Full wwPDB X-ray Structure Validation Report (i)

Mar 12, 2026 – 08:27 AM UTC

PDB ID	:	8GN2 / pdb_00008gn2
Title	:	Crystal structure of PPBQ-bound photosystem II complex
Authors	:	Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on	:	2022-08-22
Resolution	:	1.95 Å(reported)

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

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

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

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

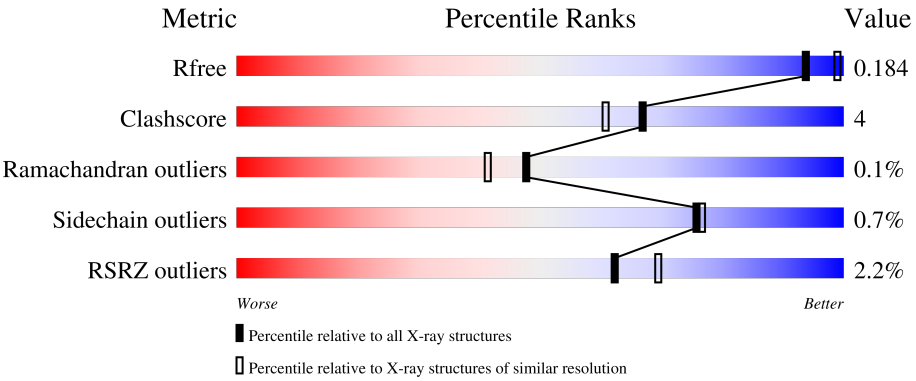
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	91% 6%
2	B	505	94% 6%
2	b	505	94% 6%
3	C	455	93% 6%

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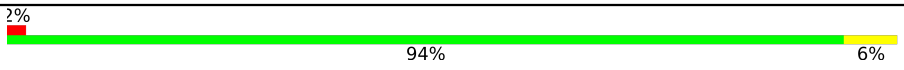
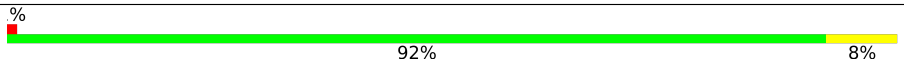
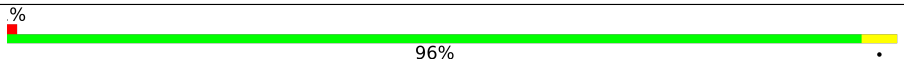
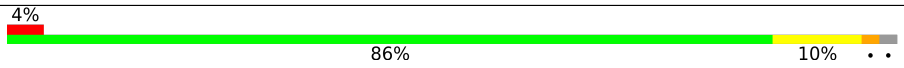
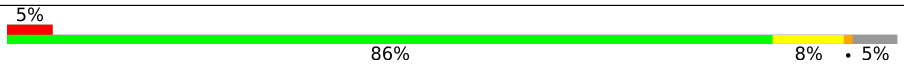
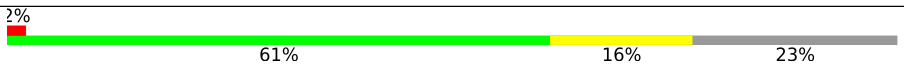
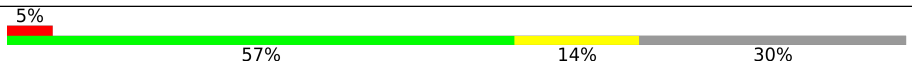
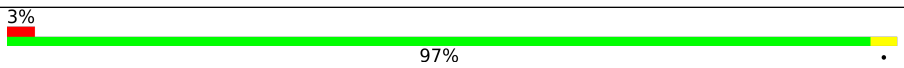
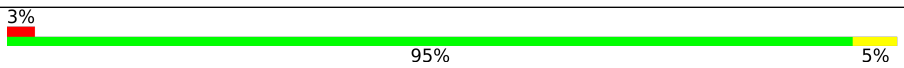
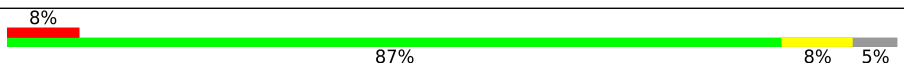
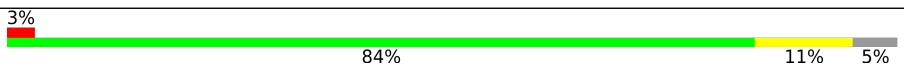
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
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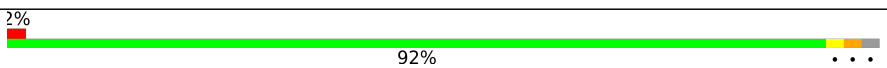
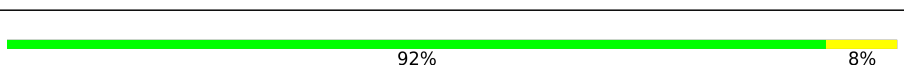
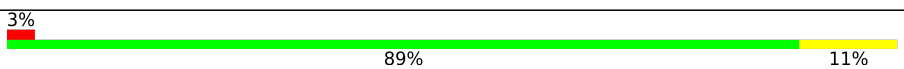
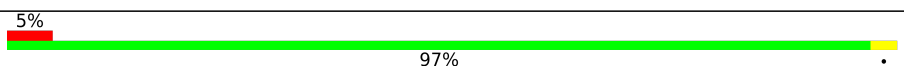
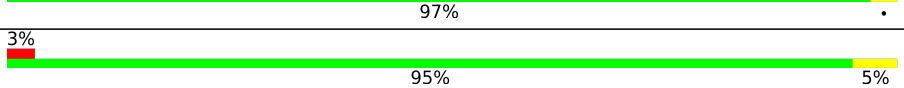
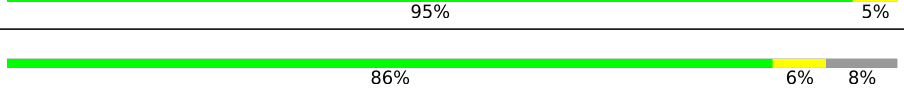
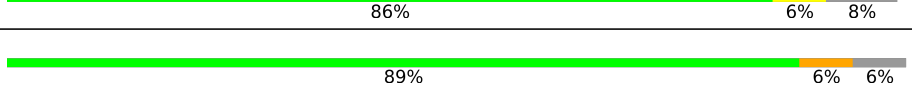
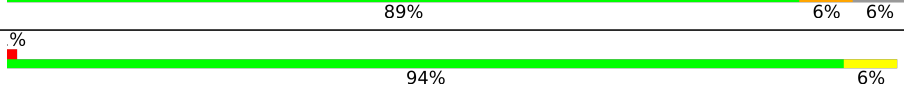
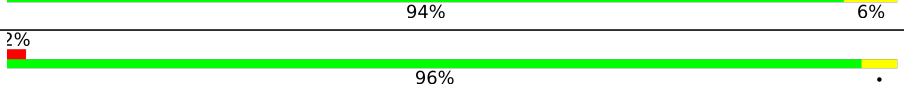
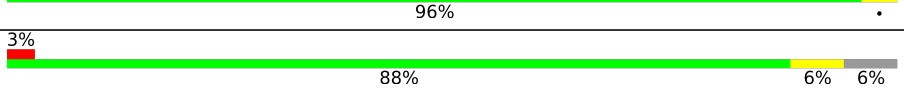
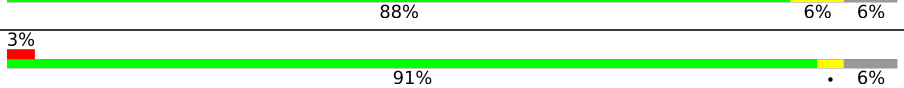
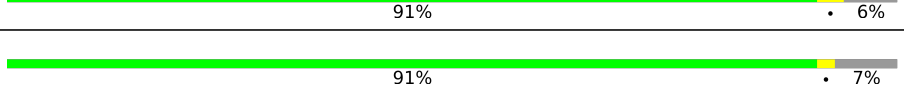
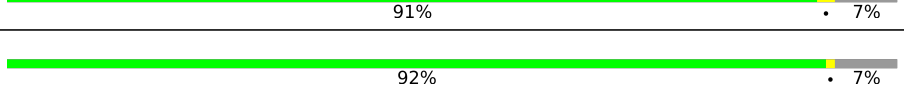
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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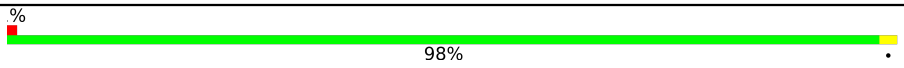
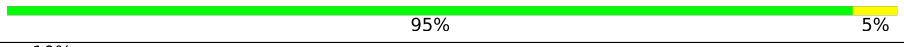
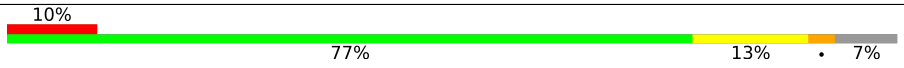
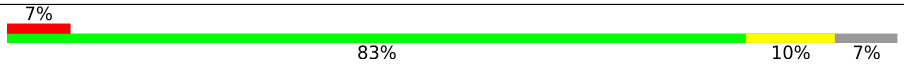
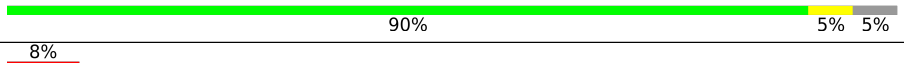
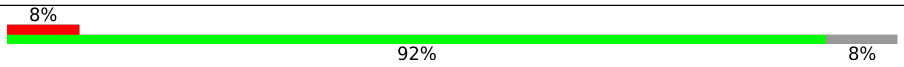
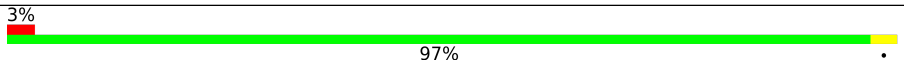
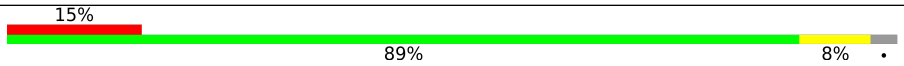
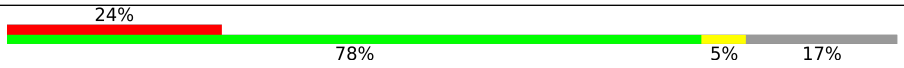
Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	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	609	X	-	-	-
24	CLA	b	610	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	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
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	c	514	X	-	-	-
24	CLA	d	404	X	-	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 55061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2624	1720	431	458	15			
1	a	334	Total	C	N	O	S	0	3	0
			2620	1717	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	9	0
			4007	2631	670	693	13			
2	b	503	Total	C	N	O	S	0	10	0
			3989	2621	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	2	0
			3516	2305	587	611	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	2	0
			2731	1812	444	463	12			
4	d	342	Total	C	N	O	S	0	3	0
			2738	1815	447	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			657	429	106	122			
5	e	79	Total	C	N	O	0	0	0
			639	419	103	117			

- 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
			274	187	45	41	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total 285	C 195	N 42	O 47	S 1	0	0	0
8	i	36	Total 296	C 200	N 46	O 49	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	39	Total 271	C 182	N 40	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 205	N 42	O 46	0	1	0
10	k	37	Total 286	C 198	N 42	O 46	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 305	C 205	N 48	O 51	S 1	0	1	0
11	l	37	Total 309	C 209	N 48	O 51	S 1	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 265	C 178	N 38	O 48	S 1	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	3	0
			281	191	39	50	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	6	0
			1884	1180	313	386	5			
13	o	243	Total	C	N	O	S	0	5	0
			1871	1172	311	382	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			776	493	130	153			
15	u	97	Total	C	N	O	0	1	0
			780	495	130	155			

- 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
			1063	676	178	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	28	Total	C	N	O	S	0	0	0
			198	130	33	32	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			279	187	45	47			
18	x	37	Total	C	N	O	0	1	0
			273	185	43	45			

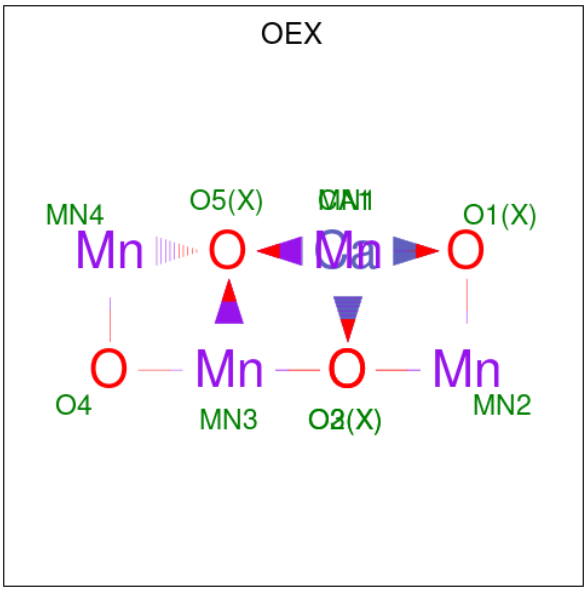
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			461	319	67	73	2			
19	z	60	Total	C	N	O	S	0	0	0
			446	306	69	70	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			240	159	42	39			

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



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

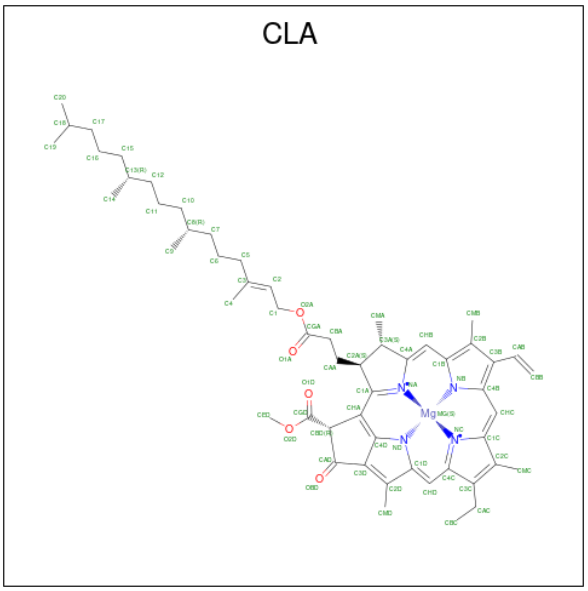
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

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

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



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

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

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

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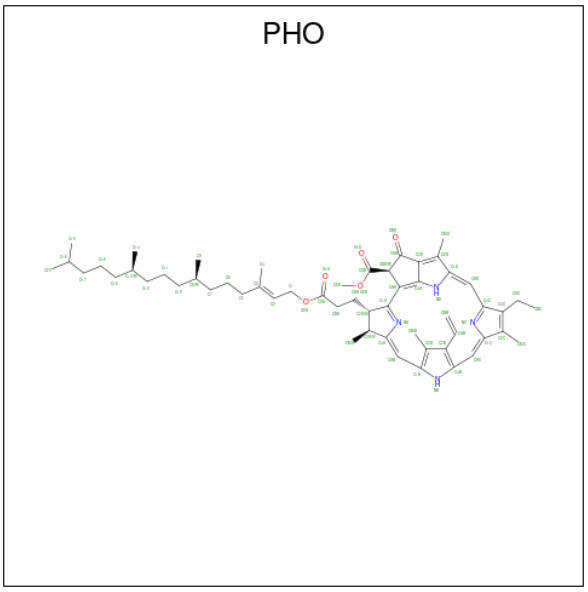
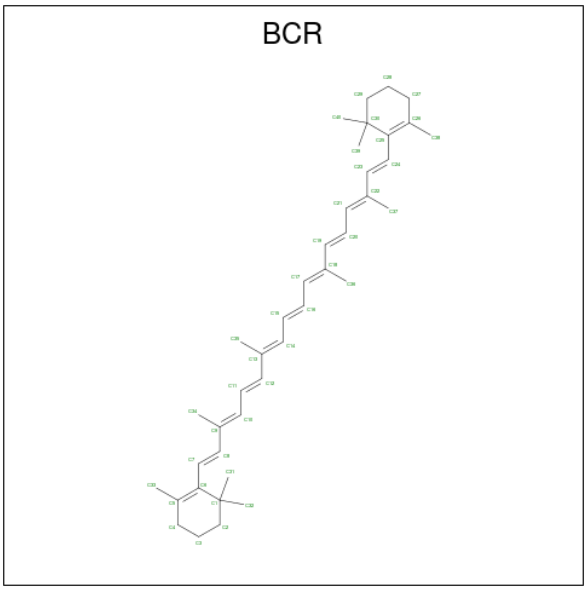
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



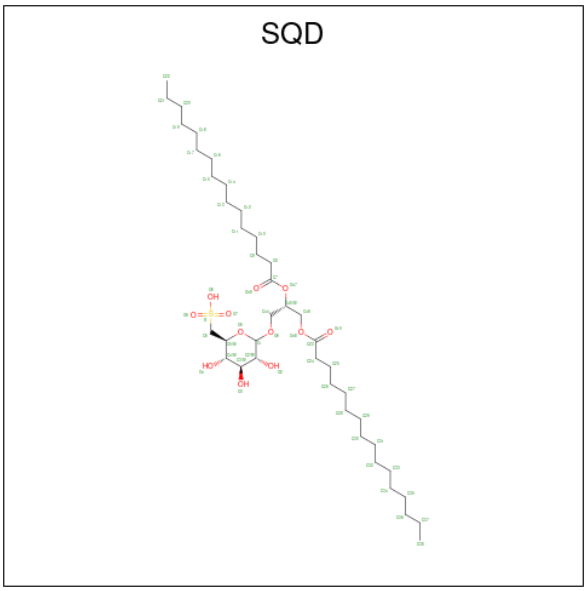
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



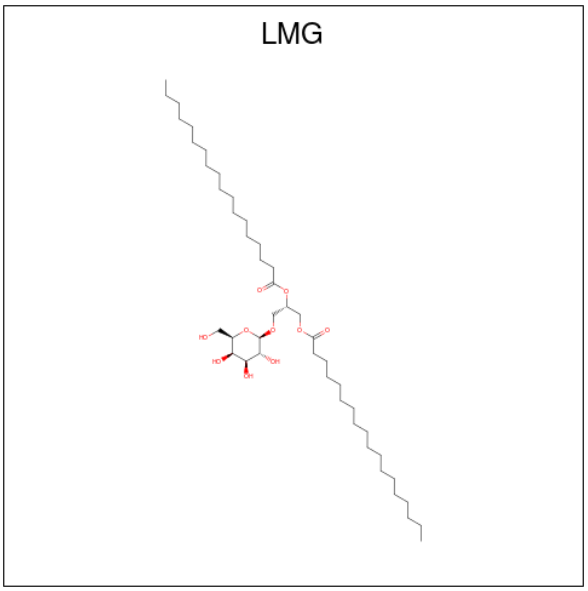
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



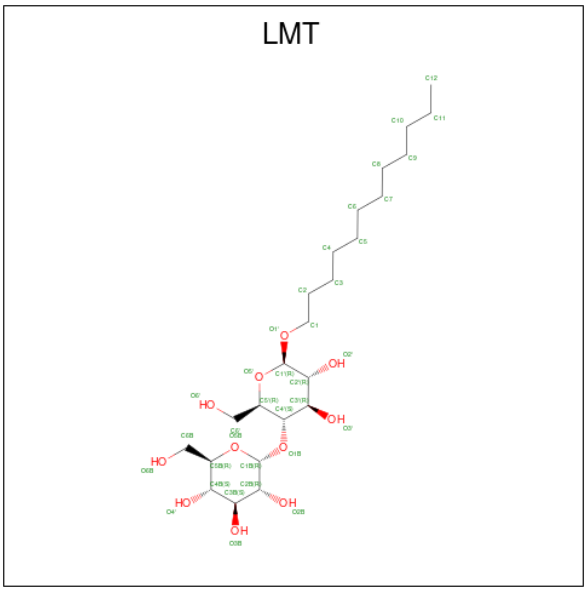
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			45	32	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			33	23	9	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 51 41 10	0	0
28	B	1	Total C O 51 41 10	0	0
28	C	1	Total C O 51 41 10	0	0
28	C	1	Total C O 51 41 10	0	0
28	D	1	Total C O 51 41 10	0	0
28	a	1	Total C O 51 41 10	0	0
28	b	1	Total C O 51 41 10	0	0
28	c	1	Total C O 51 41 10	0	0
28	c	1	Total C O 51 41 10	0	0
28	d	1	Total C O 51 41 10	0	0

- Molecule 29 is 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	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			24	18	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			24	18	6		
29	J	1	Total	C	O	0	0
			24	18	6		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			24	18	6		
29	Z	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	c	1	Total	C	O	0	0
			35	24	11		
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

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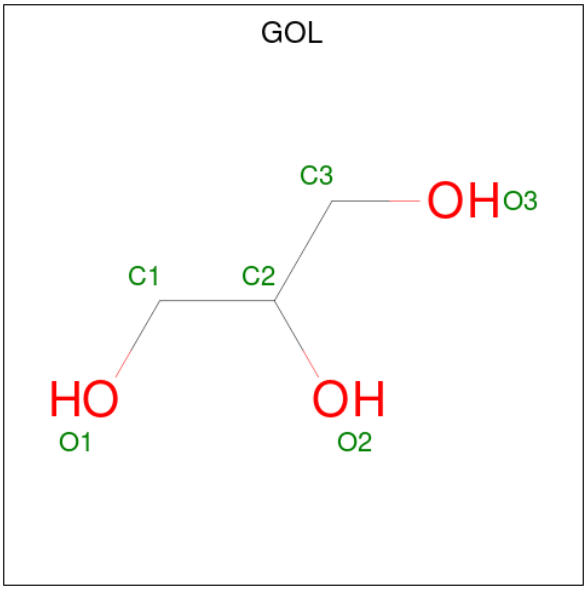
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	z	1	Total C O 32 21 11	0	0

- Molecule 30 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	E	1	Total	C	O	0	0
			6	3	3		
30	L	1	Total	C	O	0	0
			6	3	3		
30	M	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	T	1	Total	C	O	0	0
			6	3	3		
30	T	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	h	1	Total	C	O	0	0
			6	3	3		
30	k	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 31 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	4	Total C O 74 69 5	0	0
31	B	7	Total C O 99 95 4	0	0
31	C	3	Total C O 73 66 7	0	0
31	D	3	Total C O 68 63 5	0	0
31	E	2	Total C 30 30	0	0
31	H	1	Total C 8 8	0	0
31	I	3	Total C 47 47	0	0
31	J	2	Total C 31 31	0	0
31	T	1	Total C 9 9	0	0
31	Y	1	Total C 12 12	0	0
31	X	1	Total C 16 16	0	0
31	a	4	Total C O 73 68 5	0	0
31	b	5	Total C 70 70	0	0
31	c	4	Total C O 74 67 7	0	0
31	d	2	Total C O 56 51 5	0	0
31	e	1	Total C 15 15	0	0
31	h	3	Total C 39 39	0	0
31	i	3	Total C O 71 66 5	0	0
31	j	2	Total C O 34 32 2	0	0
31	k	1	Total C 16 16	0	0
31	l	1	Total C O 16 14 2	0	0
31	t	1	Total C 8 8	0	0

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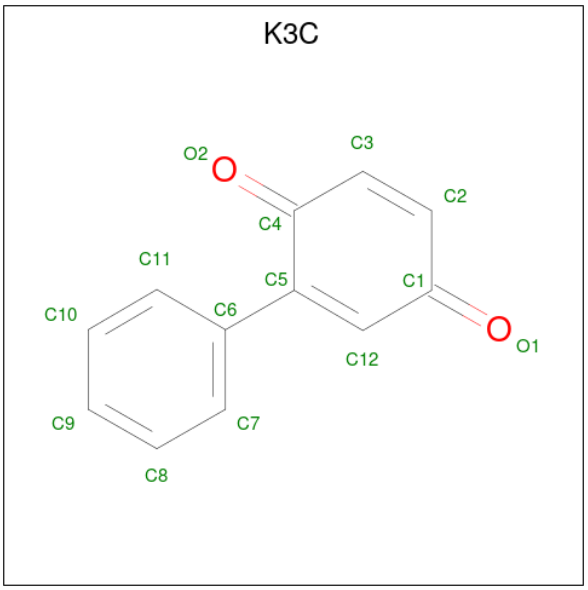
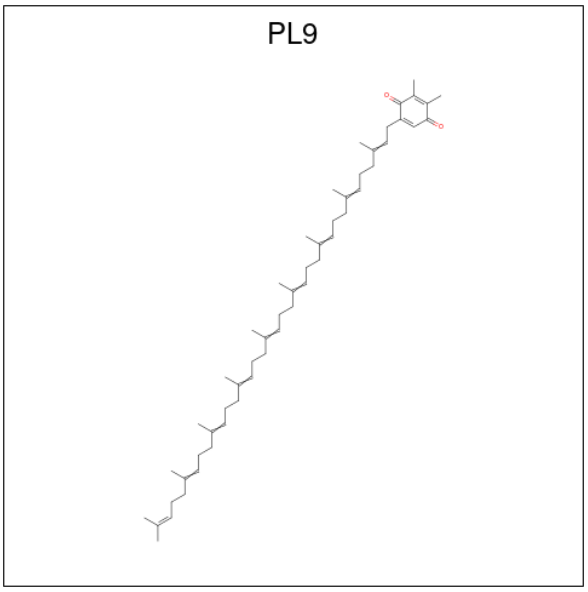
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	x	2	Total C O 30 28 2	0	0

- Molecule 32 is 2-phenylcyclohexa-2,5-diene-1,4-dione (CCD ID: K3C) (formula: $C_{12}H_8O_2$) (labeled as "Ligand of Interest" by depositor).



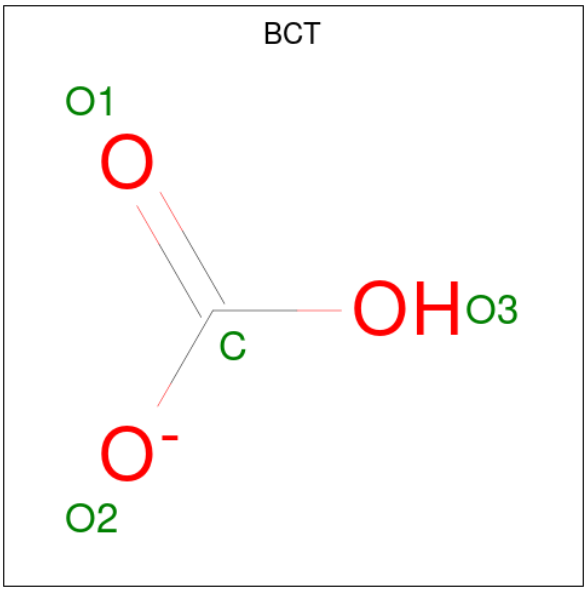
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 14 12 2	0	1
32	a	1	Total C O 14 12 2	0	1

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).

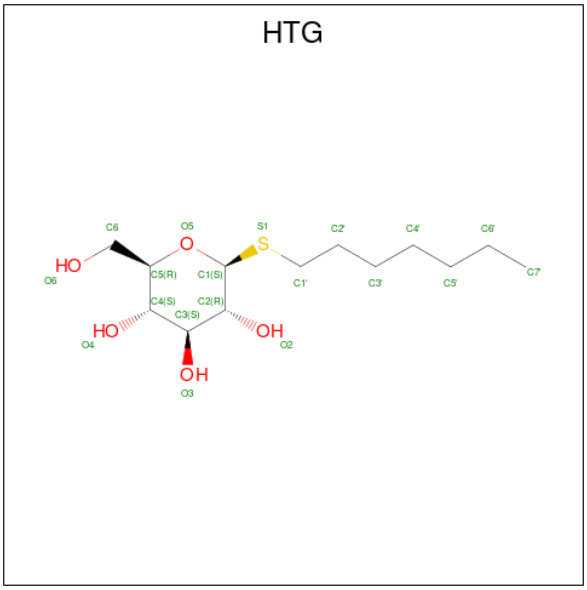


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	1	Total C O 4 1 3	0	0
34	a	1	Total C O 4 1 3	0	0

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

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

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



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

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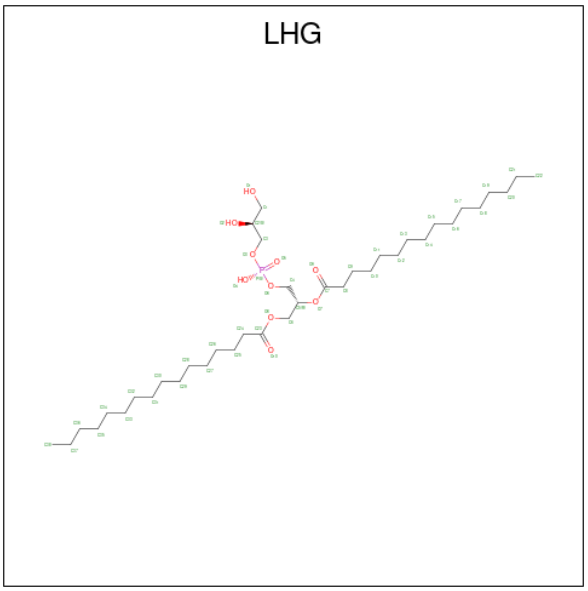
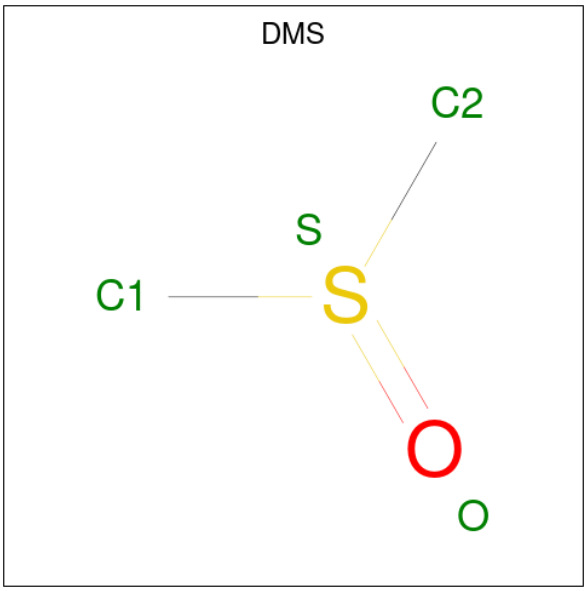
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0
36	D	1	Total C O S 19 13 5 1	0	0
36	I	1	Total C O S 19 13 5 1	0	0
36	O	1	Total C O S 19 13 5 1	0	0
36	U	1	Total C S 9 8 1	0	0
36	V	1	Total C O S 13 7 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	c	1	Total C O S 19 13 5 1	0	0
36	c	1	Total C O S 19 13 5 1	0	0
36	d	1	Total C O S 19 13 5 1	0	0
36	h	1	Total C O S 19 13 5 1	0	0
36	o	1	Total C O S 19 13 5 1	0	0
36	u	1	Total C O S 14 10 3 1	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	B	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			46	35	10	1		
37	E	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			39	28	10	1		
37	e	1	Total	C	O	P	0	0
			40	29	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	C	1	Total	C	O	S	0	0
			4	2	1	1		
38	C	1	Total	C	O	S	0	0
			4	2	1	1		
38	D	1	Total	C	O	S	0	0
			4	2	1	1		
38	E	1	Total	C	O	S	0	0
			4	2	1	1		
38	O	1	Total	C	O	S	0	0
			4	2	1	1		
38	V	1	Total	C	O	S	0	0
			4	2	1	1		
38	Y	1	Total	C	O	S	0	0
			4	2	1	1		
38	a	1	Total	C	O	S	0	0
			4	2	1	1		
38	b	1	Total	C	O	S	0	0
			4	2	1	1		

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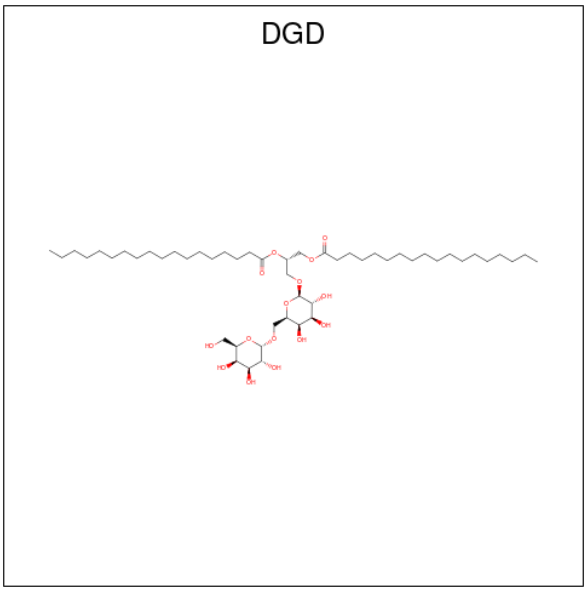
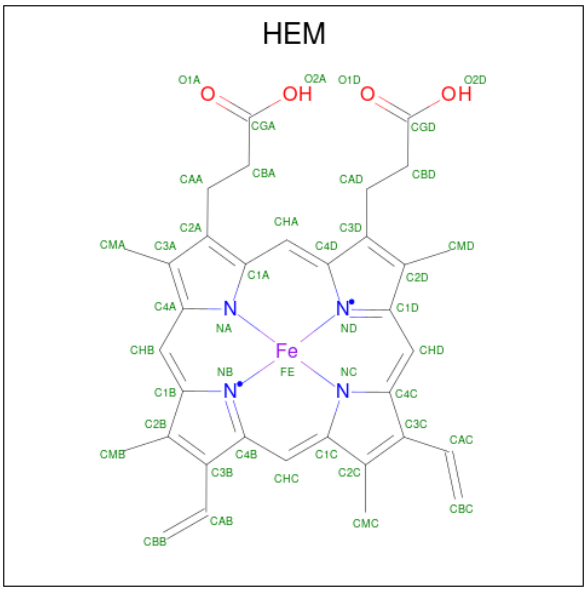
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total	C	O	S	0	0
			4	2	1	1		
38	b	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	d	1	Total	C	O	S	0	0
			4	2	1	1		
38	d	1	Total	C	O	S	0	0
			4	2	1	1		
38	i	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	v	1	Total	C	O	S	0	0
			4	2	1	1		
38	z	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



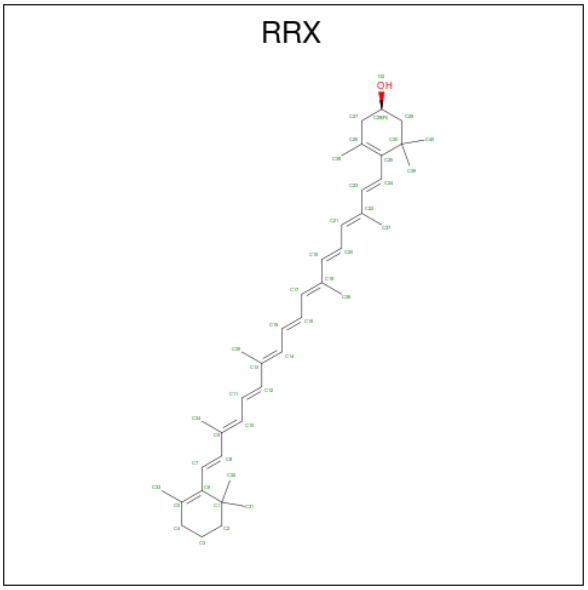
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	C	1	Total C O 62 47 15	0	0
39	C	1	Total C O 62 47 15	0	0
39	C	1	Total C O 62 47 15	0	0
39	D	1	Total C O 53 42 11	0	0
39	H	1	Total C O 62 47 15	0	0
39	c	1	Total C O 62 47 15	0	0
39	c	1	Total C O 62 47 15	0	0
39	c	1	Total C O 62 47 15	0	0
39	h	1	Total C O 62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

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



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

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

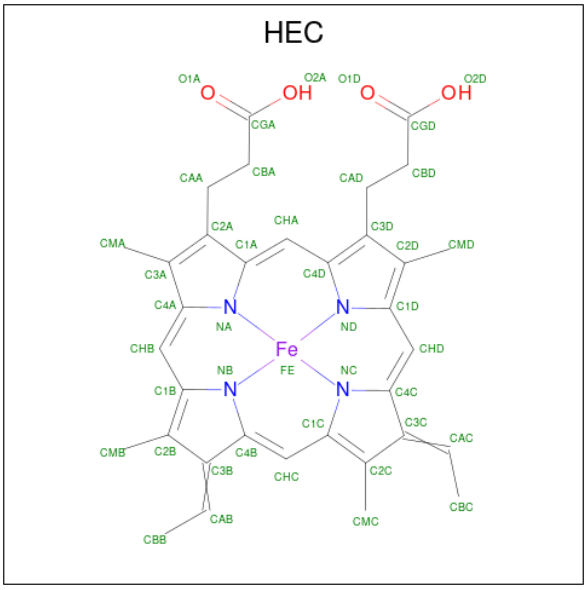


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
41	H	1	Total	C	O	0	0
			41	40	1		
41	h	1	Total	C	O	0	0
			41	40	1		

