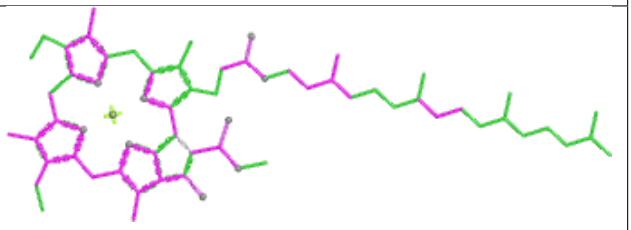


Rings

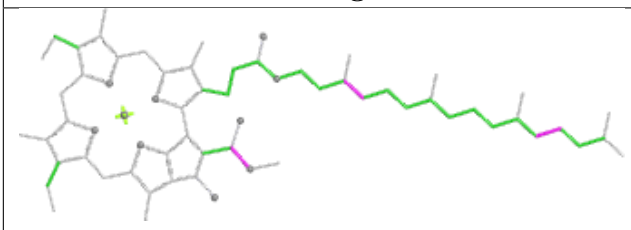
Ligand CLA B 605



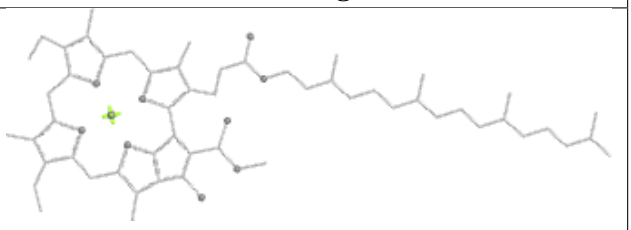
Bond lengths



Bond angles

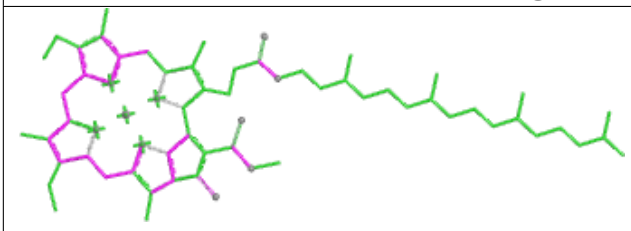


Torsions

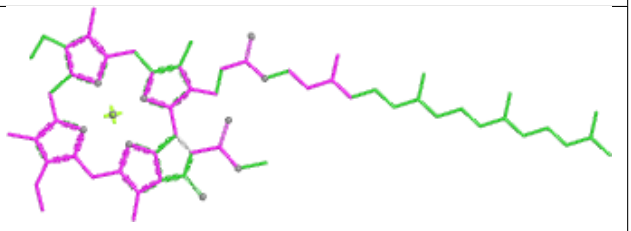


Rings

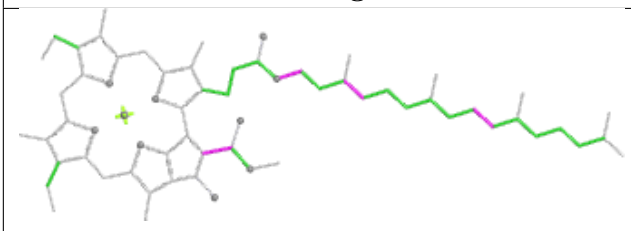
Ligand CLA c 518



Bond lengths



Bond angles



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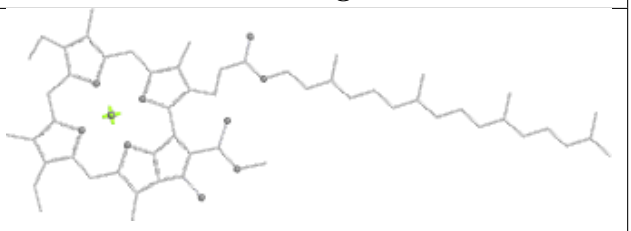
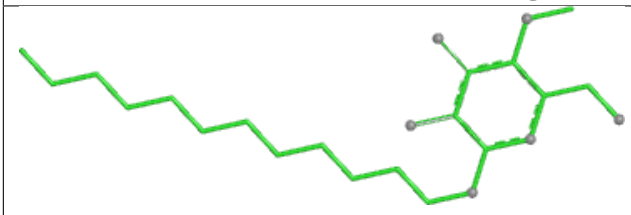


Rings

Ligand LMT b 630



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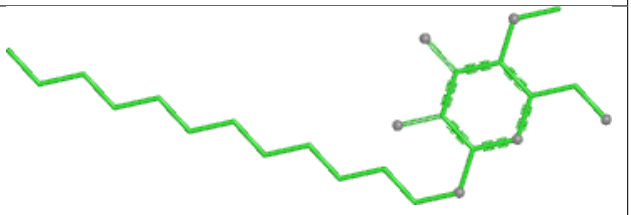
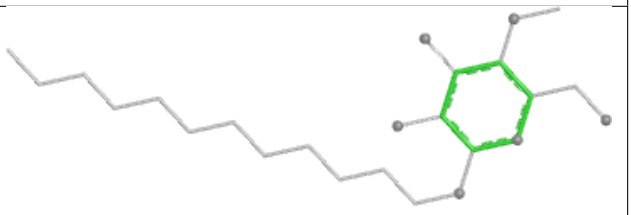


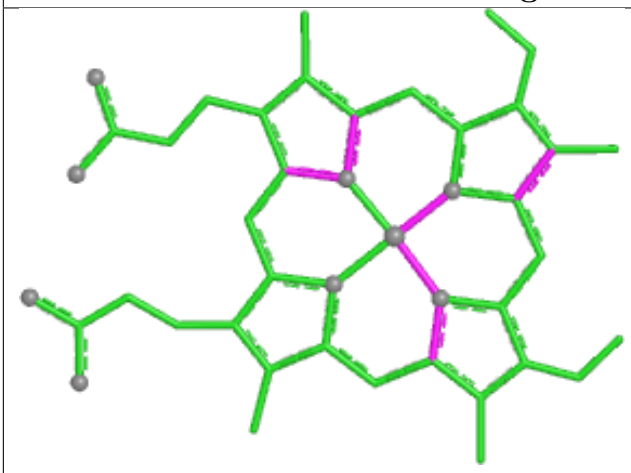
Bond angles

Torsions

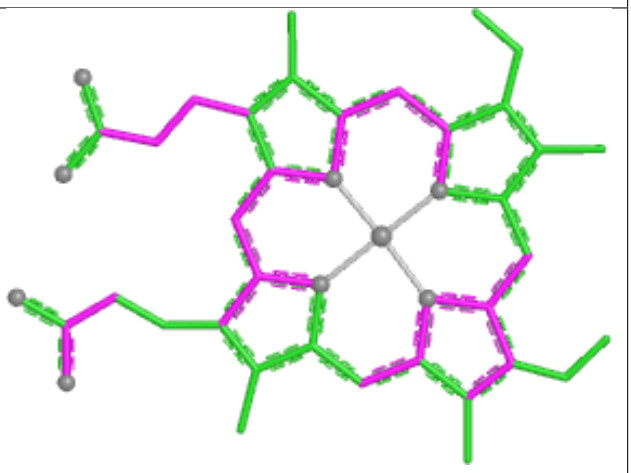


Rings

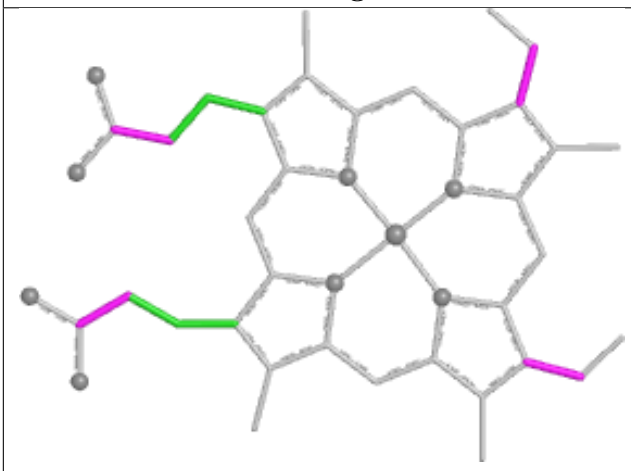
Ligand HEM F 102



Bond lengths



Bond angles



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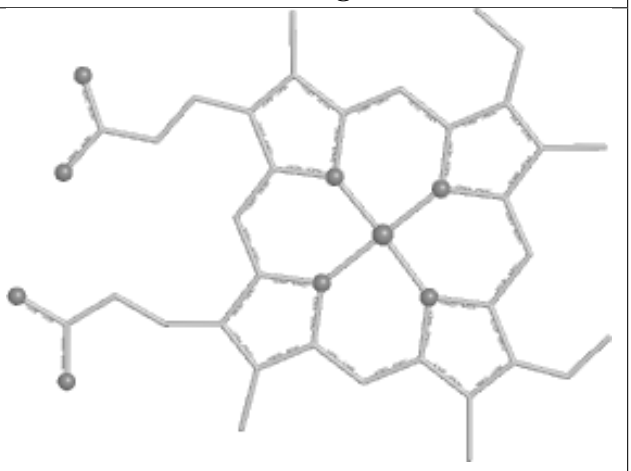
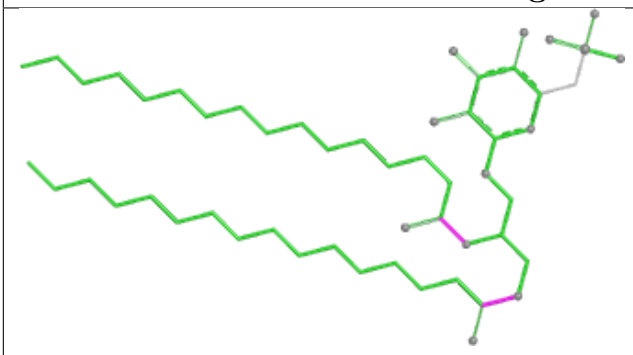


Rings

Ligand SQD a 414



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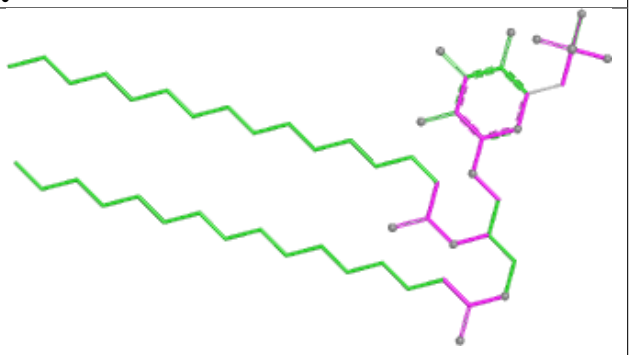
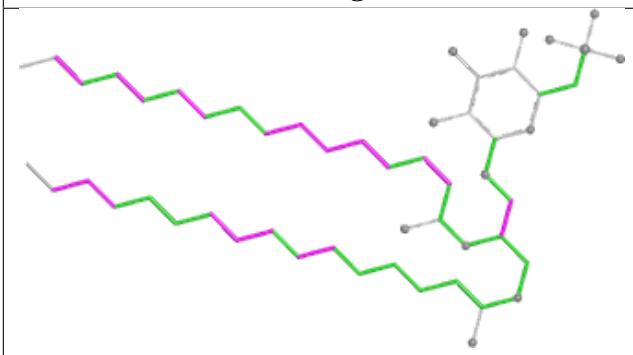
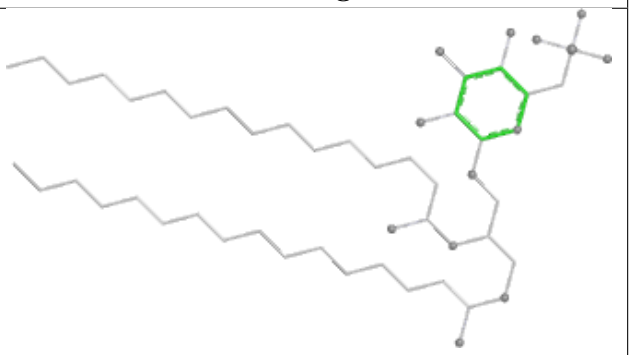


Bond angles

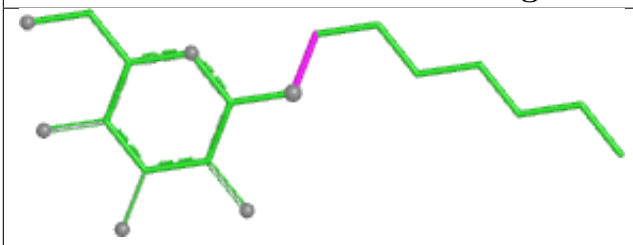


Torsions

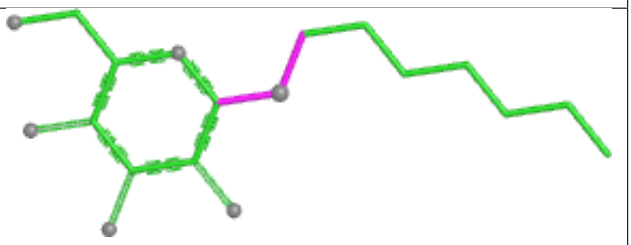


Rings

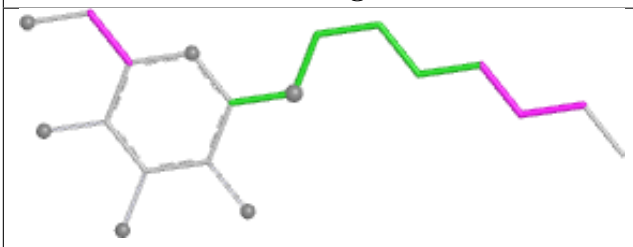
Ligand HTG B 623



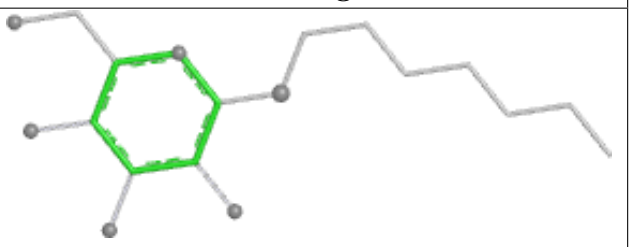
Bond lengths



Bond angles

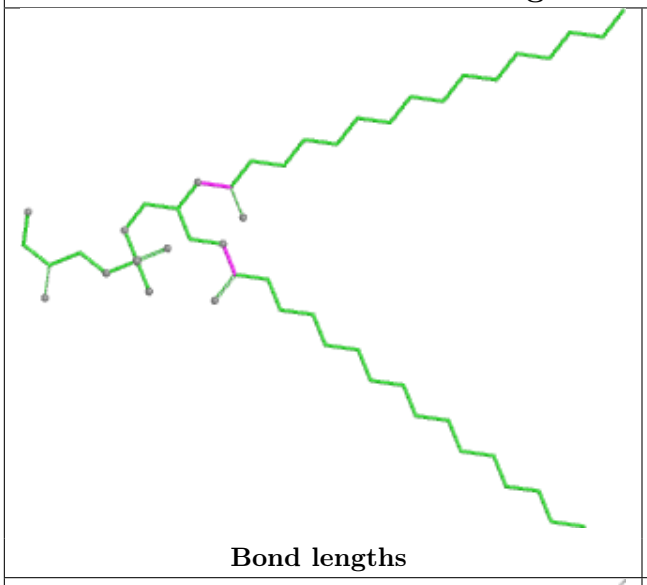


Torsions

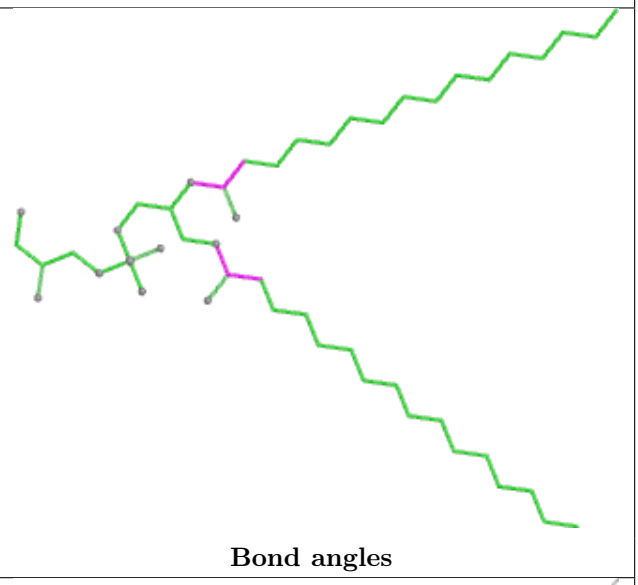


Rings

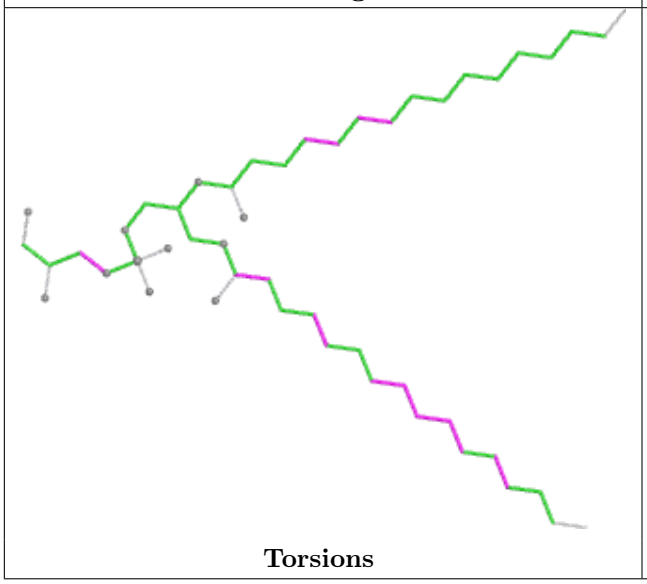
Ligand LHG d 408



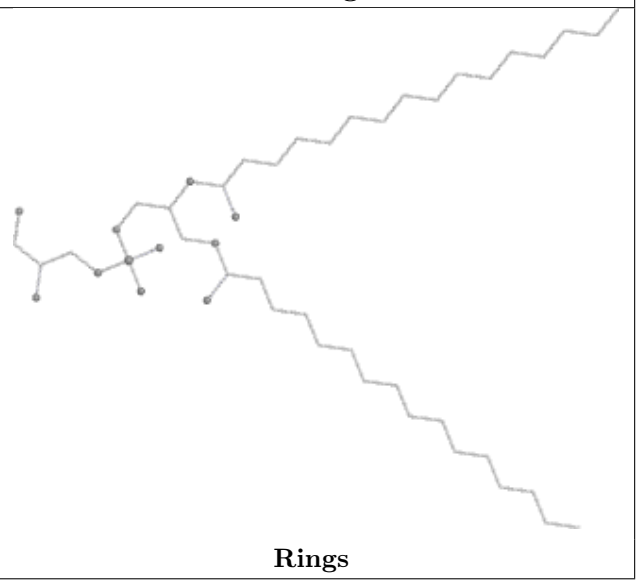
Bond lengths



Bond angles



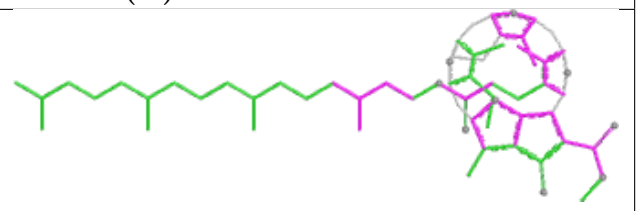
Torsions



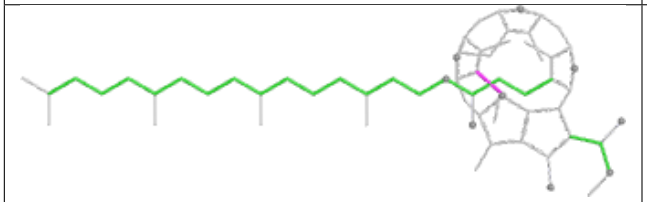
Rings

Ligand PHO a 418 (B)

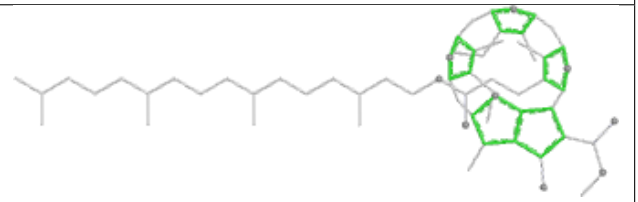
Bond lengths



Bond angles

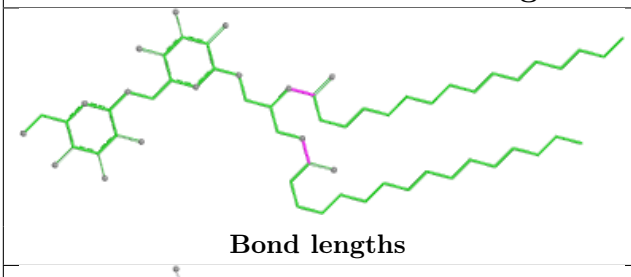


Torsions

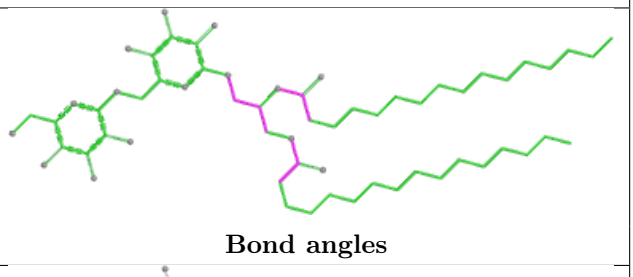


Rings

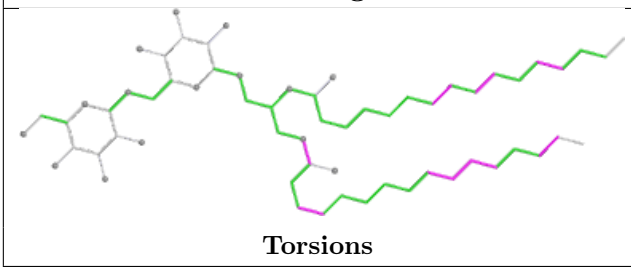
Ligand DGD C 518



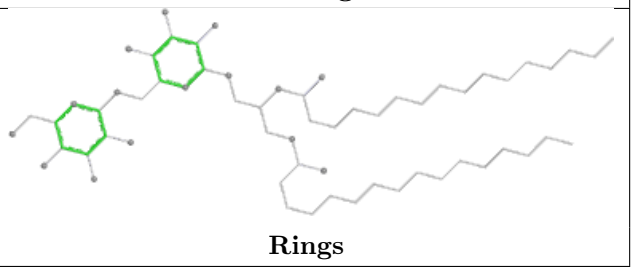
Bond lengths



Bond angles

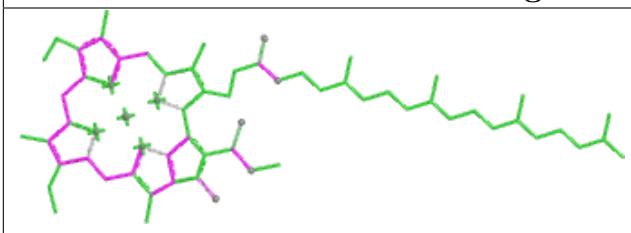


Torsions

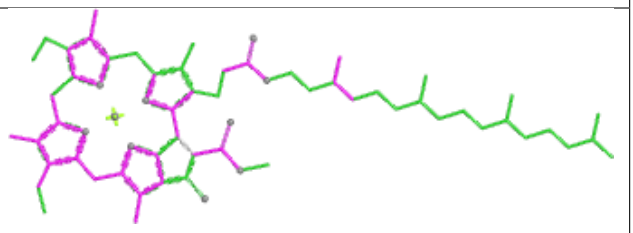


Rings

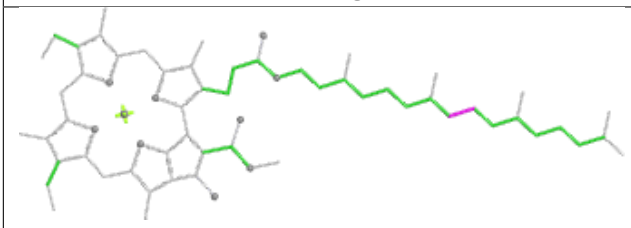
Ligand CLA C 503



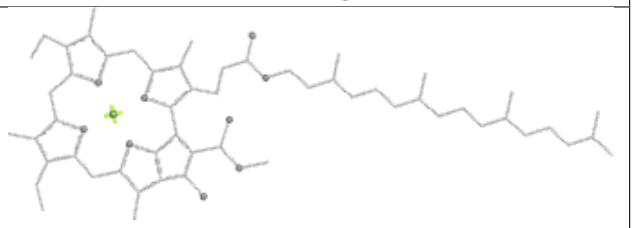
Bond lengths



Bond angles

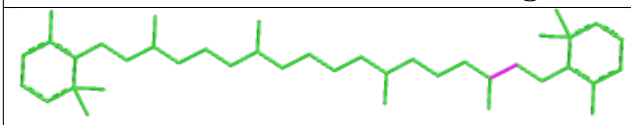


Torsions

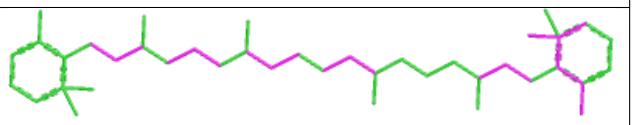


Rings

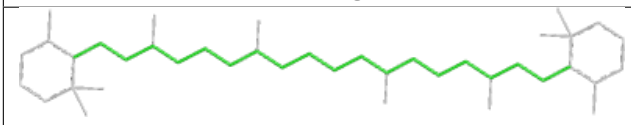
Ligand BCR H 101



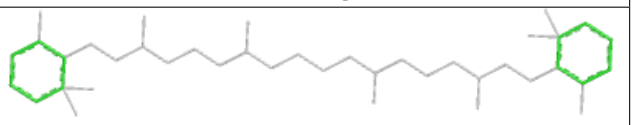
Bond lengths



Bond angles

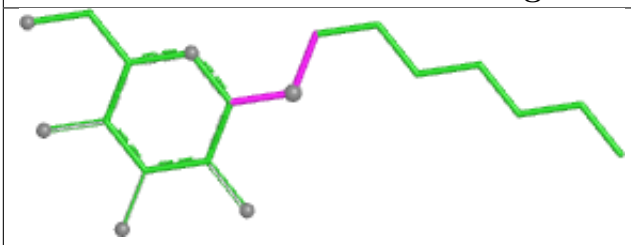


Torsions



Rings

Ligand HTG b 607



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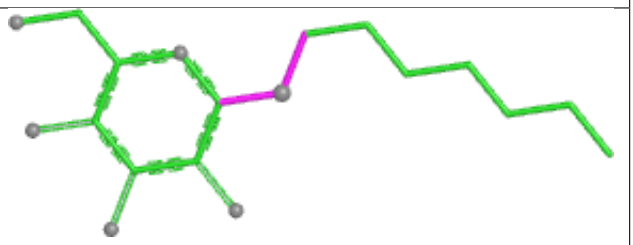
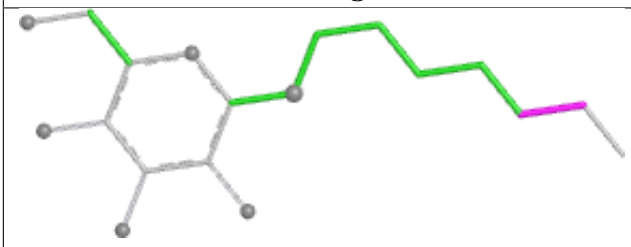


Bond angles



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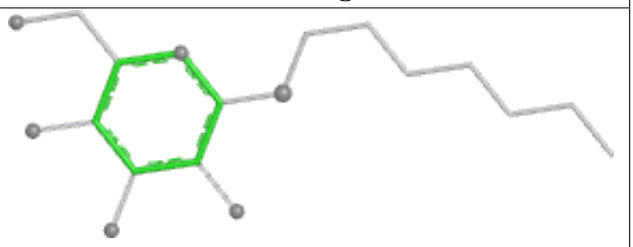
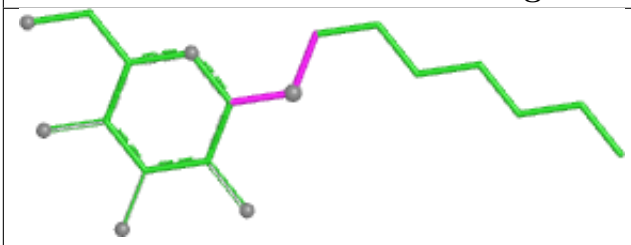
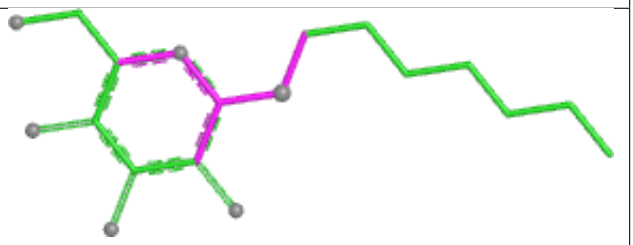


Rings

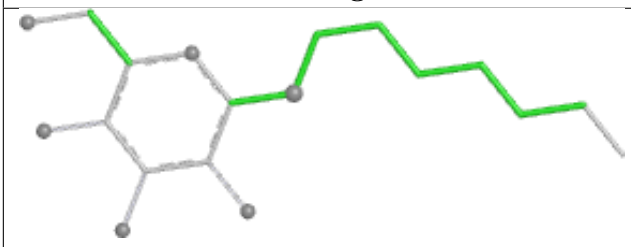
Ligand HTG b 608



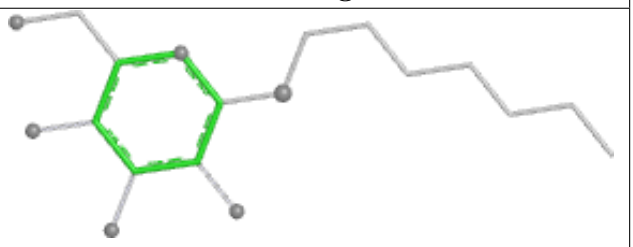
Bond lengths



Bond angles

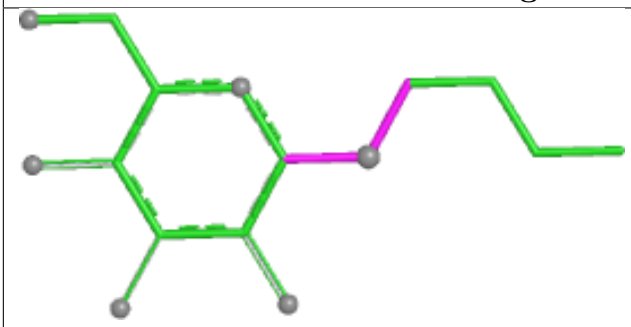


Torsions



Rings

Ligand HTG D 412



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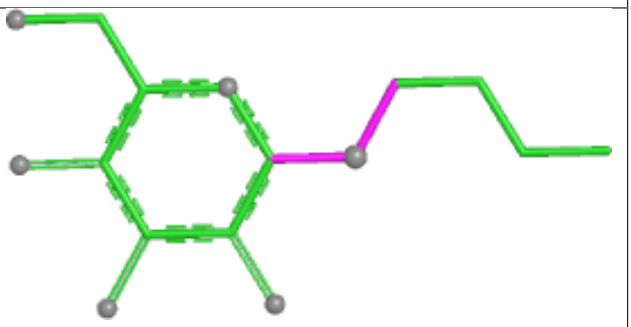
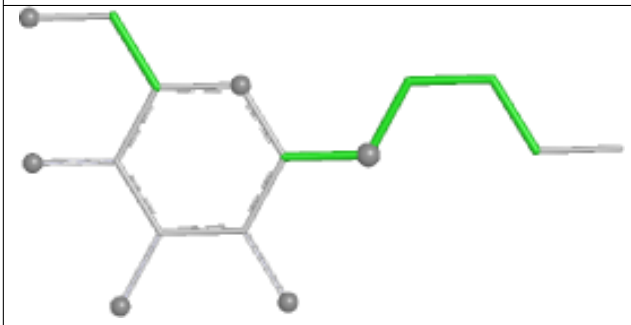
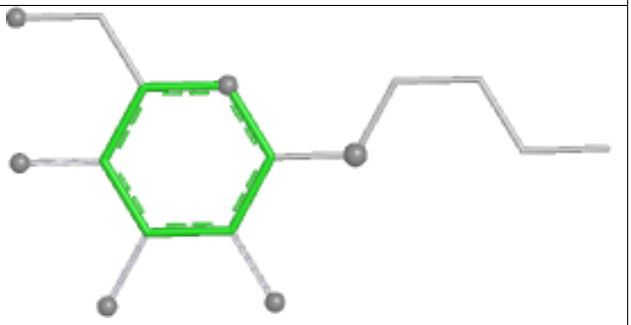


Bond angles

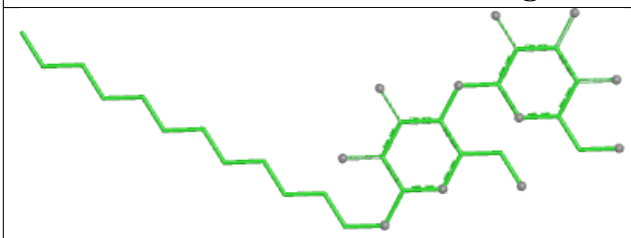


Torsions



Rings

Ligand LMT C 521



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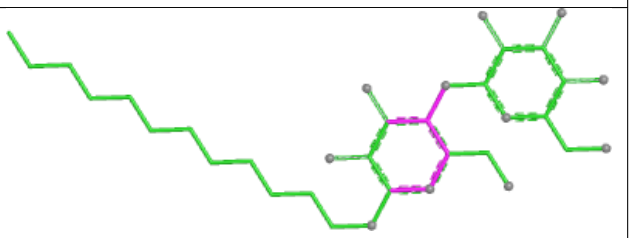
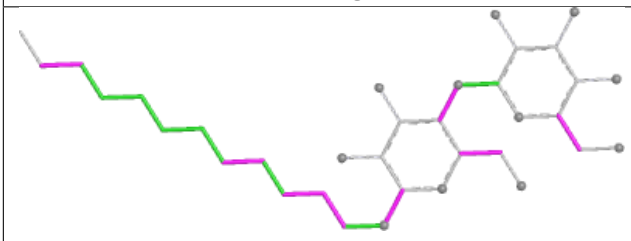
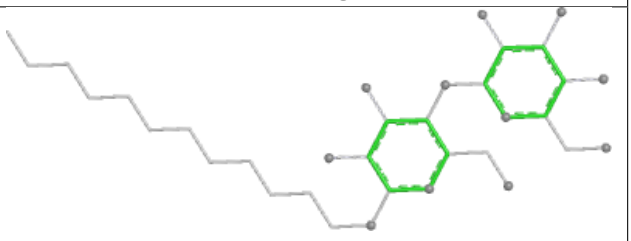


Bond angles

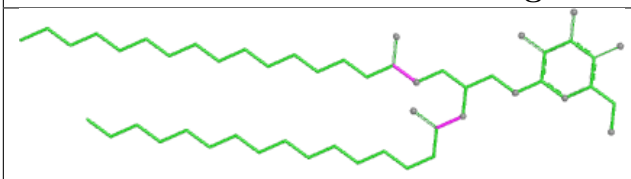


Torsions



Rings

Ligand LMG c 524



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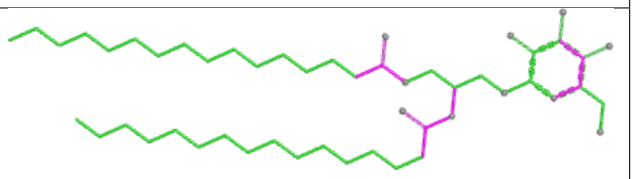
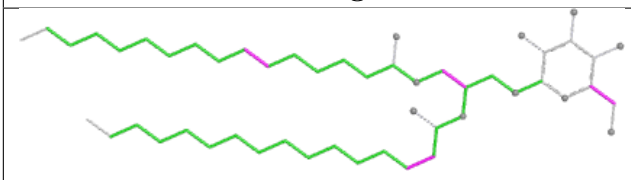
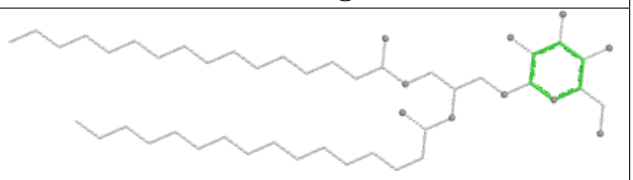


Bond angles

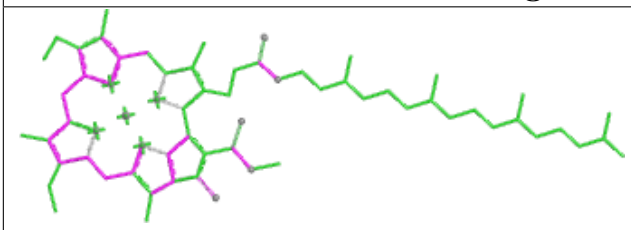


Torsions



Rings

Ligand CLA C 501



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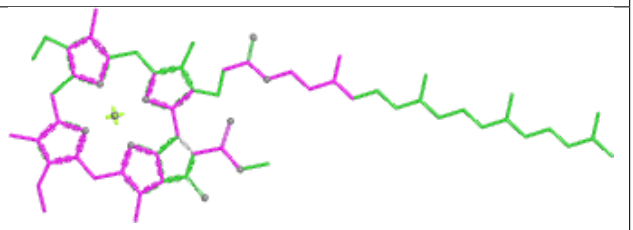
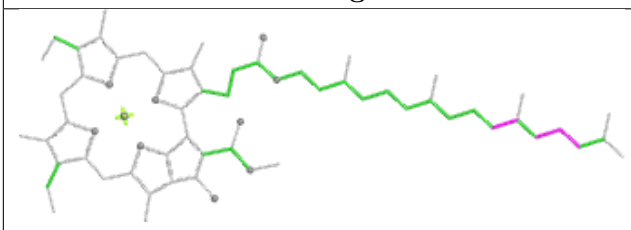
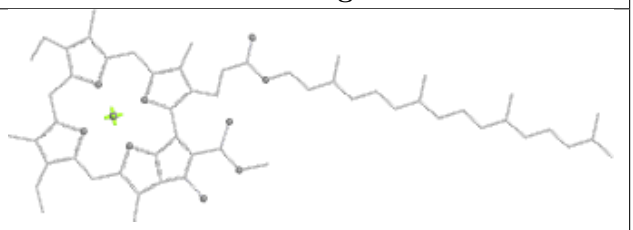


Bond angles

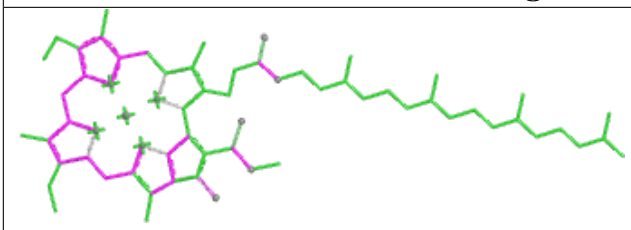


Torsions

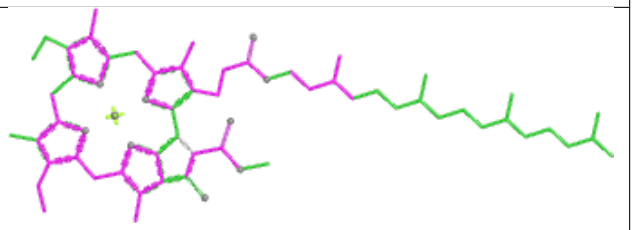


Rings

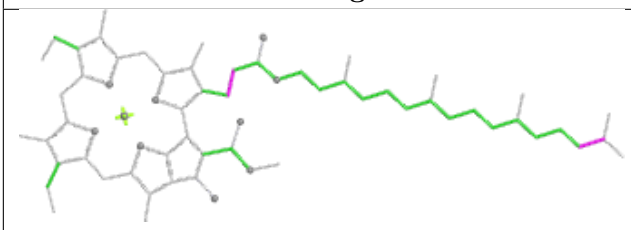
Ligand CLA B 611



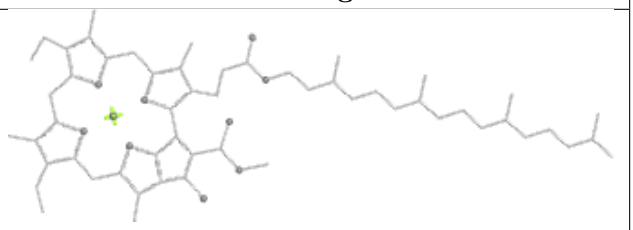
Bond lengths



Bond angles

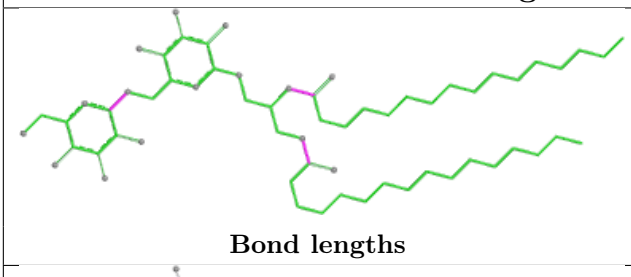


Torsions



Rings

Ligand DGD H 102



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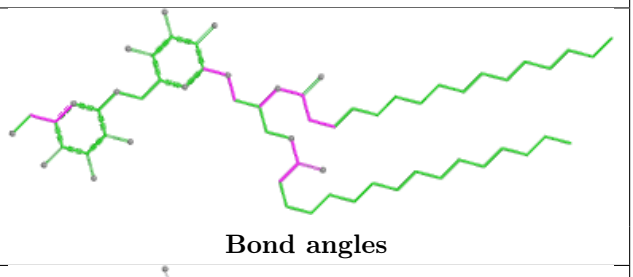
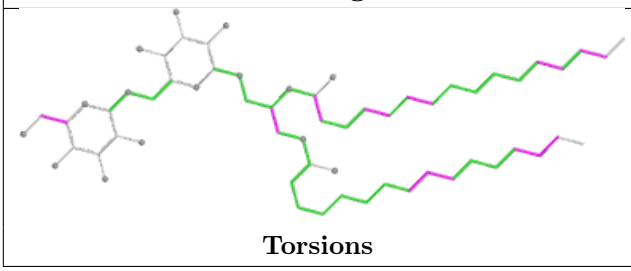
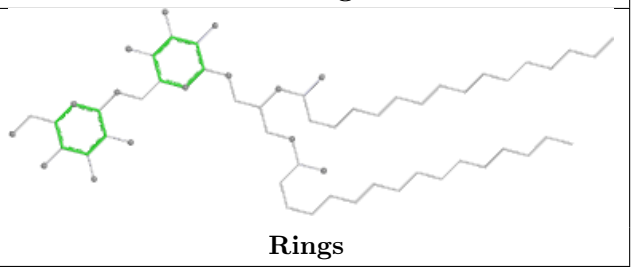


Bond angles

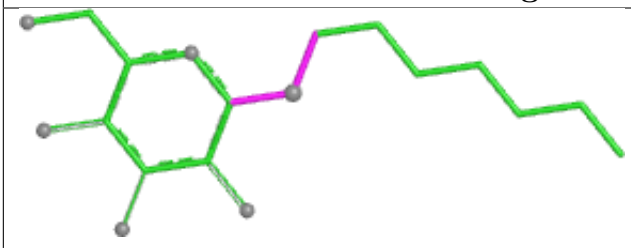


Torsions



Rings

Ligand HTG C 522



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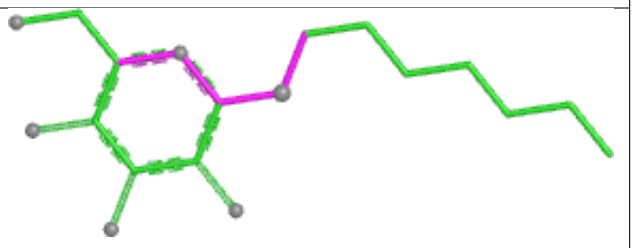
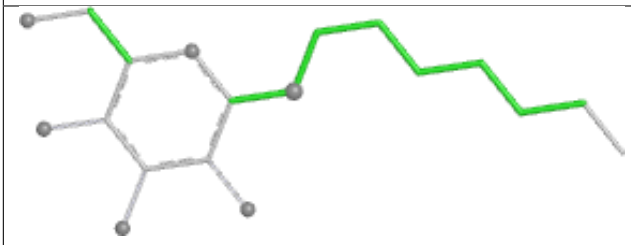
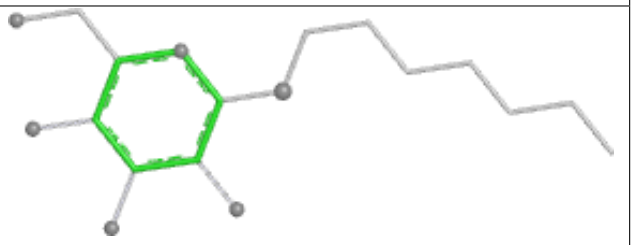


Bond angles

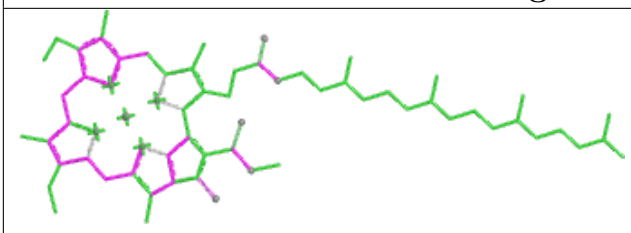


Torsions



Rings

Ligand CLA c 517



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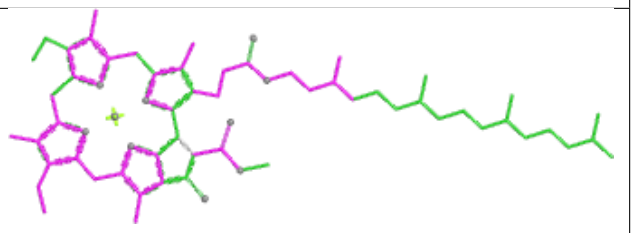
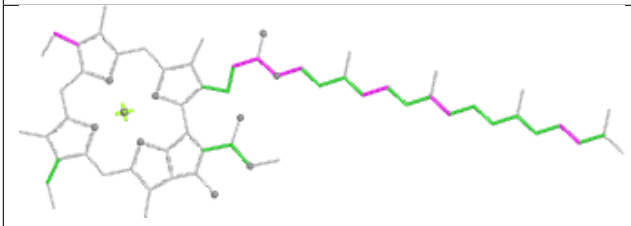
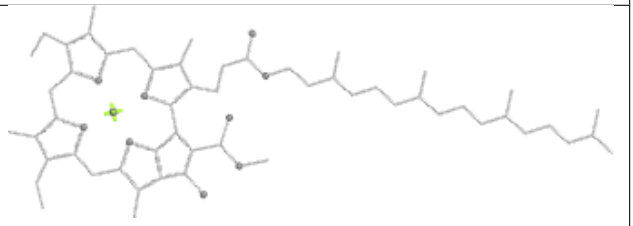


Bond angles

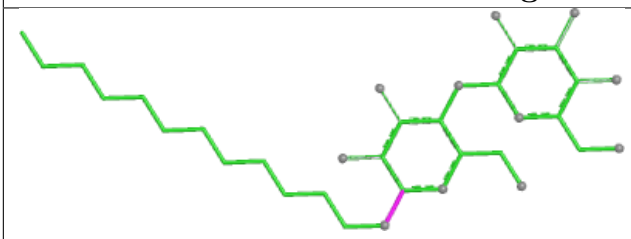


Torsions

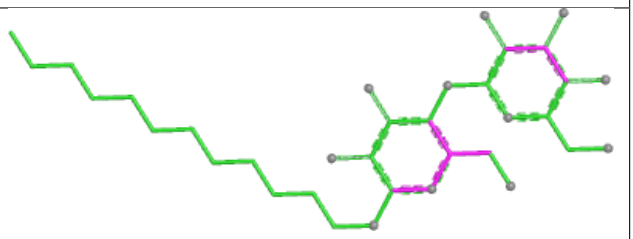


Rings

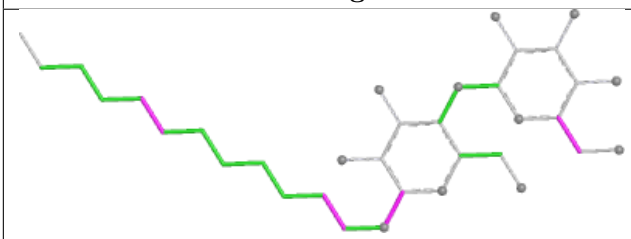
Ligand LMT A 417



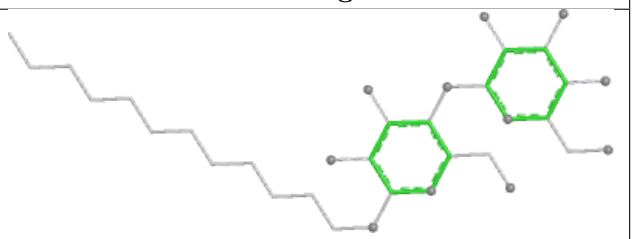
Bond lengths



Bond angles

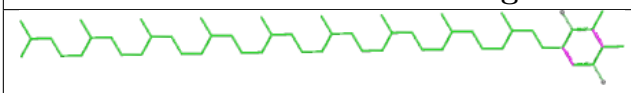


Torsions

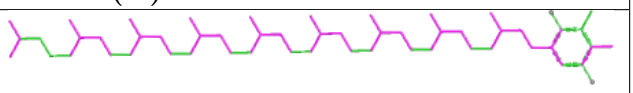


Rings

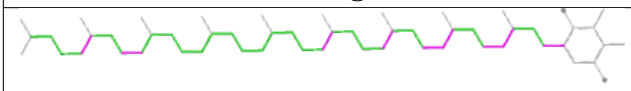
Ligand PL9 a 415 (B)



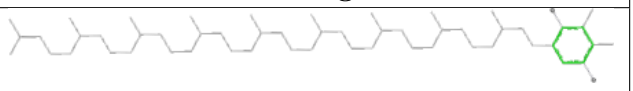
Bond lengths



Bond angles

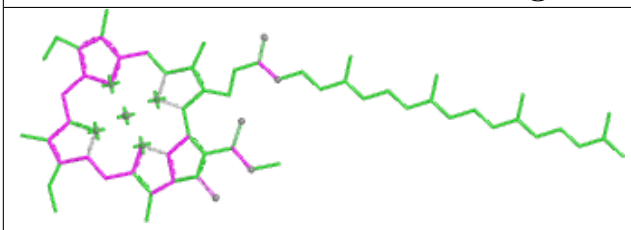


Torsions

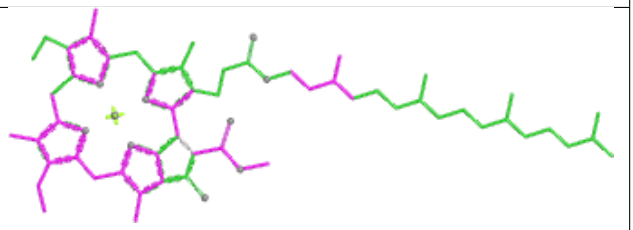


Rings

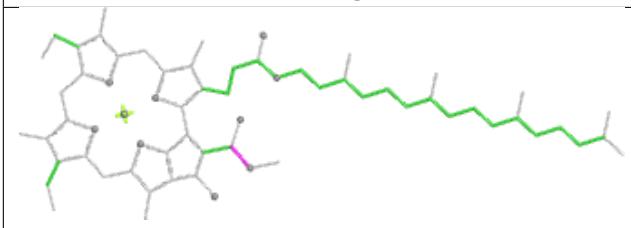
Ligand CLA c 510



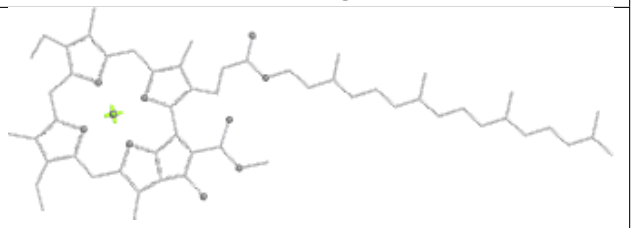
Bond lengths



Bond angles

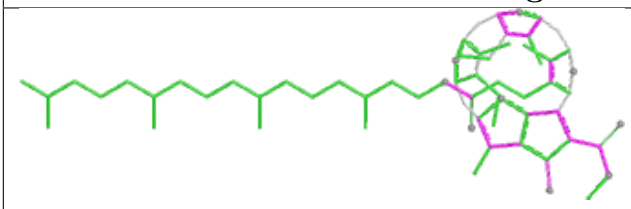


Torsions



Rings

Ligand PHO a 411



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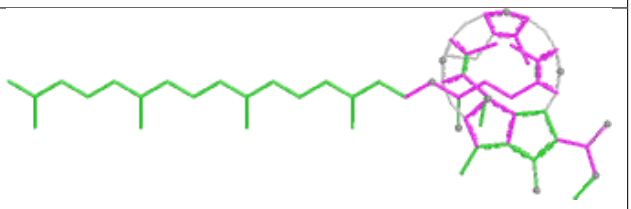
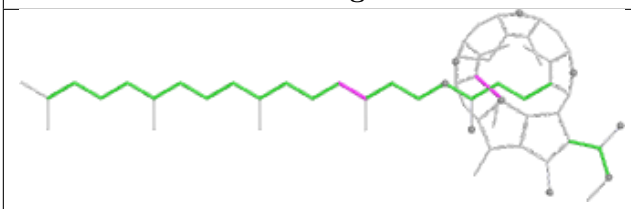


Bond angles



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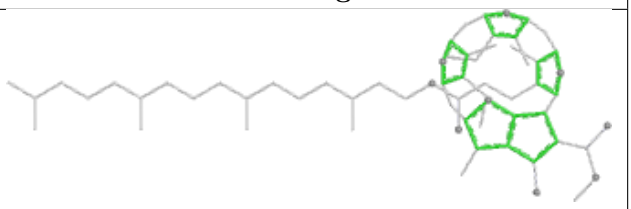
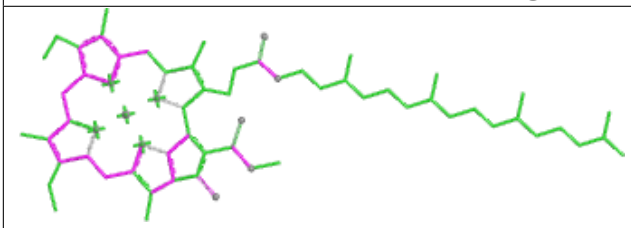


Rings

Ligand CLA B 607



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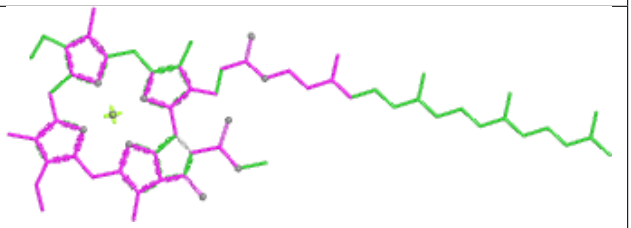
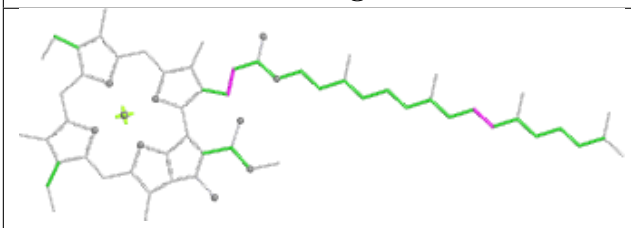


Bond angles



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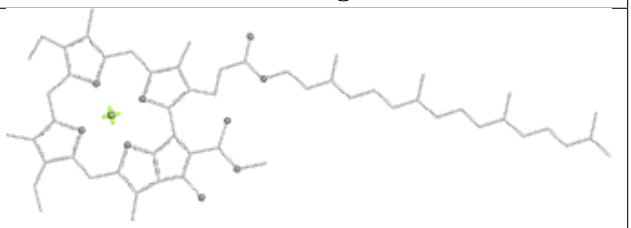
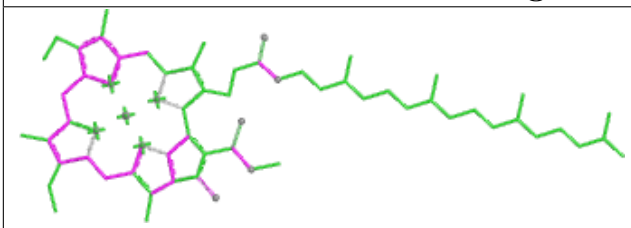


Rings

Ligand CLA b 617



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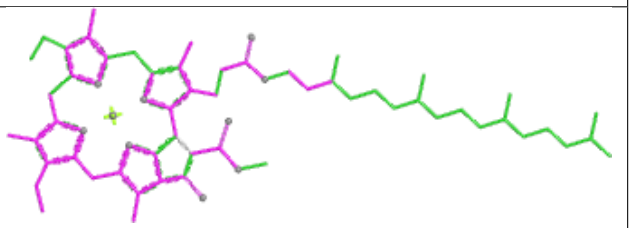
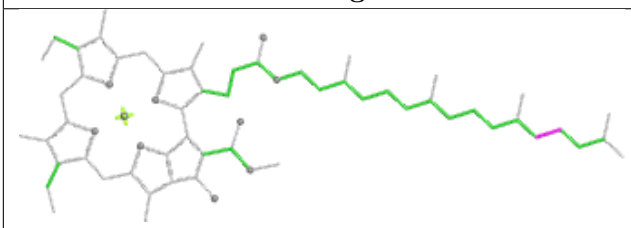


Bond angles



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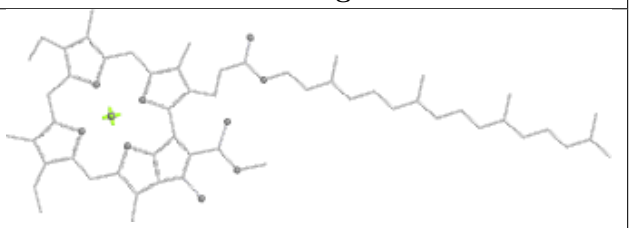
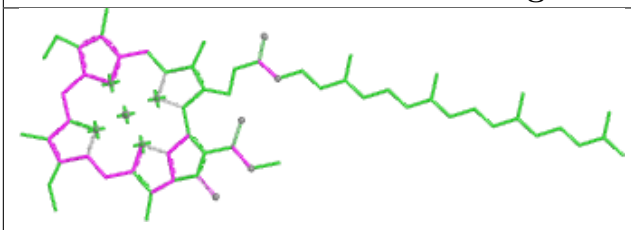


Rings

Ligand CLA b 612



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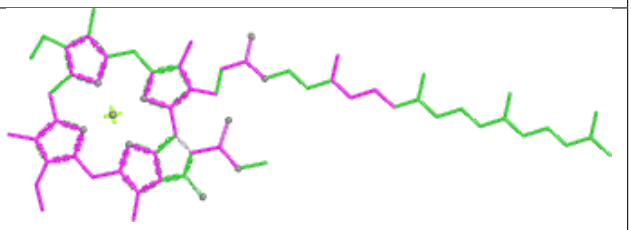
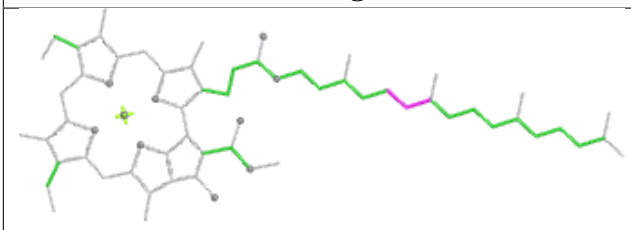


Bond angles



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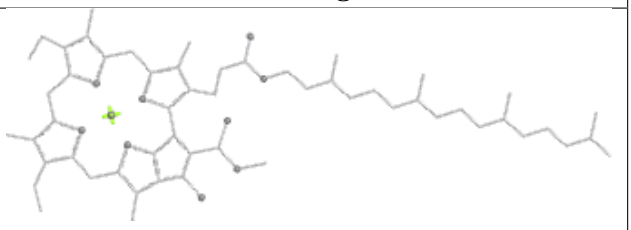
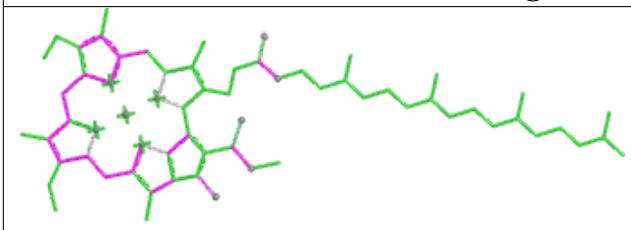


Rings

Ligand CLA B 614



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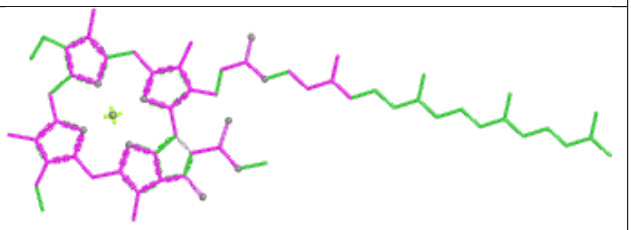
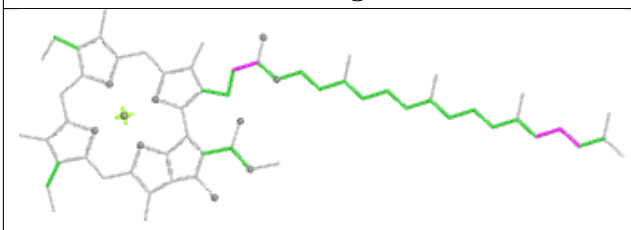


Bond angles



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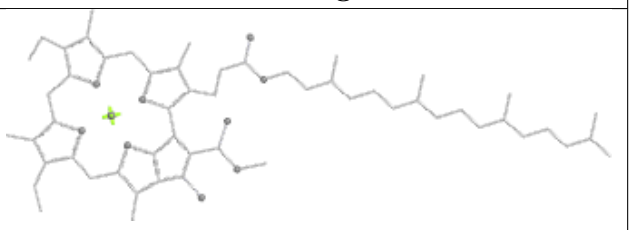
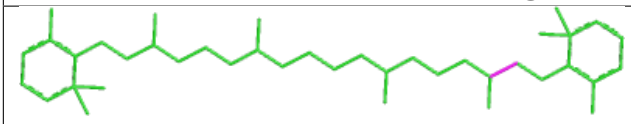


Rings

Ligand BCR A 411



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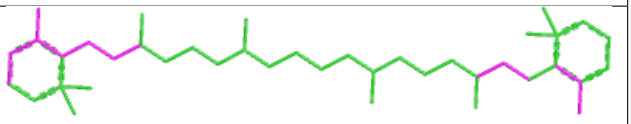
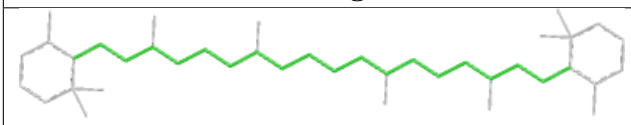
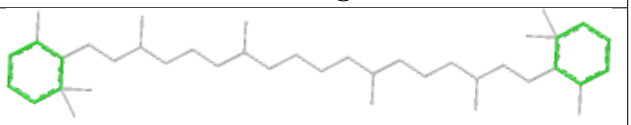


Bond angles

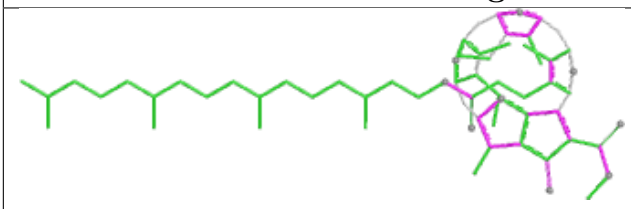


Torsions



Rings

Ligand PHO A 409 (A)



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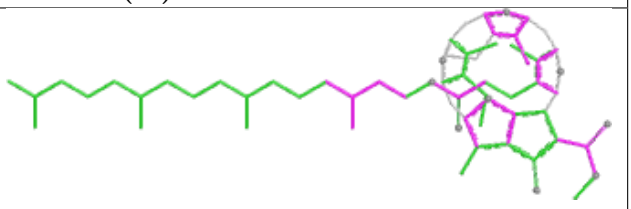
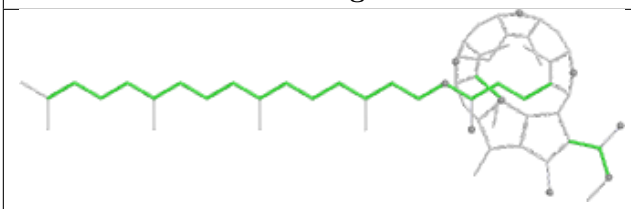
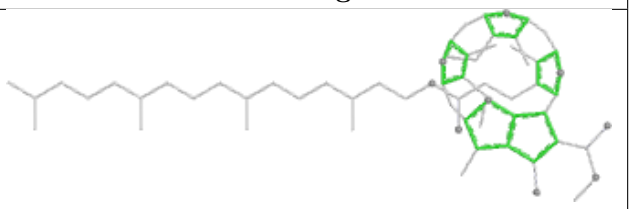


Bond angles

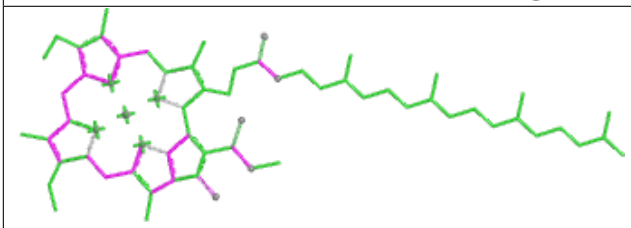


Torsions



Rings

Ligand CLA b 616



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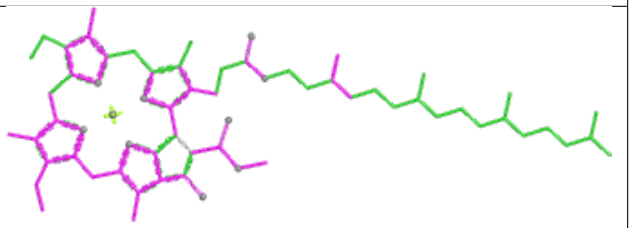
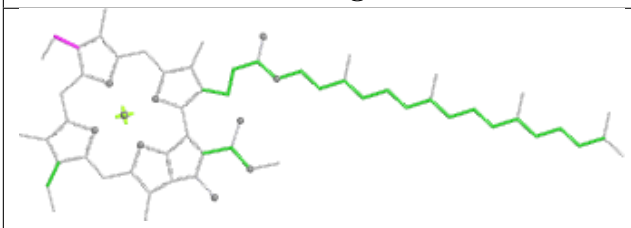
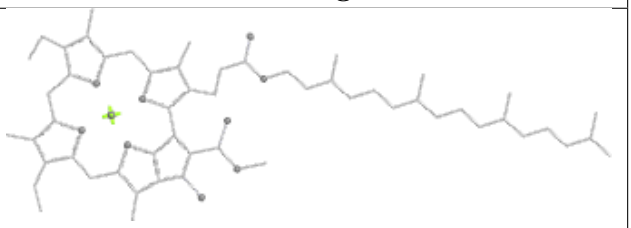


Bond angles

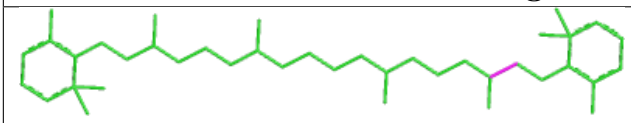


Torsions



Rings

Ligand BCR b 626



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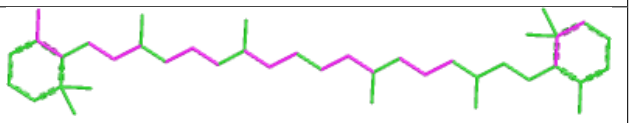
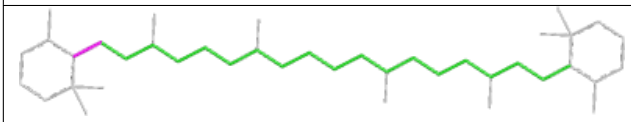
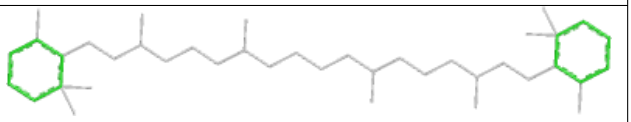


Bond angles

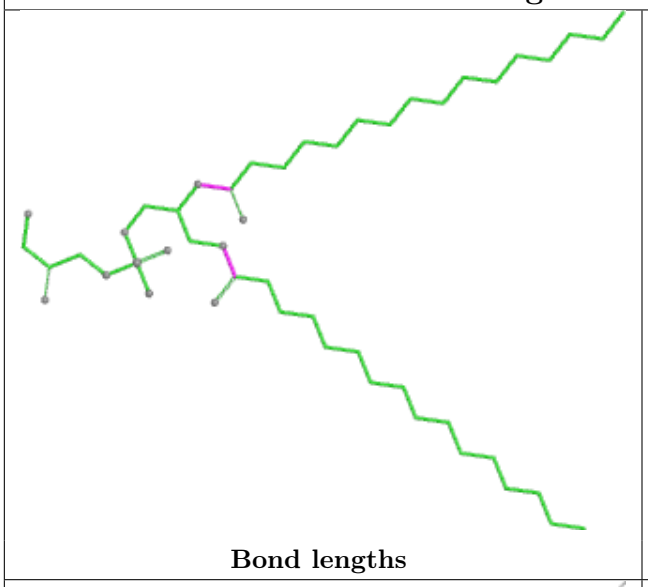


Torsions



Rings

Ligand LHG L 101



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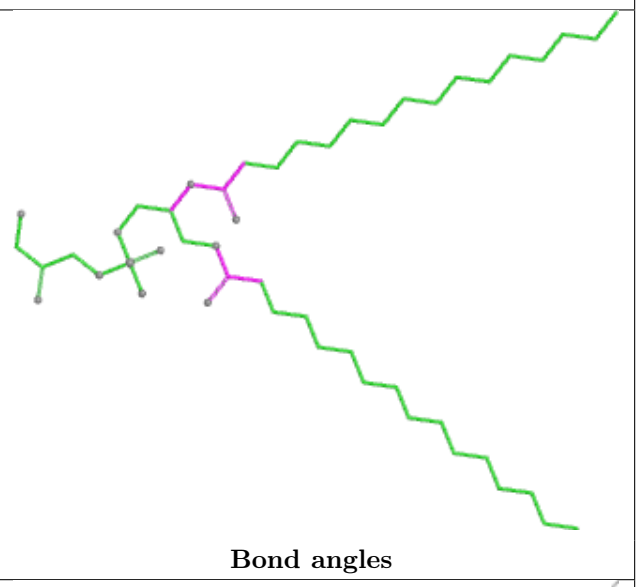
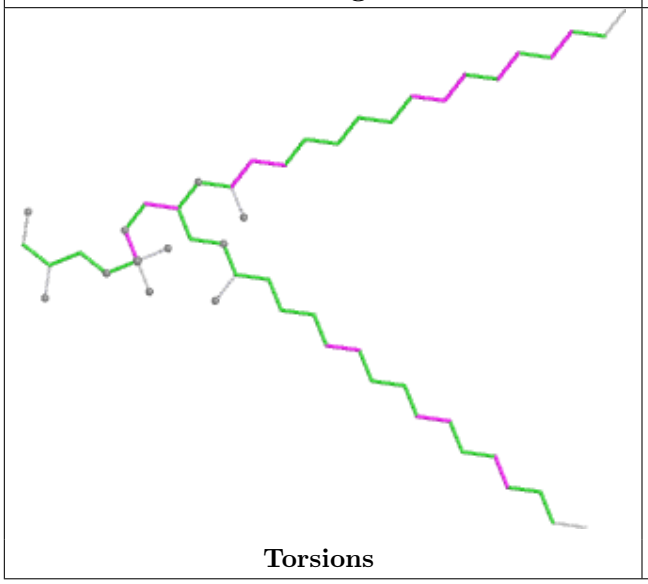
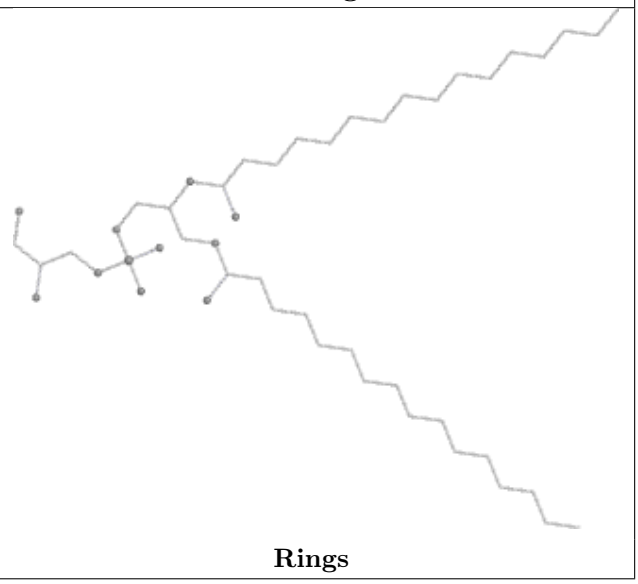


Bond angles

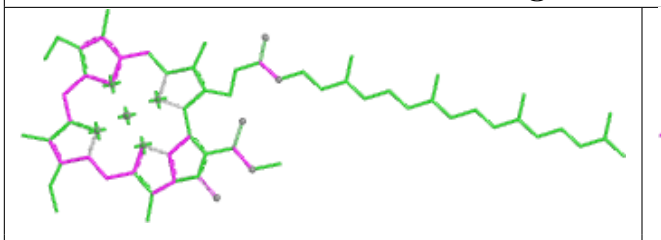


Torsions



Rings

Ligand CLA d 402



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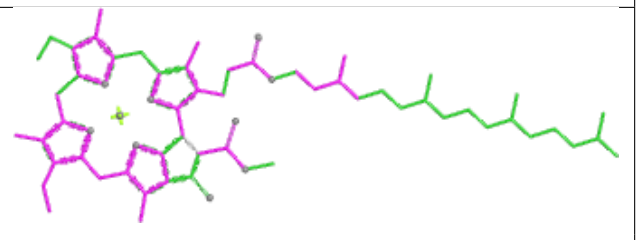
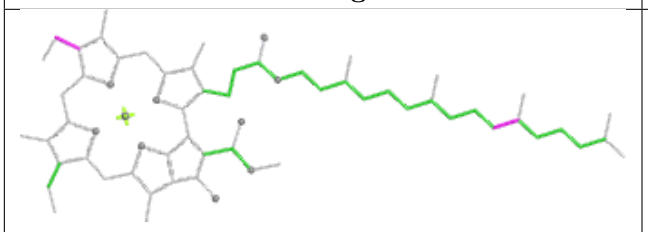
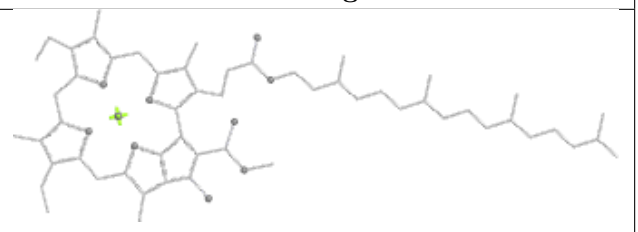


Bond angles

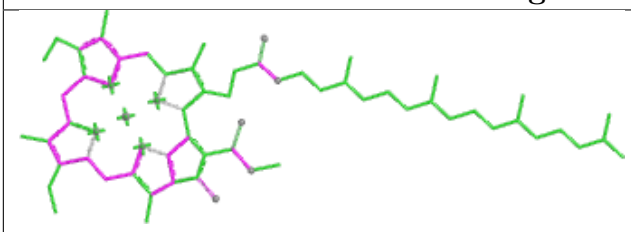


Torsions



Rings

Ligand CLA a 409



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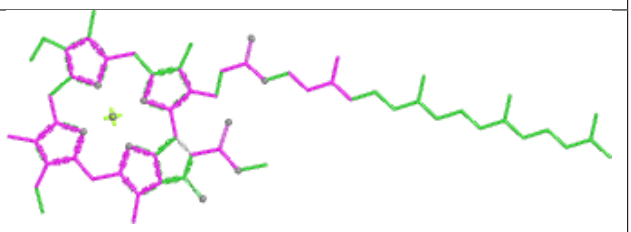
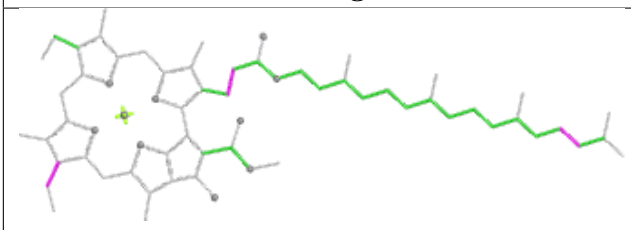


Bond angles



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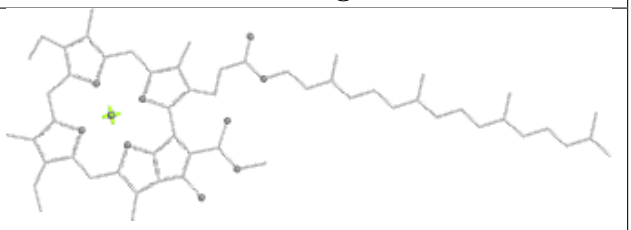
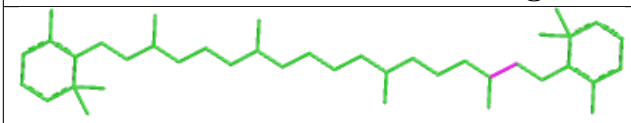


Rings

Ligand BCR b 627



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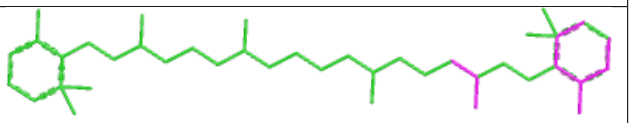
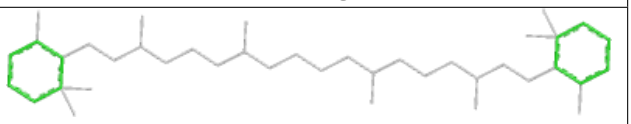


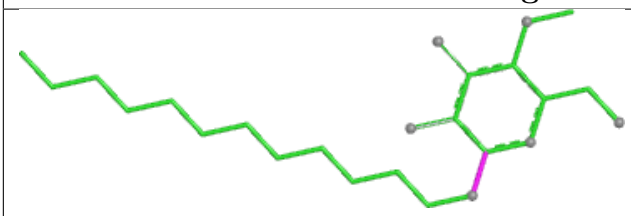
Bond angles

Torsions

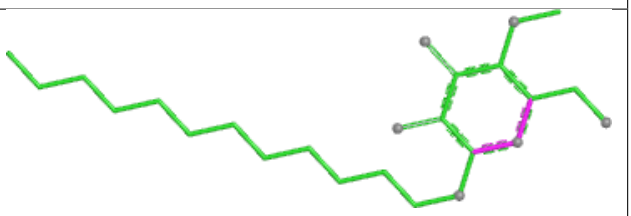


Rings

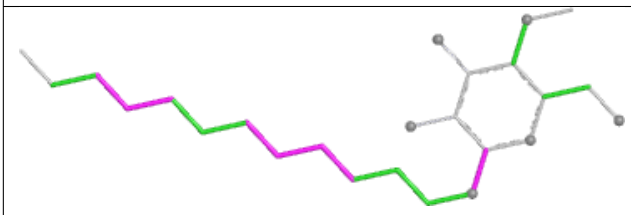
Ligand LMT B 635



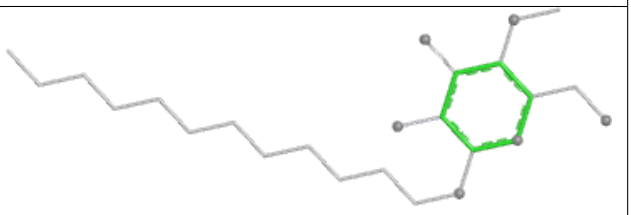
Bond lengths



Bond angles

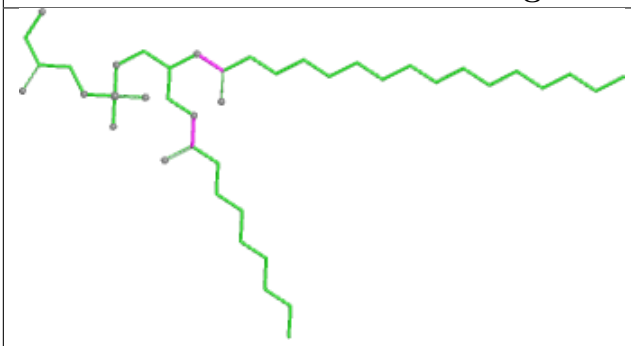


Torsions

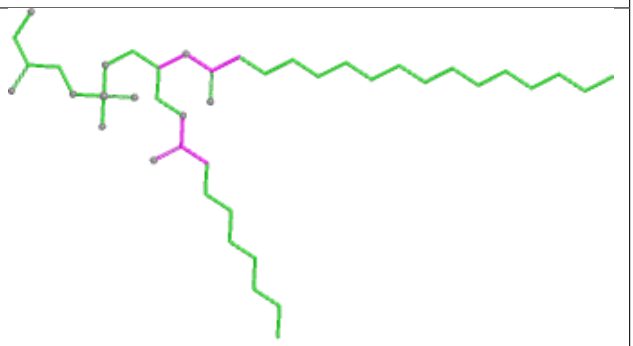


Rings

Ligand LHG E 101



Bond lengths



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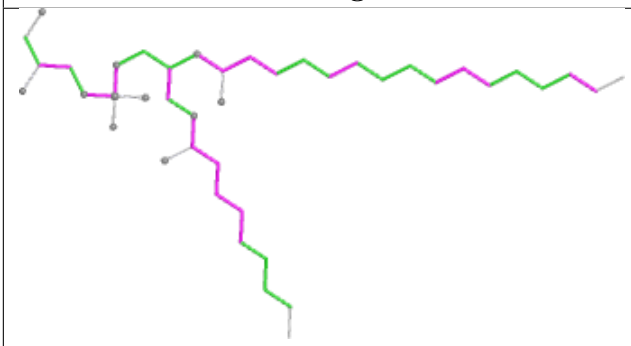
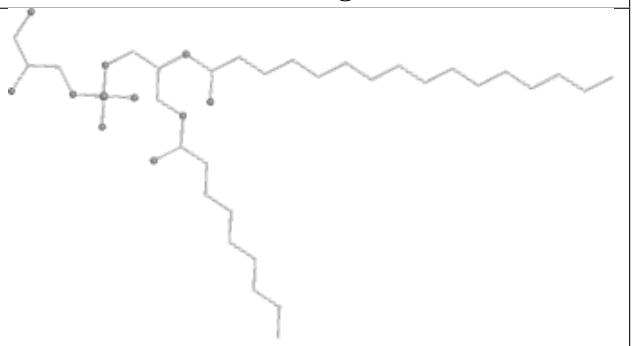


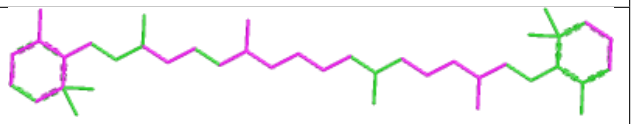
Torsions



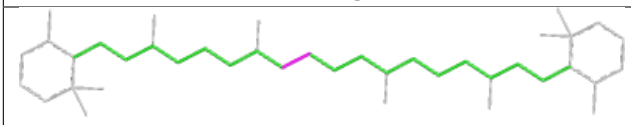
Rings

Ligand BCR t 101

Bond lengths



Bond angles



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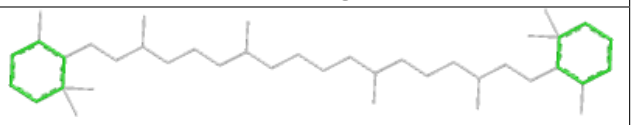
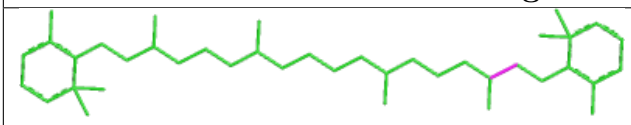


Rings

Ligand BCR C 515



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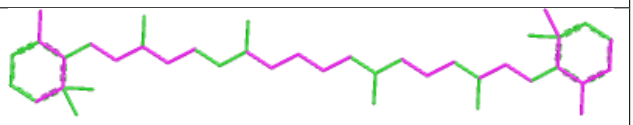
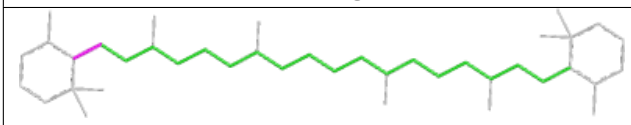


Bond angles



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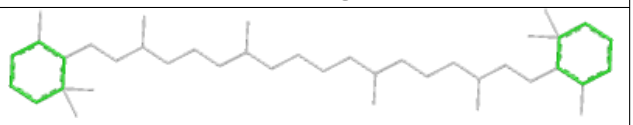
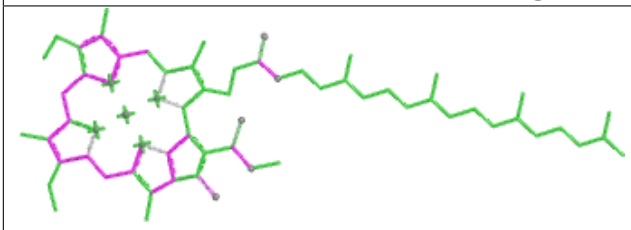


Rings

Ligand CLA c 514



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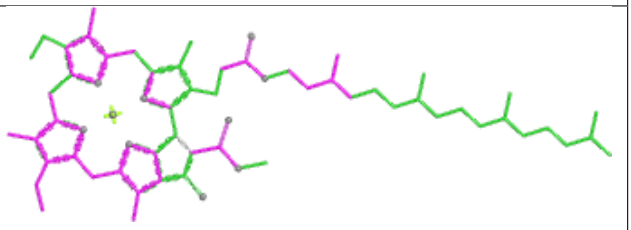
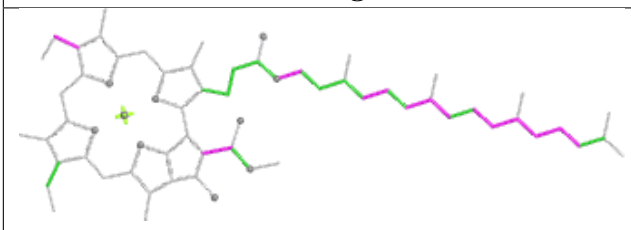


Bond angles



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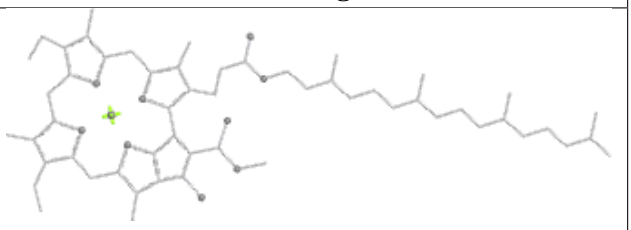
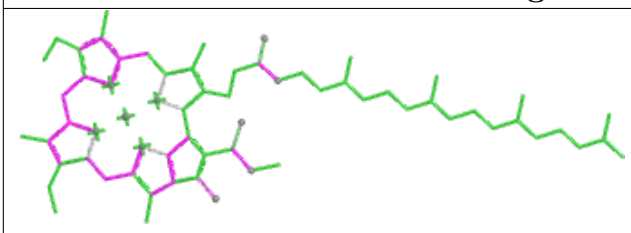


Rings

Ligand CLA d 401



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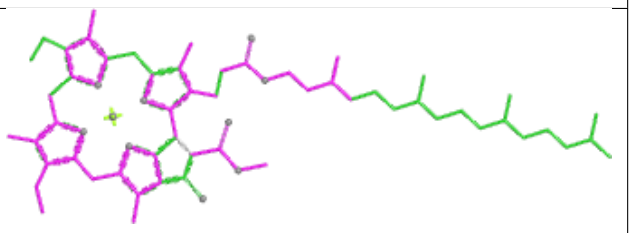
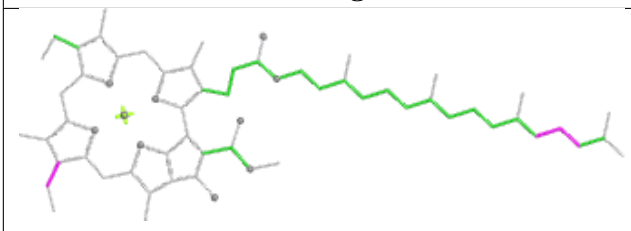


Bond angles



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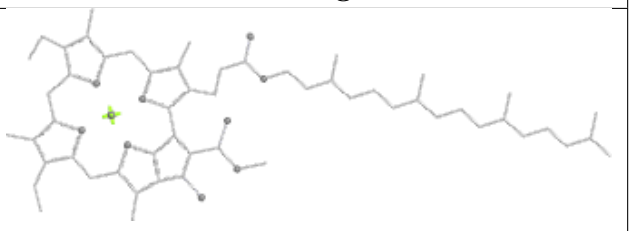
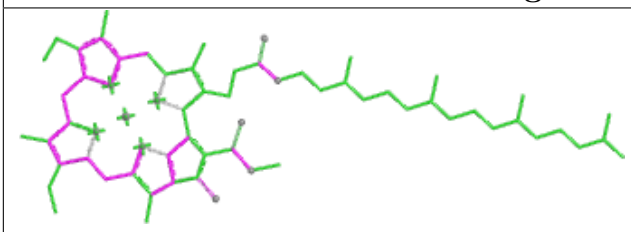


Rings

Ligand CLA B 609



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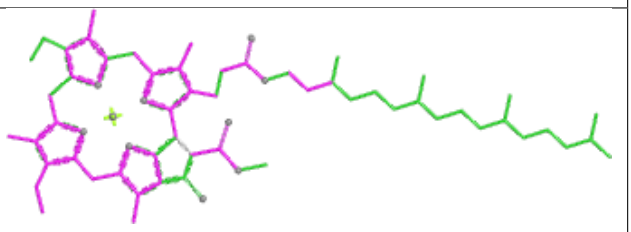
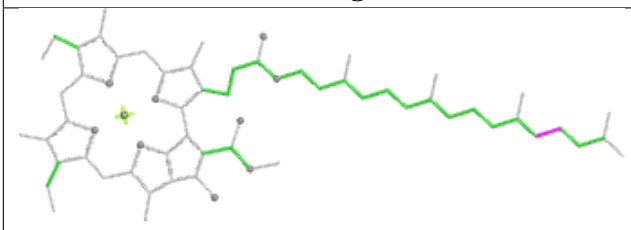


Bond angles



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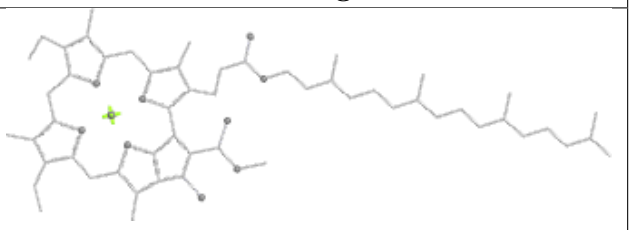
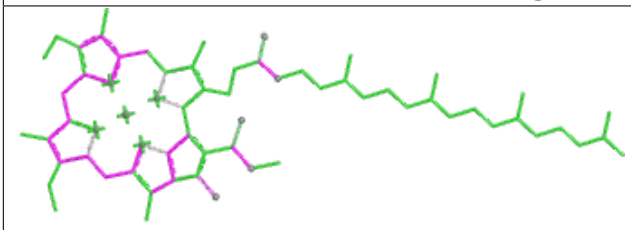


Rings

Ligand CLA c 509



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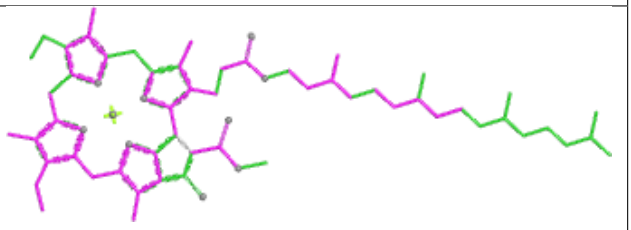
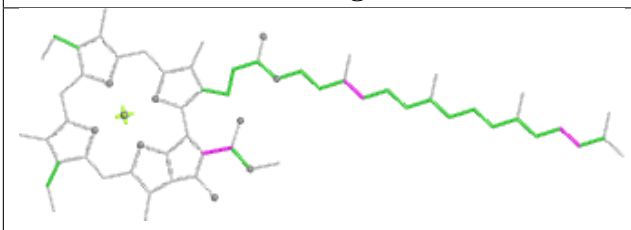


Bond angles



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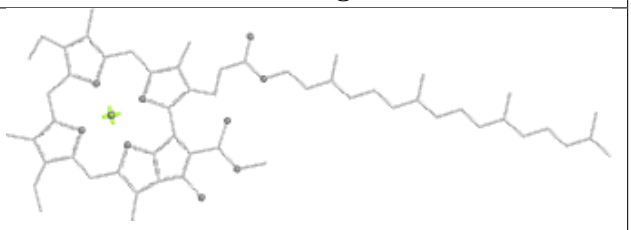
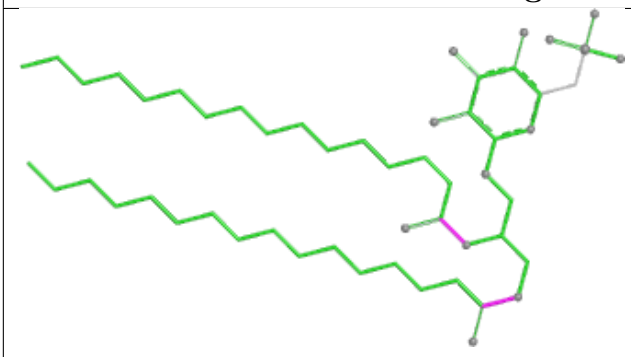


Rings

Ligand SQD B 621



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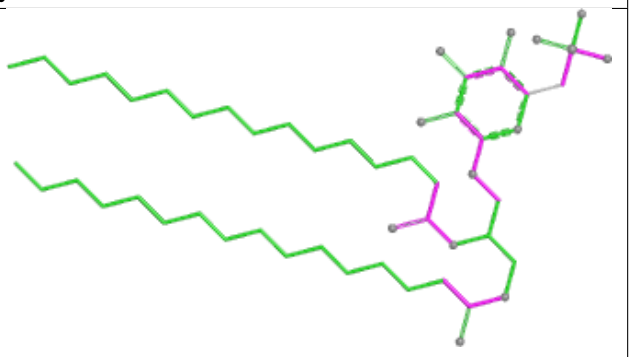
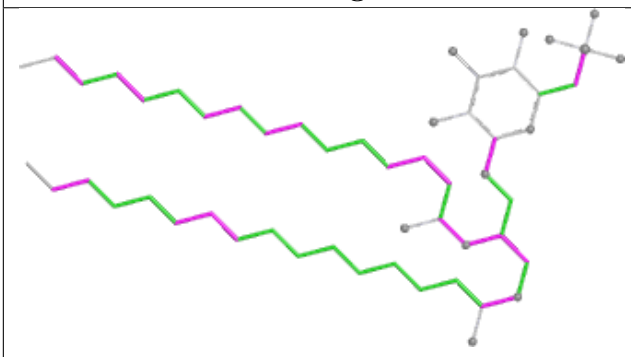
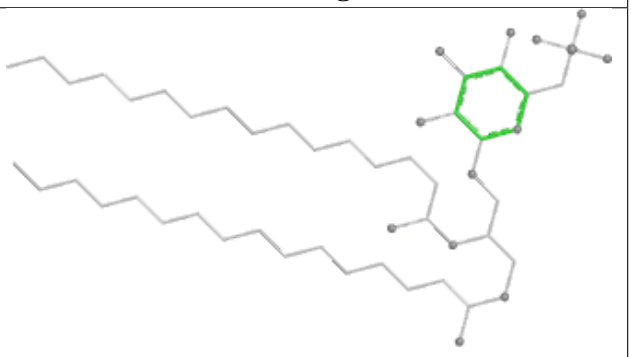


Bond angles

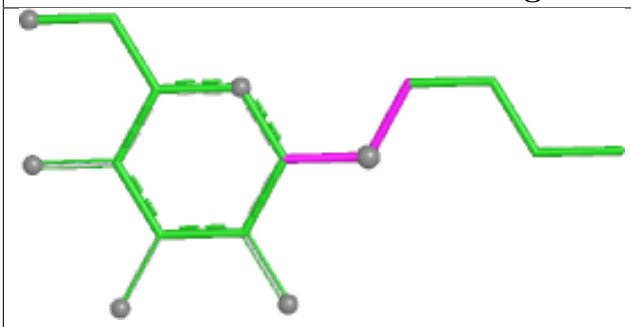


Torsions



Rings

Ligand HTG d 411



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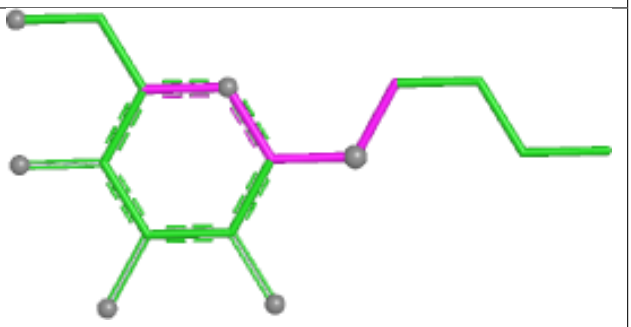
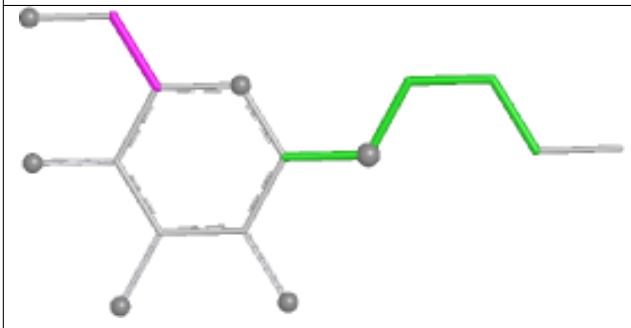
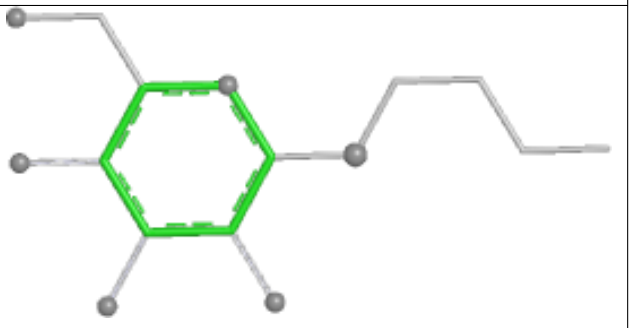


Bond angles

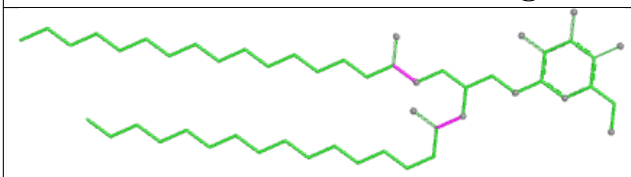


Torsions



Rings

Ligand LMG B 622



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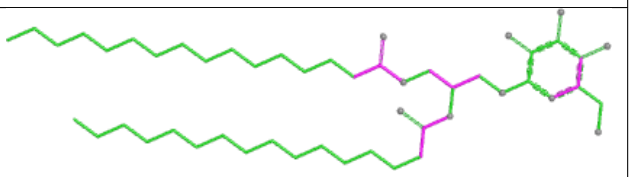
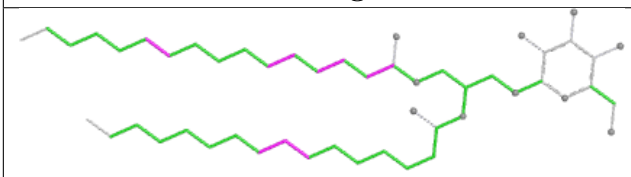


Bond angles



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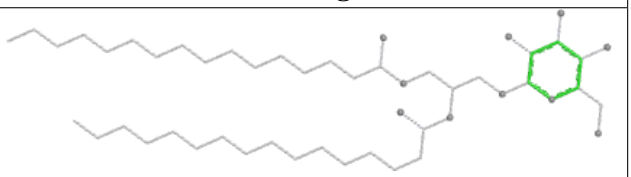
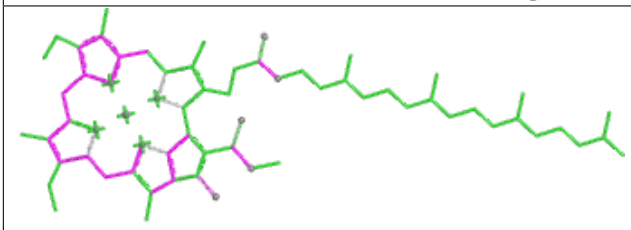


Rings

Ligand CLA C 512



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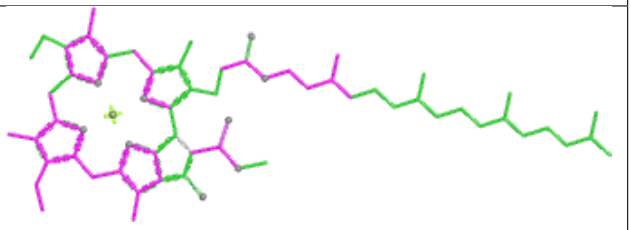
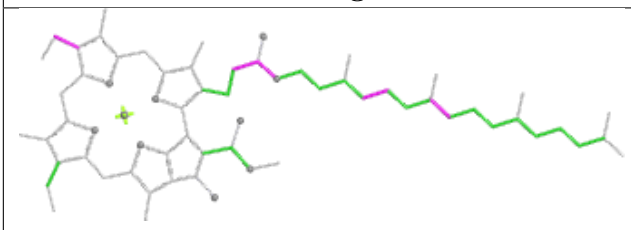
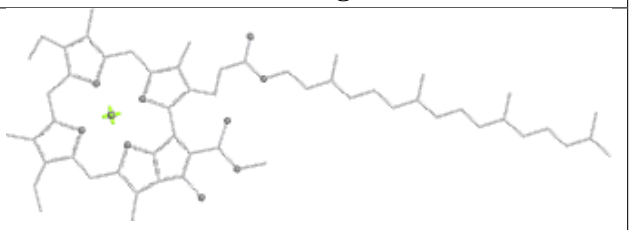


Bond angles

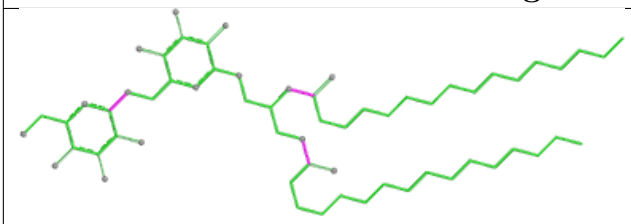


Torsions

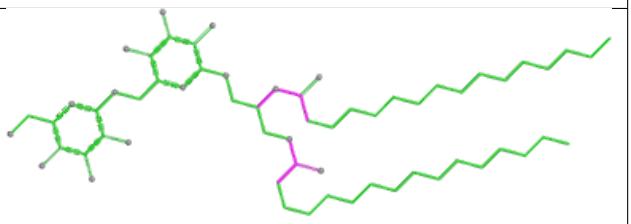


Rings

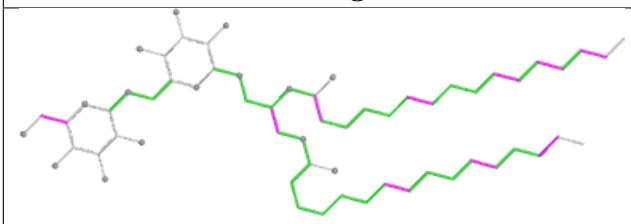
Ligand DGD h 102



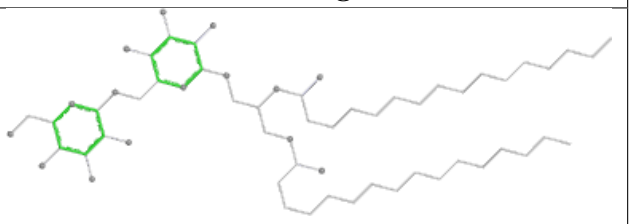
Bond lengths



Bond angles

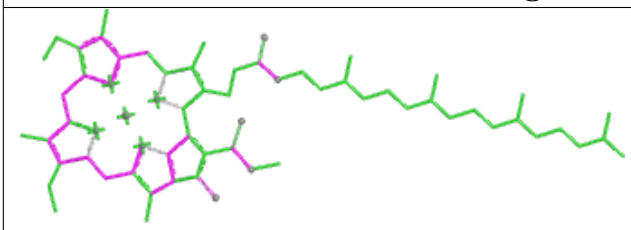


Torsions

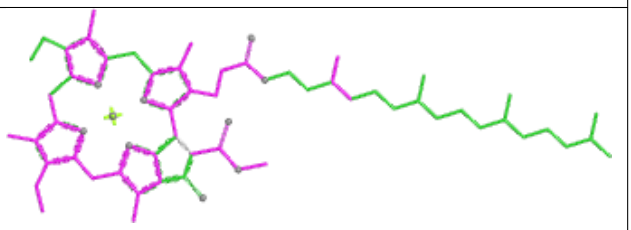


Rings

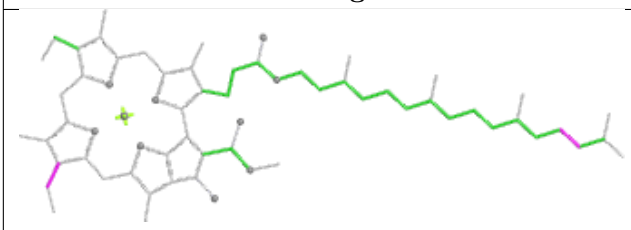
Ligand CLA A 406



Bond lengths



Bond angles



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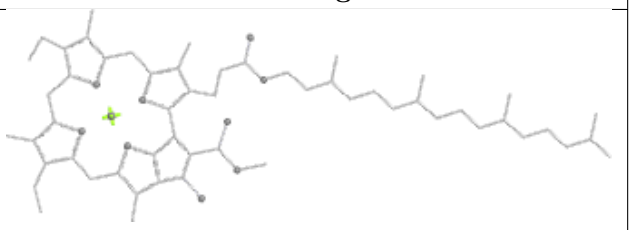
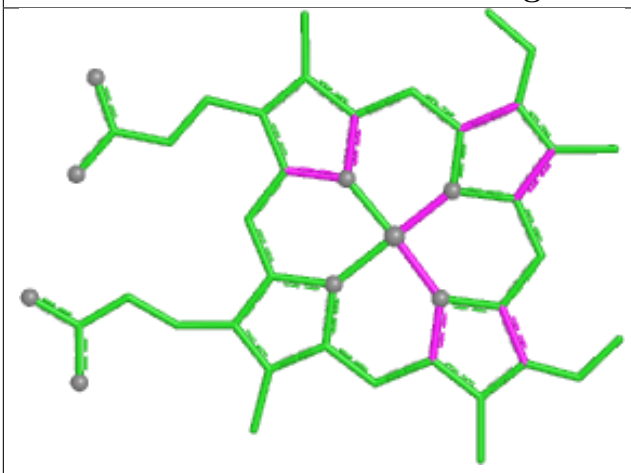
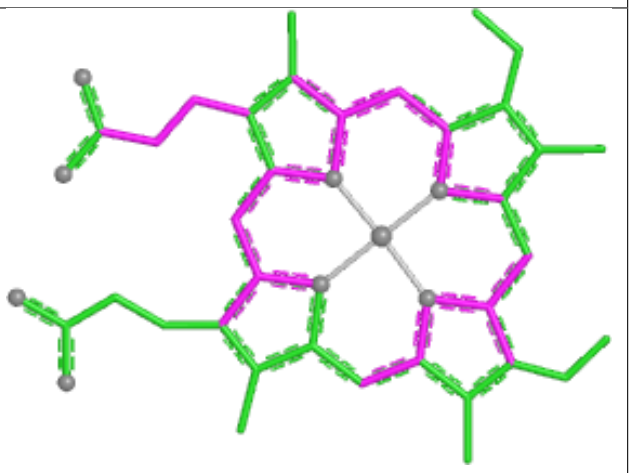


Rings

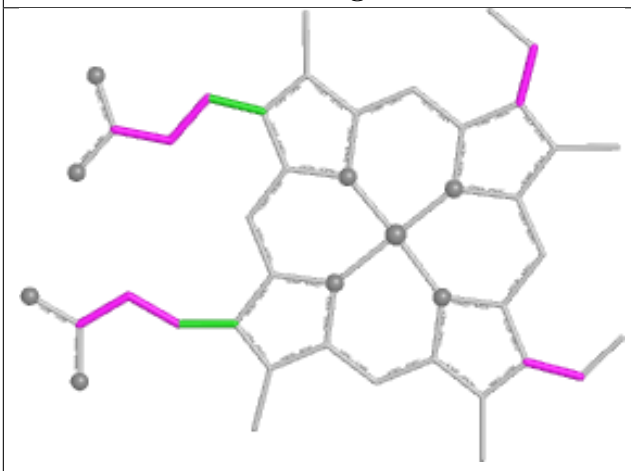
Ligand HEM e 103



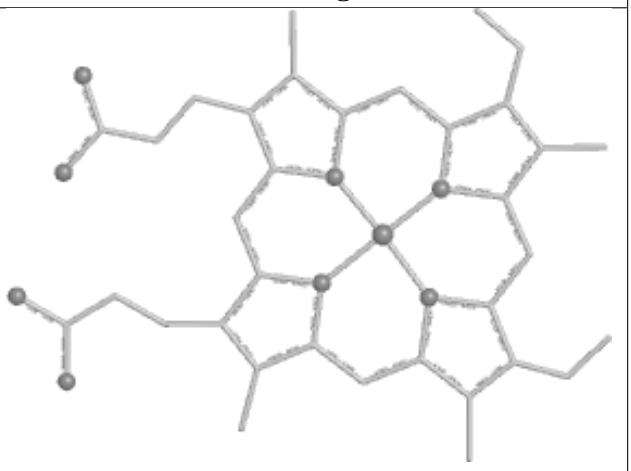
Bond lengths



Bond angles

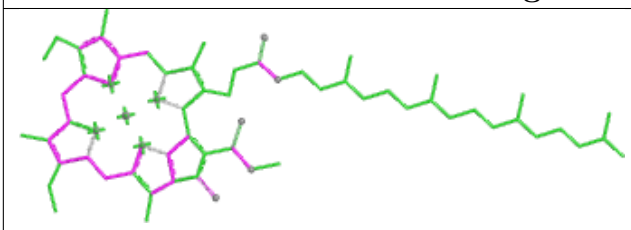


Torsions



Rings

Ligand CLA D 402



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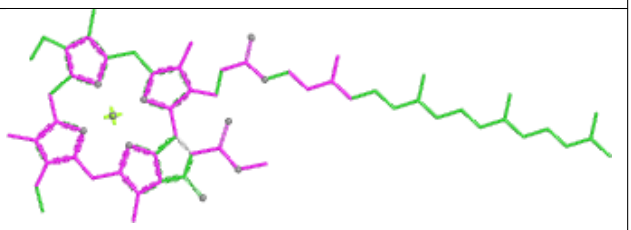
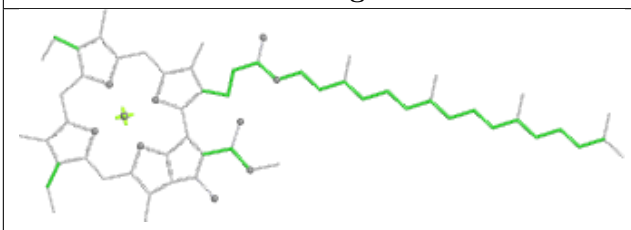
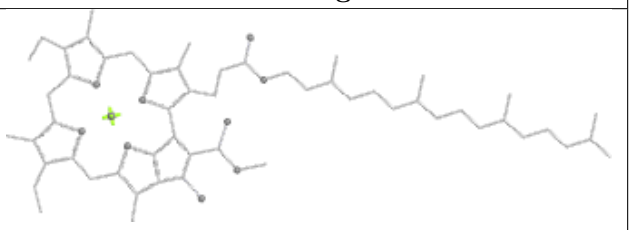


Bond angles

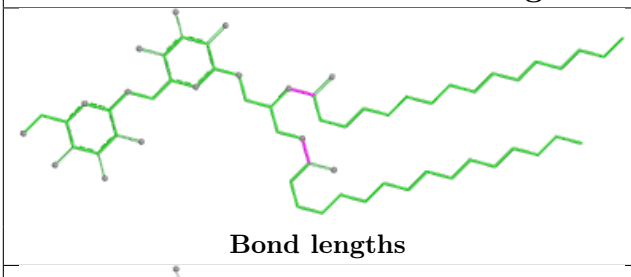


Torsions



Rings

Ligand DGD c 520



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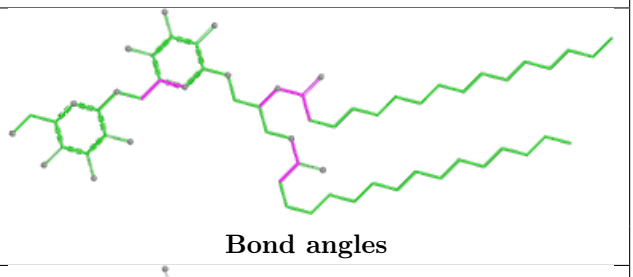
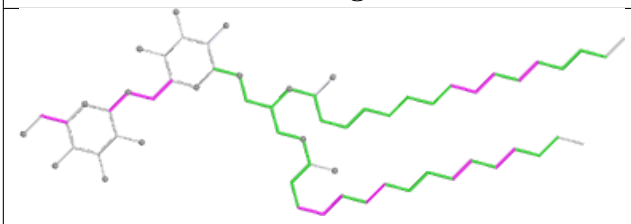


Bond angles



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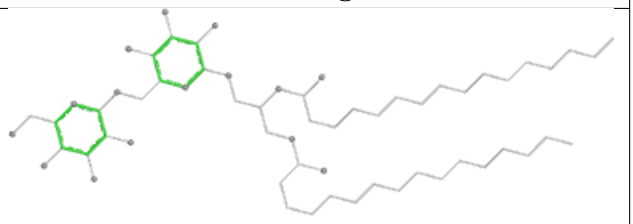
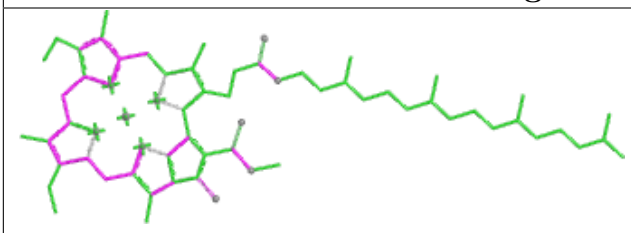


Rings

Ligand CLA B 612



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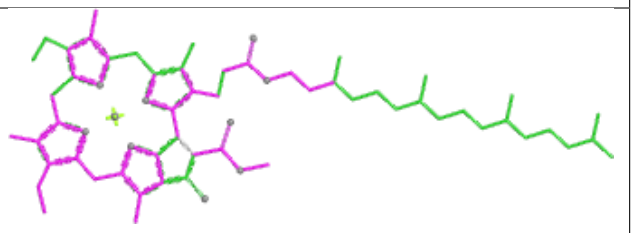
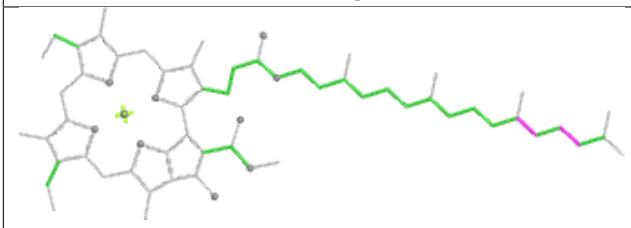
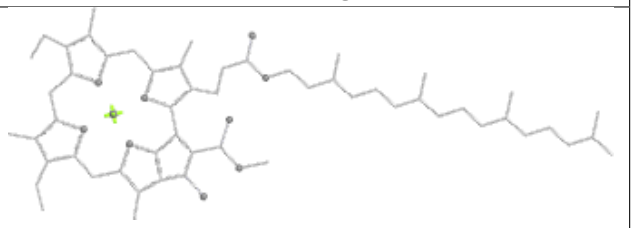


Bond angles

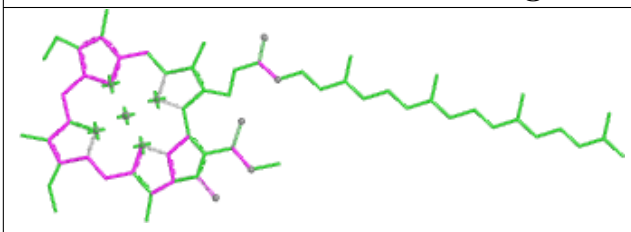


Torsions



Rings

Ligand CLA C 510



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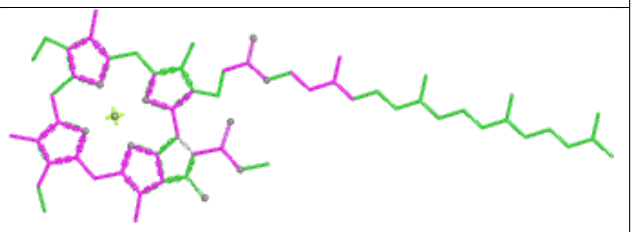
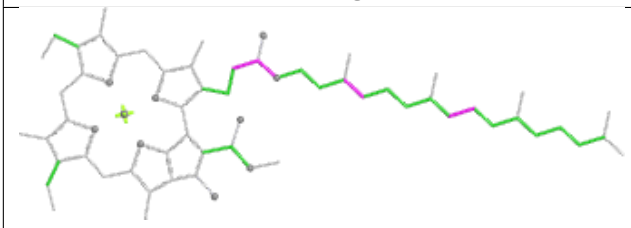
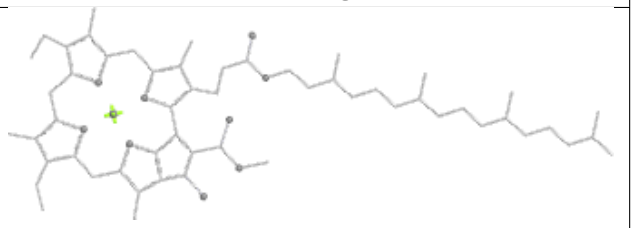


Bond angles

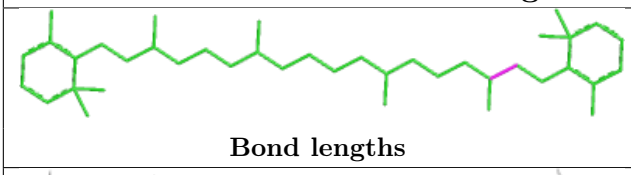


Torsions



Rings

Ligand BCR K 101



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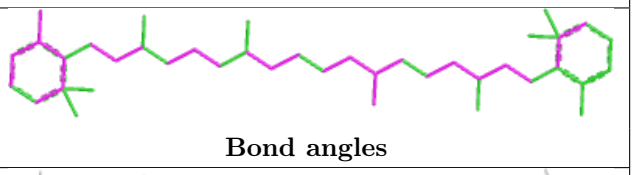
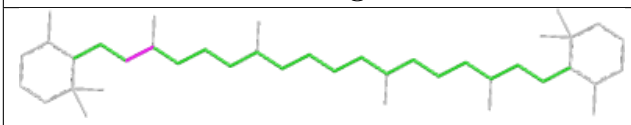
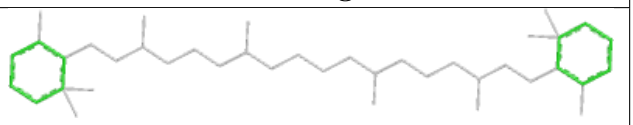


Bond angles

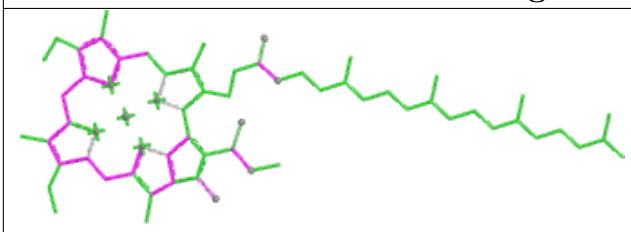


Torsions



Rings

Ligand CLA a 410



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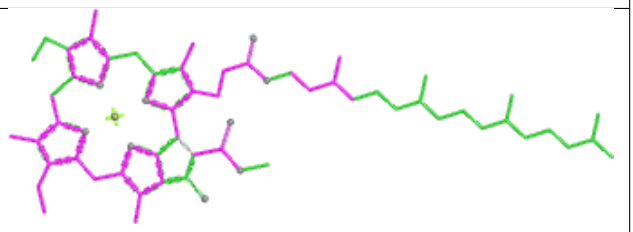
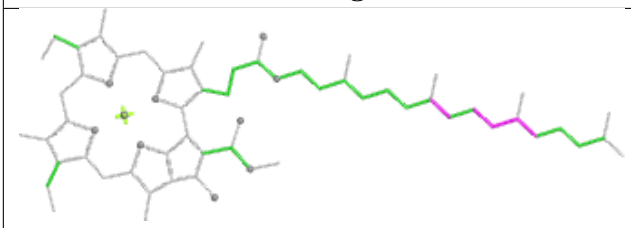
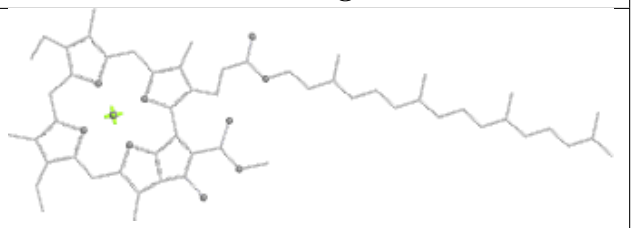


Bond angles

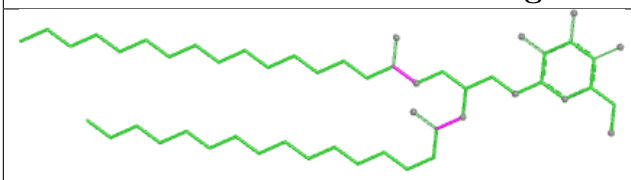


Torsions



Rings

Ligand LMG c 523



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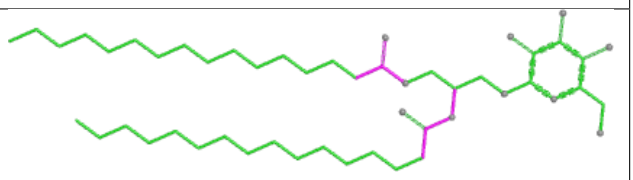
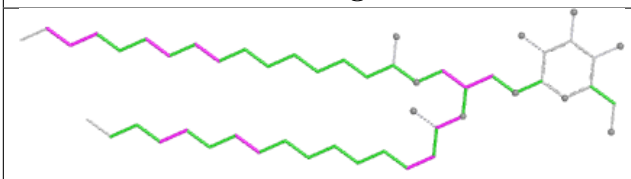


Bond angles



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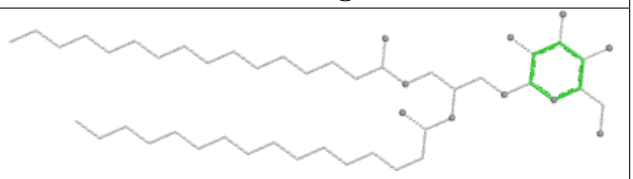
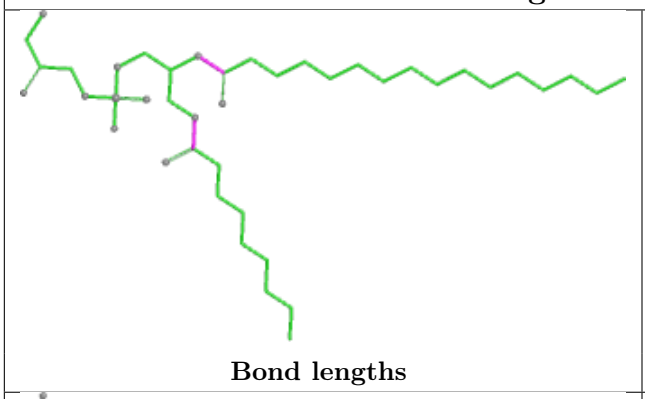
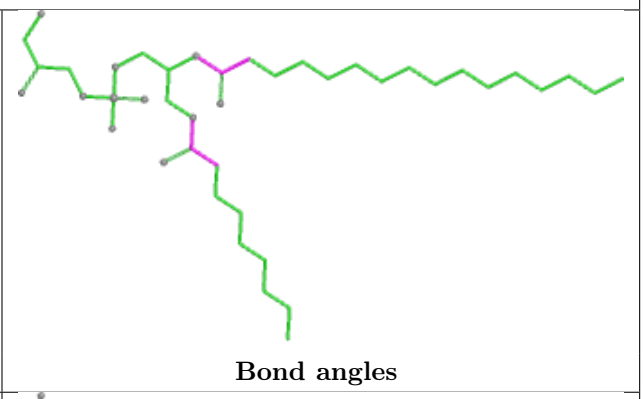


Rings

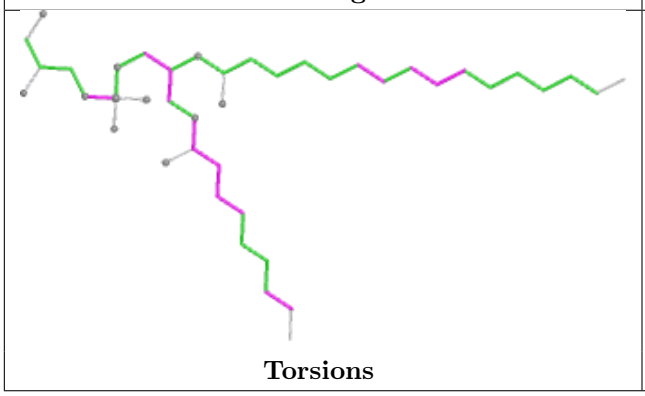
Ligand LHG e 102



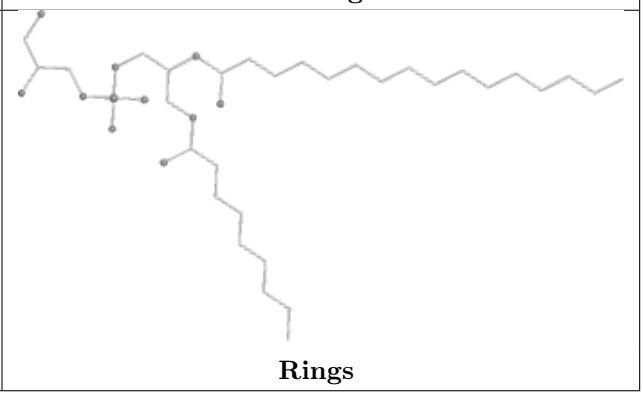
Bond lengths



Bond angles

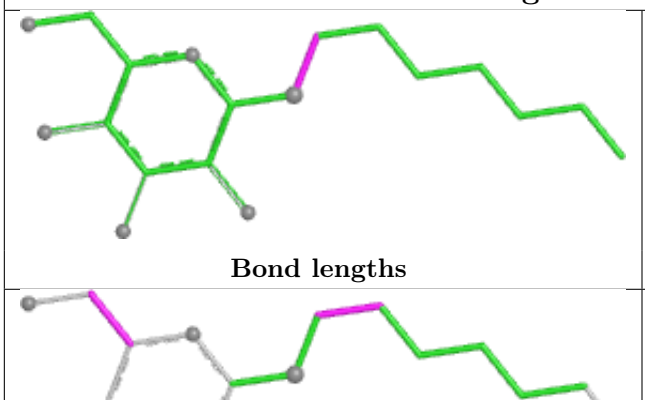


Torsions



Rings

Ligand HTG C 523



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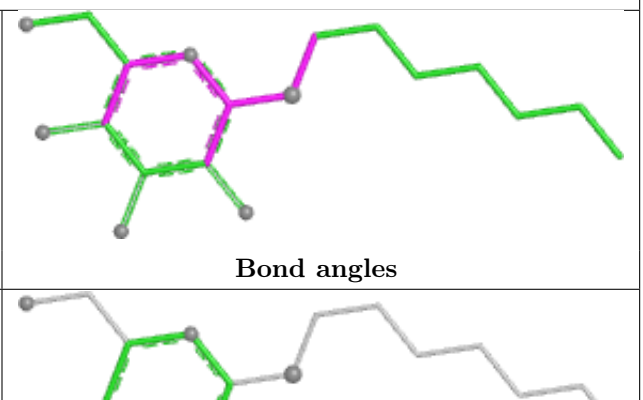
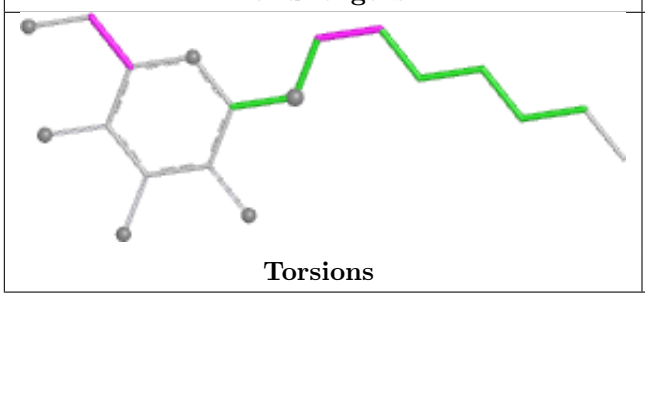
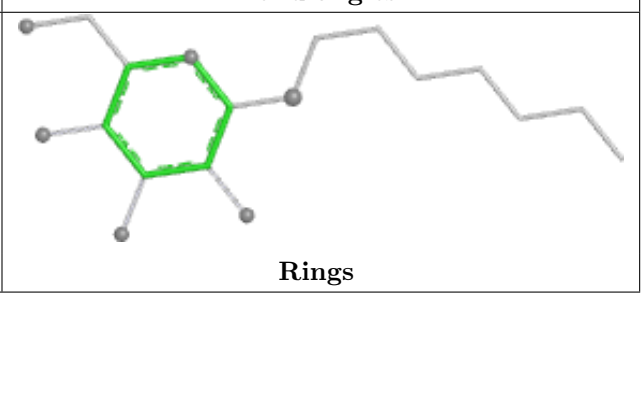


Bond angles

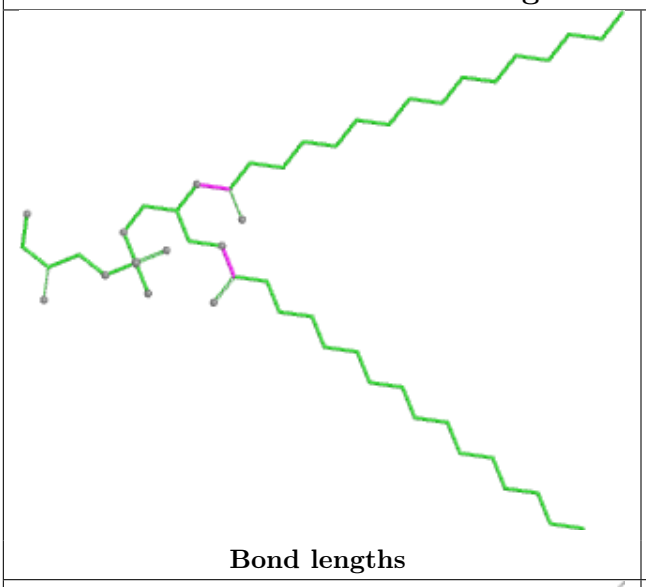


Torsions



Rings

Ligand LHG D 409



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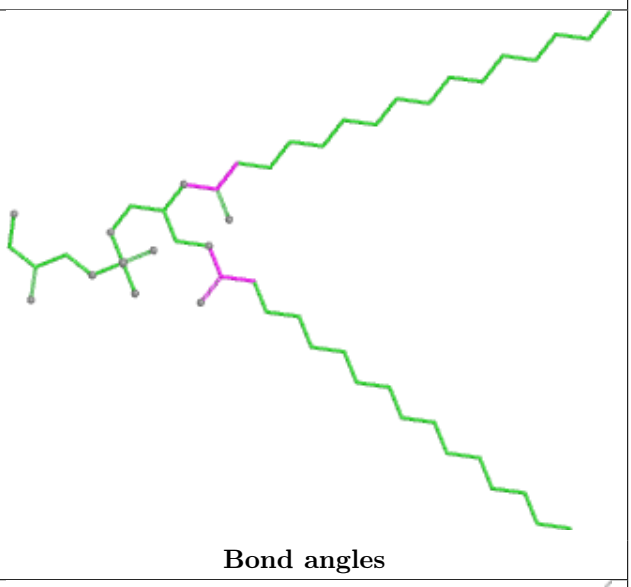
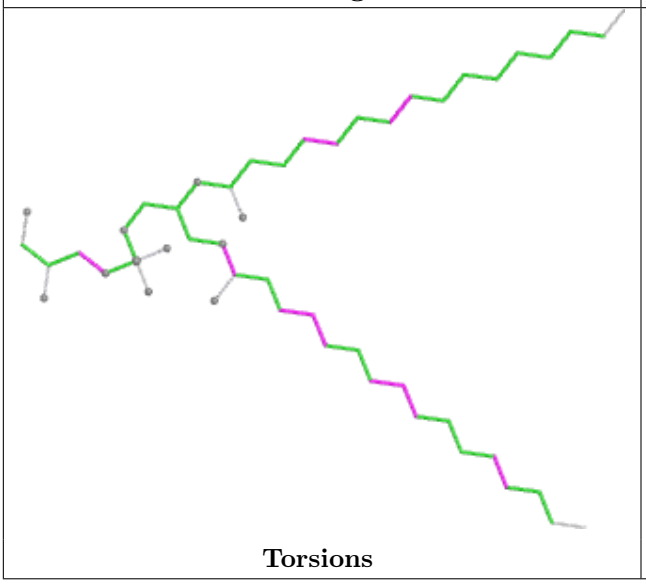
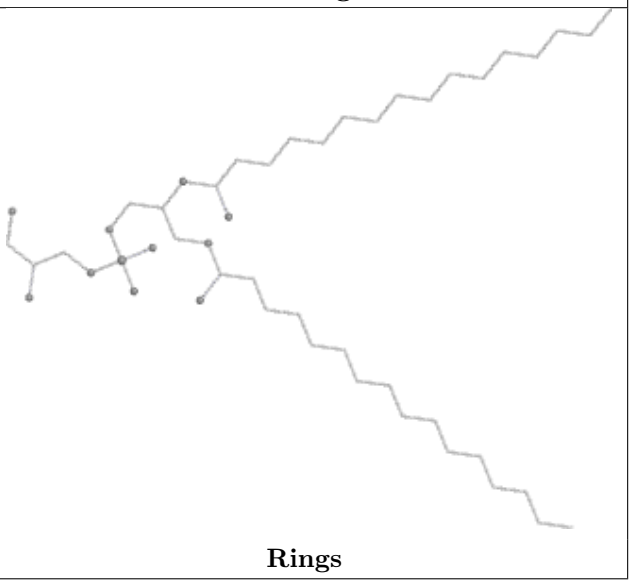


Bond angles

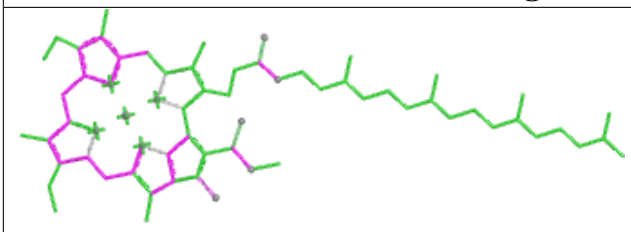


Torsions



Rings

Ligand CLA D 403



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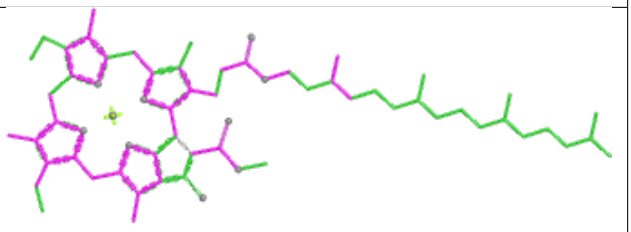
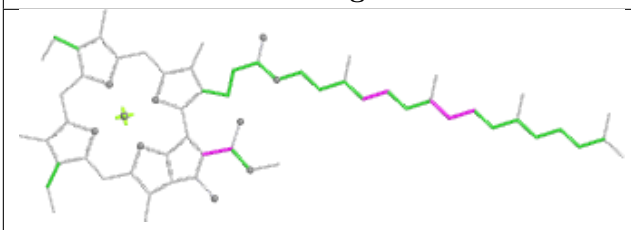
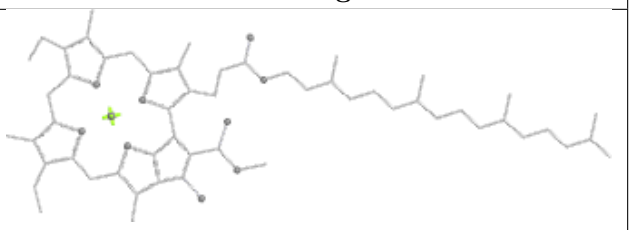


Bond angles

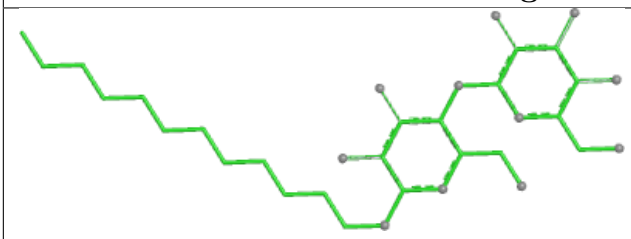


Torsions

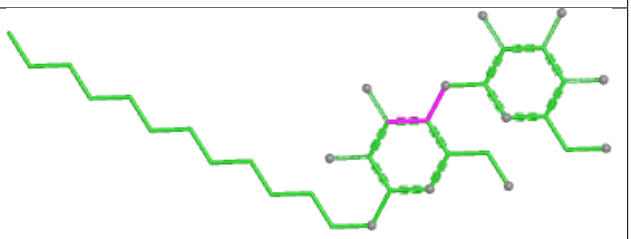


Rings

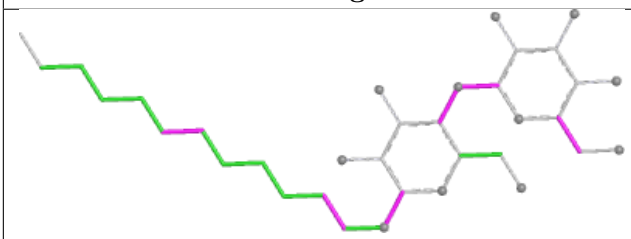
Ligand LMT D 401



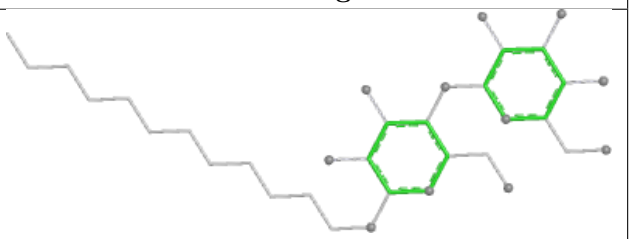
Bond lengths



Bond angles

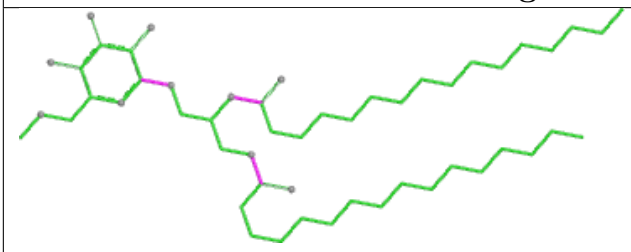


Torsions

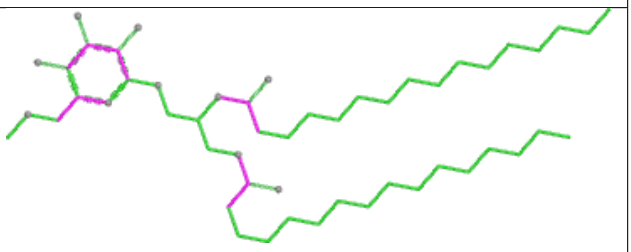


Rings

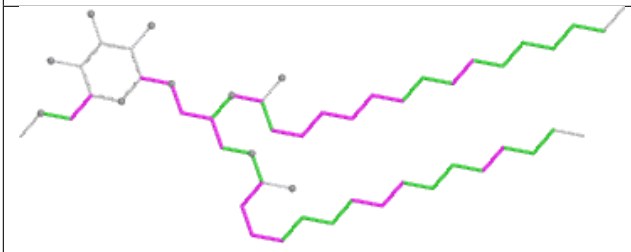
Ligand DGD D 406



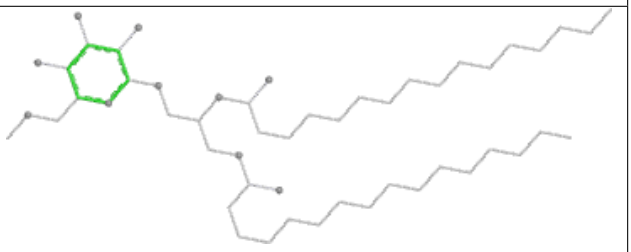
Bond lengths



Bond angles

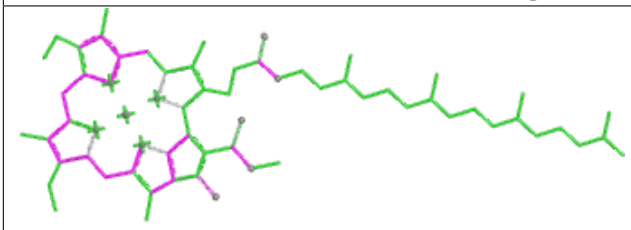


Torsions

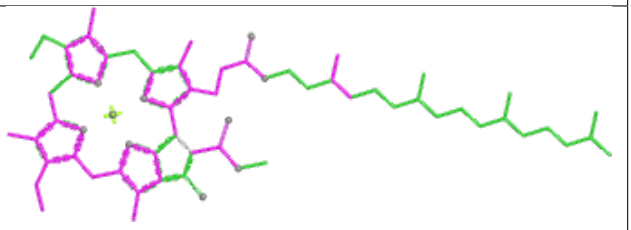


Rings

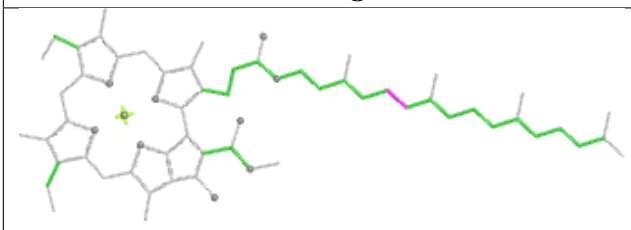
Ligand CLA B 604



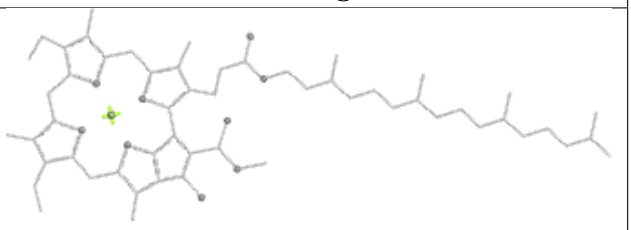
Bond lengths



Bond angles



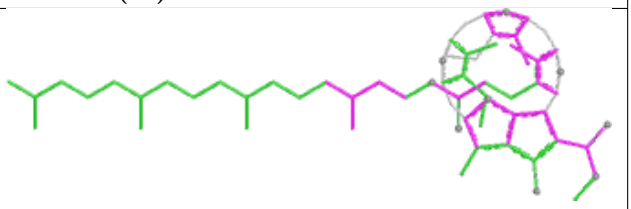
Torsions



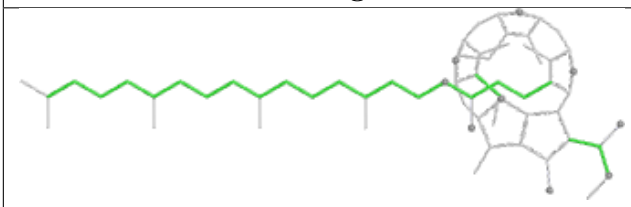
Rings

Ligand PHO a 418 (A)