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

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

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



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

- Molecule 44 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	A	176	Total O 176 176	0	0
44	B	363	Total O 364 364	0	1
44	C	284	Total O 284 284	0	0
44	D	166	Total O 166 166	0	0
44	E	47	Total O 47 47	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	F	18	Total O 18 18	0	0
44	H	62	Total O 62 62	0	0
44	I	18	Total O 18 18	0	0
44	J	15	Total O 15 15	0	0
44	K	11	Total O 11 11	0	0
44	L	31	Total O 31 31	0	0
44	M	17	Total O 17 17	0	0
44	O	195	Total O 196 196	0	1
44	T	20	Total O 20 20	0	0
44	U	102	Total O 102 102	0	0
44	V	158	Total O 159 159	0	1
44	Y	9	Total O 9 9	0	0
44	X	16	Total O 16 16	0	0
44	a	164	Total O 164 164	0	0
44	b	323	Total O 325 325	0	2
44	c	273	Total O 275 275	0	2
44	d	157	Total O 157 157	0	0
44	e	29	Total O 29 29	0	0
44	f	11	Total O 11 11	0	0
44	h	45	Total O 45 45	0	0
44	i	10	Total O 10 10	0	0

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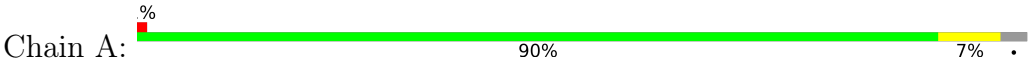
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	j	13	Total O 13 13	0	0
44	k	11	Total O 11 11	0	0
44	l	15	Total O 15 15	0	0
44	m	26	Total O 26 26	0	0
44	o	184	Total O 184 184	0	0
44	t	18	Total O 19 19	0	1
44	u	105	Total O 106 106	0	1
44	v	106	Total O 109 109	0	3
44	y	12	Total O 12 12	0	0
44	x	18	Total O 18 18	0	0
44	z	7	Total O 7 7	0	0
44	R	2	Total O 2 2	0	0

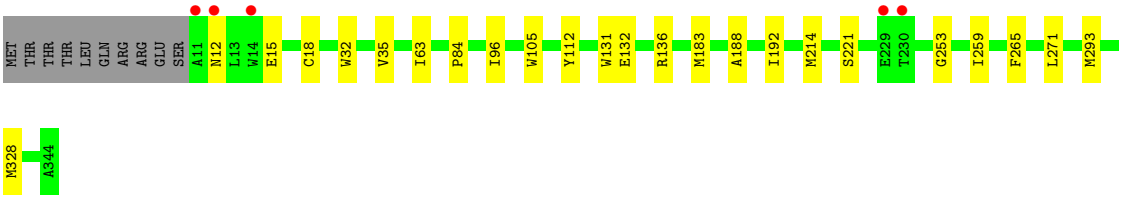
3 Residue-property plots

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

• Molecule 1: Photosystem II protein D1

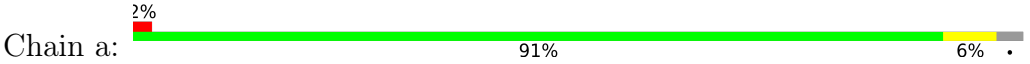
Chain A:

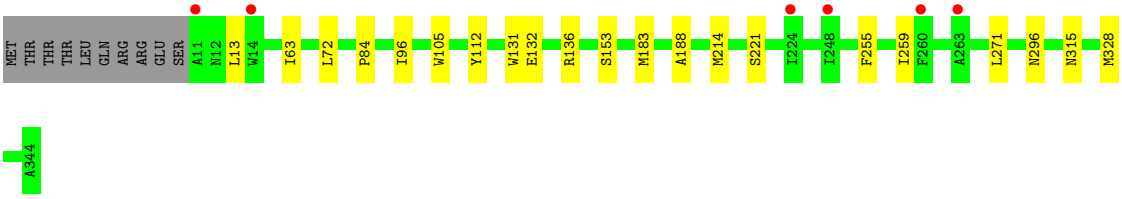




• Molecule 1: Photosystem II protein D1

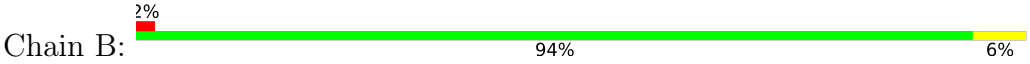
Chain a:





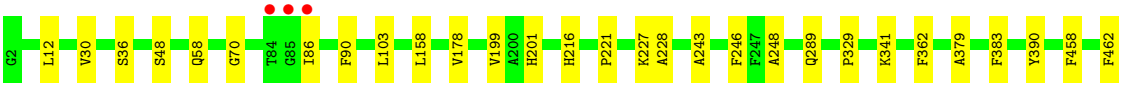
• Molecule 2: Photosystem II CP47 reaction center protein

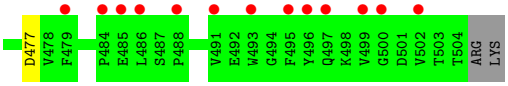
Chain B:



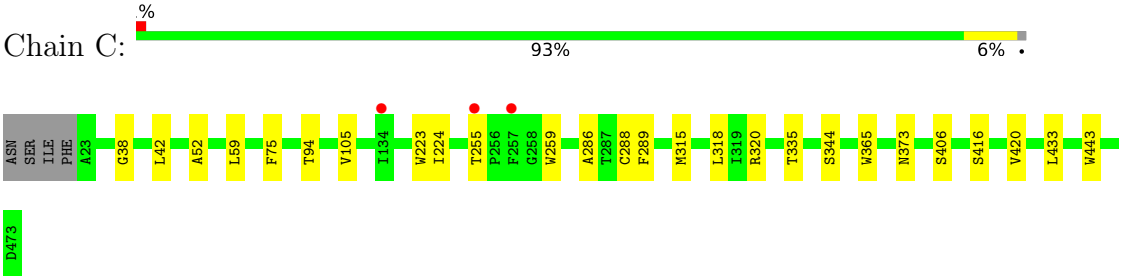
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

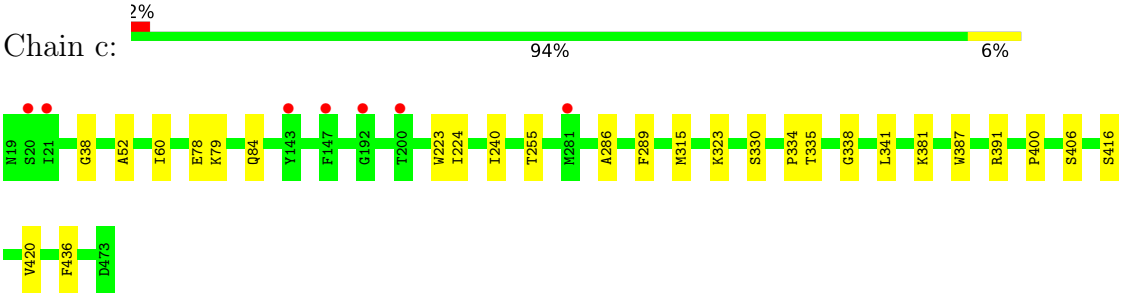




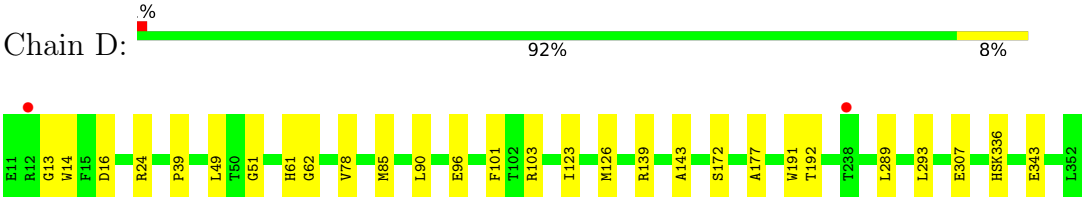
• Molecule 3: Photosystem II CP43 reaction center protein



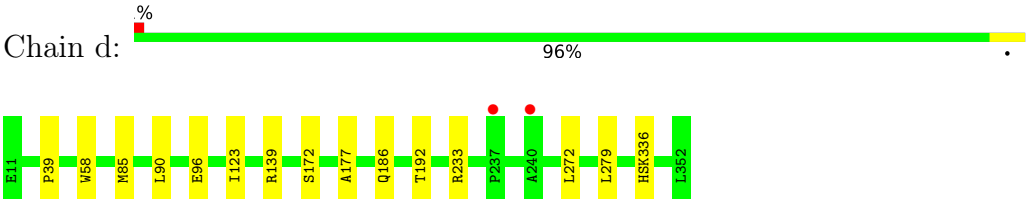
• Molecule 3: Photosystem II CP43 reaction center protein



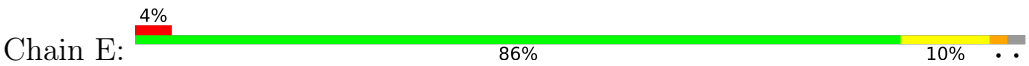
• Molecule 4: Photosystem II D2 protein

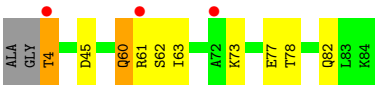


• Molecule 4: Photosystem II D2 protein



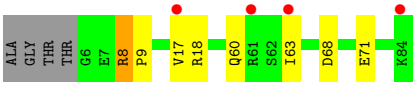
• Molecule 5: Cytochrome b559 subunit alpha





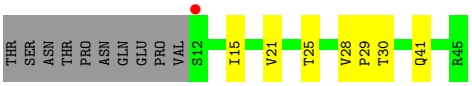
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



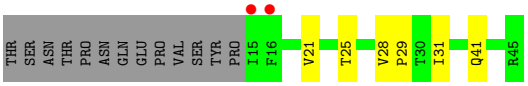
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



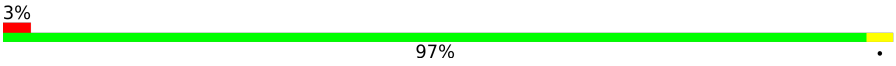
• Molecule 6: Cytochrome b559 subunit beta

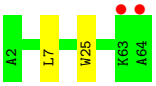
Chain f:



• Molecule 7: Photosystem II reaction center protein H

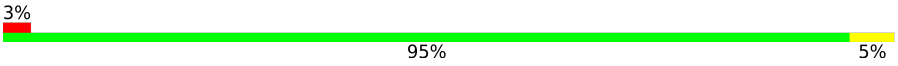
Chain H:

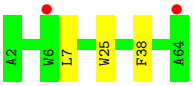




• Molecule 7: Photosystem II reaction center protein H

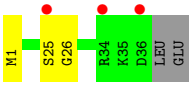
Chain h:





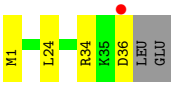
• Molecule 8: Photosystem II reaction center protein I

Chain I:



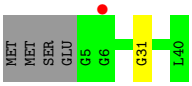
• Molecule 8: Photosystem II reaction center protein I

Chain i:



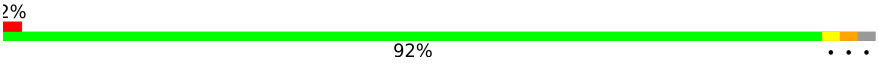
• Molecule 9: Photosystem II reaction center protein J

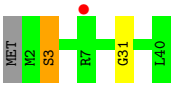
Chain J:



• Molecule 9: Photosystem II reaction center protein J

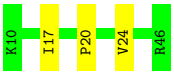
Chain j:





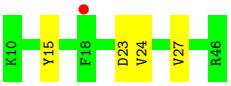
• Molecule 10: Photosystem II reaction center protein K

Chain K:



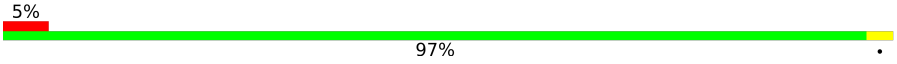
• Molecule 10: Photosystem II reaction center protein K

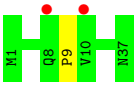
Chain k:



• Molecule 11: Photosystem II reaction center protein L

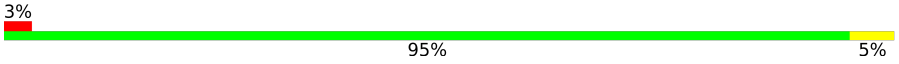
Chain L:

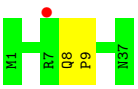




• Molecule 11: Photosystem II reaction center protein L

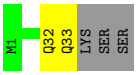
Chain l:





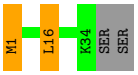
• Molecule 12: Photosystem II reaction center protein M

Chain M:



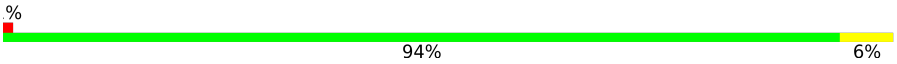
• Molecule 12: Photosystem II reaction center protein M

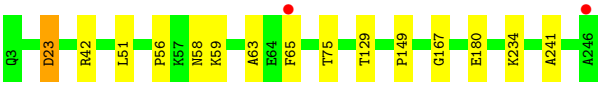
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

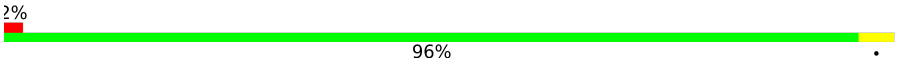
Chain O:

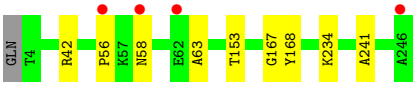




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

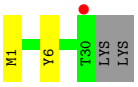
Chain o:





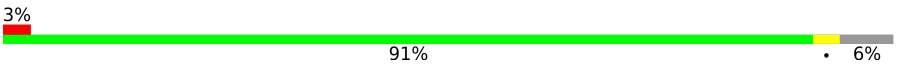
• Molecule 14: Photosystem II reaction center protein T

Chain T:



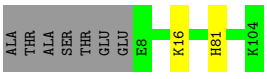
• Molecule 14: Photosystem II reaction center protein T

Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

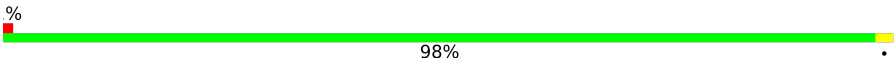


• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

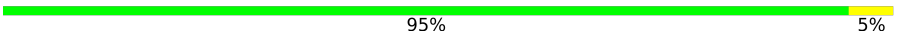
• Molecule 16: Cytochrome c-550

Chain V:



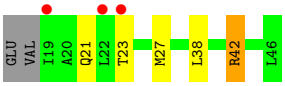
• Molecule 16: Cytochrome c-550

Chain v:



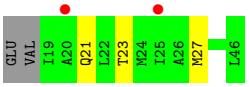
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



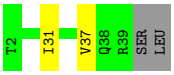
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



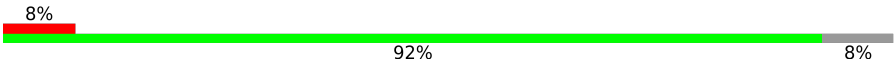
• Molecule 18: Photosystem II reaction center protein X

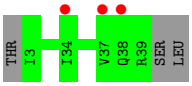
Chain X:



• Molecule 18: Photosystem II reaction center protein X

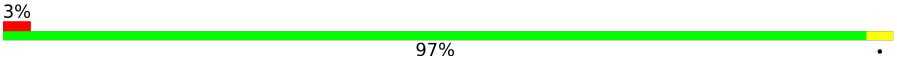
Chain x:

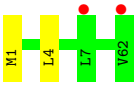




• Molecule 19: Photosystem II reaction center protein Z

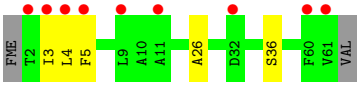
Chain Z:





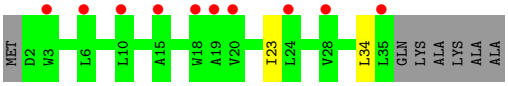
• Molecule 19: Photosystem II reaction center protein Z

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	124.02Å 229.58Å 287.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 1.95 49.22 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.22-1.95) 88.5 (49.22-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.153 , 0.181 0.157 , 0.184	Depositor DCC
R_{free} test set	29246 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55061	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: CA, HEC, PHO, GOL, CL, MG, RRX, LHG, LMG, BCR, BCT, HSK, FME, UNL, SQD, LMT, CLA, HEM, OEX, DMS, DGD, FE2, PL9, K3C, HTG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/2718	0.52	0/3707
1	a	0.34	0/2713	0.51	0/3700
2	B	0.33	1/4174 (0.0%)	0.48	0/5687
2	b	0.30	1/4158 (0.0%)	0.48	2/5667 (0.0%)
3	C	0.28	0/3613	0.44	0/4919
3	c	0.27	0/3636	0.43	0/4952
4	D	0.35	0/2809	0.50	0/3827
4	d	0.33	0/2819	0.47	0/3840
5	E	0.25	0/676	0.47	0/924
5	e	0.21	0/658	0.39	0/899
6	F	0.28	0/283	0.44	0/386
6	f	0.24	0/257	0.43	0/349
7	H	0.27	0/511	0.43	0/697
7	h	0.22	0/511	0.43	0/697
8	I	0.20	0/282	0.39	0/383
8	i	0.24	0/293	0.43	0/396
9	J	0.22	0/257	0.34	0/349
9	j	0.19	0/277	0.36	0/376
10	K	0.24	0/306	0.42	0/422
10	k	0.23	0/296	0.40	0/408
11	L	0.33	0/315	0.48	0/428
11	l	0.33	0/322	0.46	0/438
12	M	0.33	0/261	0.56	0/357
12	m	0.32	0/283	0.44	0/386
13	O	0.29	0/1933	0.49	0/2623
13	o	0.26	0/1917	0.49	0/2601
14	T	0.34	0/255	0.42	0/346
14	t	0.34	0/255	0.45	0/346
15	U	0.28	0/790	0.47	0/1071
15	u	0.30	0/794	0.48	0/1076
16	V	0.31	0/1090	0.45	0/1481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.27	0/1084	0.43	0/1475
17	Y	0.20	0/199	0.42	0/266
17	y	0.18	0/197	0.41	0/264
18	X	0.19	0/282	0.31	0/381
18	x	0.16	0/279	0.30	0/377
19	Z	0.18	0/462	0.34	0/635
19	z	0.18	0/457	0.41	0/626
20	R	0.17	0/246	0.29	0/341
All	All	0.30	2/42668 (0.0%)	0.46	2/58103 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	PRO	CA-C	6.46	1.55	1.51
2	b	221	PRO	CA-C	-6.27	1.48	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	48	SER	CA-C-N	-6.24	115.26	122.00
2	b	48	SER	C-N-CA	-6.24	115.26	122.00

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	2624	0	2525	16	0
1	a	2620	0	2527	15	0
2	B	4007	0	3875	23	0
2	b	3989	0	3850	24	0
3	C	3494	0	3418	19	0
3	c	3516	0	3430	21	0
4	D	2731	0	2631	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	2738	0	2643	12	0
5	E	657	0	637	8	0
5	e	639	0	617	5	0
6	F	274	0	279	5	0
6	f	250	0	261	4	0
7	H	498	0	518	2	0
7	h	498	0	518	4	0
8	I	285	0	291	2	0
8	i	296	0	311	1	0
9	J	251	0	257	1	0
9	j	271	0	270	3	0
10	K	293	0	303	2	0
10	k	286	0	285	3	0
11	L	305	0	323	1	0
11	l	309	0	332	1	0
12	M	265	0	286	1	0
12	m	281	0	310	3	0
13	O	1884	0	1856	11	0
13	o	1871	0	1841	6	0
14	T	256	0	256	1	0
14	t	256	0	256	0	0
15	U	776	0	777	2	0
15	u	780	0	781	0	0
16	V	1063	0	1069	2	0
16	v	1060	0	1053	5	0
17	Y	198	0	212	3	0
17	y	196	0	208	2	0
18	X	279	0	307	3	0
18	x	273	0	303	0	0
19	Z	461	0	483	0	0
19	z	446	0	457	2	0
20	R	240	0	218	1	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	24	0
24	C	845	0	936	24	0
24	D	130	0	144	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	260	0	288	4	0
24	b	1040	0	1152	31	0
24	c	845	0	936	22	0
24	d	130	0	144	3	0
25	A	64	0	74	0	0
25	D	64	0	74	2	0
25	a	64	0	74	0	0
25	d	64	0	74	2	0
26	A	40	0	56	3	0
26	B	160	0	224	10	0
26	C	80	0	112	3	0
26	D	40	0	56	3	0
26	K	40	0	56	2	0
26	T	40	0	56	3	0
26	Y	40	0	56	1	0
26	a	40	0	56	3	0
26	b	120	0	168	8	0
26	c	80	0	112	4	0
26	d	40	0	56	1	0
26	k	80	0	112	5	0
27	A	108	0	156	3	0
27	D	45	0	56	2	0
27	L	108	0	156	3	0
27	a	108	0	156	1	0
27	f	33	0	39	1	0
28	A	51	0	72	0	0
28	B	51	0	72	1	0
28	C	102	0	144	2	0
28	D	51	0	72	2	0
28	a	51	0	72	2	0
28	b	51	0	72	2	0
28	c	102	0	144	1	0
28	d	51	0	72	1	0
29	A	35	0	46	1	0
29	B	59	0	81	1	0
29	C	35	0	46	4	0
29	E	24	0	35	0	0
29	J	24	0	35	1	0
29	M	35	0	46	1	0
29	T	24	0	35	0	0
29	Z	35	0	46	0	0
29	a	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	25	0	35	1	0
29	c	35	0	46	2	0
29	f	35	0	46	1	0
29	m	105	0	138	1	0
29	z	32	0	33	2	0
30	A	12	0	16	0	0
30	B	36	0	48	0	0
30	C	30	0	40	2	0
30	E	6	0	8	0	0
30	L	6	0	8	0	0
30	M	6	0	8	0	0
30	O	6	0	8	0	0
30	T	12	0	16	1	0
30	V	24	0	30	0	0
30	a	24	0	32	3	0
30	b	24	0	32	0	0
30	c	24	0	32	1	0
30	d	12	0	16	2	0
30	h	6	0	8	0	0
30	k	6	0	8	0	0
30	o	12	0	16	1	0
30	u	6	0	8	0	0
30	v	36	0	46	1	0
31	A	74	0	0	0	0
31	B	99	0	0	0	0
31	C	73	0	0	0	0
31	D	68	0	0	0	0
31	E	30	0	0	0	0
31	H	8	0	0	0	0
31	I	47	0	0	0	0
31	J	31	0	0	0	0
31	T	9	0	0	0	0
31	X	16	0	0	0	0
31	Y	12	0	0	0	0
31	a	73	0	0	0	0
31	b	70	0	0	0	0
31	c	74	0	0	1	0
31	d	56	0	0	0	0
31	e	15	0	0	0	0
31	h	39	0	0	0	0
31	i	71	0	0	0	0
31	j	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	k	16	0	0	0	0
31	l	16	0	0	0	0
31	t	8	0	0	0	0
31	x	30	0	0	0	0
32	A	14	0	0	0	0
32	a	14	0	0	0	0
33	A	55	0	80	6	0
33	D	55	0	80	0	0
33	a	55	0	80	6	0
33	d	55	0	80	0	0
34	A	4	0	0	0	0
34	a	4	0	0	0	0
35	B	1	0	0	0	0
35	F	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	f	1	0	0	0	0
35	o	1	0	0	0	0
36	B	95	0	130	4	0
36	C	38	0	52	0	0
36	D	19	0	26	3	0
36	I	19	0	26	0	0
36	O	19	0	26	1	0
36	U	9	0	15	0	0
36	V	13	0	11	0	0
36	b	76	0	104	6	0
36	c	38	0	52	0	0
36	d	19	0	26	0	0
36	h	19	0	26	2	0
36	o	19	0	26	0	0
36	u	14	0	19	0	0
37	B	49	0	74	1	0
37	D	144	0	213	8	0
37	E	49	0	74	1	0
37	d	137	0	196	0	0
37	e	40	0	53	1	0
37	l	49	0	74	1	0
38	B	20	0	30	1	0
38	C	8	0	12	0	0
38	D	4	0	6	0	0
38	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	O	4	0	6	0	0
38	V	4	0	6	0	0
38	Y	4	0	6	0	0
38	a	4	0	6	0	0
38	b	12	0	18	3	0
38	c	20	0	30	2	0
38	d	8	0	12	0	0
38	i	4	0	6	0	0
38	o	20	0	30	1	0
38	v	4	0	6	0	0
38	z	4	0	6	0	0
39	C	186	0	246	4	0
39	D	53	0	71	6	0
39	H	62	0	82	1	0
39	c	186	0	246	5	0
39	h	62	0	82	1	0
40	F	43	0	30	1	0
40	f	43	0	30	3	0
41	H	41	0	56	3	0
41	h	41	0	56	5	0
42	J	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	0	0
43	v	43	0	30	0	0
44	A	176	0	0	0	0
44	B	364	0	0	2	0
44	C	284	0	0	1	0
44	D	166	0	0	2	0
44	E	47	0	0	0	0
44	F	18	0	0	0	0
44	H	62	0	0	1	0
44	I	18	0	0	0	0
44	J	15	0	0	0	0
44	K	11	0	0	0	0
44	L	31	0	0	1	0
44	M	17	0	0	0	0
44	O	196	0	0	2	0
44	R	2	0	0	0	0
44	T	20	0	0	0	0
44	U	102	0	0	2	0
44	V	159	0	0	1	0
44	X	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Y	9	0	0	0	0
44	a	164	0	0	0	0
44	b	325	0	0	2	0
44	c	275	0	0	5	0
44	d	157	0	0	0	0
44	e	29	0	0	0	0
44	f	11	0	0	0	0
44	h	45	0	0	0	0
44	i	10	0	0	0	0
44	j	13	0	0	0	0
44	k	11	0	0	0	0
44	l	15	0	0	0	0
44	m	26	0	0	0	0
44	o	184	0	0	1	0
44	t	19	0	0	0	0
44	u	106	0	0	0	0
44	v	109	0	0	0	0
44	x	18	0	0	0	0
44	y	12	0	0	0	0
44	z	7	0	0	0	0
All	All	55061	0	52295	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (381) 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)
39:D:407:DGD:HD62	5:E:45:ASP:HB3	1.59	0.85
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.71	0.72
39:c:519:DGD:HB62	28:c:521:LMG:H402	1.71	0.71
4:D:101:PHE:H	39:D:407:DGD:HB32	1.55	0.70
3:c:391[B]:ARG:NH2	44:c:601:HOH:O	2.24	0.69
40:f:101:HEM:HHD	40:f:101:HEM:HBC2	1.74	0.69
4:D:13:GLY:HA3	36:D:413:HTG:H62	1.75	0.69
24:a:410:CLA:H151	33:a:425[B]:PL9:H262	1.76	0.66
28:b:623:LMG:H421	37:l:302:LHG:H383	1.77	0.66
24:b:618:CLA:H2	24:b:619:CLA:HBB2	1.78	0.66
27:L:102:SQD:H1	27:L:102:SQD:H462	1.77	0.66
24:c:503:CLA:C4D	24:c:505:CLA:H2	2.26	0.66
36:D:413:HTG:H1	7:H:25:TRP:CD1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:D:407:DGD:O5D	39:D:407:DGD:O4D	2.14	0.65
24:C:507:CLA:HMC2	24:C:508:CLA:H102	1.81	0.62
2:B:227:LYS:HG2	38:B:643:DMS:H21	1.81	0.61
24:C:503:CLA:H61	24:C:513:CLA:H42	1.82	0.61
29:b:624:LMT:H11	38:b:638:DMS:H21	1.81	0.61
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.82	0.61
5:e:18:ARG:NH1	9:j:3:SER:OG	2.34	0.60
26:T:102:BCR:H321	26:T:102:BCR:HC8	1.83	0.60
4:D:62:GLY:HA3	5:E:63:ILE:HD13	1.84	0.60
24:b:604:CLA:H203	41:h:1204:RRX:H37	1.83	0.58
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.86	0.58
24:b:612:CLA:HBB1	24:b:612:CLA:HMB1	1.86	0.58
5:e:8:ARG:NH2	9:j:3:SER:O	2.37	0.58
26:B:619:BCR:H363	26:B:641:BCR:H19C	1.85	0.58
13:O:23:ASP:OD2	13:O:23:ASP:N	2.32	0.58
13:O:58:ASN:HB2	44:b:710:HOH:O	2.03	0.58
24:b:609:CLA:H72	26:b:622:BCR:H311	1.85	0.58
40:F:101:HEM:HBB2	40:F:101:HEM:HMB1	1.86	0.57
28:D:412:LMG:H412	6:F:30:THR:HG21	1.87	0.57
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.86	0.57
24:c:515:CLA:HAB	26:c:516:BCR:H24C	1.87	0.57
29:c:523:LMT:H2O1	29:c:523:LMT:H3O2	1.52	0.57
24:B:605:CLA:H43	24:B:606:CLA:H2	1.87	0.57
27:a:414:SQD:H302	24:c:510:CLA:H71	1.86	0.57
39:D:407:DGD:O2G	39:D:407:DGD:O2D	2.23	0.57
24:c:503:CLA:C3D	24:c:505:CLA:H2	2.35	0.56
2:B:248:ALA:HA	24:B:604:CLA:H42	1.87	0.56
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.86	0.56
2:B:223[B]:GLN:NE2	44:B:701:HOH:O	2.30	0.56
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.88	0.56
4:d:233:ARG:HH11	30:d:402:GOL:H12	1.69	0.55
26:T:102:BCR:H19C	26:b:621:BCR:H363	1.87	0.55
5:E:60:GLN:NE2	5:E:62:SER:O	2.27	0.55
3:c:391[A]:ARG:NH2	44:c:601:HOH:O	2.34	0.55
26:Y:302:BCR:H321	26:Y:302:BCR:HC8	1.87	0.55
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.89	0.54
24:b:608:CLA:HHC	24:b:608:CLA:HBB1	1.89	0.54
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.08	0.54
24:b:604:CLA:HAA2	36:b:626:HTG:H62	1.89	0.54
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.89	0.53
1:a:183:MET:HA	24:a:408:CLA:HMD1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:279:LEU:HD22	25:d:401:PHO:HBC3	1.91	0.53
30:a:417:GOL:H12	12:m:1:FME:HG2	1.91	0.53
30:C:530:GOL:H31	44:V:302:HOH:O	2.08	0.53
24:B:611:CLA:H122	24:B:616:CLA:HAA1	1.90	0.53
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.38	0.53
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.90	0.52
6:F:21:VAL:O	6:F:25:THR:HG23	2.09	0.52
24:b:617:CLA:H8	26:b:620:BCR:H362	1.92	0.52
24:b:618:CLA:H2	24:b:619:CLA:CBB	2.39	0.52
3:c:38:GLY:HA3	24:c:513:CLA:HMD2	1.91	0.52
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.91	0.52
2:B:162:PHE:O	24:B:607:CLA:HHD	2.10	0.52
2:b:227:LYS:HE3	38:b:638:DMS:H23	1.92	0.52
24:c:510:CLA:HBC3	24:c:512:CLA:H71	1.91	0.52
13:o:168:TYR:HB3	38:o:308:DMS:H12	1.91	0.52
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.91	0.52
7:h:25:TRP:CD2	36:h:1202:HTG:H1	2.45	0.51
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.11	0.51
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.92	0.51
33:a:425[B]:PL9:H502	4:d:39:PRO:HG3	1.92	0.51
1:A:18:CYS:SG	44:C:750:HOH:O	2.60	0.51
2:b:228:ALA:HA	38:b:638:DMS:H22	1.92	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.51
36:b:601:HTG:O2	36:b:602:HTG:S1	2.63	0.51
29:c:523:LMT:H12	8:i:24:LEU:HD13	1.91	0.51
24:b:605:CLA:HMB1	24:b:605:CLA:HBB1	1.93	0.51
6:f:21:VAL:O	6:f:25:THR:HG23	2.12	0.50
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.44	0.50
26:B:641:BCR:HC8	26:B:641:BCR:H321	1.93	0.50
24:C:513:CLA:HBB1	24:C:513:CLA:HMB1	1.92	0.50
29:M:101:LMT:H6D	11:l:9:PRO:HA	1.93	0.50
2:b:90:PHE:CZ	24:b:609:CLA:H141	2.47	0.50
24:b:607:CLA:H43	24:b:608:CLA:H2	1.93	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.49
1:a:131:TRP:CH2	24:c:507:CLA:HAA2	2.47	0.49
24:c:515:CLA:HMD3	29:z:101:LMT:H5'	1.94	0.49
24:B:610:CLA:HBB1	24:B:610:CLA:HMB1	1.93	0.49
33:A:422[B]:PL9:H502	4:D:39:PRO:HG3	1.95	0.49
26:k:302:BCR:H321	26:k:302:BCR:HC8	1.93	0.49
13:O:56:PRO:HG3	13:O:63:ALA:HB2	1.95	0.49
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:25:TRP:NE1	36:h:1202:HTG:H5	2.26	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.93	0.49
24:B:605:CLA:H101	24:B:616:CLA:H42	1.93	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.47	0.49
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.48	0.49
1:A:12:ASN:OD1	1:A:15:GLU:HB2	2.13	0.49
24:b:612:CLA:NC	41:h:1204:RRX:H56	2.27	0.49
24:c:514:CLA:H121	24:c:515:CLA:H142	1.95	0.49
40:f:101:HEM:HBB2	40:f:101:HEM:HMB2	1.93	0.49
29:f:104:LMT:O3'	29:f:104:LMT:O2B	2.24	0.49
2:b:36:SER:OG	26:b:621:BCR:H362	2.13	0.48
4:D:85:MET:CE	4:D:96:GLU:HG2	2.42	0.48
24:b:613:CLA:HHC	24:b:613:CLA:HBB1	1.96	0.48
26:b:621:BCR:H331	26:b:621:BCR:C8	2.43	0.48
29:C:521:LMT:H6'1	8:I:26:GLY:HA3	1.95	0.48
3:c:334:PRO:HA	13:o:153:THR:OG1	2.13	0.48
4:D:61:HIS:HD2	44:D:652:HOH:O	1.95	0.48
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.43	0.48
27:A:411:SQD:H322	24:C:509:CLA:H193	1.95	0.48
24:C:509:CLA:H92	37:D:411:LHG:H141	1.95	0.48
36:b:625:HTG:O2	36:b:625:HTG:H7'3	2.14	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.96	0.48
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.96	0.48
5:e:68:ASP:OD2	5:e:71:GLU:HB2	2.14	0.48
27:L:102:SQD:O2	44:L:201:HOH:O	2.20	0.48
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.95	0.47
28:a:415:LMG:H201	39:c:518:DGD:HA82	1.95	0.47
33:a:425[B]:PL9:H422	27:f:102:SQD:H262	1.96	0.47
3:C:315:MET:HE2	3:C:365:TRP:CZ3	2.49	0.47
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.96	0.47
15:U:81:HIS:HE1	44:U:380:HOH:O	1.97	0.47
1:a:132:GLU:O	1:a:136:ARG:HG2	2.13	0.47
2:B:494:GLY:HA3	5:E:4:THR:O	2.15	0.47
33:a:425[B]:PL9:H13	33:a:425[B]:PL9:H172	1.70	0.47
3:c:391[A]:ARG:HD3	44:c:604:HOH:O	2.14	0.47
3:C:406:SER:HA	3:C:420:VAL:HG23	1.96	0.47
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.96	0.47
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.55	0.47
3:C:288:CYS:SG	39:C:517:DGD:HB32	2.55	0.47
2:B:461:LEU:HD22	37:D:409:LHG:H301	1.97	0.46
24:D:404:CLA:HBB1	24:D:404:CLA:HMB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:60:ILE:HG22	24:c:505:CLA:HHD	1.97	0.46
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.30	0.46
1:A:32:TRP:O	1:A:35:VAL:HG22	2.15	0.46
39:c:519:DGD:HA81	39:c:519:DGD:HAE2	1.63	0.46
4:d:58:TRP:CH2	5:e:63:ILE:HD12	2.50	0.46
3:C:286:ALA:HB2	24:C:503:CLA:HMD2	1.97	0.46
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.46
5:E:78:THR:O	5:E:82:GLN:HG3	2.15	0.46
12:M:32:GLN:O	12:M:33:GLN:HG3	2.15	0.46
24:c:503:CLA:H192	24:c:508:CLA:C1B	2.45	0.46
28:d:411:LMG:H241	28:d:411:LMG:H192	1.97	0.46
3:C:259:TRP:CG	29:C:521:LMT:H42	2.50	0.46
25:D:401:PHO:NC	25:D:401:PHO:ND	2.62	0.46
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.98	0.46
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.97	0.46
1:A:214:MET:HB3	1:A:214:MET:HE3	1.73	0.46
33:A:422[B]:PL9:H13	33:A:422[B]:PL9:H171	1.66	0.46
24:C:502:CLA:C3D	24:C:504:CLA:H2	2.46	0.46
24:b:604:CLA:H51	44:b:954:HOH:O	2.15	0.46
1:a:63:ILE:HB	3:c:335:THR:HG21	1.98	0.46
4:d:123:ILE:HD11	39:h:1205:DGD:HAE1	1.98	0.46
24:B:605:CLA:H93	24:B:606:CLA:HAB	1.98	0.45
3:C:94:THR:HG22	24:C:502:CLA:HED1	1.97	0.45
27:L:101:SQD:H341	27:L:101:SQD:H311	1.51	0.45
3:C:443:TRP:CZ2	24:C:509:CLA:HMD1	2.51	0.45
24:C:511:CLA:H112	24:C:511:CLA:H152	1.63	0.45
2:b:216:HIS:HE1	24:b:612:CLA:C1A	2.29	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.45
3:C:320:ARG:CB	30:C:530:GOL:H32	2.46	0.45
24:c:505:CLA:H101	24:c:505:CLA:H62	1.65	0.45
24:d:405:CLA:HMB1	24:d:405:CLA:HBB1	1.97	0.45
37:B:640:LHG:HC81	37:D:409:LHG:HC91	1.98	0.45
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.51	0.45
16:v:57:GLU:H	16:v:57:GLU:CD	2.24	0.45
1:A:63:ILE:HB	3:C:335:THR:HG21	1.99	0.45
37:D:411:LHG:H341	37:D:411:LHG:H142	1.98	0.45
2:b:248:ALA:HA	24:b:606:CLA:H42	1.98	0.45
29:C:521:LMT:H2B	8:I:25:SER:HB3	1.98	0.45
30:a:417:GOL:C1	12:m:1:FME:HG2	2.47	0.45
24:A:406:CLA:HBB1	24:A:406:CLA:HMB1	1.99	0.45
3:c:223:TRP:CG	3:c:224:ILE:H	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:323:LYS:HD2	30:c:527:GOL:O2	2.16	0.45
29:z:101:LMT:O3'	29:z:101:LMT:H2B	2.16	0.45
1:A:131:TRP:CH2	24:C:506:CLA:HAA2	2.52	0.45
11:L:9:PRO:HA	29:m:102:LMT:H6D	1.99	0.45
26:A:410:BCR:H15C	26:A:410:BCR:H351	1.88	0.45
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.52	0.45
24:c:504:CLA:H61	24:c:514:CLA:H42	1.98	0.45
24:C:505:CLA:C4B	39:C:518:DGD:HB71	2.47	0.44
41:H:101:RRX:H32	41:H:101:RRX:H28	1.87	0.44
2:b:201:HIS:HB2	24:b:605:CLA:CHB	2.48	0.44
24:b:604:CLA:H141	41:h:1204:RRX:C17	2.47	0.44
4:d:85:MET:CE	4:d:96:GLU:HG2	2.48	0.44
3:C:59:LEU:HD21	26:K:101:BCR:H372	2.00	0.44
15:U:16:LYS:NZ	44:U:302:HOH:O	2.38	0.44
33:A:422[B]:PL9:H262	37:E:101:LHG:H223	1.98	0.44
24:B:603:CLA:H101	24:B:610:CLA:H193	2.00	0.44
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.48	0.44
3:c:406:SER:HA	3:c:420:VAL:HG23	1.98	0.44
24:b:612:CLA:HMA3	24:b:613:CLA:C1C	2.48	0.44
24:c:511:CLA:H112	24:c:511:CLA:H142	1.59	0.44
24:B:616:CLA:H111	24:B:616:CLA:H152	1.64	0.44
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.88	0.44
5:E:60:GLN:HG2	5:E:61:ARG:N	2.33	0.44
5:e:8:ARG:HG3	5:e:9:PRO:HD2	1.99	0.44
29:A:414:LMT:H121	36:O:302:HTG:H7'2	1.99	0.44
2:B:419:SER:HB3	36:B:623[A]:HTG:H2'1	2.00	0.44
2:B:464:PHE:CZ	37:D:409:LHG:H252	2.53	0.44
3:C:52:ALA:HB2	24:C:512:CLA:HMA2	1.98	0.44
17:Y:23:THR:O	17:Y:27:MET:HG3	2.17	0.44
13:o:58:ASN:ND2	44:o:408:HOH:O	2.49	0.44
2:B:341:LYS:NZ	36:B:623[A]:HTG:S1	2.91	0.44
3:C:318:LEU:C	3:C:318:LEU:HD23	2.43	0.44
39:D:407:DGD:HB21	39:D:407:DGD:HG2	1.86	0.44
2:b:30:VAL:HG12	24:b:608:CLA:HHD	1.99	0.44
24:b:616:CLA:HBB1	24:b:616:CLA:HMB3	1.99	0.44
24:b:618:CLA:H161	7:h:7:LEU:HD21	2.00	0.44
1:a:13:LEU:HD12	1:a:13:LEU:HA	1.80	0.44
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.99	0.44
3:c:286:ALA:HB2	24:c:504:CLA:HMD2	1.99	0.44
29:B:622:LMT:O6'	4:D:16:ASP:OD1	2.35	0.43
24:c:514:CLA:HBB1	24:c:514:CLA:HMB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:407:CLA:HBB1	25:D:401:PHO:H122	1.99	0.43
24:b:606:CLA:HAB	24:b:608:CLA:H171	1.99	0.43
26:d:406:BCR:H15C	26:d:406:BCR:H351	1.87	0.43
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.99	0.43
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.80	0.43
13:O:180:GLU:CD	13:O:180:GLU:H	2.26	0.43
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.54	0.43
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.54	0.43
33:a:425[B]:PL9:H321	33:a:425[B]:PL9:H301	1.46	0.43
1:A:265:PHE:HE1	27:A:411:SQD:H81	1.83	0.43
26:a:413:BCR:H24C	26:a:413:BCR:H371	1.85	0.43
3:c:436:PHE:CE2	24:c:506:CLA:H162	2.54	0.43
26:c:516:BCR:H15C	26:c:516:BCR:H351	1.78	0.43
16:v:53:ASP:CG	16:v:55[B]:ARG:HG3	2.43	0.43
24:B:606:CLA:HMC3	24:B:616:CLA:H43	2.00	0.43
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.91	0.43
24:b:616:CLA:H72	24:b:616:CLA:H111	1.82	0.43
26:k:302:BCR:H323	26:k:302:BCR:HC31	1.84	0.43
33:A:422[B]:PL9:C20	33:A:422[B]:PL9:H162	2.49	0.43
39:C:518:DGD:HA32	29:J:102:LMT:H101	2.00	0.43
3:c:381:LYS:NZ	44:c:615:HOH:O	2.52	0.43
31:c:501:UNL:O7	30:d:402:GOL:O2	2.29	0.43
24:c:510:CLA:HBB1	24:c:510:CLA:HMB3	2.01	0.43
24:b:606:CLA:CGA	24:b:606:CLA:H3A	2.49	0.43
3:c:52:ALA:HB2	24:c:513:CLA:HMA1	2.01	0.43
6:f:31:ILE:HG13	40:f:101:HEM:HMC2	2.00	0.43
26:B:619:BCR:C8	26:B:619:BCR:H331	2.48	0.43
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.01	0.43
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.54	0.43
10:k:24:VAL:O	10:k:27:VAL:HG22	2.19	0.43
26:A:410:BCR:H24C	26:A:410:BCR:H371	1.87	0.42
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.01	0.42
39:c:519:DGD:HAT1	39:c:520:DGD:HBE1	2.00	0.42
1:A:271:LEU:HD11	33:A:422[B]:PL9:HC71	2.01	0.42
4:D:126:MET:HE3	4:D:143:ALA:O	2.18	0.42
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.19	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.42
1:a:315:ASN:ND2	30:a:418:GOL:H2	2.34	0.42
24:b:610:CLA:H122	28:b:623:LMG:H232	2.01	0.42
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.87	0.42
3:c:330:SER:OG	30:o:305:GOL:H32	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PHE:CE2	24:B:607:CLA:H151	2.54	0.42
24:B:617:CLA:H92	24:B:617:CLA:H51	2.01	0.42
26:B:620:BCR:H331	26:B:620:BCR:C8	2.49	0.42
24:c:511:CLA:HBB1	24:c:511:CLA:HMB1	2.00	0.42
27:A:411:SQD:H171	37:D:411:LHG:H212	2.01	0.42
39:C:517:DGD:HA82	39:C:517:DGD:HAE1	1.88	0.42
1:a:271:LEU:HD11	33:a:425[B]:PL9:HC71	2.01	0.42
39:c:520:DGD:HA81	39:c:520:DGD:HAE2	1.70	0.42
26:k:303:BCR:H24C	26:k:303:BCR:H371	1.77	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.18	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.02	0.42
24:B:603:CLA:H203	24:B:603:CLA:H162	1.87	0.42
24:B:614:CLA:H122	28:B:621:LMG:H232	2.01	0.42
27:D:408:SQD:H112	18:X:31:ILE:HD11	2.02	0.42
2:B:127[A]:ARG:NH2	44:B:715:HOH:O	2.51	0.42
24:B:616:CLA:H161	7:H:7:LEU:HD21	2.02	0.42
3:C:38:GLY:HA3	24:C:512:CLA:HMD2	2.00	0.42
27:D:408:SQD:H241	18:X:31:ILE:HD13	2.01	0.42
37:D:411:LHG:H161	37:D:411:LHG:H191	1.70	0.42
24:C:502:CLA:H42	24:C:503:CLA:HMD3	2.02	0.42
24:C:514:CLA:H3A	24:C:514:CLA:HBA1	1.79	0.42
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.02	0.42
2:b:341:LYS:NZ	36:b:625:HTG:O2	2.29	0.42
2:b:462:PHE:CE2	24:b:616:CLA:HMB2	2.55	0.42
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.01	0.42
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.19	0.42
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.85	0.42
37:D:411:LHG:H171	37:D:411:LHG:H332	2.01	0.42
17:Y:38:LEU:O	17:Y:42:ARG:HG3	2.20	0.42
2:b:103:LEU:HB2	24:b:609:CLA:H62	2.02	0.42
24:C:506:CLA:HBC2	26:C:516:BCR:H341	2.01	0.42
39:D:407:DGD:HB51	39:D:407:DGD:HB81	1.85	0.42
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.50	0.42
26:D:405:BCR:H381	28:D:412:LMG:H231	2.02	0.42
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.42
13:O:149:PRO:HB2	44:O:489:HOH:O	2.20	0.42
2:b:86:ILE:H	2:b:86:ILE:HG13	1.75	0.42
26:b:620:BCR:H24C	26:b:620:BCR:H371	1.86	0.42
4:d:186:GLN:HB2	24:d:404:CLA:HBC1	2.02	0.42
17:y:23:THR:O	17:y:27:MET:HG3	2.20	0.42
36:B:625:HTG:O2	36:B:626:HTG:S1	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:613:CLA:H122	24:b:618:CLA:HAA1	2.02	0.41
26:b:622:BCR:H15C	26:b:622:BCR:H351	1.91	0.41
3:c:387:TRP:CD1	38:c:533:DMS:H12	2.55	0.41
38:c:536:DMS:S	44:c:718:HOH:O	2.62	0.41
26:k:302:BCR:HC7	26:k:302:BCR:H331	1.93	0.41
13:o:56:PRO:HD3	13:o:63:ALA:HB2	2.01	0.41
24:B:617:CLA:H161	24:B:617:CLA:H122	1.76	0.41
3:C:433:LEU:HD13	24:C:503:CLA:CHC	2.50	0.41
4:D:49:LEU:HD13	26:D:405:BCR:C15	2.50	0.41
41:H:101:RRX:H43	41:H:101:RRX:H47	1.85	0.41
28:a:415:LMG:H241	28:a:415:LMG:H422	2.01	0.41
37:e:101:LHG:H241	37:e:101:LHG:HC61	1.64	0.41
24:B:616:CLA:H71	24:B:617:CLA:H203	2.03	0.41
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.20	0.41
26:B:641:BCR:H20C	26:B:641:BCR:H361	1.94	0.41
28:C:520:LMG:H142	10:K:24[B]:VAL:HG12	2.03	0.41
28:C:532:LMG:H321	28:C:532:LMG:H352	1.91	0.41
26:D:405:BCR:H20C	26:D:405:BCR:H361	1.90	0.41
36:b:625:HTG:H5'1	36:b:625:HTG:H2'1	1.79	0.41
24:c:507:CLA:HAA1	24:c:507:CLA:HBD	2.02	0.41
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.32	0.41
1:a:153:SER:HB2	24:a:408:CLA:H43	2.02	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.41
3:c:78:GLU:O	16:v:102:PRO:HB2	2.20	0.41
24:c:513:CLA:HAA1	24:c:513:CLA:HBD	2.03	0.41
26:c:517:BCR:H20C	26:c:517:BCR:H361	1.96	0.41
26:B:641:BCR:HC7	26:B:641:BCR:H331	1.47	0.41
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.01	0.41
1:A:253:GLY:HA3	2:B:491:VAL:HB	2.02	0.41
24:A:409:CLA:H111	24:A:409:CLA:H151	1.83	0.41
2:b:12:LEU:HB2	24:b:615:CLA:HMC2	2.02	0.41
4:d:272:LEU:C	4:d:272:LEU:HD23	2.45	0.41
25:d:401:PHO:NC	25:d:401:PHO:ND	2.69	0.41
10:k:15:TYR:CE2	19:z:5:PHE:HZ	2.39	0.41
29:C:521:LMT:H31	29:C:521:LMT:H62	1.50	0.41
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.41
1:a:72:LEU:HD11	29:a:402:LMT:H52	2.03	0.41
1:a:296:ASN:HB2	3:c:400:PRO:O	2.21	0.41
7:h:38:PHE:HB2	41:h:1204:RRX:C10	2.50	0.41
1:A:132:GLU:O	1:A:136:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:406:CLA:H162	24:A:406:CLA:H203	1.79	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.03	0.41
4:D:307:GLU:HG3	44:D:605:HOH:O	2.21	0.41
24:a:408:CLA:CBD	24:a:409:CLA:HAC2	2.51	0.41
26:a:413:BCR:H20C	26:a:413:BCR:H361	1.95	0.41
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.54	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.56	0.41
26:b:622:BCR:H20C	26:b:622:BCR:H361	1.93	0.41
26:c:517:BCR:H15C	26:c:517:BCR:H351	1.90	0.41
33:A:422[B]:PL9:H301	33:A:422[B]:PL9:H322	1.87	0.40
4:D:14:TRP:CD1	36:D:413:HTG:H61	2.56	0.40
2:b:341:LYS:HZ1	36:b:625:HTG:C2	2.31	0.40
12:m:16[A]:LEU:HD12	12:m:16[A]:LEU:HA	1.84	0.40
26:B:620:BCR:H24C	26:B:620:BCR:H371	1.94	0.40
2:b:458:PHE:HB3	24:b:607:CLA:HBC2	2.03	0.40
41:h:1204:RRX:H32	41:h:1204:RRX:H28	1.89	0.40
24:A:409:CLA:HMC2	26:A:410:BCR:H12C	2.03	0.40
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.57	0.40
2:B:324:LEU:HA	4:D:293[A]:LEU:HG	2.03	0.40
24:B:616:CLA:H112	24:B:616:CLA:H91	1.76	0.40
26:B:619:BCR:H20C	26:B:619:BCR:H361	1.89	0.40
3:C:373:ASN:HB3	44:O:507:HOH:O	2.21	0.40
26:C:515:BCR:H11C	26:C:515:BCR:H341	1.87	0.40
41:H:101:RRX:H26	41:H:101:RRX:H22	1.91	0.40
14:T:6:TYR:HE2	30:T:101:GOL:H11	1.87	0.40
26:a:413:BCR:H11C	26:a:413:BCR:H341	1.93	0.40
2:b:477:ASP:N	2:b:477:ASP:OD1	2.54	0.40
24:A:406:CLA:C4A	24:A:406:CLA:HBA1	2.52	0.40
2:B:416:THR:HG23	36:B:623[A]:HTG:H7'1	2.03	0.40
13:O:234:LYS:HB2	13:O:234:LYS:HE2	1.93	0.40
26:k:302:BCR:H15C	26:k:302:BCR:H351	1.81	0.40
24:B:602:CLA:H41	44:H:256:HOH:O	2.21	0.40
3:C:344:SER:O	13:O:75:THR:HG22	2.22	0.40
4:D:123:ILE:HD11	39:H:102:DGD:HAE1	2.03	0.40
3:c:338:GLY:HA3	3:c:341:LEU:O	2.21	0.40
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.04	0.40
16:v:68:ASN:HD22	30:v:1606:GOL:C1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36	28
1	a	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36	28
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	511/505 (101%)	505 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	443 (98%)	7 (2%)	1 (0%)	43	36
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	43	36
4	D	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	77/83 (93%)	77 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	35/36 (97%)	35 (100%)	0	0	100	100
13	O	248/244 (102%)	244 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	135 (98%)	2 (2%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
17	y	26/30 (87%)	26 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	58/62 (94%)	56 (97%)	1 (2%)	1 (2%)	7	2
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5258/5387 (98%)	5169 (98%)	84 (2%)	5 (0%)	48	41

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	270 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	270/279 (97%)	270 (100%)	0	100 100
2	B	406/403 (101%)	404 (100%)	2 (0%)	81 82
2	b	405/403 (100%)	404 (100%)	1 (0%)	87 89
3	C	354/356 (99%)	352 (99%)	2 (1%)	78 79
3	c	353/356 (99%)	350 (99%)	3 (1%)	73 74
4	D	275/276 (100%)	274 (100%)	1 (0%)	84 85
4	d	277/276 (100%)	276 (100%)	1 (0%)	84 85
5	E	71/72 (99%)	69 (97%)	2 (3%)	38 30
5	e	68/72 (94%)	65 (96%)	3 (4%)	25 15
6	F	27/38 (71%)	27 (100%)	0	100 100
6	f	25/38 (66%)	25 (100%)	0	100 100
7	H	53/53 (100%)	53 (100%)	0	100 100
7	h	53/53 (100%)	53 (100%)	0	100 100
8	I	29/34 (85%)	29 (100%)	0	100 100
8	i	32/34 (94%)	30 (94%)	2 (6%)	16 6
9	J	23/28 (82%)	23 (100%)	0	100 100
9	j	25/28 (89%)	24 (96%)	1 (4%)	28 17
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 24
10	k	28/30 (93%)	28 (100%)	0	100 100
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 30
12	M	30/32 (94%)	30 (100%)	0	100 100
12	m	32/32 (100%)	30 (94%)	2 (6%)	16 6
13	O	209/207 (101%)	207 (99%)	2 (1%)	68 67
13	o	207/207 (100%)	206 (100%)	1 (0%)	81 82
14	T	25/28 (89%)	25 (100%)	0	100 100
14	t	25/28 (89%)	25 (100%)	0	100 100
15	U	84/89 (94%)	84 (100%)	0	100 100
15	u	85/89 (96%)	84 (99%)	1 (1%)	63 61
16	V	115/117 (98%)	115 (100%)	0	100 100
16	v	115/117 (98%)	115 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	18/23 (78%)	17 (94%)	1 (6%)	19 8
17	y	18/23 (78%)	18 (100%)	0	100 100
18	X	30/33 (91%)	30 (100%)	0	100 100
18	x	29/33 (88%)	29 (100%)	0	100 100
19	Z	46/51 (90%)	45 (98%)	1 (2%)	45 40
19	z	44/51 (86%)	43 (98%)	1 (2%)	44 38
20	R	19/33 (58%)	18 (95%)	1 (5%)	20 9
All	All	4276/4401 (97%)	4246 (99%)	30 (1%)	76 76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	14	ASN
2	B	86	ILE
3	C	255	THR
3	C	289	PHE
4	D	90	LEU
5	E	4	THR
5	E	60	GLN
10	K	17	ILE
13	O	23	ASP
13	O	59	LYS
17	Y	42	ARG
19	Z	4	LEU
2	b	362	PHE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	90	LEU
5	e	8	ARG
5	e	17	VAL
5	e	60	GLN
8	i	34	ARG
8	i	36	ASP
9	j	3	SER
11	l	8	GLN
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	234	LYS
15	u	9	LEU

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Mol	Chain	Res	Type
19	z	4	LEU
20	R	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	296	ASN
1	A	315	ASN
2	B	331	ASN
4	D	186	GLN
4	D	255	GLN
11	L	6	ASN
11	L	8	GLN
13	O	130	GLN
13	O	132	ASN
1	a	165	GLN
1	a	296	ASN
1	a	315	ASN
2	b	289	GLN
2	b	331	ASN
3	c	311	GLN
3	c	382	ASN
4	d	186	GLN
5	e	82	GLN
11	l	8	GLN
15	u	78	ASN
15	u	81	HIS
16	v	86	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

11 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	0.64	0	8,9,11	1.36	1 (12%)
12	FME	m	1	12	8,9,10	0.67	0	8,9,11	1.36	2 (25%)
19	FME	Z	1	19	8,9,10	0.66	0	8,9,11	1.42	2 (25%)
4	HSK	D	336[B]	-	10,11,12	2.44	3 (30%)	5,14,16	3.52	4 (80%)
4	HSK	d	336[B]	-	10,11,12	2.33	3 (30%)	5,14,16	3.60	4 (80%)
14	FME	T	1	14	8,9,10	0.60	0	8,9,11	1.65	2 (25%)
4	HSK	D	336[A]	-	10,10,12	13.46	2 (20%)	5,12,16	1.85	2 (40%)
4	HSK	d	336[A]	-	10,10,12	2.90	2 (20%)	5,12,16	1.79	3 (60%)
14	FME	t	1	14	8,9,10	0.63	0	8,9,11	1.32	1 (12%)
8	FME	I	1	8	8,9,10	0.67	0	8,9,11	1.68	3 (37%)
12	FME	M	1	12	8,9,10	0.64	0	8,9,11	1.25	0