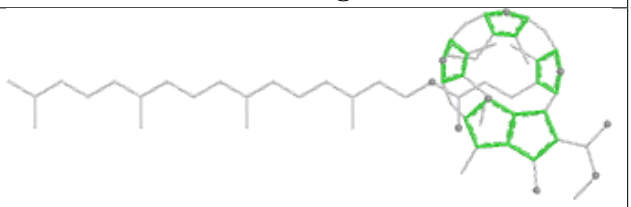
Bond lengths



Bond angles

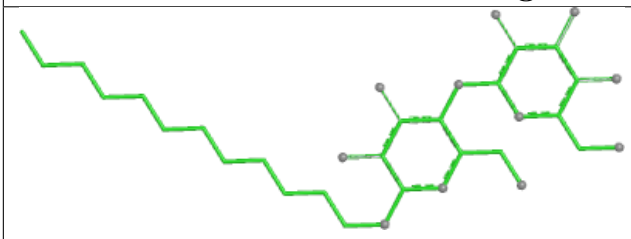


Torsions

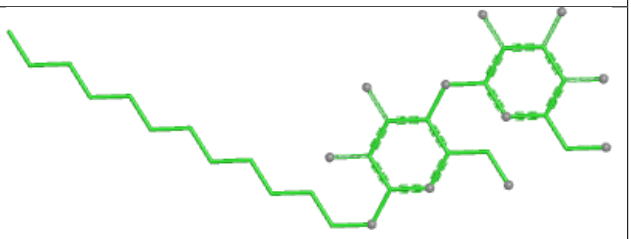


Rings

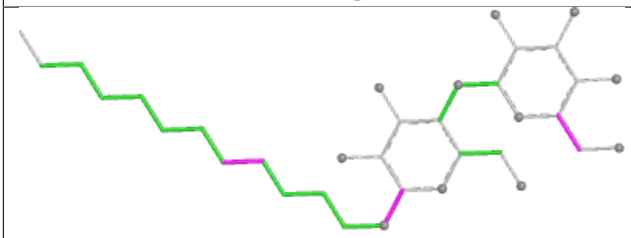
Ligand LMT M 101



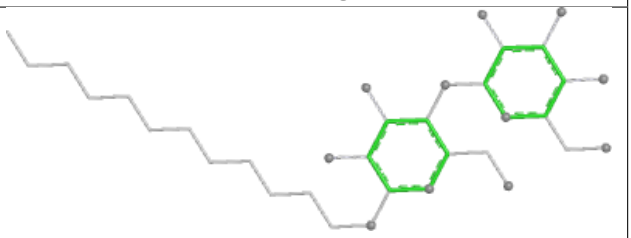
Bond lengths



Bond angles

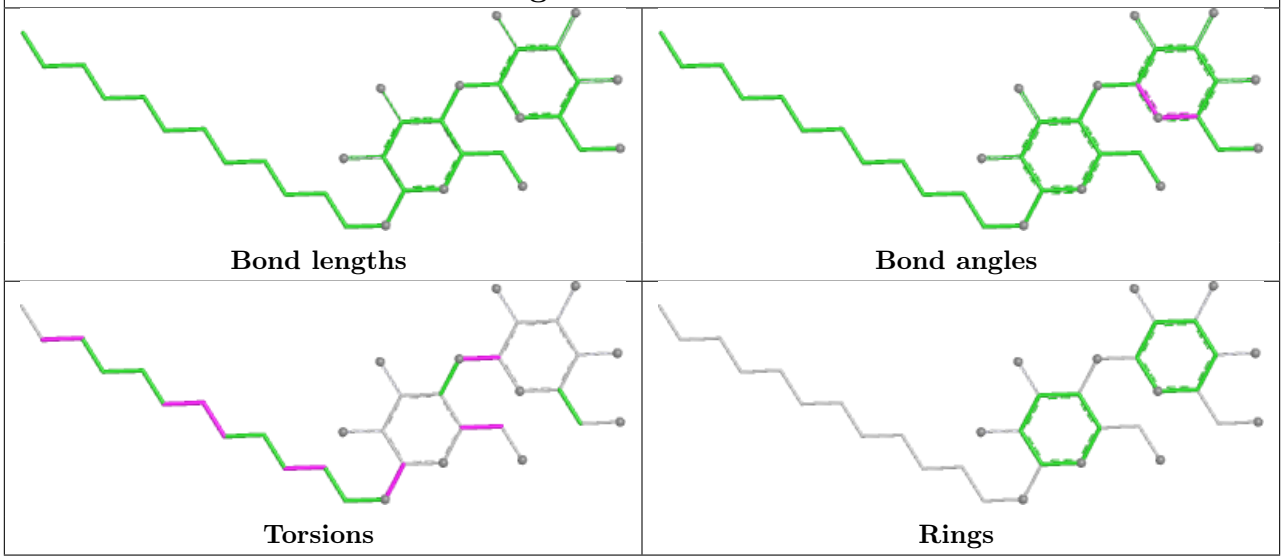


Torsions

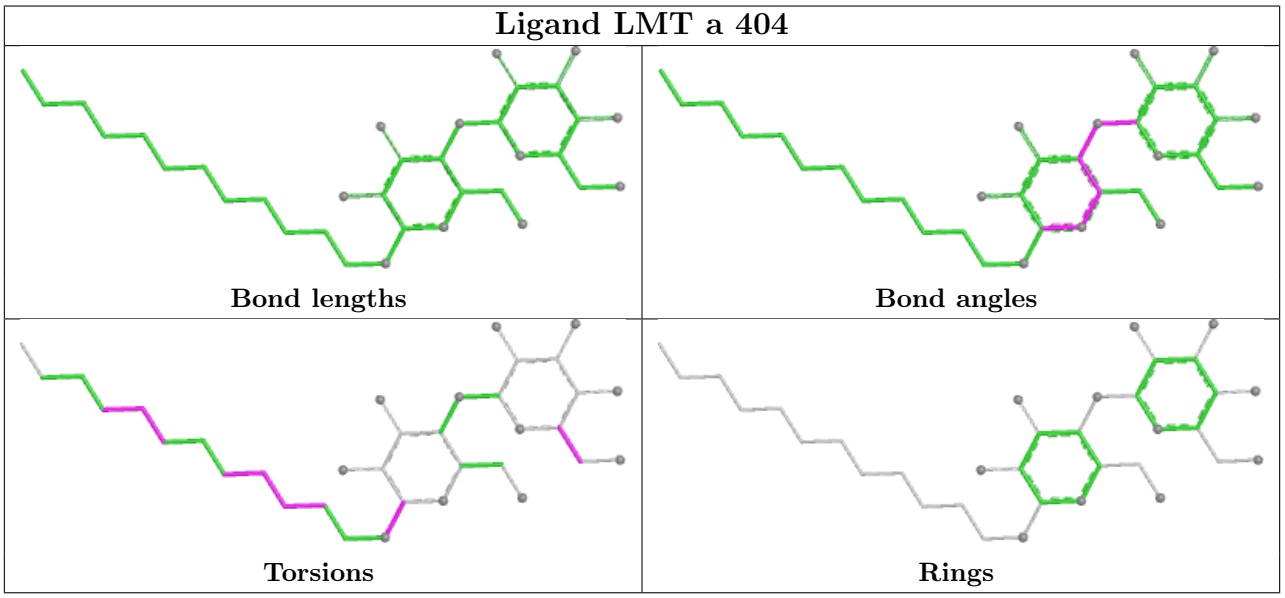


Rings

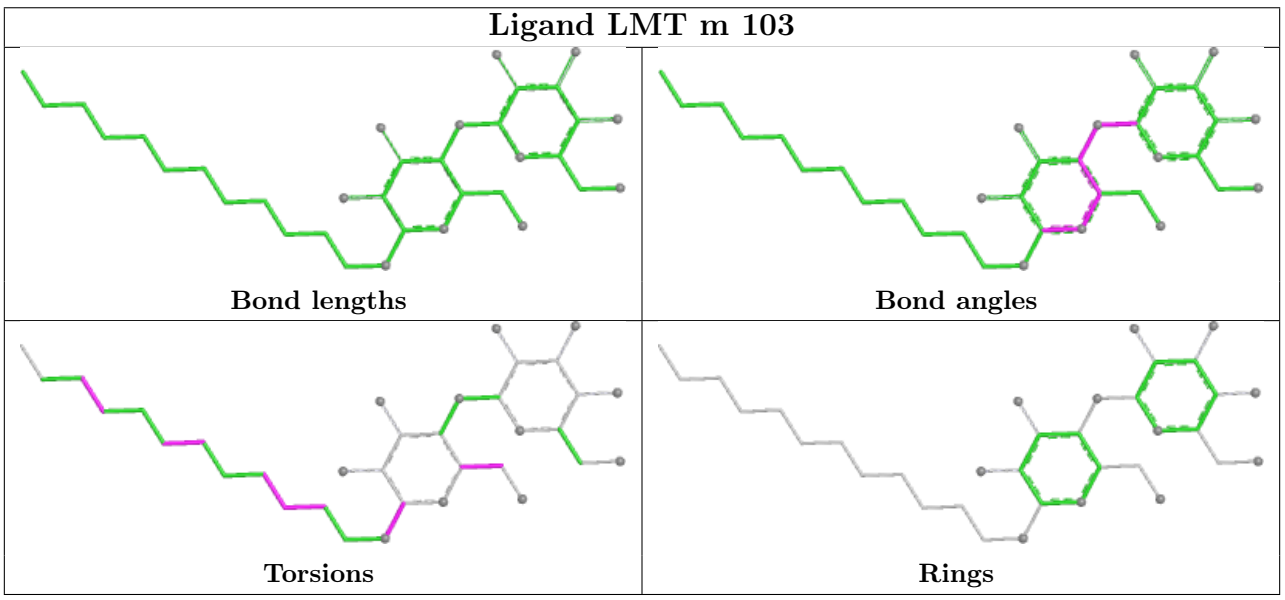
Ligand LMT f 102



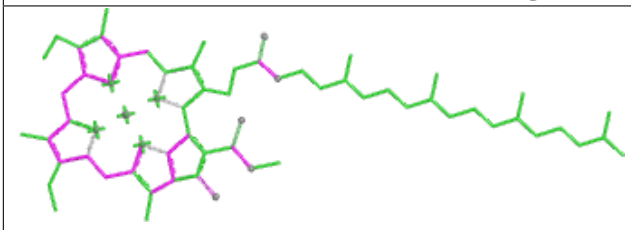
Ligand LMT a 404



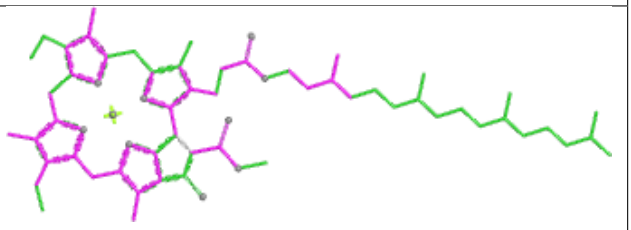
Ligand LMT m 103



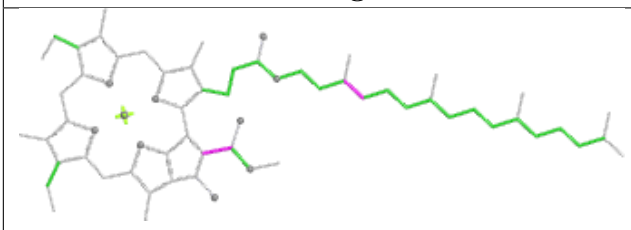
Ligand CLA B 606



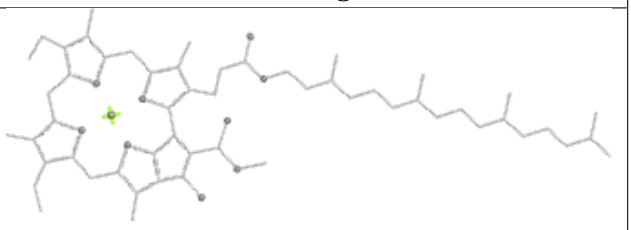
Bond lengths



Bond angles

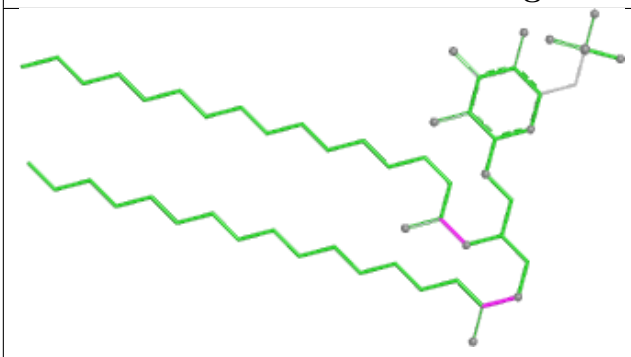


Torsions

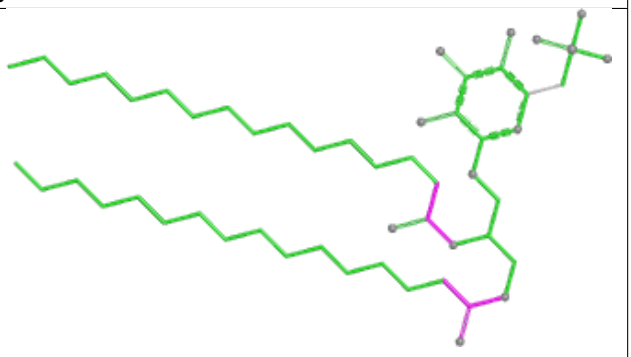


Rings

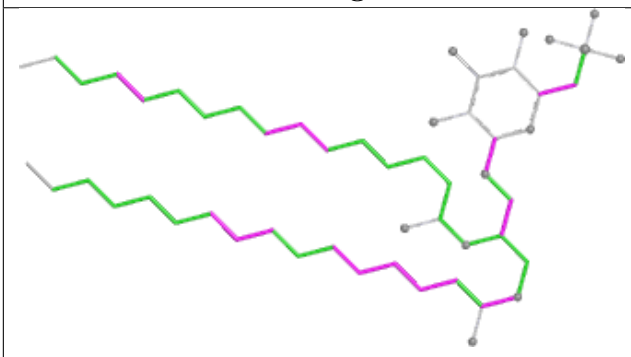
Ligand SQD A 416



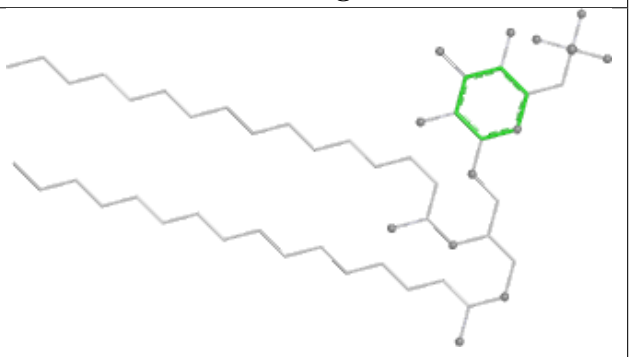
Bond lengths



Bond angles

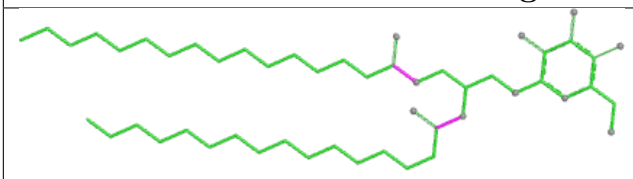


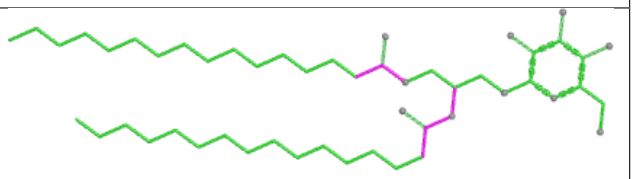
Torsions

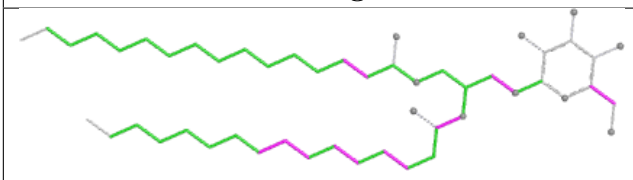


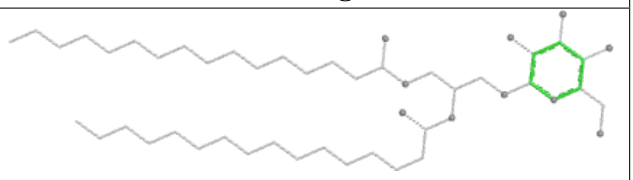
Rings

Ligand LMG C 520

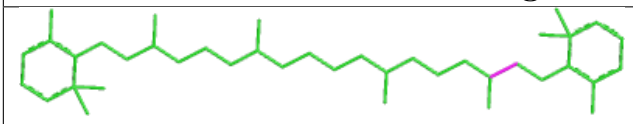

Bond lengths

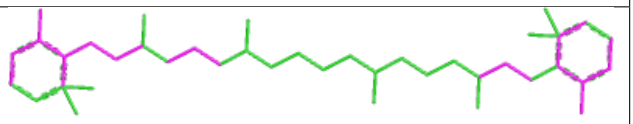

Bond angles

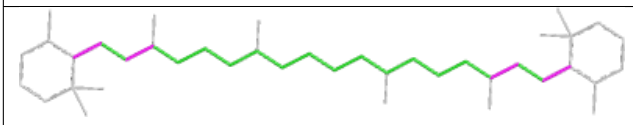

Torsions

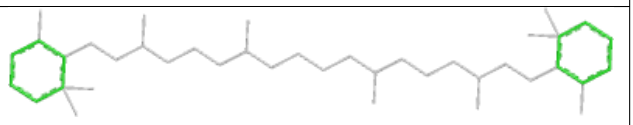

Rings

Ligand BCR D 404

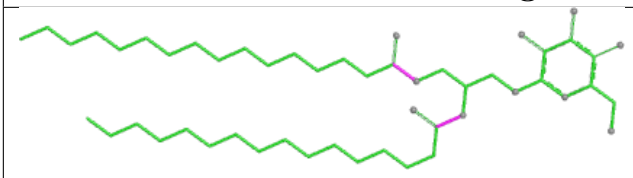

Bond lengths

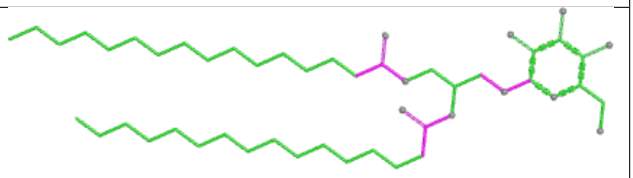

Bond angles

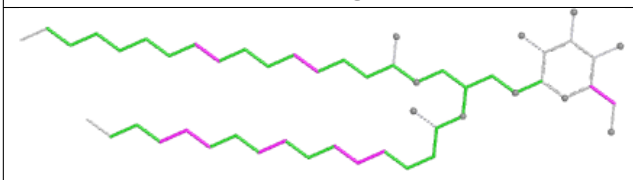

Torsions

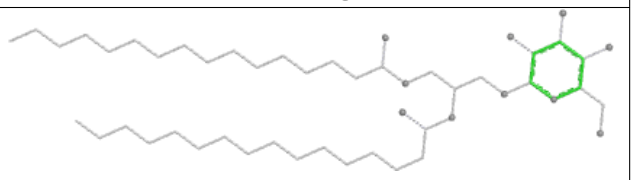

Rings

Ligand LMG D 413


Bond lengths

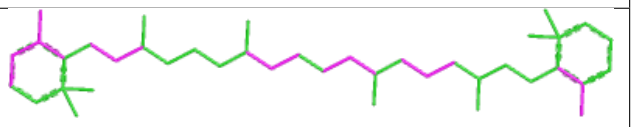

Bond angles

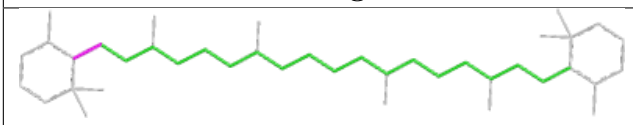

Torsions

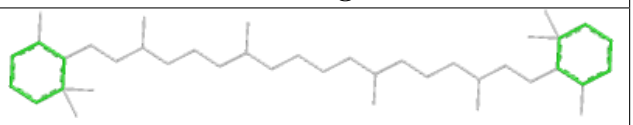

Rings

Ligand BCR c 519

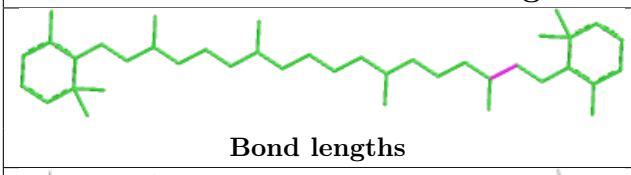
Bond lengths


Bond angles

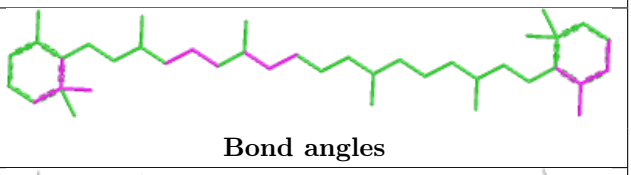

Torsions


Rings

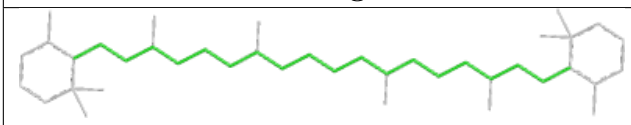
Ligand BCR B 620



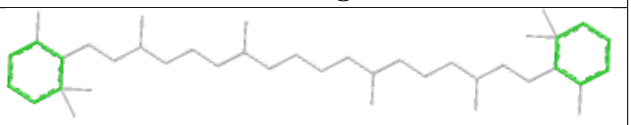
Bond lengths



Bond angles

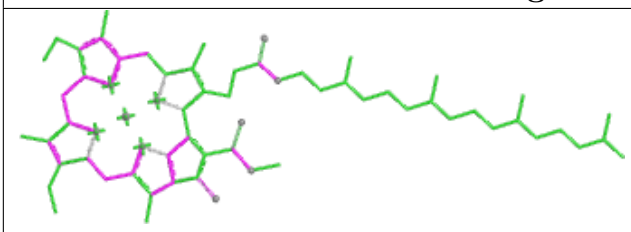


Torsions



Rings

Ligand CLA b 625



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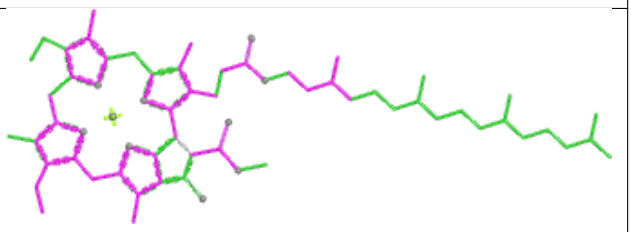
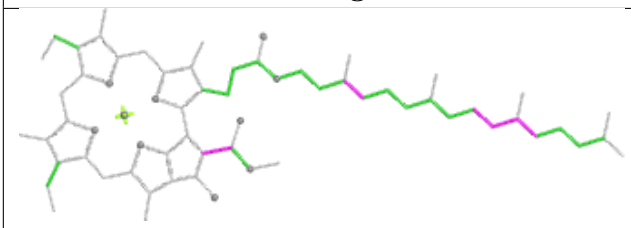
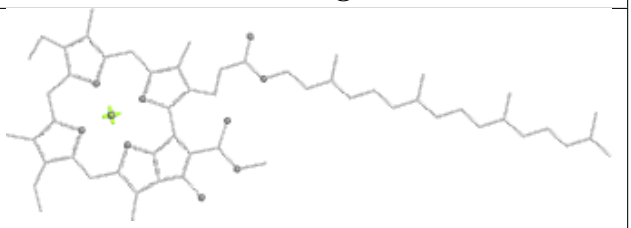


Bond angles

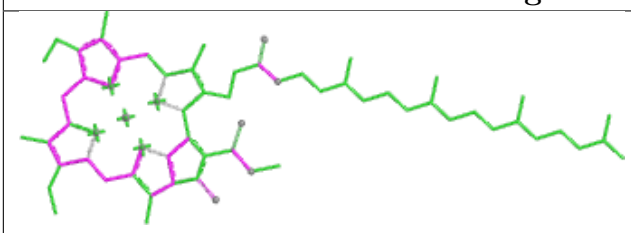


Torsions

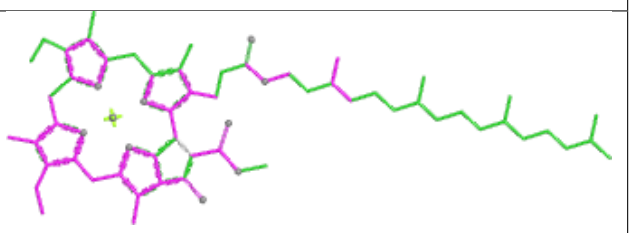


Rings

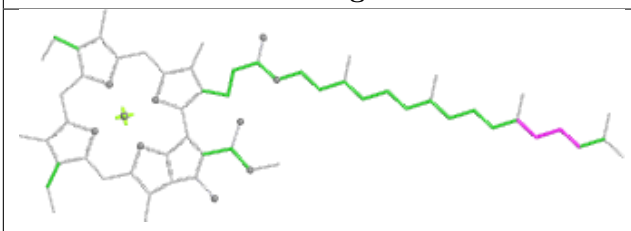
Ligand CLA C 504



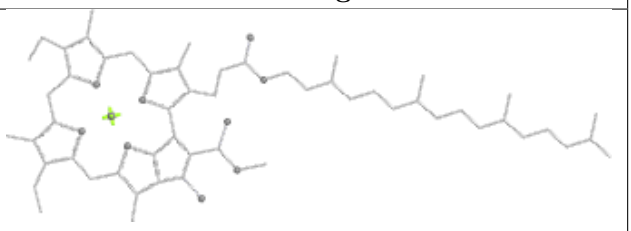
Bond lengths



Bond angles



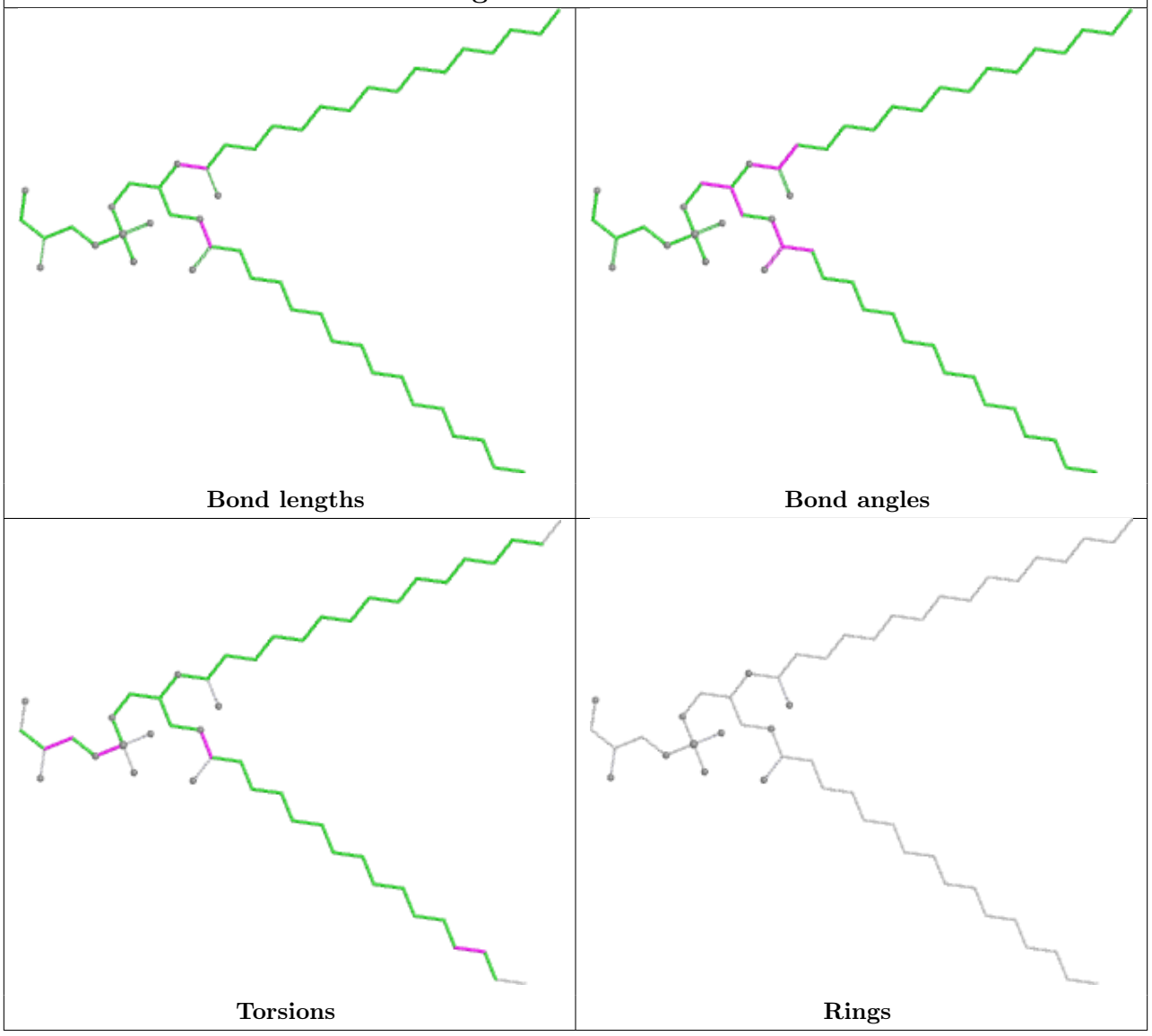
Torsions



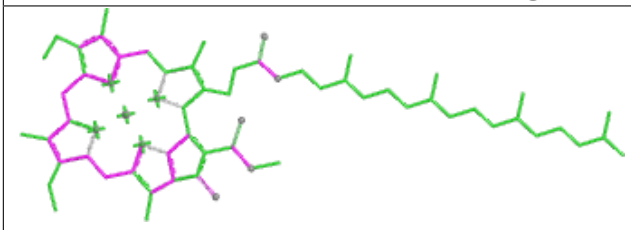
Rings

Ligand PL9 d 405 (A)

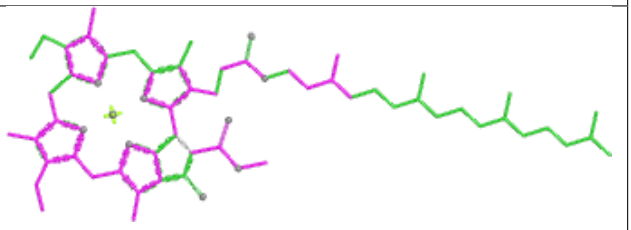
Ligand LHG d 407



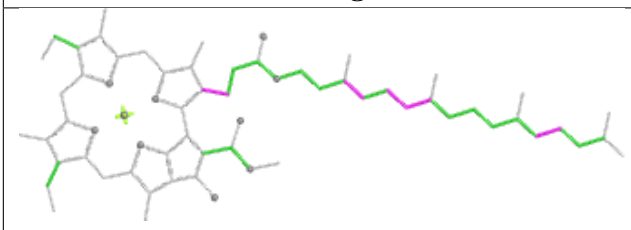
Ligand CLA C 506



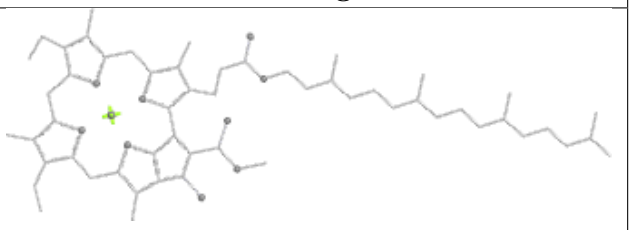
Bond lengths



Bond angles

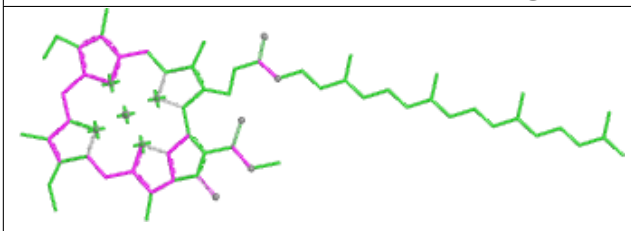


Torsions

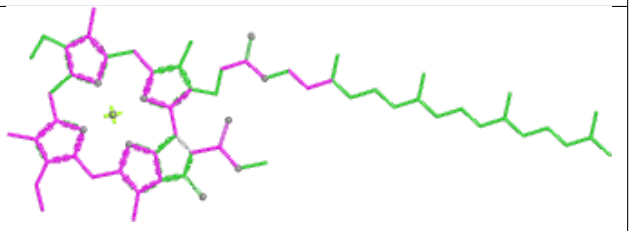


Rings

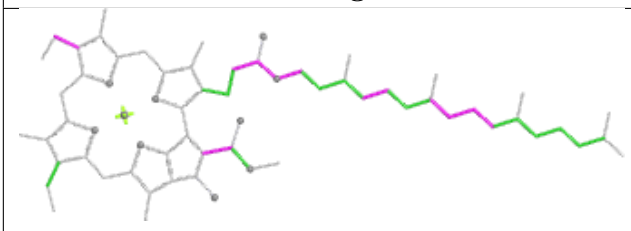
Ligand CLA B 602



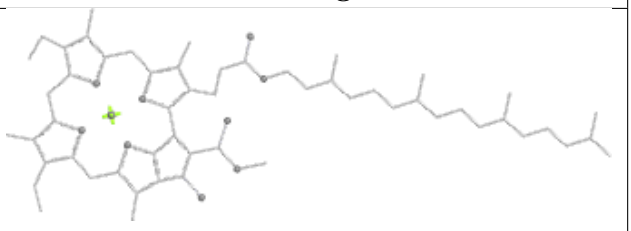
Bond lengths



Bond angles

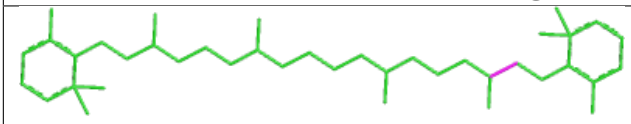


Torsions

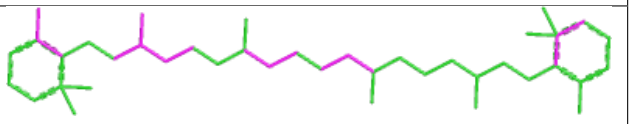


Rings

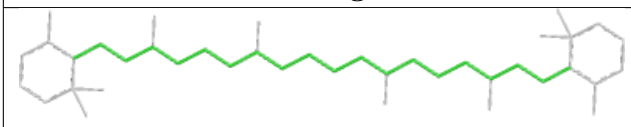
Ligand BCR c 528



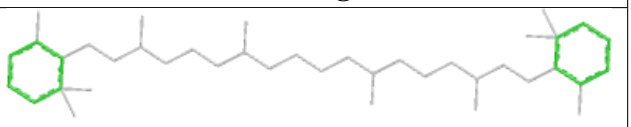
Bond lengths



Bond angles

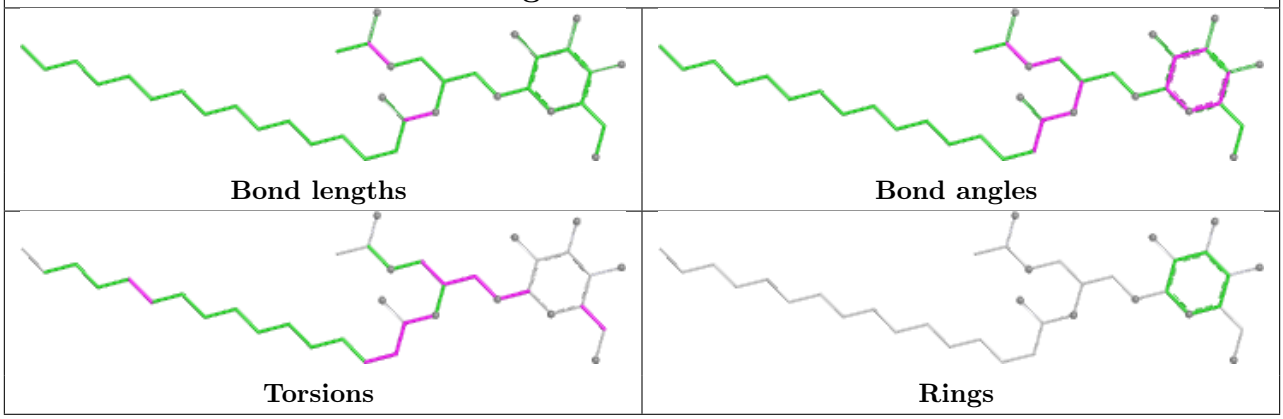


Torsions

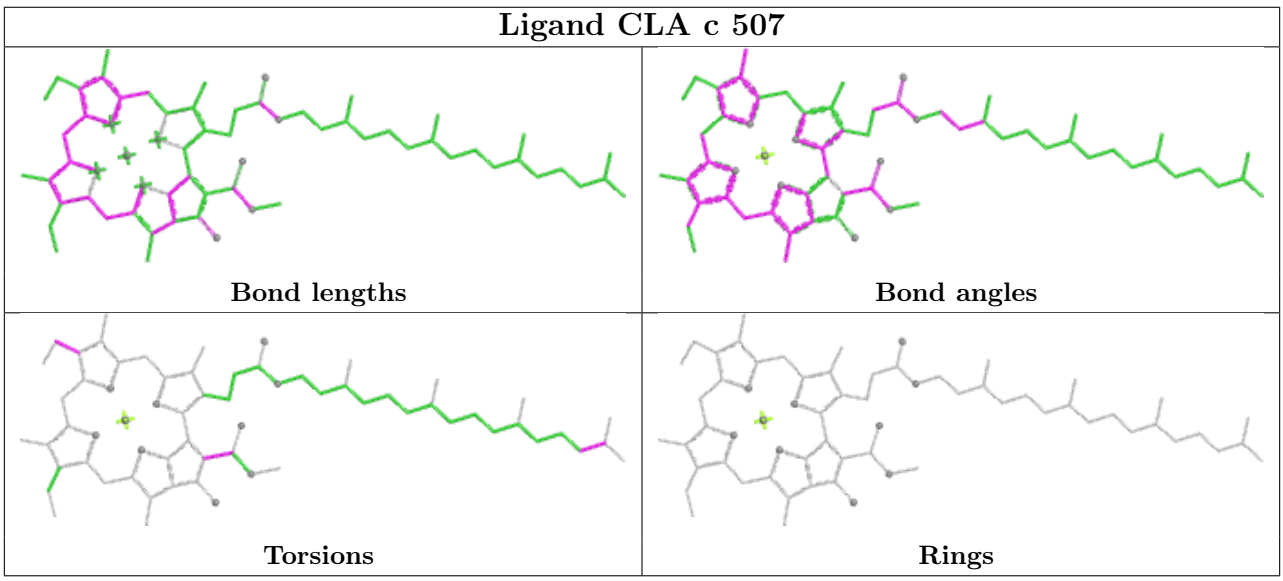


Rings

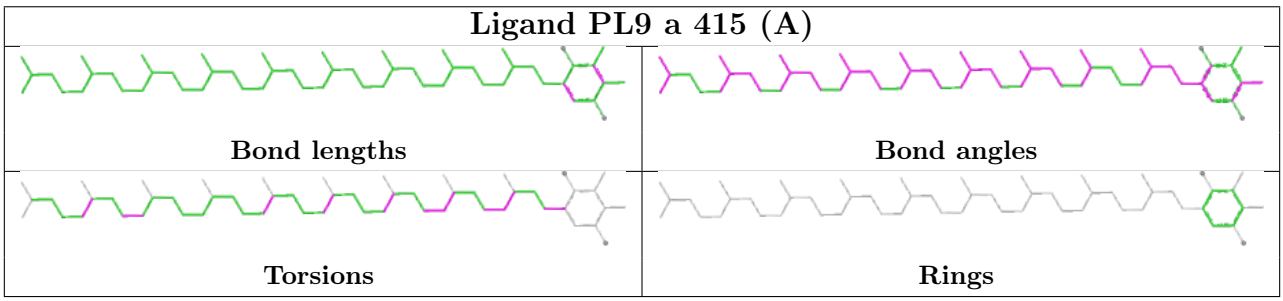
Ligand LMG Z 101



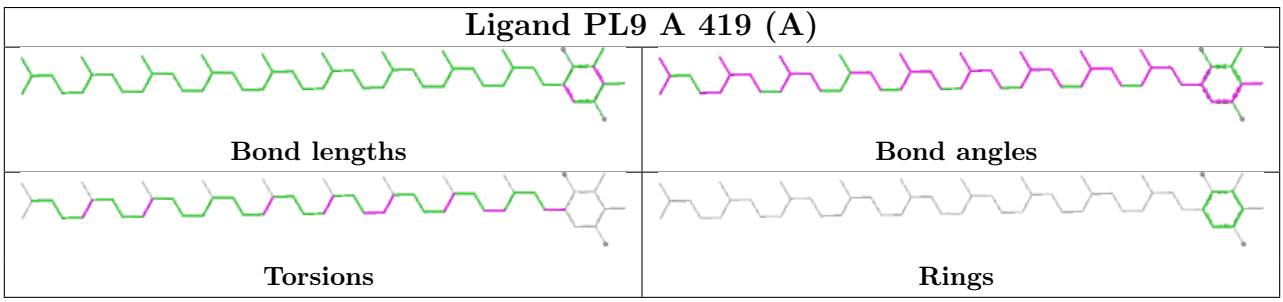
Ligand CLA c 507



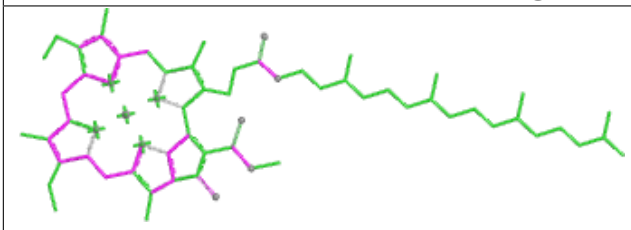
Ligand PL9 a 415 (A)



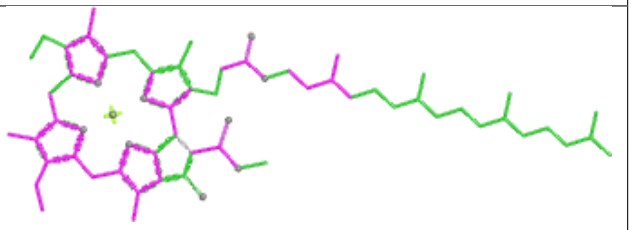
Ligand PL9 A 419 (A)



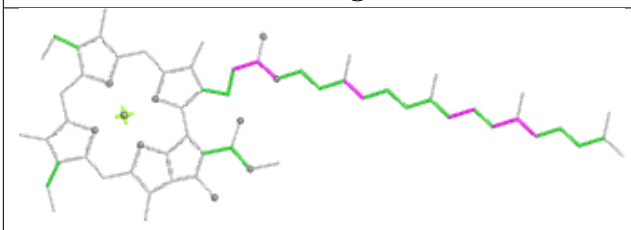
Ligand CLA c 515



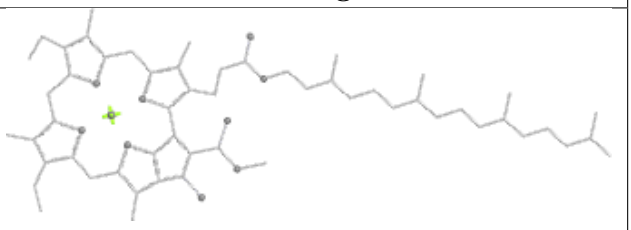
Bond lengths



Bond angles

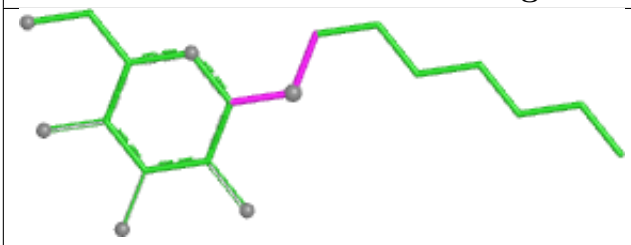


Torsions

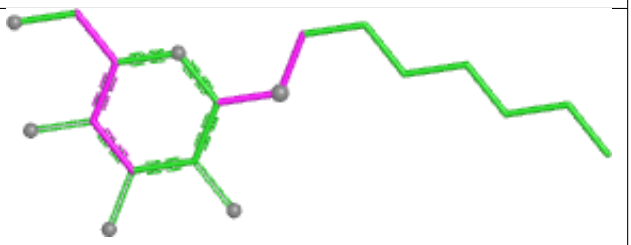


Rings

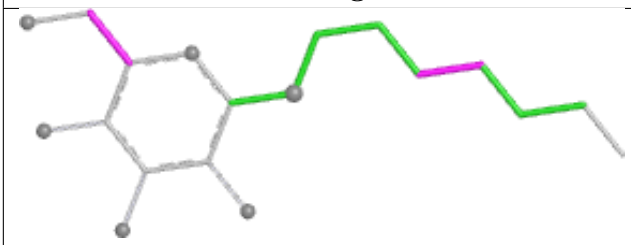
Ligand HTG B 632



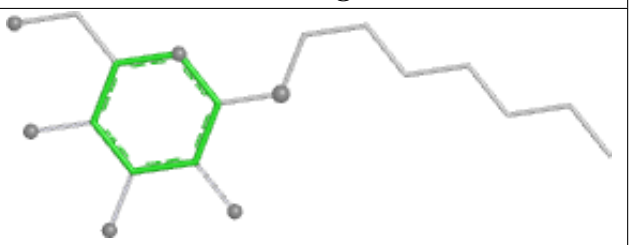
Bond lengths



Bond angles

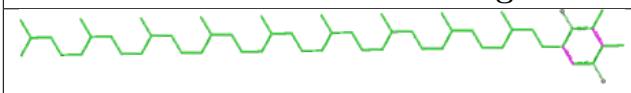


Torsions



Rings

Ligand PL9 D 405 (B)



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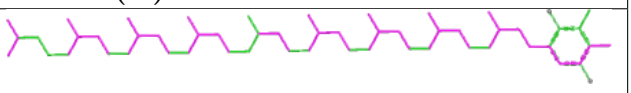
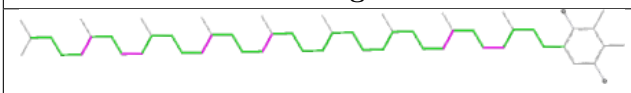
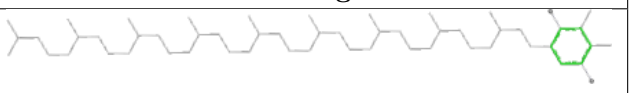


Bond angles

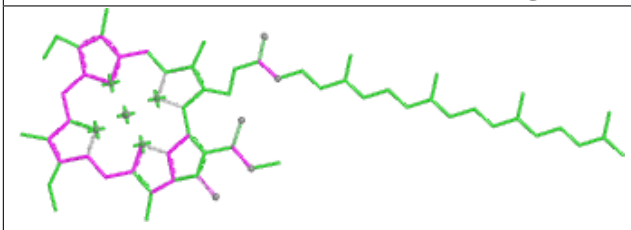


Torsions

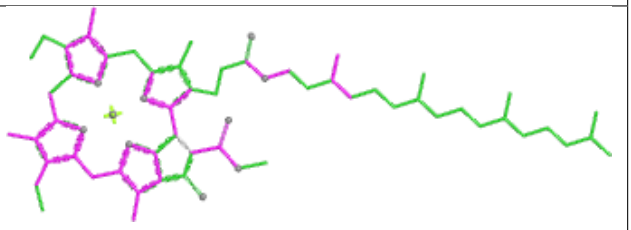


Rings

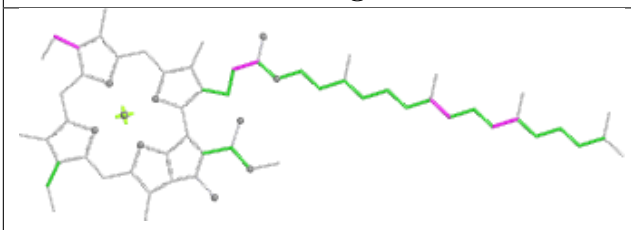
Ligand CLA C 505



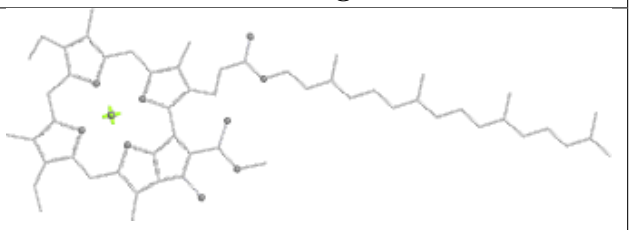
Bond lengths



Bond angles

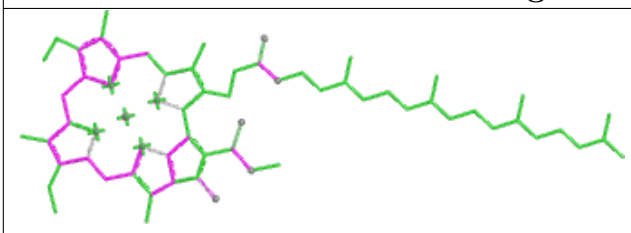


Torsions

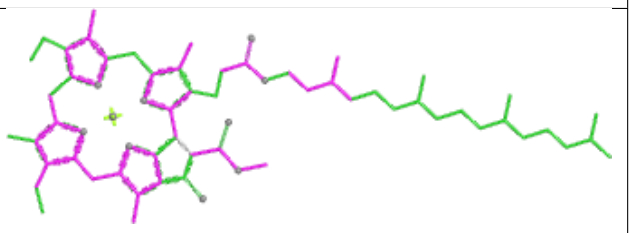


Rings

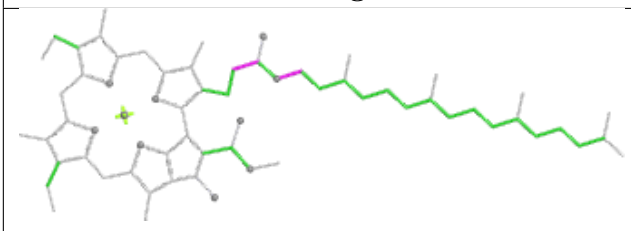
Ligand CLA b 622



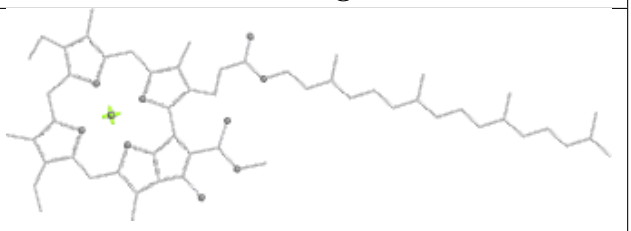
Bond lengths



Bond angles

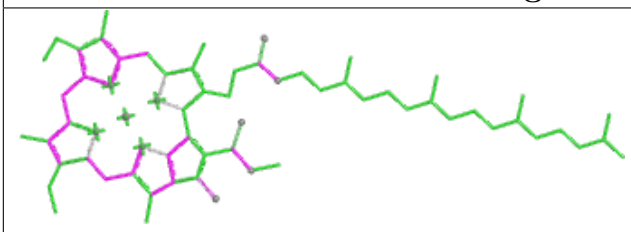


Torsions

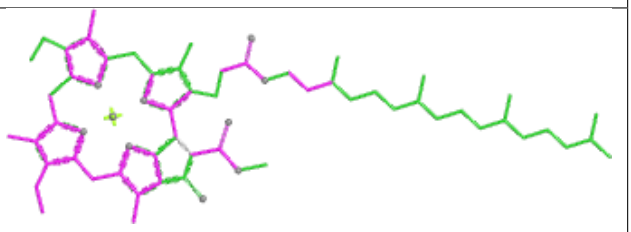


Rings

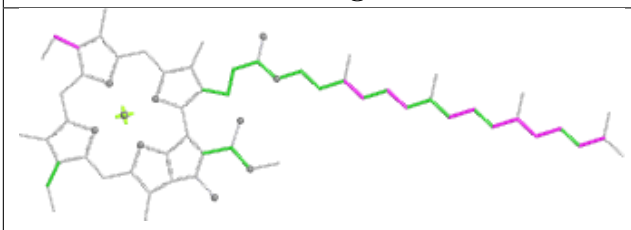
Ligand CLA B 616



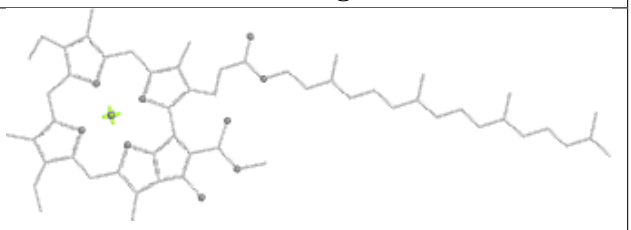
Bond lengths



Bond angles

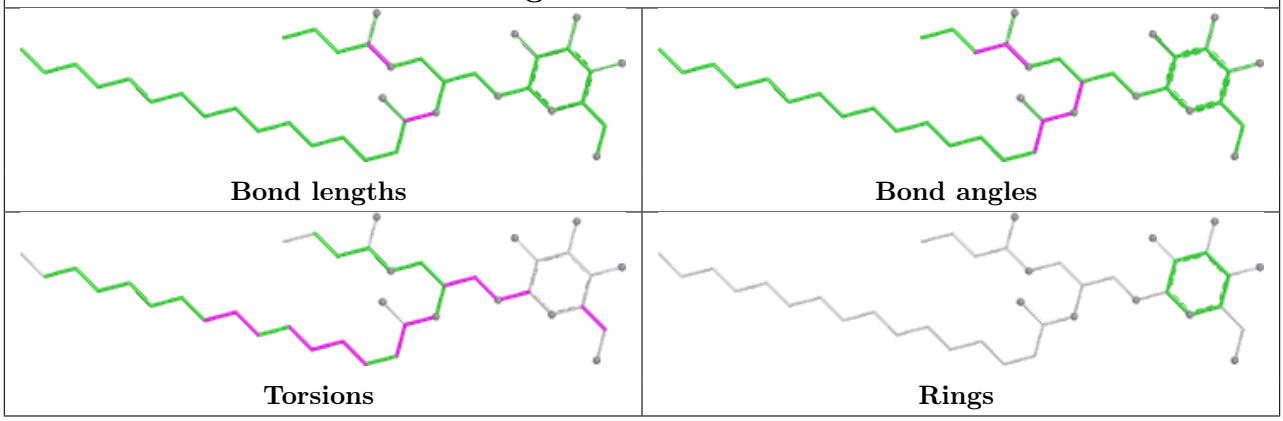


Torsions

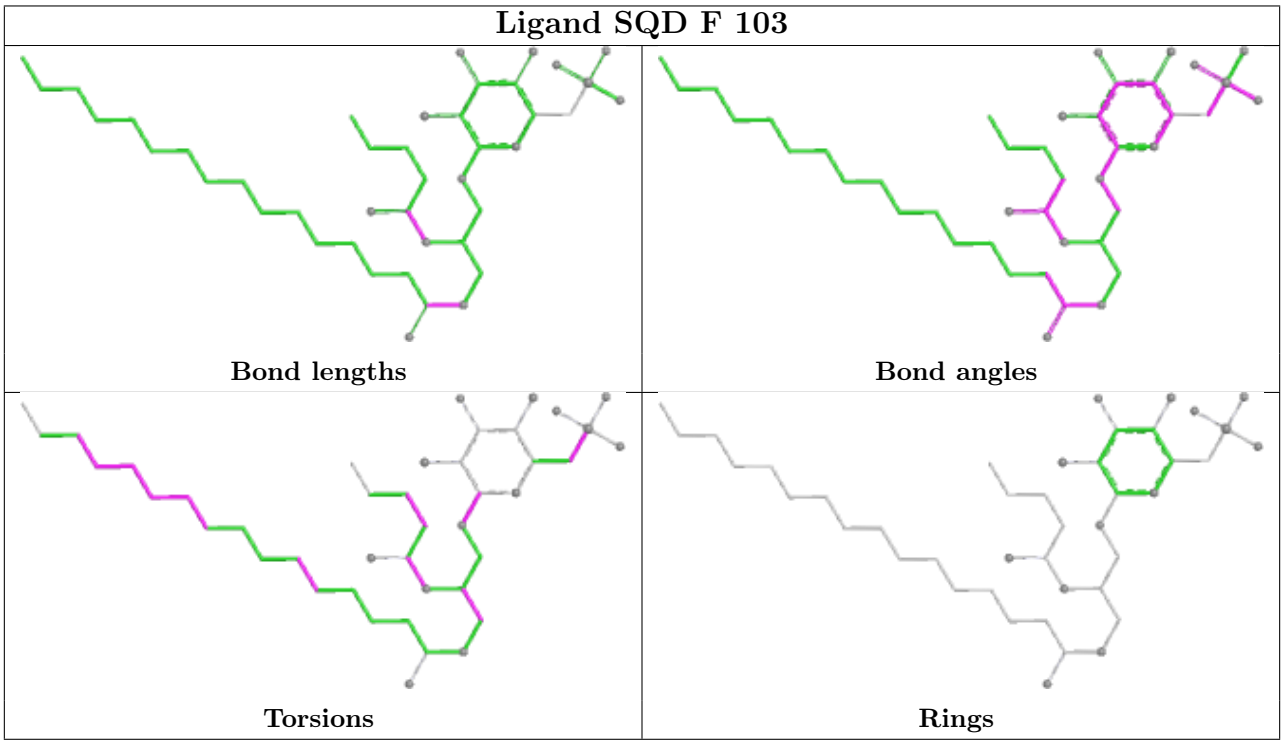


Rings

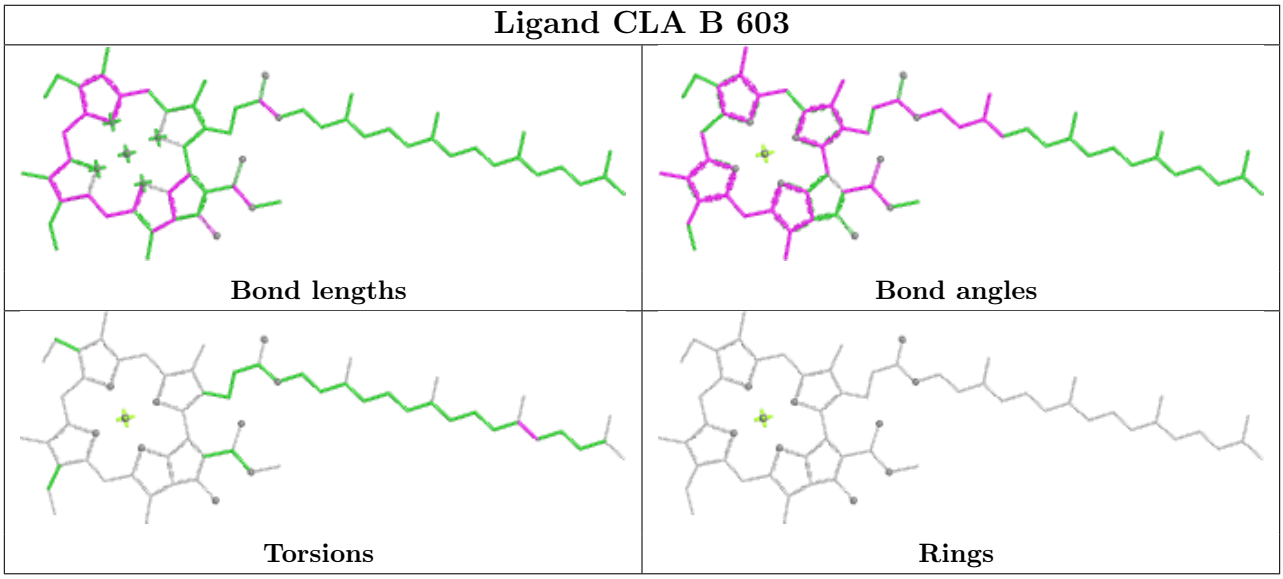
Ligand LMG z 101



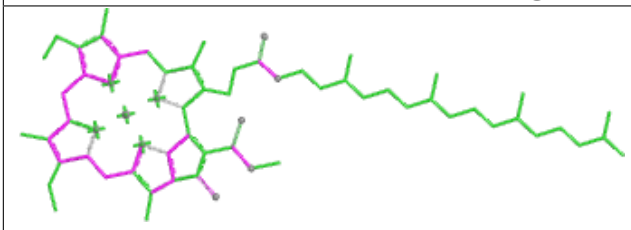
Ligand SQD F 103



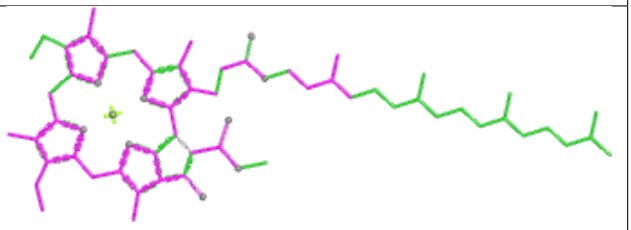
Ligand CLA B 603



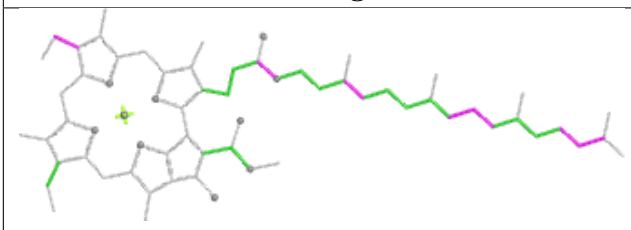
Ligand CLA a 412



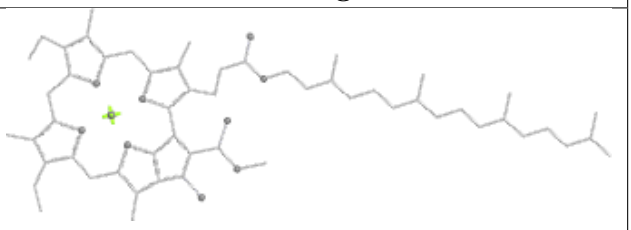
Bond lengths



Bond angles

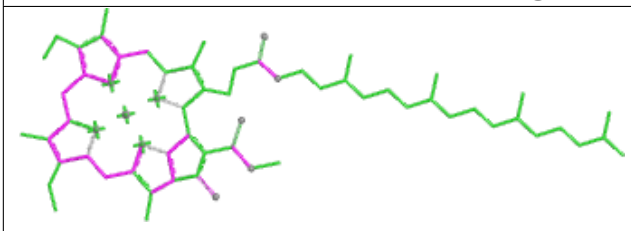


Torsions



Rings

Ligand CLA c 508



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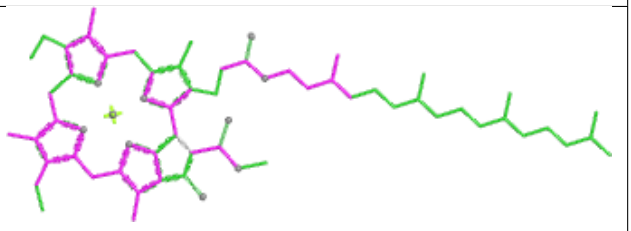
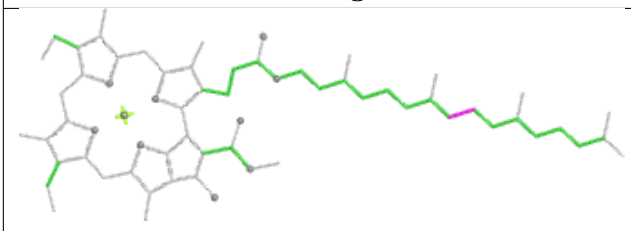


Bond angles



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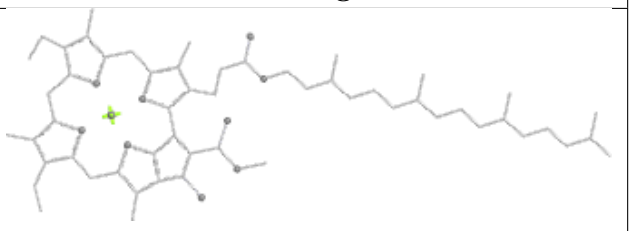
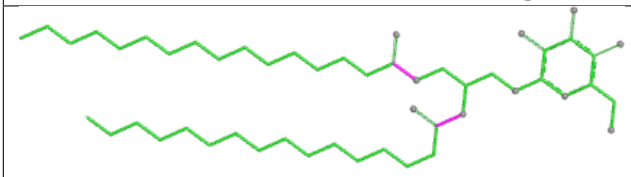
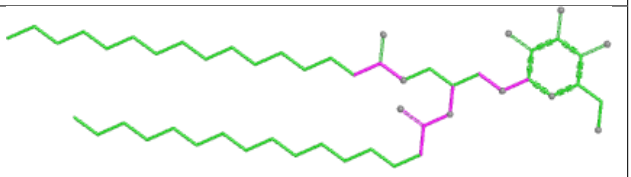


Rings

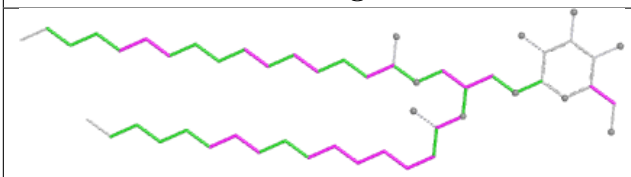
Ligand LMG A 421



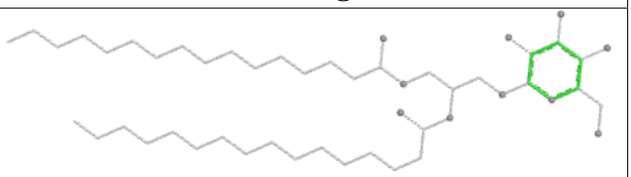
Bond lengths



Bond angles

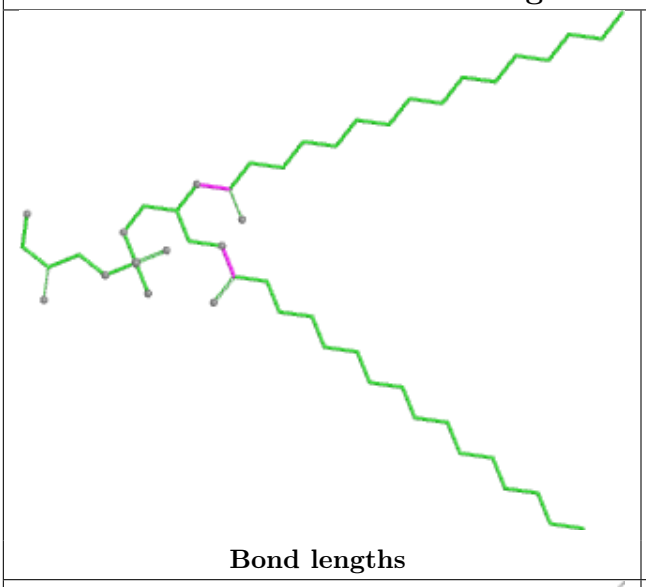


Torsions

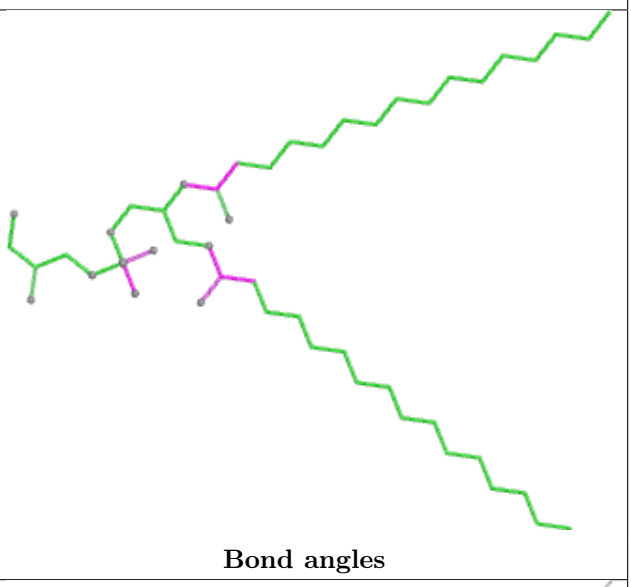


Rings

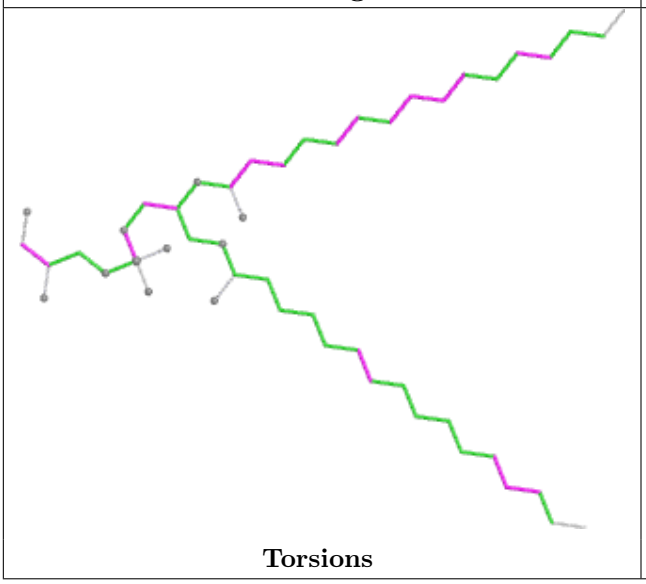
Ligand LHG b 634



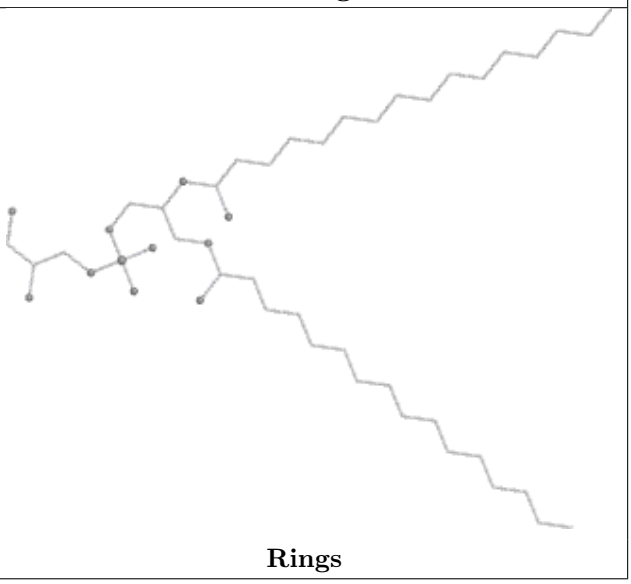
Bond lengths



Bond angles

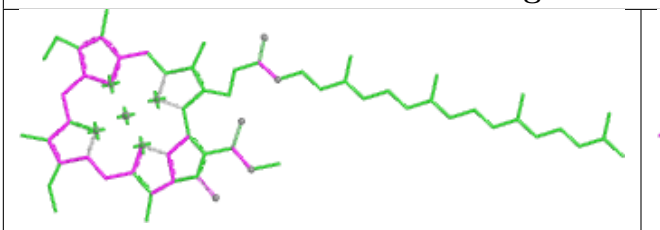


Torsions

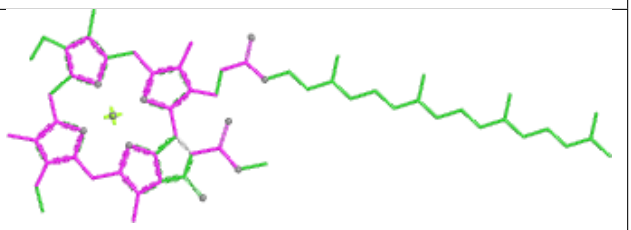


Rings

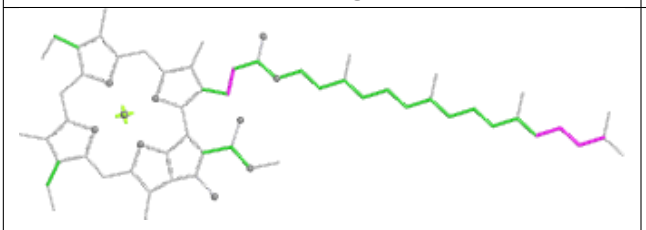
Ligand CLA A 405



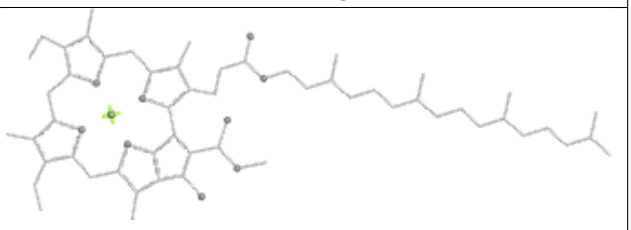
Bond lengths



Bond angles

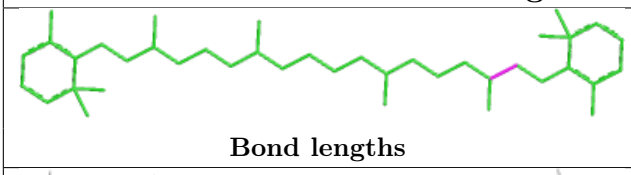


Torsions

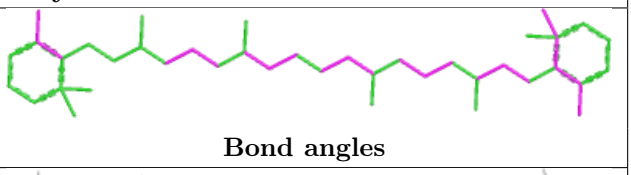


Rings

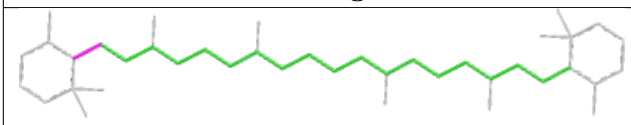
Ligand BCR y 101



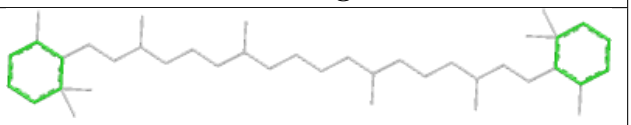
Bond lengths



Bond angles

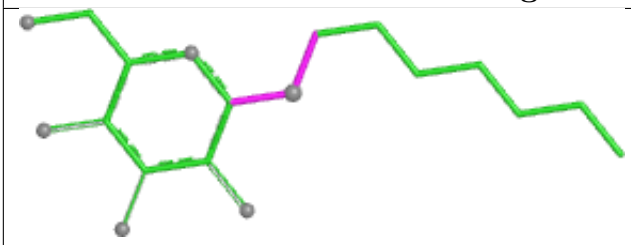


Torsions

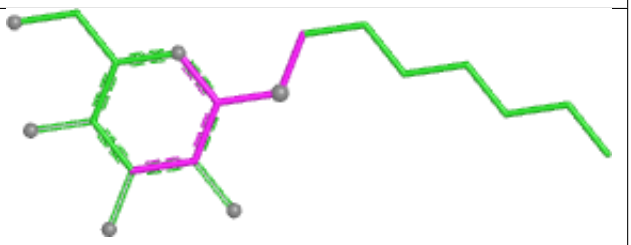


Rings

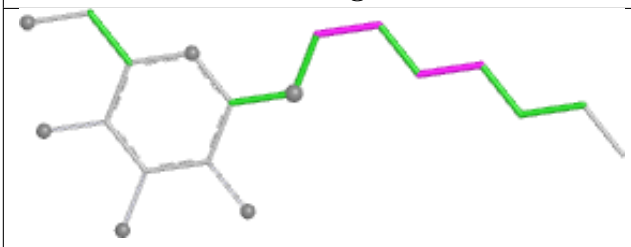
Ligand HTG V 206



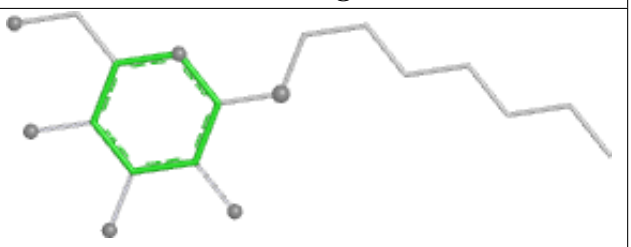
Bond lengths



Bond angles

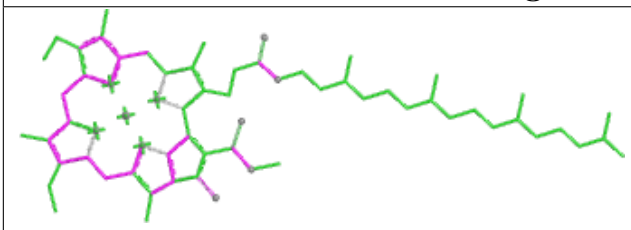


Torsions

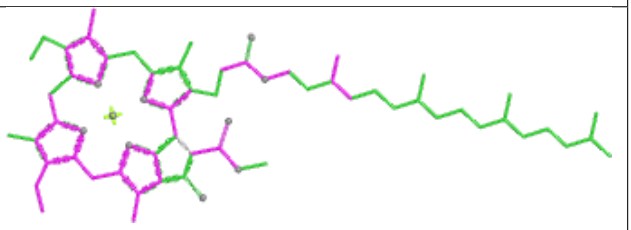


Rings

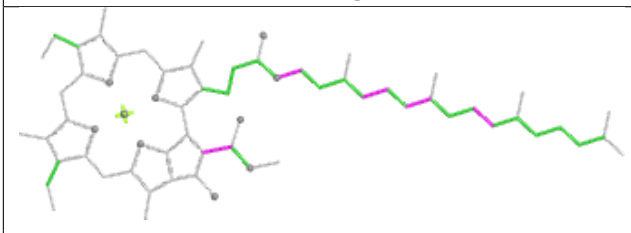
Ligand CLA B 617



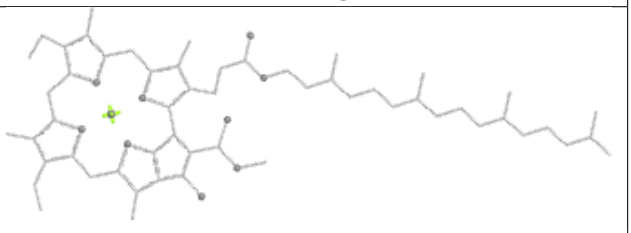
Bond lengths



Bond angles

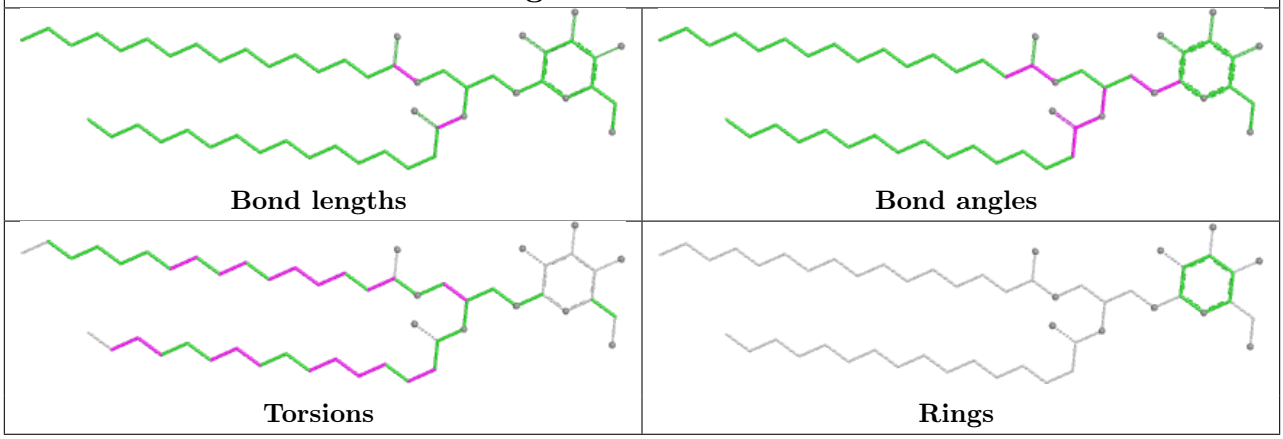


Torsions

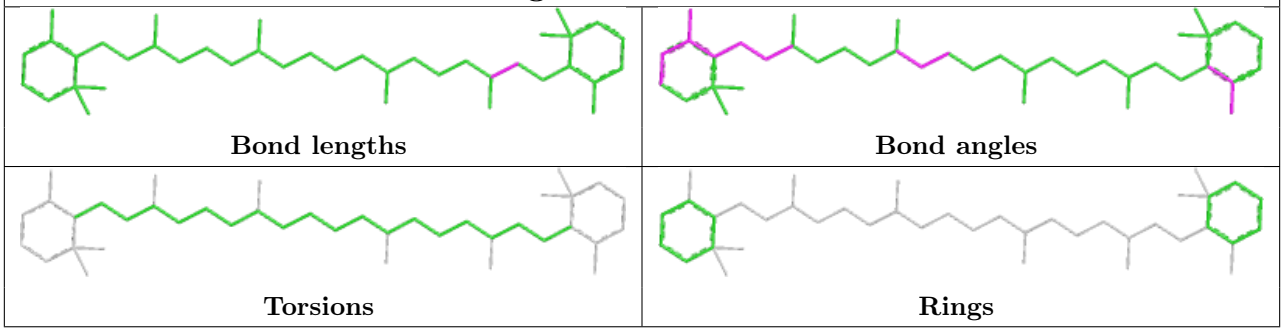


Rings

Ligand LMG c 501



Ligand BCR a 413



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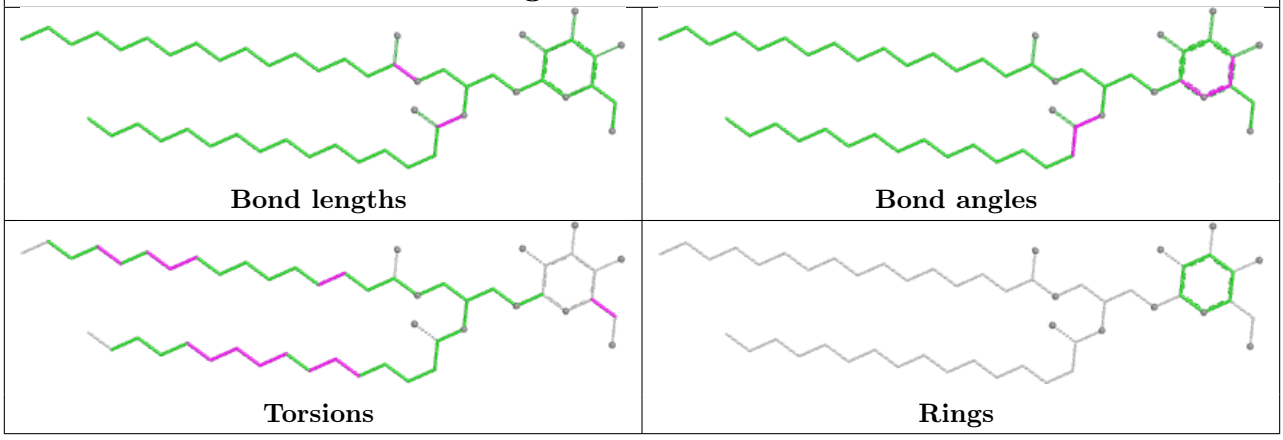
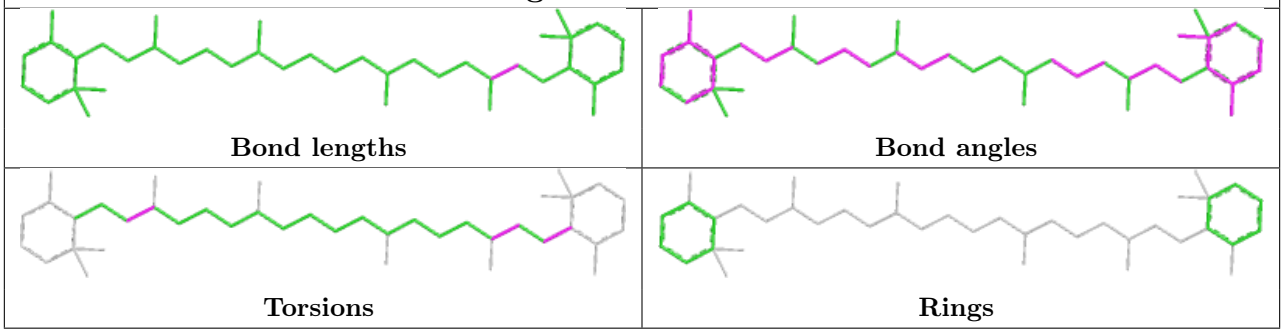
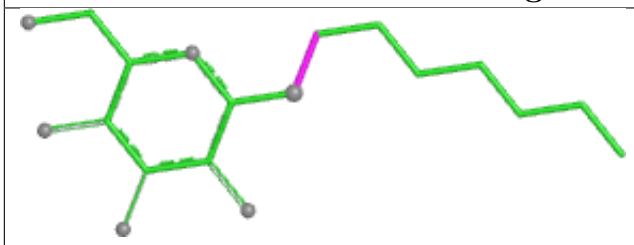


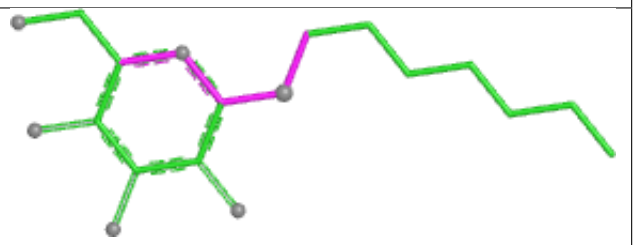
Ligand BCR d 404



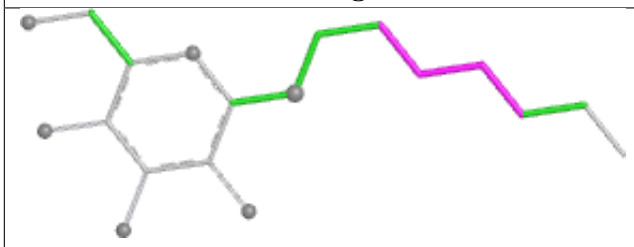
Ligand HTG b 601



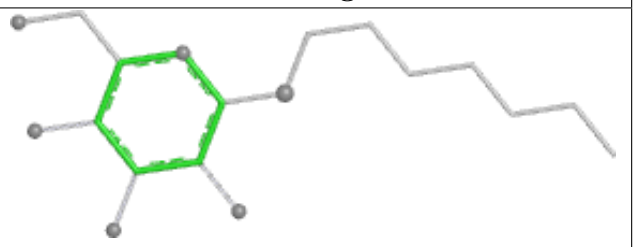
Bond lengths



Bond angles

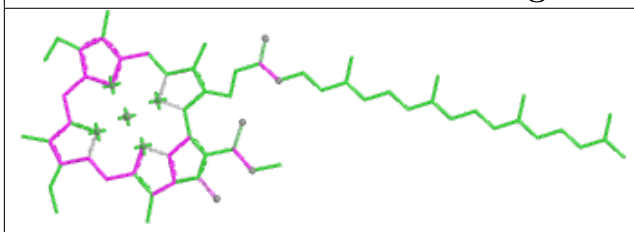


Torsions



Rings

Ligand CLA b 610



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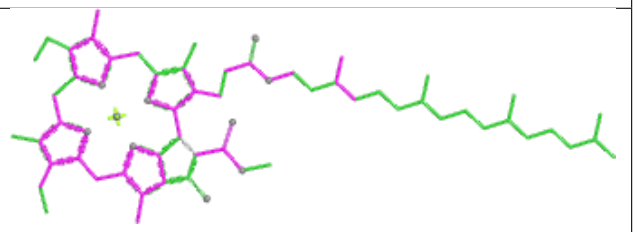
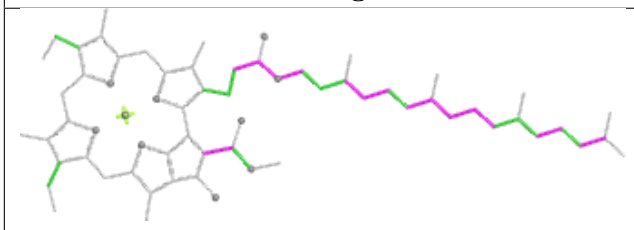
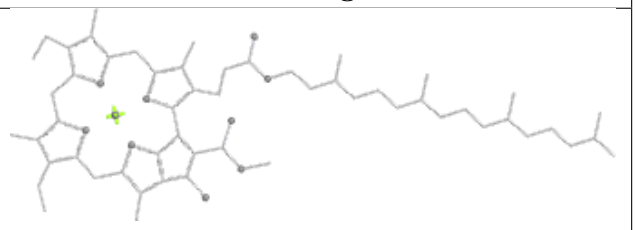


Bond angles

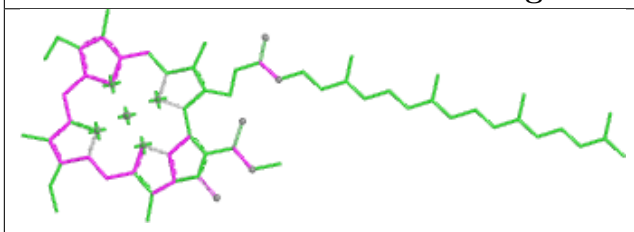


Torsions



Rings

Ligand CLA C 508



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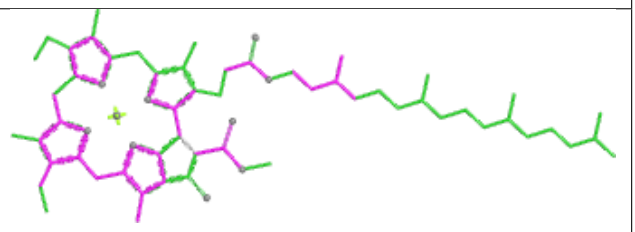
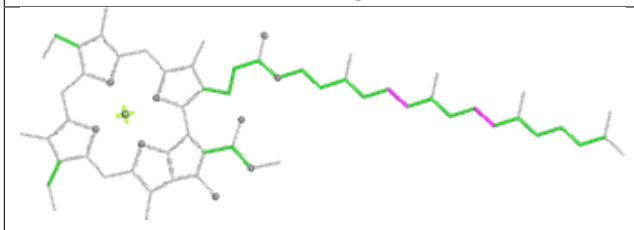
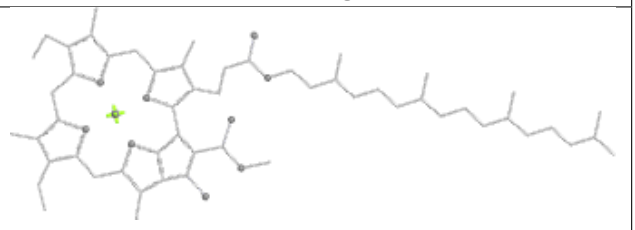


Bond angles

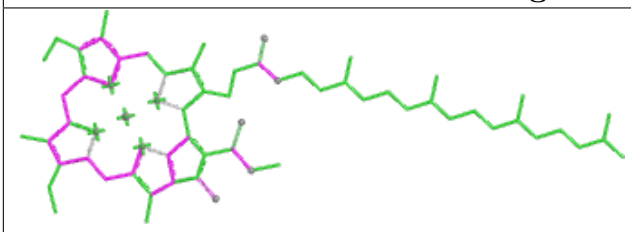


Torsions

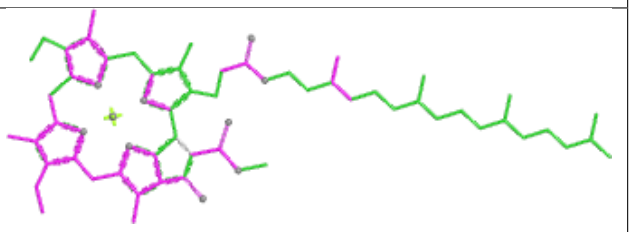


Rings

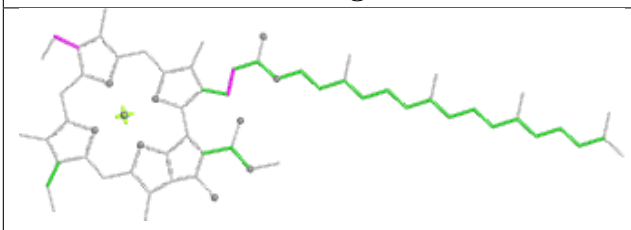
Ligand CLA c 506



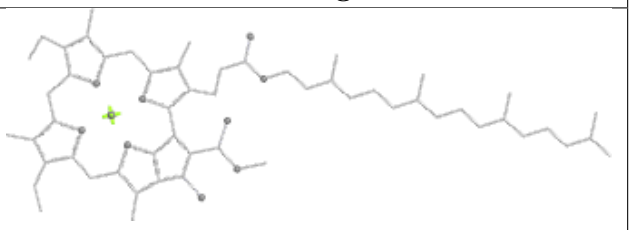
Bond lengths



Bond angles

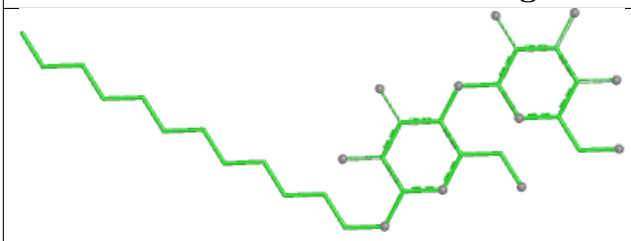


Torsions



Rings

Ligand LMT m 102



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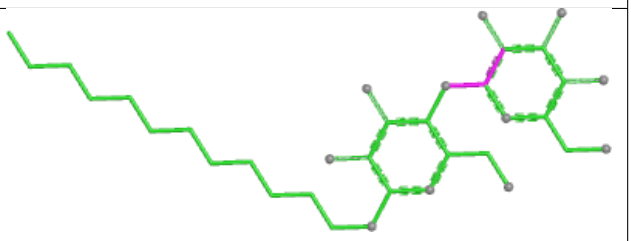
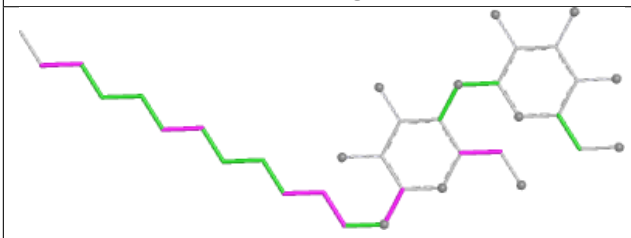
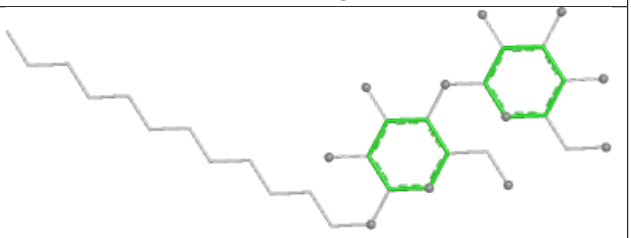


Bond angles

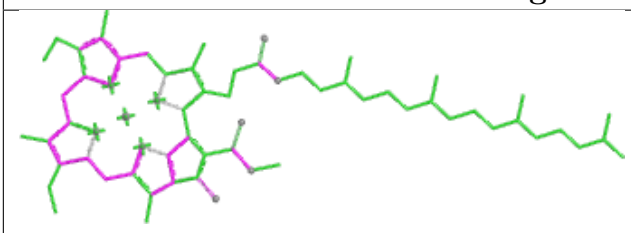


Torsions



Rings

Ligand CLA c 511



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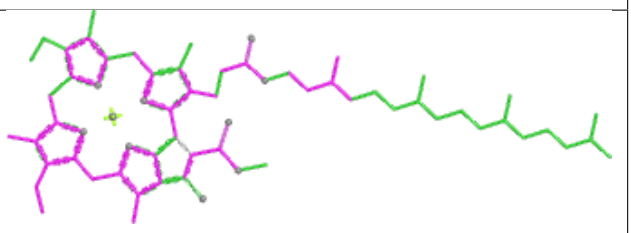
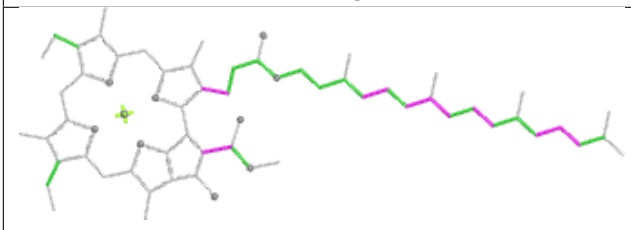
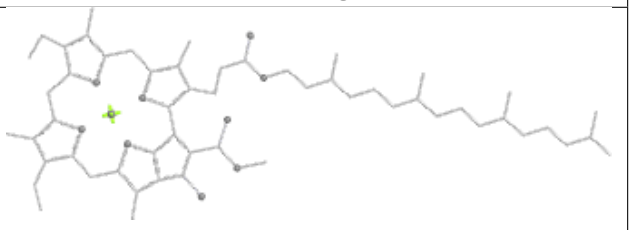


Bond angles

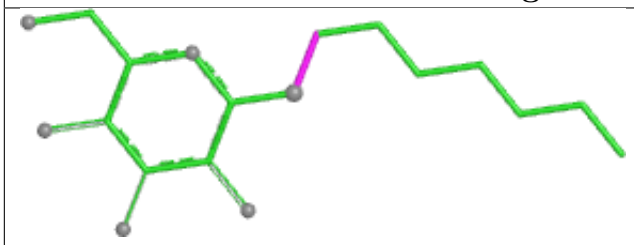


Torsions



Rings

Ligand HTG B 633



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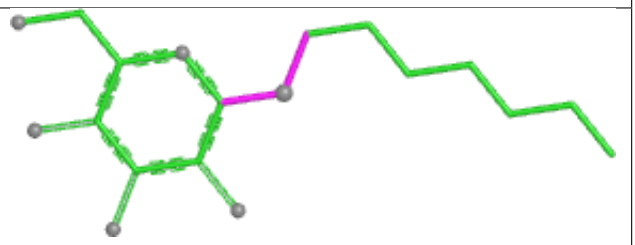
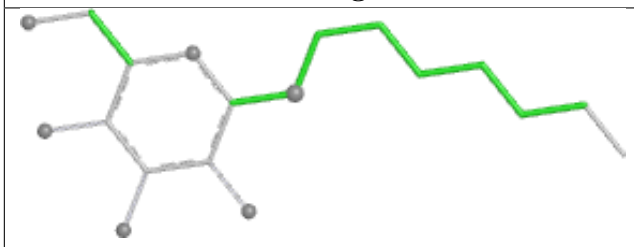
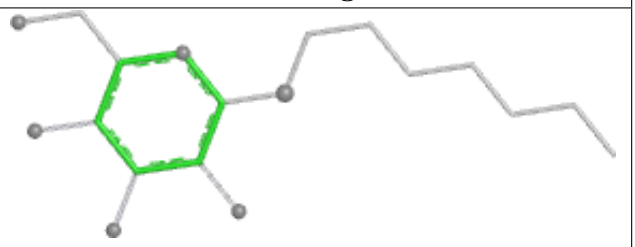


Bond angles

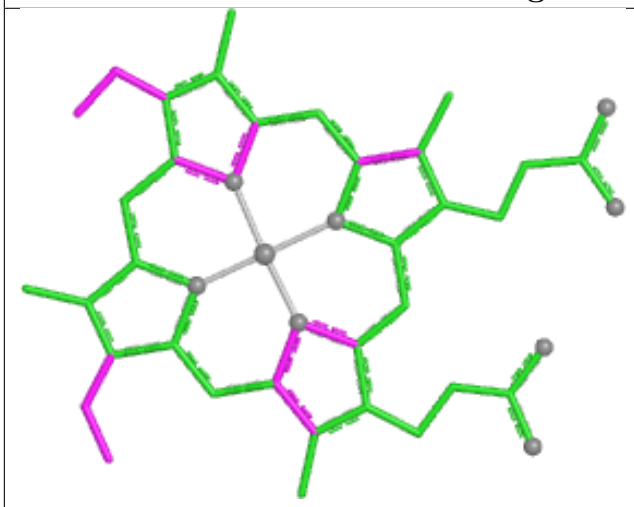


Torsions

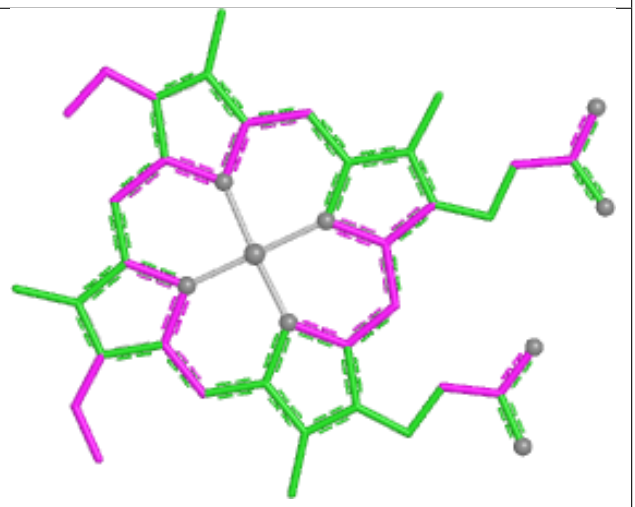


Rings

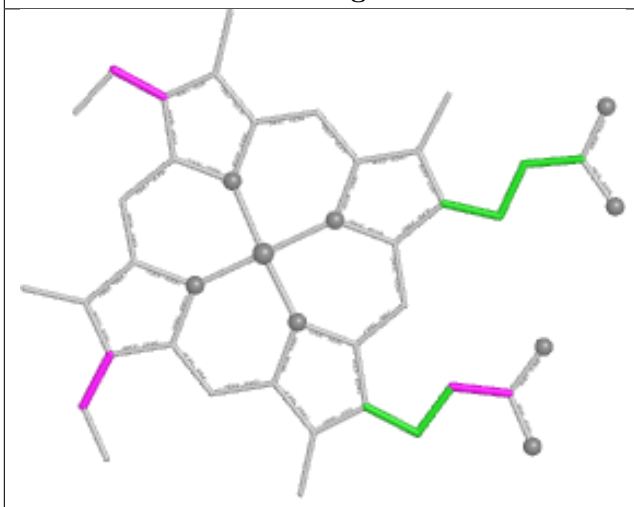
Ligand HEC v 205



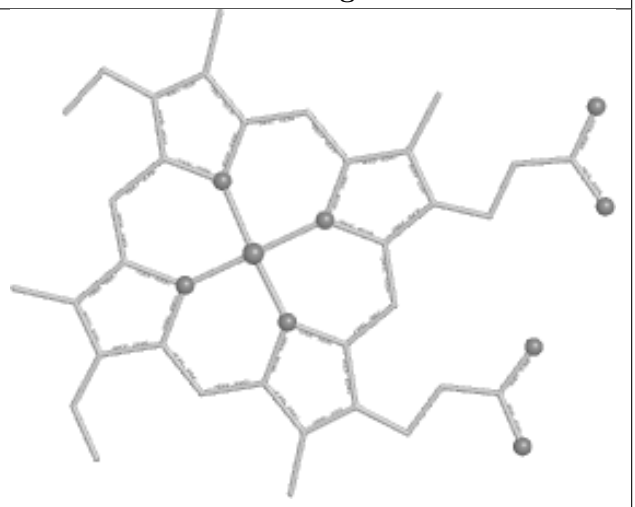
Bond lengths



Bond angles

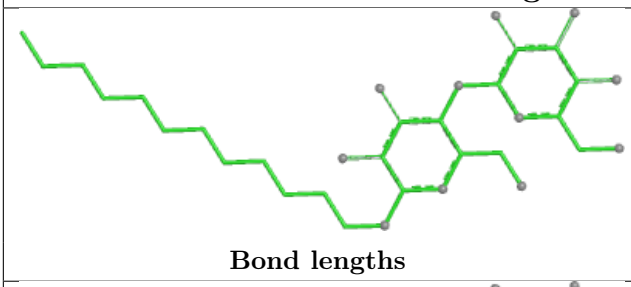


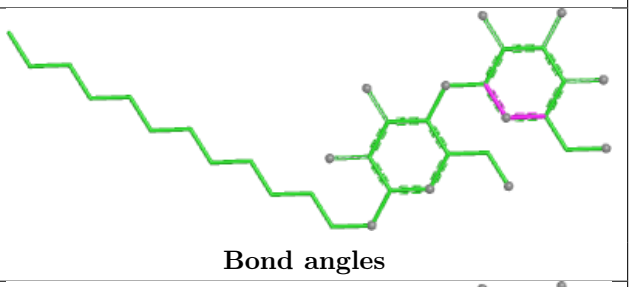
Torsions

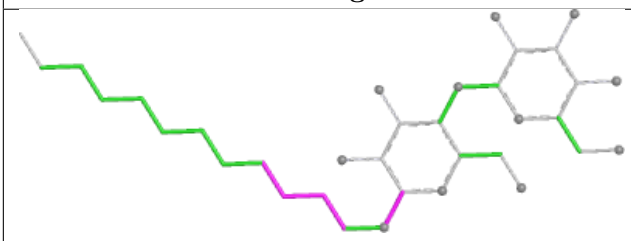


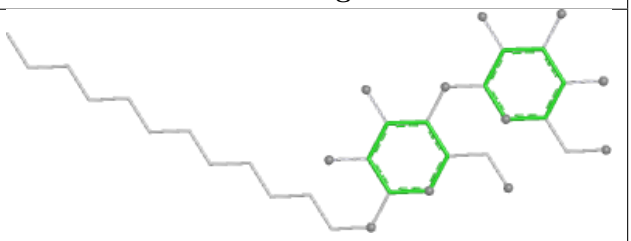
Rings

Ligand LMT F 101

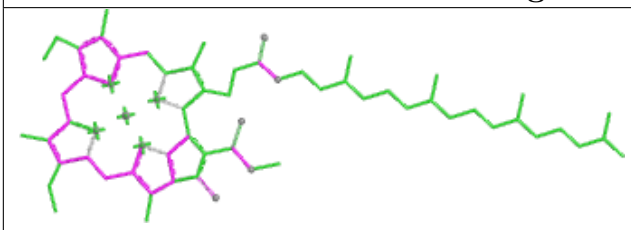

Bond lengths

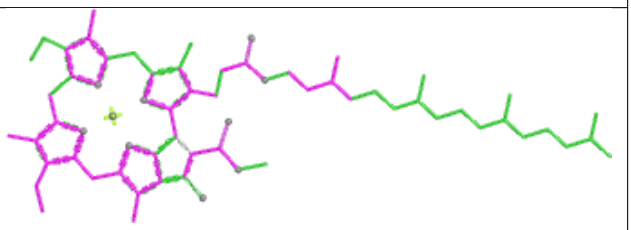

Bond angles

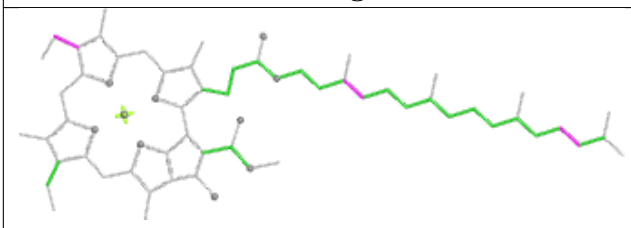

Torsions

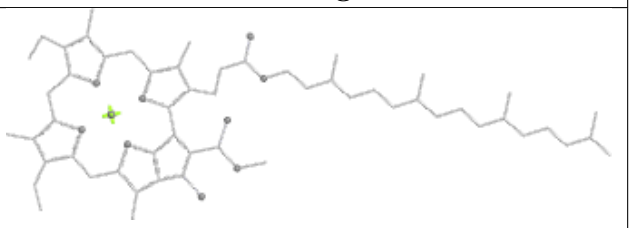

Rings

Ligand CLA d 403


Bond lengths

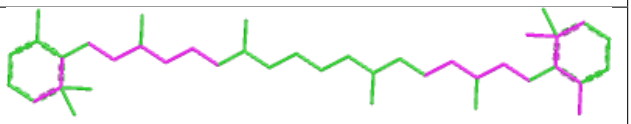

Bond angles

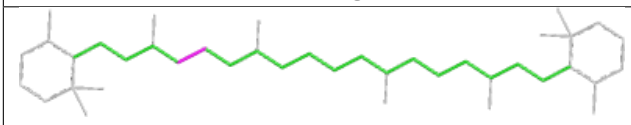

Torsions

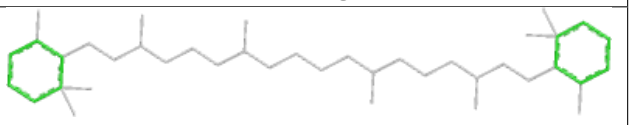

Rings

Ligand BCR k 101

Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.70	0 100 100	16, 37, 62, 117	53 (15%)
1	a	334/344 (97%)	-0.66	4 (1%) 76 79	17, 38, 70, 152	55 (16%)
2	B	504/505 (99%)	-0.63	2 (0%) 88 90	23, 43, 77, 123	10 (1%)
2	b	503/505 (99%)	-0.54	6 (1%) 76 79	26, 43, 78, 180	12 (2%)
3	C	451/455 (99%)	-0.52	0 100 100	17, 51, 70, 116	7 (1%)
3	c	455/455 (100%)	-0.52	0 100 100	19, 53, 70, 115	13 (2%)
4	D	341/342 (99%)	-0.74	0 100 100	18, 39, 61, 131	16 (4%)
4	d	341/342 (99%)	-0.72	1 (0%) 90 91	19, 41, 60, 122	16 (4%)
5	E	81/84 (96%)	-0.09	1 (1%) 76 79	32, 63, 94, 130	2 (2%)
5	e	81/84 (96%)	-0.00	2 (2%) 58 62	36, 64, 115, 176	2 (2%)
6	F	34/44 (77%)	-0.18	0 100 100	46, 56, 90, 105	0
6	f	32/44 (72%)	-0.15	1 (3%) 51 55	47, 57, 116, 141	0
7	H	65/65 (100%)	-0.31	2 (3%) 51 55	35, 52, 72, 150	1 (1%)
7	h	65/65 (100%)	-0.39	2 (3%) 51 55	42, 55, 75, 163	0
8	I	37/38 (97%)	-0.26	0 100 100	43, 54, 108, 151	0
8	i	37/38 (97%)	-0.23	1 (2%) 56 60	42, 52, 98, 131	0
9	J	38/39 (97%)	0.09	2 (5%) 32 36	46, 61, 135, 169	0
9	j	39/39 (100%)	-0.05	1 (2%) 57 61	47, 61, 131, 171	0
10	K	37/37 (100%)	-0.29	0 100 100	51, 61, 77, 101	0
10	k	37/37 (100%)	-0.32	0 100 100	52, 61, 77, 102	0
11	L	37/37 (100%)	-0.72	0 100 100	18, 35, 100, 120	1 (2%)
11	l	37/37 (100%)	-0.65	0 100 100	22, 35, 99, 120	1 (2%)
12	M	33/36 (91%)	-0.72	0 100 100	22, 37, 63, 113	1 (3%)
12	m	33/36 (91%)	-0.67	0 100 100	32, 38, 68, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.57	2 (0%)	82	84	24, 48, 91, 137	8 (3%)
13	o	243/244 (99%)	-0.48	2 (0%)	82	84	27, 50, 104, 170	5 (2%)
14	T	29/32 (90%)	-0.74	1 (3%)	48	52	31, 37, 64, 133	1 (3%)
14	t	29/32 (90%)	-0.67	1 (3%)	48	52	29, 37, 64, 133	1 (3%)
15	U	97/104 (93%)	-0.65	0	100	100	37, 48, 77, 116	0
15	u	97/104 (93%)	-0.64	0	100	100	39, 49, 71, 116	0
16	V	137/137 (100%)	-0.54	0	100	100	20, 49, 78, 116	2 (1%)
16	v	137/137 (100%)	-0.54	1 (0%)	84	85	21, 55, 84, 118	1 (0%)
17	Y	29/30 (96%)	0.76	3 (10%)	12	13	66, 80, 141, 149	0
17	y	29/30 (96%)	0.42	3 (10%)	12	13	66, 81, 142, 149	0
18	X	39/40 (97%)	0.09	1 (2%)	57	61	51, 61, 115, 136	0
18	x	38/40 (95%)	0.19	2 (5%)	32	36	53, 62, 116, 137	0
19	Z	62/62 (100%)	0.28	4 (6%)	25	28	66, 78, 125, 165	0
19	z	62/62 (100%)	0.44	3 (4%)	35	40	68, 80, 126, 166	0
20	R	18/34 (52%)	2.74	12 (66%)	0	0	106, 137, 176, 178	0
All	All	5275/5384 (97%)	-0.50	60 (1%)	78	80	16, 47, 90, 180	208 (3%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	5.2
20	R	3	TRP	4.3
19	z	3	ILE	4.0
2	b	499	VAL	3.9
20	R	13	LEU	3.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.96	0.06	35,38,64,74	0
12	FME	m	1	10/11	0.96	0.08	34,43,98,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.97	0.07	37,45,52,53	0
8	FME	i	1	10/11	0.97	0.06	41,51,56,58	0
12	FME	M	1	10/11	0.97	0.07	31,47,81,85	0
14	FME	t	1	10/11	0.97	0.05	28,38,44,87	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	e	101	62/66	0.69	0.16	70,118,175,181	0
36	DGD	D	406	52/66	0.70	0.15	65,108,147,157	0
37	LHG	e	102	42/49	0.70	0.13	69,134,167,172	0
29	LMT	F	101	35/35	0.73	0.15	86,125,152,156	0
34	CA	b	609	1/1	0.75	0.12	134,134,134,134	0
29	LMT	b	630	25/35	0.75	0.14	72,92,147,149	0
29	LMT	C	521	35/35	0.76	0.14	90,123,152,162	0
32	UNL	M	102	10/-	0.76	0.12	47,64,75,75	0
29	LMT	a	419	35/35	0.77	0.14	87,111,130,134	0
32	UNL	a	403	30/-	0.77	0.14	69,91,126,131	0
27	SQD	f	101	43/54	0.77	0.14	86,120,144,145	0
32	UNL	m	101	10/-	0.78	0.15	49,60,85,88	0
35	HTG	D	412	16/19	0.79	0.14	75,142,157,157	0
32	UNL	j	101	10/-	0.79	0.14	70,82,96,99	0
28	GOL	V	201	6/6	0.79	0.14	64,77,86,93	0
29	LMT	f	102	35/35	0.79	0.13	72,121,149,154	0
29	LMT	M	103	35/35	0.80	0.14	41,102,141,150	0
32	UNL	A	420	28/-	0.80	0.14	61,86,104,106	0
35	HTG	c	526	19/19	0.80	0.12	66,105,123,137	0
32	UNL	C	527	34/-	0.81	0.13	73,108,129,134	0
32	UNL	I	101	40/-	0.81	0.14	41,84,142,153	0
29	LMT	A	417	35/35	0.82	0.12	40,80,108,129	0
35	HTG	V	206	19/19	0.82	0.12	66,94,116,209	0
32	UNL	J	101	10/-	0.82	0.13	47,72,89,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMG	C	520	51/55	0.82	0.12	56,109,125,129	0
32	UNL	i	101	40/-	0.82	0.13	48,78,138,141	0
37	LHG	E	101	42/49	0.82	0.12	67,101,123,128	0
35	HTG	B	625	19/19	0.82	0.11	70,112,141,147	0
35	HTG	b	608	19/19	0.83	0.12	56,108,148,148	0
29	LMT	D	401	35/35	0.83	0.12	67,118,146,155	0
32	UNL	D	411	40/-	0.83	0.12	52,79,130,139	0
35	HTG	d	411	16/19	0.84	0.11	65,109,124,127	0
28	GOL	c	503	6/6	0.84	0.17	76,80,97,101	0
32	UNL	b	633	33/-	0.84	0.14	50,94,155,158	0
32	UNL	c	527	32/-	0.84	0.13	67,100,136,144	0
35	HTG	B	633	19/19	0.84	0.11	56,109,139,175	0
33	LMG	z	101	39/55	0.85	0.13	67,115,138,158	0
34	CA	B	601	1/1	0.85	0.08	130,130,130,130	0
31	PL9	A	419[A]	55/55	0.85	0.14	68,94,108,110	55
31	PL9	A	419[B]	55/55	0.85	0.14	69,94,108,111	55
31	PL9	a	415[A]	55/55	0.85	0.15	75,104,117,119	55
31	PL9	a	415[B]	55/55	0.85	0.15	73,103,117,120	55
29	LMT	a	404	35/35	0.85	0.12	47,82,112,131	0
32	UNL	d	410	36/-	0.85	0.11	51,76,129,142	0
32	UNL	B	634	33/-	0.85	0.14	56,87,134,138	0
27	SQD	B	621	54/54	0.85	0.12	51,88,147,155	0
28	GOL	O	301	6/6	0.85	0.10	64,79,82,85	0
27	SQD	F	103	43/54	0.85	0.11	76,102,119,129	0
33	LMG	Z	101	37/55	0.85	0.14	54,111,132,135	0
33	LMG	c	524	51/55	0.85	0.11	49,106,129,132	0
35	HTG	C	523	19/19	0.86	0.10	79,91,124,126	0
27	SQD	a	405	54/54	0.86	0.10	47,77,116,122	0
35	HTG	b	632	19/19	0.86	0.11	66,118,148,149	0
28	GOL	C	524	6/6	0.87	0.12	59,63,76,80	0
27	SQD	A	416	54/54	0.87	0.11	52,73,111,128	0
35	HTG	B	624	19/19	0.87	0.12	48,64,89,93	0
29	LMT	B	635	25/35	0.87	0.12	40,80,134,138	0
28	GOL	T	102	6/6	0.87	0.13	94,108,113,115	0
27	SQD	L	102	54/54	0.87	0.10	50,77,123,141	0
29	LMT	m	103	35/35	0.87	0.11	40,96,125,132	0
28	GOL	a	402	6/6	0.87	0.12	70,93,94,94	0
34	CA	f	103	1/1	0.88	0.07	106,106,106,106	0
28	GOL	v	201	6/6	0.89	0.12	68,88,90,92	0
29	LMT	T	104	25/35	0.89	0.12	37,79,133,138	0
35	HTG	C	522	19/19	0.89	0.09	72,85,101,107	0
35	HTG	b	631	19/19	0.89	0.12	56,71,84,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	T	101	6/6	0.89	0.14	58,74,93,97	0
35	HTG	c	525	19/19	0.89	0.09	87,92,102,120	0
28	GOL	A	415	6/6	0.90	0.11	52,75,79,82	0
33	LMG	c	523	51/55	0.90	0.10	48,86,111,115	0
28	GOL	B	630	6/6	0.90	0.12	48,59,72,76	0
22	CL	U	201	1/1	0.90	0.11	92,92,92,92	0
28	GOL	t	102	6/6	0.90	0.14	51,80,90,96	0
33	LMG	A	421	51/55	0.90	0.09	57,82,106,115	0
33	LMG	C	519	51/55	0.90	0.10	49,83,108,117	0
29	LMT	m	102	35/35	0.90	0.09	42,81,100,107	0
33	LMG	c	501	51/55	0.91	0.10	57,79,98,99	0
28	GOL	B	626	6/6	0.91	0.10	44,54,59,80	0
28	GOL	b	606	6/6	0.91	0.10	64,79,86,86	0
29	LMT	M	101	35/35	0.91	0.09	41,80,99,100	0
38	HEM	F	102	43/43	0.91	0.09	44,66,89,137	0
28	GOL	v	202	6/6	0.92	0.10	70,79,96,112	0
23	BCT	a	417[A]	4/4	0.92	0.08	59,60,62,70	4
32	UNL	X	101	18/-	0.92	0.10	54,73,97,100	0
28	GOL	B	636	6/6	0.92	0.08	48,56,62,62	0
28	GOL	b	605	6/6	0.92	0.14	70,80,101,103	0
23	BCT	a	417[B]	4/4	0.92	0.08	50,59,61,66	4
24	CLA	c	518	65/65	0.92	0.09	56,80,99,108	0
32	UNL	d	412	18/-	0.92	0.10	60,72,112,113	0
27	SQD	A	412	54/54	0.92	0.09	45,78,95,98	0
28	GOL	B	628	6/6	0.92	0.10	54,73,79,84	0
24	CLA	C	506	65/65	0.93	0.08	46,62,105,114	0
28	GOL	A	414	6/6	0.93	0.12	49,59,62,64	0
24	CLA	C	513	65/65	0.93	0.08	52,66,102,109	0
28	GOL	A	422	6/6	0.93	0.07	68,73,74,82	0
24	CLA	b	610	65/65	0.93	0.09	44,68,104,134	0
35	HTG	B	632	19/19	0.93	0.08	45,72,101,109	0
24	CLA	B	602	65/65	0.93	0.09	41,62,95,124	0
32	UNL	d	409	17/-	0.93	0.10	47,69,97,101	0
37	LHG	D	409	49/49	0.93	0.10	39,55,116,129	0
28	GOL	a	420	6/6	0.93	0.09	78,80,91,92	0
26	BCR	C	514	40/40	0.93	0.08	49,67,81,84	0
26	BCR	y	101	40/40	0.93	0.08	43,63,72,80	0
33	LMG	B	622	51/55	0.94	0.07	33,50,74,90	0
26	BCR	t	101	40/40	0.94	0.06	34,47,64,65	0
28	GOL	A	413	6/6	0.94	0.09	45,49,54,58	0
33	LMG	D	413	51/55	0.94	0.09	38,60,105,128	0
24	CLA	C	504	65/65	0.94	0.07	34,47,81,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMG	b	629	51/55	0.94	0.08	42,51,72,94	0
24	CLA	b	615	65/65	0.94	0.07	32,44,88,106	0
23	BCT	A	404[B]	4/4	0.94	0.08	47,48,62,72	4
23	BCT	A	404[A]	4/4	0.94	0.08	47,55,60,72	4
33	LMG	d	413	51/55	0.94	0.08	45,58,100,110	0
28	GOL	B	627	6/6	0.94	0.11	52,62,79,94	0
36	DGD	C	517	62/66	0.94	0.07	42,54,96,112	0
26	BCR	D	404	40/40	0.94	0.07	41,50,92,105	0
26	BCR	c	528	40/40	0.94	0.08	60,73,83,85	0
37	LHG	D	407	49/49	0.94	0.08	31,49,62,73	0
28	GOL	o	301	6/6	0.94	0.09	65,78,89,107	0
32	UNL	D	410	17/-	0.94	0.08	40,70,83,89	0
26	BCR	d	404	40/40	0.94	0.07	40,52,79,83	0
27	SQD	a	414	54/54	0.94	0.09	57,80,103,109	0
34	CA	F	104	1/1	0.95	0.04	84,84,84,84	0
26	BCR	h	101	40/40	0.95	0.06	38,55,66,68	0
28	GOL	B	631	6/6	0.95	0.10	43,76,84,87	0
26	BCR	k	101	40/40	0.95	0.07	44,59,73,75	0
24	CLA	b	623	65/65	0.95	0.07	26,40,88,115	0
24	CLA	b	625	65/65	0.95	0.08	35,52,101,109	0
24	CLA	c	508	65/65	0.95	0.07	41,52,62,86	0
24	CLA	c	511	65/65	0.95	0.07	43,63,91,107	0
24	CLA	c	512	65/65	0.95	0.07	42,54,67,72	0
24	CLA	c	517	65/65	0.95	0.06	49,63,82,86	0
24	CLA	C	512	65/65	0.95	0.07	48,64,81,92	0
28	GOL	b	602	6/6	0.95	0.09	56,58,65,89	0
26	BCR	A	411	40/40	0.95	0.06	28,39,46,48	0
24	CLA	B	615	65/65	0.95	0.07	26,40,90,99	0
24	CLA	C	505	65/65	0.95	0.07	38,47,68,78	0
26	BCR	H	101	40/40	0.95	0.06	35,51,65,67	0
31	PL9	d	405[A]	55/55	0.95	0.06	27,37,46,57	55
36	DGD	C	516	62/66	0.95	0.07	33,47,88,96	0
31	PL9	d	405[B]	55/55	0.95	0.06	24,38,46,57	55
26	BCR	K	101	40/40	0.95	0.07	43,57,65,68	0
36	DGD	H	102	62/66	0.95	0.07	35,48,66,78	0
36	DGD	c	521	62/66	0.95	0.07	41,52,105,128	0
36	DGD	c	522	62/66	0.95	0.07	38,52,87,96	0
26	BCR	T	103	40/40	0.95	0.06	31,46,61,62	0
26	BCR	Y	101	40/40	0.95	0.06	47,60,71,80	0
28	GOL	v	203	6/6	0.95	0.10	48,49,57,59	0
26	BCR	b	627	40/40	0.95	0.06	31,42,60,67	0
37	LHG	d	408	49/49	0.95	0.09	34,53,104,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	617	65/65	0.95	0.09	36,49,116,118	0
24	CLA	b	618	65/65	0.95	0.06	37,49,58,71	0
24	CLA	c	510	65/65	0.96	0.06	36,48,67,78	0
24	CLA	C	508	65/65	0.96	0.06	36,48,114,125	0
24	CLA	C	509	65/65	0.96	0.07	43,55,74,81	0
24	CLA	c	513	65/65	0.96	0.07	35,48,113,129	0
24	CLA	c	515	65/65	0.96	0.06	39,52,65,71	0
24	CLA	c	516	65/65	0.96	0.07	43,55,75,88	0
24	CLA	C	510	65/65	0.96	0.06	39,51,62,71	0
24	CLA	C	511	65/65	0.96	0.07	41,58,69,83	0
24	CLA	d	403	65/65	0.96	0.07	41,51,103,111	0
25	PHO	a	418[A]	64/64	0.96	0.05	28,41,47,50	64
25	PHO	a	418[B]	64/64	0.96	0.05	28,41,48,51	64
28	GOL	B	629	6/6	0.96	0.09	50,52,55,60	0
24	CLA	A	410	65/65	0.96	0.07	30,45,122,130	0
31	PL9	D	405[A]	55/55	0.96	0.05	26,37,44,57	55
31	PL9	D	405[B]	55/55	0.96	0.05	28,36,45,62	55
26	BCR	B	619	40/40	0.96	0.05	27,40,56,63	0
26	BCR	B	620	40/40	0.96	0.06	35,46,58,60	0
24	CLA	A	407	65/65	0.96	0.06	28,39,101,116	0
26	BCR	C	515	40/40	0.96	0.06	39,54,63,65	0
24	CLA	D	403	65/65	0.96	0.07	38,51,101,119	0
24	CLA	a	412	65/65	0.96	0.08	31,46,114,124	0
35	HTG	b	601	19/19	0.96	0.07	40,47,70,71	0
35	HTG	b	607	19/19	0.96	0.06	47,71,80,81	0
24	CLA	C	501	65/65	0.96	0.06	38,50,73,81	0
28	GOL	V	202	6/6	0.96	0.07	39,47,52,62	0
28	GOL	V	203	6/6	0.96	0.08	54,59,59,63	0
28	GOL	V	204	6/6	0.96	0.08	72,78,80,89	0
24	CLA	C	503	65/65	0.96	0.06	40,50,61,64	0
24	CLA	b	616	65/65	0.96	0.05	24,35,44,54	0
24	CLA	B	607	65/65	0.96	0.07	32,44,93,103	0
28	GOL	b	604	6/6	0.96	0.07	58,63,68,86	0
36	DGD	C	518	62/66	0.96	0.06	35,51,74,87	0
26	BCR	c	519	40/40	0.96	0.06	39,54,66,70	0
24	CLA	b	619	65/65	0.96	0.06	36,45,53,62	0
36	DGD	c	520	62/66	0.96	0.07	36,48,94,107	0
24	CLA	b	620	65/65	0.96	0.06	29,39,49,55	0
24	CLA	b	622	65/65	0.96	0.06	27,39,56,62	0
24	CLA	B	611	65/65	0.96	0.06	36,46,54,69	0
36	DGD	h	102	62/66	0.96	0.06	39,50,67,79	0
24	CLA	b	624	65/65	0.96	0.05	33,46,62,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	614	65/65	0.96	0.06	27,36,66,74	0
24	CLA	c	506	65/65	0.96	0.06	41,55,65,70	0
37	LHG	d	406	49/49	0.96	0.07	37,51,59,74	0
24	CLA	c	507	65/65	0.96	0.06	40,51,66,73	0
24	CLA	C	507	65/65	0.96	0.07	41,56,68,70	0
24	CLA	c	509	65/65	0.96	0.06	38,53,74,79	0
25	PHO	a	411	64/64	0.97	0.04	28,36,41,47	0
24	CLA	B	613	65/65	0.97	0.05	27,37,46,54	0
24	CLA	A	406	65/65	0.97	0.04	25,32,42,51	0
24	CLA	b	621	65/65	0.97	0.05	28,40,49,52	0
24	CLA	B	603	65/65	0.97	0.05	35,43,50,53	0
24	CLA	B	616	65/65	0.97	0.06	34,45,65,77	0
24	CLA	B	604	65/65	0.97	0.05	34,43,49,63	0
22	CL	v	204	1/1	0.97	0.07	95,95,95,95	0
24	CLA	C	502	65/65	0.97	0.05	36,46,61,78	0
24	CLA	a	409	65/65	0.97	0.05	27,35,49,58	0
24	CLA	a	410	65/65	0.97	0.06	31,41,105,114	0
24	CLA	B	608	65/65	0.97	0.05	24,35,47,52	0
24	CLA	B	609	65/65	0.97	0.05	35,43,56,60	0
26	BCR	a	413	40/40	0.97	0.04	28,39,48,56	0
26	BCR	b	626	40/40	0.97	0.04	32,41,47,49	0
24	CLA	b	611	65/65	0.97	0.06	32,46,52,57	0
26	BCR	b	628	40/40	0.97	0.05	35,50,62,66	0
24	CLA	b	612	65/65	0.97	0.05	33,44,54,59	0
24	CLA	b	613	65/65	0.97	0.05	27,38,73,79	0
24	CLA	c	514	65/65	0.97	0.07	43,54,74,85	0
24	CLA	b	614	65/65	0.97	0.06	28,39,52,55	0
24	CLA	B	610	65/65	0.97	0.05	34,46,55,64	0
28	GOL	a	401	6/6	0.97	0.08	49,63,68,76	0
24	CLA	A	405	65/65	0.97	0.05	25,33,45,67	0
24	CLA	b	617	65/65	0.97	0.05	32,45,53,60	0
24	CLA	d	401	65/65	0.97	0.04	26,33,43,52	0
37	LHG	D	408	49/49	0.97	0.06	33,43,61,89	0
28	GOL	b	603	6/6	0.97	0.06	45,63,75,80	0
24	CLA	B	612	65/65	0.97	0.05	26,38,50,57	0
37	LHG	L	101	49/49	0.97	0.06	33,45,56,59	0
37	LHG	b	634	49/49	0.97	0.06	36,45,58,64	0
25	PHO	A	408	64/64	0.97	0.05	28,34,40,40	0
25	PHO	A	409[A]	64/64	0.97	0.05	33,40,47,49	64
35	HTG	B	623	19/19	0.97	0.07	40,56,72,76	0
25	PHO	A	409[B]	64/64	0.97	0.05	27,40,48,49	64
38	HEM	e	103	43/43	0.97	0.10	55,81,121,150	0

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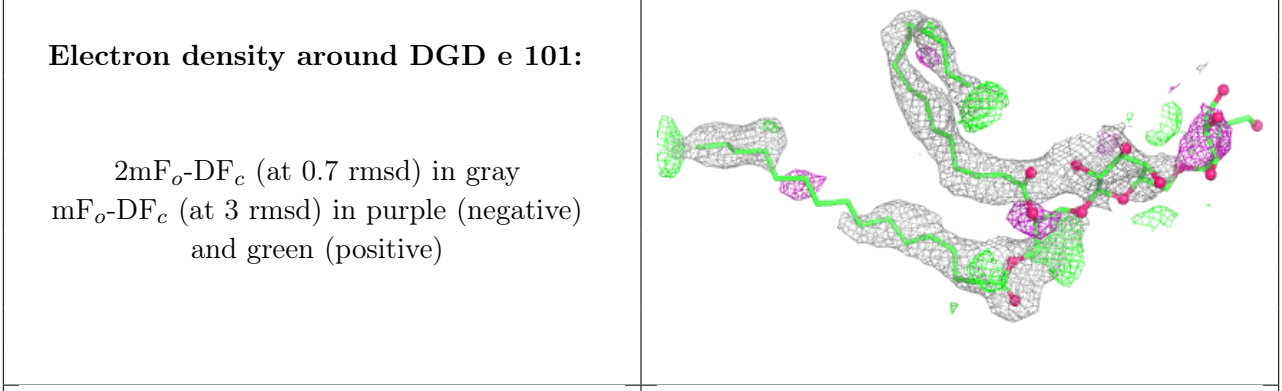
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CL	A	403[B]	1/1	0.98	0.08	35,35,35,35	1
26	BCR	B	618	40/40	0.98	0.04	27,39,46,48	0
22	CL	A	403[A]	1/1	0.98	0.08	33,33,33,33	1
24	CLA	B	605	65/65	0.98	0.05	27,36,71,75	0
24	CLA	B	606	65/65	0.98	0.05	29,39,54,58	0
37	LHG	d	407	49/49	0.98	0.06	32,42,57,88	0
24	CLA	d	402	65/65	0.98	0.05	26,36,60,71	0
24	CLA	D	402	65/65	0.98	0.05	24,34,55,61	0
28	GOL	c	502	6/6	0.98	0.05	38,44,46,48	0
28	GOL	C	525	6/6	0.98	0.04	32,42,44,45	0
39	MG	j	102	1/1	0.98	0.09	57,57,57,57	0
30	OEX	A	418[A]	10/10	0.99	0.03	30,36,43,56	10
34	CA	C	526	1/1	0.99	0.07	70,70,70,70	0
30	OEX	A	418[B]	10/10	0.99	0.03	33,37,39,39	10
22	CL	a	407[A]	1/1	0.99	0.05	36,36,36,36	1
34	CA	c	504	1/1	0.99	0.07	67,67,67,67	0
34	CA	c	505	1/1	0.99	0.03	75,75,75,75	0
22	CL	a	407[B]	1/1	0.99	0.05	37,37,37,37	1
39	MG	J	102	1/1	0.99	0.03	52,52,52,52	0
34	CA	o	302	1/1	0.99	0.03	90,90,90,90	0
40	HEC	V	205	43/43	0.99	0.05	34,40,51,56	0
40	HEC	v	205	43/43	0.99	0.05	41,52,56,60	0
22	CL	a	408[B]	1/1	1.00	0.01	40,40,40,40	1
22	CL	A	402[B]	1/1	1.00	0.01	32,32,32,32	1
21	FE2	A	401[A]	1/1	1.00	0.01	47,47,47,47	1
30	OEX	a	416[A]	10/10	1.00	0.02	34,37,40,52	10
30	OEX	a	416[B]	10/10	1.00	0.02	32,38,43,46	10
21	FE2	A	401[B]	1/1	1.00	0.01	50,50,50,50	1
34	CA	O	302	1/1	1.00	0.03	81,81,81,81	0
21	FE2	a	406[A]	1/1	1.00	0.02	48,48,48,48	1
21	FE2	a	406[B]	1/1	1.00	0.02	48,48,48,48	1
22	CL	A	402[A]	1/1	1.00	0.01	32,32,32,32	1
22	CL	a	408[A]	1/1	1.00	0.01	40,40,40,40	1

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.

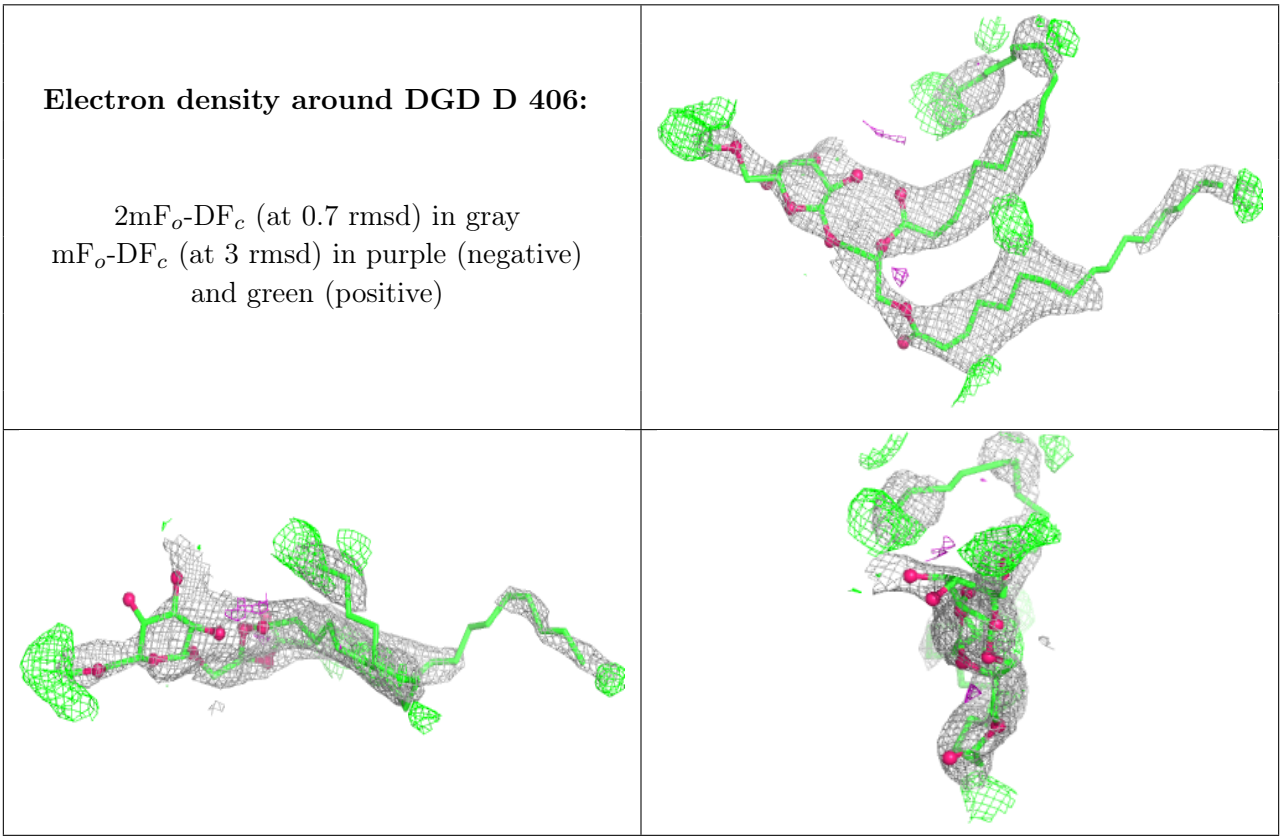
Electron density around DGD e 101:

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



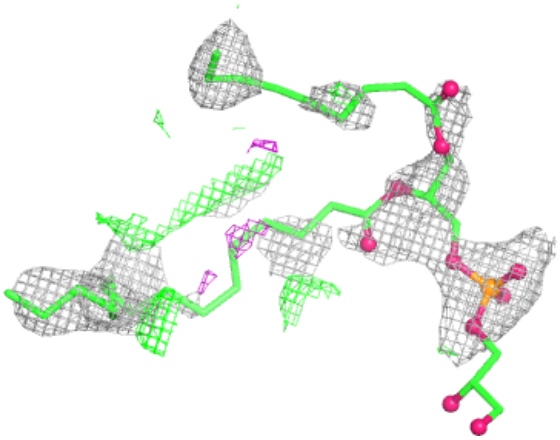
Electron density around DGD D 406:

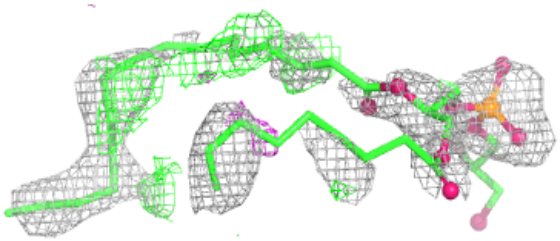
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

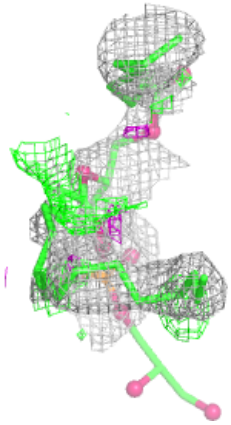


Electron density around LHG e 102:

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

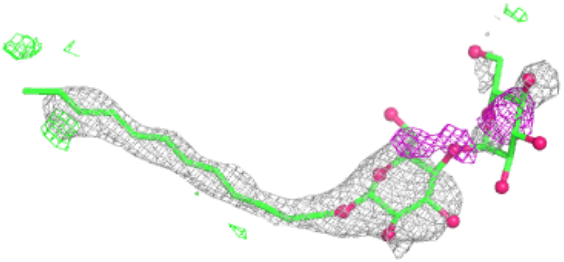


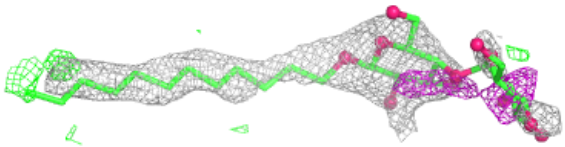


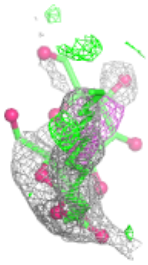


Electron density around LMT F 101:

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

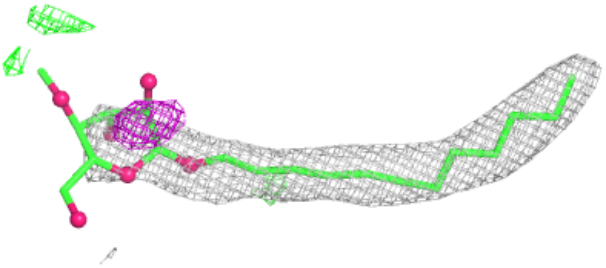


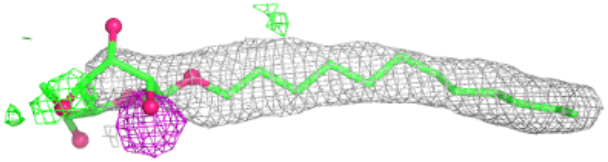


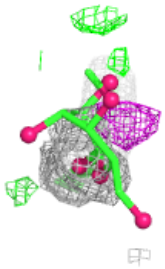


Electron density around LMT b 630:

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

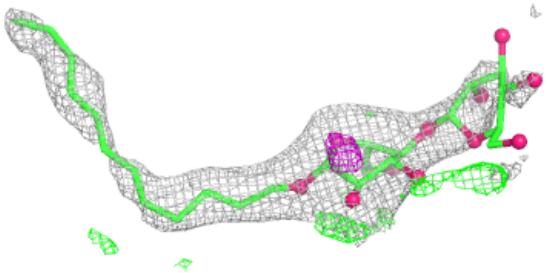


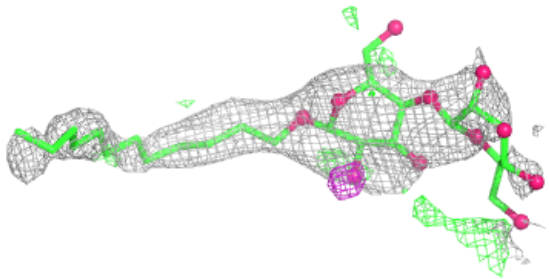


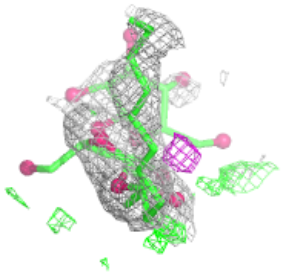


Electron density around LMT C 521:

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

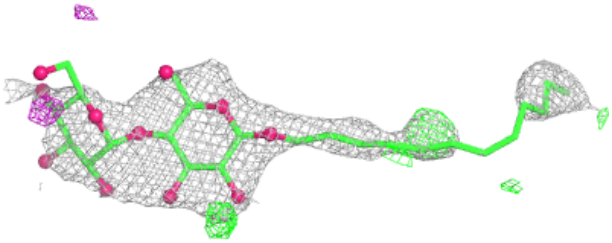


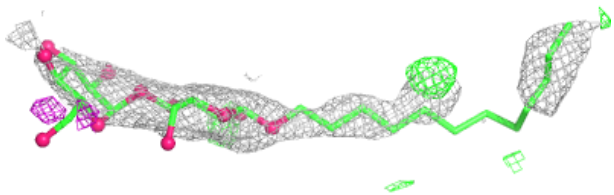




Electron density around LMT a 419:

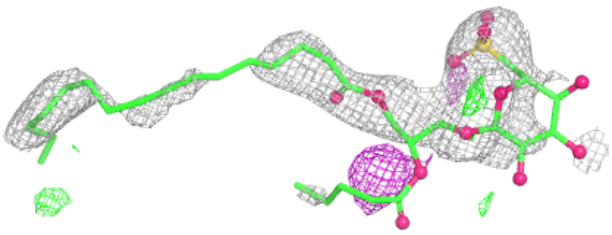
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

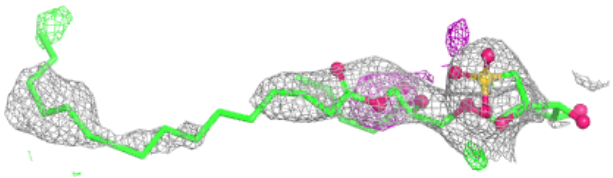


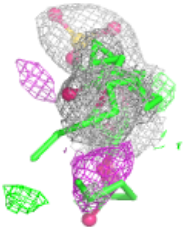


Electron density around SQD f 101:

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

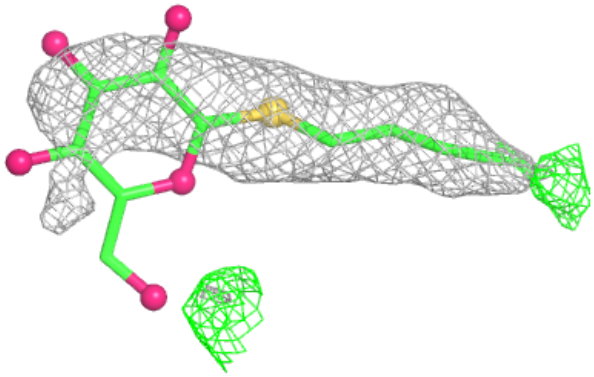


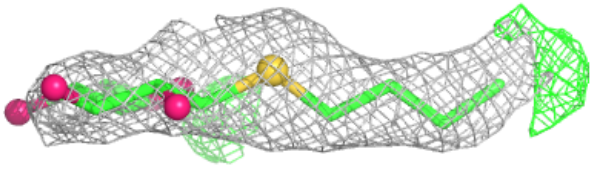


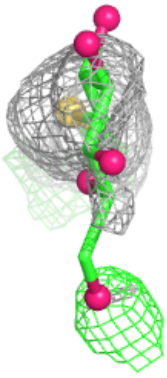


Electron density around HTG D 412:

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

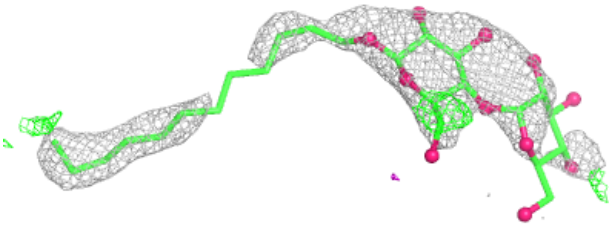


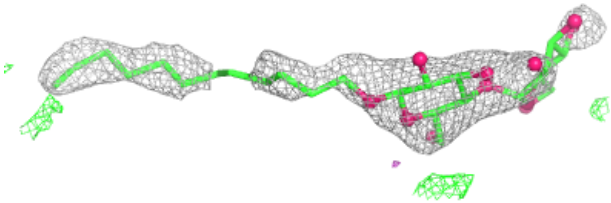


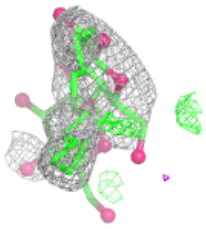


Electron density around LMT f 102:

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

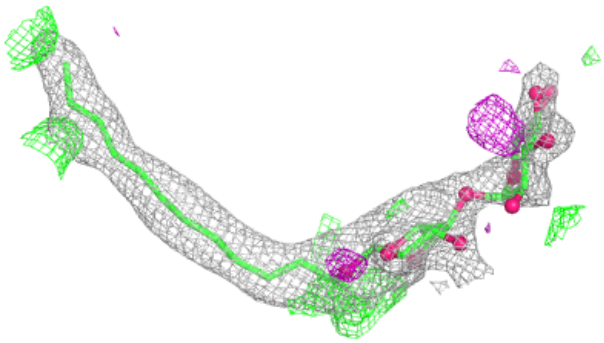


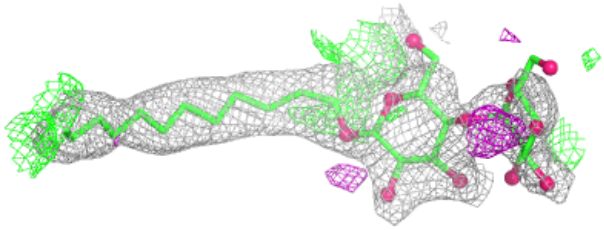


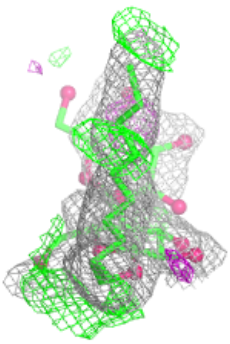


Electron density around LMT M 103:

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

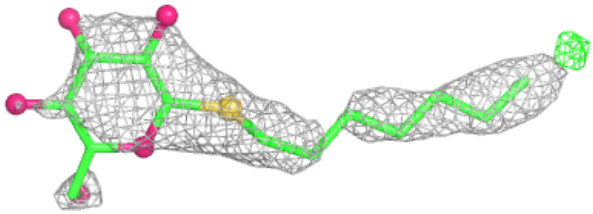


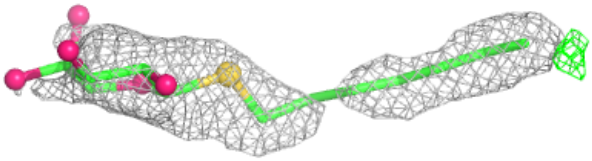


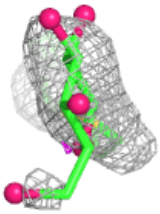


Electron density around HTG c 526:

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

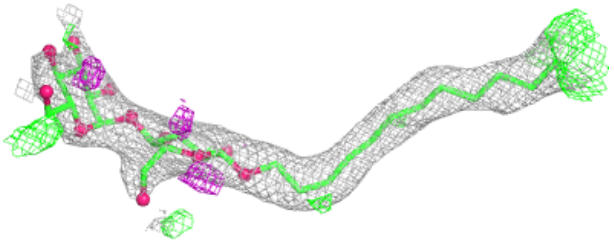


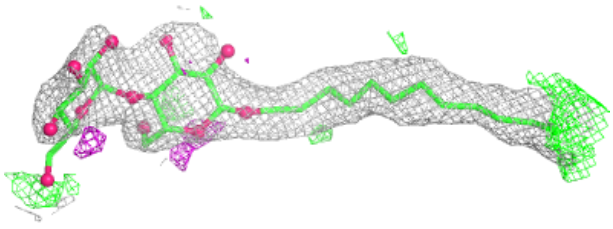


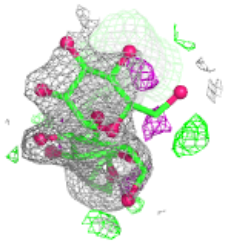


Electron density around LMT A 417:

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

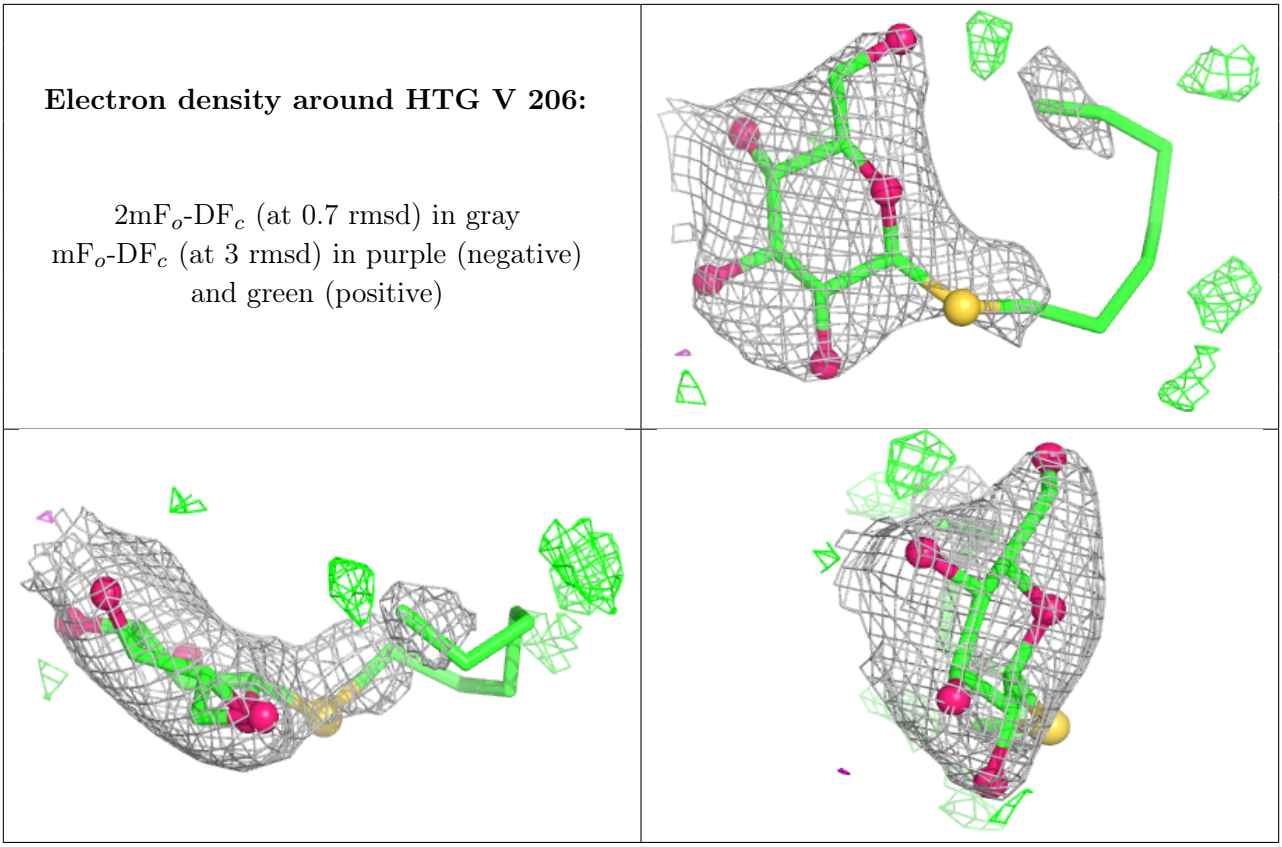






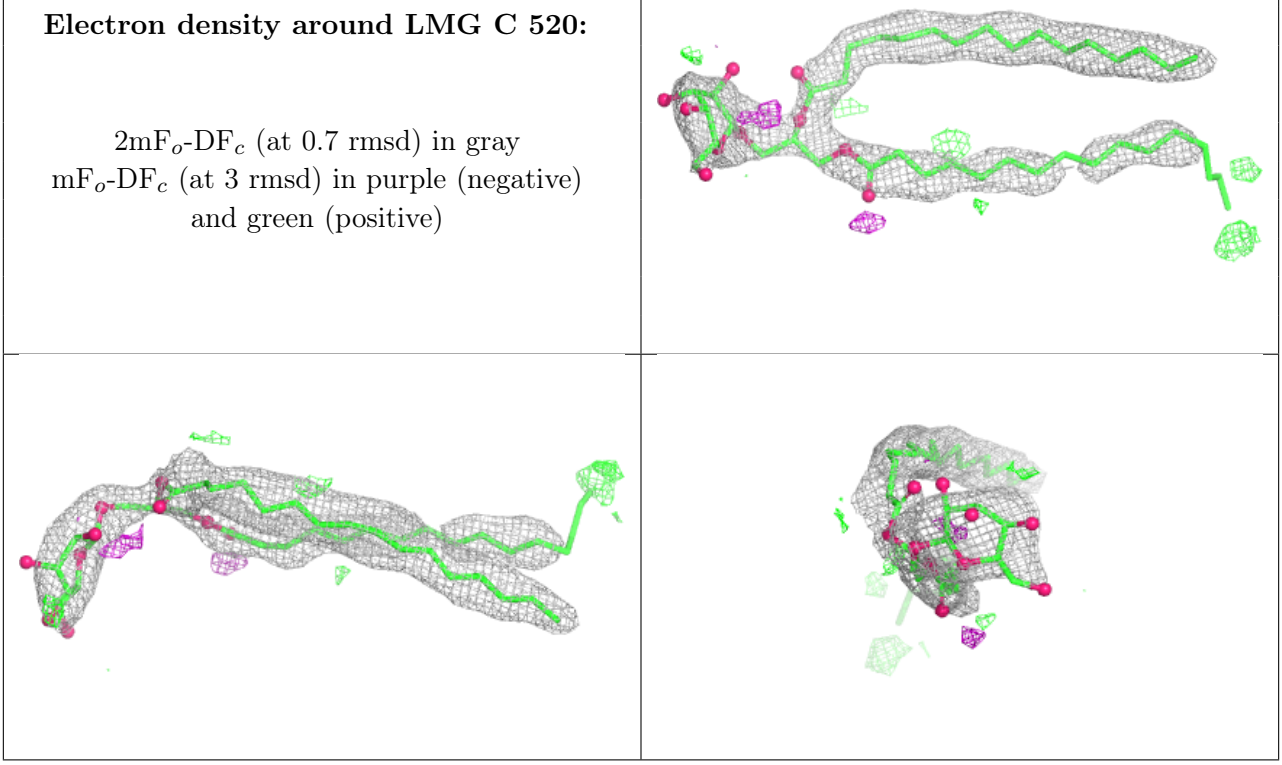
Electron density around HTG V 206:

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



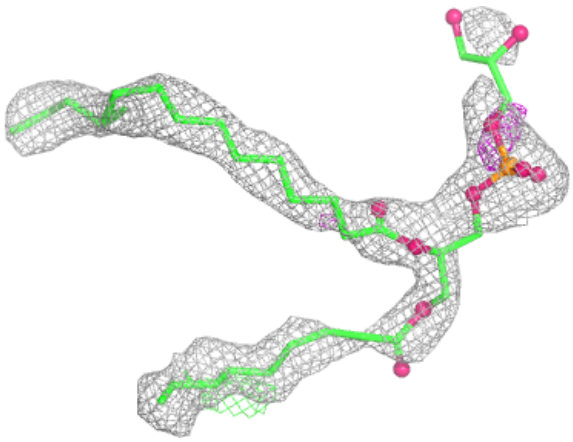
Electron density around LMG C 520:

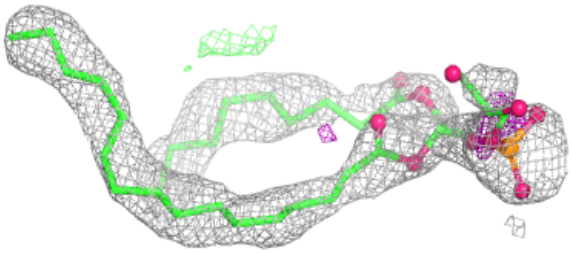
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

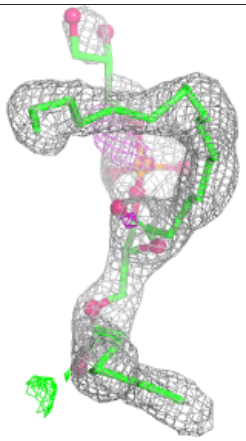


Electron density around LHG E 101:

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

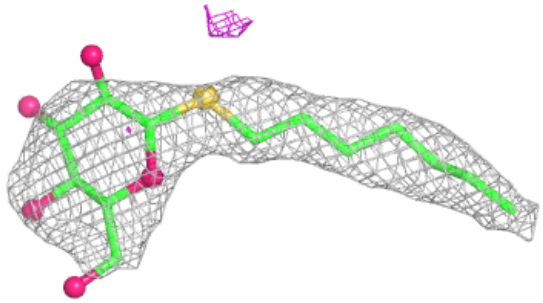


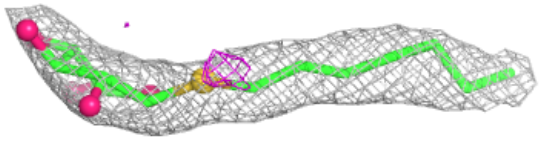


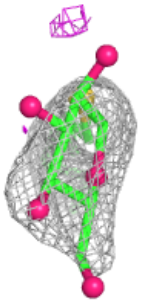


Electron density around HTG B 625:

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

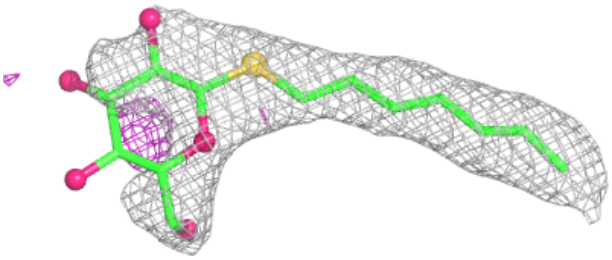


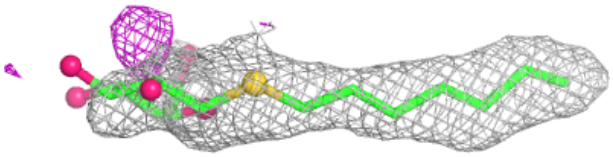


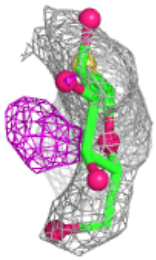


Electron density around HTG b 608:

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

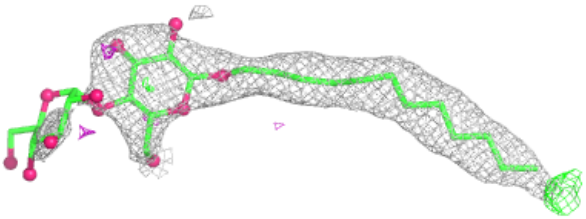


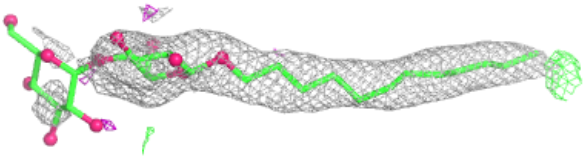


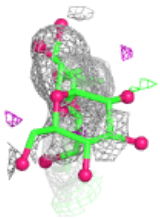


Electron density around LMT D 401:

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

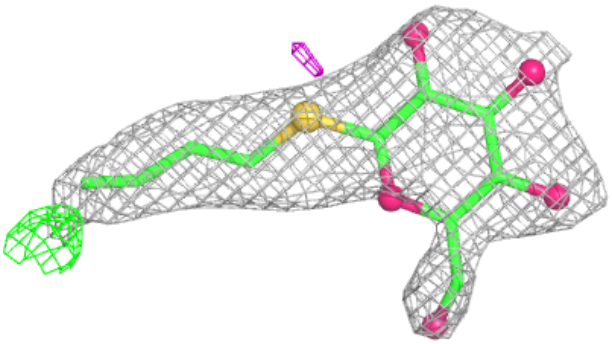


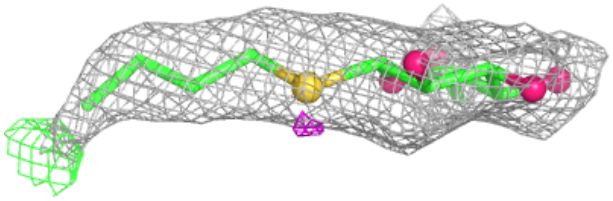


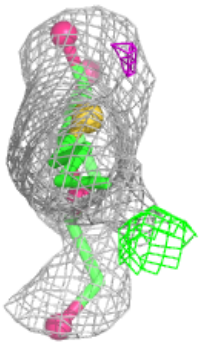


Electron density around HTG d 411:

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

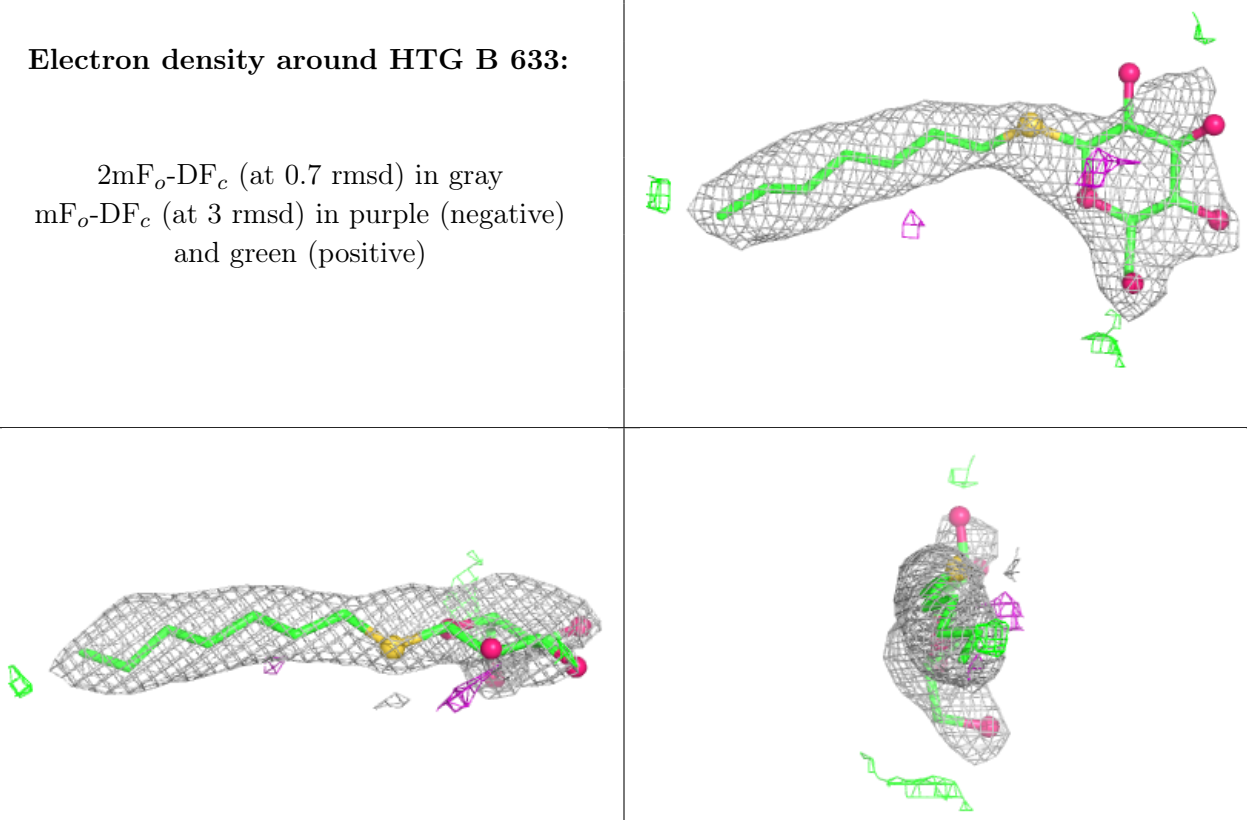






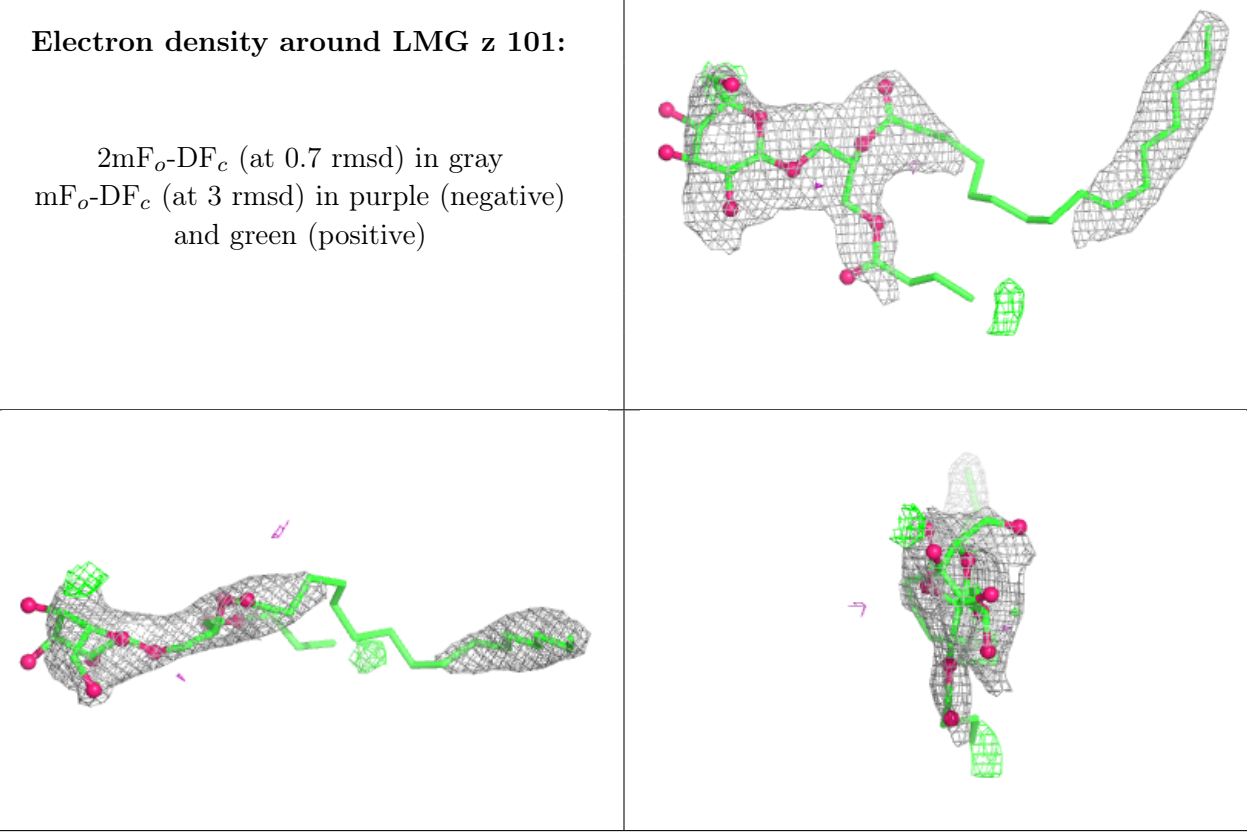
Electron density around HTG B 633:

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



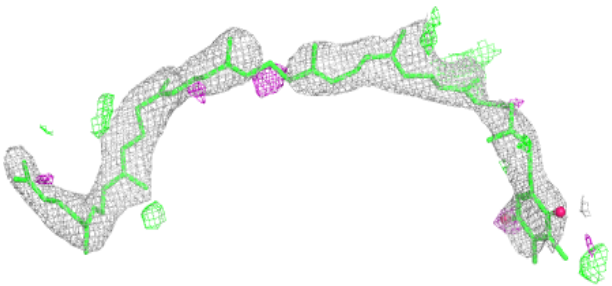
Electron density around LMG z 101:

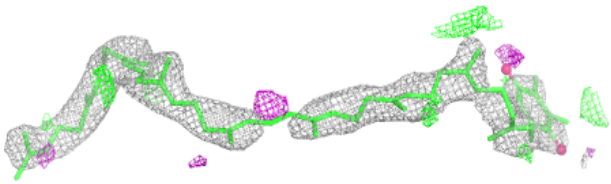
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

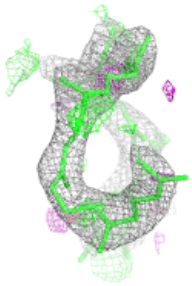


Electron density around PL9 A 419 (A):

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

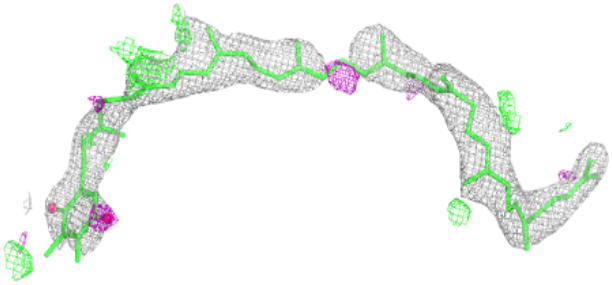


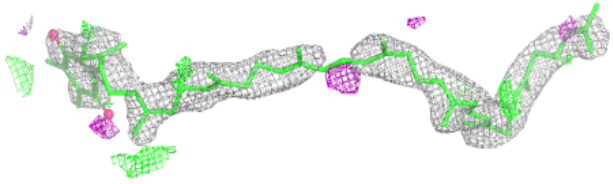


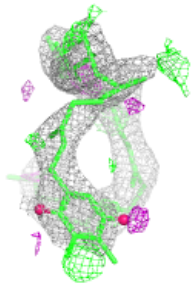


Electron density around PL9 A 419 (B):

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

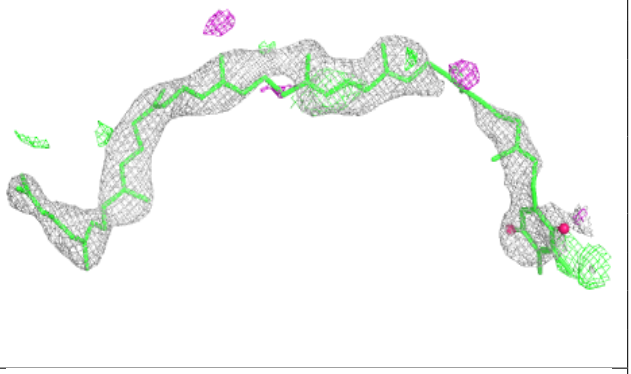


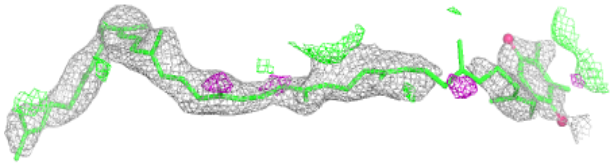


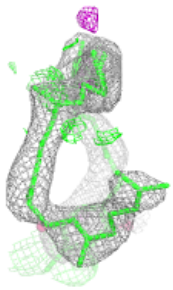


Electron density around PL9 a 415 (A):

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

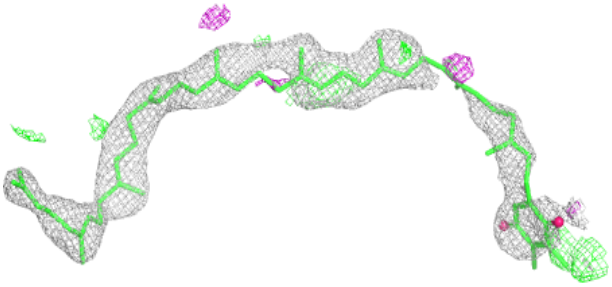


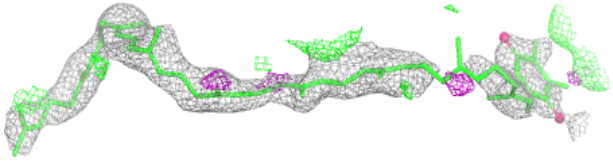


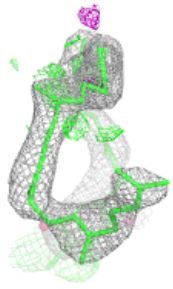


Electron density around PL9 a 415 (B):

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

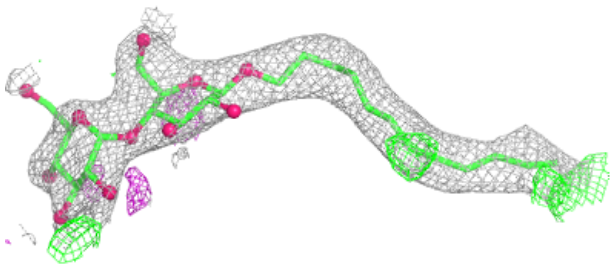


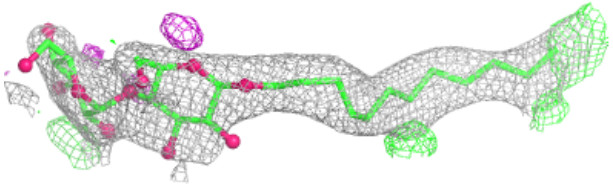


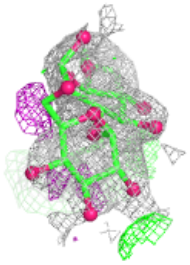


Electron density around LMT a 404:

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

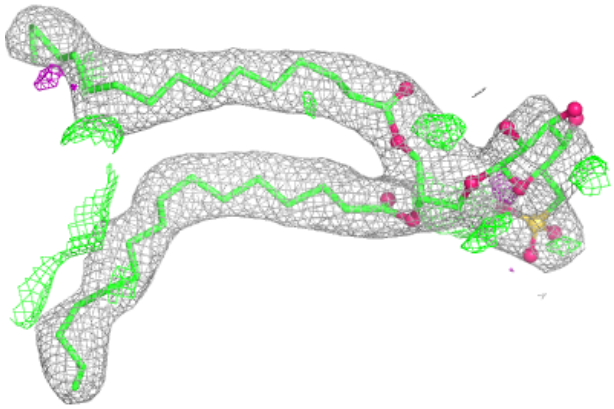


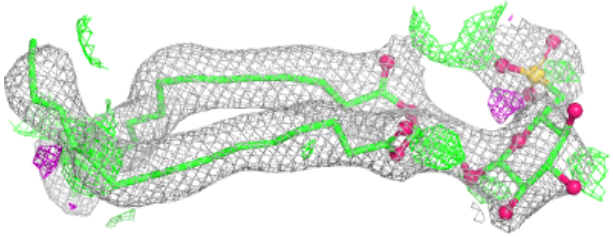


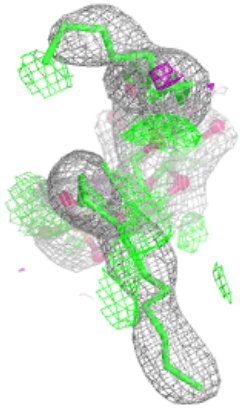


Electron density around SQD B 621:

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

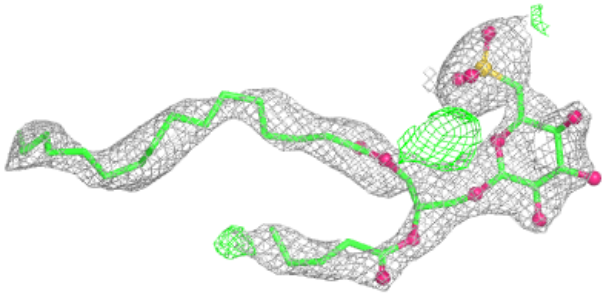


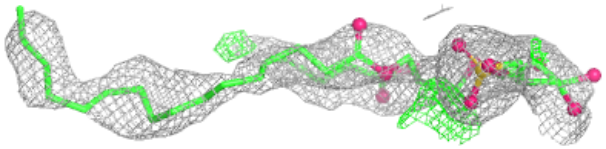


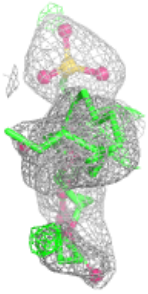


Electron density around SQD F 103:

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

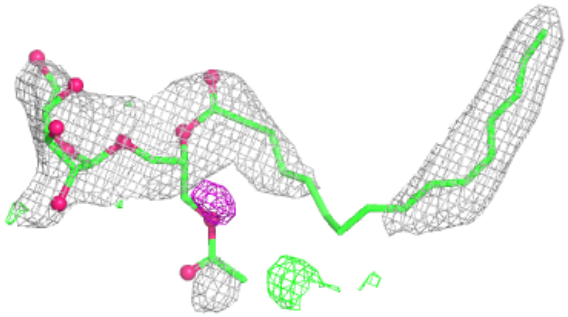


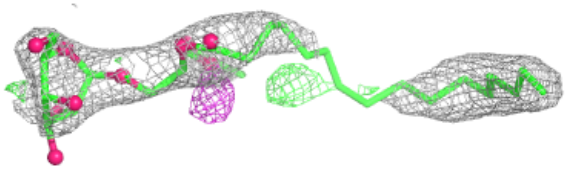


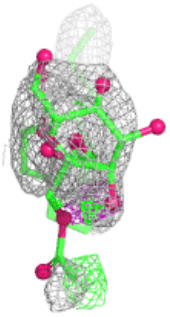


Electron density around LMG Z 101:

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

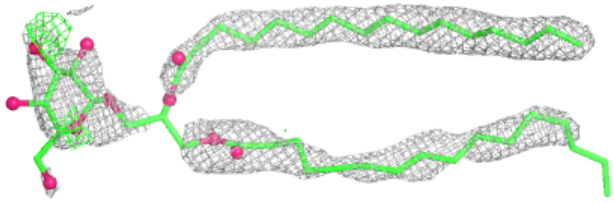


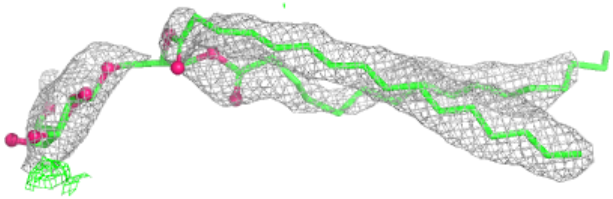


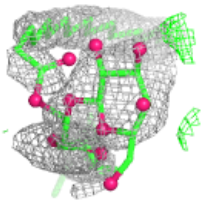


Electron density around LMG c 524:

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

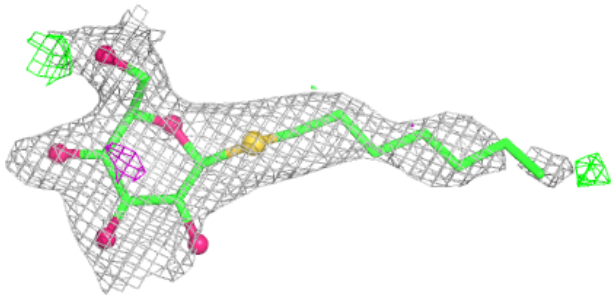


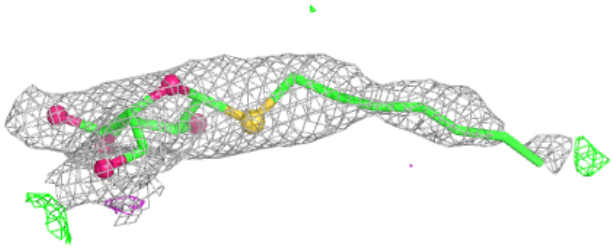


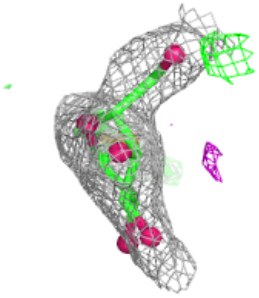


Electron density around HTG C 523:

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

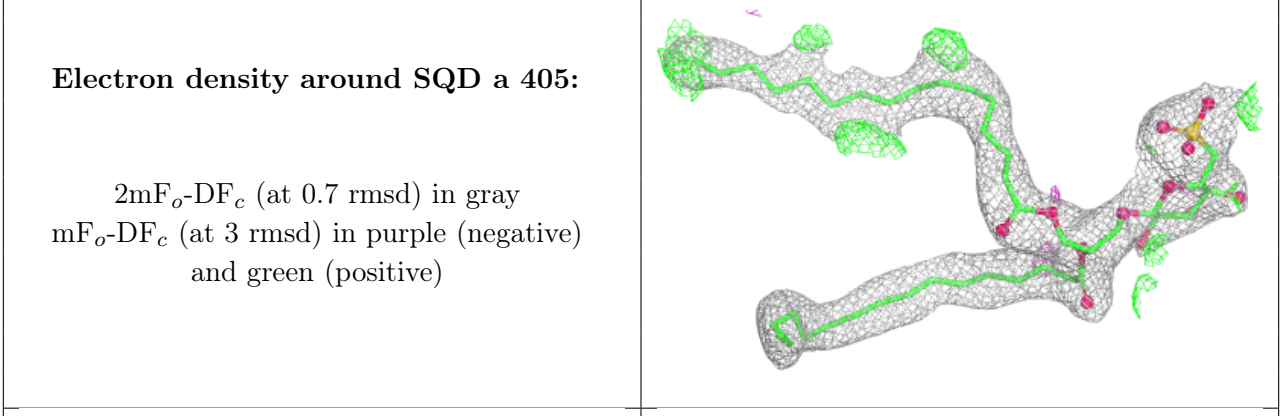






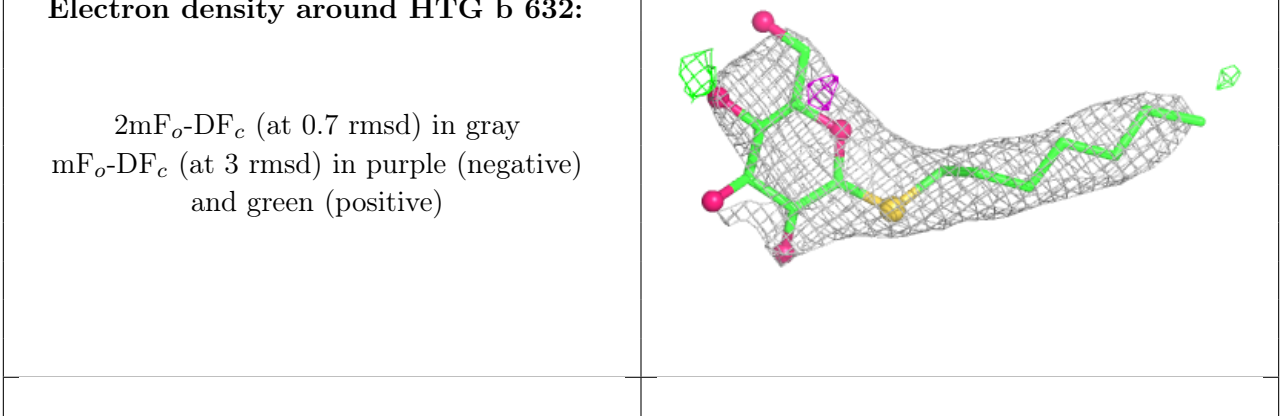
Electron density around SQD a 405:

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



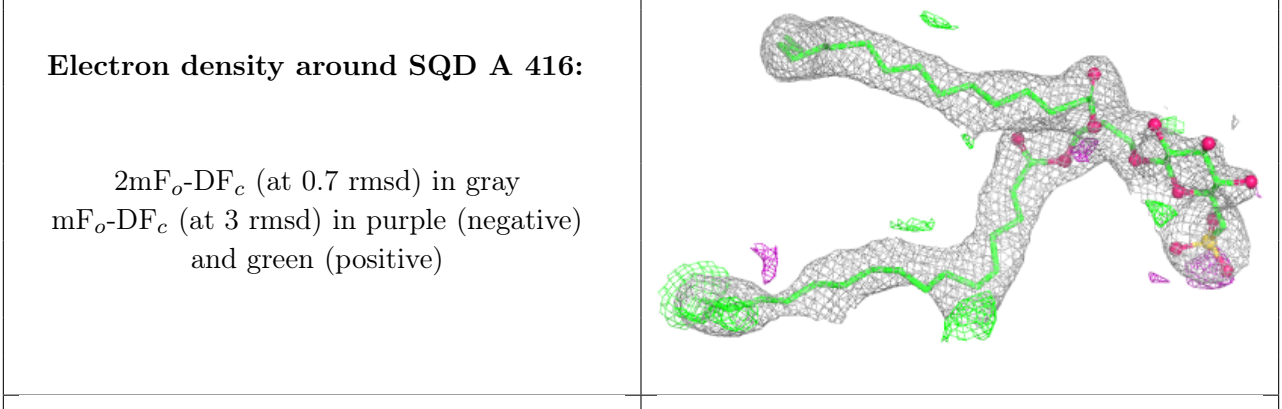
Electron density around HTG b 632:

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



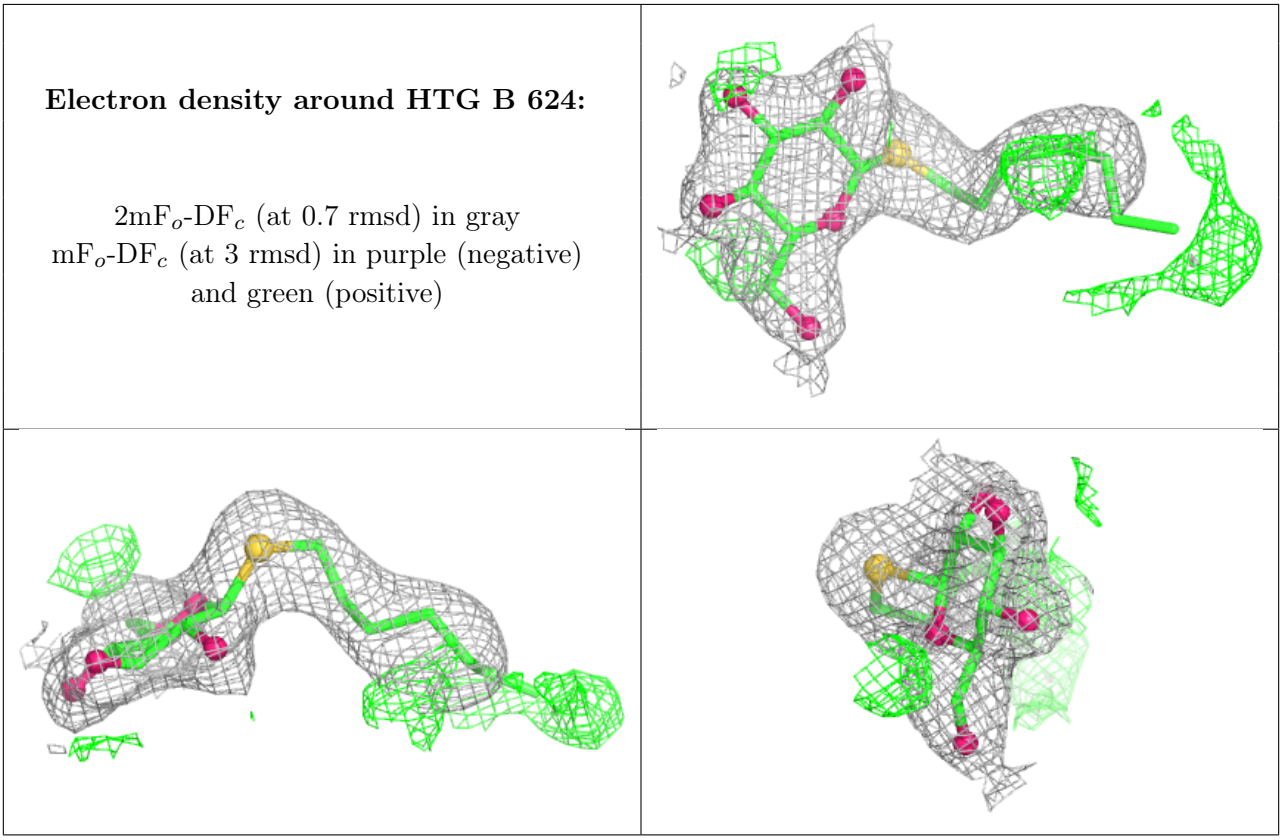
Electron density around SQD A 416:

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



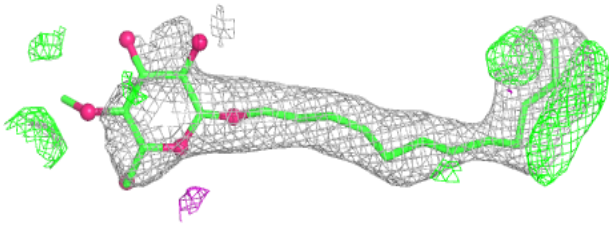
Electron density around HTG B 624:

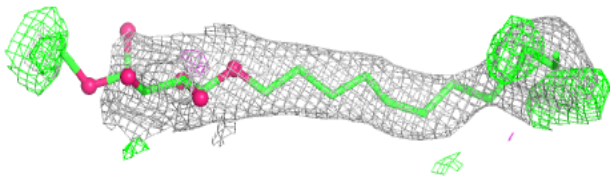
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

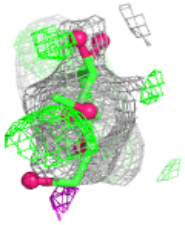


Electron density around LMT B 635:

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

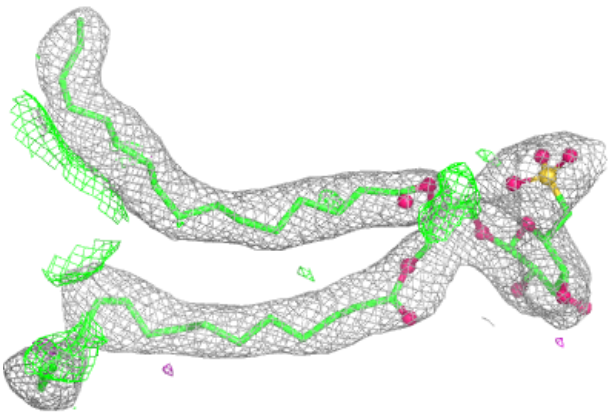


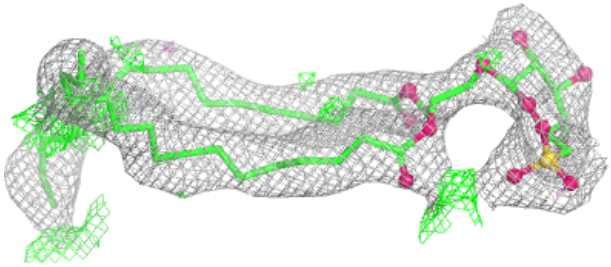


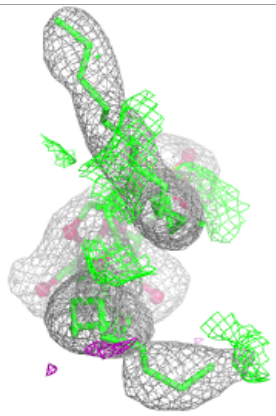


Electron density around SQD L 102:

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

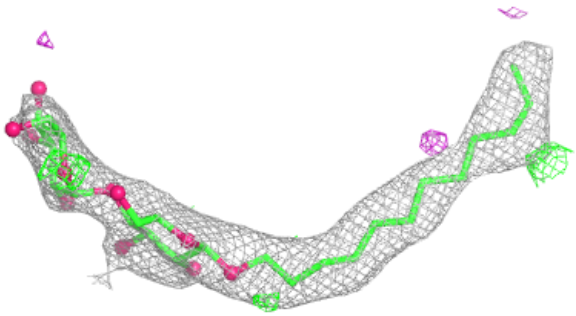


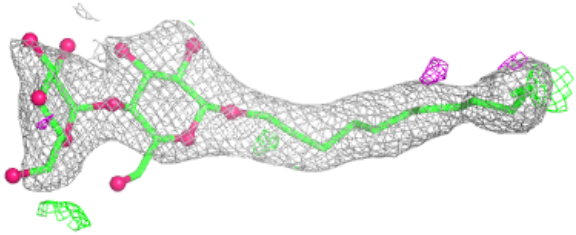


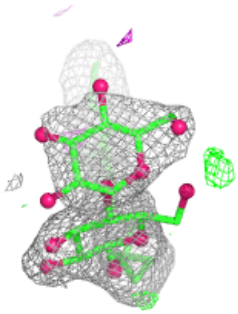


Electron density around LMT m 103:

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

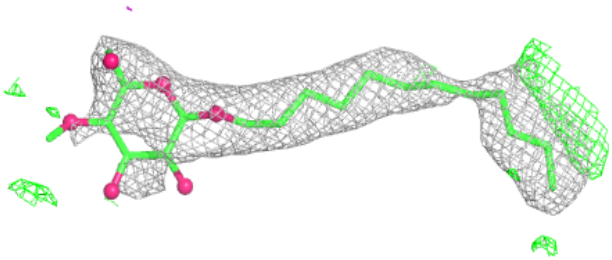


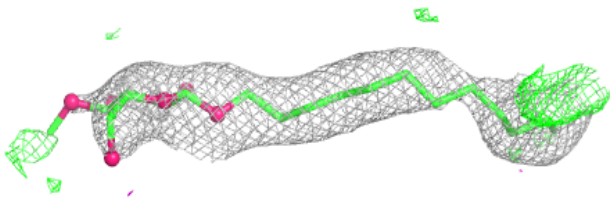


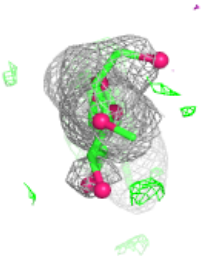


Electron density around LMT T 104:

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

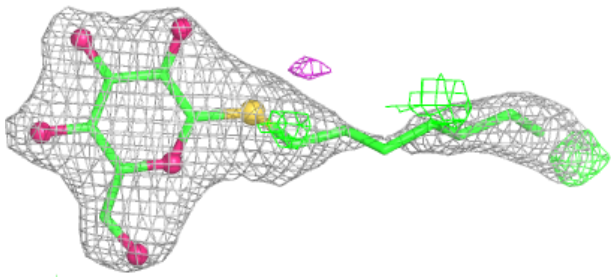


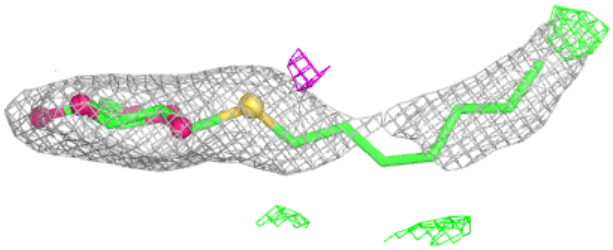


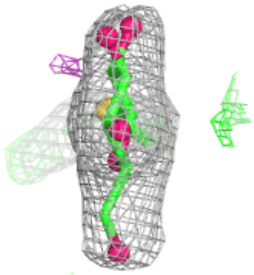


Electron density around HTG C 522:

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

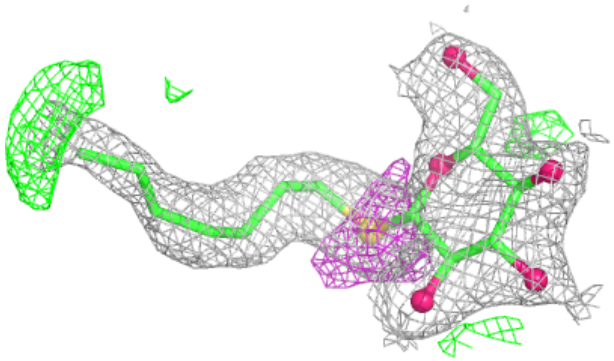


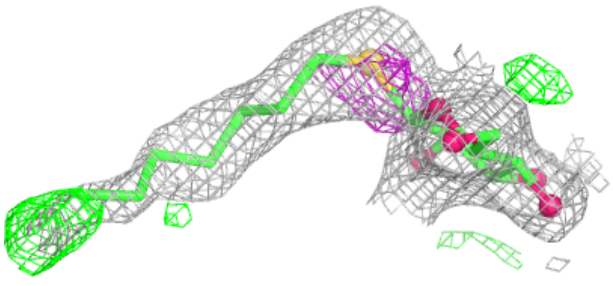


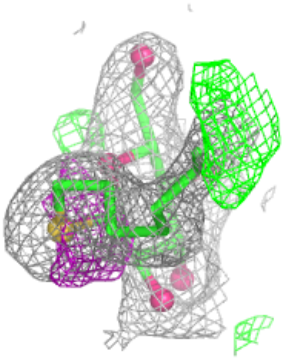


Electron density around HTG b 631:

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

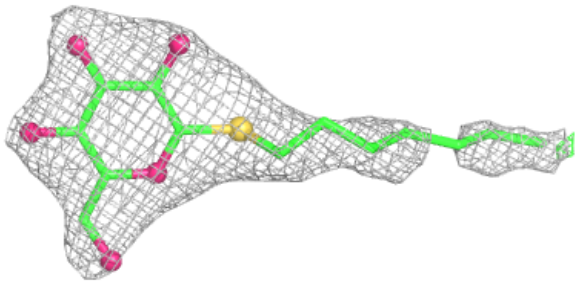


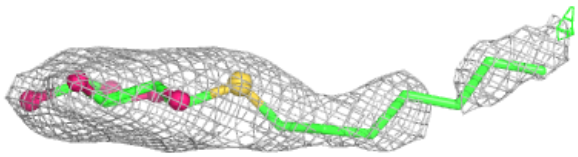


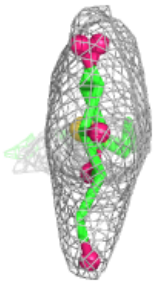


Electron density around HTG c 525:

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

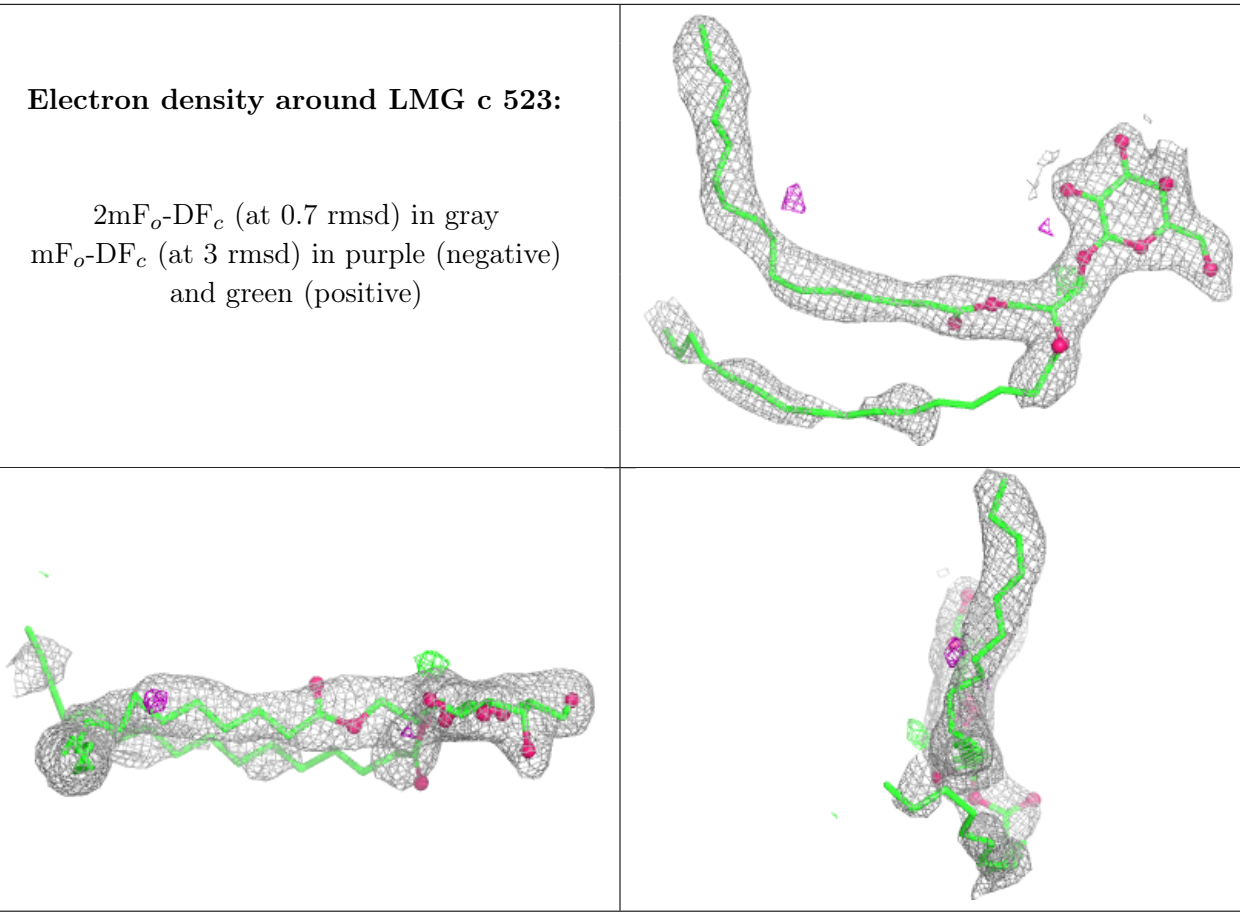






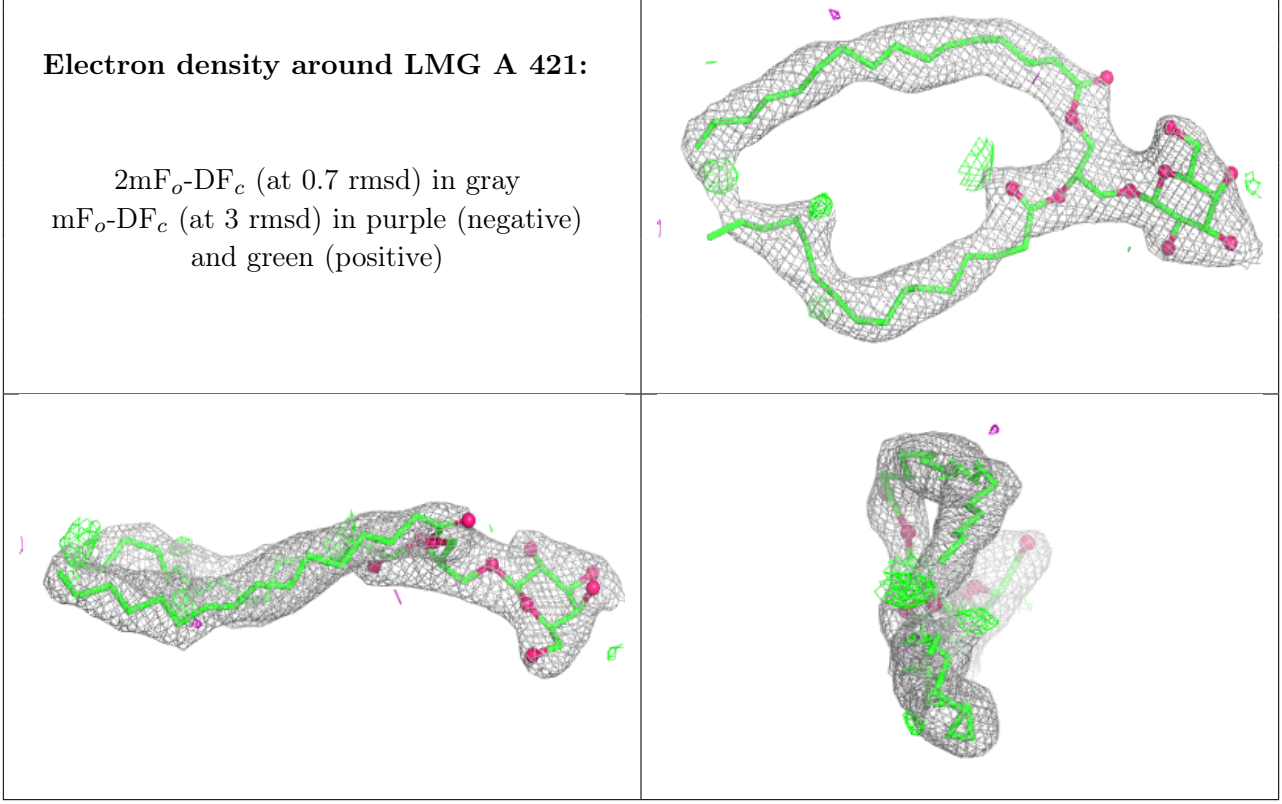
Electron density around LMG c 523:

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



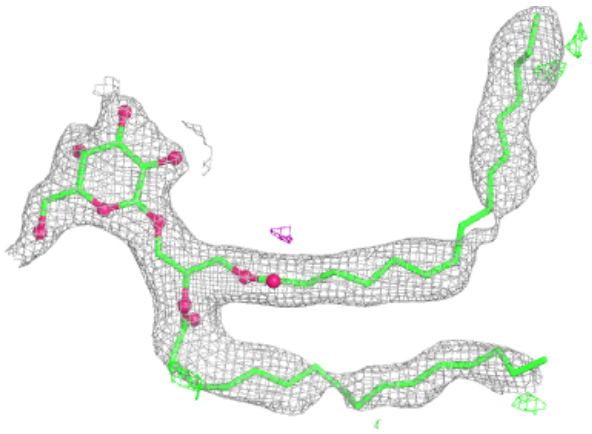
Electron density around LMG A 421:

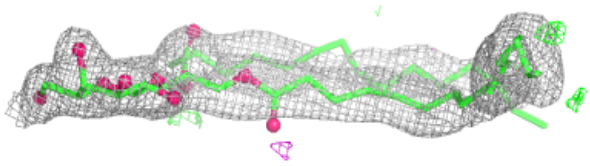
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

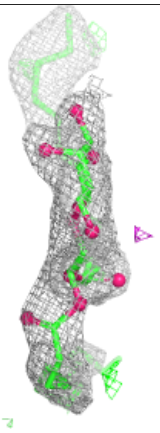


Electron density around LMG C 519:

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

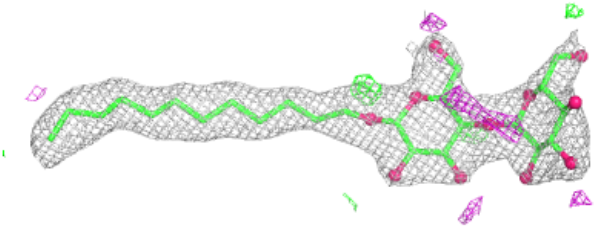


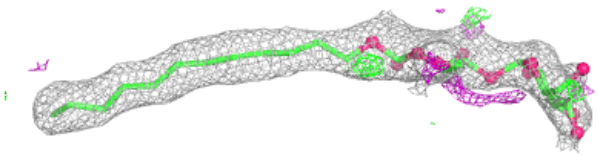


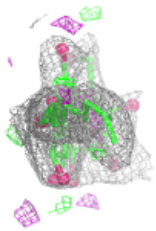


Electron density around LMT m 102:

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

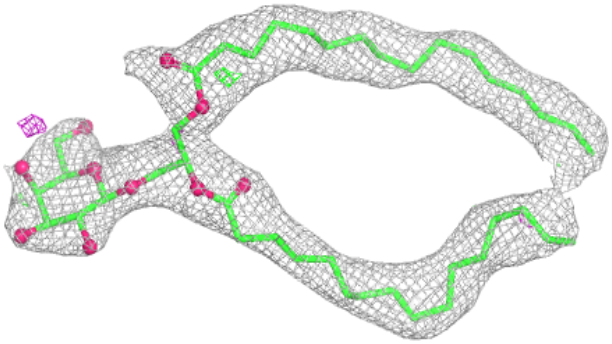


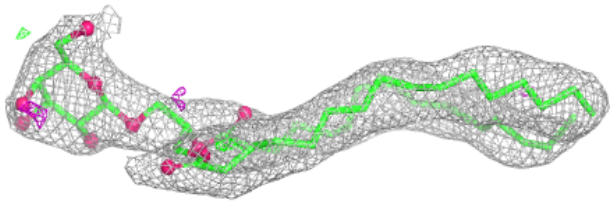


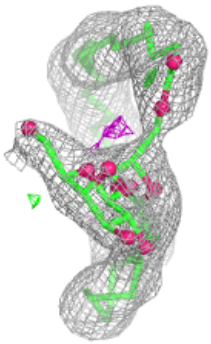


Electron density around LMG c 501:

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

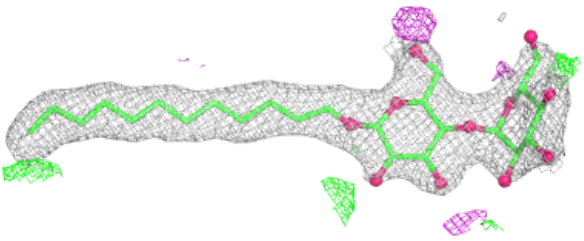


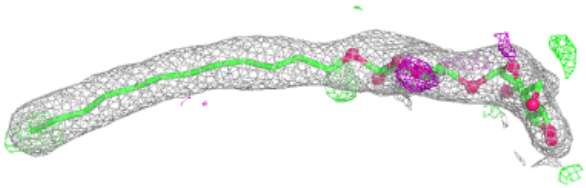


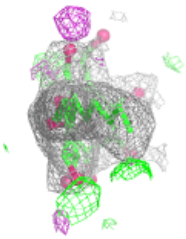


Electron density around LMT M 101:

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

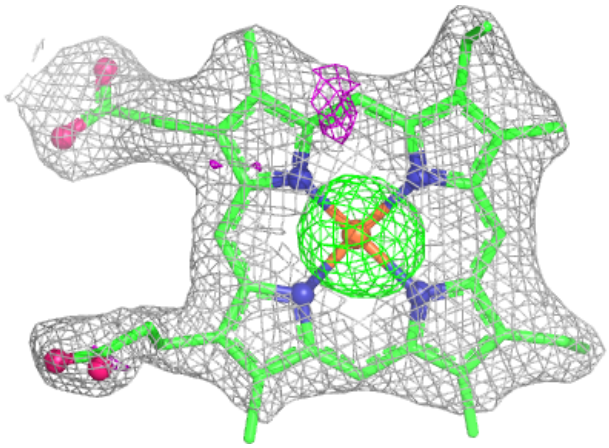


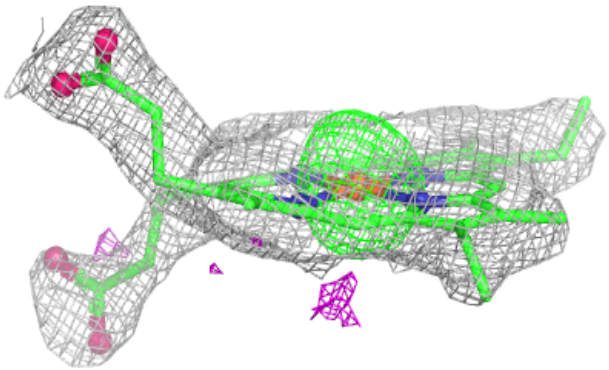


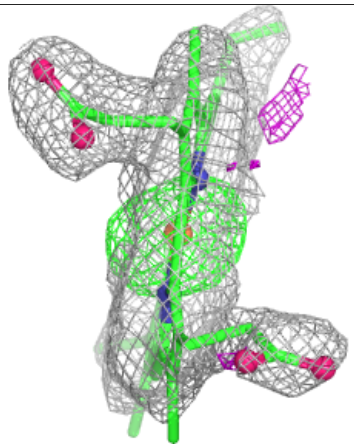


Electron density around HEM F 102:

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

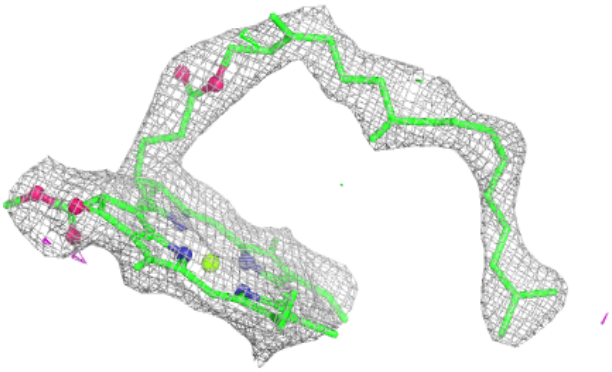


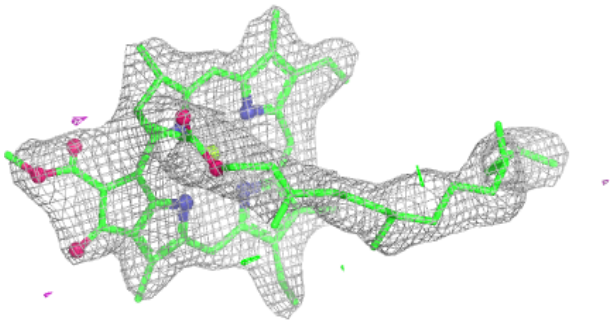


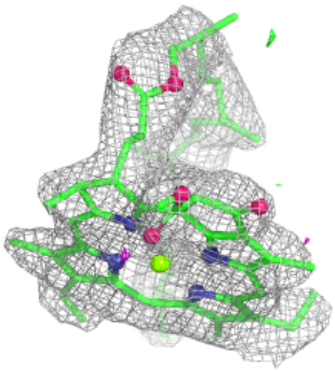


Electron density around CLA c 518:

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

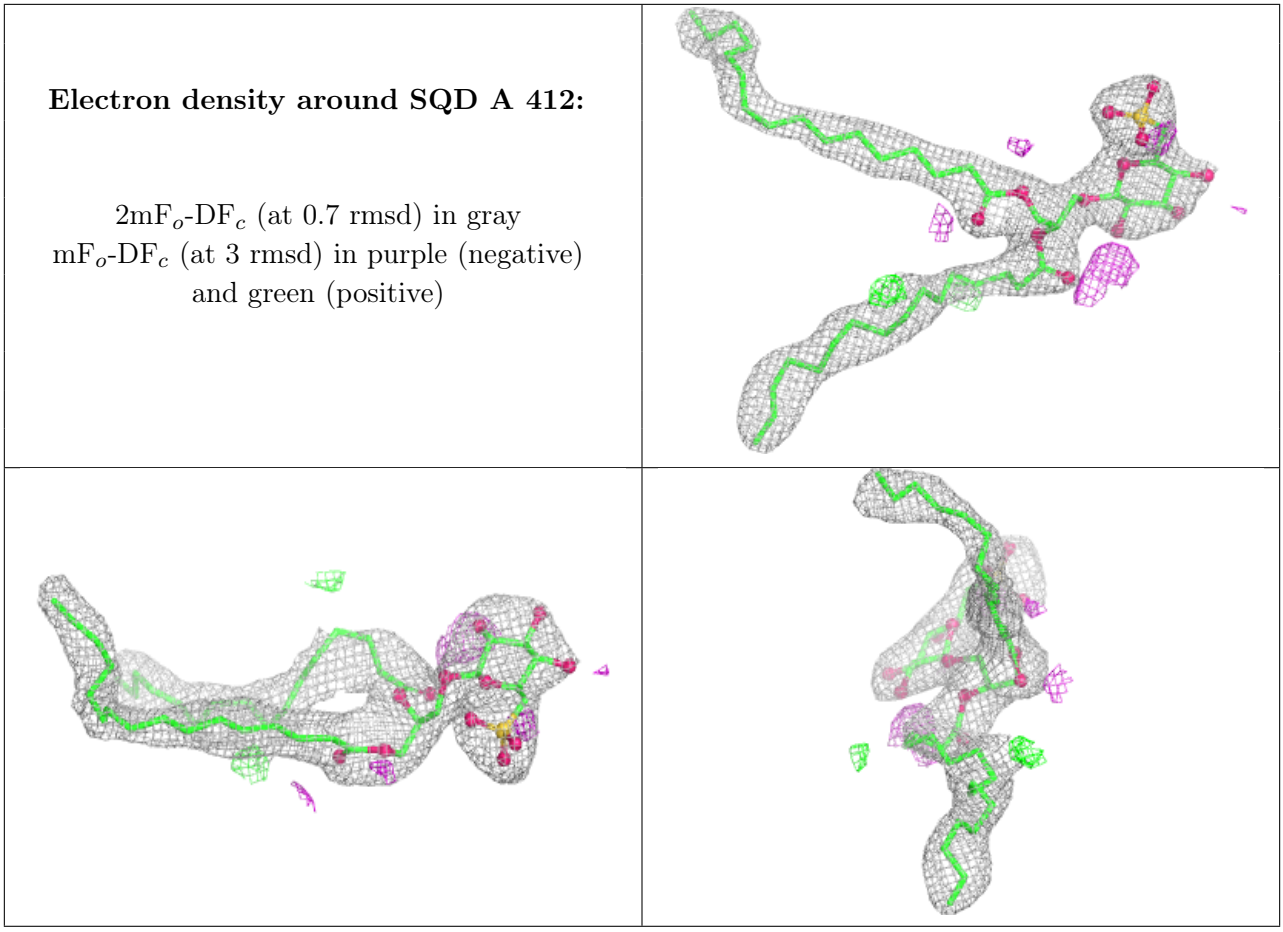






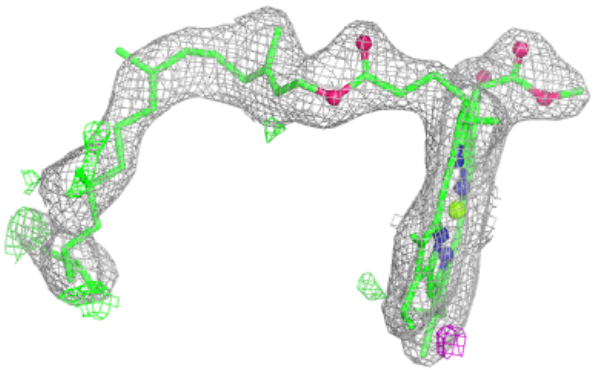
Electron density around SQD A 412:

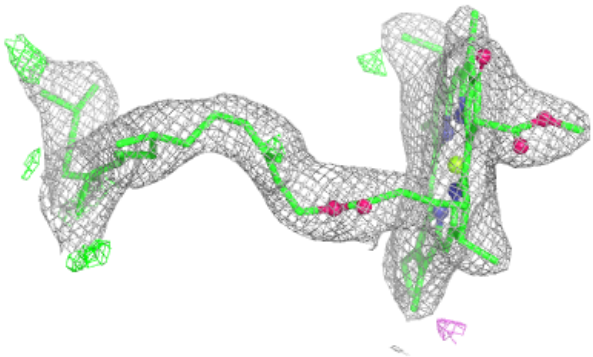
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

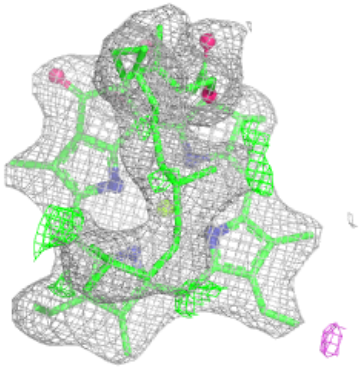


Electron density around CLA C 506:

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

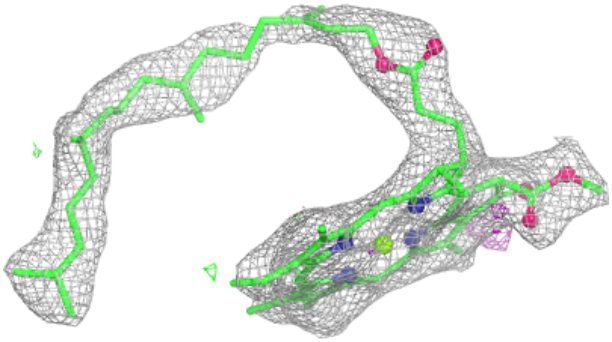


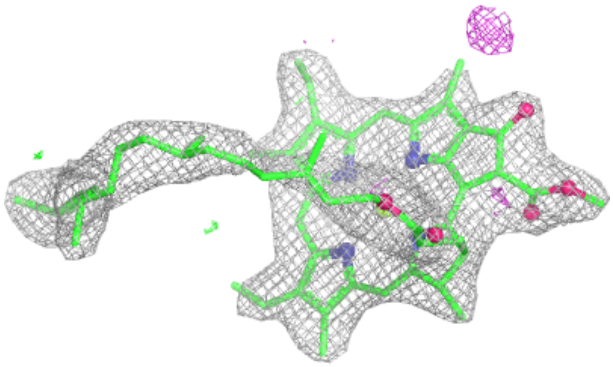


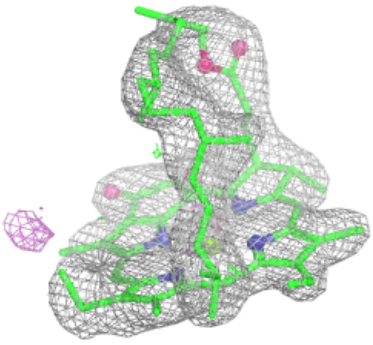


Electron density around CLA C 513:

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

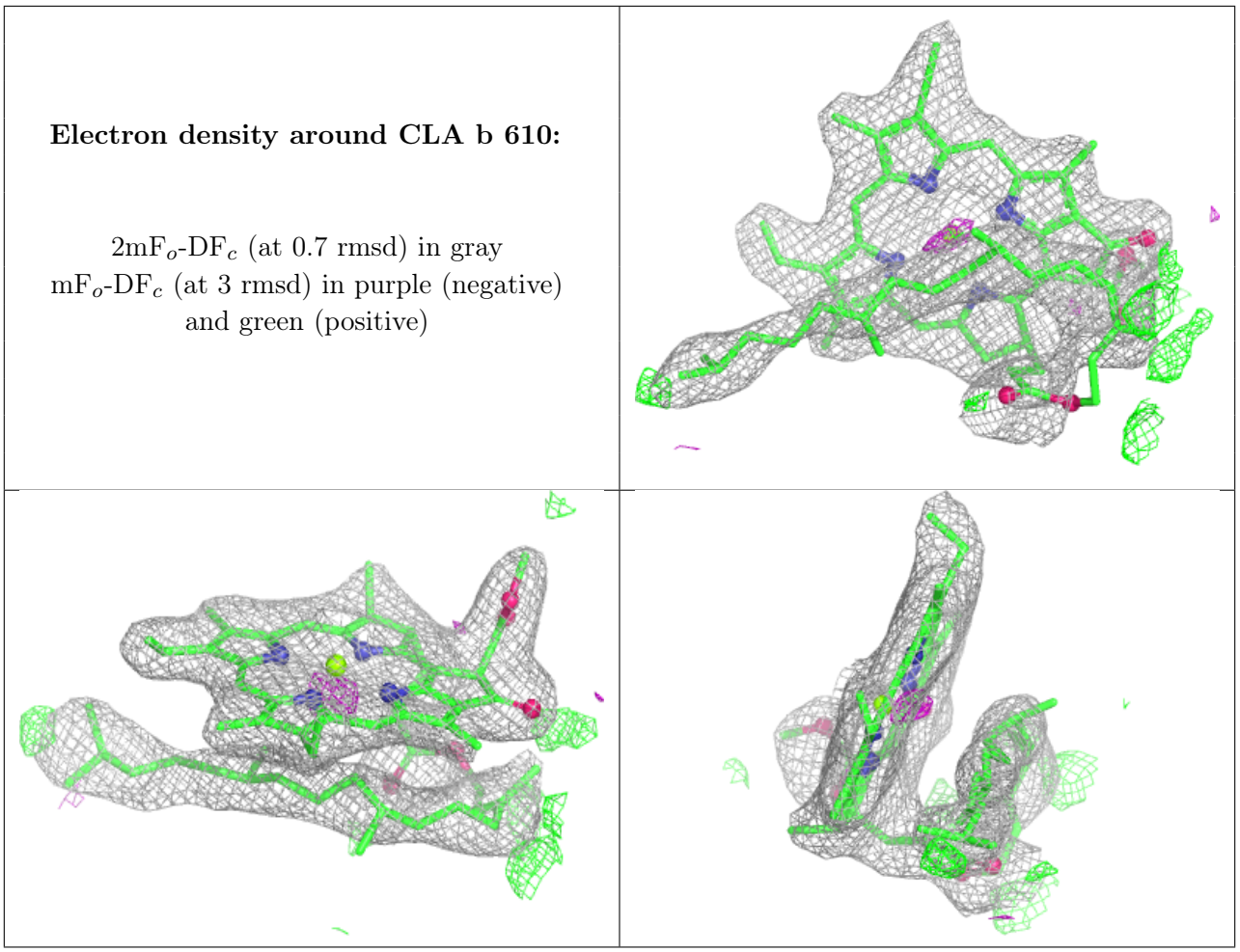






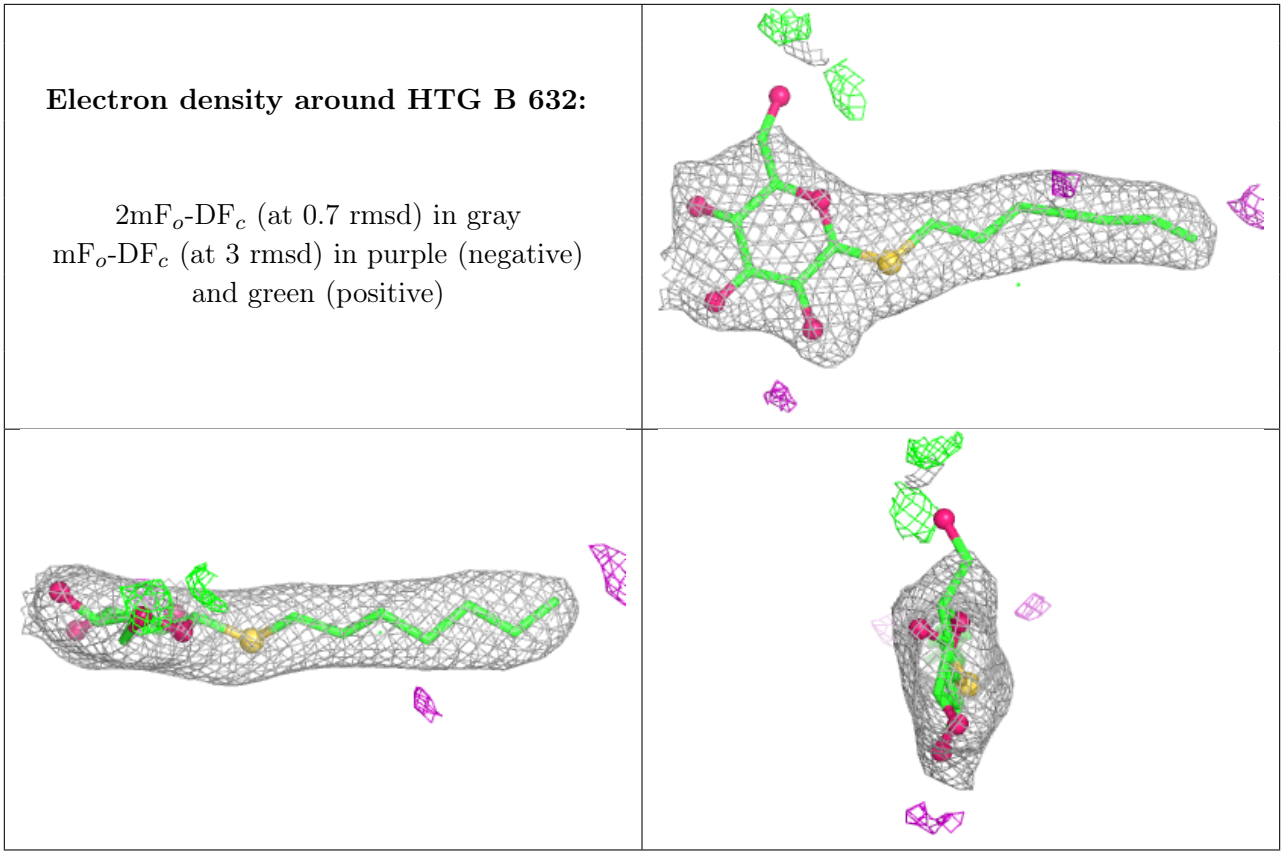
Electron density around CLA b 610:

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



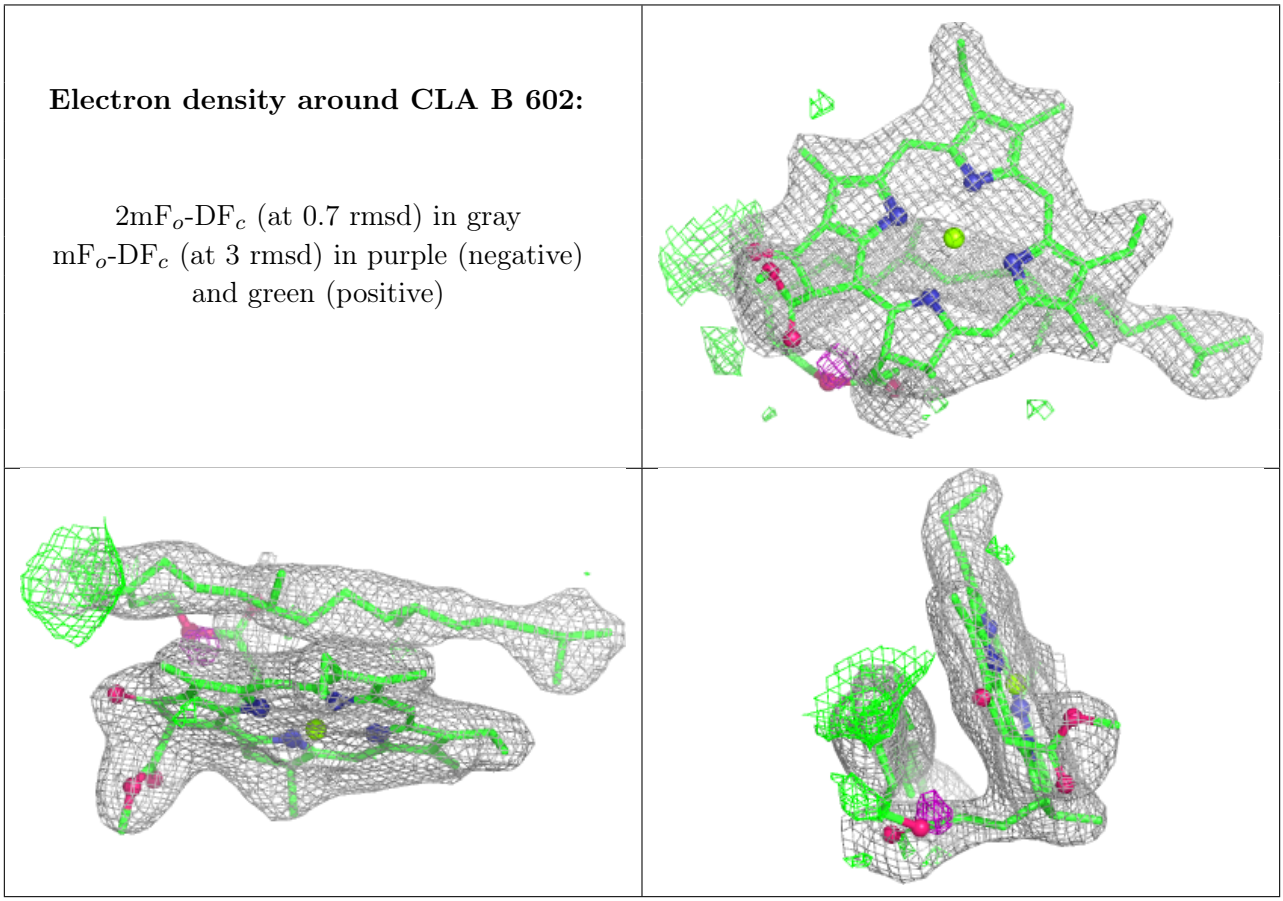
Electron density around HTG B 632:

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



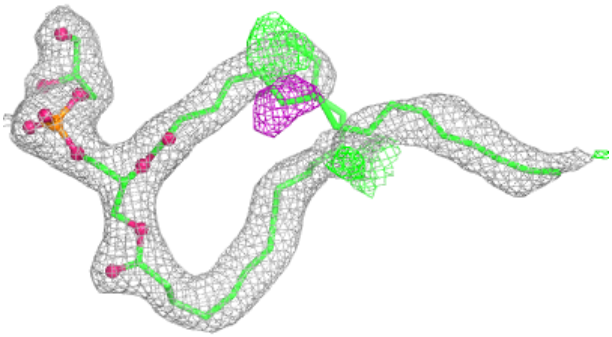
Electron density around CLA B 602:

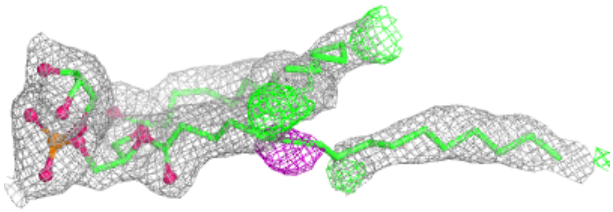
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

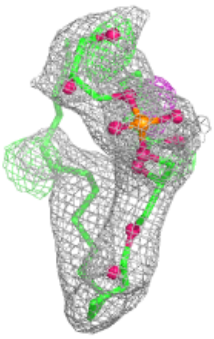


Electron density around LHG D 409:

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

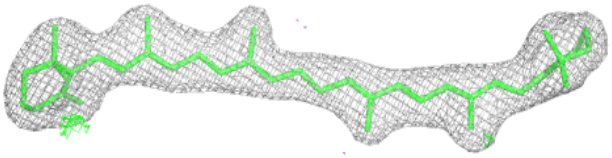


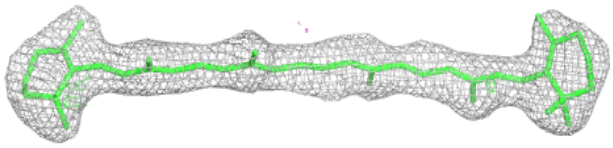


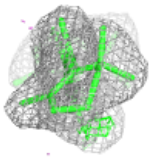


Electron density around BCR C 514:

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

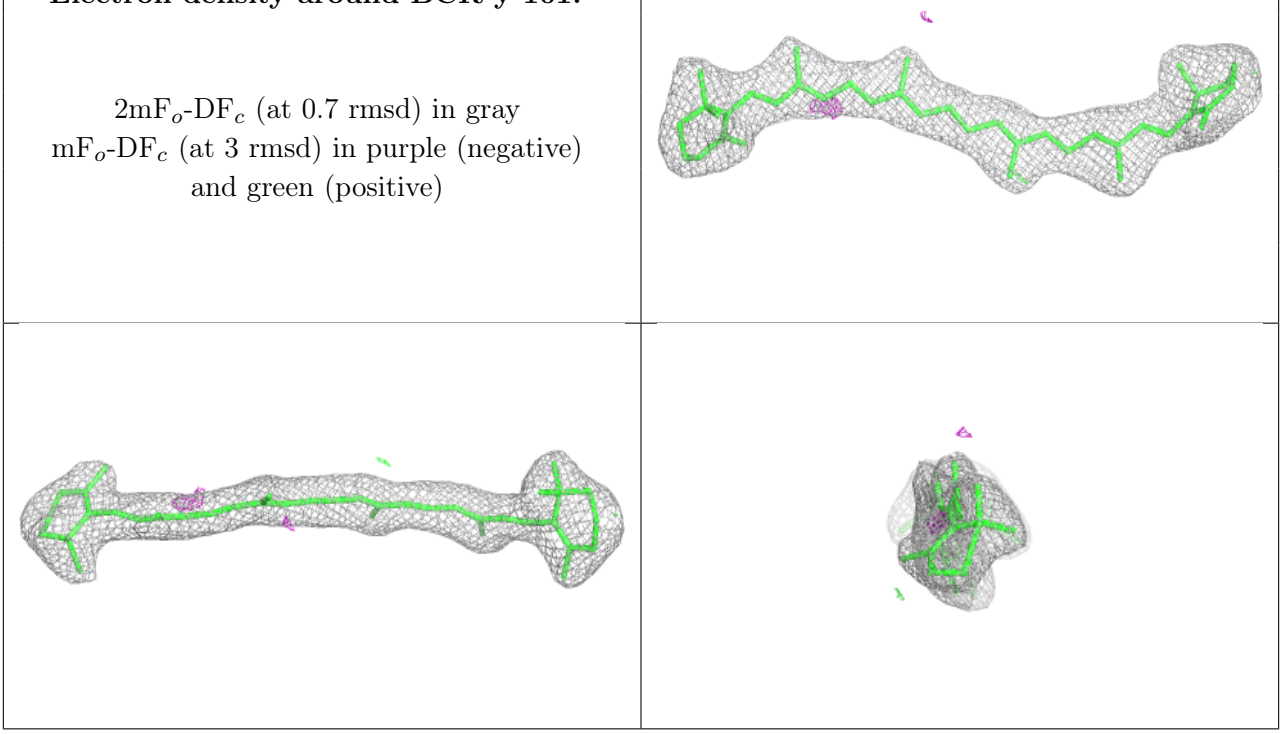






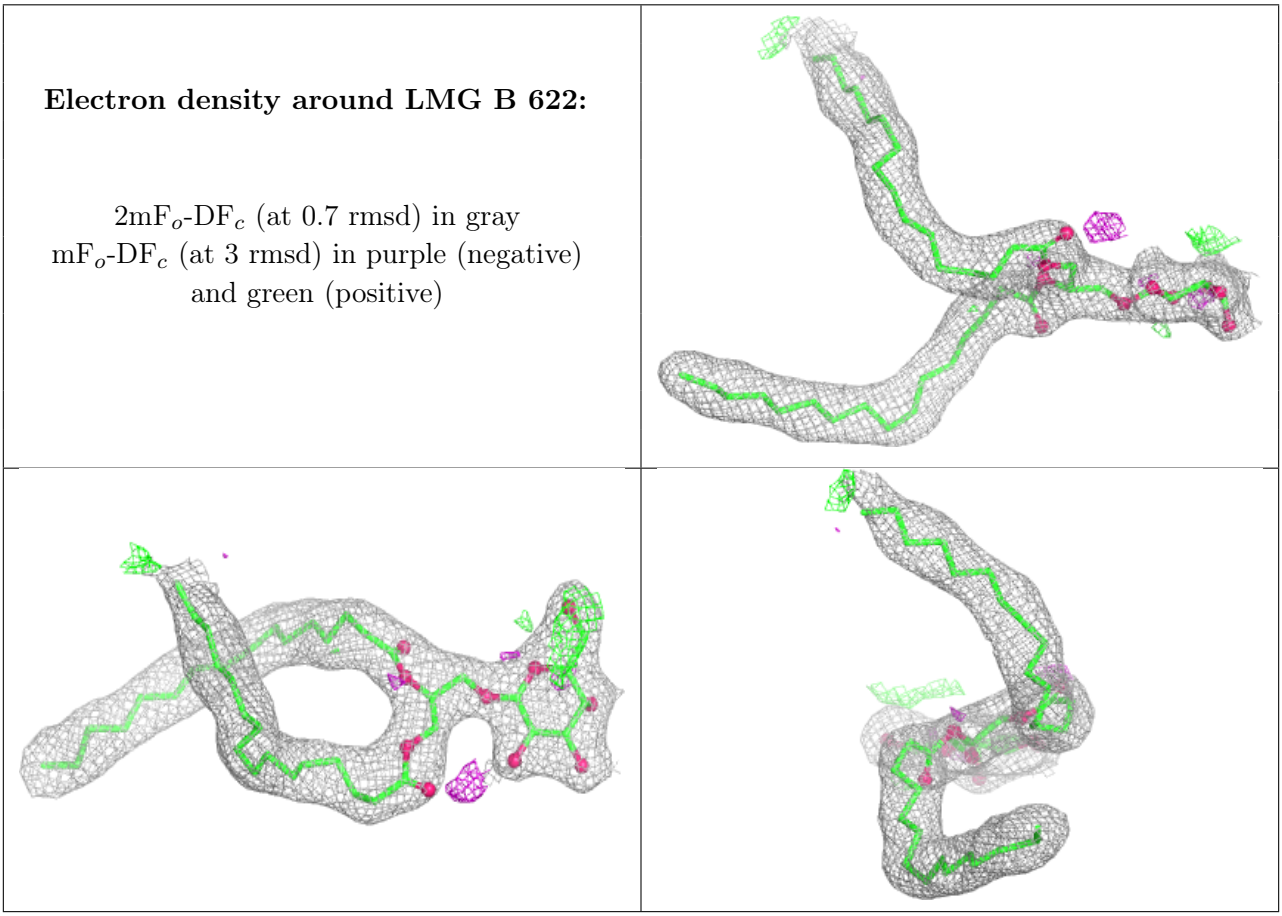
Electron density around BCR y 101:

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



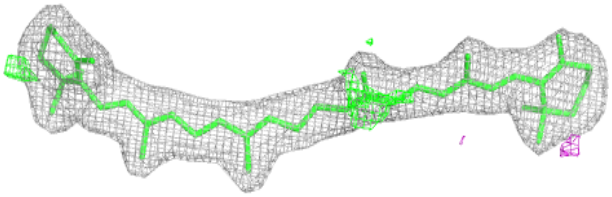
Electron density around LMG B 622:

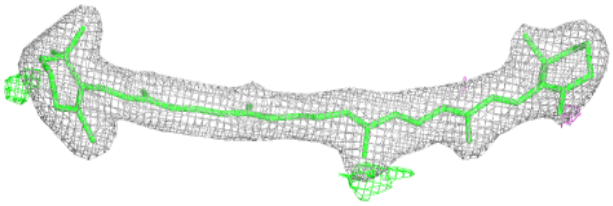
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

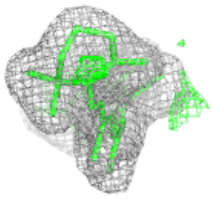


Electron density around BCR t 101:

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

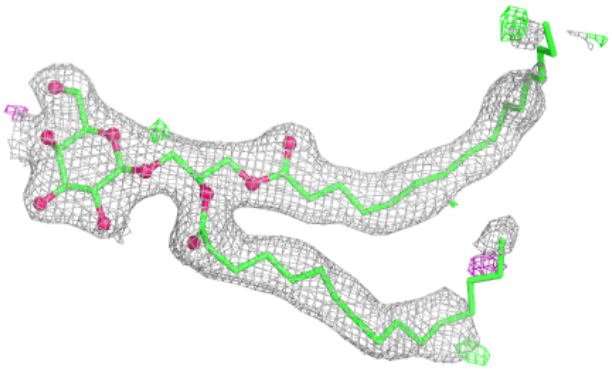


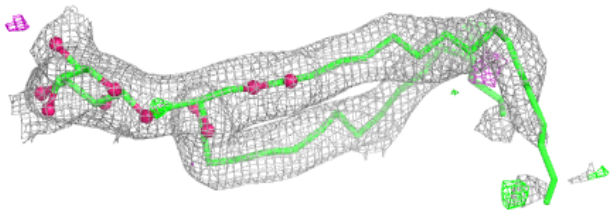




Electron density around LMG D 413:

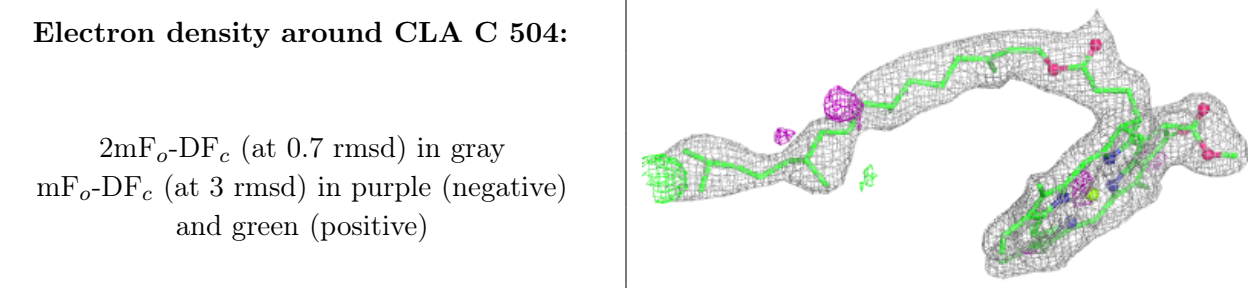
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

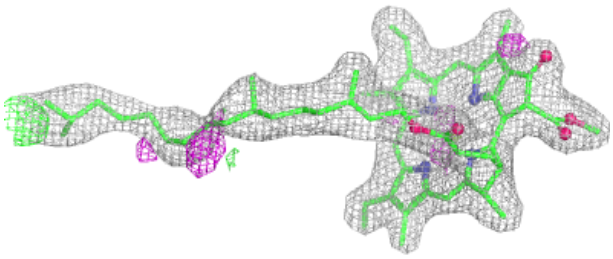


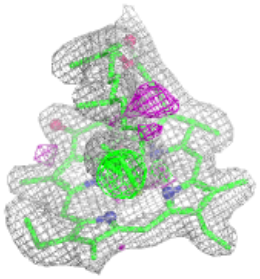


Electron density around CLA C 504:

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

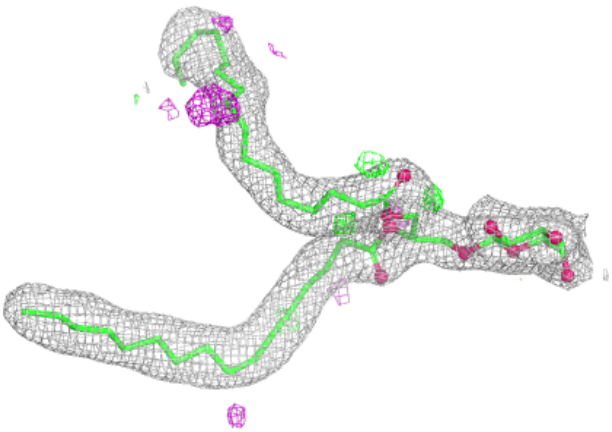


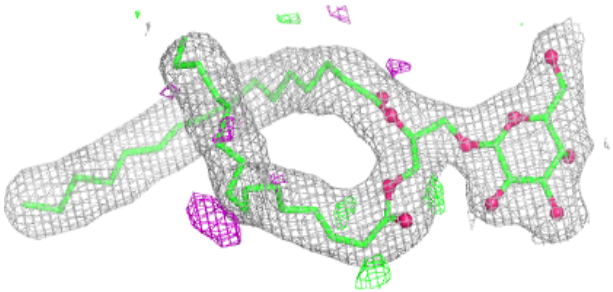


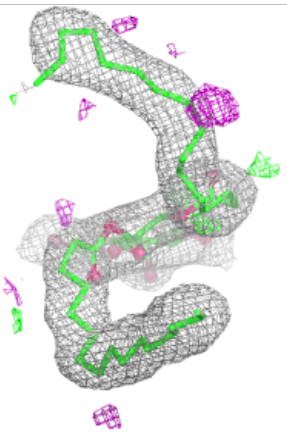


Electron density around LMG b 629:

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

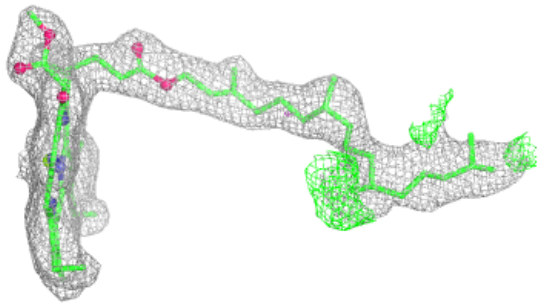


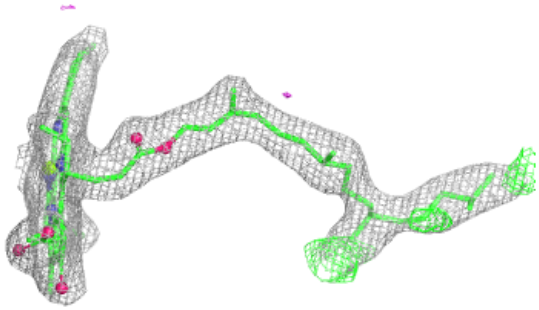


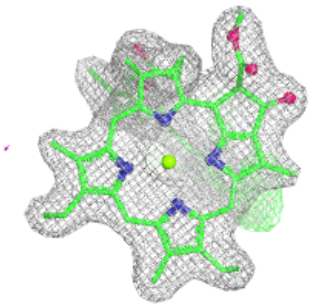


Electron density around CLA b 615:

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

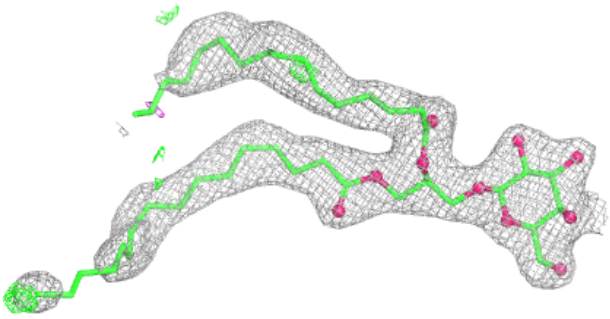


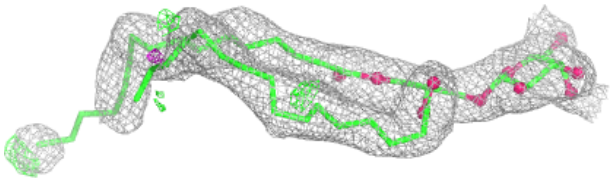


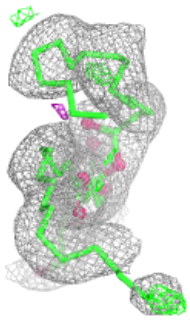


Electron density around LMG d 413:

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

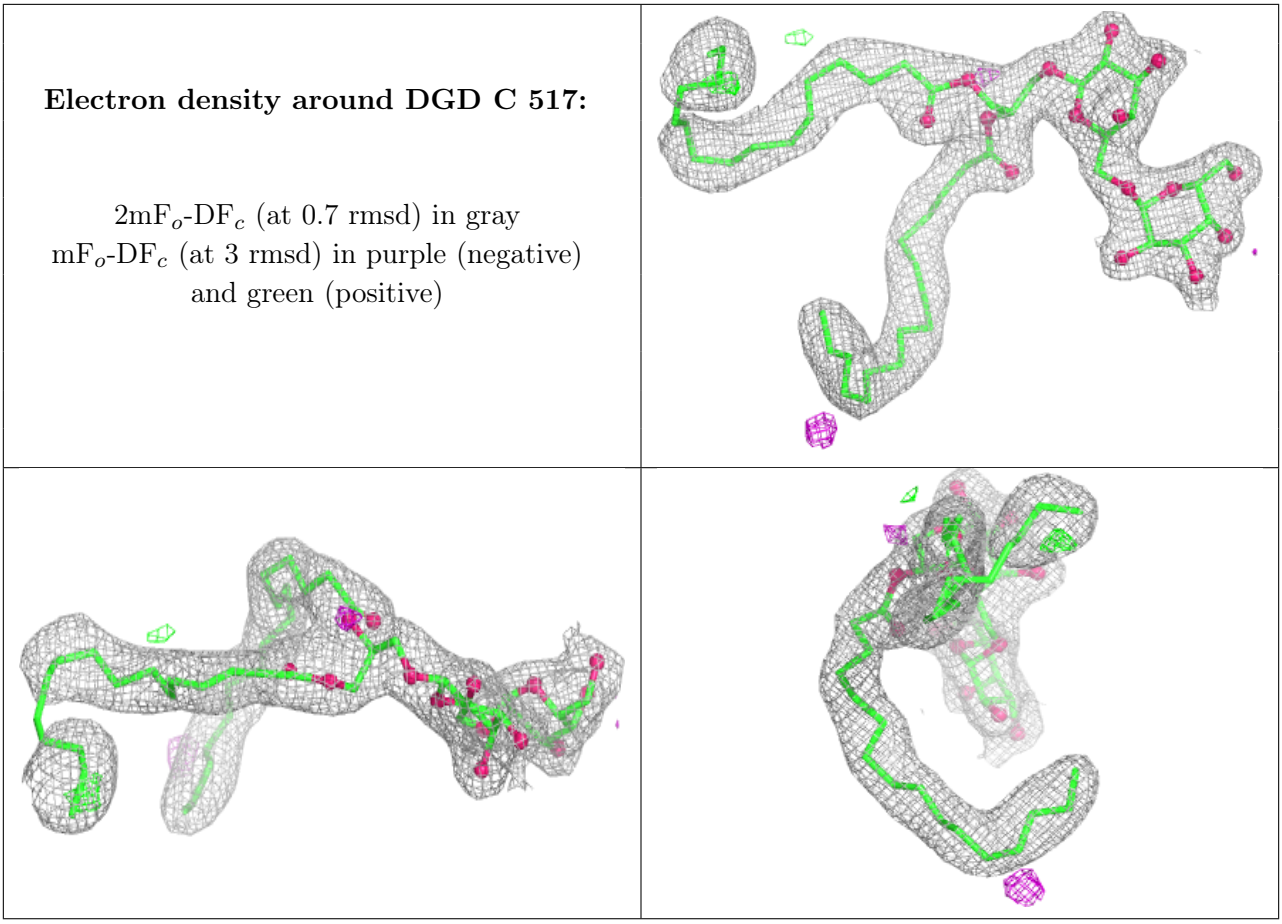






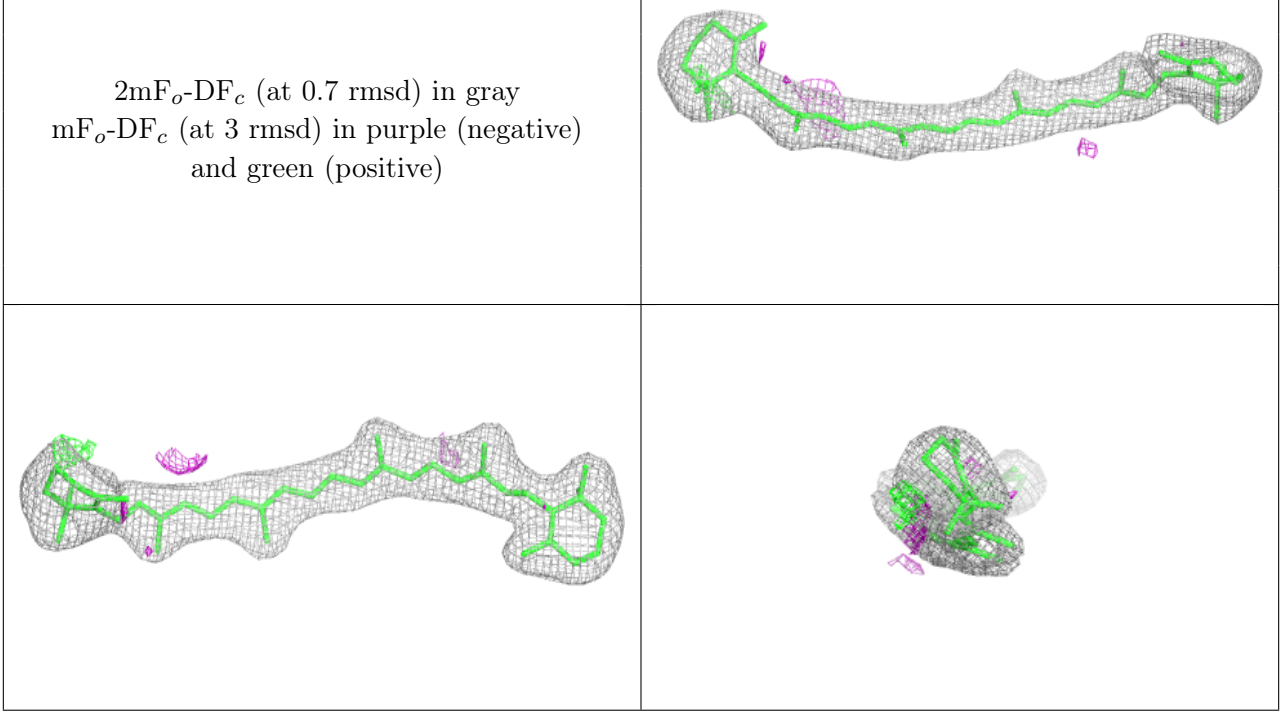
Electron density around DGD C 517:

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



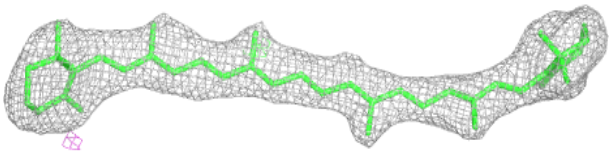
Electron density around BCR D 404:

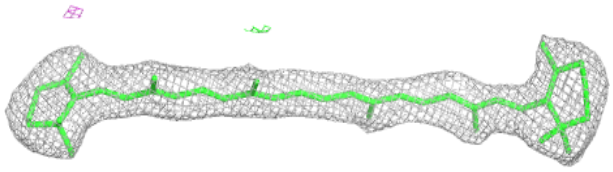
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

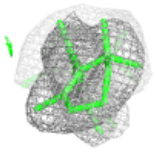


Electron density around BCR c 528:

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

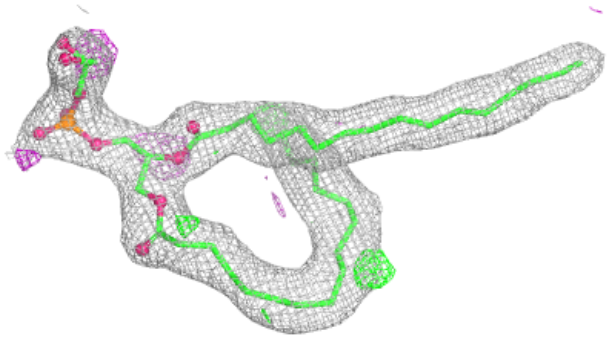


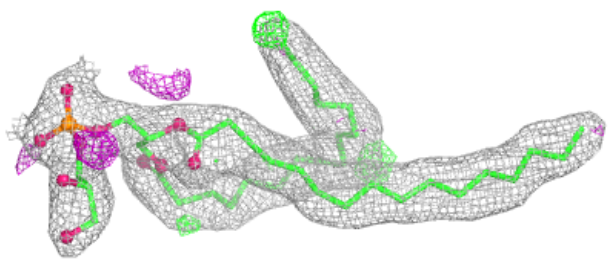


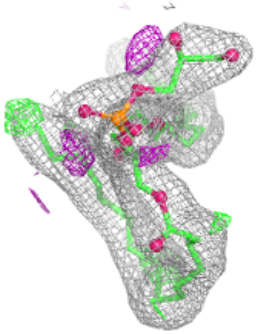


Electron density around LHG D 407:

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

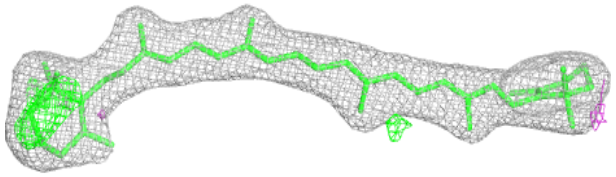


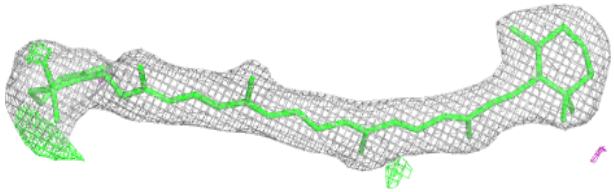


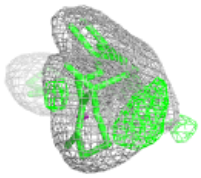


Electron density around BCR d 404:

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

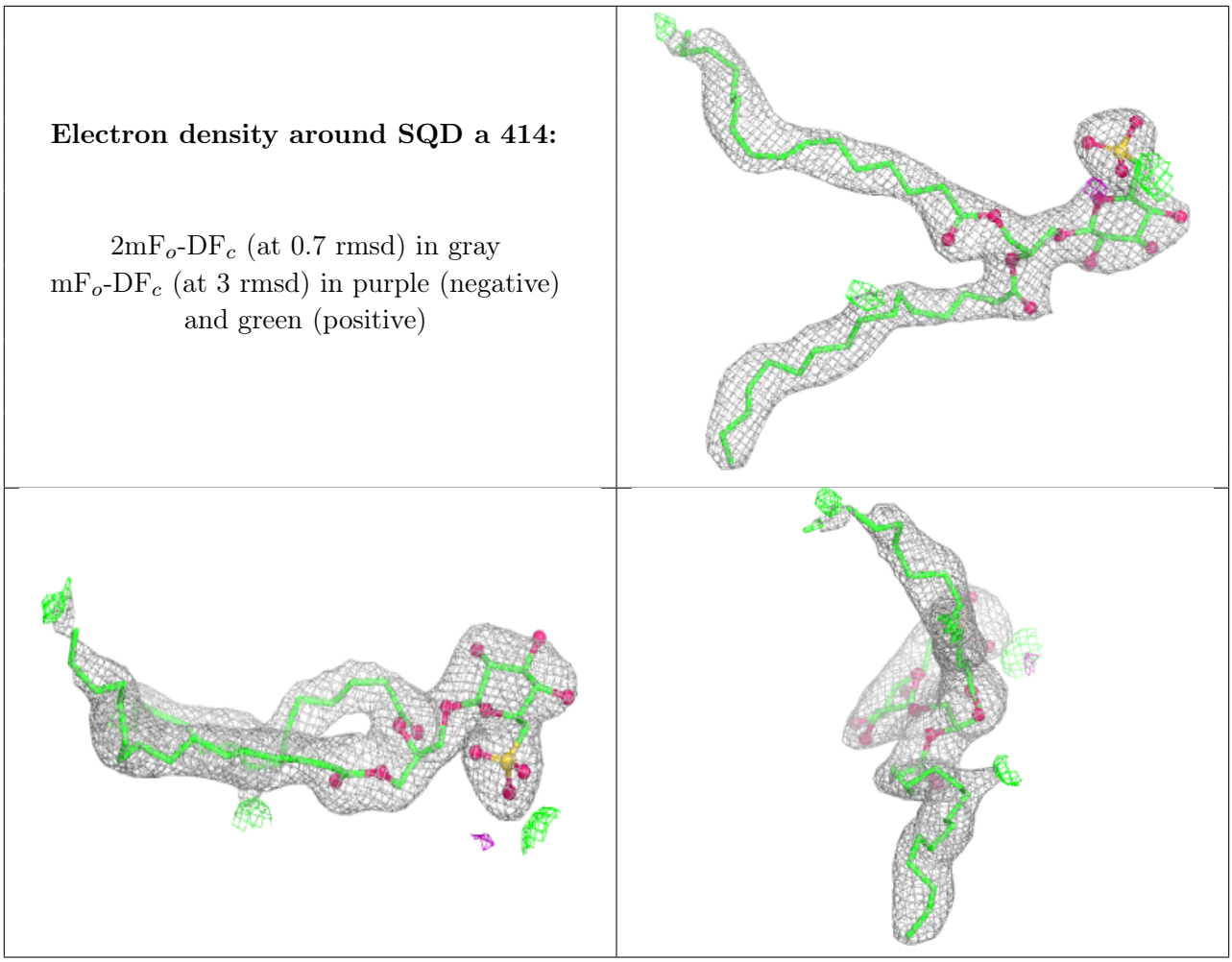






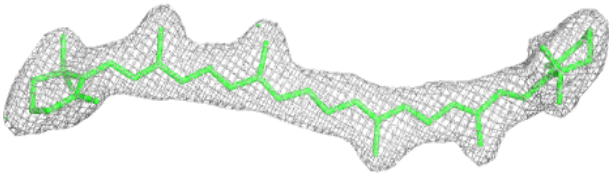
Electron density around SQD a 414:

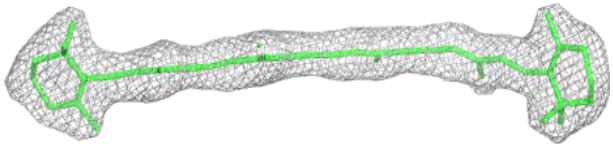
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

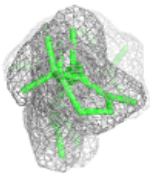


Electron density around BCR h 101:

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

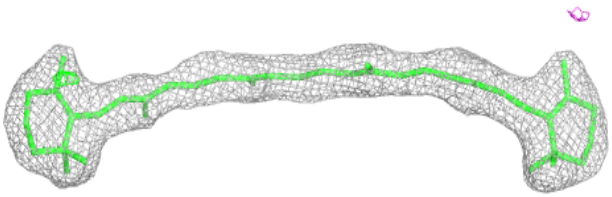


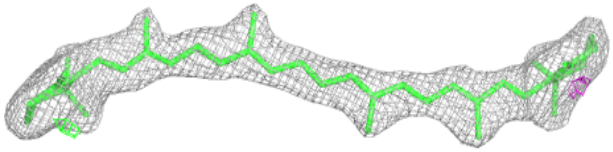


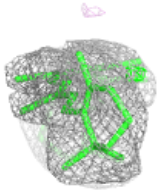


Electron density around BCR k 101:

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

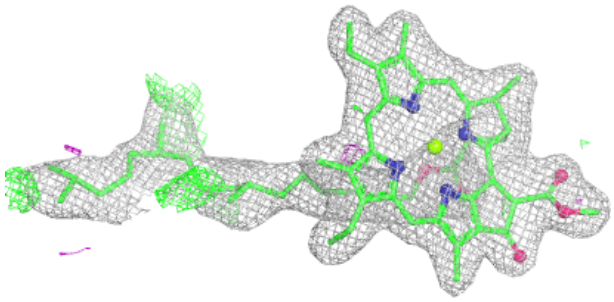


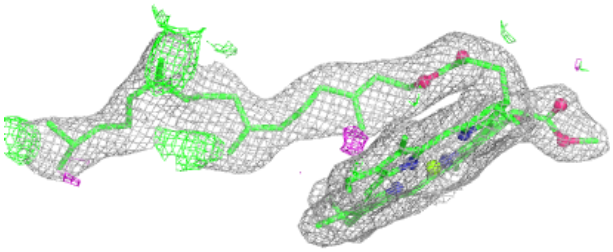


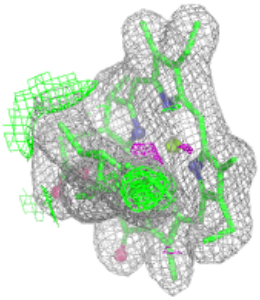


Electron density around CLA b 623:

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

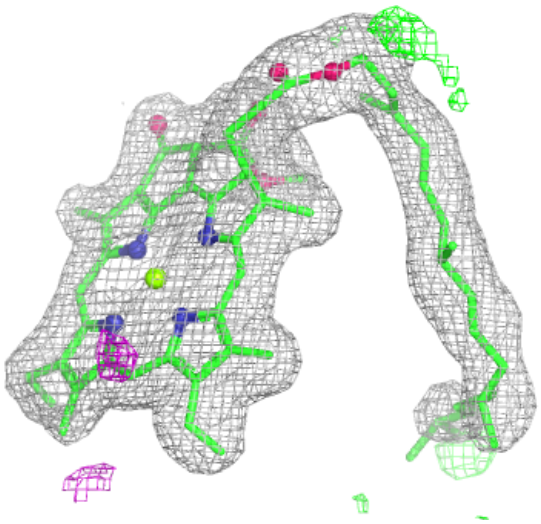


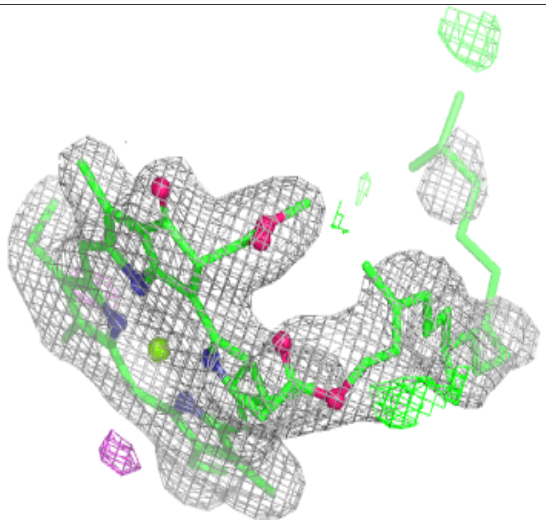


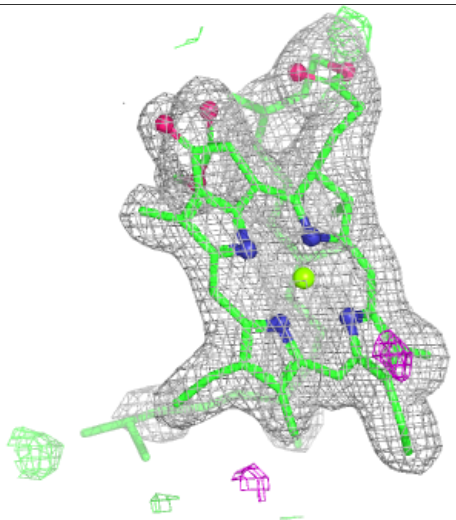


Electron density around CLA b 625:

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

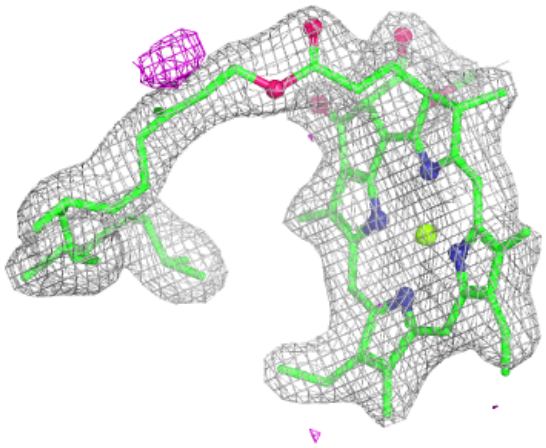


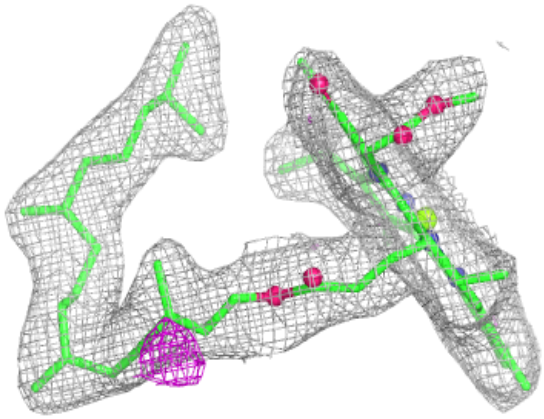


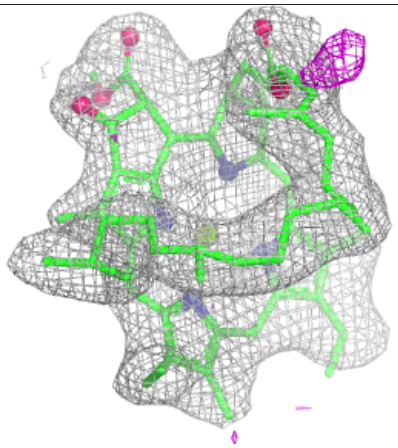


Electron density around CLA c 508:

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

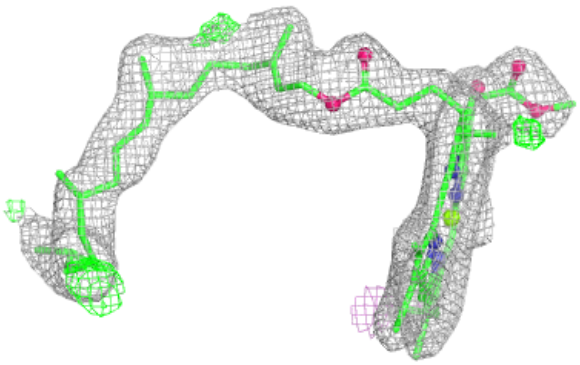


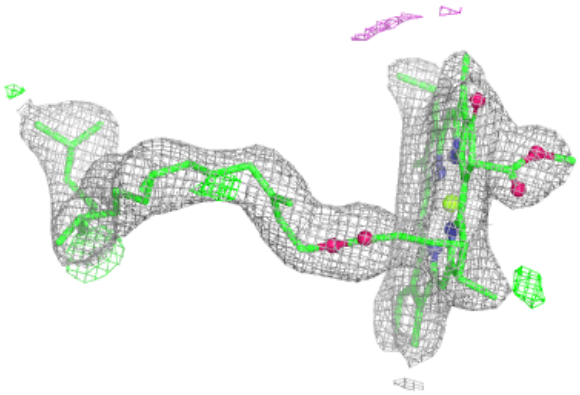


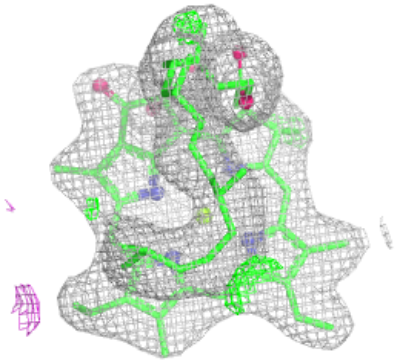


Electron density around CLA c 511:

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

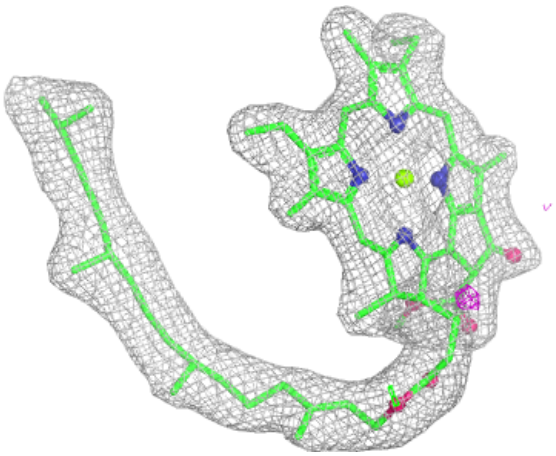


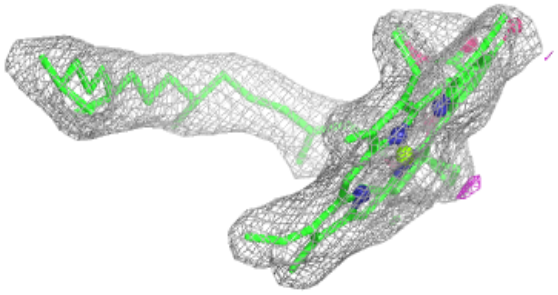


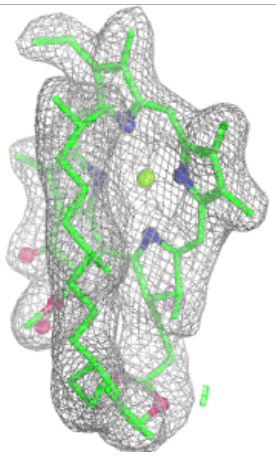


Electron density around CLA c 512:

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

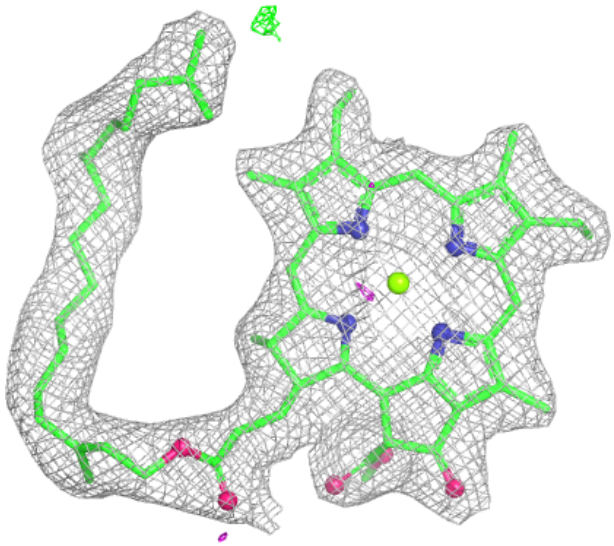


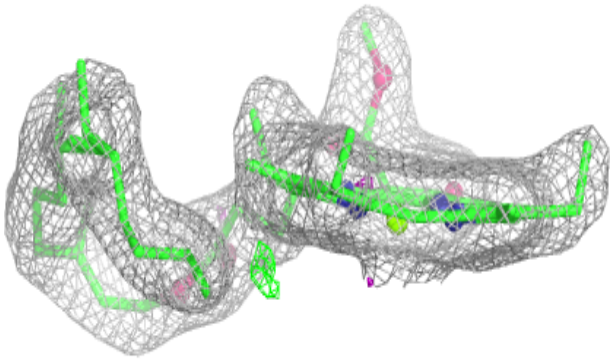


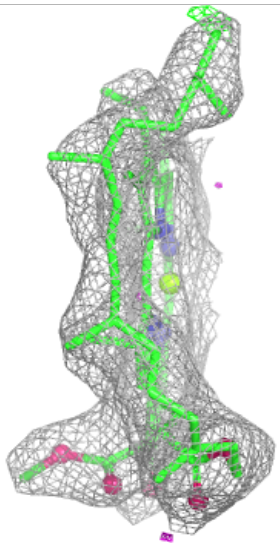


Electron density around CLA c 517:

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

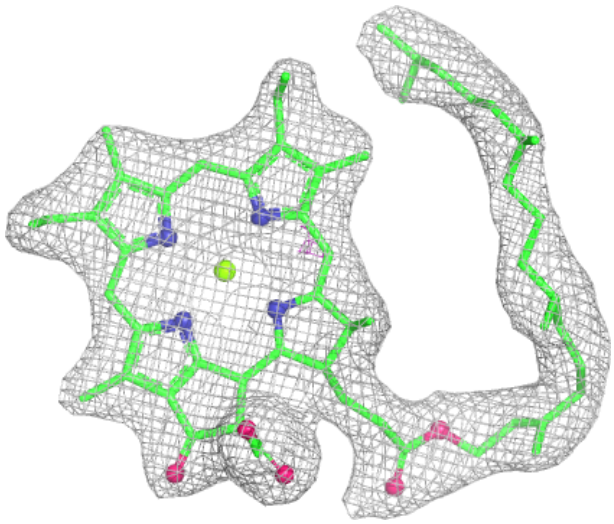


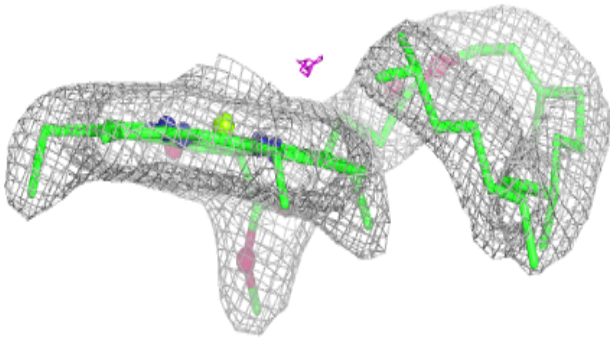


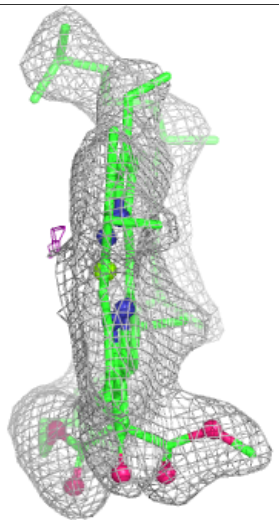


Electron density around CLA C 512:

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

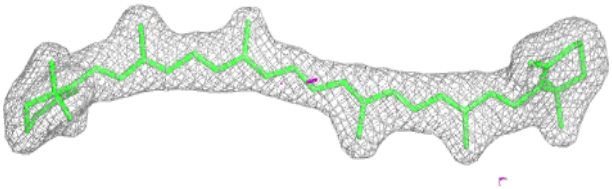


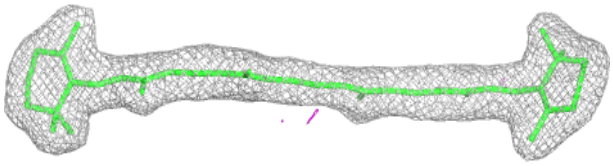


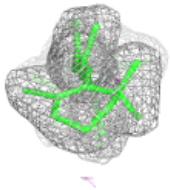


Electron density around BCR A 411:

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

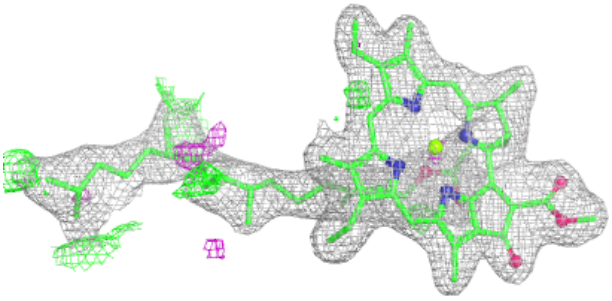


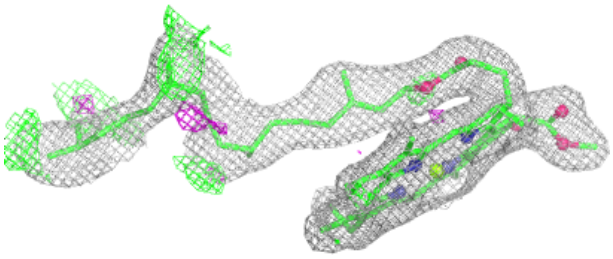


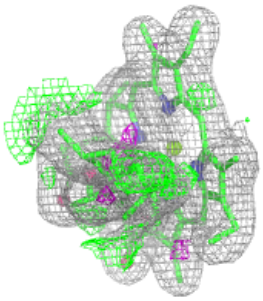


Electron density around CLA B 615:

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

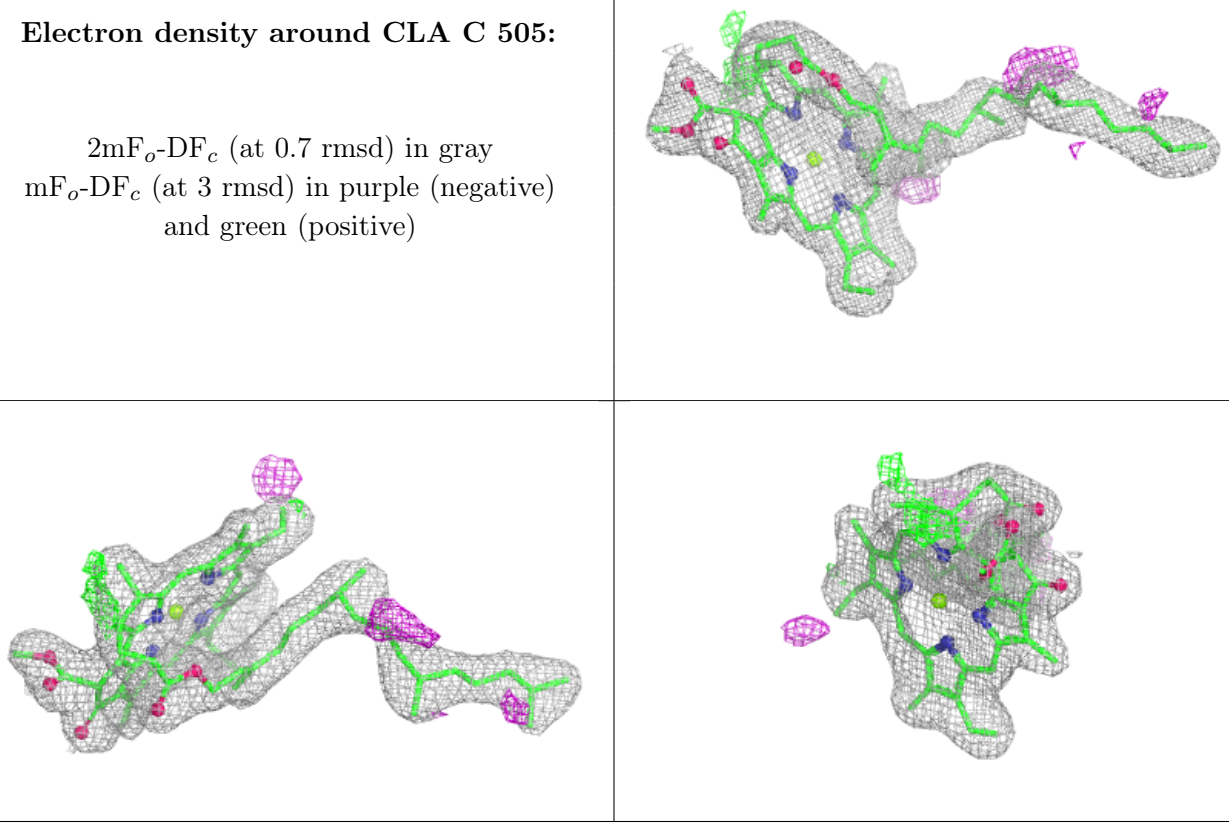






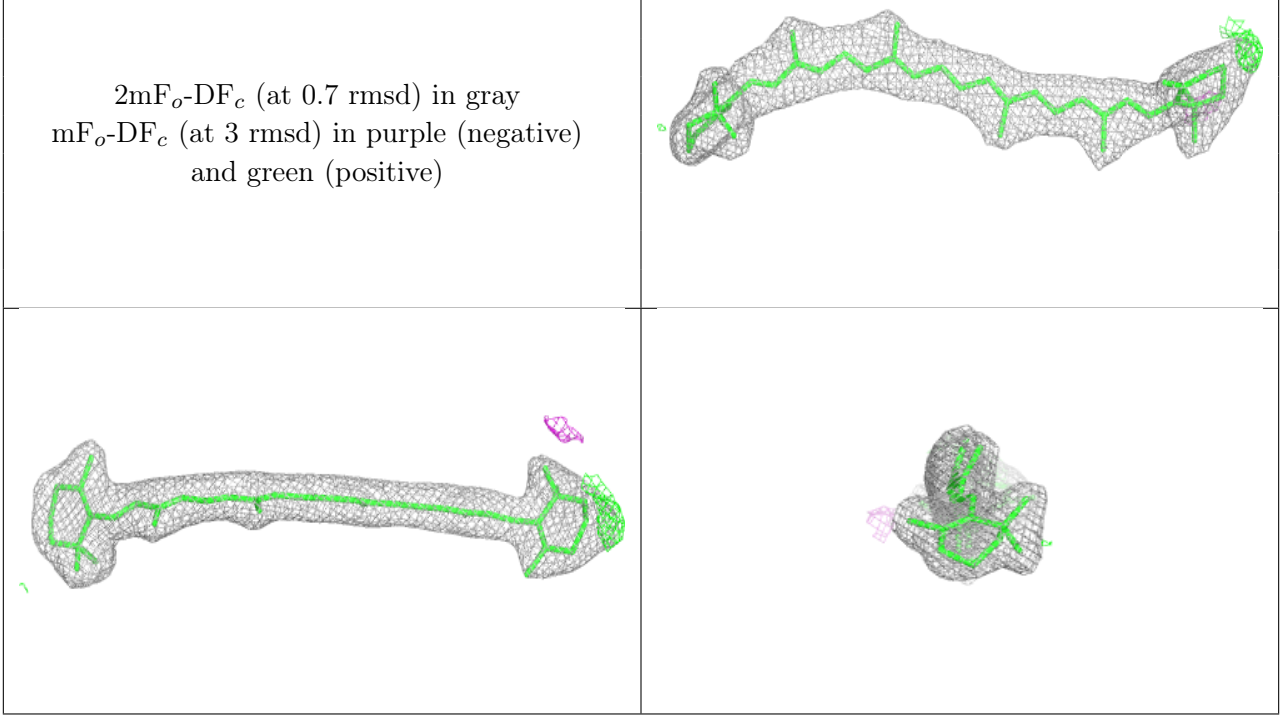
Electron density around CLA C 505:

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



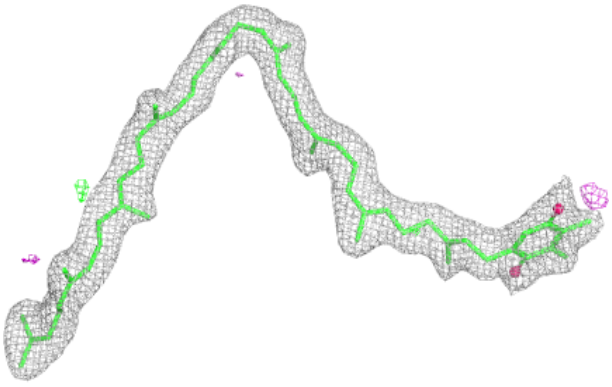
Electron density around BCR H 101:

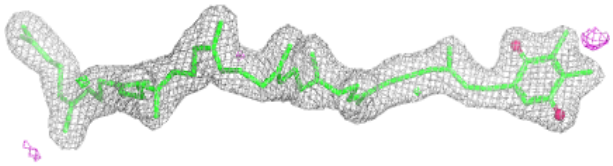
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

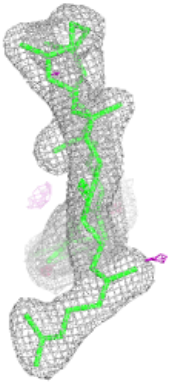


Electron density around PL9 d 405 (A):

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

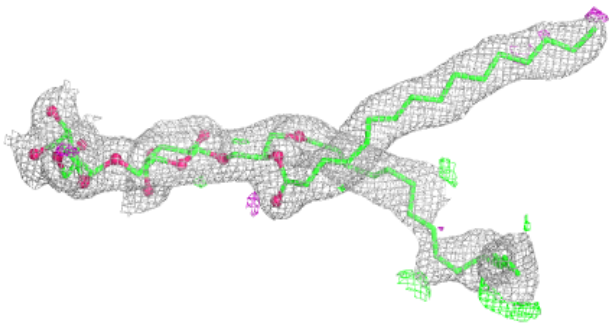


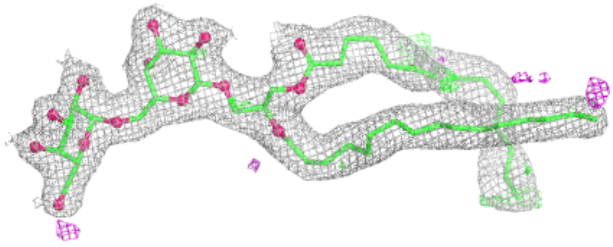


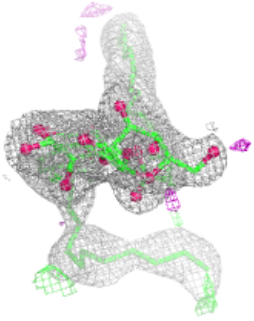


Electron density around DGD C 516:

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

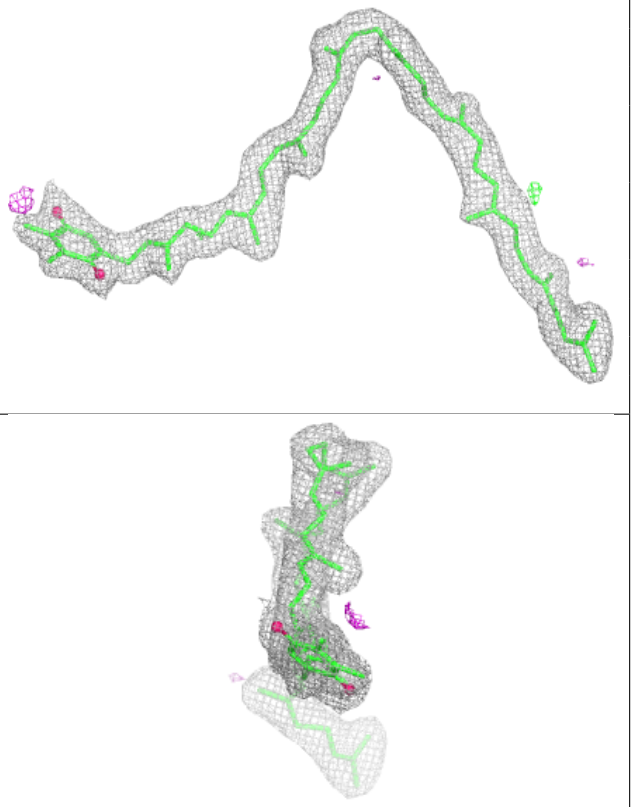






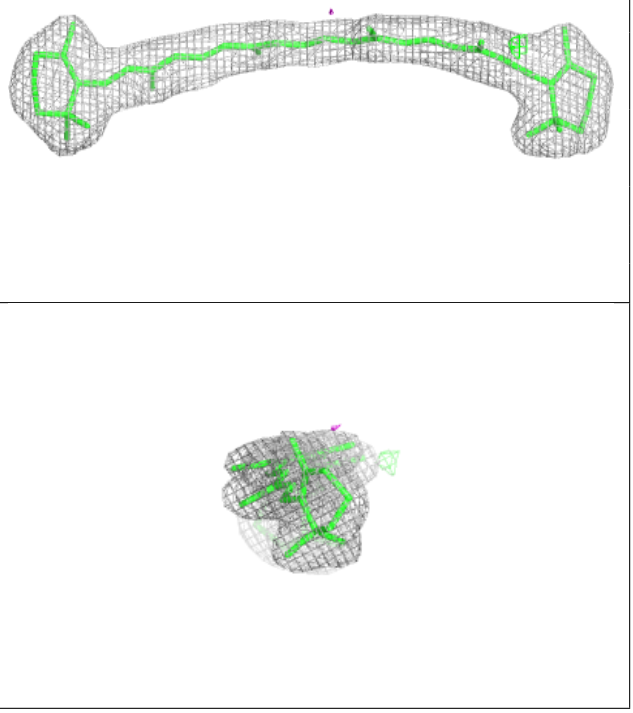
Electron density around PL9 d 405 (B):

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



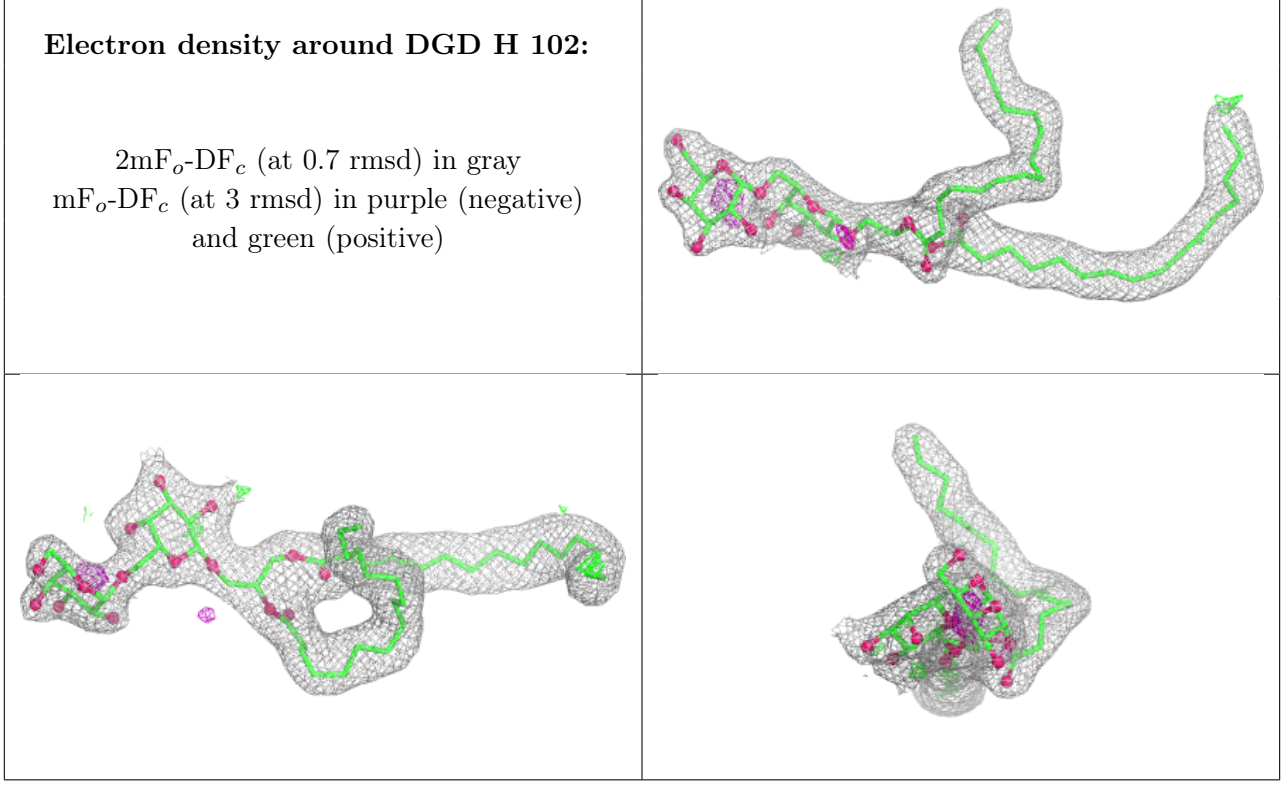
Electron density around BCR K 101:

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



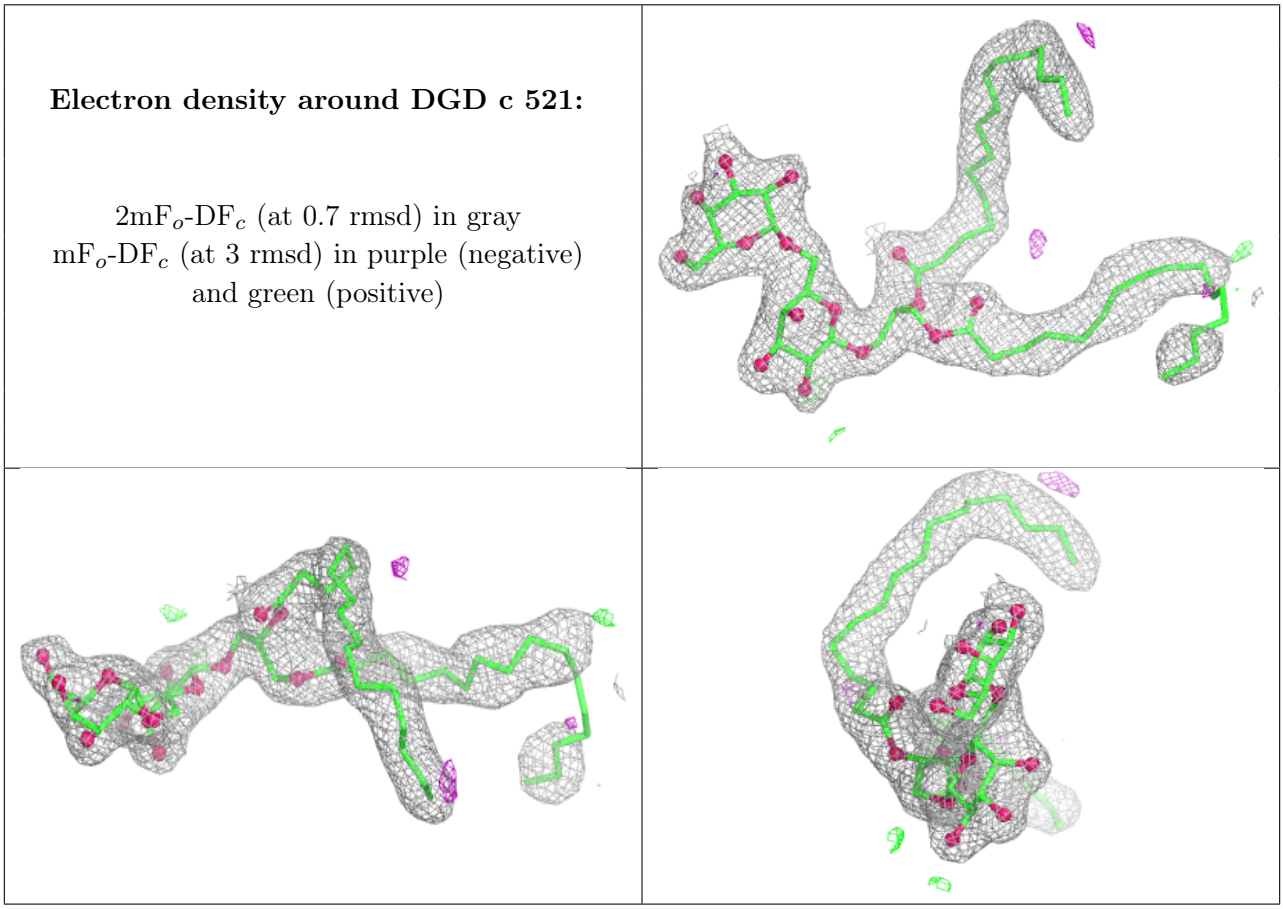
Electron density around DGD H 102:

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



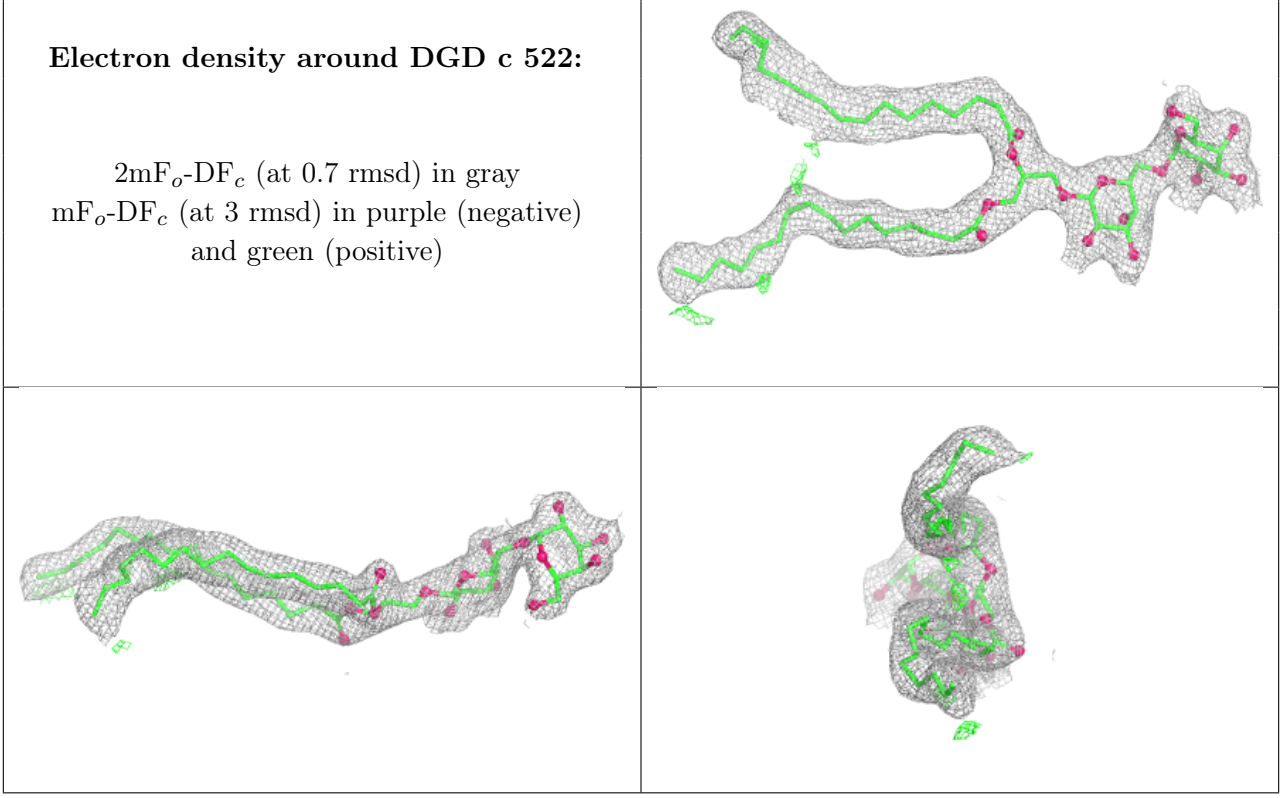
Electron density around DGD c 521:

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



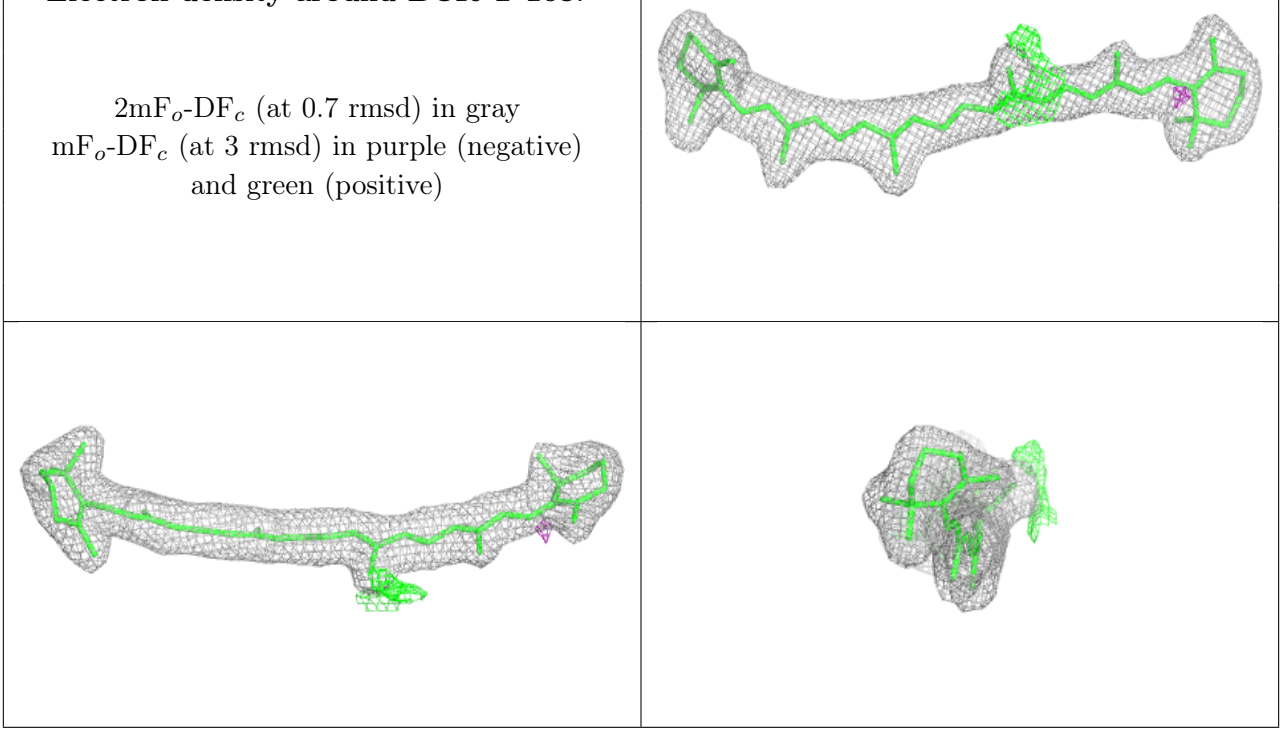
Electron density around DGD c 522:

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



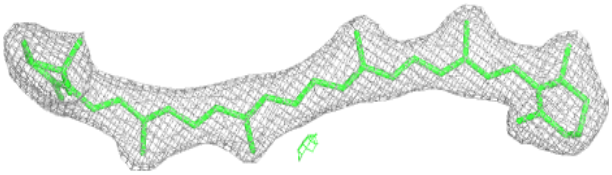
Electron density around BCR T 103:

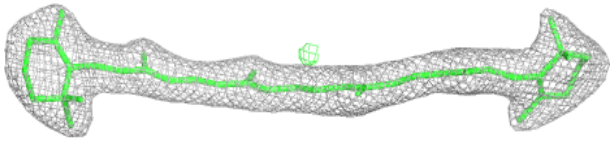
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

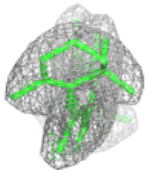


Electron density around BCR Y 101:

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

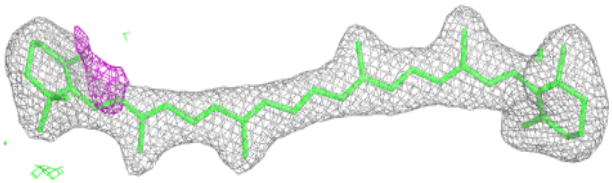


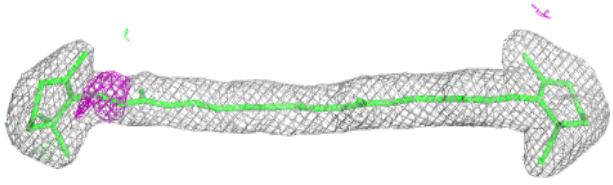


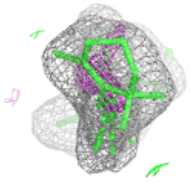


Electron density around BCR b 627:

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

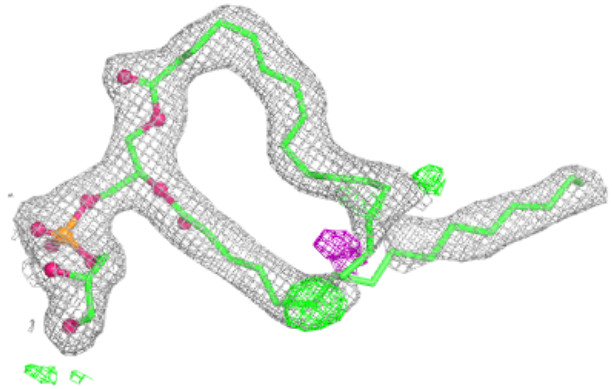


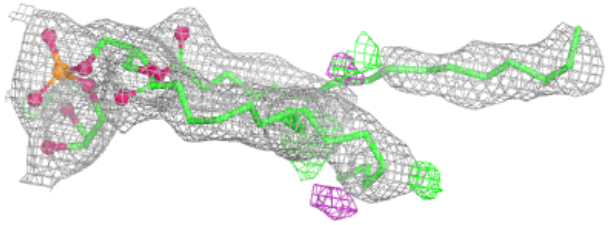


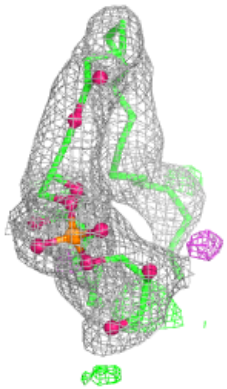


Electron density around LHG d 408:

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

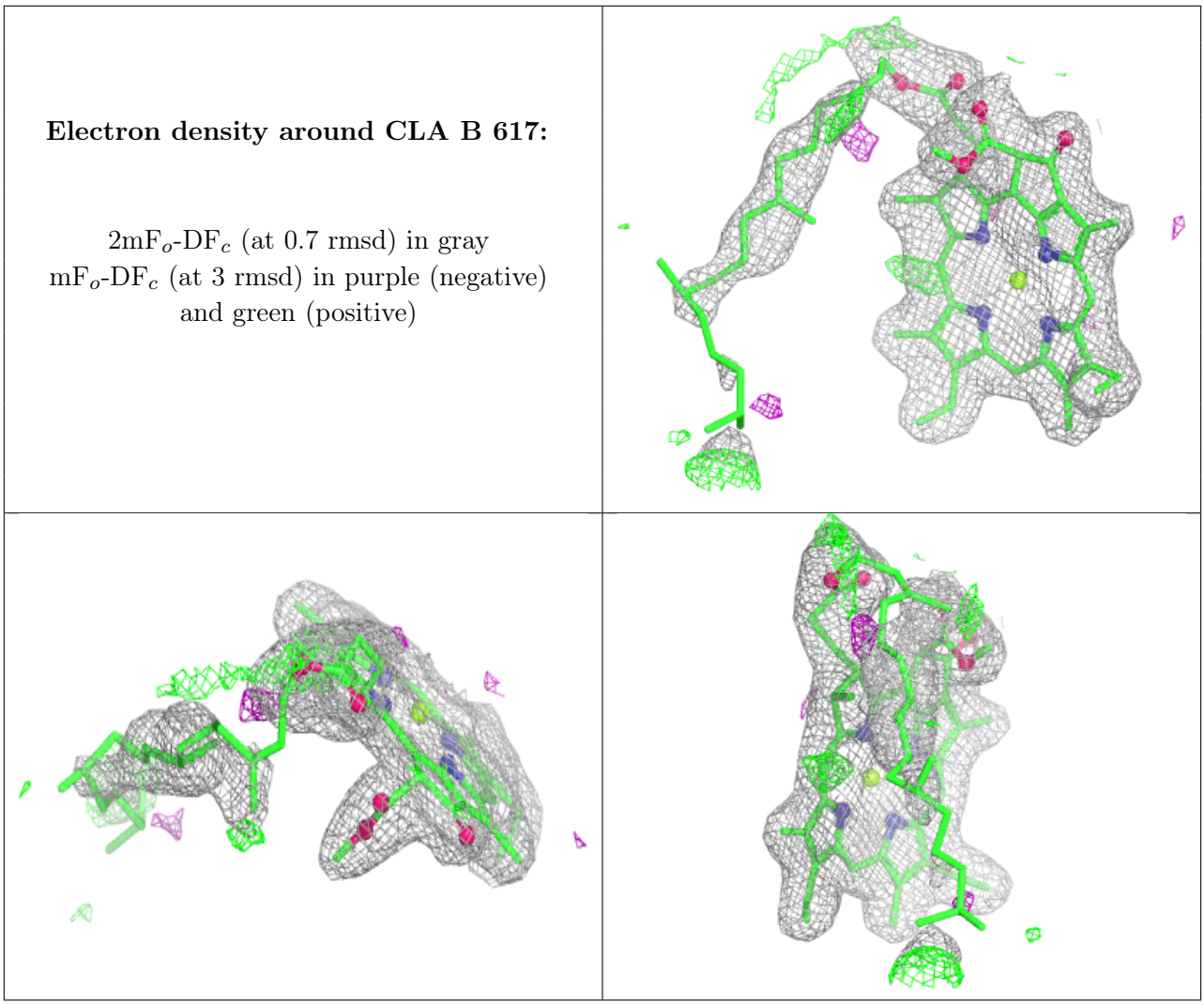






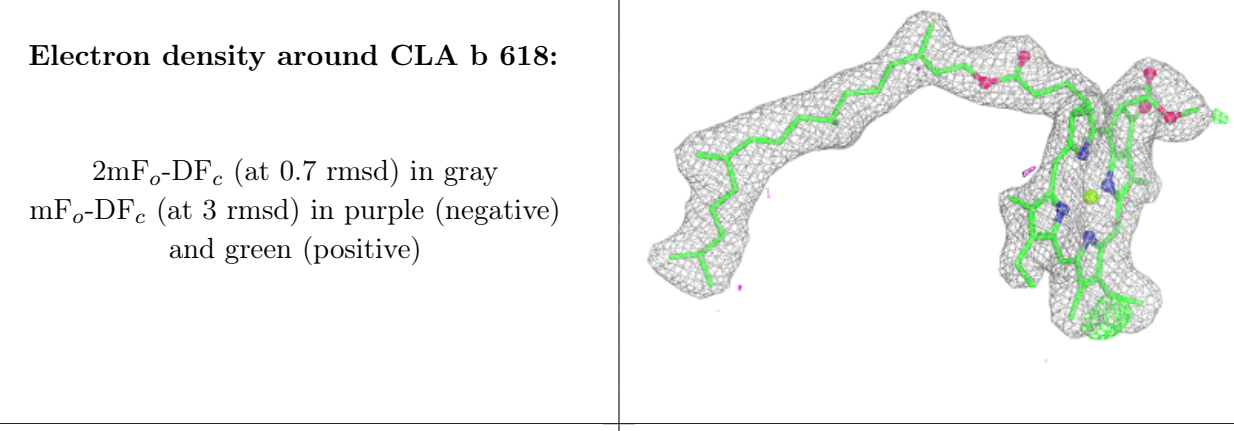
Electron density around CLA B 617:

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



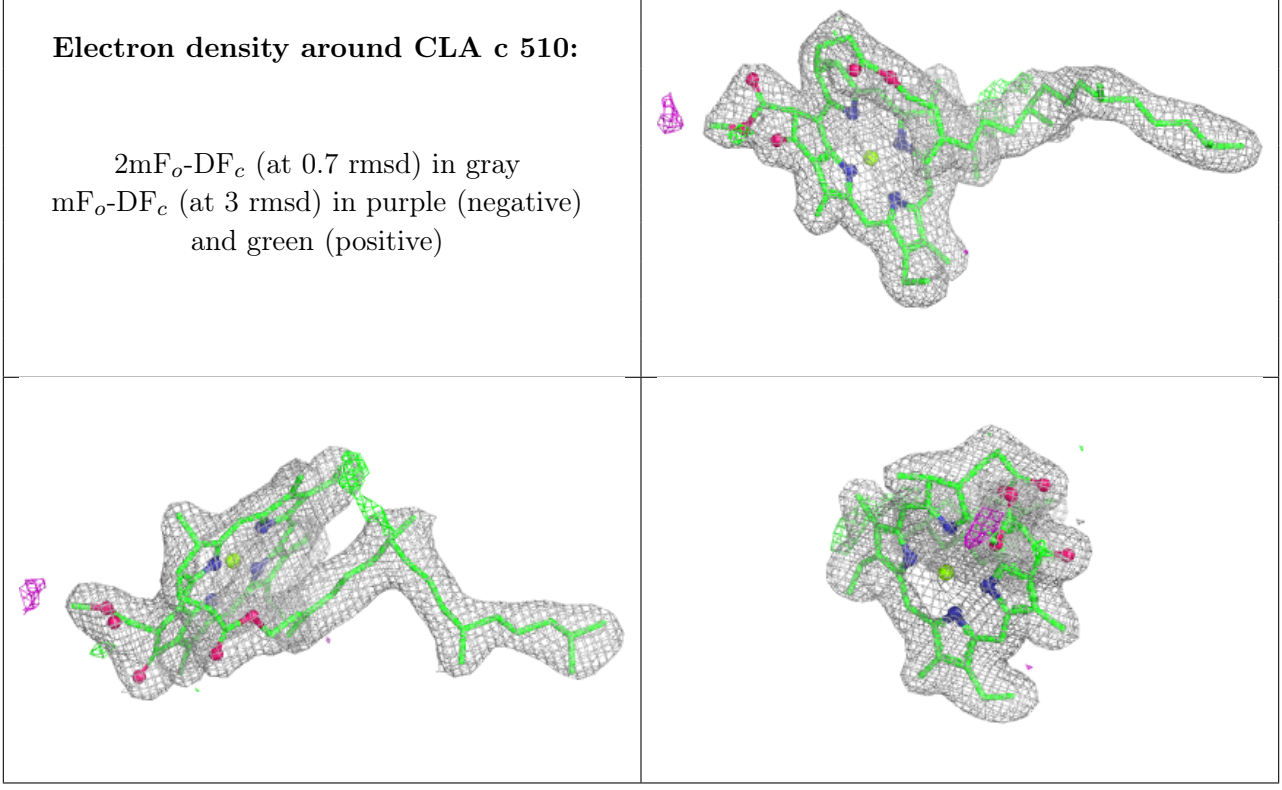
Electron density around CLA b 618:

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



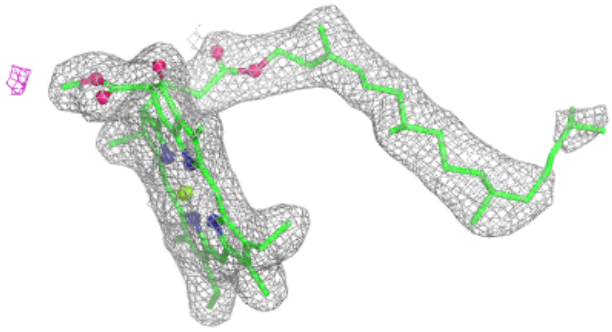
Electron density around CLA c 510:

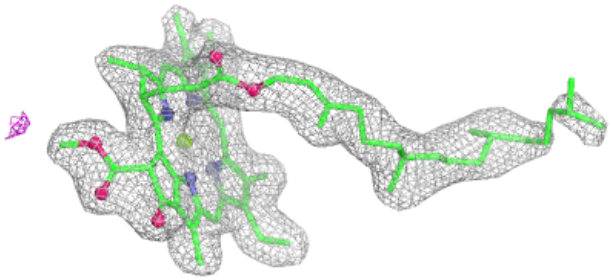
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

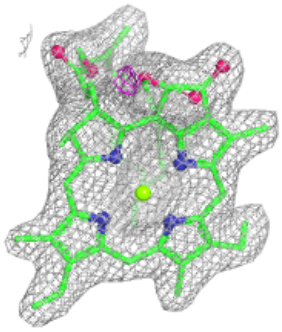


Electron density around CLA C 508:

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

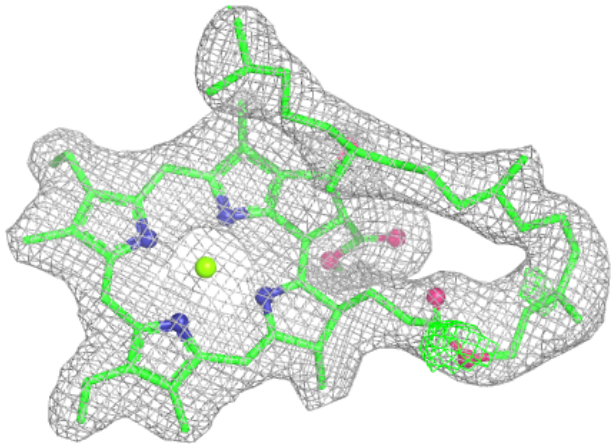


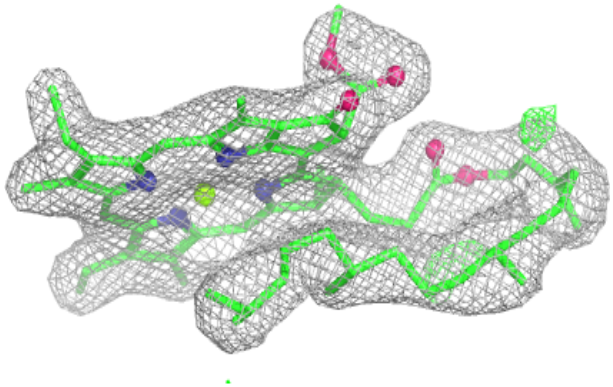


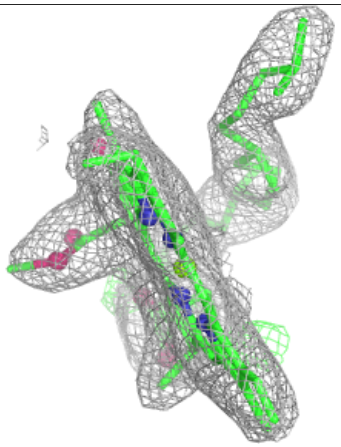


Electron density around CLA C 509:

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

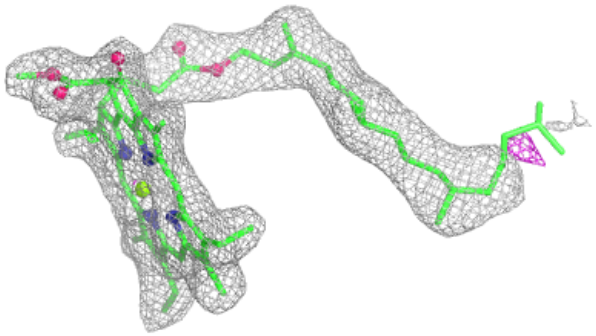


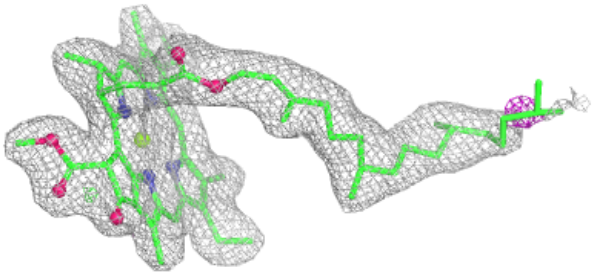


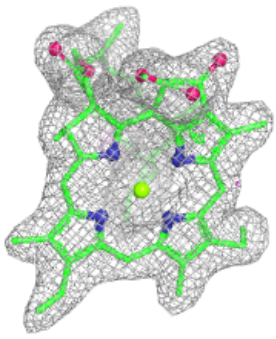


Electron density around CLA c 513:

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

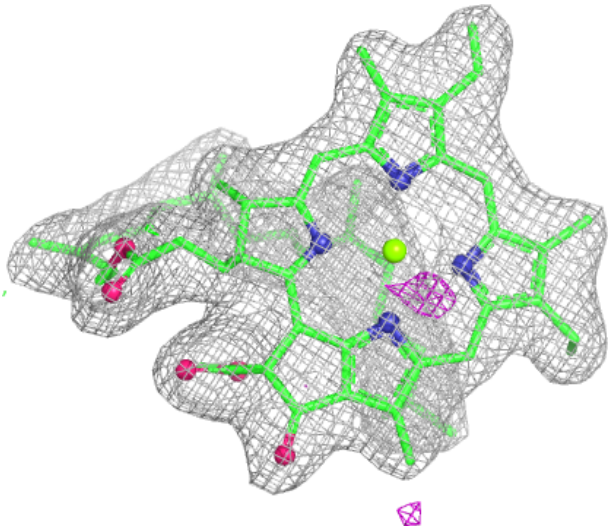


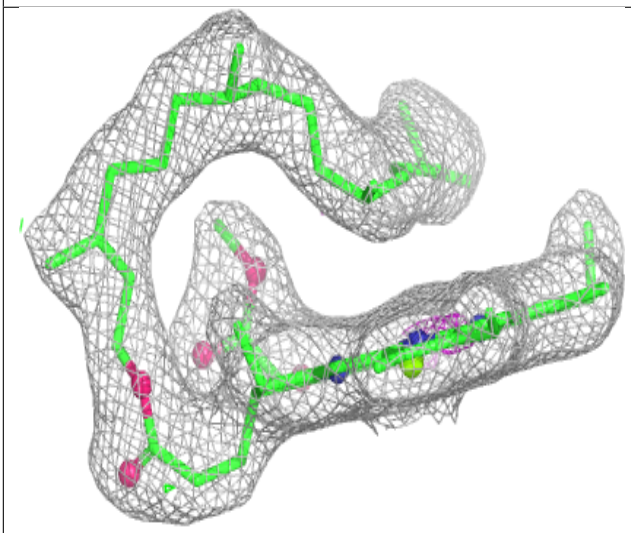


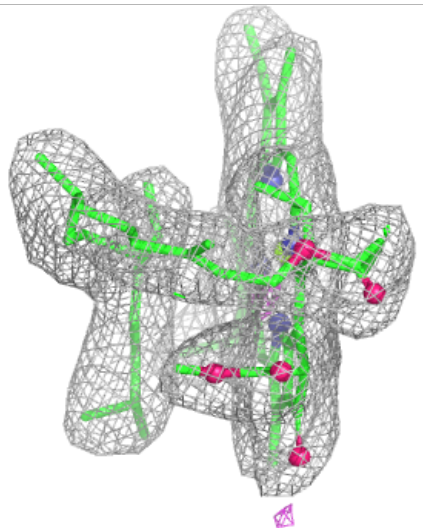


Electron density around CLA c 515:

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

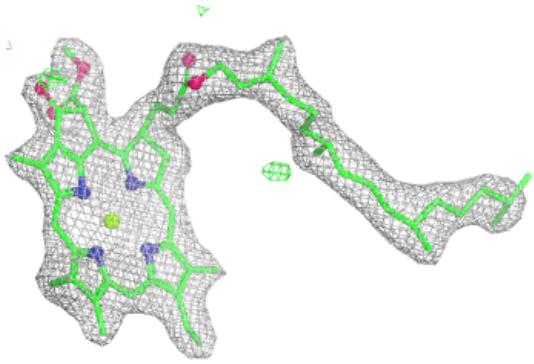


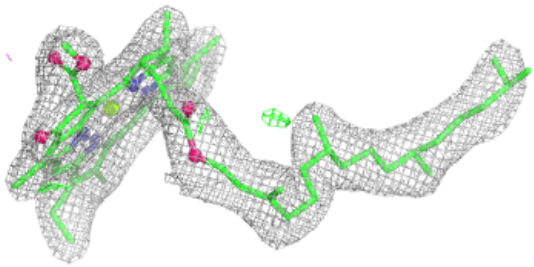


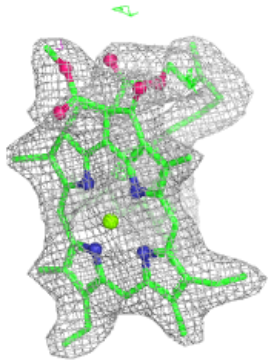


Electron density around CLA c 516:

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

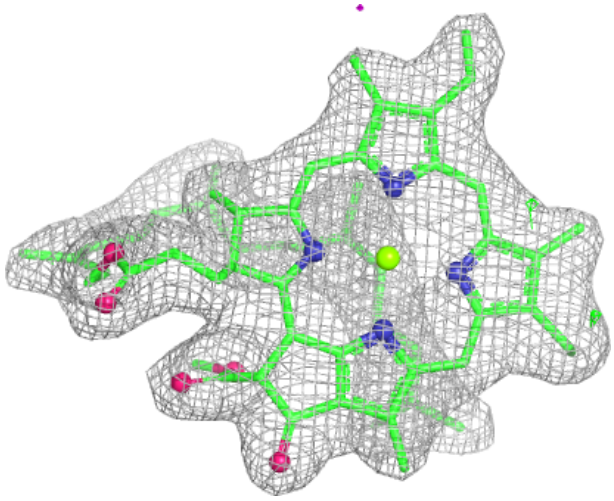


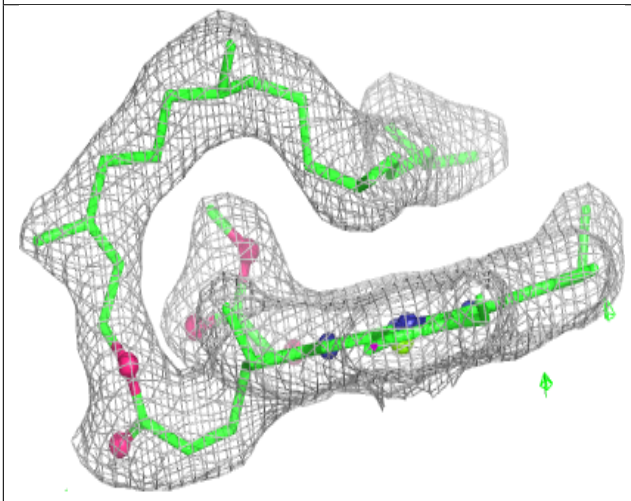


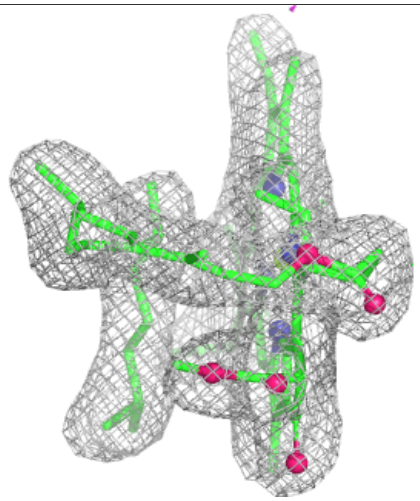


Electron density around CLA C 510:

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

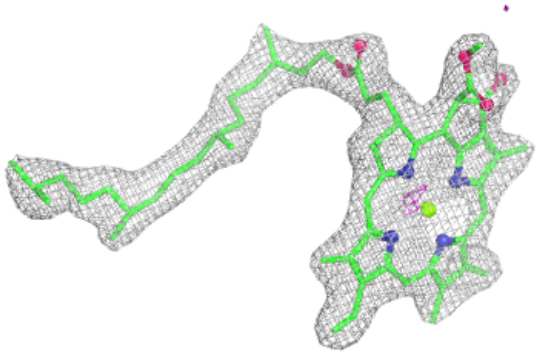


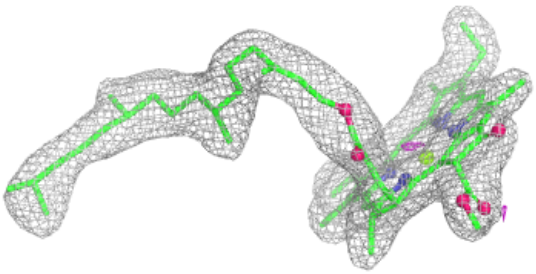


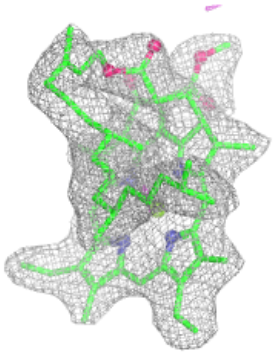


Electron density around CLA C 511:

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

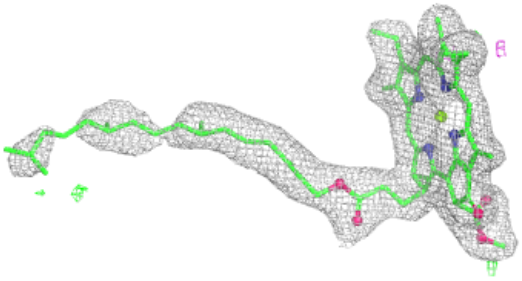


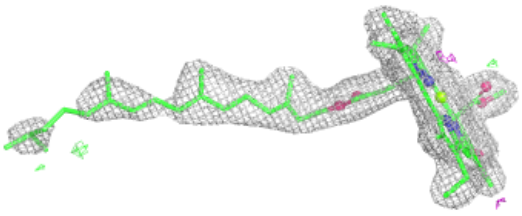


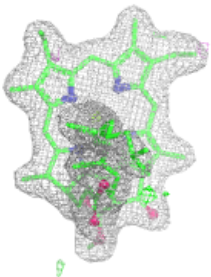


Electron density around CLA d 403:

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

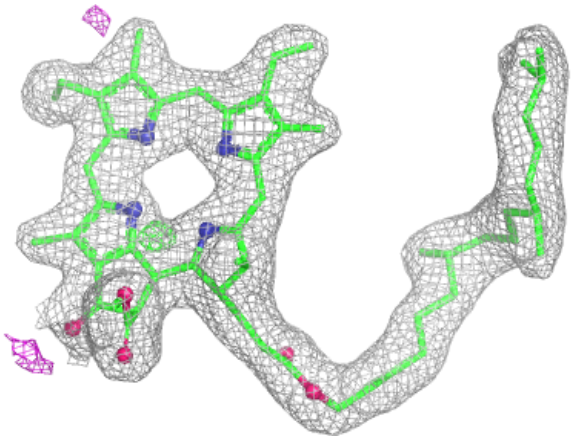


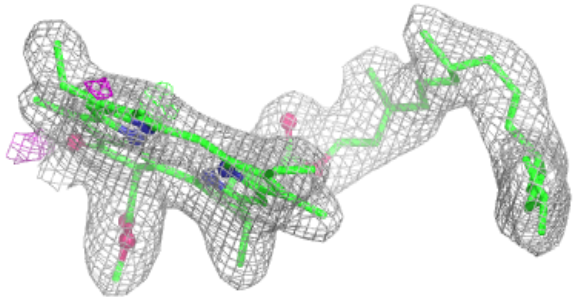


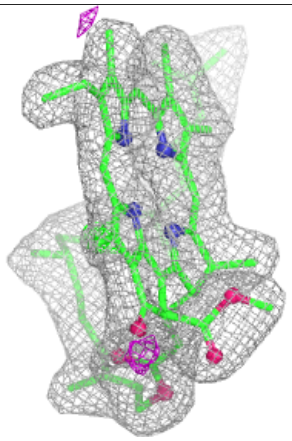


Electron density around PHO a 418 (A):

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

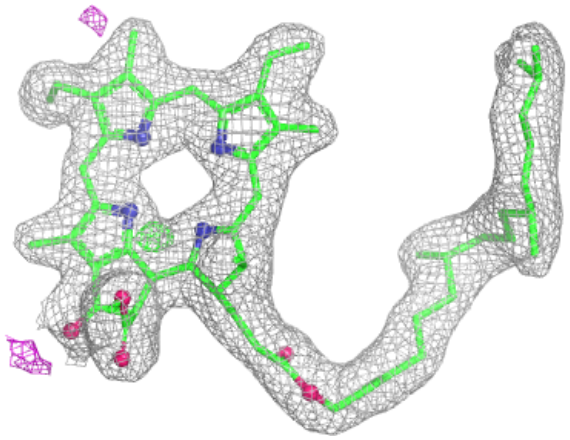


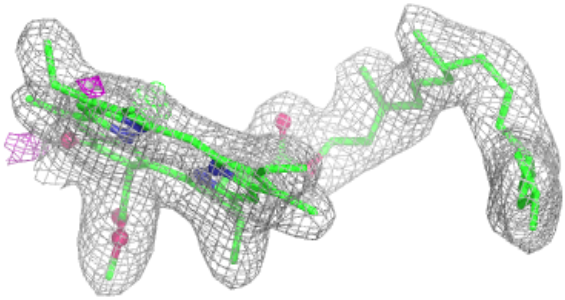


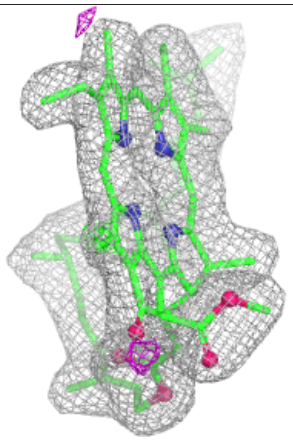


Electron density around PHO a 418 (B):

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

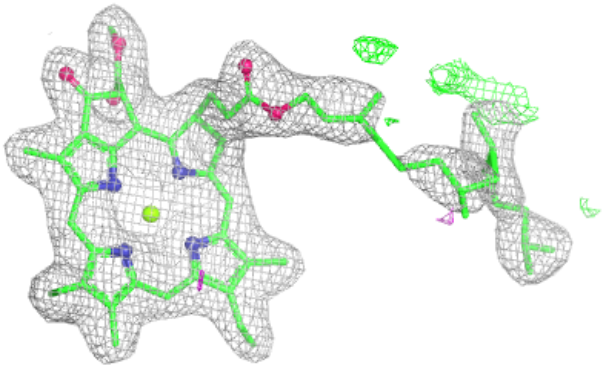


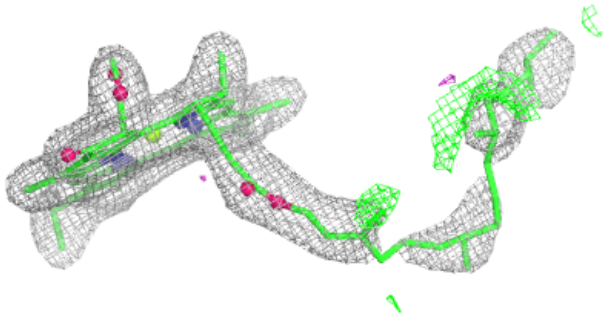


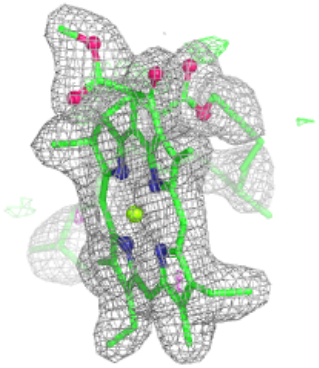


Electron density around CLA A 410:

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

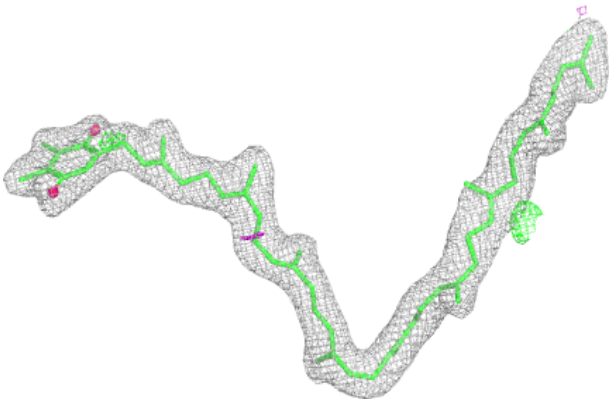


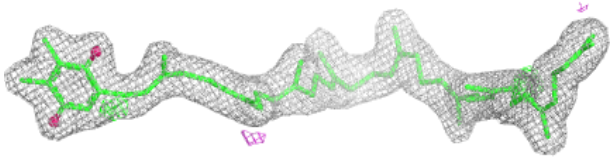




Electron density around PL9 D 405 (A):

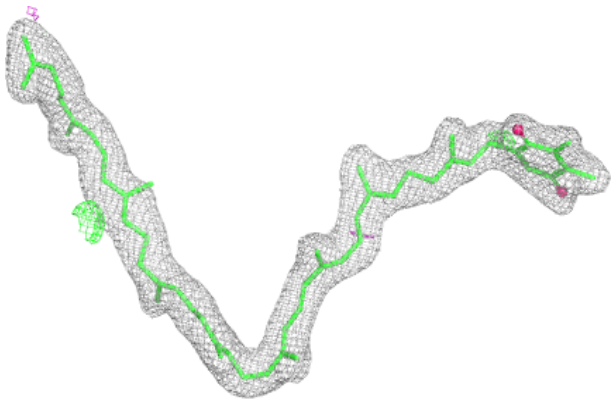
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

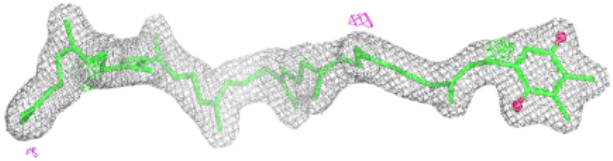


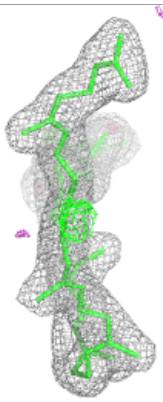


Electron density around PL9 D 405 (B):

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

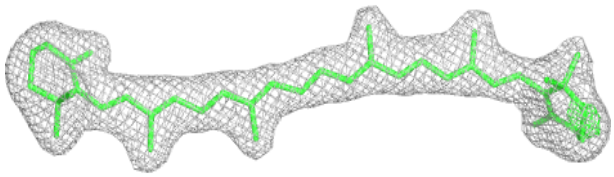


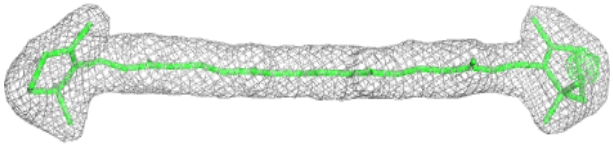


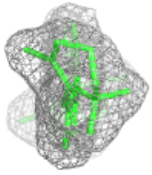


Electron density around BCR B 619:

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

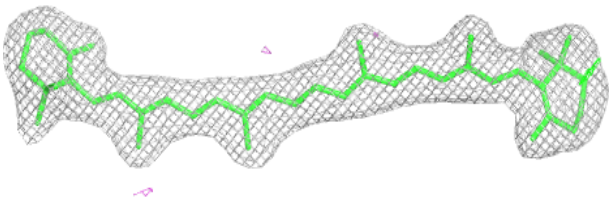


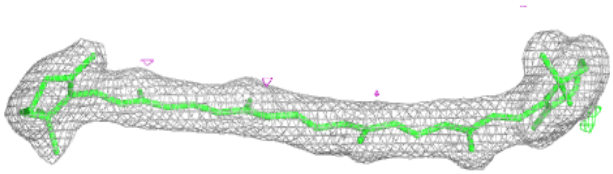


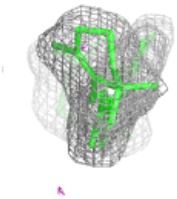


Electron density around BCR B 620:

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

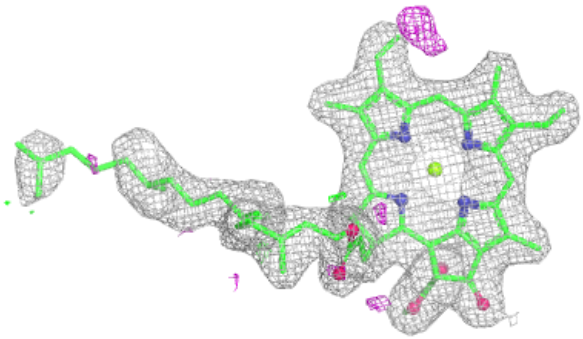


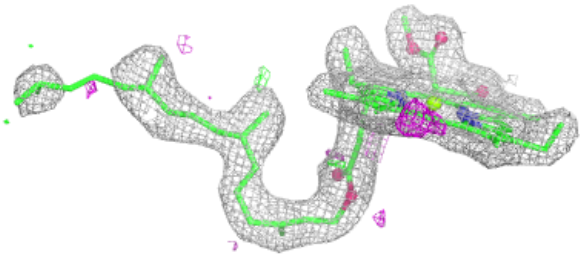


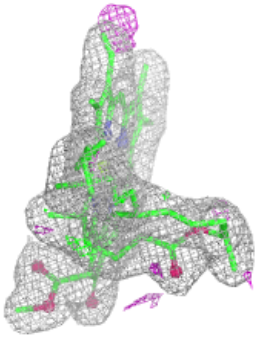


Electron density around CLA A 407:

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

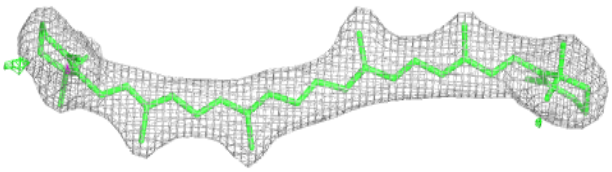


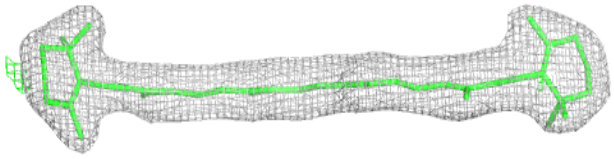


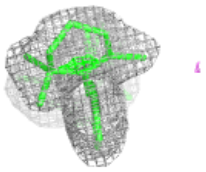


Electron density around BCR C 515:

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

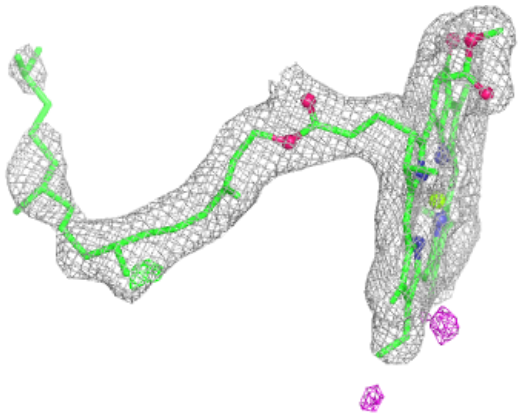


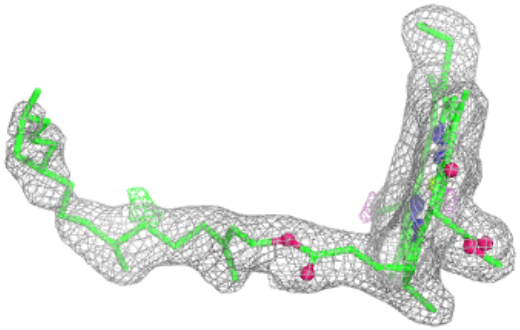


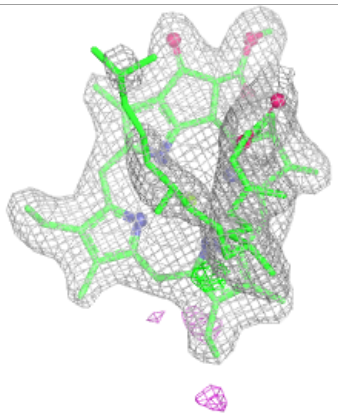


Electron density around CLA D 403:

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

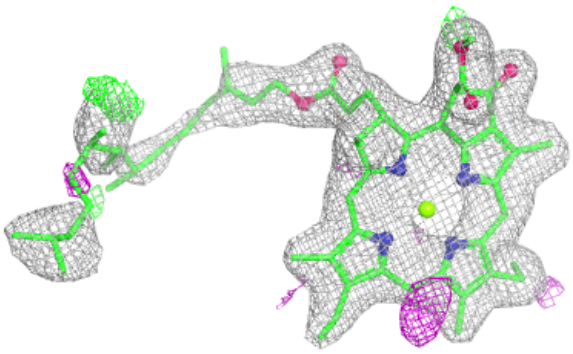


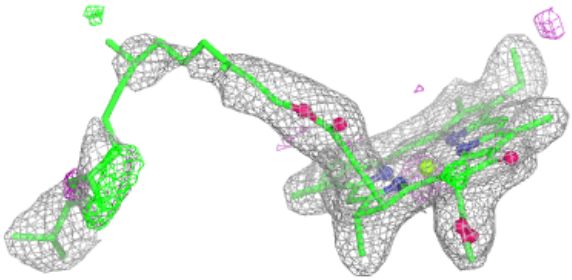


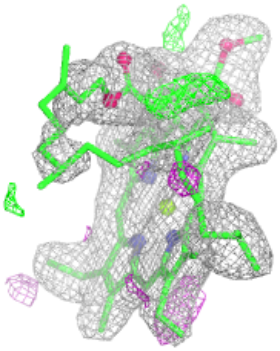


Electron density around CLA a 412:

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

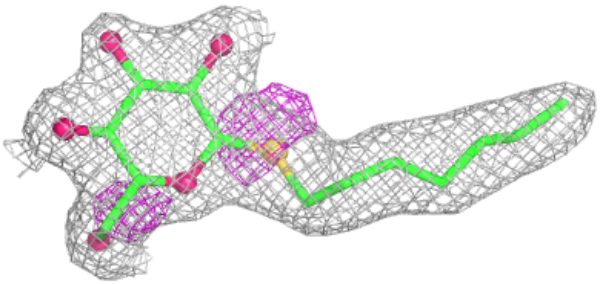


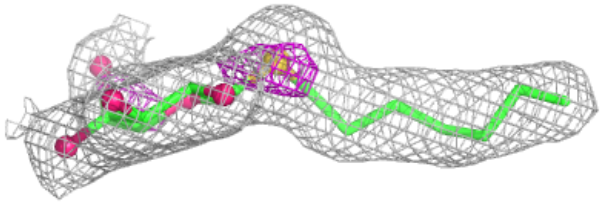


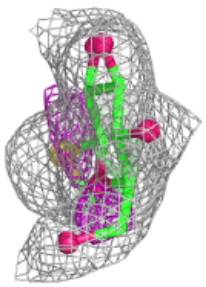


Electron density around HTG b 601:

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

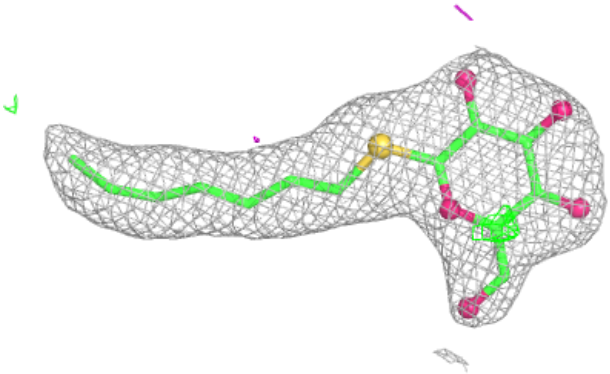


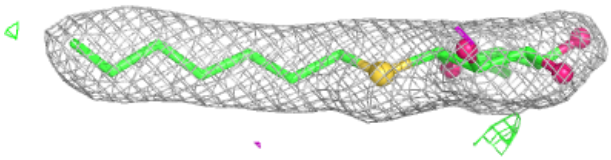


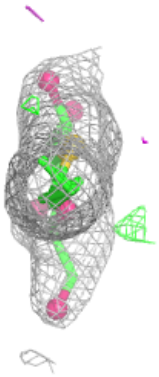


Electron density around HTG b 607:

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

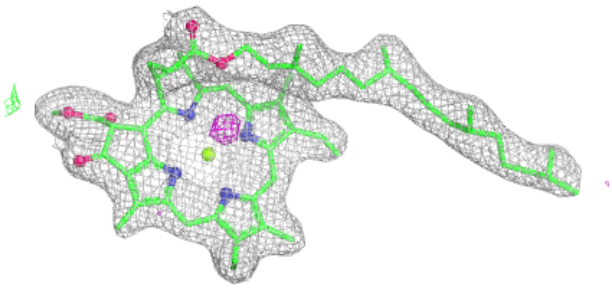


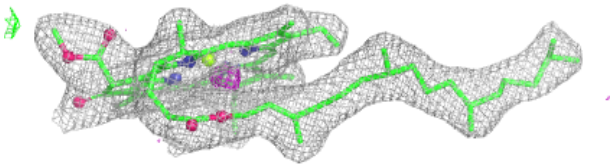


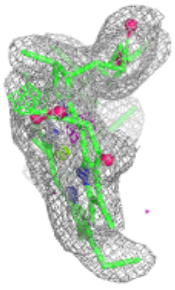


Electron density around CLA C 501:

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

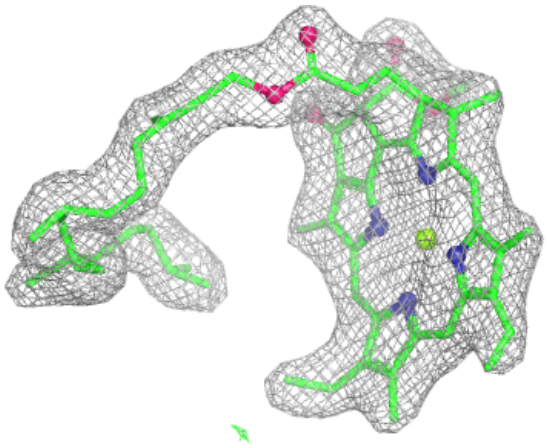


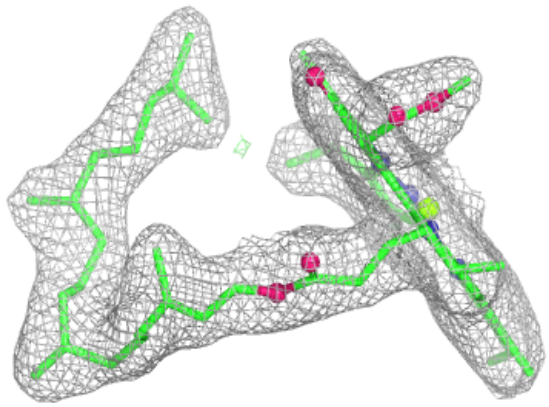


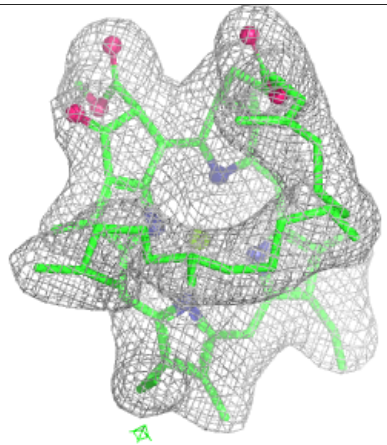


Electron density around CLA C 503:

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

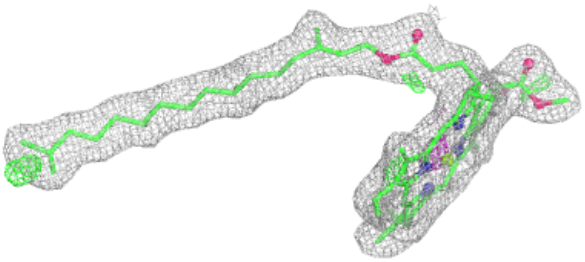


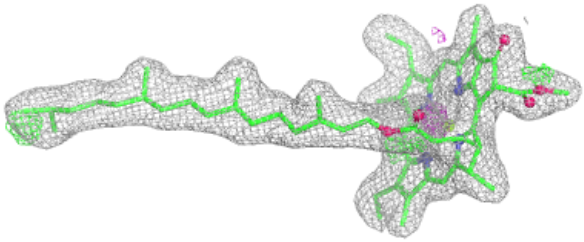


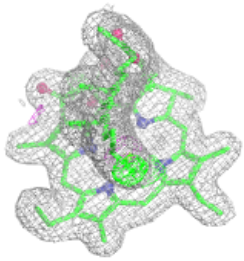


Electron density around CLA b 616:

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

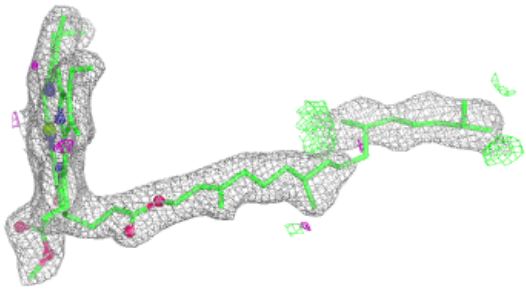


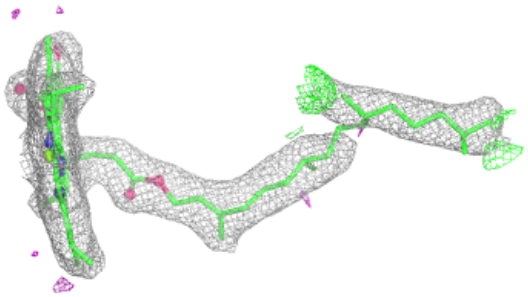


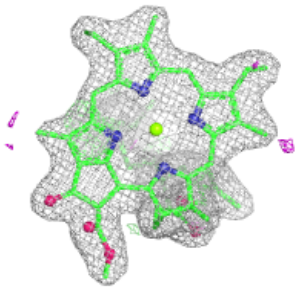


Electron density around CLA B 607:

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

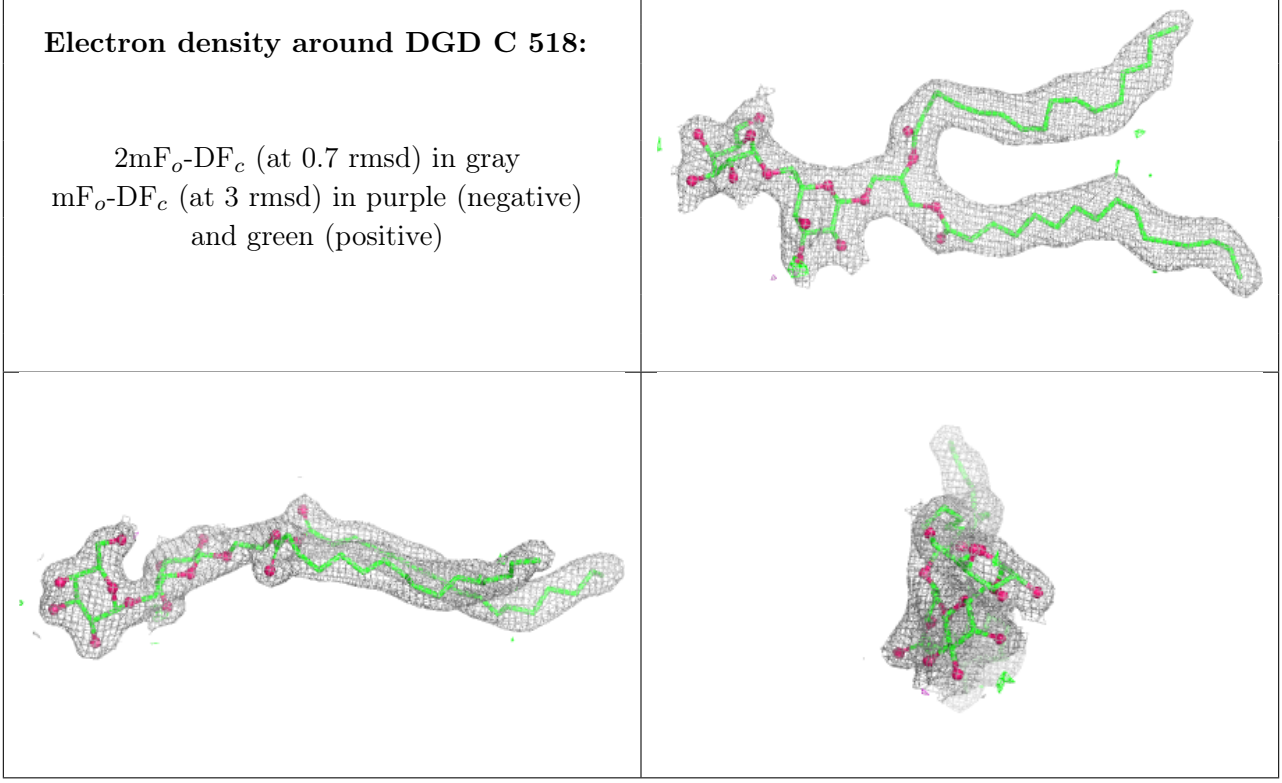






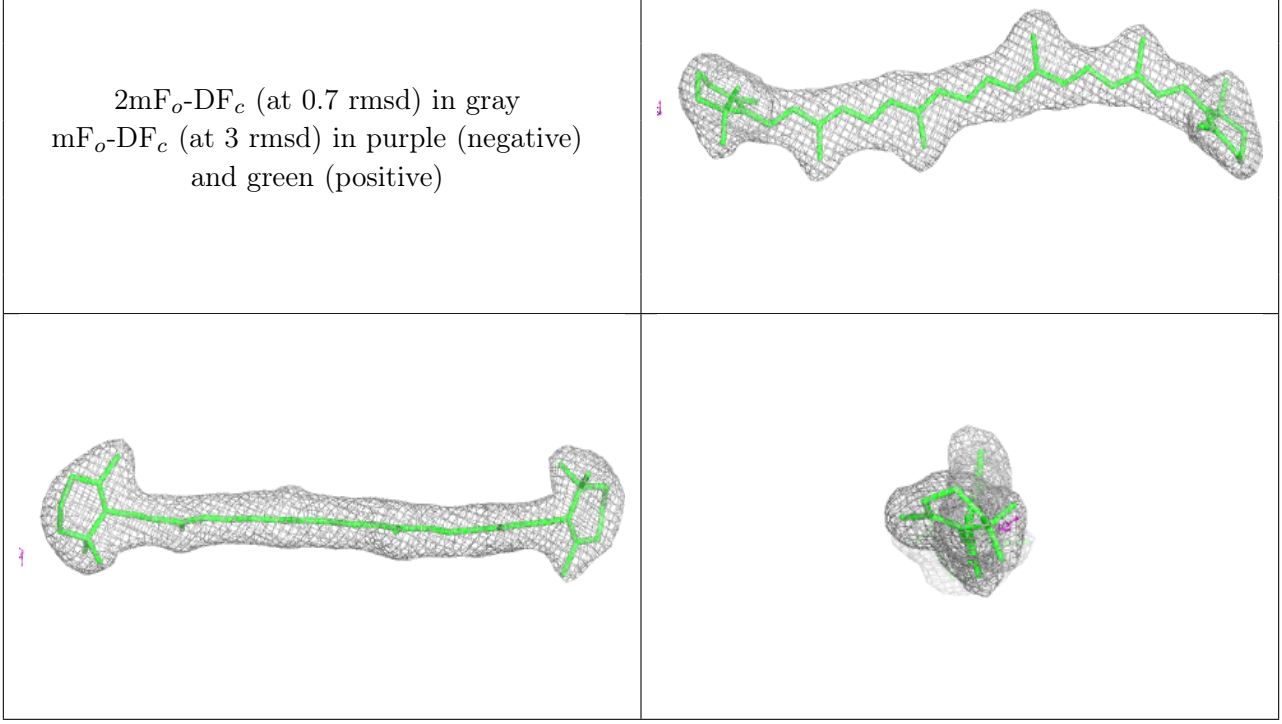
Electron density around DGD C 518:

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



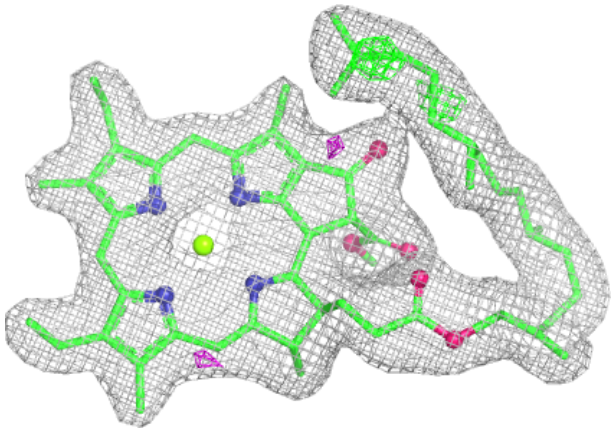
Electron density around BCR c 519:

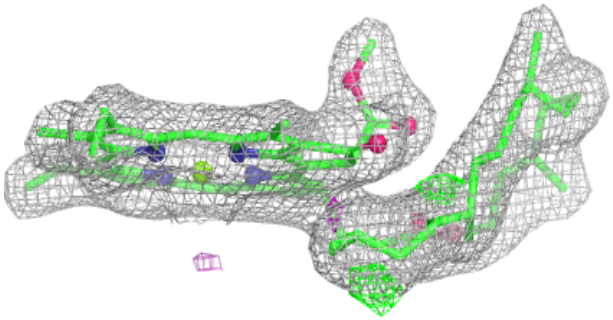
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

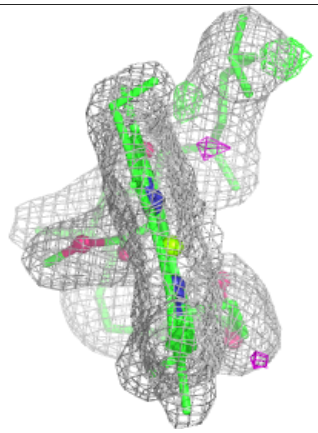


Electron density around CLA b 619:

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

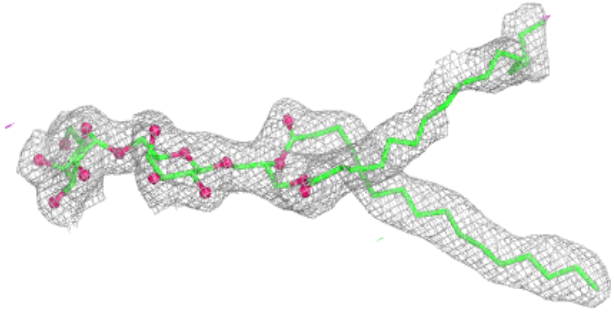


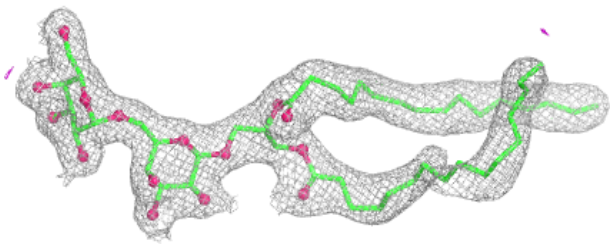


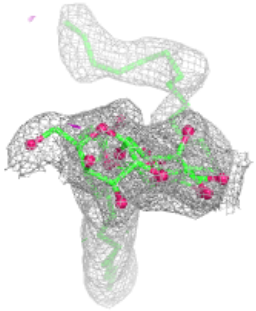


Electron density around DGD c 520:

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

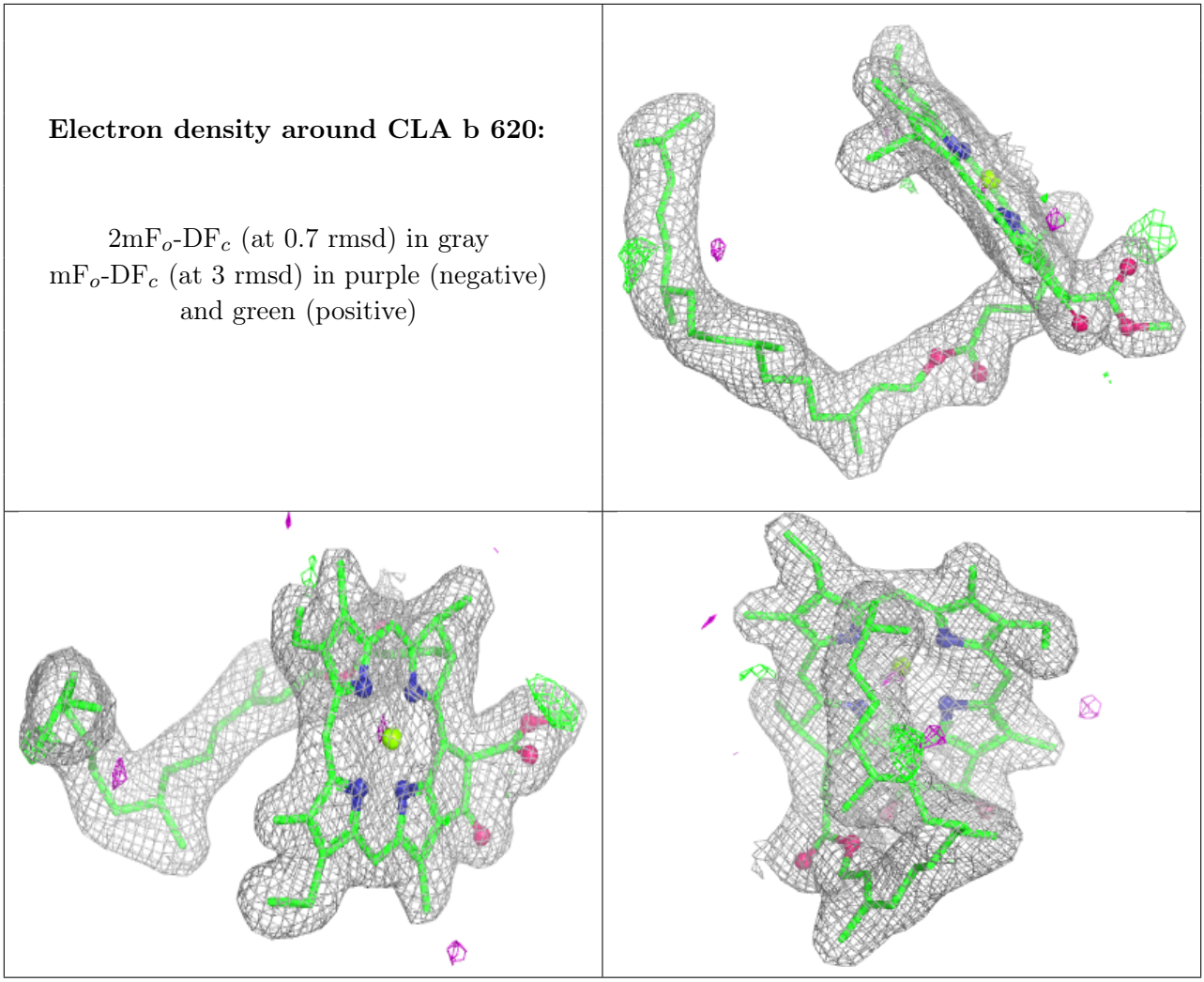






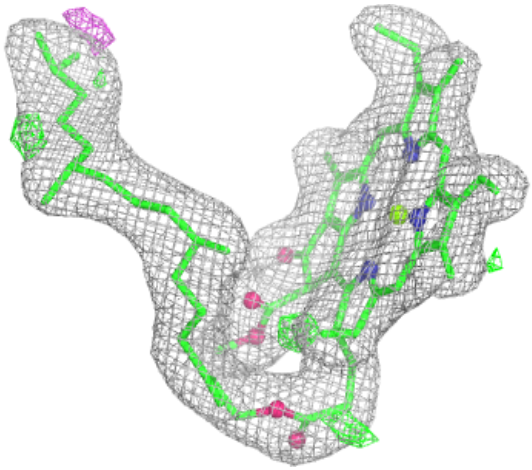
Electron density around CLA b 620:

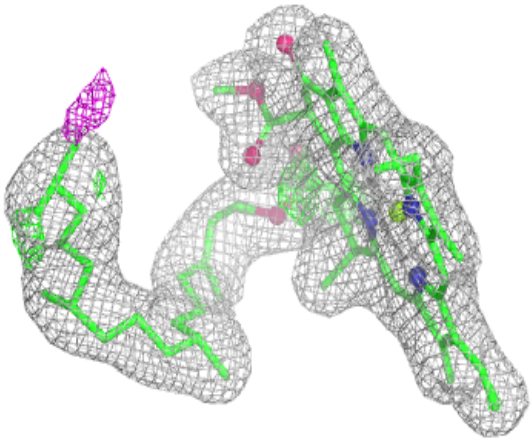
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

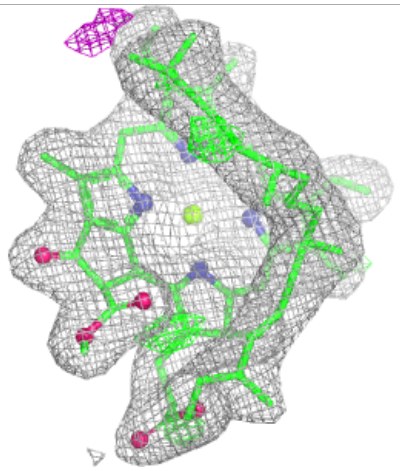


Electron density around CLA b 622:

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

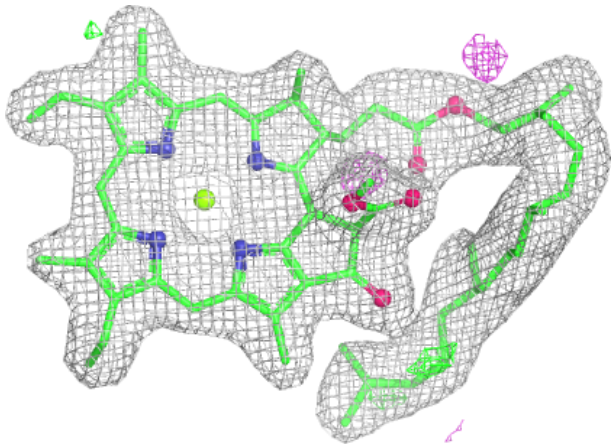


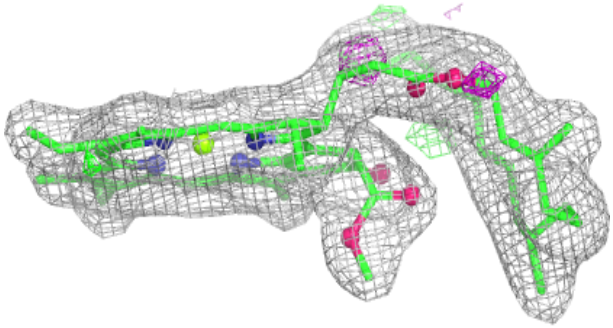


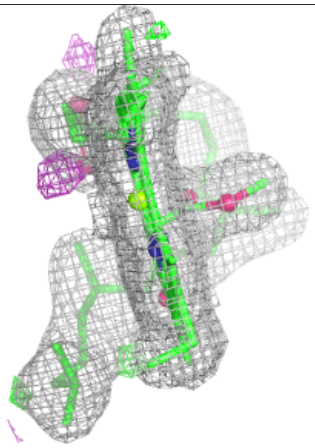


Electron density around CLA B 611:

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

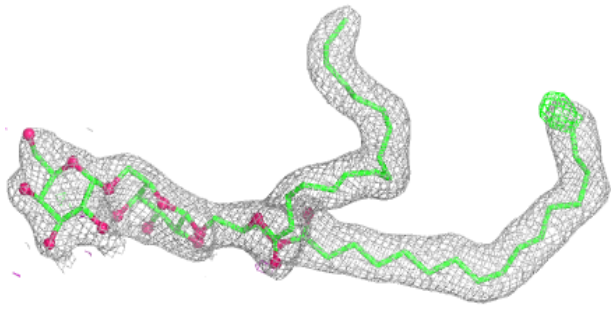


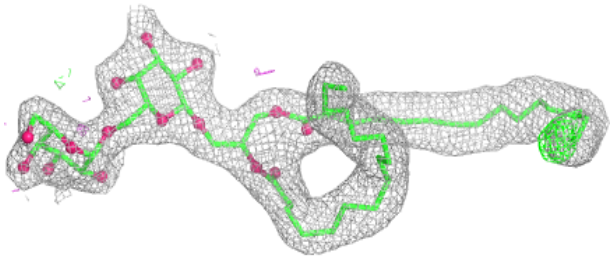




Electron density around DGD h 102:

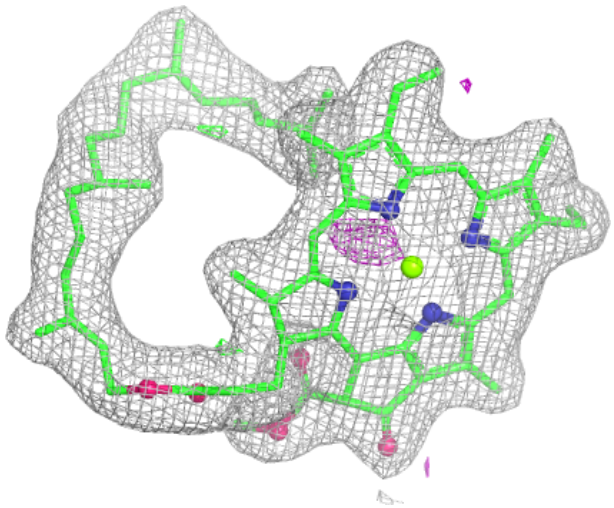
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

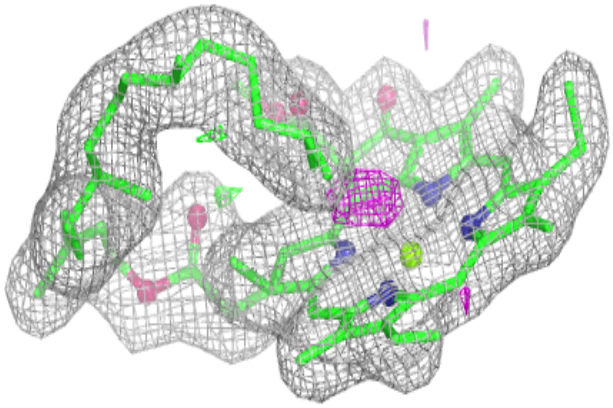


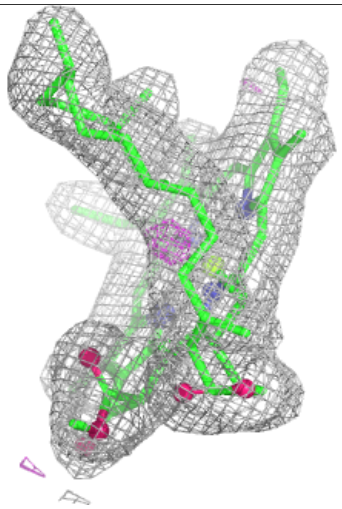


Electron density around CLA b 624:

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

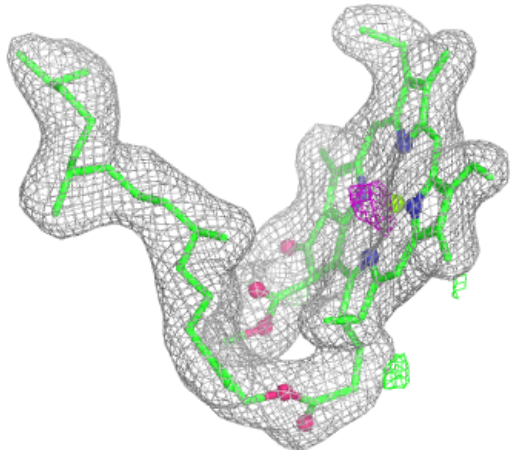


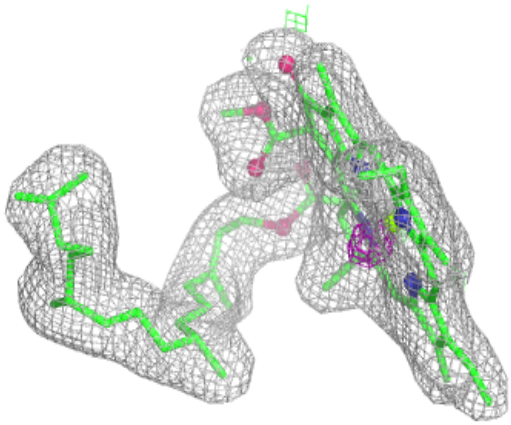


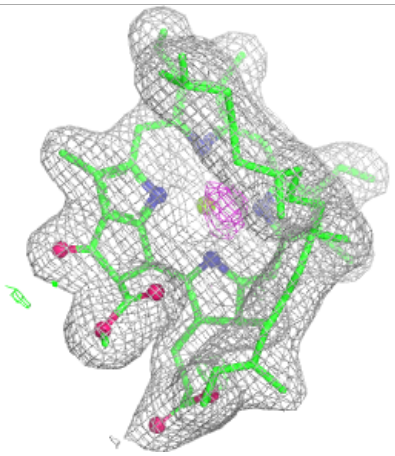


Electron density around CLA B 614:

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

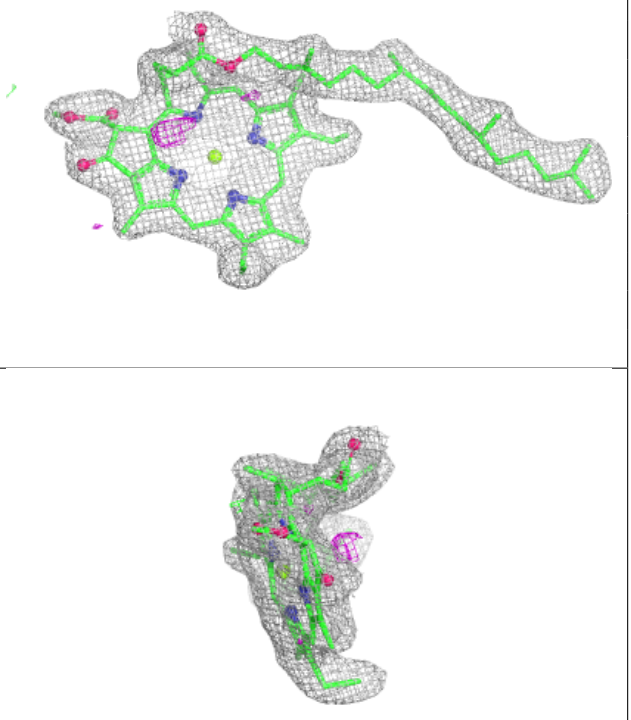






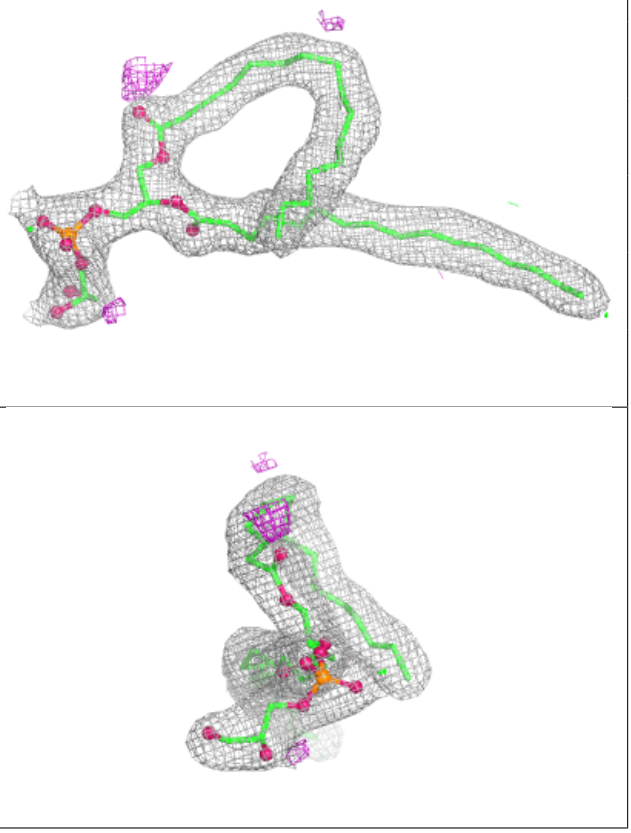
Electron density around CLA c 506:

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



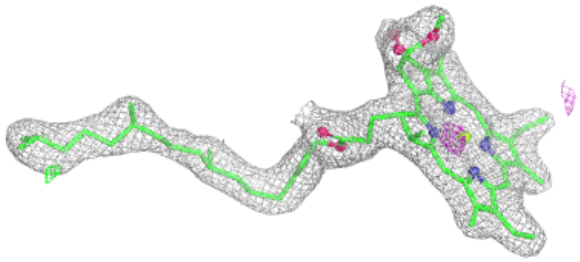
Electron density around LHG d 406:

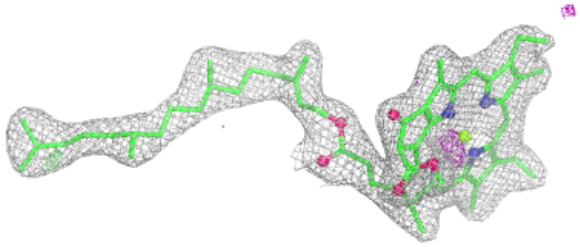
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

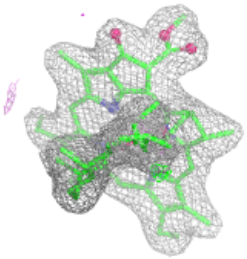


Electron density around CLA c 507:

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

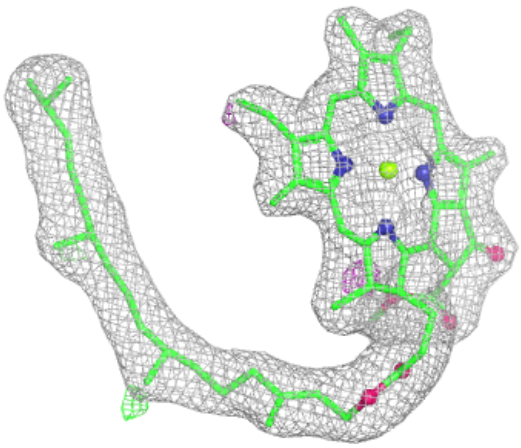


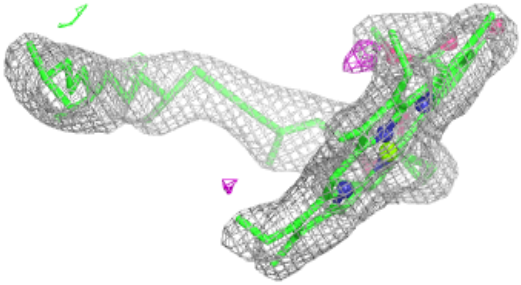


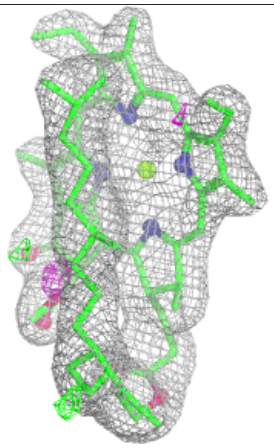


Electron density around CLA C 507:

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

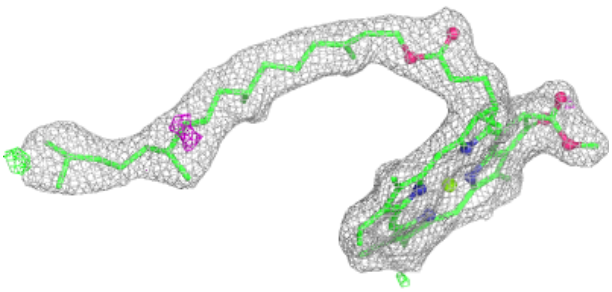


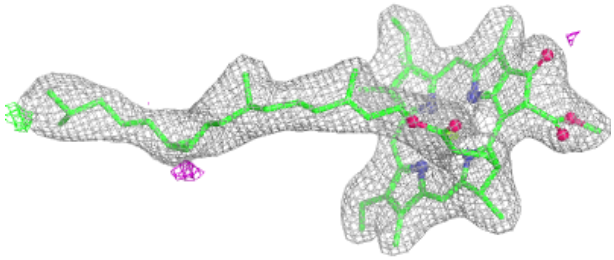


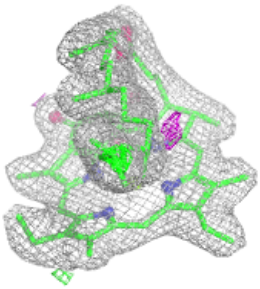


Electron density around CLA c 509:

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

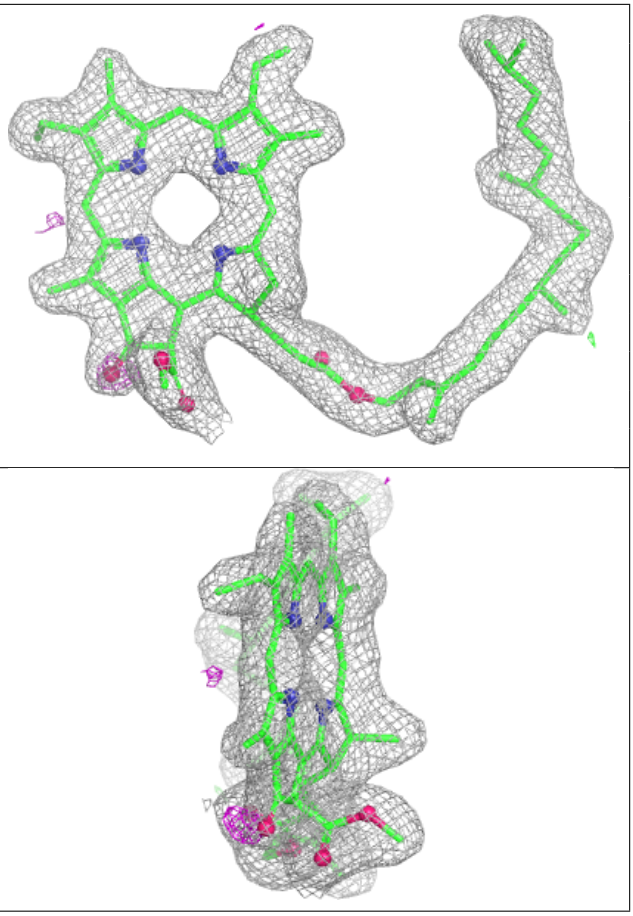






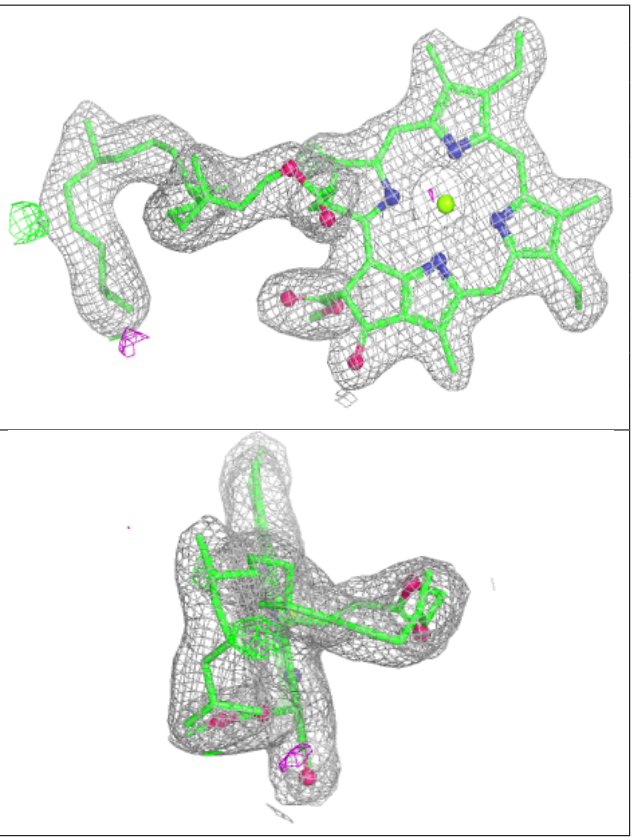
Electron density around PHO a 411:

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



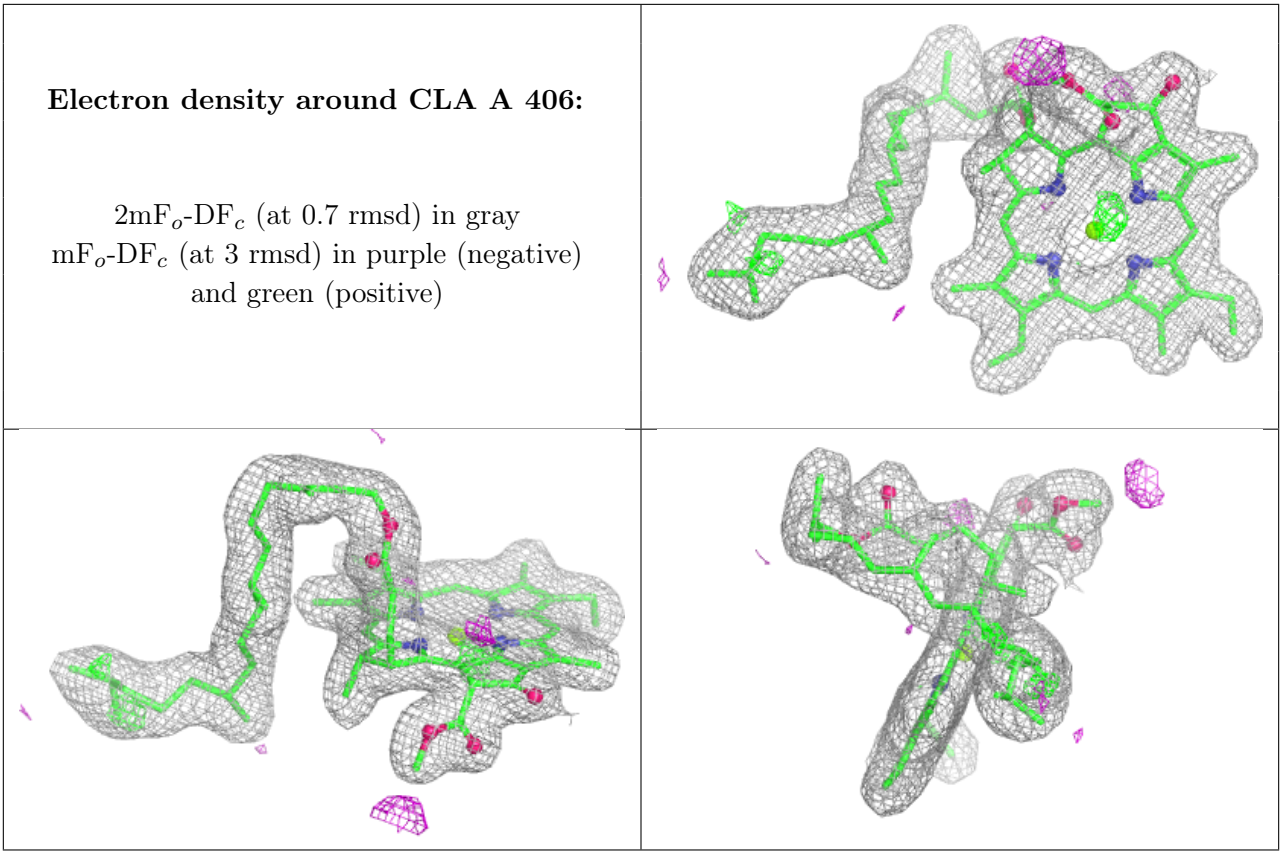
Electron density around CLA B 613:

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



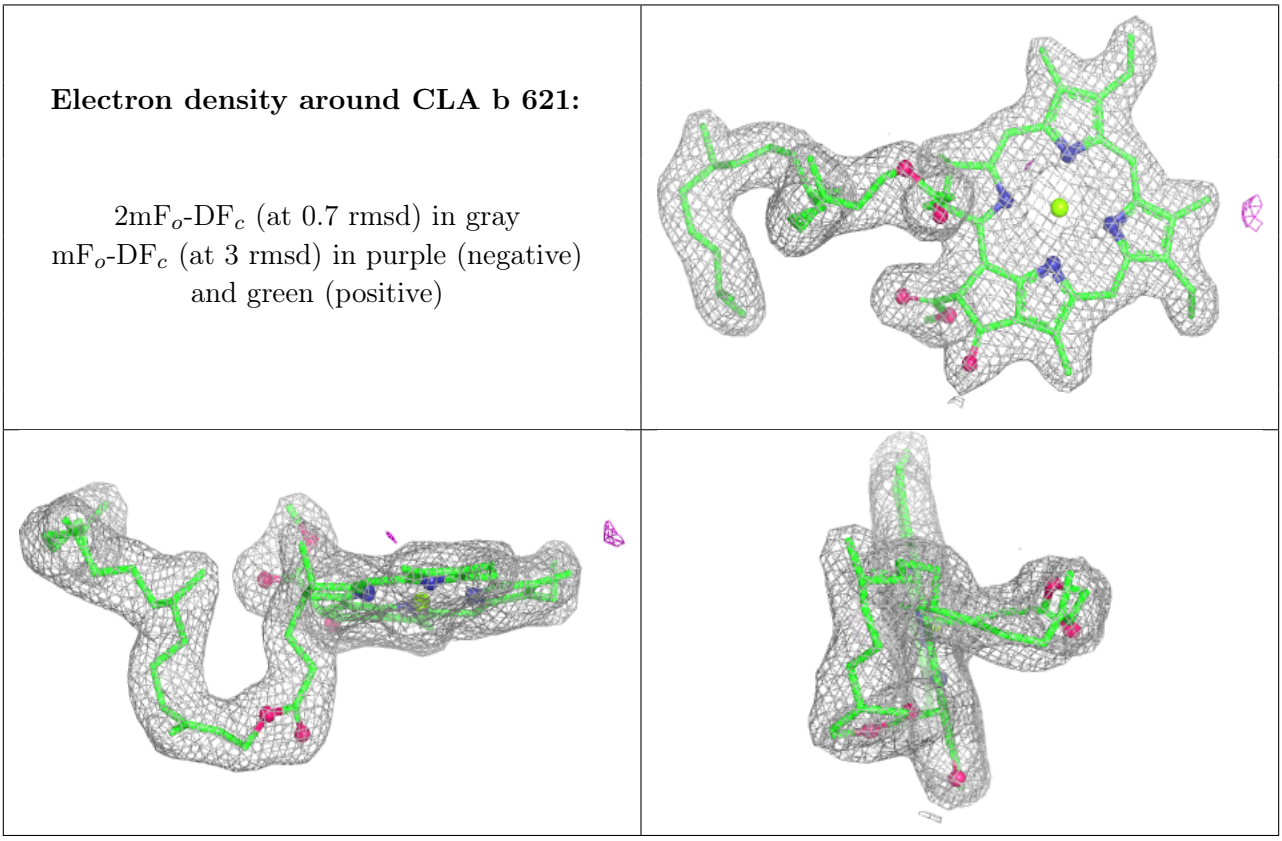
Electron density around CLA A 406:

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



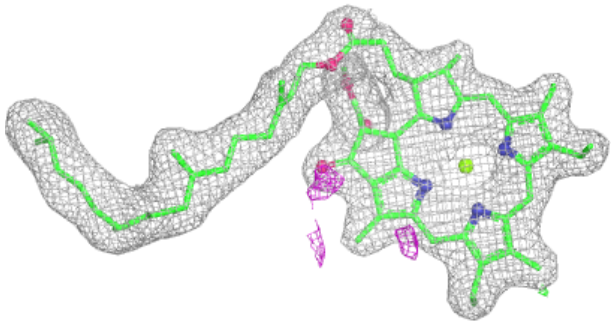
Electron density around CLA b 621:

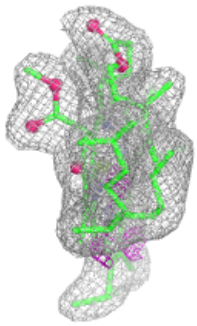
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 603:

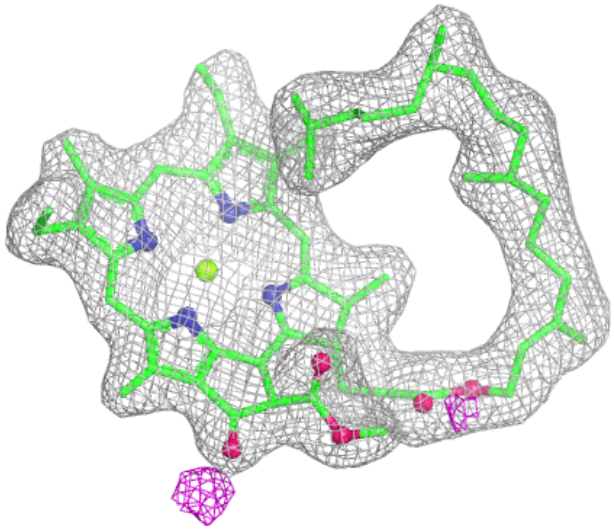
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

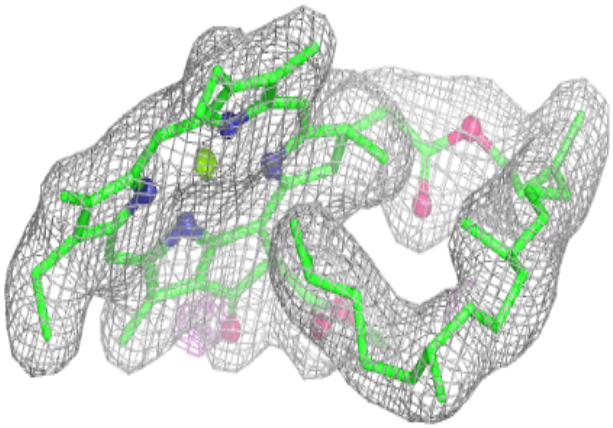




Electron density around CLA B 616:

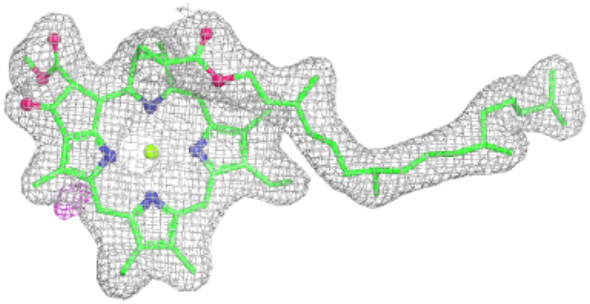
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

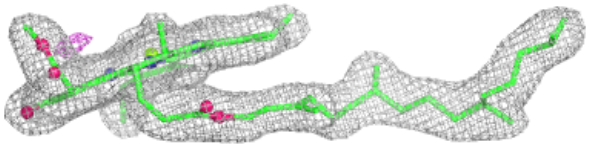


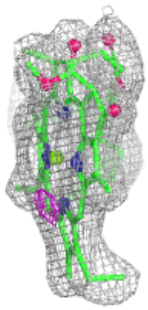


Electron density around CLA B 604:

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

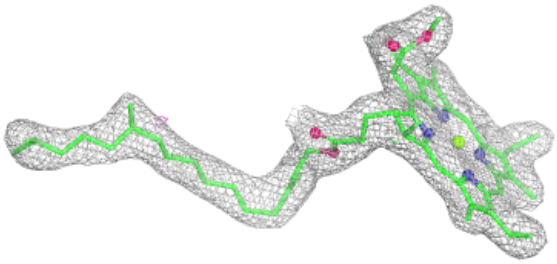


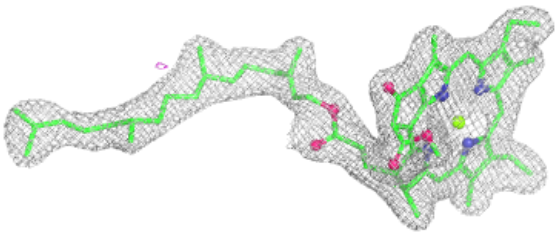


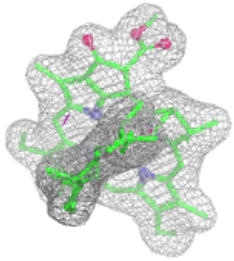


Electron density around CLA C 502:

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

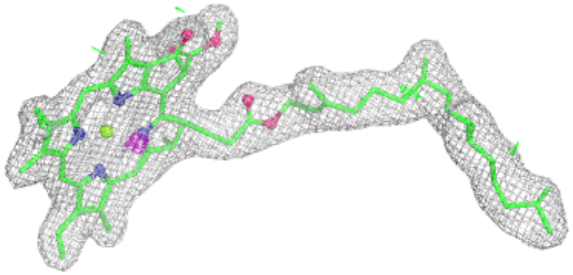


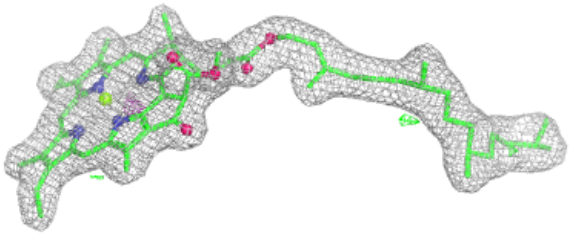


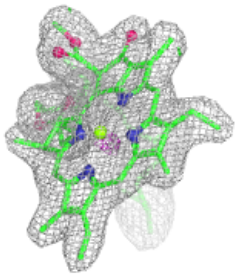


Electron density around CLA a 409:

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

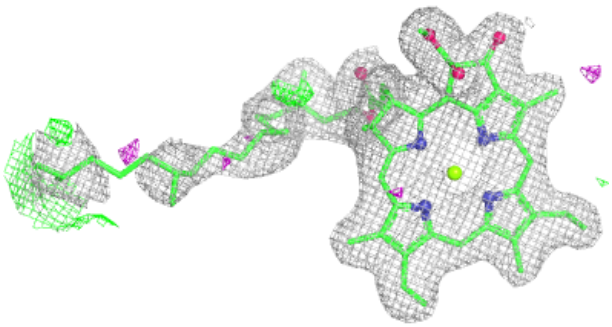


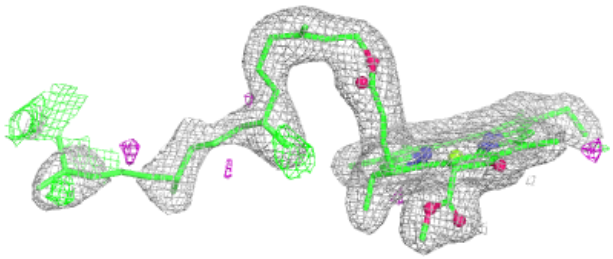




Electron density around CLA a 410:

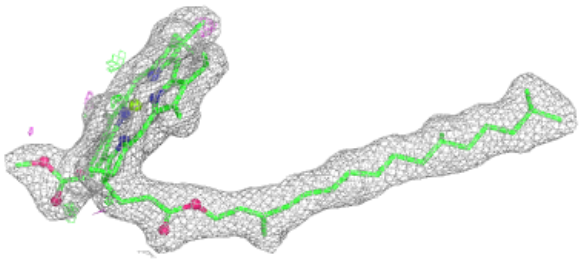
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

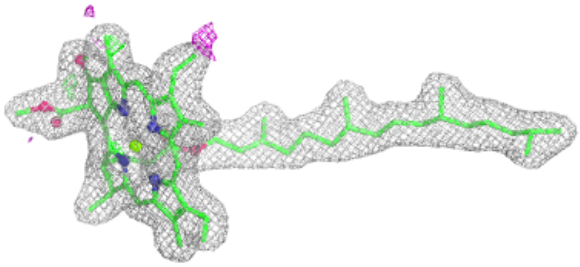


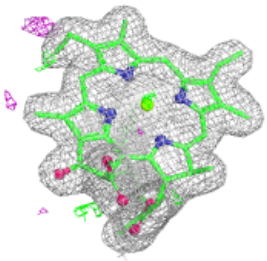


Electron density around CLA B 608:

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

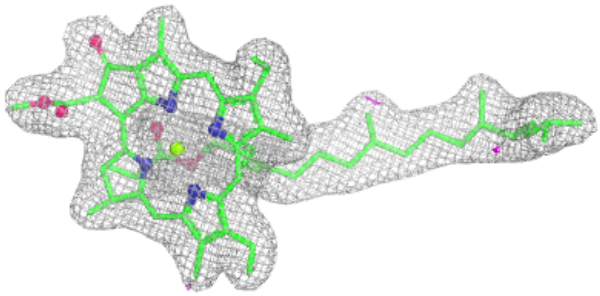


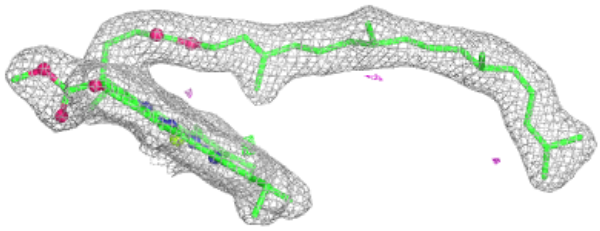


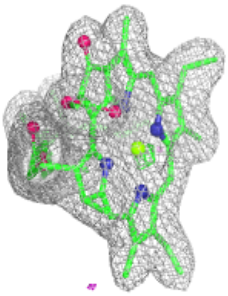


Electron density around CLA B 609:

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

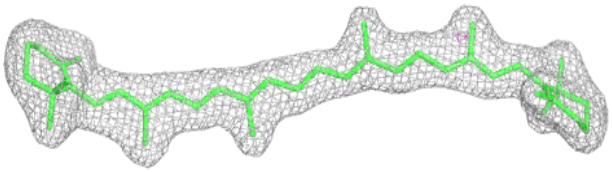


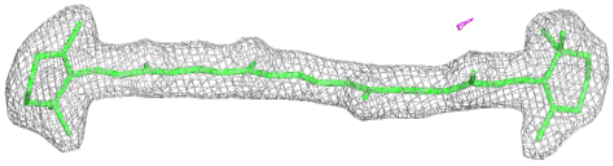


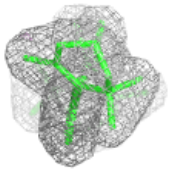


Electron density around BCR a 413:

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

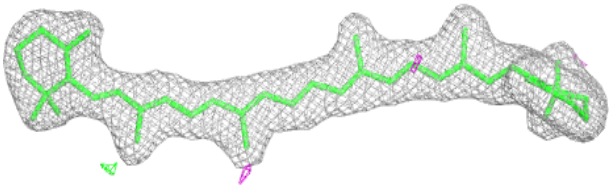


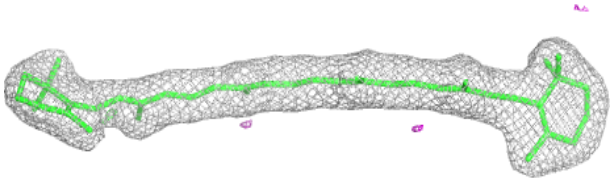


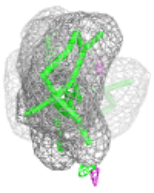


Electron density around BCR b 626:

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

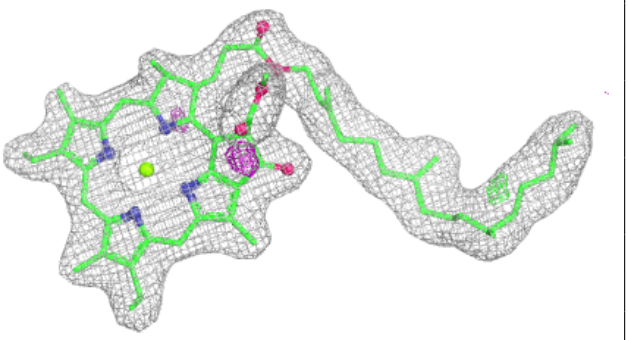


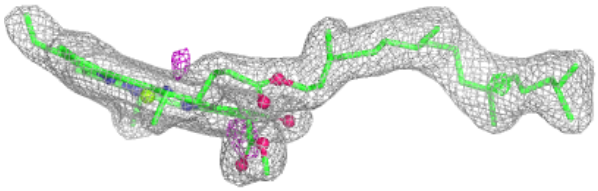




Electron density around CLA b 611:

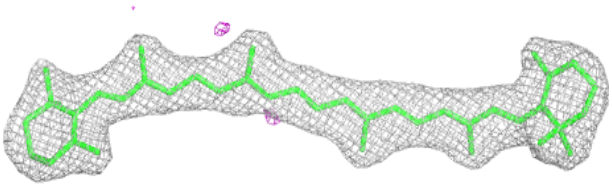
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

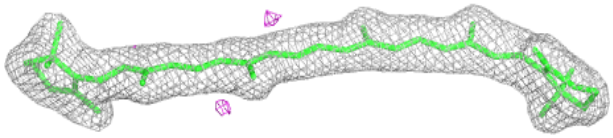


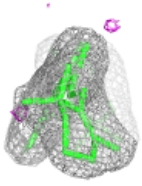


Electron density around BCR b 628:

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

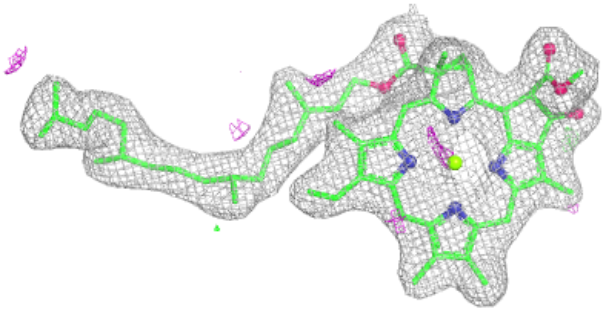


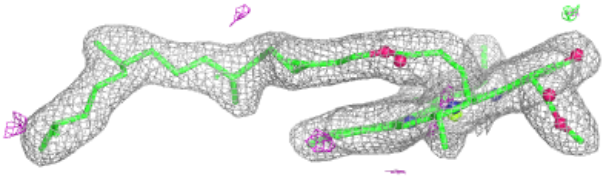


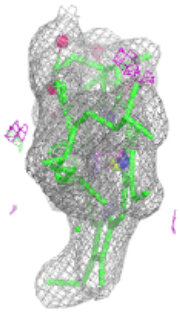


Electron density around CLA b 612:

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

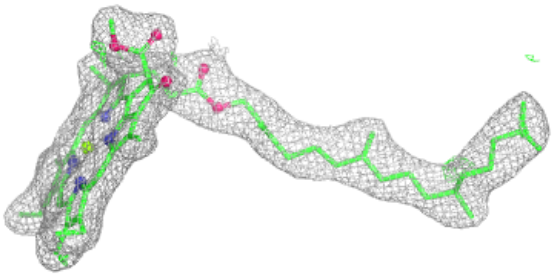


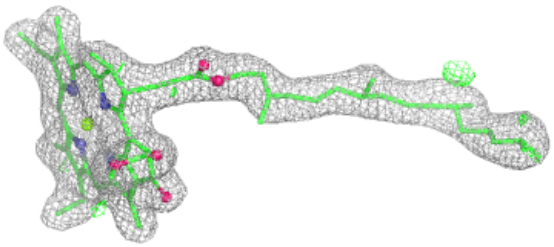


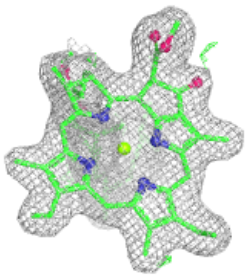


Electron density around CLA b 613:

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

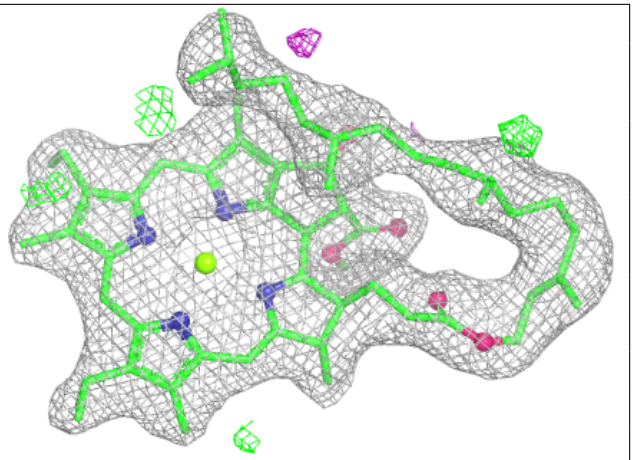


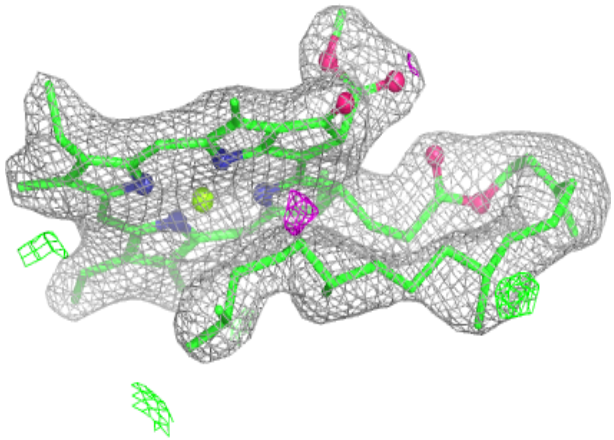


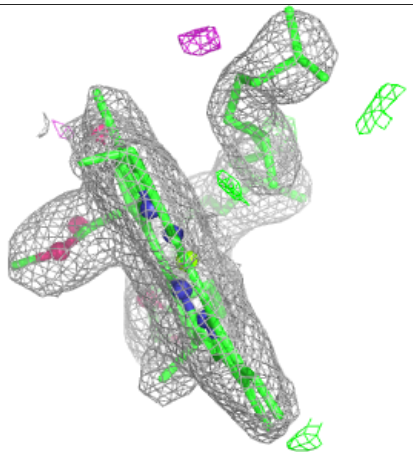


Electron density around CLA c 514:

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

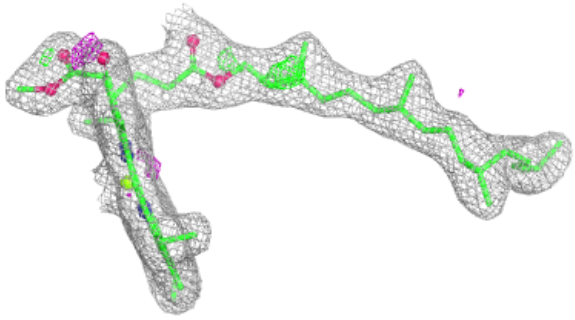


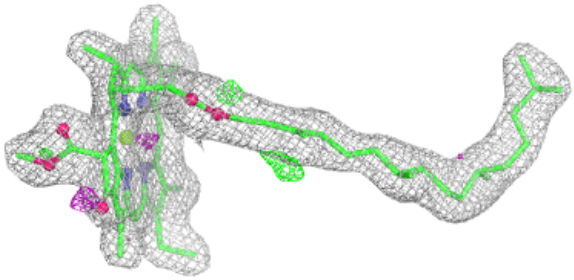


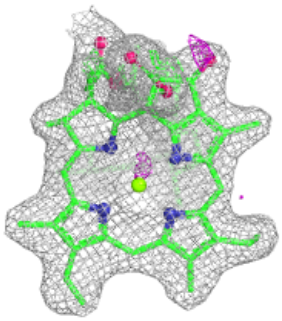


Electron density around CLA b 614:

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

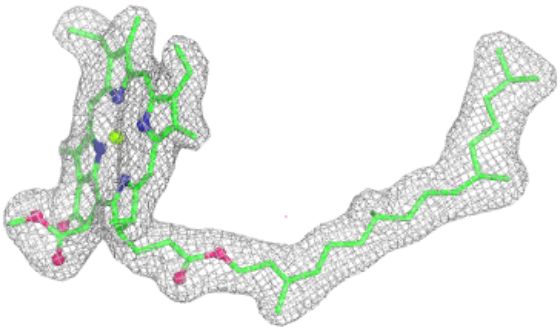


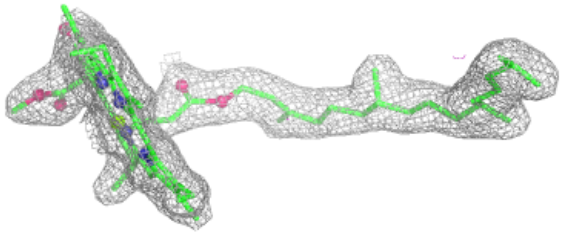


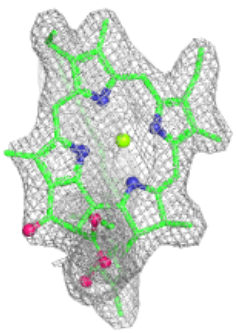


Electron density around CLA B 610:

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

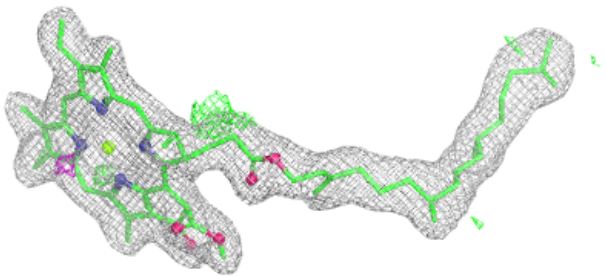


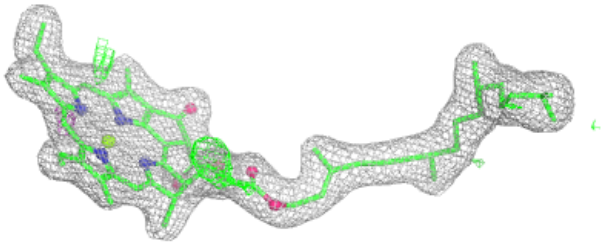




Electron density around CLA A 405:

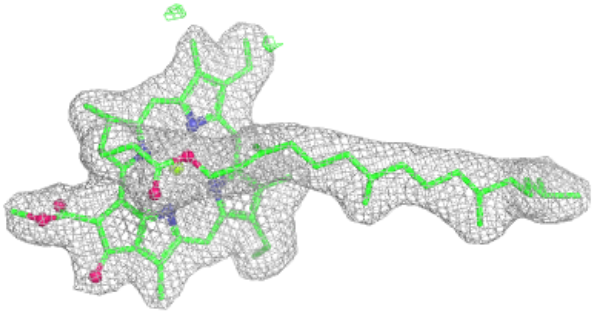
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

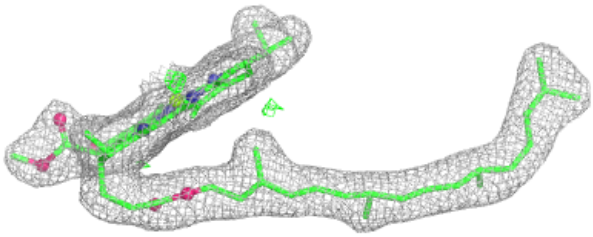




Electron density around CLA b 617:

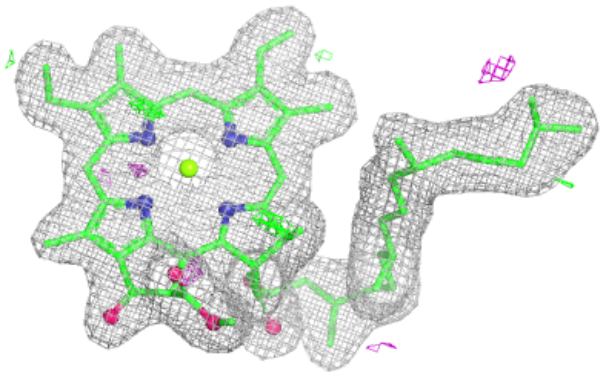
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

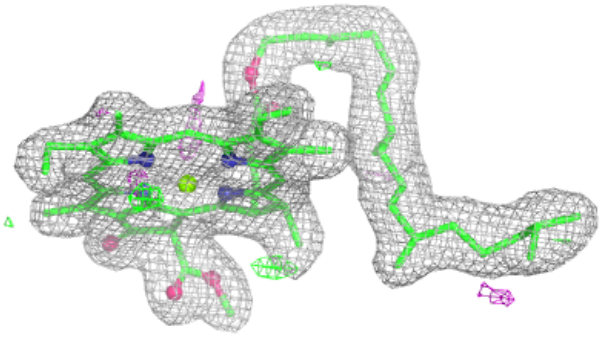


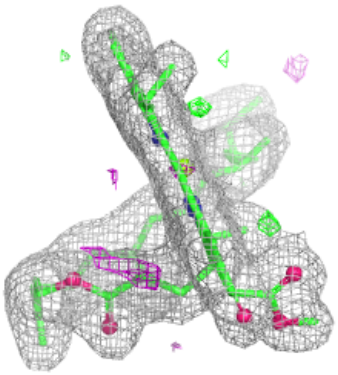


Electron density around CLA d 401:

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

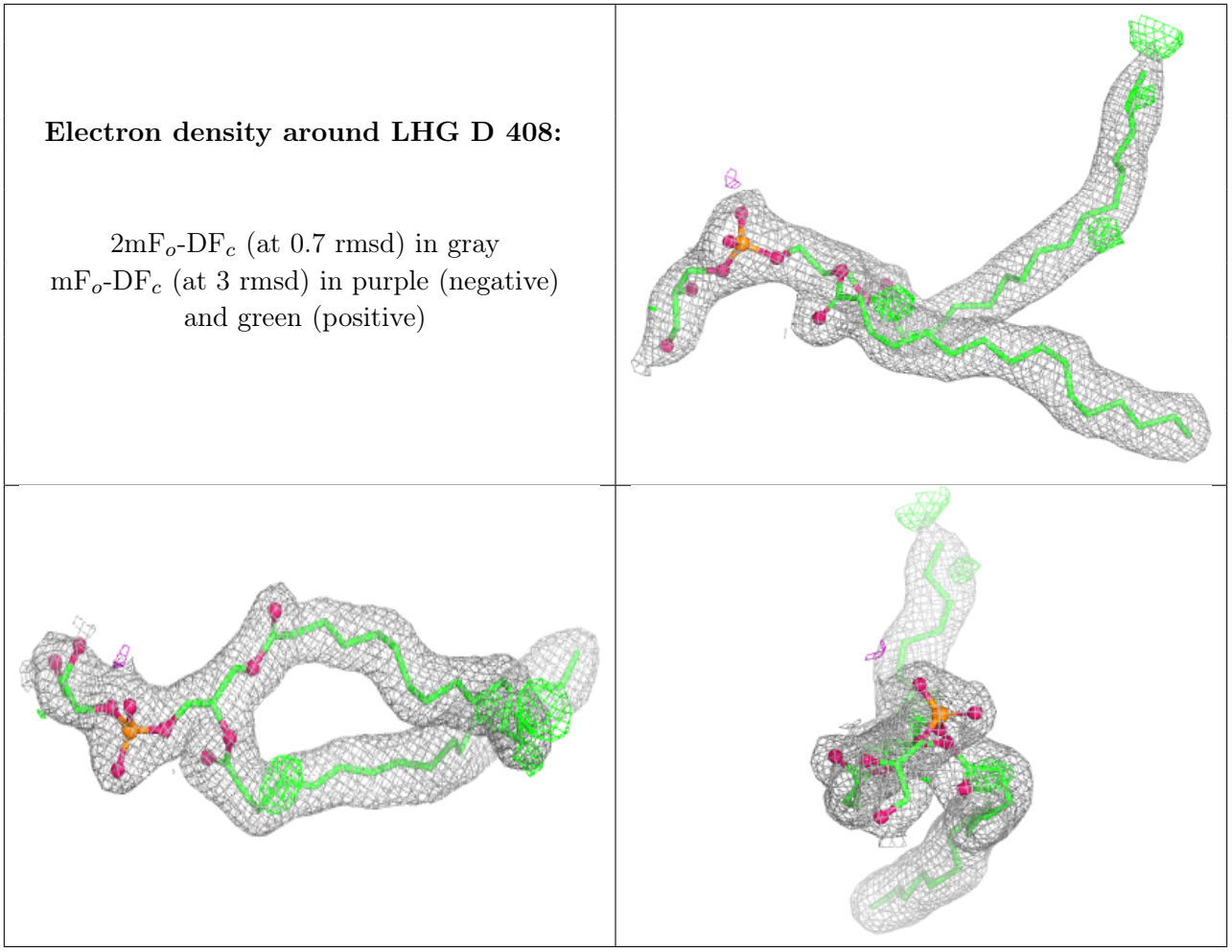






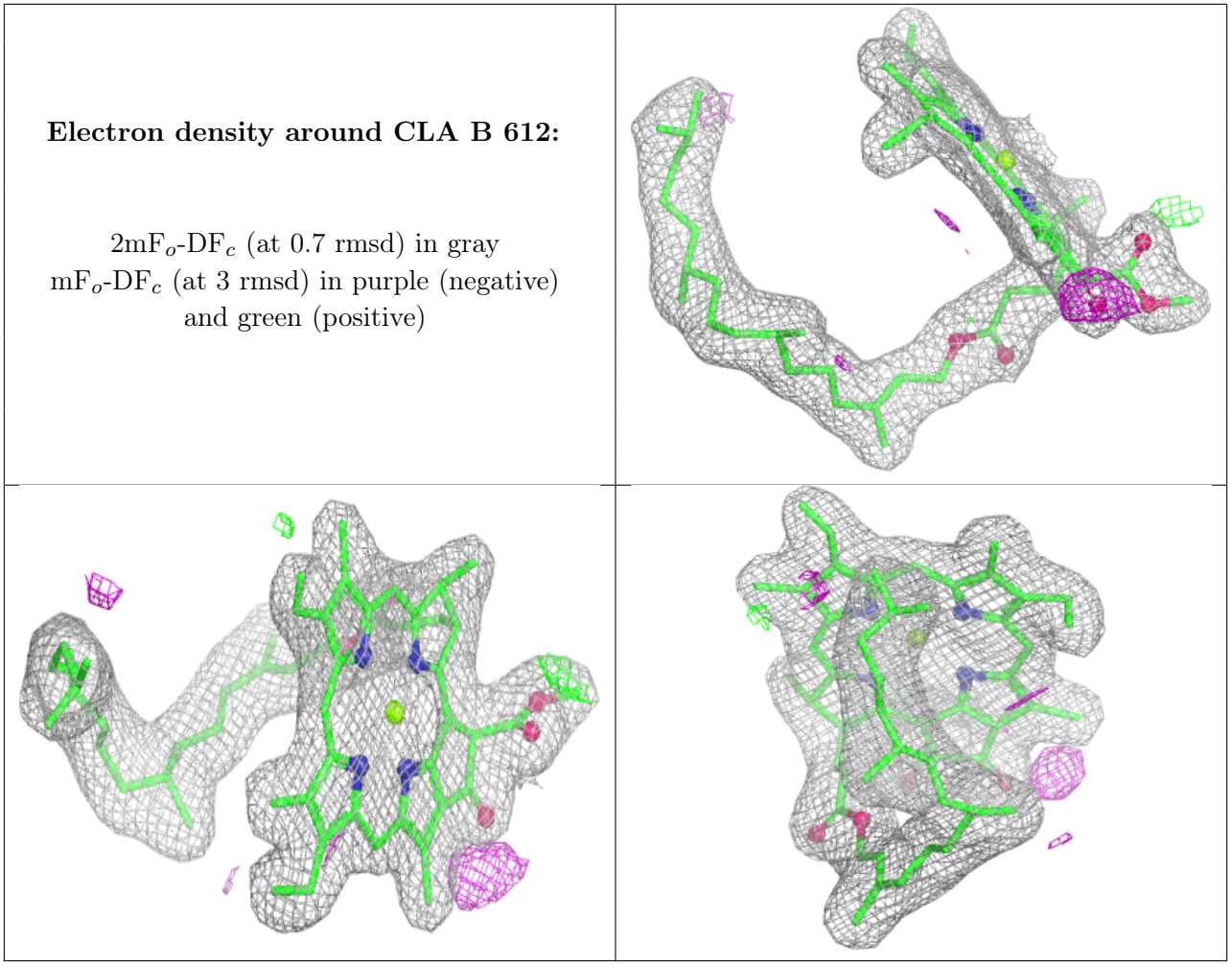
Electron density around LHG D 408:

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



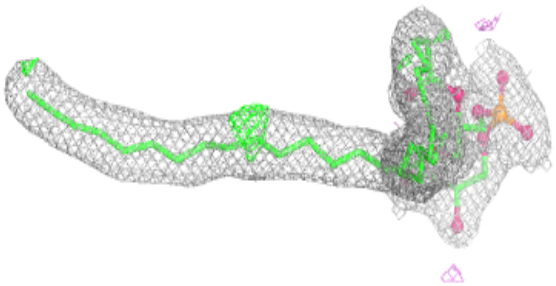
Electron density around CLA B 612:

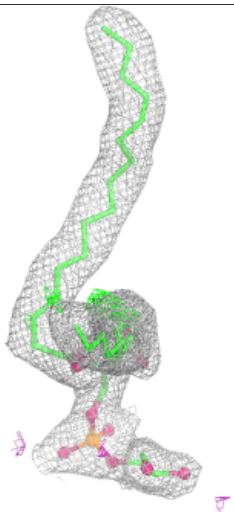
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG L 101:

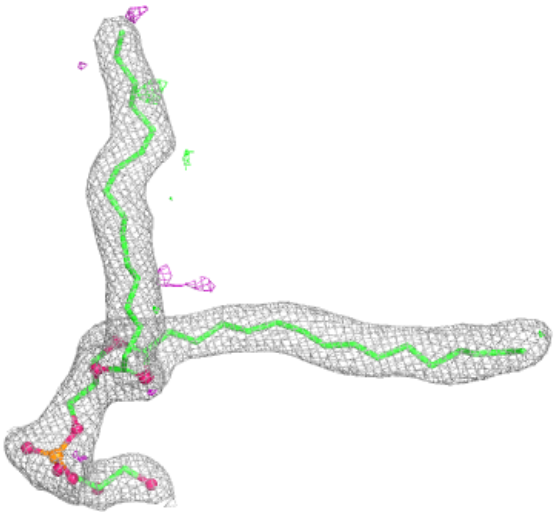
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

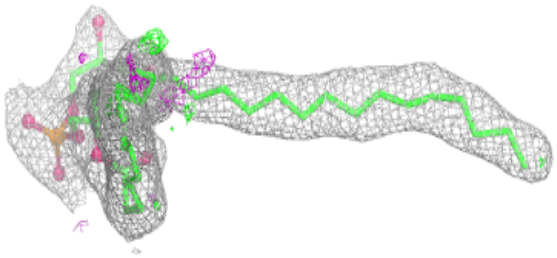


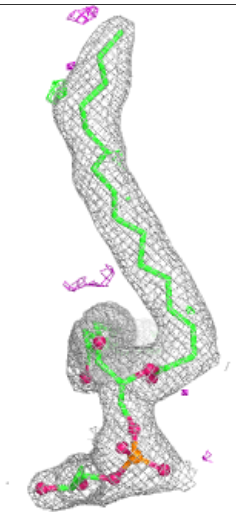


Electron density around LHG b 634:

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

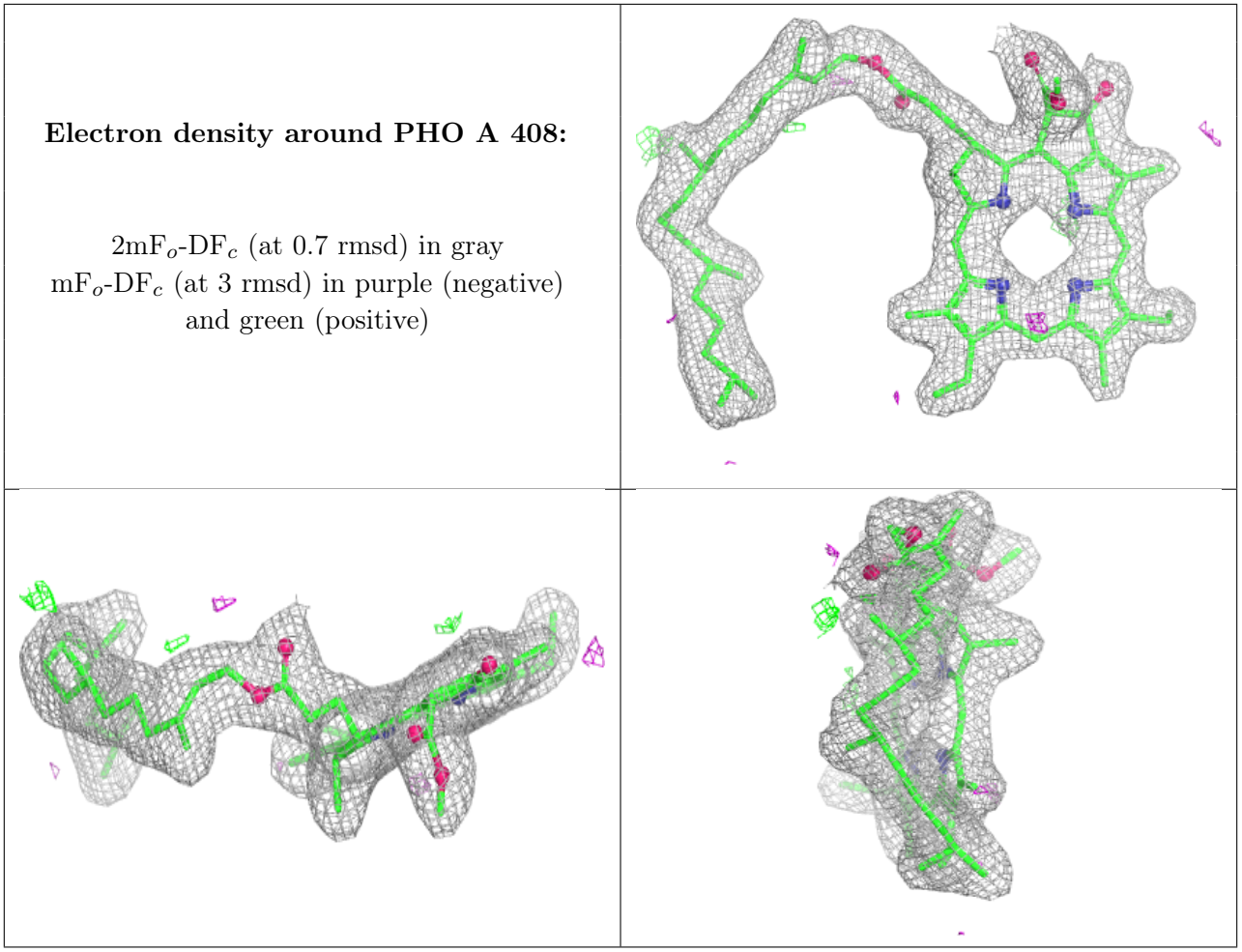






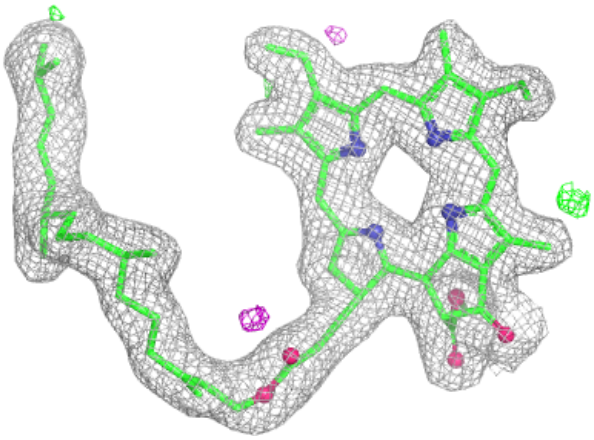
Electron density around PHO A 408:

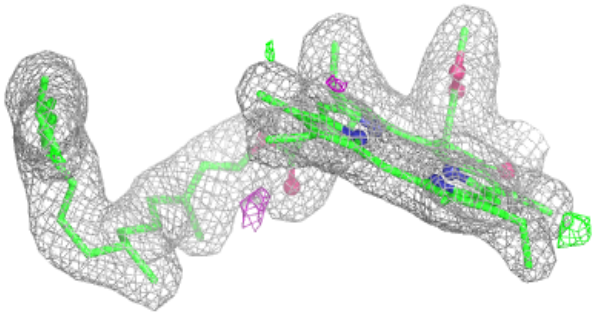
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO A 409 (A):

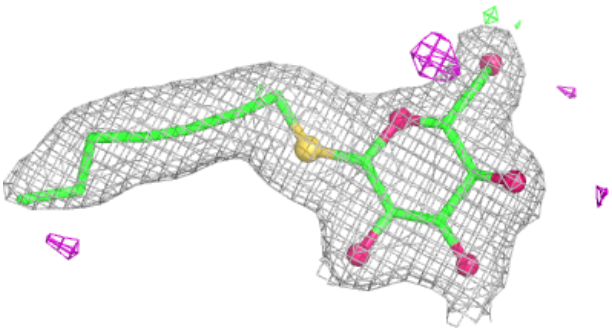
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

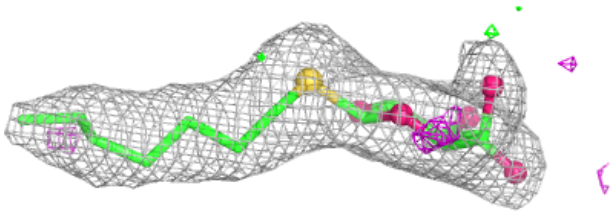


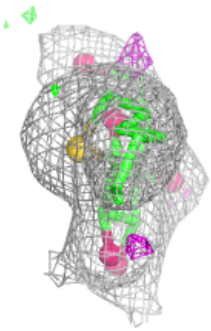


Electron density around HTG B 623:

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

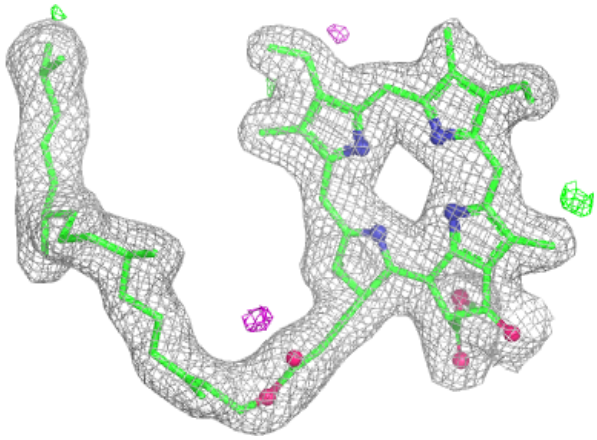


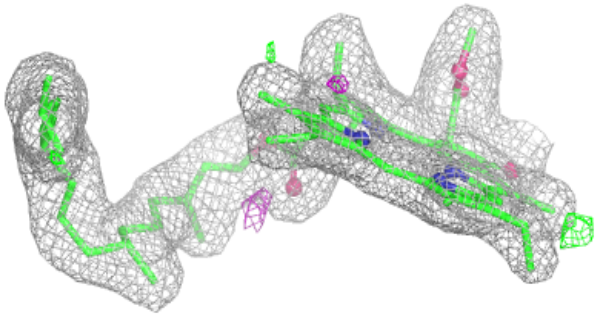


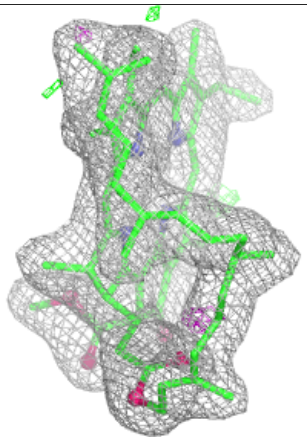


Electron density around PHO A 409 (B):

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

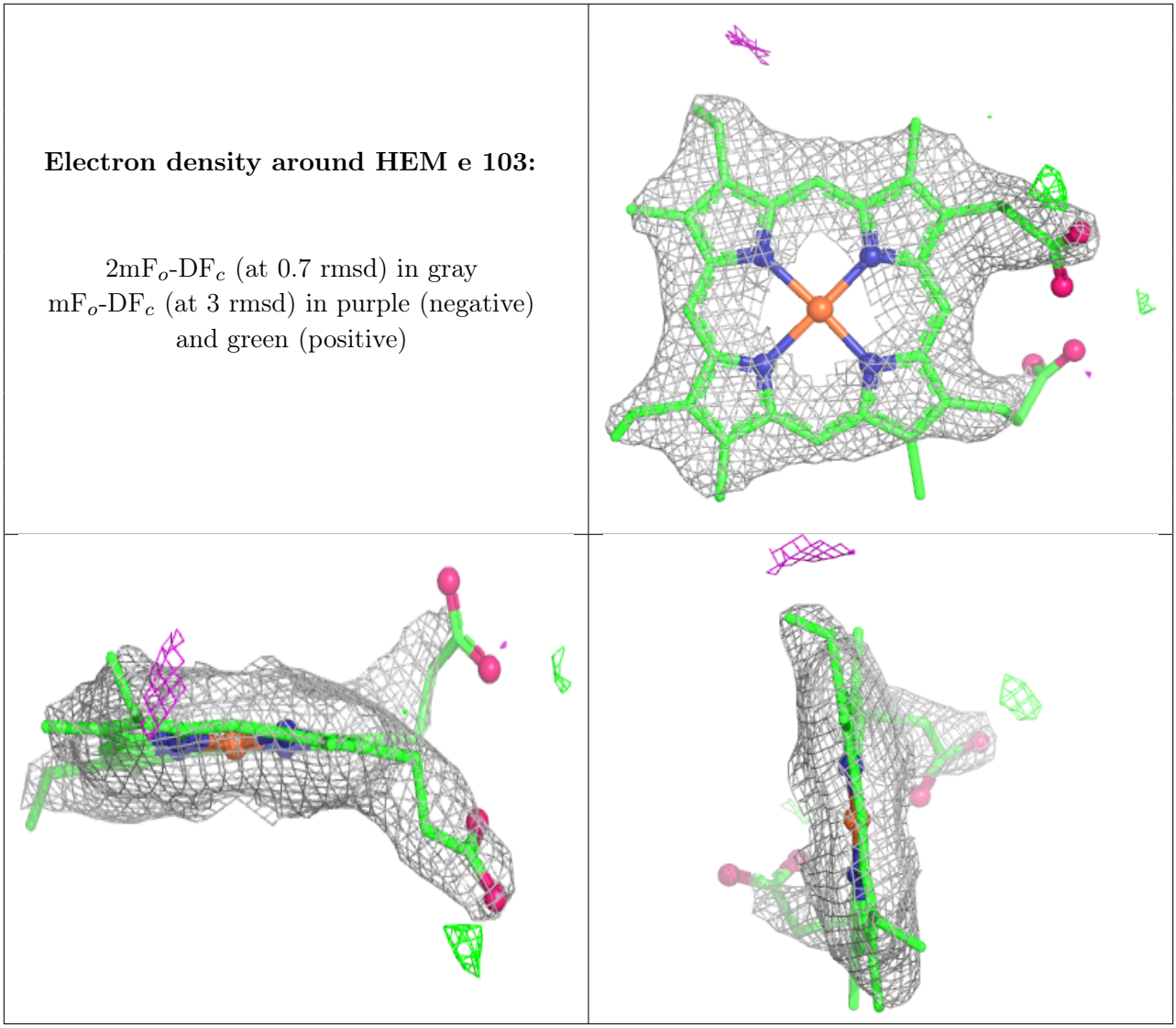






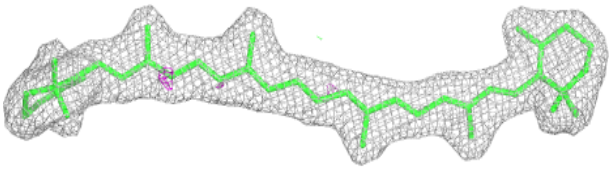
Electron density around HEM e 103:

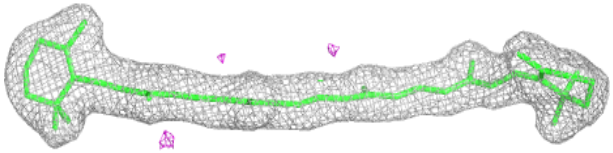
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

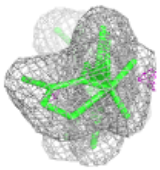


Electron density around BCR B 618:

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

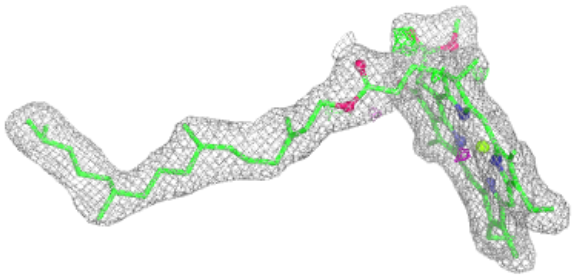


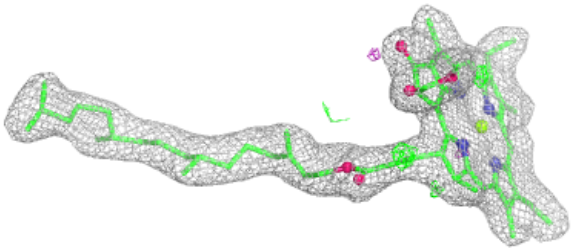


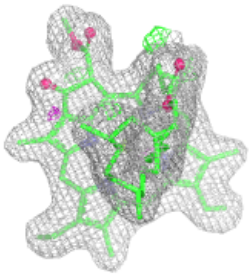


Electron density around CLA B 605:

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

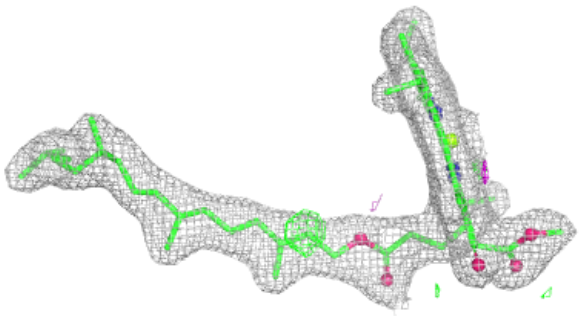


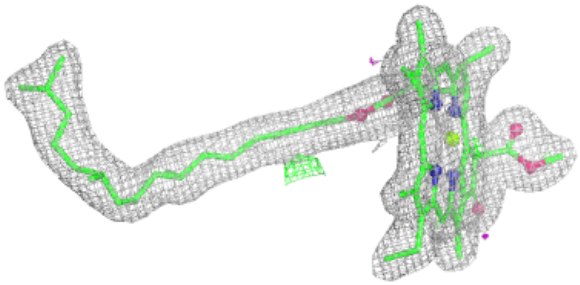


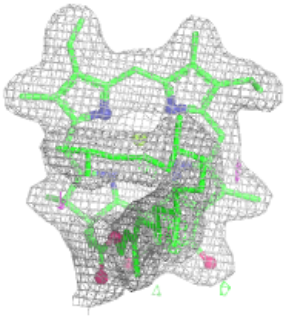


Electron density around CLA B 606:

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

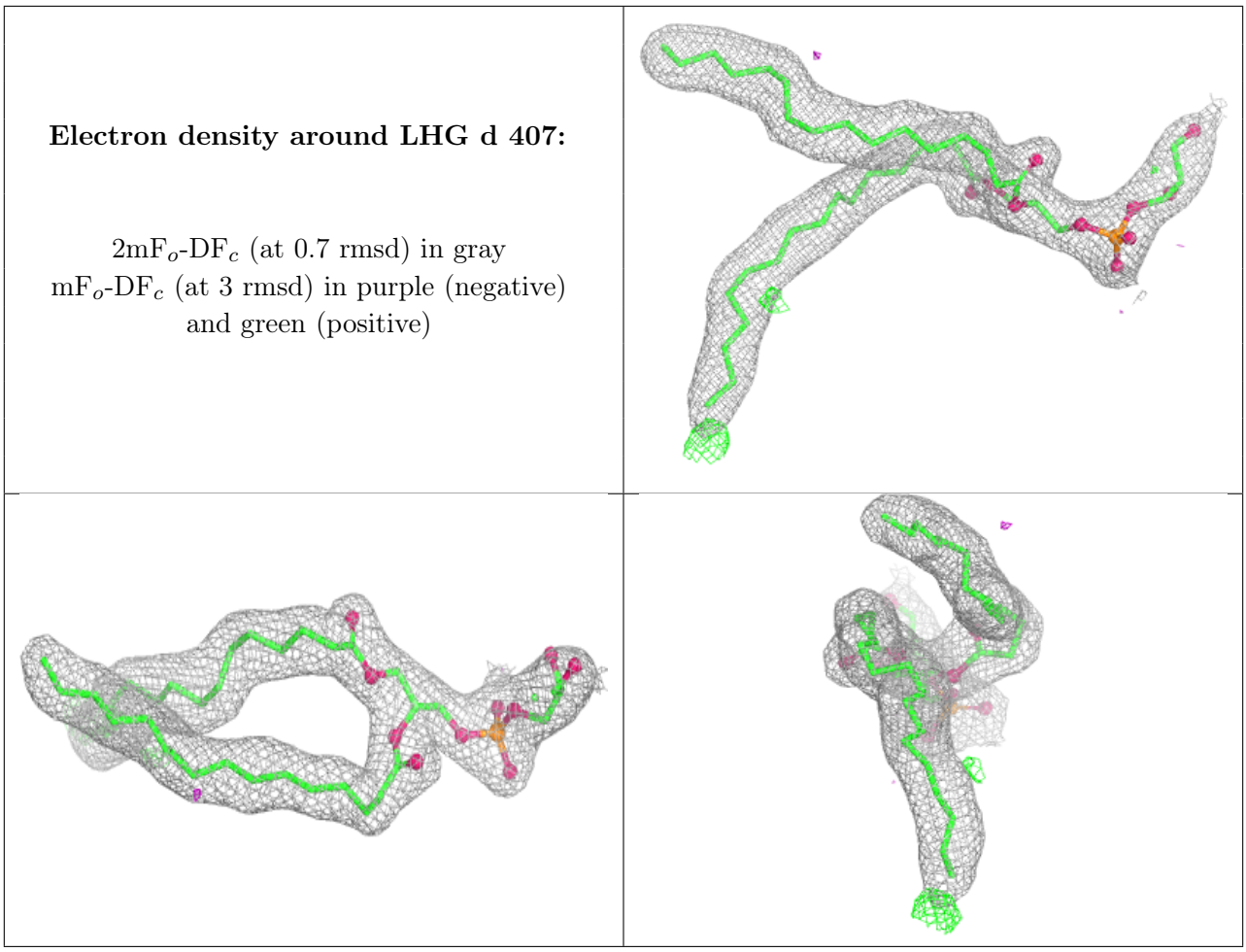






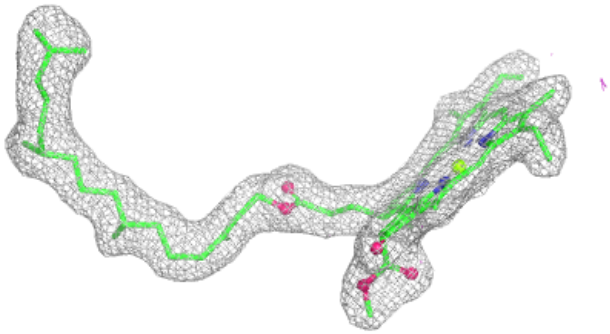
Electron density around LHG d 407:

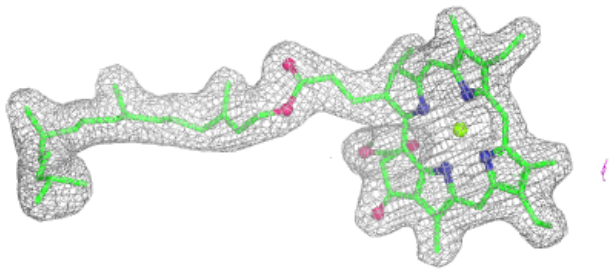
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

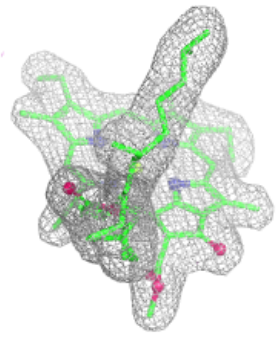


Electron density around CLA d 402:

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

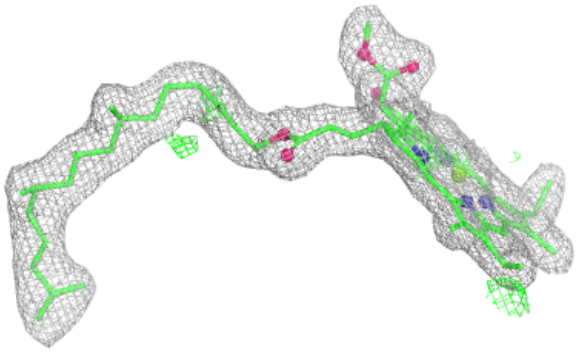


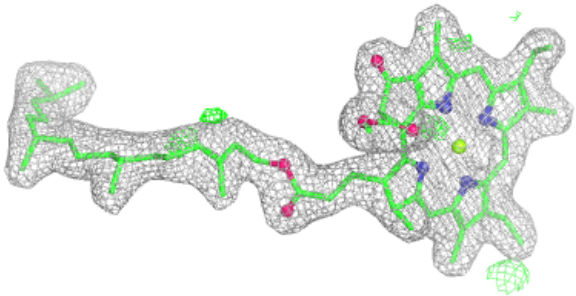




Electron density around CLA D 402:

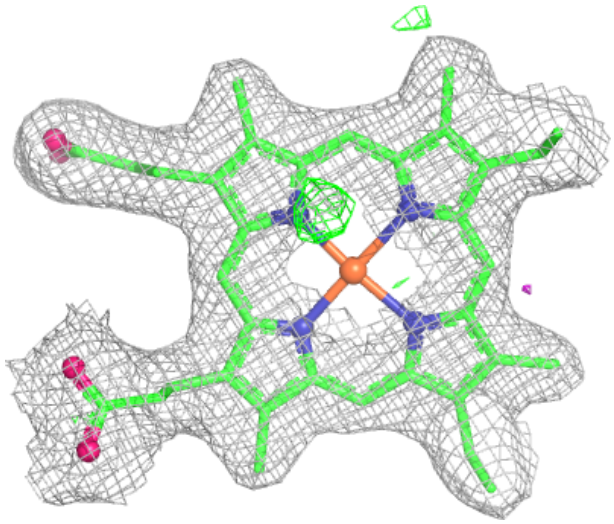
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

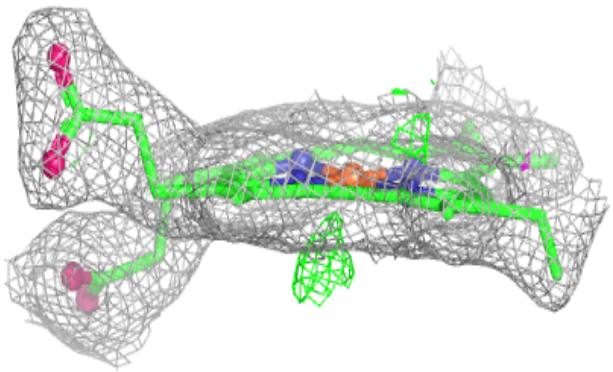




Electron density around HEC V 205:

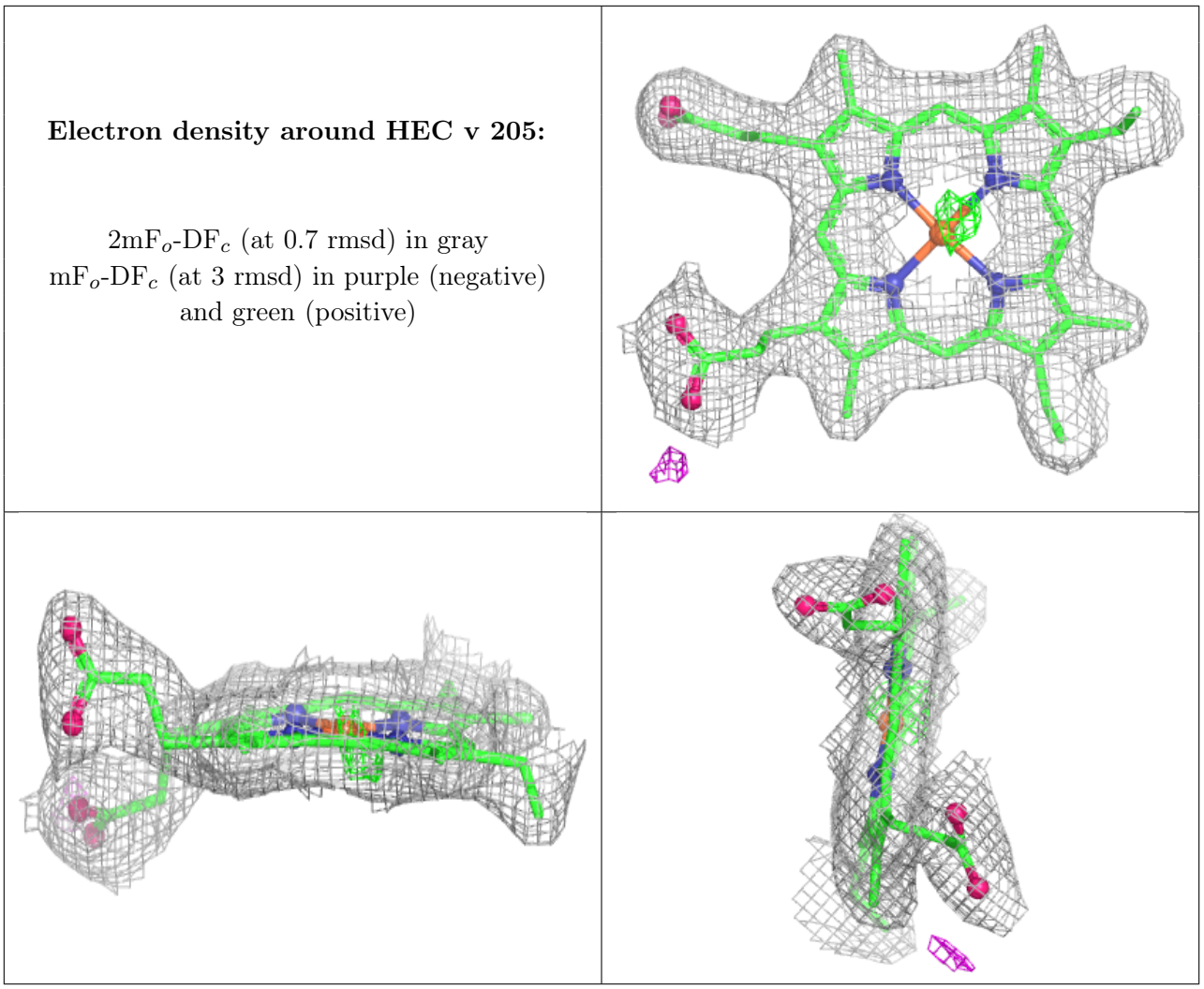
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC v 205:

$2mF_o$-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

There are no such residues in this entry.