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-42.19	0.59	1.38
4	d	336[A]	HSK	OM-ND1	-7.12	1.25	1.38
4	D	336[B]	HSK	CG-ND1	-5.92	1.32	1.40
4	d	336[B]	HSK	CG-ND1	-5.65	1.33	1.40
4	D	336[A]	HSK	CG-ND1	-4.68	1.34	1.40
4	d	336[A]	HSK	CG-ND1	-4.57	1.34	1.40
4	D	336[B]	HSK	OM-ND1	3.17	1.44	1.38
4	d	336[B]	HSK	OM-ND1	2.95	1.43	1.38
4	d	336[B]	HSK	CE1-ND1	-2.41	1.33	1.37
4	D	336[B]	HSK	CE1-ND1	-2.31	1.33	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	336[B]	HSK	ND1-CE1-NE2	-6.13	104.46	111.54
4	d	336[B]	HSK	ND1-CE1-NE2	-6.12	104.47	111.54
8	I	1	FME	CA-N-CN	-3.42	117.57	122.82
4	d	336[B]	HSK	CD2-NE2-CE1	3.17	109.39	105.24
4	D	336[B]	HSK	CD2-NE2-CE1	3.12	109.32	105.24
4	d	336[B]	HSK	CB-CG-ND1	2.98	127.91	122.89
14	T	1	FME	O-C-CA	-2.85	117.43	124.77
4	d	336[B]	HSK	CE1-ND1-CG	2.72	114.46	108.87
4	D	336[B]	HSK	CE1-ND1-CG	2.70	114.41	108.87
14	T	1	FME	CA-N-CN	-2.52	118.95	122.82
4	D	336[B]	HSK	CB-CG-ND1	2.49	127.09	122.89
4	D	336[A]	HSK	ND1-CE1-NE2	-2.49	108.67	111.54
14	t	1	FME	O-C-CA	-2.39	118.62	124.77
4	d	336[A]	HSK	ND1-CE1-NE2	-2.39	108.78	111.54
12	m	1	FME	CE-SD-CG	2.32	112.35	100.32
4	D	336[A]	HSK	CD2-NE2-CE1	2.31	108.27	105.24
8	i	1	FME	O-C-CA	-2.14	119.27	124.77
4	d	336[A]	HSK	CD2-NE2-CE1	2.13	108.03	105.24
8	I	1	FME	O-C-CA	-2.09	119.38	124.77
19	Z	1	FME	O-C-CA	-2.08	119.42	124.77
8	I	1	FME	O1-CN-N	-2.08	119.95	125.32
19	Z	1	FME	O1-CN-N	-2.04	120.04	125.32
4	d	336[A]	HSK	CB-CG-ND1	2.02	126.30	122.89
12	m	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
19	Z	1	FME	O1-CN-N-CA
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CG-SD-CE
12	M	1	FME	CA-CB-CG-SD
12	m	1	FME	CA-CB-CG-SD
8	I	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
19	Z	1	FME	CA-CB-CG-SD
12	m	1	FME	N-CA-CB-CG
19	Z	1	FME	CB-CG-SD-CE
8	I	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 337 ligands modelled in this entry, 15 are monoatomic and 57 are unknown - leaving 265 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	616	-	69,73,73	2.41	22 (31%)	82,113,113	2.49	32 (39%)
29	LMT	a	402	-	36,36,36	0.43	1 (2%)	47,47,47	0.90	1 (2%)
38	DMS	o	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	SQD	A	413	-	52,54,54	0.95	2 (3%)	62,65,65	1.29	9 (14%)
32	K3C	A	421[A]	-	15,15,15	0.95	1 (6%)	20,20,20	1.18	2 (10%)
24	CLA	B	613	-	69,73,73	2.33	22 (31%)	82,113,113	2.50	27 (32%)
36	HTG	U	201	-	8,8,19	0.39	0	7,7,24	0.79	0
26	BCR	c	516	-	41,41,41	0.80	0	56,56,56	1.43	6 (10%)
38	DMS	o	308	-	3,3,3	2.75	1 (33%)	3,3,3	0.49	0
38	DMS	o	304	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	0.86	0
24	CLA	C	503	-	69,73,73	2.54	25 (36%)	82,113,113	2.34	28 (34%)
29	LMT	Z	101	-	36,36,36	0.45	0	47,47,47	0.84	1 (2%)
26	BCR	d	406	-	41,41,41	0.82	1 (2%)	56,56,56	1.85	14 (25%)
38	DMS	i	104	-	3,3,3	2.71	1 (33%)	3,3,3	0.61	0
24	CLA	C	512	3	69,73,73	2.53	23 (33%)	82,113,113	2.32	27 (32%)
25	PHO	d	401	-	58,69,69	2.77	14 (24%)	55,99,99	2.91	18 (32%)
38	DMS	v	1608	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
26	BCR	C	515	-	41,41,41	0.71	0	56,56,56	1.48	7 (12%)
21	OEX	a	403	44,1,3	0,15,15	-	-	-		
39	DGD	c	520	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	5 (6%)
36	HTG	O	302	-	19,19,19	1.01	1 (5%)	23,24,24	0.89	1 (4%)
30	GOL	L	103	-	5,5,5	1.06	0	5,5,5	0.96	0
39	DGD	D	407	-	53,53,67	1.01	3 (5%)	61,61,81	1.41	6 (9%)
26	BCR	a	413	-	41,41,41	0.79	0	56,56,56	1.23	4 (7%)
24	CLA	C	510	-	69,73,73	2.38	23 (33%)	82,113,113	2.35	28 (34%)
24	CLA	c	511	-	69,73,73	2.52	23 (33%)	82,113,113	2.37	30 (36%)
28	LMG	C	532	-	51,51,55	0.99	2 (3%)	59,59,63	1.30	4 (6%)
24	CLA	B	617	-	69,73,73	2.26	21 (30%)	82,113,113	2.44	26 (31%)
30	GOL	k	304	-	5,5,5	0.91	0	5,5,5	0.98	0
29	LMT	C	521	-	36,36,36	0.46	0	47,47,47	1.20	4 (8%)
26	BCR	Y	302	-	41,41,41	0.80	0	56,56,56	1.62	10 (17%)
30	GOL	b	629	-	5,5,5	1.01	0	5,5,5	1.05	0
28	LMG	c	521	-	51,51,55	0.94	2 (3%)	59,59,63	1.00	4 (6%)
38	DMS	c	537	-	3,3,3	2.79	1 (33%)	3,3,3	0.58	0
27	SQD	L	101	-	52,54,54	0.98	3 (5%)	62,65,65	1.33	7 (11%)
30	GOL	O	303	-	5,5,5	0.86	0	5,5,5	1.12	0
26	BCR	B	619	-	41,41,41	0.85	0	56,56,56	1.19	4 (7%)
30	GOL	b	630	-	5,5,5	1.27	1 (20%)	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
36	HTG	h	1202	-	19,19,19	0.98	2 (10%)	23,24,24	1.59	1 (4%)
30	GOL	A	415	-	5,5,5	0.86	0	5,5,5	1.14	1 (20%)
24	CLA	A	405	-	69,73,73	2.42	22 (31%)	82,113,113	2.23	26 (31%)
36	HTG	C	522	-	19,19,19	0.88	2 (10%)	23,24,24	1.04	1 (4%)
24	CLA	D	403	-	69,73,73	2.16	23 (33%)	82,113,113	2.60	33 (40%)
24	CLA	b	611	-	69,73,73	2.56	25 (36%)	82,113,113	2.28	27 (32%)
24	CLA	b	605	-	69,73,73	2.43	24 (34%)	82,113,113	2.33	28 (34%)
30	GOL	v	1605	-	5,5,5	1.15	0	5,5,5	0.88	0
38	DMS	E	106	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
39	DGD	H	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.93	5 (6%)
26	BCR	A	410	-	41,41,41	0.79	0	56,56,56	1.30	8 (14%)
30	GOL	V	206	-	5,5,5	1.02	0	5,5,5	1.03	0
38	DMS	o	309	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
24	CLA	C	507	-	69,73,73	2.47	22 (31%)	82,113,113	2.46	33 (40%)
24	CLA	b	607	-	69,73,73	2.57	24 (34%)	82,113,113	2.42	29 (35%)
24	CLA	B	608	44	69,73,73	2.24	23 (33%)	82,113,113	2.44	26 (31%)
30	GOL	d	402	-	5,5,5	0.95	0	5,5,5	1.03	0
36	HTG	b	602	-	19,19,19	1.00	2 (10%)	23,24,24	1.12	1 (4%)
24	CLA	c	505	-	69,73,73	2.60	23 (33%)	82,113,113	2.21	26 (31%)
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.91	0
26	BCR	b	622	-	41,41,41	0.72	0	56,56,56	1.38	11 (19%)
28	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.25	5 (8%)
36	HTG	B	625	-	19,19,19	0.94	1 (5%)	23,24,24	1.23	1 (4%)
24	CLA	d	404	-	69,73,73	2.27	21 (30%)	82,113,113	2.49	30 (36%)
24	CLA	c	503	-	69,73,73	2.47	23 (33%)	82,113,113	2.56	28 (34%)
24	CLA	B	606	-	69,73,73	2.34	24 (34%)	82,113,113	2.29	26 (31%)
38	DMS	o	306	-	3,3,3	2.75	1 (33%)	3,3,3	0.52	0
39	DGD	h	1205	-	63,63,67	0.93	3 (4%)	77,77,81	0.99	4 (5%)
30	GOL	h	1206	-	5,5,5	0.99	0	5,5,5	0.97	0
28	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.06	4 (6%)
24	CLA	b	615	-	69,73,73	2.32	22 (31%)	82,113,113	2.46	27 (32%)
34	BCT	A	423	22	3,3,3	0.50	0	2,3,3	0.78	0
27	SQD	L	102	-	52,54,54	0.99	2 (3%)	62,65,65	1.60	10 (16%)
25	PHO	D	401	-	58,69,69	2.73	12 (20%)	55,99,99	3.01	14 (25%)
24	CLA	c	514	-	69,73,73	2.55	24 (34%)	82,113,113	2.53	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	DMS	c	535	-	3,3,3	2.77	1 (33%)	3,3,3	0.66	0
37	LHG	e	101	-	39,39,48	1.04	2 (5%)	42,45,54	1.08	3 (7%)
24	CLA	a	410	44	69,73,73	2.37	23 (33%)	82,113,113	2.42	31 (37%)
37	LHG	d	410	-	38,38,48	1.07	2 (5%)	41,44,54	1.09	4 (9%)
36	HTG	d	414	-	19,19,19	0.94	1 (5%)	23,24,24	1.64	3 (13%)
30	GOL	B	633	-	5,5,5	0.90	0	5,5,5	1.06	0
24	CLA	b	617	-	69,73,73	2.32	24 (34%)	82,113,113	2.52	28 (34%)
26	BCR	B	618	-	41,41,41	0.77	0	56,56,56	1.32	5 (8%)
26	BCR	b	620	-	41,41,41	0.83	0	56,56,56	1.40	7 (12%)
29	LMT	z	101	-	32,32,36	0.56	1 (3%)	42,42,47	1.48	4 (9%)
37	LHG	D	411	-	45,45,48	0.91	2 (4%)	48,51,54	1.01	3 (6%)
38	DMS	b	636	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
24	CLA	B	602	44	69,73,73	2.49	26 (37%)	82,113,113	2.32	26 (31%)
24	CLA	b	606	-	69,73,73	2.43	24 (34%)	82,113,113	2.44	27 (32%)
39	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.03	5 (6%)
30	GOL	c	526	-	5,5,5	1.11	0	5,5,5	0.90	0
21	OEX	A	401	44,1,3	0,15,15	-	-	-		
24	CLA	B	603	-	69,73,73	2.51	24 (34%)	82,113,113	2.41	31 (37%)
30	GOL	T	103	-	5,5,5	0.85	0	5,5,5	1.15	0
30	GOL	a	421	-	5,5,5	1.02	0	5,5,5	1.02	0
24	CLA	c	508	-	69,73,73	2.59	24 (34%)	82,113,113	2.35	31 (37%)
38	DMS	B	645	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
30	GOL	M	102	-	5,5,5	0.61	0	5,5,5	1.26	1 (20%)
30	GOL	b	627	-	5,5,5	0.99	0	5,5,5	0.91	0
30	GOL	a	418	-	5,5,5	0.95	0	5,5,5	1.01	0
27	SQD	a	401	-	52,54,54	0.97	2 (3%)	62,65,65	1.23	6 (9%)
24	CLA	A	409	-	69,73,73	2.25	23 (33%)	82,113,113	2.50	30 (36%)
24	CLA	b	610	44	69,73,73	2.42	23 (33%)	82,113,113	2.31	29 (35%)
39	DGD	c	518	-	63,63,67	0.80	2 (3%)	77,77,81	1.11	6 (7%)
26	BCR	B	620	-	41,41,41	0.72	0	56,56,56	1.26	5 (8%)
24	CLA	A	407	44	69,73,73	2.30	22 (31%)	82,113,113	2.47	27 (32%)
38	DMS	B	646	-	3,3,3	2.76	1 (33%)	3,3,3	0.61	0
38	DMS	d	415	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
39	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	8 (10%)
24	CLA	B	612	-	69,73,73	2.38	24 (34%)	82,113,113	2.45	32 (39%)
27	SQD	a	414	-	52,54,54	0.87	2 (3%)	62,65,65	1.68	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	0.87	0
24	CLA	c	506	44	69,73,73	2.25	24 (34%)	82,113,113	2.50	30 (36%)
38	DMS	C	533	-	3,3,3	2.75	1 (33%)	3,3,3	0.53	0
30	GOL	C	524	-	5,5,5	0.90	0	5,5,5	1.22	1 (20%)
38	DMS	z	102	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
29	LMT	T	104	-	24,24,36	0.46	0	29,29,47	1.04	3 (10%)
36	HTG	b	626	-	19,19,19	0.97	1 (5%)	23,24,24	1.45	1 (4%)
36	HTG	u	201	-	10,13,19	1.03	1 (10%)	13,14,24	1.48	1 (7%)
37	LHG	d	408	-	48,48,48	0.85	2 (4%)	51,54,54	1.09	4 (7%)
24	CLA	b	604	44	69,73,73	2.45	24 (34%)	82,113,113	2.25	27 (32%)
30	GOL	E	105	-	5,5,5	0.92	0	5,5,5	1.08	0
30	GOL	u	202	-	5,5,5	1.01	0	5,5,5	1.02	0
30	GOL	V	205	-	5,5,5	0.89	0	5,5,5	1.06	0
26	BCR	b	621	-	41,41,41	0.79	0	56,56,56	1.18	5 (8%)
24	CLA	b	609	-	69,73,73	2.52	23 (33%)	82,113,113	2.30	28 (34%)
28	LMG	A	412	-	51,51,55	0.93	2 (3%)	59,59,63	1.16	6 (10%)
24	CLA	b	618	-	69,73,73	2.35	24 (34%)	82,113,113	2.27	28 (34%)
30	GOL	v	1606	-	5,5,5	0.78	0	5,5,5	1.16	1 (20%)
36	HTG	C	523	-	19,19,19	0.90	1 (5%)	23,24,24	1.58	4 (17%)
26	BCR	k	303	-	41,41,41	0.74	0	56,56,56	1.39	7 (12%)
30	GOL	o	302	-	5,5,5	1.10	0	5,5,5	0.84	0
27	SQD	A	411	-	52,54,54	0.90	2 (3%)	62,65,65	1.70	12 (19%)
24	CLA	c	512	-	69,73,73	2.55	25 (36%)	82,113,113	2.38	28 (34%)
43	HEC	v	1603	16	46,50,50	2.03	9 (19%)	58,82,82	1.33	6 (10%)
36	HTG	B	626	-	19,19,19	0.93	1 (5%)	23,24,24	1.71	5 (21%)
25	PHO	A	408	-	58,69,69	2.64	12 (20%)	55,99,99	2.91	15 (27%)
24	CLA	c	509	44	69,73,73	2.43	21 (30%)	82,113,113	2.48	31 (37%)
29	LMT	B	642	-	24,24,36	0.57	1 (4%)	29,29,47	0.72	0
30	GOL	v	1602	35	5,5,5	0.92	0	5,5,5	1.01	0
30	GOL	B	627	-	5,5,5	1.03	0	5,5,5	0.94	0
36	HTG	o	301	-	19,19,19	1.06	1 (5%)	23,24,24	1.09	1 (4%)
37	LHG	E	101	-	48,48,48	0.97	2 (4%)	51,54,54	1.14	3 (5%)
38	DMS	O	304	-	3,3,3	2.80	1 (33%)	3,3,3	0.58	0
24	CLA	B	611	44	69,73,73	2.52	25 (36%)	82,113,113	2.32	26 (31%)
30	GOL	C	527	-	5,5,5	0.87	0	5,5,5	1.14	0
24	CLA	C	502	-	69,73,73	2.32	24 (34%)	82,113,113	2.31	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	BCT	a	407	22	3,3,3	0.51	0	2,3,3	0.67	0
24	CLA	C	504	-	69,73,73	2.43	23 (33%)	82,113,113	2.27	27 (32%)
30	GOL	d	413	-	5,5,5	0.90	0	5,5,5	1.06	0
32	K3C	a	424[A]	-	15,15,15	0.95	1 (6%)	20,20,20	1.17	2 (10%)
24	CLA	C	506	-	69,73,73	2.49	23 (33%)	82,113,113	2.26	24 (29%)
24	CLA	c	510	-	69,73,73	2.55	25 (36%)	82,113,113	2.44	27 (32%)
30	GOL	C	528	-	5,5,5	0.76	0	5,5,5	1.21	1 (20%)
38	DMS	B	644	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
38	DMS	c	536	-	3,3,3	2.72	1 (33%)	3,3,3	0.47	0
29	LMT	E	104	-	24,24,36	0.49	0	29,29,47	0.71	0
38	DMS	B	643	-	3,3,3	2.73	1 (33%)	3,3,3	0.48	0
29	LMT	B	622	-	36,36,36	0.40	0	47,47,47	1.18	4 (8%)
36	HTG	D	413	-	19,19,19	1.01	2 (10%)	23,24,24	0.99	2 (8%)
30	GOL	c	532	-	5,5,5	0.85	0	5,5,5	1.12	0
37	LHG	D	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.19	5 (9%)
38	DMS	D	416	-	3,3,3	2.77	1 (33%)	3,3,3	0.66	0
30	GOL	B	630	-	5,5,5	0.60	0	5,5,5	1.13	0
36	HTG	B	623[B]	-	19,19,19	0.85	1 (5%)	23,24,24	1.33	2 (8%)
24	CLA	B	610	-	69,73,73	2.52	21 (30%)	82,113,113	2.31	31 (37%)
38	DMS	C	525	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
24	CLA	B	614	-	69,73,73	2.40	22 (31%)	82,113,113	2.37	32 (39%)
24	CLA	B	607	-	69,73,73	2.37	22 (31%)	82,113,113	2.44	30 (36%)
30	GOL	B	631	-	5,5,5	1.12	0	5,5,5	1.04	0
38	DMS	Y	303	-	3,3,3	2.79	1 (33%)	3,3,3	0.66	0
30	GOL	B	628	-	5,5,5	1.07	0	5,5,5	0.96	0
37	LHG	B	640	-	48,48,48	0.94	3 (6%)	51,54,54	1.02	3 (5%)
27	SQD	D	408	-	43,45,54	1.05	2 (4%)	53,56,65	1.69	11 (20%)
24	CLA	b	614	-	69,73,73	2.54	25 (36%)	82,113,113	2.31	29 (35%)
30	GOL	B	629	-	5,5,5	1.08	0	5,5,5	0.81	0
24	CLA	D	404	-	69,73,73	2.46	23 (33%)	82,113,113	2.36	29 (35%)
30	GOL	V	204	-	5,5,5	1.19	0	5,5,5	0.96	0
38	DMS	V	207	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
24	CLA	B	609	-	69,73,73	2.52	21 (30%)	82,113,113	2.34	29 (35%)
36	HTG	B	624	-	19,19,19	0.99	2 (10%)	23,24,24	1.56	2 (8%)
30	GOL	V	201	35	5,5,5	0.80	0	5,5,5	1.10	0
24	CLA	C	511	-	69,73,73	2.43	23 (33%)	82,113,113	2.40	30 (36%)
37	LHG	d	409	-	48,48,48	0.86	2 (4%)	51,54,54	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LHG	D	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.92	3 (5%)
26	BCR	K	101	-	41,41,41	0.78	0	56,56,56	1.51	10 (17%)
24	CLA	c	504	-	69,73,73	2.32	24 (34%)	82,113,113	2.42	26 (31%)
26	BCR	B	641	-	41,41,41	0.70	0	56,56,56	1.63	13 (23%)
27	SQD	f	102	-	31,32,54	1.99	4 (12%)	33,36,65	1.40	3 (9%)
37	LHG	l	302	-	48,48,48	0.88	2 (4%)	51,54,54	0.86	1 (1%)
26	BCR	c	517	-	41,41,41	0.78	0	56,56,56	1.41	7 (12%)
24	CLA	B	605	-	69,73,73	2.54	19 (27%)	82,113,113	2.46	27 (32%)
24	CLA	b	608	-	69,73,73	2.23	23 (33%)	82,113,113	2.46	29 (35%)
39	DGD	C	519	-	63,63,67	0.88	2 (3%)	77,77,81	1.08	5 (6%)
33	PL9	D	406	-	55,55,55	0.73	2 (3%)	68,69,69	1.52	12 (17%)
28	LMG	b	623	-	51,51,55	0.90	2 (3%)	59,59,63	1.07	3 (5%)
41	RRX	H	101	-	42,42,42	0.75	0	56,58,58	1.30	6 (10%)
41	RRX	h	1204	-	42,42,42	0.75	0	56,58,58	1.34	6 (10%)
24	CLA	A	406	44	69,73,73	2.24	24 (34%)	82,113,113	2.55	30 (36%)
33	PL9	a	425[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.86	21 (30%)
38	DMS	a	426	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
40	HEM	F	101	6,5	50,50,50	1.91	9 (18%)	67,82,82	1.45	8 (11%)
40	HEM	f	101	6,5	50,50,50	1.88	8 (16%)	67,82,82	1.38	5 (7%)
36	HTG	c	524	-	19,19,19	0.91	2 (10%)	23,24,24	1.25	1 (4%)
30	GOL	v	1601	-	5,5,5	0.98	0	5,5,5	0.99	0
36	HTG	B	623[A]	-	19,19,19	0.93	1 (5%)	23,24,24	1.23	2 (8%)
24	CLA	c	515	-	69,73,73	2.36	24 (34%)	82,113,113	2.28	27 (32%)
29	LMT	A	414	-	36,36,36	0.40	0	47,47,47	0.98	2 (4%)
30	GOL	T	101	-	5,5,5	1.01	0	5,5,5	0.86	0
38	DMS	b	637	-	3,3,3	2.75	1 (33%)	3,3,3	0.67	0
29	LMT	f	104	-	36,36,36	0.44	0	47,47,47	0.78	0
38	DMS	B	647	-	3,3,3	2.70	1 (33%)	3,3,3	0.43	0
36	HTG	V	203	-	12,13,19	0.48	0	17,18,24	2.19	5 (29%)
30	GOL	C	529	-	5,5,5	1.02	0	5,5,5	0.86	0
24	CLA	C	509	-	69,73,73	2.52	24 (34%)	82,113,113	2.29	26 (31%)
24	CLA	C	505	44	69,73,73	2.32	22 (31%)	82,113,113	2.37	28 (34%)
38	DMS	b	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
26	BCR	C	516	-	41,41,41	0.79	0	56,56,56	1.35	6 (10%)
24	CLA	C	513	-	69,73,73	2.61	23 (33%)	82,113,113	2.43	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	616	-	69,73,73	2.53	25 (36%)	82,113,113	2.46	28 (34%)
30	GOL	v	1604	-	5,5,5	0.97	0	5,5,5	1.05	0
24	CLA	B	604	-	69,73,73	2.37	23 (33%)	82,113,113	2.57	27 (32%)
26	BCR	k	302	-	41,41,41	0.79	1 (2%)	56,56,56	1.58	14 (25%)
38	DMS	c	533	-	3,3,3	2.76	1 (33%)	3,3,3	0.62	0
36	HTG	I	102	-	19,19,19	1.02	2 (10%)	23,24,24	1.75	4 (17%)
36	HTG	b	625	-	19,19,19	0.74	1 (5%)	23,24,24	1.11	1 (4%)
30	GOL	b	628	-	5,5,5	0.88	0	5,5,5	1.01	0
26	BCR	D	405	-	41,41,41	0.87	1 (2%)	56,56,56	1.79	11 (19%)
24	CLA	C	514	-	69,73,73	2.47	24 (34%)	82,113,113	2.38	26 (31%)
38	DMS	c	534	-	3,3,3	2.73	1 (33%)	3,3,3	0.45	0
24	CLA	B	615	-	69,73,73	2.28	20 (28%)	82,113,113	2.54	31 (37%)
24	CLA	d	405	-	69,73,73	2.41	23 (33%)	82,113,113	2.38	31 (37%)
24	CLA	b	612	-	69,73,73	2.46	22 (31%)	82,113,113	2.29	27 (32%)
26	BCR	T	102	-	41,41,41	0.74	0	56,56,56	1.57	15 (26%)
29	LMT	J	102	-	24,24,36	0.51	0	29,29,47	1.18	3 (10%)
30	GOL	a	417	-	5,5,5	1.09	0	5,5,5	0.99	0
29	LMT	m	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.86	0
29	LMT	b	624	-	25,25,36	0.45	0	30,30,47	0.77	0
29	LMT	c	523	-	36,36,36	0.49	1 (2%)	47,47,47	1.07	4 (8%)
33	PL9	d	407	-	55,55,55	0.70	1 (1%)	68,69,69	1.47	11 (16%)
25	PHO	a	411	-	58,69,69	2.63	12 (20%)	55,99,99	2.86	14 (25%)
39	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.98	5 (6%)
24	CLA	c	507	-	69,73,73	2.58	23 (33%)	82,113,113	2.35	26 (31%)
24	CLA	C	508	44	69,73,73	2.66	22 (31%)	82,113,113	2.37	29 (35%)
43	HEC	V	202	16	46,50,50	1.99	9 (19%)	58,82,82	1.44	6 (10%)
24	CLA	a	408	-	69,73,73	2.37	24 (34%)	82,113,113	2.42	28 (34%)
28	LMG	d	411	42	51,51,55	0.92	3 (5%)	59,59,63	0.91	2 (3%)
28	LMG	a	415	-	51,51,55	0.94	2 (3%)	59,59,63	1.28	8 (13%)
30	GOL	a	416	-	5,5,5	1.06	0	5,5,5	1.20	1 (20%)
36	HTG	b	601	-	19,19,19	1.00	2 (10%)	23,24,24	1.38	3 (13%)
24	CLA	b	619	-	69,73,73	2.40	22 (31%)	82,113,113	2.43	27 (32%)
30	GOL	c	527	-	5,5,5	1.06	0	5,5,5	0.95	0
33	PL9	A	422[B]	-	55,55,55	0.68	2 (3%)	68,69,69	1.70	14 (20%)
30	GOL	C	530	-	5,5,5	1.24	0	5,5,5	1.21	1 (20%)
24	CLA	a	412	-	69,73,73	2.21	21 (30%)	82,113,113	2.47	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	GOL	o	305	-	5,5,5	1.14	0	5,5,5	0.86	0
38	DMS	d	416	-	3,3,3	2.78	1 (33%)	3,3,3	0.63	0
24	CLA	b	613	44	69,73,73	2.49	25 (36%)	82,113,113	2.29	26 (31%)
24	CLA	c	513	3	69,73,73	2.48	20 (28%)	82,113,113	2.36	32 (39%)
36	HTG	c	525	-	19,19,19	0.94	2 (10%)	23,24,24	1.35	3 (13%)
28	LMG	D	412	42	51,51,55	0.84	2 (3%)	59,59,63	0.89	3 (5%)
30	GOL	v	1607	-	5,5,5	0.86	0	5,5,5	1.02	0
24	CLA	a	409	44	69,73,73	2.41	22 (31%)	82,113,113	2.59	29 (35%)
30	GOL	A	416	-	5,5,5	1.05	0	5,5,5	0.97	0
30	GOL	c	528	-	5,5,5	1.00	0	5,5,5	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	616	-	1/1/15/20	6/39/115/115	-
29	LMT	a	402	-	-	8/21/61/61	0/2/2/2
27	SQD	A	413	-	-	10/49/69/69	0/1/1/1
32	K3C	A	421[A]	-	-	4/4/17/17	0/2/2/2
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
36	HTG	U	201	-	-	3/6/6/30	-
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
29	LMT	m	102	-	-	1/21/61/61	0/2/2/2
24	CLA	C	503	-	-	5/39/115/115	-
29	LMT	Z	101	-	-	12/21/61/61	0/2/2/2
26	BCR	d	406	-	-	6/29/63/63	0/2/2/2
24	CLA	C	512	3	1/1/15/20	3/39/115/115	-
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6
26	BCR	C	515	-	-	3/29/63/63	0/2/2/2
39	DGD	c	520	-	-	13/51/91/95	0/2/2/2
36	HTG	O	302	-	-	2/10/30/30	0/1/1/1
30	GOL	L	103	-	-	0/4/4/4	-
39	DGD	D	407	-	-	19/47/68/95	0/1/1/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
24	CLA	C	510	-	1/1/15/20	5/39/115/115	-
24	CLA	c	511	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	C	532	-	-	10/46/66/70	0/1/1/1
24	CLA	B	617	-	1/1/15/20	10/39/115/115	-
30	GOL	k	304	-	-	4/4/4/4	-
29	LMT	C	521	-	-	12/21/61/61	0/2/2/2
26	BCR	Y	302	-	-	5/29/63/63	0/2/2/2
30	GOL	b	629	-	-	1/4/4/4	-
28	LMG	c	521	-	-	16/46/66/70	0/1/1/1
27	SQD	L	101	-	-	24/49/69/69	0/1/1/1
30	GOL	O	303	-	-	0/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	GOL	b	630	-	-	2/4/4/4	-
28	LMG	C	520	-	-	18/46/66/70	0/1/1/1
36	HTG	h	1202	-	-	4/10/30/30	0/1/1/1
30	GOL	A	415	-	-	0/4/4/4	-
24	CLA	A	405	-	1/1/15/20	2/39/115/115	-
36	HTG	C	522	-	-	1/10/30/30	0/1/1/1
24	CLA	D	403	-	1/1/15/20	2/39/115/115	-
24	CLA	b	611	-	-	3/39/115/115	-
24	CLA	b	605	-	1/1/15/20	2/39/115/115	-
30	GOL	v	1605	-	-	2/4/4/4	-
39	DGD	H	102	-	-	8/51/91/95	0/2/2/2
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
30	GOL	V	206	-	-	0/4/4/4	-
24	CLA	C	507	-	1/1/15/20	14/39/115/115	-
24	CLA	b	607	-	1/1/15/20	3/39/115/115	-
24	CLA	B	608	44	1/1/15/20	4/39/115/115	-
30	GOL	d	402	-	-	0/4/4/4	-
36	HTG	b	602	-	-	1/10/30/30	0/1/1/1
24	CLA	c	505	-	1/1/15/20	3/39/115/115	-
29	LMT	M	101	-	-	1/21/61/61	0/2/2/2
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
28	LMG	c	522	-	-	6/46/66/70	0/1/1/1
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	d	404	-	1/1/15/20	3/39/115/115	-
24	CLA	c	503	-	1/1/15/20	3/39/115/115	-
24	CLA	B	606	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGD	h	1205	-	-	8/51/91/95	0/2/2/2
30	GOL	h	1206	-	-	0/4/4/4	-
28	LMG	B	621	-	-	9/46/66/70	0/1/1/1
24	CLA	b	615	-	1/1/15/20	0/39/115/115	-
27	SQD	L	102	-	-	24/49/69/69	0/1/1/1
25	PHO	D	401	-	-	1/37/103/103	0/5/6/6
24	CLA	c	514	-	1/1/15/20	5/39/115/115	-
37	LHG	e	101	-	-	22/44/44/53	-
24	CLA	a	410	44	-	7/39/115/115	-
37	LHG	d	410	-	-	8/43/43/53	-
36	HTG	d	414	-	-	1/10/30/30	0/1/1/1
30	GOL	B	633	-	-	0/4/4/4	-
24	CLA	b	617	-	1/1/15/20	8/39/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	b	620	-	-	2/29/63/63	0/2/2/2
29	LMT	z	101	-	-	5/15/55/61	0/2/2/2
37	LHG	D	411	-	-	11/50/50/53	-
39	DGD	C	518	-	-	19/51/91/95	0/2/2/2
24	CLA	B	602	44	1/1/15/20	14/39/115/115	-
24	CLA	b	606	-	1/1/15/20	4/39/115/115	-
30	GOL	c	526	-	-	3/4/4/4	-
24	CLA	B	603	-	1/1/15/20	2/39/115/115	-
30	GOL	T	103	-	-	0/4/4/4	-
30	GOL	a	421	-	-	4/4/4/4	-
24	CLA	c	508	-	1/1/15/20	6/39/115/115	-
30	GOL	M	102	-	-	0/4/4/4	-
30	GOL	b	627	-	-	0/4/4/4	-
30	GOL	a	418	-	-	2/4/4/4	-
27	SQD	a	401	-	-	12/49/69/69	0/1/1/1
24	CLA	A	409	-	-	7/39/115/115	-
24	CLA	b	610	44	1/1/15/20	2/39/115/115	-
39	DGD	c	518	-	-	16/51/91/95	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	A	407	44	-	4/39/115/115	-
39	DGD	C	517	-	-	12/51/91/95	0/2/2/2
24	CLA	B	612	-	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	a	414	-	-	12/49/69/69	0/1/1/1
29	LMT	m	103	-	-	2/21/61/61	0/2/2/2
24	CLA	c	506	44	1/1/15/20	5/39/115/115	-
30	GOL	C	524	-	-	0/4/4/4	-
29	LMT	T	104	-	-	8/15/35/61	0/1/1/2
36	HTG	b	626	-	-	3/10/30/30	0/1/1/1
36	HTG	u	201	-	-	2/12/14/30	-
37	LHG	d	408	-	-	6/53/53/53	-
24	CLA	b	604	44	1/1/15/20	15/39/115/115	-
30	GOL	E	105	-	-	1/4/4/4	-
30	GOL	u	202	-	-	2/4/4/4	-
30	GOL	V	205	-	-	0/4/4/4	-
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	CLA	b	609	-	1/1/15/20	8/39/115/115	-
28	LMG	A	412	-	-	21/46/66/70	0/1/1/1
24	CLA	b	618	-	1/1/15/20	11/39/115/115	-
30	GOL	v	1606	-	-	2/4/4/4	-
36	HTG	C	523	-	-	4/10/30/30	0/1/1/1
26	BCR	k	303	-	-	0/29/63/63	0/2/2/2
30	GOL	o	302	-	-	4/4/4/4	-
27	SQD	A	411	-	-	9/49/69/69	0/1/1/1
24	CLA	c	512	-	1/1/15/20	3/39/115/115	-
43	HEC	v	1603	16	-	6/14/54/54	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
24	CLA	c	509	44	1/1/15/20	6/39/115/115	-
29	LMT	B	642	-	-	7/15/35/61	0/1/1/2
30	GOL	v	1602	35	-	2/4/4/4	-
30	GOL	B	627	-	-	2/4/4/4	-
36	HTG	o	301	-	-	0/10/30/30	0/1/1/1
37	LHG	E	101	-	-	25/53/53/53	-
24	CLA	B	611	44	1/1/15/20	7/39/115/115	-
30	GOL	C	527	-	-	1/4/4/4	-
24	CLA	C	502	-	1/1/15/20	4/39/115/115	-
24	CLA	C	504	-	-	5/39/115/115	-
30	GOL	d	413	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	K3C	a	424[A]	-	-	4/4/17/17	0/2/2/2
24	CLA	C	506	-	1/1/15/20	0/39/115/115	-
24	CLA	c	510	-	1/1/15/20	2/39/115/115	-
30	GOL	C	528	-	-	0/4/4/4	-
29	LMT	E	104	-	-	6/15/35/61	0/1/1/2
29	LMT	B	622	-	-	8/21/61/61	0/2/2/2
36	HTG	D	413	-	-	1/10/30/30	0/1/1/1
30	GOL	c	532	-	-	0/4/4/4	-
37	LHG	D	409	-	-	10/53/53/53	-
30	GOL	B	630	-	-	0/4/4/4	-
36	HTG	B	623[B]	-	-	1/10/30/30	0/1/1/1
24	CLA	B	610	-	1/1/15/20	0/39/115/115	-
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
24	CLA	B	607	-	1/1/15/20	3/39/115/115	-
30	GOL	B	631	-	-	1/4/4/4	-
30	GOL	B	628	-	-	0/4/4/4	-
37	LHG	B	640	-	-	12/53/53/53	-
27	SQD	D	408	-	-	15/40/60/69	0/1/1/1
24	CLA	b	614	-	1/1/15/20	4/39/115/115	-
30	GOL	B	629	-	-	2/4/4/4	-
24	CLA	D	404	-	1/1/15/20	5/39/115/115	-
30	GOL	V	204	-	-	2/4/4/4	-
24	CLA	B	609	-	-	2/39/115/115	-
36	HTG	B	624	-	-	3/10/30/30	0/1/1/1
30	GOL	V	201	35	-	0/4/4/4	-
24	CLA	C	511	-	1/1/15/20	3/39/115/115	-
37	LHG	d	409	-	-	10/53/53/53	-
37	LHG	D	410	-	-	8/53/53/53	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	CLA	c	504	-	1/1/15/20	8/39/115/115	-
26	BCR	B	641	-	-	1/29/63/63	0/2/2/2
27	SQD	f	102	-	-	10/33/33/69	-
37	LHG	l	302	-	-	13/53/53/53	-
26	BCR	c	517	-	-	0/29/63/63	0/2/2/2
24	CLA	B	605	-	1/1/15/20	3/39/115/115	-
24	CLA	b	608	-	1/1/15/20	4/39/115/115	-
39	DGD	C	519	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PL9	D	406	-	-	2/53/73/73	0/1/1/1
28	LMG	b	623	-	-	18/46/66/70	0/1/1/1
41	RRX	H	101	-	-	2/29/65/65	0/2/2/2
41	RRX	h	1204	-	-	1/29/65/65	0/2/2/2
24	CLA	A	406	44	-	1/39/115/115	-
33	PL9	a	425[B]	-	-	10/53/73/73	0/1/1/1
40	HEM	f	101	6,5	-	3/14/54/54	-
40	HEM	F	101	6,5	-	2/14/54/54	-
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
30	GOL	v	1601	-	-	0/4/4/4	-
36	HTG	B	623[A]	-	-	1/10/30/30	0/1/1/1
24	CLA	c	515	-	-	8/39/115/115	-
29	LMT	A	414	-	-	5/21/61/61	0/2/2/2
30	GOL	T	101	-	-	3/4/4/4	-
29	LMT	f	104	-	-	7/21/61/61	0/2/2/2
36	HTG	V	203	-	-	1/4/24/30	0/1/1/1
30	GOL	C	529	-	-	0/4/4/4	-
24	CLA	C	509	-	1/1/15/20	3/39/115/115	-
24	CLA	C	505	44	1/1/15/20	5/39/115/115	-
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
24	CLA	C	513	-	1/1/15/20	5/39/115/115	-
24	CLA	b	616	-	1/1/15/20	0/39/115/115	-
30	GOL	v	1604	-	-	0/4/4/4	-
24	CLA	B	604	-	1/1/15/20	2/39/115/115	-
26	BCR	k	302	-	-	4/29/63/63	0/2/2/2
36	HTG	I	102	-	-	5/10/30/30	0/1/1/1
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
30	GOL	b	628	-	-	0/4/4/4	-
26	BCR	D	405	-	-	6/29/63/63	0/2/2/2
24	CLA	C	514	-	-	4/39/115/115	-
24	CLA	B	615	-	1/1/15/20	8/39/115/115	-
24	CLA	d	405	-	-	5/39/115/115	-
24	CLA	b	612	-	1/1/15/20	2/39/115/115	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
29	LMT	J	102	-	-	2/15/35/61	0/1/1/2
30	GOL	a	417	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	m	101	-	-	4/21/61/61	0/2/2/2
29	LMT	b	624	-	-	4/17/37/61	0/1/1/2
29	LMT	c	523	-	-	6/21/61/61	0/2/2/2
33	PL9	d	407	-	-	5/53/73/73	0/1/1/1
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6
39	DGD	c	519	-	-	16/51/91/95	0/2/2/2
24	CLA	c	507	-	1/1/15/20	7/39/115/115	-
24	CLA	C	508	44	1/1/15/20	11/39/115/115	-
43	HEC	V	202	16	-	6/14/54/54	-
24	CLA	a	408	-	1/1/15/20	4/39/115/115	-
28	LMG	d	411	42	-	10/46/66/70	0/1/1/1
28	LMG	a	415	-	-	14/46/66/70	0/1/1/1
30	GOL	a	416	-	-	2/4/4/4	-
36	HTG	b	601	-	-	1/10/30/30	0/1/1/1
24	CLA	b	619	-	1/1/15/20	8/39/115/115	-
30	GOL	c	527	-	-	0/4/4/4	-
33	PL9	A	422[B]	-	-	13/53/73/73	0/1/1/1
30	GOL	C	530	-	-	0/4/4/4	-
24	CLA	a	412	-	1/1/15/20	9/39/115/115	-
30	GOL	o	305	-	-	2/4/4/4	-
24	CLA	b	613	44	1/1/15/20	6/39/115/115	-
24	CLA	c	513	3	1/1/15/20	0/39/115/115	-
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1
28	LMG	D	412	42	-	10/46/66/70	0/1/1/1
30	GOL	v	1607	-	-	4/4/4/4	-
24	CLA	a	409	44	1/1/15/20	2/39/115/115	-
30	GOL	A	416	-	-	0/4/4/4	-
30	GOL	c	528	-	-	0/4/4/4	-

All (1860) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	11.28	2.33	2.06
24	c	513	CLA	MG-NA	10.92	2.32	2.06
24	C	508	CLA	MG-NA	10.64	2.31	2.06
24	B	605	CLA	MG-ND	-10.09	1.85	2.05
24	c	505	CLA	MG-NA	9.46	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	MG-NA	9.21	2.28	2.06
24	a	409	CLA	MG-ND	-9.17	1.87	2.05
25	D	401	PHO	C1B-C2B	9.09	1.49	1.39
25	d	401	PHO	C1D-C2D	9.02	1.49	1.39
24	c	511	CLA	MG-NA	9.00	2.27	2.06
25	A	408	PHO	C1D-C2D	8.90	1.49	1.39
25	a	411	PHO	C1D-C2D	8.87	1.49	1.39
24	B	607	CLA	MG-NA	8.87	2.27	2.06
24	C	504	CLA	MG-NA	8.80	2.27	2.06
24	b	616	CLA	MG-ND	-8.78	1.88	2.05
25	d	401	PHO	C1B-C2B	8.75	1.49	1.39
24	B	609	CLA	MG-NA	8.75	2.27	2.06
24	c	507	CLA	MG-NA	8.72	2.27	2.06
24	b	618	CLA	MG-NA	8.70	2.26	2.06
24	c	514	CLA	MG-ND	-8.65	1.88	2.05
24	c	508	CLA	MG-ND	-8.60	1.88	2.05
24	B	610	CLA	MG-NA	8.57	2.26	2.06
24	C	513	CLA	MG-ND	-8.49	1.89	2.05
24	b	607	CLA	MG-NA	8.32	2.26	2.06
24	B	616	CLA	MG-NA	8.28	2.25	2.06
24	c	512	CLA	MG-ND	-8.24	1.89	2.05
25	a	411	PHO	C1B-C2B	8.19	1.48	1.39
24	B	612	CLA	MG-NA	8.17	2.25	2.06
24	B	602	CLA	MG-NA	8.12	2.25	2.06
24	b	609	CLA	MG-NA	8.10	2.25	2.06
24	c	507	CLA	MG-ND	-8.09	1.89	2.05
25	A	408	PHO	C1B-C2B	8.07	1.48	1.39
24	c	510	CLA	MG-ND	-8.05	1.89	2.05
25	D	401	PHO	C1D-C2D	7.95	1.48	1.39
25	d	401	PHO	C3B-C4B	7.95	1.49	1.41
24	C	511	CLA	MG-NA	7.93	2.25	2.06
25	D	401	PHO	C3B-C4B	7.92	1.49	1.41
24	b	605	CLA	MG-NC	7.75	2.24	2.06
24	B	613	CLA	MG-NA	7.56	2.24	2.06
24	c	505	CLA	MG-NC	7.56	2.24	2.06
24	b	612	CLA	MG-NA	7.55	2.24	2.06
24	b	614	CLA	MG-NA	7.55	2.24	2.06
24	C	506	CLA	MG-NA	7.54	2.24	2.06
40	f	101	HEM	C3D-C2D	7.54	1.53	1.36
24	c	509	CLA	MG-NA	7.51	2.24	2.06
27	f	102	SQD	C6-S	-7.47	1.67	1.77
40	F	101	HEM	C3D-C2D	7.43	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	MG-NA	7.43	2.23	2.06
24	C	508	CLA	MG-ND	-7.43	1.91	2.05
24	C	506	CLA	MG-ND	-7.41	1.91	2.05
24	b	607	CLA	MG-ND	-7.33	1.91	2.05
24	B	603	CLA	MG-ND	-7.29	1.91	2.05
24	D	404	CLA	MG-NC	7.28	2.23	2.06
24	C	503	CLA	MG-ND	-7.24	1.91	2.05
24	b	608	CLA	MG-NA	7.20	2.23	2.06
24	c	503	CLA	MG-ND	-7.19	1.91	2.05
24	C	513	CLA	MG-NA	7.17	2.23	2.06
24	B	615	CLA	MG-NA	7.11	2.23	2.06
24	A	405	CLA	MG-NA	7.11	2.23	2.06
24	d	405	CLA	MG-NC	7.11	2.23	2.06
24	b	611	CLA	MG-NA	7.11	2.23	2.06
24	a	410	CLA	MG-NA	7.09	2.23	2.06
25	D	401	PHO	C4D-CHA	7.08	1.50	1.39
25	A	408	PHO	C4D-CHA	7.05	1.50	1.39
25	a	411	PHO	C3B-C4B	7.02	1.48	1.41
24	b	611	CLA	MG-ND	-7.01	1.91	2.05
24	b	604	CLA	MG-NA	7.00	2.22	2.06
24	c	508	CLA	MG-NC	6.96	2.22	2.06
24	C	507	CLA	MG-NA	6.94	2.22	2.06
24	b	619	CLA	MG-NA	6.91	2.22	2.06
24	B	614	CLA	MG-NA	6.90	2.22	2.06
24	B	609	CLA	MG-ND	-6.89	1.92	2.05
24	b	607	CLA	MG-NC	6.73	2.22	2.06
24	c	514	CLA	MG-NA	6.72	2.22	2.06
25	d	401	PHO	C4D-CHA	6.71	1.49	1.39
24	B	611	CLA	MG-NC	6.66	2.22	2.06
24	c	515	CLA	MG-NC	6.64	2.22	2.06
24	B	604	CLA	MG-ND	-6.64	1.92	2.05
24	B	603	CLA	MG-NA	6.61	2.22	2.06
24	C	507	CLA	MG-ND	-6.61	1.92	2.05
24	B	611	CLA	MG-ND	-6.57	1.92	2.05
24	C	509	CLA	MG-NA	6.57	2.21	2.06
24	B	616	CLA	MG-ND	-6.55	1.92	2.05
24	b	613	CLA	MG-NC	6.55	2.21	2.06
25	A	408	PHO	C3B-C2B	6.54	1.49	1.40
24	b	606	CLA	MG-NC	6.54	2.21	2.06
24	C	503	CLA	MG-NC	6.53	2.21	2.06
24	b	616	CLA	MG-NC	6.53	2.21	2.06
25	D	401	PHO	C3B-C2B	6.49	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	MG-ND	-6.49	1.92	2.05
24	B	610	CLA	MG-ND	-6.47	1.93	2.05
24	b	609	CLA	MG-NC	6.47	2.21	2.06
24	b	610	CLA	MG-NA	6.40	2.21	2.06
24	b	613	CLA	MG-ND	-6.37	1.93	2.05
43	V	202	HEC	CAC-C3C	6.36	1.55	1.35
43	v	1603	HEC	CAB-C3B	6.36	1.55	1.35
25	a	411	PHO	C4D-CHA	6.35	1.49	1.39
24	b	619	CLA	MG-ND	-6.34	1.93	2.05
25	d	401	PHO	C3B-C2B	6.33	1.48	1.40
24	A	405	CLA	MG-NC	6.29	2.21	2.06
24	A	407	CLA	MG-NC	6.28	2.21	2.06
24	c	509	CLA	MG-NC	6.28	2.21	2.06
24	C	510	CLA	MG-NA	6.26	2.21	2.06
24	b	614	CLA	MG-NC	6.24	2.21	2.06
43	v	1603	HEC	CAC-C3C	6.24	1.55	1.35
24	c	510	CLA	MG-NC	6.24	2.21	2.06
25	a	411	PHO	C3B-C2B	6.23	1.48	1.40
43	V	202	HEC	CAB-C3B	6.20	1.55	1.35
24	C	511	CLA	MG-ND	-6.17	1.93	2.05
24	b	611	CLA	MG-NC	6.17	2.20	2.06
24	b	614	CLA	MG-ND	-6.15	1.93	2.05
24	c	504	CLA	MG-ND	-6.15	1.93	2.05
24	C	514	CLA	MG-NA	6.12	2.20	2.06
25	A	408	PHO	C3B-C4B	6.11	1.47	1.41
24	b	615	CLA	MG-NA	6.11	2.20	2.06
24	C	505	CLA	MG-NA	6.11	2.20	2.06
24	c	512	CLA	MG-NC	6.10	2.20	2.06
24	B	611	CLA	MG-NA	6.10	2.20	2.06
24	C	514	CLA	MG-ND	-6.10	1.93	2.05
24	C	514	CLA	MG-NC	6.09	2.20	2.06
24	B	606	CLA	MG-NC	6.09	2.20	2.06
24	B	606	CLA	MG-NA	6.07	2.20	2.06
24	b	612	CLA	MG-NC	6.06	2.20	2.06
24	C	502	CLA	MG-NA	6.05	2.20	2.06
24	C	509	CLA	MG-NB	6.05	2.17	2.05
24	a	410	CLA	MG-ND	-6.05	1.93	2.05
24	C	509	CLA	MG-ND	-6.05	1.93	2.05
27	f	102	SQD	O47-C7	5.99	1.46	1.33
24	C	505	CLA	MG-NC	5.96	2.20	2.06
24	C	510	CLA	MG-NC	5.93	2.20	2.06
24	c	508	CLA	C1D-ND	5.88	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	MG-NA	5.83	2.20	2.06
24	a	408	CLA	MG-ND	-5.81	1.94	2.05
24	b	606	CLA	MG-ND	-5.81	1.94	2.05
24	c	510	CLA	C3C-C2C	5.80	1.49	1.36
24	c	508	CLA	MG-NA	5.80	2.20	2.06
24	c	511	CLA	MG-NC	5.80	2.20	2.06
24	c	512	CLA	MG-NA	5.80	2.20	2.06
24	B	611	CLA	C3C-C2C	5.78	1.49	1.36
24	c	512	CLA	C3C-C2C	5.78	1.49	1.36
24	b	604	CLA	C3C-C2C	5.78	1.49	1.36
24	C	503	CLA	MG-NA	5.76	2.20	2.06
24	d	404	CLA	MG-NA	5.75	2.19	2.06
24	B	617	CLA	MG-NA	5.75	2.19	2.06
24	b	613	CLA	C3C-C2C	5.74	1.49	1.36
24	b	610	CLA	MG-NC	5.73	2.19	2.06
24	B	617	CLA	MG-ND	-5.73	1.94	2.05
24	b	616	CLA	C1D-ND	5.72	1.45	1.37
24	C	513	CLA	C3C-C2C	5.72	1.49	1.36
24	D	404	CLA	C3C-C2C	5.72	1.49	1.36
24	a	409	CLA	C3C-C2C	5.70	1.49	1.36
24	b	604	CLA	MG-NC	5.68	2.19	2.06
24	C	504	CLA	C3C-C2C	5.68	1.49	1.36
24	B	613	CLA	MG-ND	-5.68	1.94	2.05
24	b	609	CLA	MG-ND	-5.67	1.94	2.05
24	b	605	CLA	C3C-C2C	5.66	1.49	1.36
24	b	616	CLA	C3C-C2C	5.66	1.49	1.36
24	b	606	CLA	MG-NA	5.66	2.19	2.06
24	B	602	CLA	C3C-C2C	5.64	1.48	1.36
24	b	610	CLA	MG-ND	-5.63	1.94	2.05
24	c	505	CLA	C3C-C2C	5.62	1.48	1.36
24	a	412	CLA	C3C-C2C	5.62	1.48	1.36
24	b	613	CLA	MG-NA	5.60	2.19	2.06
24	B	604	CLA	MG-NC	5.60	2.19	2.06
24	b	611	CLA	C3C-C2C	5.59	1.48	1.36
24	C	506	CLA	MG-NC	5.58	2.19	2.06
24	c	509	CLA	C3C-C2C	5.57	1.48	1.36
24	c	511	CLA	C1D-ND	5.57	1.45	1.37
24	B	606	CLA	C3C-C2C	5.56	1.48	1.36
24	C	509	CLA	C3C-C2C	5.56	1.48	1.36
24	c	505	CLA	C1D-ND	5.55	1.45	1.37
24	C	508	CLA	C1D-ND	5.55	1.45	1.37
24	C	507	CLA	C1D-ND	5.54	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C3C-C2C	5.53	1.48	1.36
24	C	502	CLA	C3C-C2C	5.53	1.48	1.36
24	C	508	CLA	C3C-C2C	5.52	1.48	1.36
24	b	610	CLA	C3C-C2C	5.50	1.48	1.36
24	a	410	CLA	C3C-C2C	5.50	1.48	1.36
24	B	603	CLA	C3C-C2C	5.50	1.48	1.36
24	c	511	CLA	C3C-C2C	5.50	1.48	1.36
24	b	616	CLA	MG-NA	5.50	2.19	2.06
24	c	508	CLA	C3C-C2C	5.49	1.48	1.36
24	c	507	CLA	C1D-ND	5.49	1.45	1.37
24	C	507	CLA	C3C-C2C	5.48	1.48	1.36
24	B	610	CLA	MG-NC	5.48	2.19	2.06
24	b	612	CLA	C1D-ND	5.47	1.45	1.37
24	b	609	CLA	C1D-ND	5.47	1.45	1.37
24	D	403	CLA	MG-NA	5.47	2.19	2.06
24	C	505	CLA	C3C-C2C	5.46	1.48	1.36
24	b	606	CLA	C3C-C2C	5.45	1.48	1.36
24	c	507	CLA	C3C-C2C	5.45	1.48	1.36
24	b	604	CLA	C1D-ND	5.45	1.45	1.37
24	C	507	CLA	MG-NC	5.44	2.19	2.06
43	v	1603	HEC	C3D-C2D	5.44	1.53	1.38
24	C	503	CLA	C3C-C2C	5.44	1.48	1.36
40	F	101	HEM	FE-ND	5.43	2.11	1.94
24	b	612	CLA	C3C-C2C	5.43	1.48	1.36
24	C	510	CLA	C3C-C2C	5.42	1.48	1.36
24	D	403	CLA	C3C-C2C	5.42	1.48	1.36
24	b	608	CLA	C3C-C2C	5.42	1.48	1.36
24	A	407	CLA	MG-ND	-5.42	1.95	2.05
24	A	405	CLA	C3C-C2C	5.42	1.48	1.36
25	A	408	PHO	C3D-C2D	5.41	1.48	1.39
24	A	409	CLA	C3C-C2C	5.41	1.48	1.36
24	a	408	CLA	C3C-C2C	5.41	1.48	1.36
24	c	513	CLA	C3C-C2C	5.40	1.48	1.36
24	C	513	CLA	MG-NC	5.40	2.19	2.06
24	B	609	CLA	C3C-C2C	5.40	1.48	1.36
24	C	514	CLA	C1D-ND	5.39	1.44	1.37
24	c	510	CLA	C1D-ND	5.39	1.44	1.37
24	C	511	CLA	C3C-C2C	5.38	1.48	1.36
24	c	504	CLA	C3C-C2C	5.38	1.48	1.36
24	c	507	CLA	MG-NC	5.38	2.19	2.06
24	c	506	CLA	MG-NA	5.37	2.19	2.06
24	B	604	CLA	C3C-C2C	5.37	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C1D-ND	5.37	1.44	1.37
24	c	514	CLA	C3C-C2C	5.37	1.48	1.36
24	c	506	CLA	C3C-C2C	5.36	1.48	1.36
24	B	602	CLA	CHC-C1C	5.36	1.49	1.38
24	b	617	CLA	CHC-C1C	5.36	1.49	1.38
24	B	609	CLA	C1D-ND	5.35	1.44	1.37
43	V	202	HEC	C3D-C2D	5.35	1.52	1.38
24	C	503	CLA	C1D-ND	5.35	1.44	1.37
24	D	404	CLA	CHC-C1C	5.35	1.49	1.38
24	B	605	CLA	MG-NC	5.35	2.19	2.06
24	b	617	CLA	MG-NC	5.34	2.19	2.06
24	d	404	CLA	MG-ND	-5.34	1.95	2.05
24	c	514	CLA	C1D-ND	5.34	1.44	1.37
24	b	615	CLA	MG-ND	-5.34	1.95	2.05
24	B	607	CLA	C3C-C2C	5.33	1.48	1.36
24	C	510	CLA	C1D-ND	5.33	1.44	1.37
24	b	607	CLA	C1D-ND	5.33	1.44	1.37
25	a	411	PHO	C3D-C2D	5.33	1.48	1.39
24	B	615	CLA	C3C-C2C	5.33	1.48	1.36
24	B	612	CLA	MG-ND	-5.33	1.95	2.05
24	A	406	CLA	C3C-C2C	5.32	1.48	1.36
24	b	617	CLA	MG-NA	5.31	2.18	2.06
24	A	407	CLA	C3C-C2C	5.30	1.48	1.36
24	D	403	CLA	MG-ND	-5.30	1.95	2.05
24	c	514	CLA	MG-NC	5.30	2.18	2.06
24	b	619	CLA	C1D-ND	5.29	1.44	1.37
24	C	514	CLA	C3C-C2C	5.29	1.48	1.36
24	b	617	CLA	C3C-C2C	5.29	1.48	1.36
24	B	611	CLA	CHC-C1C	5.28	1.49	1.38
24	A	406	CLA	MG-ND	-5.28	1.95	2.05
24	C	514	CLA	CHC-C1C	5.27	1.49	1.38
24	C	502	CLA	MG-NC	5.27	2.18	2.06
24	c	515	CLA	C3C-C2C	5.26	1.48	1.36
24	b	611	CLA	C1D-ND	5.26	1.44	1.37
24	d	405	CLA	C1D-ND	5.26	1.44	1.37
24	B	613	CLA	C3C-C2C	5.25	1.48	1.36
24	B	608	CLA	C3C-C2C	5.25	1.48	1.36
24	d	405	CLA	C3C-C2C	5.25	1.48	1.36
24	B	614	CLA	C3C-C2C	5.25	1.48	1.36
24	C	513	CLA	CHC-C1C	5.24	1.49	1.38
24	C	504	CLA	MG-NC	5.23	2.18	2.06
25	D	401	PHO	C3D-C2D	5.22	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C3C-C2C	5.21	1.48	1.36
24	c	503	CLA	C3C-C2C	5.21	1.48	1.36
24	B	613	CLA	CHC-C1C	5.21	1.48	1.38
24	d	404	CLA	C3C-C2C	5.21	1.48	1.36
24	b	613	CLA	C1D-ND	5.20	1.44	1.37
24	b	617	CLA	MG-ND	-5.19	1.95	2.05
24	b	619	CLA	C3C-C2C	5.19	1.48	1.36
24	A	409	CLA	MG-ND	-5.19	1.95	2.05
24	b	606	CLA	C1D-ND	5.19	1.44	1.37
24	b	612	CLA	O2D-CGD	5.18	1.46	1.33
24	b	618	CLA	C3C-C2C	5.17	1.47	1.36
24	a	410	CLA	CHC-C1C	5.17	1.48	1.38
24	B	604	CLA	CHC-C1C	5.17	1.48	1.38
24	c	506	CLA	O2D-CGD	5.17	1.45	1.33
24	C	506	CLA	C1D-ND	5.15	1.44	1.37
24	D	404	CLA	C1D-ND	5.15	1.44	1.37
24	C	512	CLA	C3C-C2C	5.15	1.47	1.36
24	b	609	CLA	C3C-C2C	5.15	1.47	1.36
24	b	607	CLA	C3C-C2C	5.14	1.47	1.36
24	b	614	CLA	CHC-C1C	5.14	1.48	1.38
24	B	617	CLA	C3C-C2C	5.14	1.47	1.36
24	B	605	CLA	C3C-C2C	5.14	1.47	1.36
24	c	515	CLA	CHC-C1C	5.14	1.48	1.38
24	b	605	CLA	CHC-C1C	5.13	1.48	1.38
24	c	504	CLA	MG-NA	5.12	2.18	2.06
24	B	602	CLA	MG-ND	-5.12	1.95	2.05
24	B	602	CLA	C1D-ND	5.12	1.44	1.37
24	B	604	CLA	C1D-ND	5.11	1.44	1.37
24	B	612	CLA	C3C-C2C	5.11	1.47	1.36
25	d	401	PHO	C3D-C2D	5.11	1.48	1.39
24	c	512	CLA	C1D-ND	5.11	1.44	1.37
24	c	513	CLA	CHC-C1C	5.11	1.48	1.38
24	a	408	CLA	MG-NA	5.10	2.18	2.06
24	B	603	CLA	CHC-C1C	5.10	1.48	1.38
24	B	610	CLA	O2D-CGD	5.09	1.45	1.33
24	a	408	CLA	MG-NC	5.09	2.18	2.06
24	b	605	CLA	C1D-ND	5.08	1.44	1.37
24	B	610	CLA	C1D-ND	5.08	1.44	1.37
24	c	510	CLA	MG-NB	5.07	2.15	2.05
24	b	614	CLA	C3C-C2C	5.07	1.47	1.36
24	B	611	CLA	C1D-ND	5.07	1.44	1.37
24	C	503	CLA	CHC-C1C	5.07	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	C1D-ND	5.06	1.44	1.37
24	B	603	CLA	C1D-ND	5.06	1.44	1.37
24	C	502	CLA	CHC-C1C	5.06	1.48	1.38
24	c	515	CLA	C1D-ND	5.05	1.44	1.37
24	b	615	CLA	MG-NC	5.05	2.18	2.06
24	b	614	CLA	C1D-ND	5.04	1.44	1.37
24	c	508	CLA	CHC-C1C	5.04	1.48	1.38
24	C	507	CLA	O2D-CGD	5.03	1.45	1.33
24	a	408	CLA	C1D-ND	5.03	1.44	1.37
24	b	615	CLA	C3C-C2C	5.03	1.47	1.36
25	d	401	PHO	OBD-CAD	5.03	1.28	1.22
24	C	504	CLA	C1D-ND	5.01	1.44	1.37
24	b	613	CLA	CHC-C1C	5.01	1.48	1.38
24	d	405	CLA	MG-ND	-5.01	1.95	2.05
24	b	604	CLA	CHD-C1D	5.00	1.48	1.38
24	B	602	CLA	O2D-CGD	5.00	1.45	1.33
24	C	505	CLA	CHC-C1C	5.00	1.48	1.38
24	b	604	CLA	O2D-CGD	5.00	1.45	1.33
24	C	513	CLA	C1D-ND	5.00	1.44	1.37
25	a	411	PHO	O2D-CGD	4.99	1.45	1.33
24	B	616	CLA	C1D-ND	4.99	1.44	1.37
24	D	404	CLA	MG-ND	-4.99	1.95	2.05
24	c	507	CLA	CHD-C1D	4.98	1.48	1.38
24	b	604	CLA	CHC-C1C	4.98	1.48	1.38
24	C	508	CLA	MG-NC	4.98	2.18	2.06
24	B	609	CLA	O2D-CGD	4.98	1.45	1.33
24	c	515	CLA	CHD-C1D	4.97	1.48	1.38
24	c	509	CLA	CHC-C1C	4.97	1.48	1.38
24	b	611	CLA	CHC-C1C	4.97	1.48	1.38
24	c	503	CLA	C1D-ND	4.97	1.44	1.37
24	b	609	CLA	CHD-C1D	4.96	1.48	1.38
24	b	605	CLA	O2D-CGD	4.96	1.45	1.33
24	b	616	CLA	O2D-CGD	4.95	1.45	1.33
24	b	605	CLA	MG-NA	4.95	2.18	2.06
24	b	612	CLA	CHC-C1C	4.94	1.48	1.38
24	A	407	CLA	CHC-C1C	4.94	1.48	1.38
24	c	504	CLA	CHC-C1C	4.93	1.48	1.38
24	B	616	CLA	O2D-CGD	4.92	1.45	1.33
24	C	510	CLA	O2D-CGD	4.92	1.45	1.33
24	c	505	CLA	CHC-C1C	4.92	1.48	1.38
24	b	619	CLA	O2D-CGD	4.91	1.45	1.33
24	b	606	CLA	CHC-C1C	4.91	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	CHC-C1C	4.91	1.48	1.38
24	a	412	CLA	CHC-C1C	4.91	1.48	1.38
24	c	510	CLA	CHC-C1C	4.90	1.48	1.38
24	B	609	CLA	CHD-C1D	4.90	1.48	1.38
24	B	602	CLA	MG-NC	4.90	2.17	2.06
24	B	604	CLA	O2D-CGD	4.90	1.45	1.33
24	c	515	CLA	O2D-CGD	4.90	1.45	1.33
24	C	503	CLA	O2D-CGD	4.90	1.45	1.33
24	B	604	CLA	MG-NA	4.89	2.17	2.06
24	C	510	CLA	CHD-C1D	4.89	1.48	1.38
24	B	607	CLA	O2D-CGD	4.88	1.45	1.33
24	B	603	CLA	O2D-CGD	4.88	1.45	1.33
24	c	503	CLA	CHC-C1C	4.88	1.48	1.38
24	b	613	CLA	O2D-CGD	4.87	1.45	1.33
24	D	404	CLA	O2D-CGD	4.86	1.45	1.33
25	d	401	PHO	O2D-CGD	4.86	1.45	1.33
24	b	615	CLA	O2D-CGD	4.86	1.45	1.33
24	a	412	CLA	O2D-CGD	4.86	1.45	1.33
24	b	608	CLA	CHC-C1C	4.86	1.48	1.38
24	A	405	CLA	C1D-ND	4.86	1.44	1.37
24	b	609	CLA	CHC-C1C	4.86	1.48	1.38
24	B	615	CLA	C1D-ND	4.85	1.44	1.37
24	B	614	CLA	CHC-C1C	4.84	1.48	1.38
24	b	610	CLA	CHC-C1C	4.84	1.48	1.38
24	b	606	CLA	O2D-CGD	4.84	1.45	1.33
24	D	404	CLA	CHD-C1D	4.84	1.47	1.38
24	c	511	CLA	CHC-C1C	4.84	1.48	1.38
24	B	608	CLA	O2D-CGD	4.83	1.45	1.33
24	B	616	CLA	C3C-C2C	4.83	1.47	1.36
24	b	617	CLA	C1D-ND	4.83	1.44	1.37
24	a	409	CLA	C1D-ND	4.83	1.44	1.37
24	B	607	CLA	C1D-ND	4.83	1.44	1.37
24	C	508	CLA	CHD-C1D	4.83	1.47	1.38
24	B	612	CLA	CHC-C1C	4.83	1.48	1.38
24	B	612	CLA	C1D-ND	4.83	1.44	1.37
24	c	514	CLA	CHC-C1C	4.83	1.48	1.38
24	B	606	CLA	O2D-CGD	4.82	1.45	1.33
24	A	409	CLA	O2D-CGD	4.81	1.45	1.33
24	C	511	CLA	CHC-C1C	4.81	1.48	1.38
24	A	407	CLA	O2D-CGD	4.81	1.45	1.33
24	B	617	CLA	O2D-CGD	4.81	1.45	1.33
24	b	614	CLA	O2D-CGD	4.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CHD-C1D	4.80	1.47	1.38
24	d	405	CLA	CHC-C1C	4.80	1.48	1.38
24	c	510	CLA	O2D-CGD	4.80	1.45	1.33
24	C	508	CLA	CHC-C1C	4.79	1.48	1.38
24	B	615	CLA	MG-ND	-4.78	1.96	2.05
24	B	614	CLA	O2D-CGD	4.78	1.45	1.33
24	b	613	CLA	CHD-C1D	4.78	1.47	1.38
24	B	606	CLA	CHC-C1C	4.78	1.48	1.38
24	b	618	CLA	O2D-CGD	4.77	1.45	1.33
24	B	610	CLA	CHC-C1C	4.77	1.48	1.38
24	C	513	CLA	O2D-CGD	4.77	1.45	1.33
24	B	616	CLA	CHC-C1C	4.76	1.48	1.38
24	B	615	CLA	CHC-C1C	4.76	1.48	1.38
24	C	504	CLA	CHC-C1C	4.76	1.48	1.38
24	b	607	CLA	CHC-C1C	4.76	1.48	1.38
24	c	506	CLA	CHC-C1C	4.76	1.48	1.38
24	C	509	CLA	O2D-CGD	4.76	1.44	1.33
24	b	617	CLA	O2D-CGD	4.75	1.44	1.33
24	c	507	CLA	CHC-C1C	4.75	1.48	1.38
24	c	508	CLA	CHD-C1D	4.75	1.47	1.38
24	c	504	CLA	MG-NC	4.75	2.17	2.06
24	a	412	CLA	C1D-ND	4.75	1.44	1.37
24	C	505	CLA	CHB-C1B	4.75	1.50	1.39
24	b	605	CLA	CHD-C1D	4.74	1.47	1.38
24	C	503	CLA	CHD-C1D	4.74	1.47	1.38
24	c	505	CLA	CHD-C1D	4.73	1.47	1.38
24	B	602	CLA	CHD-C1D	4.73	1.47	1.38
25	D	401	PHO	O2D-CGD	4.73	1.44	1.33
24	b	614	CLA	CHD-C1D	4.73	1.47	1.38
24	C	512	CLA	O2D-CGD	4.73	1.44	1.33
24	B	606	CLA	C1D-ND	4.72	1.44	1.37
24	C	514	CLA	O2D-CGD	4.72	1.44	1.33
24	c	512	CLA	CHB-C1B	4.71	1.50	1.39
24	c	508	CLA	O2D-CGD	4.71	1.44	1.33
24	d	405	CLA	O2D-CGD	4.71	1.44	1.33
24	C	512	CLA	CHC-C1C	4.71	1.47	1.38
24	c	511	CLA	O2D-CGD	4.71	1.44	1.33
24	c	511	CLA	CHB-C1B	4.71	1.50	1.39
24	b	612	CLA	CHD-C1D	4.71	1.47	1.38
24	a	408	CLA	CHC-C1C	4.71	1.47	1.38
24	B	610	CLA	CHD-C1D	4.71	1.47	1.38
38	O	304	DMS	O-S	4.70	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	O2D-CGD	4.69	1.44	1.33
25	A	408	PHO	O2D-CGD	4.69	1.44	1.33
24	B	610	CLA	CHB-C1B	4.69	1.49	1.39
38	c	537	DMS	O-S	4.68	1.81	1.50
24	b	615	CLA	C1D-ND	4.68	1.44	1.37
24	c	503	CLA	CHB-C1B	4.68	1.49	1.39
24	A	409	CLA	C1D-ND	4.68	1.44	1.37
24	B	613	CLA	CHB-C1B	4.68	1.49	1.39
38	Y	303	DMS	O-S	4.68	1.81	1.50
24	d	404	CLA	O2D-CGD	4.67	1.44	1.33
24	B	617	CLA	CHC-C1C	4.67	1.47	1.38
24	b	611	CLA	O2D-CGD	4.67	1.44	1.33
24	C	511	CLA	C1D-ND	4.67	1.44	1.37
24	c	504	CLA	O2D-CGD	4.67	1.44	1.33
24	C	506	CLA	CHC-C1C	4.67	1.47	1.38
24	C	510	CLA	CHC-C1C	4.67	1.47	1.38
24	C	512	CLA	C1D-ND	4.66	1.44	1.37
24	b	615	CLA	CHC-C1C	4.66	1.47	1.38
24	b	610	CLA	C1D-ND	4.66	1.44	1.37
24	C	505	CLA	C1D-ND	4.66	1.44	1.37
24	c	503	CLA	O2D-CGD	4.66	1.44	1.33
24	C	507	CLA	CHD-C1D	4.66	1.47	1.38
25	D	401	PHO	OBD-CAD	4.65	1.28	1.22
38	D	416	DMS	O-S	4.65	1.80	1.50
38	o	308	DMS	O-S	4.65	1.80	1.50
24	c	509	CLA	O2D-CGD	4.65	1.44	1.33
24	c	513	CLA	O2D-CGD	4.65	1.44	1.33
38	d	416	DMS	O-S	4.65	1.80	1.50
38	c	535	DMS	O-S	4.64	1.80	1.50
24	C	511	CLA	O2D-CGD	4.64	1.44	1.33
24	A	405	CLA	CHB-C1B	4.64	1.49	1.39
38	B	646	DMS	O-S	4.64	1.80	1.50
24	b	611	CLA	CHD-C1D	4.64	1.47	1.38
24	a	409	CLA	O2D-CGD	4.64	1.44	1.33
38	b	637	DMS	O-S	4.63	1.80	1.50
24	A	407	CLA	CHD-C1D	4.63	1.47	1.38
24	c	512	CLA	CHC-C1C	4.63	1.47	1.38
38	b	638	DMS	O-S	4.63	1.80	1.50
38	o	304	DMS	O-S	4.63	1.80	1.50
28	C	520	LMG	O8-C28	4.63	1.46	1.33
24	A	405	CLA	O2D-CGD	4.63	1.44	1.33
38	c	533	DMS	O-S	4.63	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C	533	DMS	O-S	4.63	1.80	1.50
38	z	102	DMS	O-S	4.63	1.80	1.50
24	A	405	CLA	MG-ND	-4.63	1.96	2.05
24	A	405	CLA	CHC-C1C	4.62	1.47	1.38
24	b	618	CLA	CHC-C1C	4.62	1.47	1.38
24	d	404	CLA	MG-NC	4.62	2.17	2.06
38	o	306	DMS	O-S	4.62	1.80	1.50
24	C	512	CLA	MG-ND	-4.62	1.96	2.05
38	a	426	DMS	O-S	4.62	1.80	1.50
24	b	610	CLA	CHD-C1D	4.62	1.47	1.38
38	v	1608	DMS	O-S	4.61	1.80	1.50
38	B	645	DMS	O-S	4.61	1.80	1.50
38	B	644	DMS	O-S	4.61	1.80	1.50
38	o	307	DMS	O-S	4.61	1.80	1.50
38	d	415	DMS	O-S	4.61	1.80	1.50
38	b	636	DMS	O-S	4.60	1.80	1.50
24	C	508	CLA	O2D-CGD	4.60	1.44	1.33
38	B	643	DMS	O-S	4.60	1.80	1.50
24	C	506	CLA	O2D-CGD	4.60	1.44	1.33
24	B	611	CLA	CHD-C1D	4.60	1.47	1.38
24	b	619	CLA	CHD-C1D	4.60	1.47	1.38
24	a	410	CLA	C1D-ND	4.60	1.43	1.37
38	o	309	DMS	O-S	4.60	1.80	1.50
24	B	606	CLA	CHD-C1D	4.59	1.47	1.38
24	C	502	CLA	CHD-C1D	4.59	1.47	1.38
24	c	513	CLA	C1D-ND	4.59	1.43	1.37
38	c	534	DMS	O-S	4.59	1.80	1.50
24	b	618	CLA	C1D-ND	4.59	1.43	1.37
38	E	106	DMS	O-S	4.58	1.80	1.50
38	C	525	DMS	O-S	4.58	1.80	1.50
24	d	404	CLA	CHC-C1C	4.58	1.47	1.38
24	b	616	CLA	CHC-C1C	4.58	1.47	1.38
24	C	502	CLA	O2D-CGD	4.58	1.44	1.33
24	b	619	CLA	CHC-C1C	4.57	1.47	1.38
38	V	207	DMS	O-S	4.57	1.80	1.50
24	c	512	CLA	CHD-C1D	4.57	1.47	1.38
24	b	607	CLA	O2D-CGD	4.56	1.44	1.33
24	C	510	CLA	CHB-C1B	4.56	1.49	1.39
24	a	409	CLA	CHC-C1C	4.56	1.47	1.38
24	C	509	CLA	CHD-C1D	4.56	1.47	1.38
24	b	614	CLA	CHB-C1B	4.55	1.49	1.39
38	c	536	DMS	O-S	4.55	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CHC-C4B	4.55	1.49	1.39
24	b	607	CLA	CHD-C1D	4.55	1.47	1.38
24	b	610	CLA	O2D-CGD	4.55	1.44	1.33
24	B	607	CLA	CHC-C1C	4.55	1.47	1.38
24	c	504	CLA	C1D-ND	4.54	1.43	1.37
38	i	104	DMS	O-S	4.54	1.80	1.50
24	C	504	CLA	O2D-CGD	4.54	1.44	1.33
38	B	647	DMS	O-S	4.54	1.80	1.50
24	A	406	CLA	MG-NA	4.54	2.17	2.06
24	B	615	CLA	O2D-CGD	4.53	1.44	1.33
24	b	608	CLA	O2D-CGD	4.53	1.44	1.33
24	C	511	CLA	CHD-C1D	4.53	1.47	1.38
24	c	507	CLA	O2D-CGD	4.53	1.44	1.33
24	C	509	CLA	MG-NC	4.53	2.17	2.06
24	C	502	CLA	C1D-ND	4.52	1.43	1.37
24	a	409	CLA	MG-NA	4.52	2.17	2.06
24	c	510	CLA	CHD-C1D	4.52	1.47	1.38
24	C	505	CLA	CHD-C1D	4.51	1.47	1.38
24	b	609	CLA	O2D-CGD	4.51	1.44	1.33
24	B	611	CLA	O2D-CGD	4.51	1.44	1.33
24	B	605	CLA	CHB-C1B	4.51	1.49	1.39
24	B	608	CLA	CHB-C1B	4.50	1.49	1.39
24	d	405	CLA	CHD-C1D	4.50	1.47	1.38
24	b	606	CLA	CHD-C1D	4.50	1.47	1.38
24	B	609	CLA	CHC-C1C	4.50	1.47	1.38
24	D	404	CLA	CHB-C1B	4.50	1.49	1.39
24	B	603	CLA	MG-NC	4.50	2.17	2.06
24	c	505	CLA	O2D-CGD	4.50	1.44	1.33
28	C	532	LMG	O7-C10	4.50	1.47	1.34
24	C	506	CLA	CHD-C1D	4.49	1.47	1.38
24	A	406	CLA	CHC-C1C	4.49	1.47	1.38
24	C	514	CLA	CHD-C1D	4.49	1.47	1.38
24	A	409	CLA	CHC-C1C	4.48	1.47	1.38
24	C	511	CLA	CHB-C1B	4.48	1.49	1.39
25	A	408	PHO	OBD-CAD	4.48	1.28	1.22
24	B	611	CLA	CHB-C1B	4.48	1.49	1.39
24	A	406	CLA	O2D-CGD	4.48	1.44	1.33
24	C	505	CLA	O2D-CGD	4.47	1.44	1.33
24	B	613	CLA	O2D-CGD	4.47	1.44	1.33
24	B	614	CLA	C1D-ND	4.46	1.43	1.37
24	A	405	CLA	CHD-C1D	4.46	1.47	1.38
24	c	514	CLA	O2D-CGD	4.46	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	D	407	DGD	O1G-C1A	4.46	1.46	1.33
24	b	619	CLA	MG-NC	4.46	2.16	2.06
24	C	512	CLA	CHB-C1B	4.45	1.49	1.39
24	c	515	CLA	MG-NA	4.44	2.16	2.06
40	f	101	HEM	FE-NB	4.44	2.08	1.94
24	b	608	CLA	C1D-ND	4.44	1.43	1.37
24	C	512	CLA	CHD-C1D	4.44	1.47	1.38
24	c	513	CLA	CHB-C1B	4.44	1.49	1.39
24	b	612	CLA	CHB-C1B	4.43	1.49	1.39
24	B	612	CLA	O2D-CGD	4.43	1.44	1.33
24	c	510	CLA	MG-NA	4.43	2.16	2.06
24	B	617	CLA	C1D-ND	4.42	1.43	1.37
24	c	504	CLA	CHB-C1B	4.42	1.49	1.39
24	B	605	CLA	O2D-CGD	4.42	1.44	1.33
24	b	619	CLA	CHB-C1B	4.41	1.49	1.39
24	c	509	CLA	CHD-C1D	4.41	1.47	1.38
24	C	504	CLA	CHD-C1D	4.41	1.47	1.38
24	C	513	CLA	CHD-C1D	4.41	1.47	1.38
24	C	514	CLA	CHB-C1B	4.41	1.49	1.39
28	a	415	LMG	O8-C28	4.41	1.46	1.33
24	b	611	CLA	CHB-C1B	4.41	1.49	1.39
24	B	602	CLA	CHC-C4B	4.40	1.49	1.39
24	a	412	CLA	MG-NC	4.40	2.16	2.06
24	b	615	CLA	CHB-C1B	4.40	1.49	1.39
24	A	409	CLA	CHD-C1D	4.40	1.47	1.38
39	D	407	DGD	O2G-C1B	4.40	1.46	1.34
24	b	613	CLA	CHB-C1B	4.39	1.49	1.39
24	b	611	CLA	CHC-C4B	4.39	1.49	1.39
37	E	101	LHG	O8-C23	4.39	1.46	1.33
24	a	408	CLA	O2D-CGD	4.39	1.44	1.33
24	b	610	CLA	CHB-C1B	4.39	1.49	1.39
24	B	610	CLA	OBD-CAD	4.38	1.30	1.22
24	B	613	CLA	MG-NC	4.37	2.16	2.06
24	a	410	CLA	O2A-CGA	4.37	1.46	1.33
24	c	514	CLA	CHD-C1D	4.37	1.46	1.38
24	C	503	CLA	CHB-C1B	4.37	1.49	1.39
28	C	532	LMG	O8-C28	4.37	1.46	1.33
24	a	412	CLA	CHD-C1D	4.37	1.46	1.38
28	c	522	LMG	O7-C10	4.37	1.46	1.34
24	a	412	CLA	O2A-CGA	4.36	1.46	1.33
24	A	406	CLA	C1D-ND	4.36	1.43	1.37
24	B	608	CLA	CHC-C1C	4.36	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	CHD-C1D	4.36	1.46	1.38
24	c	511	CLA	CHD-C1D	4.36	1.46	1.38
24	C	509	CLA	CHC-C4B	4.36	1.49	1.39
24	d	404	CLA	CHB-C1B	4.36	1.49	1.39
24	B	607	CLA	CHD-C1D	4.36	1.46	1.38
24	b	604	CLA	MG-ND	-4.36	1.97	2.05
24	C	507	CLA	CHB-C1B	4.35	1.49	1.39
40	f	101	HEM	FE-ND	4.35	2.08	1.94
28	B	621	LMG	O8-C28	4.35	1.46	1.33
24	b	604	CLA	O2A-CGA	4.35	1.46	1.33
24	b	617	CLA	CHD-C1D	4.34	1.46	1.38
24	B	602	CLA	O2A-CGA	4.34	1.46	1.33
24	B	604	CLA	O2A-CGA	4.33	1.46	1.33
24	b	613	CLA	CHC-C4B	4.33	1.49	1.39
27	L	101	SQD	O47-C7	4.33	1.46	1.34
24	d	404	CLA	O2A-CGA	4.33	1.46	1.33
24	D	403	CLA	CHC-C1C	4.33	1.47	1.38
24	C	507	CLA	CHC-C1C	4.33	1.47	1.38
24	b	612	CLA	OBD-CAD	4.33	1.29	1.22
24	C	509	CLA	C1D-ND	4.33	1.43	1.37
24	c	515	CLA	O2A-CGA	4.32	1.45	1.33
24	a	410	CLA	O2D-CGD	4.32	1.43	1.33
24	C	509	CLA	O2A-CGA	4.32	1.45	1.33
24	c	514	CLA	O2A-CGA	4.32	1.45	1.33
24	c	505	CLA	CHB-C1B	4.31	1.49	1.39
27	a	401	SQD	O48-C23	4.31	1.45	1.33
27	a	401	SQD	O47-C7	4.31	1.46	1.34
24	B	614	CLA	CHB-C1B	4.31	1.49	1.39
24	A	407	CLA	C1D-ND	4.30	1.43	1.37
24	A	409	CLA	MG-NC	4.30	2.16	2.06
27	A	413	SQD	O48-C23	4.30	1.45	1.33
24	D	404	CLA	OBD-CAD	4.30	1.29	1.22
24	d	404	CLA	C1D-ND	4.30	1.43	1.37
24	C	507	CLA	O2A-CGA	4.29	1.45	1.33
24	B	613	CLA	C1D-ND	4.29	1.43	1.37
27	L	102	SQD	O47-C7	4.29	1.46	1.34
24	D	404	CLA	MG-NA	4.29	2.16	2.06
24	C	509	CLA	CHB-C1B	4.29	1.49	1.39
24	B	615	CLA	CHD-C1D	4.29	1.46	1.38
24	B	614	CLA	CHD-C1D	4.28	1.46	1.38
28	b	623	LMG	O8-C28	4.28	1.45	1.33
27	A	413	SQD	O47-C7	4.28	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	CHD-C1D	4.28	1.46	1.38
24	C	513	CLA	CHC-C4B	4.27	1.49	1.39
24	A	406	CLA	O2A-CGA	4.27	1.45	1.33
24	c	506	CLA	MG-ND	-4.27	1.97	2.05
27	D	408	SQD	O48-C23	4.27	1.45	1.33
25	a	411	PHO	OBD-CAD	4.27	1.27	1.22
24	C	504	CLA	CHC-C4B	4.27	1.49	1.39
24	c	511	CLA	O2A-CGA	4.27	1.45	1.33
37	E	101	LHG	O7-C7	4.26	1.46	1.34
24	b	608	CLA	CHC-C4B	4.26	1.49	1.39
24	B	608	CLA	OBD-CAD	4.26	1.29	1.22
24	c	506	CLA	C1D-ND	4.26	1.43	1.37
24	D	403	CLA	O2A-CGA	4.26	1.45	1.33
28	c	522	LMG	O8-C28	4.26	1.45	1.33
24	C	502	CLA	CHC-C4B	4.26	1.49	1.39
24	C	510	CLA	O2A-CGA	4.26	1.45	1.33
24	b	604	CLA	CHD-C4C	4.25	1.48	1.39
24	b	607	CLA	CHB-C1B	4.25	1.49	1.39
24	B	609	CLA	MG-NC	4.25	2.16	2.06
24	c	506	CLA	CHD-C1D	4.25	1.46	1.38
24	b	605	CLA	CHB-C1B	4.24	1.48	1.39
24	C	512	CLA	O2A-CGA	4.23	1.45	1.33
24	b	616	CLA	CHB-C1B	4.23	1.48	1.39
28	a	415	LMG	O7-C10	4.23	1.46	1.34
24	B	608	CLA	CHD-C1D	4.23	1.46	1.38
40	F	101	HEM	FE-NA	4.22	2.09	1.95
24	B	614	CLA	CHC-C4B	4.22	1.48	1.39
24	B	606	CLA	CHB-C1B	4.22	1.48	1.39
24	B	615	CLA	CHB-C1B	4.22	1.48	1.39
24	C	514	CLA	O2A-CGA	4.22	1.45	1.33
24	b	619	CLA	O2A-CGA	4.22	1.45	1.33
24	b	618	CLA	O2A-CGA	4.22	1.45	1.33
27	D	408	SQD	O47-C7	4.21	1.46	1.34
37	e	101	LHG	O8-C23	4.21	1.45	1.33
24	c	513	CLA	CHD-C1D	4.21	1.46	1.38
27	L	101	SQD	O48-C23	4.21	1.45	1.33
27	f	102	SQD	O48-C23	4.20	1.45	1.33
24	c	509	CLA	MG-ND	-4.20	1.97	2.05
27	L	102	SQD	O48-C23	4.20	1.45	1.33
24	c	507	CLA	CHB-C1B	4.20	1.48	1.39
24	B	612	CLA	CHC-C4B	4.19	1.48	1.39
24	B	617	CLA	CHD-C1D	4.19	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	d	410	LHG	O7-C7	4.19	1.46	1.34
24	c	504	CLA	CHD-C1D	4.19	1.46	1.38
24	d	405	CLA	CHB-C1B	4.19	1.48	1.39
24	B	608	CLA	C1D-ND	4.19	1.43	1.37
24	b	605	CLA	O2A-CGA	4.19	1.45	1.33
24	b	609	CLA	CHB-C1B	4.19	1.48	1.39
24	b	616	CLA	CHD-C1D	4.19	1.46	1.38
24	c	515	CLA	CHC-C4B	4.19	1.48	1.39
28	A	412	LMG	O7-C10	4.18	1.46	1.34
28	c	521	LMG	O8-C28	4.18	1.45	1.33
24	B	602	CLA	CHB-C1B	4.18	1.48	1.39
24	B	605	CLA	CHD-C1D	4.18	1.46	1.38
24	c	510	CLA	O2A-CGA	4.17	1.45	1.33
24	B	603	CLA	CHC-C4B	4.17	1.48	1.39
24	c	511	CLA	CHC-C4B	4.17	1.48	1.39
24	A	406	CLA	CHD-C1D	4.17	1.46	1.38
24	D	403	CLA	O2D-CGD	4.17	1.43	1.33
24	c	509	CLA	CHB-C1B	4.16	1.48	1.39
24	c	508	CLA	CHB-C1B	4.16	1.48	1.39
24	C	513	CLA	MG-NB	4.16	2.14	2.05
24	a	410	CLA	CHD-C1D	4.15	1.46	1.38
24	A	409	CLA	O2A-CGA	4.15	1.45	1.33
24	c	509	CLA	O2A-CGA	4.15	1.45	1.33
24	B	607	CLA	MG-NC	4.15	2.16	2.06
24	b	614	CLA	CHC-C4B	4.15	1.48	1.39
24	b	606	CLA	CHB-C1B	4.14	1.48	1.39
24	b	614	CLA	MG-NB	4.14	2.14	2.05
24	c	505	CLA	CHC-C4B	4.14	1.48	1.39
24	c	505	CLA	MG-ND	-4.14	1.97	2.05
24	B	607	CLA	CHB-C1B	4.14	1.48	1.39
24	b	618	CLA	CHB-C1B	4.14	1.48	1.39
24	c	511	CLA	MG-ND	-4.13	1.97	2.05
24	C	513	CLA	O2A-CGA	4.13	1.45	1.33
24	c	513	CLA	O2A-CGA	4.13	1.45	1.33
24	b	617	CLA	CHC-C4B	4.13	1.48	1.39
24	a	410	CLA	CHB-C1B	4.13	1.48	1.39
24	B	605	CLA	CHC-C1C	4.12	1.46	1.38
24	c	506	CLA	C3D-C2D	4.12	1.50	1.39
24	b	611	CLA	O2A-CGA	4.12	1.45	1.33
24	b	608	CLA	O2A-CGA	4.12	1.45	1.33
40	f	101	HEM	FE-NC	4.12	2.08	1.95
24	B	612	CLA	MG-NB	4.12	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	CHB-C1B	4.12	1.48	1.39
24	B	617	CLA	CHB-C1B	4.12	1.48	1.39
24	C	508	CLA	O2A-CGA	4.11	1.45	1.33
24	d	405	CLA	O2A-CGA	4.11	1.45	1.33
24	C	509	CLA	C3D-C2D	4.11	1.50	1.39
24	b	616	CLA	O2A-CGA	4.11	1.45	1.33
24	c	504	CLA	CHC-C4B	4.11	1.48	1.39
43	v	1603	HEC	CBC-CAC	-4.10	1.34	1.49
24	b	605	CLA	MG-ND	-4.10	1.97	2.05
24	b	604	CLA	CHC-C4B	4.10	1.48	1.39
24	c	508	CLA	CHC-C4B	4.10	1.48	1.39
24	C	506	CLA	CHB-C1B	4.10	1.48	1.39
28	A	412	LMG	O8-C28	4.09	1.45	1.33
24	B	603	CLA	CHB-C1B	4.09	1.48	1.39
24	b	612	CLA	O2A-CGA	4.09	1.45	1.33
24	b	604	CLA	C3D-C2D	4.09	1.50	1.39
24	D	403	CLA	CHB-C1B	4.08	1.48	1.39
24	B	612	CLA	CHD-C1D	4.08	1.46	1.38
24	B	612	CLA	CHB-C1B	4.08	1.48	1.39
24	b	615	CLA	CHC-C4B	4.08	1.48	1.39
24	C	503	CLA	O2A-CGA	4.08	1.45	1.33
24	B	610	CLA	CHC-C4B	4.08	1.48	1.39
39	c	520	DGD	O1G-C1A	4.07	1.45	1.33
39	h	1205	DGD	O1G-C1A	4.07	1.45	1.33
37	d	410	LHG	O8-C23	4.07	1.45	1.33
24	C	502	CLA	O2A-CGA	4.07	1.45	1.33
24	b	615	CLA	OBD-CAD	4.07	1.29	1.22
24	c	514	CLA	CHB-C1B	4.07	1.48	1.39
24	C	514	CLA	CHC-C4B	4.06	1.48	1.39
24	b	606	CLA	O2A-CGA	4.06	1.45	1.33
24	a	408	CLA	CHB-C1B	4.06	1.48	1.39
24	B	609	CLA	O2A-CGA	4.06	1.45	1.33
24	B	604	CLA	CHC-C4B	4.06	1.48	1.39
24	c	505	CLA	O2A-CGA	4.06	1.45	1.33
37	e	101	LHG	O7-C7	4.06	1.45	1.34
24	D	404	CLA	O2A-CGA	4.06	1.45	1.33
24	B	606	CLA	OBD-CAD	4.06	1.29	1.22
24	A	405	CLA	CHC-C4B	4.06	1.48	1.39
24	A	409	CLA	CHB-C1B	4.06	1.48	1.39
24	c	509	CLA	CHC-C4B	4.06	1.48	1.39
24	a	408	CLA	CHC-C4B	4.05	1.48	1.39
24	b	604	CLA	CHB-C1B	4.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	CHC-C4B	4.05	1.48	1.39
39	h	1205	DGD	O2G-C1B	4.05	1.45	1.34
39	C	517	DGD	O2G-C1B	4.05	1.45	1.34
24	b	611	CLA	OBD-CAD	4.05	1.29	1.22
28	C	520	LMG	O7-C10	4.04	1.45	1.34
24	C	503	CLA	CHC-C4B	4.04	1.48	1.39
24	B	606	CLA	CHC-C4B	4.04	1.48	1.39
24	c	513	CLA	CHC-C4B	4.04	1.48	1.39
39	C	519	DGD	O1G-C1A	4.04	1.45	1.33
24	a	409	CLA	CHD-C1D	4.04	1.46	1.38
24	c	506	CLA	CHB-C1B	4.04	1.48	1.39
24	C	511	CLA	CHC-C4B	4.04	1.48	1.39
28	c	521	LMG	O7-C10	4.03	1.45	1.34
24	B	606	CLA	C3D-C2D	4.03	1.50	1.39
24	a	409	CLA	OBD-CAD	4.03	1.29	1.22
24	C	502	CLA	CHB-C1B	4.03	1.48	1.39
24	a	412	CLA	CHB-C1B	4.03	1.48	1.39
24	B	603	CLA	O2A-CGA	4.03	1.45	1.33
24	B	609	CLA	C3D-C2D	4.03	1.50	1.39
24	c	503	CLA	CHD-C1D	4.03	1.46	1.38
24	b	608	CLA	CHD-C1D	4.02	1.46	1.38
24	b	614	CLA	O2A-CGA	4.02	1.45	1.33
39	c	519	DGD	O1G-C1A	4.02	1.45	1.33
24	A	406	CLA	OBD-CAD	4.02	1.29	1.22
24	B	616	CLA	CHB-C1B	4.02	1.48	1.39
24	C	512	CLA	CHD-C4C	4.02	1.48	1.39
24	C	503	CLA	C3D-C2D	4.01	1.49	1.39
39	H	102	DGD	O1G-C1A	4.01	1.45	1.33
27	A	411	SQD	O47-C7	4.01	1.45	1.34
24	C	513	CLA	CHB-C1B	4.01	1.48	1.39
28	d	411	LMG	O8-C28	4.01	1.45	1.33
24	C	504	CLA	CHB-C1B	4.01	1.48	1.39
24	B	614	CLA	MG-NC	4.00	2.15	2.06
24	B	617	CLA	O2A-CGA	4.00	1.45	1.33
24	c	508	CLA	O2A-CGA	4.00	1.45	1.33
24	c	515	CLA	CHB-C1B	4.00	1.48	1.39
24	b	617	CLA	O2A-CGA	3.99	1.45	1.33
24	b	605	CLA	CHC-C4B	3.99	1.48	1.39
24	b	615	CLA	CHD-C1D	3.99	1.46	1.38
24	a	408	CLA	CHD-C4C	3.99	1.48	1.39
37	B	640	LHG	O8-C23	3.99	1.45	1.33
24	c	513	CLA	C3D-C2D	3.99	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHC-C4B	3.99	1.48	1.39
43	V	202	HEC	CBC-CAC	-3.98	1.34	1.49
37	D	411	LHG	O7-C7	3.98	1.45	1.34
36	o	301	HTG	C1'-S1	-3.98	1.75	1.81
24	B	614	CLA	C3D-C2D	3.97	1.49	1.39
24	C	505	CLA	CHC-C4B	3.97	1.48	1.39
24	c	508	CLA	CHD-C4C	3.97	1.48	1.39
24	B	602	CLA	CHD-C4C	3.97	1.48	1.39
24	c	513	CLA	OBD-CAD	3.97	1.29	1.22
24	a	408	CLA	CHD-C1D	3.97	1.46	1.38
24	C	505	CLA	CHD-C4C	3.97	1.48	1.39
24	C	510	CLA	CHD-C4C	3.96	1.48	1.39
24	c	503	CLA	O2A-CGA	3.96	1.44	1.33
24	c	513	CLA	CHD-C4C	3.96	1.48	1.39
24	c	510	CLA	CHC-C4B	3.96	1.48	1.39
24	a	412	CLA	C3D-C2D	3.96	1.49	1.39
24	c	512	CLA	CHC-C4B	3.96	1.48	1.39
24	C	510	CLA	C3D-C2D	3.96	1.49	1.39
24	C	502	CLA	C3D-C2D	3.96	1.49	1.39
24	d	405	CLA	CHD-C4C	3.96	1.48	1.39
24	B	616	CLA	O2A-CGA	3.95	1.44	1.33
24	A	405	CLA	CHD-C4C	3.95	1.48	1.39
24	A	405	CLA	C3D-C2D	3.95	1.49	1.39
24	b	610	CLA	O2A-CGA	3.95	1.44	1.33
24	b	612	CLA	CHC-C4B	3.95	1.48	1.39
24	d	405	CLA	CHC-C4B	3.94	1.48	1.39
24	B	606	CLA	O2A-CGA	3.94	1.44	1.33
24	c	515	CLA	C3D-C2D	3.94	1.49	1.39
24	b	607	CLA	CHC-C4B	3.94	1.48	1.39
24	c	507	CLA	CHC-C4B	3.93	1.48	1.39
24	C	510	CLA	CHC-C4B	3.93	1.48	1.39
24	C	513	CLA	C3D-C2D	3.92	1.49	1.39
24	C	505	CLA	O2A-CGA	3.92	1.44	1.33
24	b	609	CLA	CHD-C4C	3.92	1.48	1.39
24	b	606	CLA	CHC-C4B	3.92	1.48	1.39
24	b	612	CLA	CHD-C4C	3.92	1.48	1.39
24	b	613	CLA	C3D-C2D	3.92	1.49	1.39
24	C	502	CLA	CHD-C4C	3.91	1.48	1.39
24	C	503	CLA	OBD-CAD	3.91	1.29	1.22
24	d	404	CLA	CHD-C1D	3.91	1.46	1.38
24	B	609	CLA	CHC-C4B	3.91	1.48	1.39
24	d	404	CLA	CHC-C4B	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	OBD-CAD	3.91	1.29	1.22
24	D	403	CLA	C1D-ND	3.91	1.43	1.37
24	b	615	CLA	O2A-CGA	3.90	1.44	1.33
24	C	508	CLA	CHB-C1B	3.89	1.48	1.39
24	C	508	CLA	CHC-C4B	3.89	1.48	1.39
24	B	616	CLA	CHC-C4B	3.89	1.48	1.39
28	B	621	LMG	O7-C10	3.89	1.45	1.34
24	B	610	CLA	C3D-C2D	3.89	1.49	1.39
24	c	514	CLA	C3D-C2D	3.89	1.49	1.39
24	b	609	CLA	O2A-CGA	3.89	1.44	1.33
24	A	407	CLA	CHB-C1B	3.88	1.48	1.39
24	b	617	CLA	CHD-C4C	3.88	1.48	1.39
37	B	640	LHG	O7-C7	3.88	1.45	1.34
24	b	605	CLA	C3D-C2D	3.88	1.49	1.39
36	O	302	HTG	C1'-S1	-3.88	1.76	1.81
24	B	608	CLA	MG-NC	3.88	2.15	2.06
24	B	607	CLA	CHC-C4B	3.88	1.48	1.39
24	c	511	CLA	C3D-C2D	3.88	1.49	1.39
24	C	512	CLA	C3D-C2D	3.87	1.49	1.39
24	c	509	CLA	CHD-C4C	3.87	1.48	1.39
24	b	608	CLA	CHB-C1B	3.87	1.48	1.39
24	C	502	CLA	OBD-CAD	3.87	1.29	1.22
24	c	511	CLA	CHD-C4C	3.87	1.48	1.39
24	C	505	CLA	C3D-C2D	3.87	1.49	1.39
24	B	616	CLA	CHD-C1D	3.87	1.46	1.38
24	C	506	CLA	CHC-C4B	3.87	1.48	1.39
24	C	507	CLA	C3D-C2D	3.87	1.49	1.39
24	B	607	CLA	O2A-CGA	3.87	1.44	1.33
24	B	608	CLA	CHC-C4B	3.87	1.48	1.39
24	B	603	CLA	CHD-C4C	3.87	1.48	1.39
24	d	405	CLA	MG-NA	3.87	2.15	2.06
24	A	405	CLA	OBD-CAD	3.87	1.29	1.22
24	c	515	CLA	CHD-C4C	3.86	1.48	1.39
24	B	617	CLA	C3D-C2D	3.86	1.49	1.39
24	C	511	CLA	C3D-C2D	3.86	1.49	1.39
24	C	504	CLA	C3D-C2D	3.86	1.49	1.39
24	a	410	CLA	C3D-C2D	3.86	1.49	1.39
27	A	411	SQD	O48-C23	3.86	1.44	1.33
24	a	410	CLA	OBD-CAD	3.85	1.29	1.22
24	C	509	CLA	CHD-C4C	3.85	1.48	1.39
24	C	504	CLA	O2A-CGA	3.85	1.44	1.33
24	a	410	CLA	CHD-C4C	3.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	CHD-C4C	3.85	1.48	1.39
24	b	605	CLA	CHD-C4C	3.84	1.47	1.39
24	b	605	CLA	OBD-CAD	3.84	1.29	1.22
24	B	615	CLA	O2A-CGA	3.84	1.44	1.33
24	a	409	CLA	CHB-C1B	3.84	1.48	1.39
24	b	618	CLA	CHD-C4C	3.84	1.47	1.39
24	b	613	CLA	CHD-C4C	3.83	1.47	1.39
24	B	604	CLA	CHB-C1B	3.83	1.48	1.39
39	c	519	DGD	O2G-C1B	3.83	1.45	1.34
24	b	614	CLA	C3D-C2D	3.83	1.49	1.39
25	A	408	PHO	O2A-CGA	3.82	1.44	1.33
39	c	518	DGD	O2G-C1B	3.82	1.45	1.34
28	b	623	LMG	O7-C10	3.82	1.45	1.34
24	a	412	CLA	MG-NA	3.82	2.15	2.06
24	B	608	CLA	CHD-C4C	3.82	1.47	1.39
24	C	507	CLA	CHD-C4C	3.82	1.47	1.39
24	B	608	CLA	O2A-CGA	3.82	1.44	1.33
24	A	406	CLA	CHC-C4B	3.82	1.48	1.39
24	a	409	CLA	O2A-CGA	3.82	1.44	1.33
24	c	509	CLA	OBD-CAD	3.81	1.29	1.22
24	b	610	CLA	CHC-C4B	3.81	1.48	1.39
24	B	610	CLA	CHD-C4C	3.81	1.47	1.39
24	b	608	CLA	CHD-C4C	3.81	1.47	1.39
24	D	403	CLA	CHD-C4C	3.81	1.47	1.39
24	B	610	CLA	O2A-CGA	3.81	1.44	1.33
24	c	510	CLA	CHB-C1B	3.80	1.47	1.39
24	A	407	CLA	O2A-CGA	3.80	1.44	1.33
24	B	606	CLA	CHD-C4C	3.80	1.47	1.39
24	c	506	CLA	O2A-CGA	3.80	1.44	1.33
24	C	514	CLA	CHD-C4C	3.80	1.47	1.39
24	c	507	CLA	CHD-C4C	3.80	1.47	1.39
24	b	617	CLA	CHB-C1B	3.80	1.47	1.39
24	a	408	CLA	OBD-CAD	3.80	1.29	1.22
37	d	408	LHG	O8-C23	3.80	1.44	1.33
24	A	407	CLA	OBD-CAD	3.80	1.29	1.22
24	d	404	CLA	CHD-C4C	3.79	1.47	1.39
25	d	401	PHO	O2A-CGA	3.79	1.44	1.33
24	C	504	CLA	CHD-C4C	3.79	1.47	1.39
24	B	608	CLA	C3D-C2D	3.79	1.49	1.39
24	c	514	CLA	CHC-C4B	3.79	1.47	1.39
24	b	609	CLA	C3D-C2D	3.79	1.49	1.39
24	c	509	CLA	C3D-C2D	3.79	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C3D-C2D	3.79	1.49	1.39
27	a	414	SQD	O48-C23	3.79	1.44	1.33
24	D	404	CLA	CHC-C4B	3.79	1.47	1.39
24	B	611	CLA	C3D-C2D	3.79	1.49	1.39
43	v	1603	HEC	CBB-CAB	-3.78	1.35	1.49
24	A	405	CLA	O2A-CGA	3.78	1.44	1.33
24	c	506	CLA	CHC-C4B	3.78	1.47	1.39
24	C	508	CLA	CHD-C4C	3.77	1.47	1.39
24	c	505	CLA	C3D-C2D	3.77	1.49	1.39
25	D	401	PHO	O2A-CGA	3.77	1.44	1.33
24	A	406	CLA	CHD-C4C	3.77	1.47	1.39
27	a	414	SQD	O47-C7	3.77	1.44	1.34
24	A	409	CLA	C3D-C2D	3.77	1.49	1.39
24	C	511	CLA	O2A-CGA	3.77	1.44	1.33
24	a	410	CLA	CHC-C4B	3.77	1.47	1.39
24	b	613	CLA	OBD-CAD	3.77	1.29	1.22
24	C	510	CLA	OBD-CAD	3.77	1.29	1.22
24	B	602	CLA	OBD-CAD	3.77	1.29	1.22
24	b	610	CLA	C3D-C2D	3.77	1.49	1.39
24	c	510	CLA	C3D-C2D	3.76	1.49	1.39
24	C	513	CLA	CHD-C4C	3.76	1.47	1.39
24	b	618	CLA	C3D-C2D	3.76	1.49	1.39
39	H	102	DGD	O2G-C1B	3.76	1.44	1.34
24	B	604	CLA	CHD-C1D	3.76	1.45	1.38
24	a	409	CLA	C3D-C2D	3.76	1.49	1.39
24	d	405	CLA	C3D-C2D	3.76	1.49	1.39
37	l	302	LHG	O8-C23	3.76	1.44	1.33
24	C	509	CLA	OBD-CAD	3.75	1.28	1.22
39	C	518	DGD	O2G-C1B	3.75	1.44	1.34
24	B	607	CLA	C3D-C2D	3.75	1.49	1.39
24	A	409	CLA	MG-NA	3.75	2.15	2.06
24	a	412	CLA	CHD-C4C	3.75	1.47	1.39
24	c	503	CLA	CHC-C4B	3.74	1.47	1.39
24	b	615	CLA	C3D-C2D	3.74	1.49	1.39
24	A	407	CLA	C1B-NB	-3.74	1.32	1.37
37	D	410	LHG	O7-C7	3.74	1.44	1.34
24	D	404	CLA	CHD-C4C	3.74	1.47	1.39
24	A	409	CLA	OBD-CAD	3.74	1.28	1.22
24	C	503	CLA	CHD-C4C	3.74	1.47	1.39
24	b	618	CLA	MG-NC	3.74	2.15	2.06
39	C	519	DGD	O2G-C1B	3.73	1.44	1.34
24	a	408	CLA	O2A-CGA	3.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	OBD-CAD	3.73	1.28	1.22
24	b	609	CLA	OBD-CAD	3.73	1.28	1.22
24	B	614	CLA	O2A-CGA	3.73	1.44	1.33
39	c	520	DGD	O2G-C1B	3.73	1.44	1.34
24	C	504	CLA	OBD-CAD	3.72	1.28	1.22
24	A	406	CLA	CHB-C1B	3.72	1.47	1.39
25	a	411	PHO	O2A-CGA	3.72	1.44	1.33
24	B	615	CLA	CHC-C4B	3.72	1.47	1.39
24	C	508	CLA	C3D-C2D	3.72	1.49	1.39
24	C	511	CLA	OBD-CAD	3.72	1.28	1.22
24	d	405	CLA	OBD-CAD	3.71	1.28	1.22
24	b	607	CLA	CHD-C4C	3.70	1.47	1.39
40	F	101	HEM	FE-NC	3.70	2.07	1.95
24	D	404	CLA	C3D-C2D	3.70	1.49	1.39
24	c	503	CLA	OBD-CAD	3.70	1.28	1.22
24	B	605	CLA	CHC-C4B	3.70	1.47	1.39
28	d	411	LMG	O7-C10	3.69	1.44	1.34
24	B	608	CLA	C1B-NB	-3.69	1.33	1.37
24	B	615	CLA	CHD-C4C	3.69	1.47	1.39
37	d	409	LHG	O8-C23	3.69	1.44	1.33
37	D	409	LHG	O8-C23	3.69	1.44	1.33
24	C	514	CLA	OBD-CAD	3.69	1.28	1.22
24	D	403	CLA	CHD-C1D	3.69	1.45	1.38
24	b	619	CLA	C3D-C2D	3.69	1.49	1.39
24	c	506	CLA	CHD-C4C	3.69	1.47	1.39
24	b	611	CLA	C3D-C2D	3.69	1.49	1.39
24	B	616	CLA	OBD-CAD	3.69	1.28	1.22
24	b	608	CLA	OBD-CAD	3.68	1.28	1.22
24	C	503	CLA	MG-NB	3.68	2.13	2.05
24	c	512	CLA	CHD-C4C	3.68	1.47	1.39
37	d	409	LHG	O7-C7	3.68	1.44	1.34
24	c	504	CLA	OBD-CAD	3.68	1.28	1.22
24	B	609	CLA	CHD-C4C	3.67	1.47	1.39
24	b	613	CLA	O2A-CGA	3.67	1.44	1.33
24	B	602	CLA	C3D-C2D	3.67	1.49	1.39
24	b	612	CLA	C3D-C2D	3.67	1.49	1.39
24	c	504	CLA	O2A-CGA	3.67	1.44	1.33
24	C	506	CLA	O2A-CGA	3.66	1.44	1.33
24	B	603	CLA	OBD-CAD	3.66	1.28	1.22
24	b	606	CLA	CHD-C4C	3.66	1.47	1.39
24	c	510	CLA	CHD-C4C	3.66	1.47	1.39
24	b	607	CLA	O2A-CGA	3.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	OBD-CAD	3.65	1.28	1.22
24	A	407	CLA	CHD-C4C	3.64	1.47	1.39
24	b	618	CLA	CHC-C4B	3.64	1.47	1.39
39	C	518	DGD	O1G-C1A	3.64	1.44	1.33
24	c	505	CLA	CHD-C4C	3.64	1.47	1.39
24	B	617	CLA	MG-NC	3.64	2.14	2.06
24	b	617	CLA	C3D-C2D	3.64	1.48	1.39
24	C	514	CLA	C3D-C2D	3.63	1.48	1.39
24	b	619	CLA	OBD-CAD	3.63	1.28	1.22
24	B	605	CLA	O2A-CGA	3.63	1.43	1.33
37	l	302	LHG	O7-C7	3.63	1.44	1.34
24	B	613	CLA	OBD-CAD	3.63	1.28	1.22
39	C	517	DGD	O1G-C1A	3.63	1.43	1.33
24	c	503	CLA	CHD-C4C	3.63	1.47	1.39
24	B	612	CLA	O2A-CGA	3.63	1.43	1.33
24	B	613	CLA	O2A-CGA	3.63	1.43	1.33
24	c	508	CLA	C3D-C2D	3.62	1.48	1.39
24	A	406	CLA	C3D-C2D	3.62	1.48	1.39
24	C	511	CLA	MG-NC	3.62	2.14	2.06
24	B	615	CLA	C3D-C2D	3.62	1.48	1.39
24	A	409	CLA	CHD-C4C	3.62	1.47	1.39
24	A	406	CLA	MG-NC	3.61	2.14	2.06
37	D	410	LHG	O8-C23	3.61	1.43	1.33
24	c	510	CLA	OBD-CAD	3.61	1.28	1.22
24	D	403	CLA	OBD-CAD	3.61	1.28	1.22
24	B	616	CLA	C3D-C2D	3.61	1.48	1.39
24	b	604	CLA	OBD-CAD	3.61	1.28	1.22
24	a	412	CLA	CHC-C4B	3.60	1.47	1.39
24	B	603	CLA	MG-NB	3.60	2.12	2.05
37	D	411	LHG	O8-C23	3.60	1.43	1.33
24	B	607	CLA	OBD-CAD	3.60	1.28	1.22
24	c	515	CLA	OBD-CAD	3.59	1.28	1.22
24	B	612	CLA	CHD-C4C	3.59	1.47	1.39
24	B	616	CLA	CHD-C4C	3.59	1.47	1.39
24	B	608	CLA	MG-ND	-3.59	1.98	2.05
24	c	512	CLA	O2A-CGA	3.59	1.43	1.33
24	C	508	CLA	OBD-CAD	3.59	1.28	1.22
24	d	405	CLA	C1B-NB	-3.59	1.33	1.37
24	b	611	CLA	CHD-C4C	3.58	1.47	1.39
28	D	412	LMG	O7-C10	3.58	1.44	1.34
24	C	512	CLA	OBD-CAD	3.58	1.28	1.22
24	c	507	CLA	O2A-CGA	3.58	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	CHD-C4C	3.58	1.47	1.39
24	c	514	CLA	CHD-C4C	3.57	1.47	1.39
24	B	603	CLA	C3D-C2D	3.57	1.48	1.39
24	b	612	CLA	MG-ND	-3.57	1.98	2.05
24	b	606	CLA	C3D-C2D	3.57	1.48	1.39
24	b	616	CLA	C3D-C2D	3.57	1.48	1.39
24	c	508	CLA	OBD-CAD	3.56	1.28	1.22
24	b	607	CLA	OBD-CAD	3.56	1.28	1.22
24	A	407	CLA	C3D-C2D	3.56	1.48	1.39
24	a	409	CLA	MG-NB	3.56	2.12	2.05
24	A	407	CLA	CHC-C4B	3.56	1.47	1.39
24	c	504	CLA	CHD-C4C	3.56	1.47	1.39
24	a	408	CLA	MG-NB	3.56	2.12	2.05
24	b	608	CLA	C3D-C2D	3.55	1.48	1.39
24	b	618	CLA	MG-ND	-3.55	1.98	2.05
24	C	506	CLA	C3D-C2D	3.55	1.48	1.39
24	B	614	CLA	OBD-CAD	3.55	1.28	1.22
24	B	615	CLA	OBD-CAD	3.55	1.28	1.22
24	d	404	CLA	C3D-C2D	3.55	1.48	1.39
39	c	518	DGD	O1G-C1A	3.55	1.43	1.33
24	c	511	CLA	OBD-CAD	3.54	1.28	1.22
24	B	611	CLA	CHD-C4C	3.54	1.47	1.39
25	D	401	PHO	CHA-CBD	-3.54	1.47	1.51
36	b	626	HTG	C1'-S1	-3.53	1.76	1.81
24	a	412	CLA	OBD-CAD	3.53	1.28	1.22
24	B	612	CLA	MG-NC	3.53	2.14	2.06
24	B	613	CLA	C3D-C2D	3.53	1.48	1.39
24	b	619	CLA	CHC-C4B	3.53	1.47	1.39
24	C	507	CLA	OBD-CAD	3.53	1.28	1.22
24	C	506	CLA	OBD-CAD	3.52	1.28	1.22
36	b	601	HTG	C1'-S1	-3.52	1.76	1.81
24	c	512	CLA	MG-NB	3.52	2.12	2.05
24	b	619	CLA	CHD-C4C	3.50	1.47	1.39
24	c	511	CLA	C4D-CHA	3.50	1.50	1.38
24	d	404	CLA	C1B-NB	-3.50	1.33	1.37
24	c	512	CLA	C3D-C2D	3.50	1.48	1.39
24	B	607	CLA	CHD-C4C	3.50	1.47	1.39
24	B	611	CLA	O2A-CGA	3.49	1.43	1.33
36	B	625	HTG	C1'-S1	-3.49	1.76	1.81
24	c	514	CLA	OBD-CAD	3.49	1.28	1.22
24	b	617	CLA	OBD-CAD	3.49	1.28	1.22
24	B	617	CLA	CHC-C4B	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	102	HTG	C1'-S1	-3.48	1.76	1.81
24	b	610	CLA	CHD-C4C	3.48	1.47	1.39
24	c	512	CLA	OBD-CAD	3.48	1.28	1.22
24	B	605	CLA	CHD-C4C	3.48	1.47	1.39
24	C	512	CLA	CHC-C4B	3.48	1.47	1.39
36	b	602	HTG	C1'-S1	-3.48	1.76	1.81
36	h	1202	HTG	C1'-S1	-3.48	1.76	1.81
24	c	504	CLA	C3D-C2D	3.48	1.48	1.39
24	C	513	CLA	OBD-CAD	3.48	1.28	1.22
36	B	624	HTG	C1'-S1	-3.47	1.76	1.81
24	a	408	CLA	C3D-C2D	3.47	1.48	1.39
24	A	406	CLA	C4B-NB	-3.47	1.33	1.37
24	b	607	CLA	C4D-CHA	3.46	1.50	1.38
28	D	412	LMG	O8-C28	3.46	1.43	1.33
36	B	623[A]	HTG	C1'-S1	-3.46	1.76	1.81
36	D	413	HTG	C1'-S1	-3.46	1.76	1.81
24	b	610	CLA	OBD-CAD	3.46	1.28	1.22
24	B	617	CLA	CHD-C4C	3.46	1.47	1.39
24	B	614	CLA	MG-NB	3.45	2.12	2.05
24	C	507	CLA	CHC-C4B	3.45	1.47	1.39
24	b	606	CLA	OBD-CAD	3.45	1.28	1.22
24	b	616	CLA	CHC-C4B	3.45	1.47	1.39
24	b	608	CLA	MG-NC	3.45	2.14	2.06
24	C	508	CLA	C4D-CHA	3.43	1.50	1.38
24	B	604	CLA	C3D-C2D	3.42	1.48	1.39
24	B	613	CLA	CHD-C4C	3.42	1.47	1.39
24	B	605	CLA	OBD-CAD	3.40	1.28	1.22
24	c	505	CLA	OBD-CAD	3.40	1.28	1.22
24	D	403	CLA	CHC-C4B	3.40	1.47	1.39
24	B	615	CLA	C4B-NB	-3.40	1.33	1.37
24	c	515	CLA	MG-ND	-3.39	1.99	2.05
24	C	506	CLA	CHD-C4C	3.39	1.46	1.39
24	C	512	CLA	C4D-CHA	3.39	1.50	1.38
24	a	412	CLA	MG-ND	-3.38	1.99	2.05
24	B	612	CLA	C3D-C2D	3.38	1.48	1.39
24	B	611	CLA	OBD-CAD	3.37	1.28	1.22
24	B	613	CLA	CHC-C4B	3.37	1.47	1.39
24	a	410	CLA	C1B-NB	-3.36	1.33	1.37
36	d	414	HTG	C1'-S1	-3.36	1.76	1.81
24	B	616	CLA	C4B-NB	-3.36	1.33	1.37
24	B	612	CLA	OBD-CAD	3.36	1.28	1.22
24	c	503	CLA	C3D-C2D	3.35	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	OBD-CAD	3.34	1.28	1.22
24	B	604	CLA	CHD-C4C	3.33	1.46	1.39
36	c	525	HTG	C1'-S1	-3.33	1.76	1.81
43	V	202	HEC	CBB-CAB	-3.33	1.37	1.49
37	d	408	LHG	O7-C7	3.33	1.43	1.34
24	B	614	CLA	CHD-C4C	3.32	1.46	1.39
24	c	507	CLA	C1B-C2B	3.31	1.50	1.43
36	B	626	HTG	C1'-S1	-3.31	1.76	1.81
24	b	616	CLA	CHD-C4C	3.31	1.46	1.39
24	b	618	CLA	C4D-CHA	3.30	1.49	1.38
24	c	507	CLA	C3D-C2D	3.30	1.48	1.39
24	B	617	CLA	OBD-CAD	3.29	1.28	1.22
24	c	512	CLA	C1B-NB	-3.29	1.33	1.37
24	B	606	CLA	C1B-C2B	3.29	1.50	1.43
24	c	504	CLA	C4B-NB	-3.29	1.33	1.37
24	B	611	CLA	C1B-NB	-3.29	1.33	1.37
24	C	504	CLA	C4D-CHA	3.28	1.49	1.38
24	B	604	CLA	OBD-CAD	3.28	1.28	1.22
24	b	615	CLA	CHD-C4C	3.27	1.46	1.39
24	c	509	CLA	C4D-CHA	3.27	1.49	1.38
24	c	506	CLA	C1B-NB	-3.26	1.33	1.37
24	a	409	CLA	CHC-C4B	3.25	1.46	1.39
24	a	412	CLA	C1B-C2B	3.25	1.50	1.43
24	C	502	CLA	MG-ND	-3.25	1.99	2.05
24	c	505	CLA	C4D-CHA	3.25	1.49	1.38
37	D	409	LHG	O7-C7	3.25	1.43	1.34
24	c	514	CLA	MG-NB	3.24	2.12	2.05
24	c	513	CLA	C4D-CHA	3.23	1.49	1.38
24	B	605	CLA	C3D-C2D	3.23	1.47	1.39
24	B	614	CLA	C4D-CHA	3.23	1.49	1.38
24	a	409	CLA	C1B-NB	-3.22	1.33	1.37
24	a	408	CLA	C1B-NB	-3.22	1.33	1.37
24	C	506	CLA	C1B-C2B	3.21	1.50	1.43
24	b	610	CLA	C1B-C2B	3.21	1.50	1.43
36	B	623[B]	HTG	C1'-S1	-3.21	1.76	1.81
24	D	404	CLA	C1B-C2B	3.20	1.50	1.43
24	B	609	CLA	C4D-CHA	3.20	1.49	1.38
24	a	412	CLA	C1B-NB	-3.19	1.33	1.37
24	b	609	CLA	C4D-CHA	3.19	1.49	1.38
24	c	504	CLA	MG-NB	3.17	2.12	2.05
36	u	201	HTG	C1'-S1	-3.16	1.77	1.81
24	c	503	CLA	MG-NC	3.16	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1B-NB	-3.16	1.33	1.37
24	a	409	CLA	CHD-C4C	3.16	1.46	1.39
24	b	615	CLA	C1B-C2B	3.16	1.50	1.43
24	C	506	CLA	C4D-CHA	3.16	1.49	1.38
24	c	505	CLA	C1B-C2B	3.15	1.50	1.43
40	f	101	HEM	CAB-C3B	3.15	1.55	1.47
24	c	506	CLA	C4B-NB	-3.15	1.33	1.37
24	B	616	CLA	C1B-C2B	3.14	1.50	1.43
24	C	512	CLA	C1B-C2B	3.14	1.50	1.43
40	F	101	HEM	CAB-C3B	3.14	1.55	1.47
24	b	609	CLA	C1B-C2B	3.14	1.50	1.43
24	D	404	CLA	MG-NB	3.13	2.12	2.05
24	C	506	CLA	C1B-NB	-3.13	1.33	1.37
24	c	513	CLA	C1B-C2B	3.12	1.50	1.43
24	B	607	CLA	C4D-CHA	3.12	1.49	1.38
24	a	409	CLA	MG-NC	3.11	2.13	2.06
24	b	616	CLA	OBD-CAD	3.11	1.27	1.22
24	a	408	CLA	C4B-NB	-3.10	1.33	1.37
24	B	615	CLA	C4D-CHA	3.10	1.49	1.38
24	B	603	CLA	C1B-NB	-3.10	1.33	1.37
24	B	610	CLA	C1B-C2B	3.10	1.50	1.43
24	c	503	CLA	C4D-CHA	3.09	1.49	1.38
24	b	614	CLA	C4D-CHA	3.09	1.49	1.38
24	C	504	CLA	MG-ND	-3.09	1.99	2.05
24	b	610	CLA	MG-NB	3.09	2.11	2.05
24	a	409	CLA	C1B-C2B	3.09	1.50	1.43
24	B	611	CLA	MG-NB	3.09	2.11	2.05
24	C	503	CLA	C4D-CHA	3.09	1.49	1.38
24	B	612	CLA	C4D-CHA	3.09	1.49	1.38
24	c	512	CLA	C4D-CHA	3.08	1.48	1.38
24	b	610	CLA	C1B-NB	-3.08	1.33	1.37
24	b	610	CLA	C4D-CHA	3.08	1.48	1.38
24	C	510	CLA	C4D-CHA	3.08	1.48	1.38
24	C	511	CLA	C4D-CHA	3.06	1.48	1.38
24	D	403	CLA	C1B-C2B	3.06	1.50	1.43
24	a	410	CLA	C4D-CHA	3.06	1.48	1.38
24	B	605	CLA	C4D-CHA	3.05	1.48	1.38
24	b	611	CLA	C4D-CHA	3.04	1.48	1.38
24	B	614	CLA	C1B-C2B	3.04	1.50	1.43
24	c	507	CLA	C4D-CHA	3.04	1.48	1.38
24	C	508	CLA	C1B-C2B	3.04	1.50	1.43
24	B	616	CLA	C1B-NB	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	MG-NA	3.04	2.13	2.06
24	B	611	CLA	C4D-CHA	3.04	1.48	1.38
24	A	409	CLA	C1B-C2B	3.03	1.50	1.43
24	c	506	CLA	OBD-CAD	3.03	1.27	1.22
24	c	512	CLA	C1B-C2B	3.03	1.50	1.43
24	B	608	CLA	C1B-C2B	3.03	1.50	1.43
24	B	615	CLA	C1B-NB	-3.03	1.33	1.37
24	b	607	CLA	C1B-C2B	3.03	1.50	1.43
24	b	604	CLA	C4D-CHA	3.02	1.48	1.38
24	b	619	CLA	C4D-CHA	3.01	1.48	1.38
24	B	608	CLA	C4D-CHA	3.01	1.48	1.38
24	C	509	CLA	C4B-NB	-3.01	1.33	1.37
24	C	510	CLA	C4B-NB	-3.00	1.33	1.37
24	B	605	CLA	C1B-C2B	3.00	1.50	1.43
36	c	524	HTG	C1'-S1	-3.00	1.77	1.81
24	C	510	CLA	C1B-C2B	3.00	1.50	1.43
24	C	505	CLA	C1B-C2B	3.00	1.50	1.43
24	C	513	CLA	C4D-CHA	3.00	1.48	1.38
24	B	602	CLA	C4D-CHA	2.99	1.48	1.38
24	b	618	CLA	C1B-C2B	2.99	1.50	1.43
36	C	523	HTG	C1'-S1	-2.99	1.77	1.81
24	b	616	CLA	C1B-C2B	2.99	1.50	1.43
24	c	511	CLA	C1B-C2B	2.99	1.50	1.43
24	d	404	CLA	OBD-CAD	2.98	1.27	1.22
36	C	522	HTG	C1'-S1	-2.98	1.77	1.81
24	b	619	CLA	C1B-C2B	2.98	1.50	1.43
24	d	405	CLA	MG-NB	2.98	2.11	2.05
24	c	514	CLA	C1B-C2B	2.98	1.50	1.43
24	D	403	CLA	MG-NC	2.97	2.13	2.06
24	d	405	CLA	C1B-C2B	2.97	1.50	1.43
40	F	101	HEM	FE-NB	2.97	2.04	1.94
24	B	609	CLA	C1B-C2B	2.97	1.50	1.43
24	B	617	CLA	C1B-C2B	2.97	1.50	1.43
24	b	606	CLA	C1B-C2B	2.97	1.50	1.43
24	A	406	CLA	C4D-CHA	2.97	1.48	1.38
24	b	606	CLA	C4D-CHA	2.97	1.48	1.38
24	c	514	CLA	C1B-NB	-2.96	1.34	1.37
24	d	405	CLA	C4B-NB	-2.96	1.34	1.37
24	B	617	CLA	C4D-CHA	2.96	1.48	1.38
24	b	614	CLA	C1B-NB	-2.96	1.34	1.37
24	c	503	CLA	C1B-C2B	2.95	1.50	1.43
24	C	502	CLA	C4D-CHA	2.95	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C1B-NB	-2.95	1.34	1.37
24	b	608	CLA	C1B-NB	-2.95	1.34	1.37
24	b	605	CLA	C4D-CHA	2.94	1.48	1.38
24	B	604	CLA	C1B-NB	-2.94	1.34	1.37
24	b	617	CLA	C1B-C2B	2.94	1.50	1.43
24	b	612	CLA	C1B-C2B	2.94	1.50	1.43
40	f	101	HEM	CAC-C3C	2.94	1.55	1.47
24	b	619	CLA	C4B-NB	-2.94	1.34	1.37
24	b	611	CLA	C1B-NB	-2.93	1.34	1.37
24	a	408	CLA	C4D-CHA	2.93	1.48	1.38
24	b	608	CLA	C4D-CHA	2.93	1.48	1.38
24	b	617	CLA	C1B-NB	-2.93	1.34	1.37
24	c	504	CLA	C1B-C2B	2.92	1.50	1.43
24	c	513	CLA	C4B-NB	-2.92	1.34	1.37
24	B	616	CLA	C4D-CHA	2.92	1.48	1.38
24	D	403	CLA	C3D-C2D	2.92	1.47	1.39
24	C	514	CLA	MG-NB	2.91	2.11	2.05
24	c	514	CLA	C4D-CHA	2.91	1.48	1.38
40	F	101	HEM	CAC-C3C	2.91	1.55	1.47
24	A	405	CLA	C4D-CHA	2.91	1.48	1.38
24	A	409	CLA	C4D-CHA	2.91	1.48	1.38
24	C	505	CLA	C1B-NB	-2.91	1.34	1.37
24	b	616	CLA	C1B-NB	-2.91	1.34	1.37
24	c	510	CLA	C4D-CHA	2.90	1.48	1.38
24	C	503	CLA	C4B-NB	-2.90	1.34	1.37
24	B	603	CLA	C1B-C2B	2.90	1.49	1.43
24	b	615	CLA	C4D-CHA	2.89	1.48	1.38
24	c	506	CLA	MG-NC	2.89	2.13	2.06
24	b	612	CLA	C4D-CHA	2.88	1.48	1.38
24	B	603	CLA	C4D-CHA	2.88	1.48	1.38
24	b	614	CLA	OBD-CAD	2.87	1.27	1.22
24	B	610	CLA	C4D-CHA	2.87	1.48	1.38
24	c	506	CLA	C4D-CHA	2.86	1.48	1.38
24	A	406	CLA	C1B-NB	-2.86	1.34	1.37
24	A	407	CLA	C4B-NB	-2.86	1.34	1.37
24	c	515	CLA	C4D-CHA	2.86	1.48	1.38
24	C	512	CLA	C4B-NB	-2.86	1.34	1.37
24	B	607	CLA	C1B-C2B	2.86	1.49	1.43
24	C	513	CLA	C1B-NB	-2.86	1.34	1.37
24	b	613	CLA	C1B-NB	-2.86	1.34	1.37
24	B	609	CLA	C4B-NB	-2.85	1.34	1.37
24	b	614	CLA	C1B-C2B	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C1B-NB	-2.85	1.34	1.37
24	C	511	CLA	C4B-NB	-2.85	1.34	1.37
24	C	514	CLA	C1B-C2B	2.85	1.49	1.43
24	c	509	CLA	C1B-C2B	2.84	1.49	1.43
24	B	613	CLA	C4D-CHA	2.84	1.48	1.38
24	C	507	CLA	C4B-NB	-2.84	1.34	1.37
24	A	407	CLA	C1B-C2B	2.84	1.49	1.43
24	B	606	CLA	C4D-CHA	2.84	1.48	1.38
24	c	508	CLA	C4D-CHA	2.84	1.48	1.38
24	D	403	CLA	C4D-CHA	2.84	1.48	1.38
24	a	409	CLA	C4D-CHA	2.83	1.48	1.38
24	B	615	CLA	C1B-C2B	2.83	1.49	1.43
24	C	505	CLA	C4D-CHA	2.83	1.48	1.38
24	C	510	CLA	C1B-NB	-2.83	1.34	1.37
24	b	617	CLA	C4D-CHA	2.83	1.48	1.38
24	C	507	CLA	C4D-CHA	2.83	1.48	1.38
24	c	506	CLA	MG-NB	2.83	2.11	2.05
24	B	607	CLA	C1B-NB	-2.82	1.34	1.37
24	c	506	CLA	C1B-C2B	2.82	1.49	1.43
24	C	507	CLA	C1B-NB	-2.82	1.34	1.37
24	B	604	CLA	C1B-C2B	2.82	1.49	1.43
24	C	514	CLA	C4D-CHA	2.81	1.48	1.38
24	C	509	CLA	C4D-CHA	2.80	1.48	1.38
24	b	613	CLA	C4D-CHA	2.80	1.48	1.38
24	A	409	CLA	C1B-NB	-2.80	1.34	1.37
24	b	606	CLA	C1B-NB	-2.80	1.34	1.37
24	b	615	CLA	C1B-NB	-2.80	1.34	1.37
24	C	507	CLA	C1C-NC	-2.79	1.33	1.37
24	C	504	CLA	C4B-NB	-2.79	1.34	1.37
24	c	512	CLA	C4B-NB	-2.79	1.34	1.37
24	A	406	CLA	C1B-C2B	2.79	1.49	1.43
24	B	613	CLA	C1B-C2B	2.78	1.49	1.43
24	c	515	CLA	C1B-C2B	2.78	1.49	1.43
24	b	616	CLA	C4D-CHA	2.78	1.47	1.38
24	C	509	CLA	C1B-NB	-2.77	1.34	1.37
24	c	511	CLA	C1B-NB	-2.77	1.34	1.37
24	c	515	CLA	C1B-NB	-2.77	1.34	1.37
24	b	619	CLA	C1B-NB	-2.77	1.34	1.37
24	C	513	CLA	C1C-C2C	2.77	1.50	1.44
25	A	408	PHO	CHA-CBD	-2.77	1.48	1.51
24	A	409	CLA	C4B-NB	-2.77	1.34	1.37
24	c	504	CLA	C4D-CHA	2.76	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	C1C-NC	-2.76	1.33	1.37
24	d	405	CLA	C4D-CHA	2.76	1.47	1.38
24	C	511	CLA	C1C-C2C	2.76	1.50	1.44
33	d	407	PL9	C6-C5	2.75	1.48	1.35
24	B	612	CLA	C1B-NB	-2.75	1.34	1.37
24	b	604	CLA	C1B-C2B	2.75	1.49	1.43
24	c	510	CLA	C1B-C2B	2.74	1.49	1.43
39	H	102	DGD	O5D-C1E	2.74	1.44	1.40
24	D	404	CLA	C4D-CHA	2.73	1.47	1.38
24	C	510	CLA	C4C-C3C	2.73	1.49	1.45
33	a	425[B]	PL9	C6-C5	2.73	1.48	1.35
24	d	404	CLA	C4D-CHA	2.73	1.47	1.38
24	C	502	CLA	C1B-C2B	2.73	1.49	1.43
24	c	513	CLA	MG-ND	-2.72	2.00	2.05
24	B	612	CLA	C1B-C2B	2.72	1.49	1.43
24	D	404	CLA	C1B-NB	-2.72	1.34	1.37
33	A	422[B]	PL9	C6-C5	2.71	1.48	1.35
24	C	514	CLA	C1B-NB	-2.71	1.34	1.37
24	a	408	CLA	C1B-C2B	2.71	1.49	1.43
24	D	403	CLA	C4B-NB	-2.71	1.34	1.37
24	C	506	CLA	C4B-NB	-2.71	1.34	1.37
24	B	617	CLA	C4B-NB	-2.70	1.34	1.37
24	C	503	CLA	C1B-C2B	2.70	1.49	1.43
24	C	503	CLA	C1B-NB	-2.70	1.34	1.37
24	C	505	CLA	MG-ND	-2.70	2.00	2.05
24	B	608	CLA	C4C-C3C	2.70	1.49	1.45
24	D	404	CLA	C4B-NB	-2.70	1.34	1.37
24	b	613	CLA	C1B-C2B	2.69	1.49	1.43
24	b	605	CLA	C1B-C2B	2.69	1.49	1.43
24	C	502	CLA	C1C-C2C	2.69	1.50	1.44
24	C	513	CLA	C1B-C2B	2.69	1.49	1.43
24	B	616	CLA	MG-NC	2.68	2.12	2.06
24	a	412	CLA	C4B-NB	-2.68	1.34	1.37
24	B	609	CLA	C4C-C3C	2.68	1.49	1.45
24	b	607	CLA	C4C-C3C	2.68	1.49	1.45
24	a	412	CLA	C4D-CHA	2.68	1.47	1.38
24	c	510	CLA	C4B-NB	-2.68	1.34	1.37
33	D	406	PL9	C6-C5	2.68	1.48	1.35
24	c	509	CLA	C4B-NB	-2.68	1.34	1.37
43	V	202	HEC	CMC-C2C	2.67	1.56	1.50
24	B	607	CLA	MG-NB	-2.67	2.00	2.05
24	b	615	CLA	C1C-NC	-2.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	625	HTG	C1'-S1	-2.67	1.77	1.81
24	c	511	CLA	C1C-C2C	2.66	1.49	1.44
24	C	511	CLA	C1B-C2B	2.66	1.49	1.43
24	B	607	CLA	C4B-NB	-2.66	1.34	1.37
24	C	511	CLA	C1B-NB	-2.66	1.34	1.37
24	b	612	CLA	C1C-NC	-2.65	1.33	1.37
24	B	606	CLA	C1B-NB	-2.65	1.34	1.37
24	C	513	CLA	C4B-NB	-2.65	1.34	1.37
24	B	613	CLA	C1B-NB	-2.65	1.34	1.37
24	b	611	CLA	C1B-C2B	2.64	1.49	1.43
24	C	509	CLA	C4C-C3C	2.64	1.49	1.45
24	C	509	CLA	C1B-C2B	2.64	1.49	1.43
24	c	505	CLA	C4B-NB	-2.64	1.34	1.37
24	a	410	CLA	C1B-C2B	2.64	1.49	1.43
25	A	408	PHO	CBD-CGD	-2.64	1.49	1.52
24	A	407	CLA	C4D-CHA	2.64	1.47	1.38
24	C	514	CLA	C4B-NB	-2.63	1.34	1.37
24	b	611	CLA	C4B-NB	-2.63	1.34	1.37
24	c	505	CLA	C4C-C3C	2.63	1.49	1.45
24	b	616	CLA	MG-NB	2.62	2.11	2.05
24	D	403	CLA	C1B-NB	-2.62	1.34	1.37
39	h	1205	DGD	O5D-C1E	2.62	1.44	1.40
24	d	404	CLA	C1B-C2B	2.62	1.49	1.43
24	c	515	CLA	C1C-C2C	2.61	1.49	1.44
24	b	611	CLA	C1C-C2C	2.61	1.49	1.44
24	C	512	CLA	MG-NC	2.60	2.12	2.06
25	d	401	PHO	C3A-C2A	-2.59	1.52	1.54
24	b	613	CLA	C4C-C3C	2.59	1.49	1.45
24	b	608	CLA	C1B-C2B	2.59	1.49	1.43
24	b	613	CLA	MG-NB	2.59	2.10	2.05
40	f	101	HEM	FE-NA	2.59	2.03	1.95
24	A	407	CLA	C1C-NC	-2.58	1.33	1.37
24	b	608	CLA	C1C-C2C	2.58	1.49	1.44
29	z	101	LMT	O1'-C1'	2.58	1.44	1.40
24	c	507	CLA	C4C-C3C	2.58	1.49	1.45
24	b	611	CLA	C4C-C3C	2.57	1.49	1.45
24	B	617	CLA	C1B-NB	-2.57	1.34	1.37
24	C	507	CLA	C1B-C2B	2.56	1.49	1.43
24	C	514	CLA	C1C-C2C	2.56	1.49	1.44
24	b	619	CLA	C1C-NC	-2.56	1.33	1.37
24	A	405	CLA	C4B-NB	-2.56	1.34	1.37
24	B	603	CLA	C4B-NB	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C4C-C3C	2.56	1.49	1.45
24	c	511	CLA	C4B-NB	-2.55	1.34	1.37
24	C	505	CLA	C4B-NB	-2.55	1.34	1.37
24	c	511	CLA	C3B-C2B	2.55	1.49	1.41
24	B	607	CLA	MG-ND	-2.55	2.00	2.05
24	A	405	CLA	C1C-C2C	2.54	1.49	1.44
24	B	617	CLA	C1C-NC	-2.54	1.33	1.37
24	B	606	CLA	MG-ND	-2.54	2.00	2.05
24	B	604	CLA	C1C-NC	-2.54	1.33	1.37
24	a	409	CLA	C4B-NB	-2.54	1.34	1.37
25	d	401	PHO	C4B-NB	-2.54	1.34	1.38
24	b	606	CLA	C4B-NB	-2.54	1.34	1.37
24	C	514	CLA	C3B-C2B	2.54	1.49	1.41
24	b	615	CLA	C1C-C2C	2.54	1.49	1.44
25	a	411	PHO	C4B-NB	-2.53	1.34	1.38
24	B	611	CLA	C1B-C2B	2.53	1.49	1.43
24	b	612	CLA	C1B-NB	-2.53	1.34	1.37
24	C	510	CLA	MG-ND	-2.53	2.00	2.05
24	c	505	CLA	C1C-C2C	2.53	1.49	1.44
25	a	411	PHO	CHA-CBD	-2.53	1.48	1.51
24	b	604	CLA	C1B-NB	-2.52	1.34	1.37
24	B	609	CLA	C1B-NB	-2.52	1.34	1.37
24	A	405	CLA	C1B-C2B	2.52	1.49	1.43
24	c	514	CLA	C4C-C3C	2.51	1.49	1.45
24	B	604	CLA	C4D-CHA	2.51	1.47	1.38
24	b	606	CLA	C3B-C4B	2.51	1.50	1.42
24	C	512	CLA	C4C-C3C	2.51	1.49	1.45
24	c	510	CLA	C4C-C3C	2.51	1.49	1.45
24	C	514	CLA	C1C-NC	-2.51	1.33	1.37
24	A	409	CLA	C1C-C2C	2.50	1.49	1.44
24	B	602	CLA	C1B-C2B	2.50	1.49	1.43
24	b	605	CLA	C3B-C2B	2.50	1.49	1.41
24	b	605	CLA	C1B-NB	-2.50	1.34	1.37
24	a	410	CLA	C4B-NB	-2.50	1.34	1.37
24	b	609	CLA	C4B-NB	-2.49	1.34	1.37
24	c	515	CLA	C4B-NB	-2.49	1.34	1.37
24	C	513	CLA	C3B-C2B	2.49	1.49	1.41
24	C	504	CLA	C1B-C2B	2.49	1.49	1.43
36	D	413	HTG	C1-S1	-2.48	1.76	1.80
24	b	610	CLA	C4B-NB	-2.48	1.34	1.37
24	B	614	CLA	C1C-C2C	2.48	1.49	1.44
24	c	506	CLA	C1C-C2C	2.48	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	C3D-C4D	-2.48	1.38	1.44
24	C	509	CLA	C3B-C2B	2.48	1.49	1.41
24	b	618	CLA	C4B-NB	-2.47	1.34	1.37
24	C	502	CLA	C1B-NB	-2.47	1.34	1.37
24	a	410	CLA	C3D-C4D	-2.47	1.38	1.44
24	B	611	CLA	C1C-C2C	2.47	1.49	1.44
24	C	506	CLA	C1C-NC	-2.46	1.34	1.37
24	C	508	CLA	C4B-NB	-2.46	1.34	1.37
24	B	602	CLA	C3B-C4B	2.46	1.49	1.42
24	b	614	CLA	C4B-NB	-2.46	1.34	1.37
24	C	504	CLA	C1C-C2C	2.46	1.49	1.44
24	B	606	CLA	C4B-NB	-2.46	1.34	1.37
24	B	612	CLA	C3B-C2B	2.46	1.49	1.41
24	b	613	CLA	C4B-NB	-2.45	1.34	1.37
24	B	604	CLA	C3B-C4B	2.45	1.49	1.42
24	b	606	CLA	C1C-C2C	2.45	1.49	1.44
24	c	508	CLA	C1B-C2B	2.45	1.48	1.43
24	B	607	CLA	C4C-C3C	2.45	1.49	1.45
24	c	510	CLA	C3B-C2B	2.45	1.49	1.41
24	B	613	CLA	C4B-NB	-2.45	1.34	1.37
24	b	609	CLA	C1C-C2C	2.45	1.49	1.44
24	C	502	CLA	C3B-C4B	2.44	1.49	1.42
24	a	408	CLA	C4C-C3C	2.44	1.49	1.45
24	C	506	CLA	C1C-C2C	2.44	1.49	1.44
24	C	511	CLA	C3B-C2B	2.44	1.49	1.41
24	c	508	CLA	C3D-C4D	-2.44	1.38	1.44
24	B	603	CLA	C1C-C2C	2.44	1.49	1.44
24	c	505	CLA	C1C-NC	-2.44	1.34	1.37
24	C	510	CLA	C1C-NC	-2.44	1.34	1.37
24	c	515	CLA	C4C-C3C	2.43	1.49	1.45
24	b	614	CLA	C3B-C2B	2.43	1.49	1.41
24	b	615	CLA	C4B-NB	-2.43	1.34	1.37
24	b	618	CLA	C3B-C2B	2.42	1.49	1.41
24	b	610	CLA	C3B-C2B	2.42	1.49	1.41
24	b	617	CLA	C4B-NB	-2.42	1.34	1.37
39	c	520	DGD	O2G-C2G	-2.42	1.40	1.46
24	C	505	CLA	C3B-C2B	2.42	1.49	1.41
24	B	616	CLA	MG-NB	2.42	2.10	2.05
24	b	619	CLA	C3B-C2B	2.41	1.49	1.41
24	c	506	CLA	C3D-C4D	-2.41	1.38	1.44
24	A	405	CLA	C1B-NB	-2.41	1.34	1.37
24	c	512	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C4C-C3C	2.41	1.49	1.45
24	B	617	CLA	C3B-C2B	2.41	1.49	1.41
24	D	404	CLA	C1C-C2C	2.41	1.49	1.44
24	B	604	CLA	C1C-C2C	2.41	1.49	1.44
24	B	611	CLA	C1C-NC	-2.41	1.34	1.37
24	c	503	CLA	C1C-NC	-2.41	1.34	1.37
24	C	506	CLA	C4C-C3C	2.41	1.49	1.45
24	d	405	CLA	C4C-C3C	2.40	1.49	1.45
24	b	607	CLA	C1C-C2C	2.40	1.49	1.44
24	c	513	CLA	C1B-NB	-2.40	1.34	1.37
24	C	512	CLA	C1C-NC	-2.40	1.34	1.37
24	d	404	CLA	C1C-C2C	2.39	1.49	1.44
24	c	512	CLA	C1C-NC	-2.39	1.34	1.37
24	B	611	CLA	C3B-C4B	2.39	1.49	1.42
24	c	503	CLA	C4B-NB	-2.39	1.34	1.37
24	c	514	CLA	C3B-C2B	2.39	1.49	1.41
24	c	515	CLA	C3B-C4B	2.39	1.49	1.42
24	b	607	CLA	C1C-NC	-2.39	1.34	1.37
24	b	612	CLA	C4B-NB	-2.38	1.34	1.37
24	B	605	CLA	C1C-NC	-2.38	1.34	1.37
24	C	504	CLA	C1C-NC	-2.37	1.34	1.37
24	D	404	CLA	C1C-NC	-2.37	1.34	1.37
24	C	508	CLA	C1C-C2C	2.37	1.49	1.44
24	b	609	CLA	C3B-C2B	2.37	1.49	1.41
27	f	102	SQD	O47-C45	-2.37	1.43	1.46
24	c	504	CLA	C1B-NB	-2.36	1.34	1.37
24	B	605	CLA	C3B-C2B	2.36	1.49	1.41
24	D	403	CLA	C4C-C3C	2.36	1.49	1.45
24	d	404	CLA	C1C-NC	-2.36	1.34	1.37
24	B	603	CLA	C3D-C4D	-2.36	1.38	1.44
43	v	1603	HEC	CMD-C2D	2.36	1.55	1.50
24	b	618	CLA	C1C-NC	-2.35	1.34	1.37
24	b	612	CLA	C1C-C2C	2.35	1.49	1.44
24	C	502	CLA	C4C-C3C	2.35	1.49	1.45
24	b	611	CLA	MG-NB	2.35	2.10	2.05
24	B	617	CLA	MG-NB	2.35	2.10	2.05
24	b	609	CLA	C4C-C3C	2.35	1.49	1.45
24	A	405	CLA	C1C-NC	-2.35	1.34	1.37
25	D	401	PHO	C3D-C4D	-2.35	1.38	1.41
24	b	606	CLA	C3B-C2B	2.35	1.49	1.41
24	C	503	CLA	C1C-C2C	2.35	1.49	1.44
24	B	614	CLA	C3B-C2B	2.35	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C1C-C2C	2.35	1.49	1.44
24	c	514	CLA	C4B-NB	-2.35	1.34	1.37
24	b	606	CLA	C4C-C3C	2.35	1.49	1.45
24	D	403	CLA	C1C-NC	-2.34	1.34	1.37
24	b	616	CLA	C1C-C2C	2.34	1.49	1.44
24	c	508	CLA	MG-NB	2.34	2.10	2.05
24	b	605	CLA	C1C-NC	-2.34	1.34	1.37
24	C	507	CLA	C4C-C3C	2.34	1.49	1.45
24	b	609	CLA	C1B-NB	-2.34	1.34	1.37
24	B	609	CLA	C3B-C2B	2.34	1.49	1.41
32	A	421[A]	K3C	O2-C4	2.34	1.30	1.24
24	C	511	CLA	C1C-NC	-2.34	1.34	1.37
24	A	405	CLA	C3B-C2B	2.33	1.49	1.41
24	c	515	CLA	C3D-C4D	-2.33	1.38	1.44
24	b	604	CLA	C4C-C3C	2.33	1.49	1.45
24	B	602	CLA	C1B-NB	-2.33	1.34	1.37
24	b	613	CLA	C3B-C4B	2.33	1.49	1.42
24	b	607	CLA	C1B-NB	-2.33	1.34	1.37
24	B	611	CLA	C4B-NB	-2.33	1.34	1.37
24	C	513	CLA	C3B-C4B	2.33	1.49	1.42
24	C	504	CLA	C1B-NB	-2.33	1.34	1.37
24	c	503	CLA	C3B-C2B	2.33	1.49	1.41
24	C	503	CLA	C3B-C2B	2.33	1.49	1.41
24	a	408	CLA	C3B-C2B	2.33	1.49	1.41
24	B	602	CLA	C1C-C2C	2.32	1.49	1.44
24	B	602	CLA	C1C-NC	-2.32	1.34	1.37
24	b	616	CLA	C4C-C3C	2.32	1.49	1.45
24	C	512	CLA	C3B-C2B	2.32	1.49	1.41
24	b	614	CLA	C3D-C4D	-2.32	1.39	1.44
24	b	605	CLA	C4B-NB	-2.32	1.34	1.37
25	d	401	PHO	C1B-NB	-2.32	1.34	1.38
24	B	614	CLA	C4B-NB	-2.31	1.34	1.37
24	c	507	CLA	C1B-NB	-2.31	1.34	1.37
24	A	409	CLA	C3B-C4B	2.31	1.49	1.42
24	b	610	CLA	C4C-C3C	2.31	1.49	1.45
24	D	404	CLA	C3B-C2B	2.31	1.49	1.41
24	a	410	CLA	C3B-C4B	2.30	1.49	1.42
24	b	615	CLA	C3B-C2B	2.30	1.48	1.41
43	V	202	HEC	CMB-C2B	2.30	1.55	1.50
24	B	603	CLA	C3B-C2B	2.30	1.48	1.41
24	B	612	CLA	C4B-NB	-2.30	1.34	1.37
24	b	606	CLA	C1C-NC	-2.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	601	HTG	C1-S1	-2.30	1.76	1.80
24	b	604	CLA	C3B-C4B	2.30	1.49	1.42
24	C	504	CLA	C3B-C2B	2.29	1.48	1.41
24	c	513	CLA	C3B-C2B	2.29	1.48	1.41
24	b	605	CLA	C1C-C2C	2.29	1.49	1.44
24	a	410	CLA	MG-NC	2.29	2.11	2.06
32	a	424[A]	K3C	O2-C4	2.29	1.30	1.24
24	d	405	CLA	C3B-C2B	2.29	1.48	1.41
24	C	508	CLA	C1C-NC	-2.29	1.34	1.37
24	b	608	CLA	C3B-C4B	2.29	1.49	1.42
24	b	614	CLA	C1C-NC	-2.28	1.34	1.37
24	B	603	CLA	C3B-C4B	2.28	1.49	1.42
24	c	506	CLA	C3B-C2B	2.28	1.48	1.41
24	c	508	CLA	C3B-C4B	2.28	1.49	1.42
26	k	302	BCR	C30-C25	-2.28	1.50	1.53
24	c	514	CLA	C1C-C2C	2.28	1.49	1.44
24	C	504	CLA	C4C-C3C	2.28	1.48	1.45
24	C	503	CLA	C3B-C4B	2.28	1.49	1.42
36	b	602	HTG	C1-S1	-2.28	1.76	1.80
24	c	504	CLA	C3D-C4D	-2.27	1.39	1.44
24	c	514	CLA	C3D-C4D	-2.27	1.39	1.44
24	c	508	CLA	C3B-C2B	2.27	1.48	1.41
24	C	505	CLA	C1C-NC	-2.27	1.34	1.37
24	A	406	CLA	MG-NB	2.27	2.10	2.05
24	b	610	CLA	C1C-C2C	2.27	1.49	1.44
24	c	507	CLA	C1C-C2C	2.27	1.49	1.44
24	B	602	CLA	C3B-C2B	2.26	1.48	1.41
24	a	410	CLA	C4C-C3C	2.26	1.48	1.45
24	B	613	CLA	C1C-C2C	2.26	1.49	1.44
24	c	506	CLA	C4C-C3C	2.26	1.48	1.45
24	C	507	CLA	C1C-C2C	2.26	1.49	1.44
24	B	615	CLA	MG-NB	2.26	2.10	2.05
29	B	642	LMT	O1'-C1'	2.26	1.44	1.40
24	C	508	CLA	C3B-C2B	2.26	1.48	1.41
24	c	507	CLA	C4B-NB	-2.26	1.34	1.37
24	A	406	CLA	C3D-C4D	-2.26	1.39	1.44
25	D	401	PHO	C4B-NB	-2.25	1.34	1.38
24	B	609	CLA	C1C-C2C	2.25	1.49	1.44
24	c	509	CLA	C1C-C2C	2.25	1.49	1.44
24	b	604	CLA	C1C-NC	-2.25	1.34	1.37
24	b	607	CLA	C4B-NB	-2.25	1.34	1.37
24	B	612	CLA	C1C-C2C	2.25	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C1C-NC	-2.25	1.34	1.37
43	v	1603	HEC	CMC-C2C	2.25	1.55	1.50
24	b	617	CLA	C3B-C4B	2.25	1.49	1.42
24	b	618	CLA	C1B-NB	-2.25	1.34	1.37
24	a	412	CLA	C1C-NC	-2.25	1.34	1.37
24	C	509	CLA	C1C-C2C	2.25	1.49	1.44
24	b	608	CLA	C1C-NC	-2.25	1.34	1.37
24	A	409	CLA	C3B-C2B	2.25	1.48	1.41
24	b	612	CLA	C3B-C2B	2.25	1.48	1.41
24	b	607	CLA	C3D-C4D	-2.24	1.39	1.44
24	c	512	CLA	C3B-C2B	2.24	1.48	1.41
24	b	616	CLA	C4B-NB	-2.24	1.34	1.37
24	B	612	CLA	C4C-C3C	2.24	1.48	1.45
24	B	606	CLA	C1C-NC	-2.24	1.34	1.37
24	b	617	CLA	C1C-NC	-2.24	1.34	1.37
24	b	605	CLA	C4C-C3C	2.24	1.48	1.45
24	c	509	CLA	C3B-C2B	2.24	1.48	1.41
24	d	404	CLA	C3D-C4D	-2.24	1.39	1.44
24	c	512	CLA	C3D-C4D	-2.23	1.39	1.44
24	b	608	CLA	MG-ND	-2.23	2.01	2.05
24	B	604	CLA	C3B-C2B	2.23	1.48	1.41
36	c	524	HTG	C1-S1	-2.23	1.77	1.80
24	C	510	CLA	C3B-C2B	2.23	1.48	1.41
24	D	404	CLA	C3B-C4B	2.23	1.49	1.42
24	a	408	CLA	C3B-C4B	2.23	1.49	1.42
24	B	604	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	507	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	611	CLA	C3B-C2B	2.23	1.48	1.41
24	B	606	CLA	C3B-C2B	2.22	1.48	1.41
24	c	510	CLA	C1C-C2C	2.22	1.49	1.44
24	d	405	CLA	C1C-C2C	2.22	1.49	1.44
24	b	604	CLA	C1C-C2C	2.22	1.49	1.44
24	B	606	CLA	C1C-C2C	2.22	1.49	1.44
24	B	616	CLA	C1C-NC	-2.22	1.34	1.37
24	c	505	CLA	C1B-NB	-2.22	1.34	1.37
24	b	604	CLA	C3B-C2B	2.22	1.48	1.41
24	c	511	CLA	C1C-NC	-2.22	1.34	1.37
24	c	515	CLA	C3B-C2B	2.22	1.48	1.41
24	b	619	CLA	C3D-C4D	-2.22	1.39	1.44
24	c	504	CLA	C3B-C2B	2.21	1.48	1.41
24	D	403	CLA	C3B-C2B	2.21	1.48	1.41
24	d	405	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C3B-C2B	2.21	1.48	1.41
24	c	508	CLA	C1C-C2C	2.21	1.49	1.44
24	A	409	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	617	CLA	C1C-C2C	2.21	1.49	1.44
24	b	611	CLA	C3B-C2B	2.21	1.48	1.41
24	b	616	CLA	C3B-C2B	2.21	1.48	1.41
24	a	408	CLA	C1C-C2C	2.20	1.49	1.44
24	b	611	CLA	C3B-C4B	2.20	1.49	1.42
24	c	510	CLA	C1C-NC	-2.20	1.34	1.37
24	B	607	CLA	C1C-C2C	2.20	1.49	1.44
24	a	410	CLA	MG-NB	2.20	2.10	2.05
24	C	511	CLA	C3D-C4D	-2.20	1.39	1.44
24	c	505	CLA	C3B-C2B	2.20	1.48	1.41
24	b	605	CLA	C3B-C4B	2.20	1.49	1.42
24	b	607	CLA	C3B-C2B	2.20	1.48	1.41
24	A	407	CLA	C3B-C2B	2.20	1.48	1.41
24	a	410	CLA	C1C-C2C	2.20	1.49	1.44
24	B	610	CLA	C3B-C2B	2.20	1.48	1.41
24	b	613	CLA	C3B-C2B	2.20	1.48	1.41
24	B	611	CLA	C4C-C3C	2.20	1.48	1.45
24	B	611	CLA	C3D-C4D	-2.19	1.39	1.44
24	D	403	CLA	C1C-C2C	2.19	1.49	1.44
24	C	514	CLA	C3D-C4D	-2.19	1.39	1.44
24	c	503	CLA	C3D-C4D	-2.19	1.39	1.44
25	d	401	PHO	CBD-CGD	-2.19	1.49	1.52
24	A	406	CLA	C3B-C4B	2.19	1.49	1.42
24	B	606	CLA	C4C-C3C	2.19	1.48	1.45
24	C	506	CLA	C3B-C2B	2.19	1.48	1.41
24	c	510	CLA	C3B-C4B	2.19	1.49	1.42
24	c	508	CLA	C1C-NC	-2.19	1.34	1.37
24	B	604	CLA	C4B-NB	-2.19	1.35	1.37
24	B	602	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	614	CLA	C3B-C4B	2.18	1.49	1.42
24	C	508	CLA	C4C-C3C	2.18	1.48	1.45
24	b	605	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	613	CLA	C1C-NC	-2.18	1.34	1.37
33	D	406	PL9	C2-C3	2.18	1.40	1.34
24	B	607	CLA	C3B-C2B	2.17	1.48	1.41
24	C	502	CLA	C3B-C2B	2.17	1.48	1.41
24	C	505	CLA	C1C-C2C	2.17	1.48	1.44
24	c	512	CLA	C4C-C3C	2.17	1.48	1.45
24	B	616	CLA	C3B-C2B	2.17	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C1C-NC	-2.17	1.34	1.37
24	b	604	CLA	C3D-C4D	-2.17	1.39	1.44
24	A	409	CLA	C4C-C3C	2.17	1.48	1.45
24	c	509	CLA	C4C-C3C	2.17	1.48	1.45
37	D	409	LHG	O7-C5	-2.17	1.41	1.46
26	D	405	BCR	C30-C25	-2.16	1.51	1.53
37	B	640	LHG	O7-C5	-2.16	1.41	1.46
24	b	608	CLA	C4B-NB	-2.16	1.35	1.37
24	b	617	CLA	C3B-C2B	2.16	1.48	1.41
24	A	406	CLA	C4C-C3C	2.16	1.48	1.45
40	F	101	HEM	CMA-C3A	2.16	1.55	1.50
24	b	609	CLA	C3B-C4B	2.16	1.49	1.42
36	I	102	HTG	C1-S1	-2.16	1.77	1.80
24	C	510	CLA	C1C-C2C	2.16	1.48	1.44
24	B	610	CLA	C1C-C2C	2.16	1.48	1.44
24	c	504	CLA	C1C-NC	-2.16	1.34	1.37
24	A	406	CLA	C3B-C2B	2.15	1.48	1.41
24	c	507	CLA	C3B-C2B	2.15	1.48	1.41
25	A	408	PHO	C4B-NB	-2.15	1.34	1.38
24	B	602	CLA	C4B-NB	-2.15	1.35	1.37
24	c	510	CLA	C3D-C4D	-2.14	1.39	1.44
24	C	513	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	602	CLA	C4C-C3C	2.14	1.48	1.45
25	a	411	PHO	C1D-ND	-2.14	1.34	1.38
24	b	618	CLA	C4C-C3C	2.14	1.48	1.45
24	C	512	CLA	C1C-C2C	2.13	1.48	1.44
24	b	618	CLA	C3D-C4D	-2.13	1.39	1.44
24	C	509	CLA	C3B-C4B	2.13	1.49	1.42
24	C	507	CLA	C3D-C4D	-2.13	1.39	1.44
24	C	504	CLA	C3B-C4B	2.13	1.49	1.42
24	b	606	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	608	CLA	C1C-C2C	2.13	1.48	1.44
24	b	615	CLA	C4C-C3C	2.13	1.48	1.45
24	b	604	CLA	C4B-NB	-2.13	1.35	1.37
24	c	506	CLA	C1C-NC	-2.13	1.34	1.37
43	V	202	HEC	CMD-C2D	2.13	1.55	1.50
36	h	1202	HTG	C1-S1	-2.12	1.77	1.80
29	m	101	LMT	O1'-C1'	2.12	1.43	1.40
24	B	606	CLA	C3D-C4D	-2.12	1.39	1.44
33	a	425[B]	PL9	C2-C3	2.12	1.40	1.34
24	B	610	CLA	C4C-C3C	2.12	1.48	1.45
24	C	509	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C1C-C2C	2.12	1.48	1.44
24	b	619	CLA	C4C-C3C	2.12	1.48	1.45
24	b	607	CLA	C3B-C4B	2.12	1.48	1.42
24	c	503	CLA	C4C-C3C	2.11	1.48	1.45
24	C	503	CLA	C3D-C4D	-2.11	1.39	1.44
40	f	101	HEM	CMB-C2B	2.11	1.55	1.50
24	a	409	CLA	C3B-C2B	2.11	1.48	1.41
24	C	505	CLA	C4C-C3C	2.11	1.48	1.45
24	B	610	CLA	C1C-NC	-2.11	1.34	1.37
43	V	202	HEC	CMA-C3A	2.11	1.55	1.50
39	D	407	DGD	O3G-C1D	2.11	1.43	1.40
24	b	617	CLA	C4C-C3C	2.10	1.48	1.45
24	c	508	CLA	C4C-C3C	2.10	1.48	1.45
24	A	406	CLA	C1C-NC	-2.10	1.34	1.37
30	b	630	GOL	C3-C2	2.10	1.59	1.51
24	c	511	CLA	C4C-C3C	2.10	1.48	1.45
33	A	422[B]	PL9	C2-C3	2.10	1.39	1.34
24	b	612	CLA	C4C-C3C	2.10	1.48	1.45
24	c	504	CLA	C3B-C4B	2.10	1.48	1.42
24	C	510	CLA	C3D-C4D	-2.09	1.39	1.44
36	c	525	HTG	C1-S1	-2.09	1.77	1.80
24	B	608	CLA	C4B-NB	-2.09	1.35	1.37
24	b	614	CLA	C1C-C2C	2.09	1.48	1.44
24	b	611	CLA	C3D-C4D	-2.09	1.39	1.44
24	c	503	CLA	C1C-C2C	2.09	1.48	1.44
24	b	617	CLA	C3D-C4D	-2.09	1.39	1.44
24	B	610	CLA	C1B-NB	-2.09	1.35	1.37
24	a	412	CLA	C3B-C4B	2.09	1.48	1.42
24	B	608	CLA	C3D-C4D	-2.09	1.39	1.44
26	d	406	BCR	C30-C25	-2.08	1.51	1.53
24	c	504	CLA	C1C-C2C	2.08	1.48	1.44
24	C	508	CLA	C3D-C4D	-2.08	1.39	1.44
24	b	608	CLA	C3D-C4D	-2.08	1.39	1.44
24	C	514	CLA	C3B-C4B	2.08	1.48	1.42
29	c	523	LMT	O1'-C1'	2.08	1.43	1.40
24	c	503	CLA	C1B-NB	-2.08	1.35	1.37
24	B	612	CLA	C3B-C4B	2.08	1.48	1.42
24	c	505	CLA	C3B-C4B	2.07	1.48	1.42
24	A	405	CLA	C4C-C3C	2.07	1.48	1.45
24	d	404	CLA	C3B-C2B	2.07	1.48	1.41
24	C	511	CLA	C4C-C3C	2.07	1.48	1.45
24	B	608	CLA	C3B-C2B	2.07	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	C1C-NC	-2.07	1.34	1.37
36	B	624	HTG	C1-S1	-2.06	1.77	1.80
24	C	503	CLA	C4C-C3C	2.06	1.48	1.45
24	a	412	CLA	C1C-C2C	2.06	1.48	1.44
24	B	616	CLA	C3D-C4D	-2.06	1.39	1.44
24	D	403	CLA	C3D-C4D	-2.06	1.39	1.44
24	B	613	CLA	C1C-NC	-2.06	1.34	1.37
40	F	101	HEM	CMB-C2B	2.06	1.55	1.50
24	a	409	CLA	C1C-C2C	2.05	1.48	1.44
24	c	512	CLA	C3B-C4B	2.05	1.48	1.42
24	b	614	CLA	C4C-C3C	2.05	1.48	1.45
24	B	615	CLA	C3B-C4B	2.05	1.48	1.42
24	C	502	CLA	C4B-NB	-2.05	1.35	1.37
24	C	502	CLA	MG-NB	2.05	2.09	2.05
24	B	602	CLA	MG-NB	2.05	2.09	2.05
43	v	1603	HEC	C3B-C2B	-2.05	1.34	1.41
24	c	507	CLA	C1C-NC	-2.05	1.34	1.37
24	b	613	CLA	C3D-C4D	-2.04	1.39	1.44
24	B	606	CLA	C3B-C4B	2.04	1.48	1.42
24	C	512	CLA	C1B-NB	-2.04	1.35	1.37
24	c	513	CLA	C1C-C2C	2.04	1.48	1.44
24	B	613	CLA	C3B-C4B	2.04	1.48	1.42
24	C	503	CLA	C1C-NC	-2.04	1.34	1.37
24	b	608	CLA	C3B-C2B	2.04	1.48	1.41
24	C	502	CLA	C1C-NC	-2.04	1.34	1.37
24	a	408	CLA	C3D-C4D	-2.04	1.39	1.44
24	b	618	CLA	C3B-C4B	2.03	1.48	1.42
24	b	616	CLA	C3D-C4D	-2.03	1.39	1.44
27	L	101	SQD	O6-C1	2.03	1.43	1.40
24	b	616	CLA	C3B-C4B	2.03	1.48	1.42
24	B	608	CLA	C3B-C4B	2.03	1.48	1.42
29	a	402	LMT	O1'-C1'	2.03	1.43	1.40
24	B	615	CLA	C3B-C2B	2.02	1.48	1.41
24	C	506	CLA	C3D-C4D	-2.02	1.39	1.44
24	A	407	CLA	C3B-C4B	2.02	1.48	1.42
24	B	602	CLA	C1D-C2D	2.02	1.49	1.45
24	c	513	CLA	C3B-C4B	2.02	1.48	1.42
24	b	609	CLA	C3D-C4D	-2.02	1.39	1.44
43	v	1603	HEC	CMB-C2B	2.02	1.54	1.50
24	b	610	CLA	C1C-NC	-2.02	1.34	1.37
24	B	612	CLA	C1C-NC	-2.01	1.34	1.37
24	c	515	CLA	C1C-NC	-2.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C3B-C4B	2.01	1.48	1.42
24	c	511	CLA	C3D-C4D	-2.01	1.39	1.44
24	b	618	CLA	C1C-C2C	2.01	1.48	1.44
28	d	411	LMG	O7-C8	-2.01	1.41	1.46
25	d	401	PHO	CHA-CBD	-2.00	1.49	1.51
24	C	512	CLA	C3B-C4B	2.00	1.48	1.42
36	C	522	HTG	C1-S1	-2.00	1.77	1.80

All (2586) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	C2D-C1D-ND	12.01	118.11	109.43
25	D	401	PHO	C2D-C1D-ND	11.67	117.87	109.43
25	a	411	PHO	C2D-C1D-ND	11.30	117.60	109.43
25	d	401	PHO	C2D-C1D-ND	10.88	117.30	109.43
24	B	604	CLA	C1D-ND-C4D	-10.79	98.74	106.31
24	D	403	CLA	C1D-ND-C4D	-10.72	98.79	106.31
24	c	503	CLA	C1D-ND-C4D	-10.60	98.88	106.31
24	a	409	CLA	C1D-ND-C4D	-10.21	99.15	106.31
24	B	605	CLA	C1D-ND-C4D	-10.08	99.24	106.31
24	B	613	CLA	C1D-ND-C4D	-10.08	99.24	106.31
24	c	504	CLA	C1D-ND-C4D	-10.05	99.26	106.31
24	A	406	CLA	C1D-ND-C4D	-9.97	99.32	106.31
24	b	615	CLA	C1D-ND-C4D	-9.91	99.36	106.31
24	A	409	CLA	C1D-ND-C4D	-9.91	99.36	106.31
24	c	510	CLA	C1D-ND-C4D	-9.81	99.43	106.31
24	b	616	CLA	C1D-ND-C4D	-9.77	99.45	106.31
24	b	617	CLA	C1D-ND-C4D	-9.68	99.52	106.31
24	a	410	CLA	C1D-ND-C4D	-9.67	99.52	106.31
24	B	612	CLA	C1D-ND-C4D	-9.64	99.55	106.31
24	c	506	CLA	C1D-ND-C4D	-9.57	99.60	106.31
24	B	616	CLA	C1D-ND-C4D	-9.57	99.60	106.31
24	a	408	CLA	C1D-ND-C4D	-9.55	99.61	106.31
24	b	608	CLA	C1D-ND-C4D	-9.51	99.64	106.31
24	d	404	CLA	C1D-ND-C4D	-9.47	99.67	106.31
24	B	614	CLA	C1D-ND-C4D	-9.39	99.72	106.31
24	C	514	CLA	C1D-ND-C4D	-9.37	99.74	106.31
24	C	507	CLA	C1D-ND-C4D	-9.37	99.74	106.31
24	c	512	CLA	C1D-ND-C4D	-9.35	99.75	106.31
24	A	407	CLA	C1D-ND-C4D	-9.34	99.76	106.31
24	C	505	CLA	C1D-ND-C4D	-9.33	99.76	106.31
24	b	612	CLA	C1D-ND-C4D	-9.28	99.80	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C1D-ND-C4D	-9.28	99.80	106.31
24	C	511	CLA	C1D-ND-C4D	-9.23	99.84	106.31
24	c	514	CLA	C1D-ND-C4D	-9.23	99.84	106.31
24	B	617	CLA	C1D-ND-C4D	-9.22	99.84	106.31
24	b	611	CLA	C1D-ND-C4D	-9.18	99.87	106.31
24	B	615	CLA	C1D-ND-C4D	-9.16	99.89	106.31
24	B	608	CLA	C1D-ND-C4D	-9.15	99.90	106.31
24	a	412	CLA	C1D-ND-C4D	-9.12	99.92	106.31
24	c	509	CLA	C1D-ND-C4D	-9.06	99.95	106.31
24	C	509	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	B	610	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	b	606	CLA	C1D-ND-C4D	-8.99	100.01	106.31
24	D	404	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	d	405	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	b	613	CLA	C1D-ND-C4D	-8.84	100.11	106.31
24	c	508	CLA	C1D-ND-C4D	-8.81	100.13	106.31
24	B	607	CLA	C1D-ND-C4D	-8.81	100.13	106.31
25	a	411	PHO	O2D-CGD-CBD	8.79	120.60	110.95
24	b	614	CLA	C1D-ND-C4D	-8.73	100.19	106.31
24	B	603	CLA	C1D-ND-C4D	-8.70	100.21	106.31
24	c	513	CLA	C1D-ND-C4D	-8.68	100.22	106.31
24	b	619	CLA	C1D-ND-C4D	-8.66	100.23	106.31
24	c	507	CLA	C1D-ND-C4D	-8.66	100.24	106.31
24	B	602	CLA	C1D-ND-C4D	-8.64	100.25	106.31
24	c	515	CLA	C1D-ND-C4D	-8.62	100.27	106.31
24	B	609	CLA	C1D-ND-C4D	-8.62	100.27	106.31
24	b	610	CLA	C1D-ND-C4D	-8.60	100.28	106.31
24	C	503	CLA	C1D-ND-C4D	-8.56	100.31	106.31
25	A	408	PHO	C3B-C4B-NB	8.55	113.04	107.46
24	C	502	CLA	C1D-ND-C4D	-8.52	100.33	106.31
24	A	405	CLA	C1D-ND-C4D	-8.47	100.37	106.31
24	B	606	CLA	C1D-ND-C4D	-8.46	100.38	106.31
24	b	618	CLA	C1D-ND-C4D	-8.46	100.38	106.31
24	C	506	CLA	C1D-ND-C4D	-8.46	100.38	106.31
24	B	611	CLA	C1D-ND-C4D	-8.44	100.39	106.31
24	b	605	CLA	C1D-ND-C4D	-8.32	100.47	106.31
25	D	401	PHO	O2D-CGD-CBD	8.32	120.09	110.95
24	b	604	CLA	C1D-ND-C4D	-8.32	100.48	106.31
24	c	511	CLA	C1D-ND-C4D	-8.20	100.56	106.31
24	b	607	CLA	C1D-ND-C4D	-8.19	100.56	106.31
24	C	510	CLA	C1D-ND-C4D	-8.17	100.58	106.31
24	C	504	CLA	C1D-ND-C4D	-8.12	100.62	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	C1D-ND-C4D	-8.09	100.63	106.31
24	C	508	CLA	C1D-ND-C4D	-8.06	100.66	106.31
25	d	401	PHO	O2D-CGD-CBD	7.95	119.68	110.95
24	C	512	CLA	C1D-ND-C4D	-7.95	100.74	106.31
24	c	505	CLA	C1D-ND-C4D	-7.86	100.80	106.31
25	a	411	PHO	C3B-C4B-NB	7.24	112.18	107.46
25	D	401	PHO	C3B-C4B-NB	7.21	112.16	107.46
25	A	408	PHO	O2D-CGD-CBD	7.15	118.81	110.95
24	D	403	CLA	C2D-C1D-ND	7.13	117.18	110.13
24	a	409	CLA	C2D-C1D-ND	7.09	117.14	110.13
25	d	401	PHO	C3B-C4B-NB	7.04	112.05	107.46
24	c	509	CLA	O2D-CGD-CBD	7.03	123.52	111.23
24	B	614	CLA	C2D-C1D-ND	6.94	117.00	110.13
25	D	401	PHO	C2B-C1B-NB	6.93	114.44	109.43
24	c	503	CLA	C2D-C1D-ND	6.92	116.97	110.13
24	c	514	CLA	O2D-CGD-CBD	6.91	123.30	111.23
24	d	404	CLA	CMD-C2D-C1D	6.87	136.83	124.73
24	c	508	CLA	CMD-C2D-C1D	6.81	136.71	124.73
24	b	616	CLA	CMD-C2D-C1D	6.80	136.70	124.73
24	B	615	CLA	CMD-C2D-C1D	6.72	136.56	124.73
24	c	506	CLA	C2D-C1D-ND	6.71	116.77	110.13
24	B	616	CLA	C2D-C1D-ND	6.62	116.67	110.13
24	B	602	CLA	CMD-C2D-C1D	6.61	136.36	124.73
24	A	409	CLA	C2D-C1D-ND	6.57	116.63	110.13
24	B	613	CLA	C2D-C1D-ND	6.54	116.60	110.13
25	a	411	PHO	C2B-C1B-NB	6.50	114.13	109.43
24	A	406	CLA	C2D-C1D-ND	6.48	116.54	110.13
24	b	607	CLA	CMD-C2D-C1D	6.48	136.13	124.73
24	c	507	CLA	O2D-CGD-CBD	6.47	122.54	111.23
24	b	615	CLA	C2D-C1D-ND	6.46	116.52	110.13
25	A	408	PHO	C2B-C1B-NB	6.45	114.09	109.43
36	h	1202	HTG	C1'-S1-C1	6.44	114.35	100.45
24	c	507	CLA	CMD-C2D-C1D	6.43	136.05	124.73
24	B	608	CLA	C2D-C1D-ND	6.43	116.49	110.13
24	B	612	CLA	C2D-C1D-ND	6.42	116.48	110.13
24	d	405	CLA	CMD-C2D-C1D	6.41	136.02	124.73
24	B	607	CLA	CMD-C2D-C1D	6.37	135.95	124.73
24	B	604	CLA	C2D-C1D-ND	6.35	116.41	110.13
24	b	617	CLA	C2D-C1D-ND	6.34	116.40	110.13
24	B	615	CLA	C2D-C1D-ND	6.32	116.38	110.13
24	c	503	CLA	CMD-C2D-C1D	6.31	135.85	124.73
24	B	612	CLA	CMD-C2D-C1D	6.30	135.82	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	CMD-C2D-C1D	6.28	135.78	124.73
24	b	607	CLA	O2D-CGD-CBD	6.27	122.19	111.23
24	c	504	CLA	C2D-C1D-ND	6.27	116.33	110.13
24	B	617	CLA	C2D-C1D-ND	6.26	116.33	110.13
24	C	508	CLA	CMD-C2D-C1D	6.25	135.74	124.73
24	b	605	CLA	O2D-CGD-CBD	6.25	122.16	111.23
24	B	604	CLA	CMD-C2D-C1D	6.25	135.73	124.73
24	b	608	CLA	C2D-C1D-ND	6.24	116.30	110.13
24	c	513	CLA	C2D-C1D-ND	6.23	116.30	110.13
24	c	509	CLA	C2D-C1D-ND	6.21	116.27	110.13
24	B	617	CLA	O2D-CGD-CBD	6.20	122.07	111.23
24	a	408	CLA	CMD-C2D-C1D	6.20	135.64	124.73
24	b	608	CLA	CMD-C2D-C1D	6.19	135.63	124.73
24	B	607	CLA	C2D-C1D-ND	6.18	116.25	110.13
25	D	401	PHO	C4D-ND-C1D	-6.18	101.47	108.87
24	B	605	CLA	CMD-C2D-C1D	6.17	135.60	124.73
24	B	603	CLA	CMD-C2D-C1D	6.17	135.59	124.73
25	d	401	PHO	C4D-ND-C1D	-6.16	101.49	108.87
24	C	514	CLA	CMD-C2D-C1D	6.15	135.55	124.73
24	b	616	CLA	C2D-C1D-ND	6.14	116.21	110.13
24	c	512	CLA	CMD-C2D-C1D	6.14	135.53	124.73
24	C	505	CLA	C2D-C1D-ND	6.11	116.18	110.13
25	d	401	PHO	C2B-C1B-NB	6.11	113.85	109.43
24	b	617	CLA	CMD-C2D-C1D	6.10	135.47	124.73
24	b	612	CLA	CMD-C2D-C1D	6.09	135.44	124.73
27	L	102	SQD	O6-C1-C2	6.07	117.50	108.27
24	D	403	CLA	CMD-C2D-C1D	6.07	135.41	124.73
25	A	408	PHO	C4D-ND-C1D	-6.06	101.62	108.87
24	D	404	CLA	CMD-C2D-C1D	6.05	135.38	124.73
24	B	602	CLA	O2D-CGD-CBD	6.05	121.81	111.23
24	C	510	CLA	CMD-C2D-C1D	6.04	135.37	124.73
24	b	619	CLA	O2D-CGD-CBD	6.04	121.79	111.23
24	B	605	CLA	C2D-C1D-ND	6.04	116.11	110.13
24	B	604	CLA	O2D-CGD-CBD	6.03	121.77	111.23
24	B	611	CLA	CMD-C2D-C1D	6.01	135.32	124.73
24	c	511	CLA	CMD-C2D-C1D	6.01	135.32	124.73
24	c	514	CLA	C2D-C1D-ND	6.01	116.08	110.13
24	b	606	CLA	O2D-CGD-CBD	6.01	121.73	111.23
27	a	414	SQD	O6-C1-C2	5.99	117.37	108.27
24	C	511	CLA	O2D-CGD-CBD	5.98	121.69	111.23
24	b	609	CLA	CMD-C2D-C1D	5.97	135.23	124.73
27	D	408	SQD	O6-C1-C2	5.96	117.32	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	C2D-C1D-ND	5.95	116.02	110.13
24	c	510	CLA	C2D-C1D-ND	5.94	116.00	110.13
24	C	502	CLA	O2D-CGD-CBD	5.92	121.59	111.23
24	C	502	CLA	CMD-C2D-C1D	5.92	135.16	124.73
24	C	507	CLA	CMD-C2D-C1D	5.92	135.15	124.73
24	b	619	CLA	C2D-C1D-ND	5.91	115.98	110.13
24	b	604	CLA	CMD-C2D-C1D	5.90	135.12	124.73
24	a	410	CLA	C2D-C1D-ND	5.88	115.94	110.13
24	b	614	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	b	605	CLA	CMD-C2D-C1D	5.86	135.04	124.73
24	C	512	CLA	C2D-C1D-ND	5.86	115.92	110.13
25	a	411	PHO	C4D-ND-C1D	-5.85	101.86	108.87
24	C	513	CLA	C2D-C1D-ND	5.81	115.88	110.13
24	C	514	CLA	C2D-C1D-ND	5.81	115.88	110.13
24	B	608	CLA	CMD-C2D-C1D	5.81	134.96	124.73
24	a	408	CLA	C2D-C1D-ND	5.80	115.87	110.13
24	b	618	CLA	C2D-C1D-ND	5.79	115.86	110.13
24	b	610	CLA	CMD-C2D-C1D	5.79	134.93	124.73
24	C	511	CLA	C2D-C1D-ND	5.79	115.86	110.13
24	C	506	CLA	CMD-C2D-C1D	5.78	134.91	124.73
36	b	626	HTG	C1'-S1-C1	5.78	112.93	100.45
24	C	509	CLA	C2D-C1D-ND	5.78	115.84	110.13
24	A	407	CLA	CMD-C2D-C1D	5.77	134.89	124.73
24	b	618	CLA	CMD-C2D-C1D	5.76	134.87	124.73
24	b	617	CLA	O2D-CGD-CBD	5.76	121.30	111.23
24	C	508	CLA	O2D-CGD-CBD	5.74	121.27	111.23
24	C	504	CLA	CMD-C2D-C1D	5.74	134.83	124.73
24	B	611	CLA	C2D-C1D-ND	5.72	115.79	110.13
24	a	410	CLA	CMD-C2D-C1D	5.72	134.80	124.73
29	z	101	LMT	O1'-C1'-C2'	5.72	114.74	108.14
24	B	613	CLA	O2D-CGD-CBD	5.72	121.22	111.23
24	b	615	CLA	O2D-CGD-CBD	5.71	121.21	111.23
24	b	606	CLA	CMD-C2D-C1D	5.69	134.76	124.73
24	a	412	CLA	C2D-C1D-ND	5.69	115.76	110.13
24	d	404	CLA	C2D-C1D-ND	5.69	115.75	110.13
24	B	609	CLA	C2D-C1D-ND	5.68	115.75	110.13
24	b	612	CLA	C2D-C1D-ND	5.68	115.75	110.13
27	A	411	SQD	O6-C1-C2	5.68	116.89	108.27
24	b	619	CLA	CMD-C2D-C1D	5.68	134.72	124.73
24	B	610	CLA	C2D-C1D-ND	5.67	115.74	110.13
24	c	515	CLA	CMD-C2D-C1D	5.66	134.70	124.73
24	c	505	CLA	C2D-C1D-ND	5.66	115.73	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	511	CLA	C2D-C1D-ND	5.64	115.70	110.13
24	C	513	CLA	O2D-CGD-CBD	5.61	121.04	111.23
25	d	401	PHO	C3D-C4D-ND	5.61	114.90	107.71
24	b	611	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	b	613	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	C	507	CLA	C2D-C1D-ND	5.60	115.66	110.13
24	c	503	CLA	O2D-CGD-CBD	5.58	120.99	111.23
24	A	406	CLA	CMD-C2D-C1D	5.58	134.55	124.73
24	A	407	CLA	C2D-C1D-ND	5.57	115.64	110.13
24	d	405	CLA	C2D-C1D-ND	5.57	115.63	110.13
24	c	510	CLA	O2D-CGD-CBD	5.55	120.94	111.23
24	C	504	CLA	C2D-C1D-ND	5.55	115.62	110.13
24	C	505	CLA	CMD-C2D-C1D	5.55	134.50	124.73
24	B	607	CLA	O2D-CGD-CBD	5.55	120.93	111.23
24	B	610	CLA	CMD-C2D-C1D	5.55	134.49	124.73
24	c	509	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	C	508	CLA	C2D-C1D-ND	5.53	115.60	110.13
24	b	613	CLA	CMD-C2D-C1D	5.51	134.44	124.73
24	D	404	CLA	C2D-C1D-ND	5.50	115.56	110.13
24	c	512	CLA	C2D-C1D-ND	5.47	115.54	110.13
24	c	505	CLA	CMD-C2D-C1D	5.47	134.36	124.73
24	B	606	CLA	CMD-C2D-C1D	5.43	134.28	124.73
24	c	504	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	c	514	CLA	CMD-C2D-C1D	5.41	134.26	124.73
24	C	502	CLA	C2D-C1D-ND	5.41	115.48	110.13
24	D	404	CLA	O2D-CGD-CBD	5.41	120.68	111.23
24	C	509	CLA	O2D-CGD-CBD	5.40	120.67	111.23
24	b	614	CLA	CMD-C2D-C1D	5.40	134.24	124.73
36	B	624	HTG	C1'-S1-C1	5.40	112.11	100.45
24	B	603	CLA	O2D-CGD-CBD	5.39	120.66	111.23
24	C	503	CLA	C2D-C1D-ND	5.39	115.46	110.13
24	a	412	CLA	CMD-C2D-C1D	5.38	134.21	124.73
24	c	506	CLA	CMD-C2D-C1D	5.38	134.20	124.73
24	a	412	CLA	O2D-CGD-CBD	5.37	120.62	111.23
24	c	506	CLA	O2D-CGD-CBD	5.37	120.61	111.23
25	a	411	PHO	C3D-C4D-ND	5.37	114.59	107.71
24	C	512	CLA	CMD-C2D-C1D	5.36	134.17	124.73
24	B	606	CLA	C2D-C1D-ND	5.36	115.43	110.13
24	C	510	CLA	O2D-CGD-CBD	5.36	120.60	111.23
24	A	405	CLA	C2D-C1D-ND	5.35	115.42	110.13
24	C	504	CLA	C1-C2-C3	-5.33	117.47	126.20
36	I	102	HTG	C1'-S1-C1	5.32	111.94	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	C2D-C1D-ND	5.30	115.37	110.13
24	b	604	CLA	O2D-CGD-CBD	5.30	120.50	111.23
36	d	414	HTG	C1'-S1-C1	5.28	111.85	100.45
24	b	607	CLA	C2D-C1D-ND	5.28	115.35	110.13
40	F	101	HEM	C4D-ND-C1D	5.27	111.45	105.21
25	D	401	PHO	C3D-C4D-ND	5.26	114.45	107.71
24	C	503	CLA	CMD-C2D-C1D	5.26	133.99	124.73
24	C	503	CLA	O2D-CGD-CBD	5.24	120.38	111.23
24	b	617	CLA	C1-C2-C3	-5.24	117.62	126.20
24	a	409	CLA	CMD-C2D-C1D	5.22	133.92	124.73
24	B	616	CLA	CMD-C2D-C1D	5.21	133.91	124.73
24	A	409	CLA	CMD-C2D-C1D	5.20	133.89	124.73
24	b	608	CLA	CHD-C4C-C3C	-5.20	117.19	124.77
26	D	405	BCR	C7-C8-C9	-5.19	118.56	126.23
24	C	506	CLA	C2D-C1D-ND	5.18	115.25	110.13
24	a	409	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
24	C	513	CLA	CMD-C2D-C1D	5.17	133.84	124.73
24	c	515	CLA	C2D-C1D-ND	5.17	115.24	110.13
24	c	512	CLA	O2D-CGD-CBD	5.15	120.23	111.23
24	B	602	CLA	C2D-C1D-ND	5.15	115.22	110.13
25	A	408	PHO	C3D-C4D-ND	5.13	114.29	107.71
24	C	510	CLA	C2D-C1D-ND	5.11	115.18	110.13
27	L	101	SQD	O47-C7-C8	5.10	122.51	111.48
25	d	401	PHO	C1-C2-C3	-5.10	117.85	126.20
24	b	609	CLA	O2D-CGD-CBD	5.09	120.13	111.23
24	c	506	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	C	514	CLA	O2D-CGD-CBD	5.06	120.08	111.23
28	a	415	LMG	O7-C10-C11	5.04	122.39	111.48
43	V	202	HEC	CBB-CAB-C3B	-5.04	117.36	127.43
36	B	626	HTG	C1'-S1-C1	5.02	111.30	100.45
24	c	504	CLA	O2D-CGD-CBD	5.02	120.01	111.23
24	c	508	CLA	C2D-C1D-ND	5.02	115.10	110.13
24	C	513	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
24	c	510	CLA	CMD-C2D-C1D	5.01	133.55	124.73
24	B	616	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
24	b	609	CLA	C2D-C1D-ND	4.99	115.06	110.13
24	C	511	CLA	CMD-C2D-C1D	4.99	133.51	124.73
24	B	603	CLA	C2D-C1D-ND	4.99	115.06	110.13
24	A	407	CLA	O2D-CGD-CBD	4.98	119.94	111.23
26	B	641	BCR	C33-C5-C6	-4.98	119.05	124.48
40	f	101	HEM	C4D-ND-C1D	4.97	111.10	105.21
24	c	513	CLA	CMD-C2D-C1D	4.96	133.46	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	O2D-CGD-CBD	4.96	119.90	111.23
24	B	605	CLA	O2D-CGD-CBD	4.96	119.90	111.23
24	D	403	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	b	604	CLA	C2D-C1D-ND	4.95	115.02	110.13
24	B	614	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
24	c	513	CLA	CHD-C4C-C3C	-4.93	117.59	124.77
24	C	507	CLA	C1-C2-C3	-4.91	118.15	126.20
36	V	203	HTG	C1-C2-C3	-4.91	100.94	110.55
24	B	612	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
33	d	407	PL9	C7-C8-C9	-4.91	118.38	126.83
24	B	609	CLA	CMD-C2D-C1D	4.90	133.36	124.73
24	C	508	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
27	f	102	SQD	O47-C7-O49	-4.87	119.45	125.70
26	D	405	BCR	C38-C26-C25	-4.87	119.17	124.48
36	u	201	HTG	C1'-S1-C1	4.86	110.95	100.45
24	B	615	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
24	b	605	CLA	C2D-C1D-ND	4.84	114.92	110.13
24	b	619	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	A	406	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
24	B	608	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	b	615	CLA	CMD-C2D-C1D	4.82	133.22	124.73
26	d	406	BCR	C38-C26-C25	-4.82	119.22	124.48
24	c	503	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
24	B	613	CLA	CMD-C2D-C1D	4.80	133.18	124.73
39	D	407	DGD	O2G-C1B-C2B	4.79	121.85	111.48
24	c	509	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
26	d	406	BCR	C24-C23-C22	-4.78	119.17	126.23
27	L	102	SQD	O47-C7-C8	4.78	121.81	111.48
24	B	607	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	B	611	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
24	A	405	CLA	CMD-C2D-C1D	4.75	133.09	124.73
24	B	616	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
24	B	615	CLA	O2D-CGD-CBD	4.74	119.53	111.23
24	A	409	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	c	507	CLA	C2D-C1D-ND	4.74	114.82	110.13
24	A	406	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	b	610	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
27	A	411	SQD	O47-C7-C8	4.73	121.72	111.48
24	B	606	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
37	E	101	LHG	O7-C7-C8	4.72	121.69	111.48
24	c	509	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	C	514	CLA	C3B-C2B-C1B	-4.71	101.62	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	405	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
24	D	404	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
27	A	411	SQD	C1-O5-C5	-4.70	104.54	113.72
24	C	504	CLA	C3B-C2B-C1B	-4.70	101.64	107.17
24	A	409	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
24	C	503	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
24	B	609	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	c	515	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	b	607	CLA	C1-C2-C3	-4.67	118.54	126.20
24	c	514	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
24	d	405	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	617	CLA	CMD-C2D-C1D	4.65	132.91	124.73
24	C	512	CLA	O2D-CGD-CBD	4.64	119.34	111.23
24	b	609	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
24	b	616	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	c	510	CLA	C3D-C4D-ND	4.63	117.51	109.99
24	B	615	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	b	618	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	b	608	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	c	504	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
24	A	407	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
24	B	614	CLA	CMD-C2D-C1D	4.61	132.84	124.73
26	D	405	BCR	C24-C23-C22	-4.61	119.42	126.23
24	B	608	CLA	C1C-C2C-C3C	-4.61	102.14	106.98
24	a	410	CLA	C3D-C4D-ND	4.61	117.47	109.99
24	C	514	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	B	612	CLA	CAC-C3C-C4C	4.60	130.78	124.79
24	B	616	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
24	B	604	CLA	C3D-C4D-ND	4.60	117.46	109.99
24	b	617	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	A	407	CLA	C3D-C4D-ND	4.59	117.44	109.99
24	c	505	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	b	617	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
24	A	406	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
26	Y	302	BCR	C33-C5-C6	-4.58	119.49	124.48
24	B	615	CLA	CHD-C4C-C3C	-4.58	118.10	124.77
24	b	616	CLA	C1-C2-C3	-4.57	118.70	126.20
24	a	408	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
28	A	412	LMG	O7-C10-C11	4.57	121.36	111.48
24	c	511	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
36	C	523	HTG	C1'-S1-C1	4.57	110.31	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	510	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
24	C	503	CLA	C1-C2-C3	-4.56	118.72	126.20
24	B	606	CLA	O2D-CGD-CBD	4.56	119.20	111.23
24	C	508	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
25	D	401	PHO	C1-C2-C3	-4.55	118.73	126.20
24	C	513	CLA	C1-C2-C3	-4.55	118.74	126.20
24	c	514	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	c	511	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	B	617	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
24	c	505	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	b	607	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	C	506	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	B	611	CLA	O2D-CGD-CBD	4.53	119.14	111.23
24	A	406	CLA	CBC-CAC-C3C	-4.52	100.18	112.42
24	C	512	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
24	d	404	CLA	O2D-CGD-CBD	4.51	119.11	111.23
24	C	509	CLA	C3D-C4D-ND	4.51	117.32	109.99
24	c	506	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
28	c	522	LMG	O7-C10-C11	4.50	121.22	111.48
24	c	507	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
24	C	505	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
27	a	414	SQD	O47-C7-C8	4.50	121.21	111.48
24	c	504	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	c	510	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
24	a	409	CLA	CHD-C4C-C3C	-4.50	118.22	124.77
24	c	513	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
24	a	409	CLA	C1C-C2C-C3C	-4.49	102.25	106.98
28	C	532	LMG	O7-C10-C11	4.49	121.20	111.48
24	b	605	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
36	c	525	HTG	C1'-S1-C1	4.48	110.12	100.45
24	C	504	CLA	O2D-CGD-CBD	4.47	119.05	111.23
26	K	101	BCR	C33-C5-C6	-4.46	119.61	124.48
24	c	504	CLA	C3D-C4D-ND	4.46	117.24	109.99
24	a	412	CLA	C3B-C2B-C1B	-4.45	101.93	107.17
24	b	619	CLA	C3B-C2B-C1B	-4.45	101.93	107.17
24	a	409	CLA	C2C-C1C-NC	4.44	114.65	109.98
24	B	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
36	V	203	HTG	O5-C1-C2	-4.44	104.20	110.32
36	b	601	HTG	C1'-S1-C1	4.43	110.03	100.45
24	A	406	CLA	C3D-C4D-ND	4.43	117.19	109.99
24	a	410	CLA	C3D-C2D-C1D	-4.43	99.78	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	403	CLA	CHD-C4C-C3C	-4.43	118.32	124.77
24	C	505	CLA	O2D-CGD-CBD	4.43	118.97	111.23
24	d	404	CLA	CHD-C4C-C3C	-4.42	118.33	124.77
24	a	412	CLA	C3D-C4D-ND	4.42	117.17	109.99
24	c	503	CLA	O2D-CGD-O1D	-4.41	115.26	123.85
24	d	404	CLA	C3D-C4D-ND	4.41	117.15	109.99
24	B	608	CLA	O2D-CGD-CBD	4.41	118.93	111.23
24	C	504	CLA	CHD-C4C-C3C	-4.41	118.35	124.77
36	I	102	HTG	C1-O5-C5	4.40	120.45	112.56
24	B	603	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
36	B	623[B]	HTG	C1'-S1-C1	4.39	109.93	100.45
26	c	517	BCR	C7-C8-C9	-4.39	119.74	126.23
24	a	408	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
24	c	506	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
24	c	508	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
24	a	412	CLA	CHD-C4C-C3C	-4.36	118.41	124.77
24	B	608	CLA	C2C-C1C-NC	4.36	114.57	109.98
24	D	403	CLA	C2C-C1C-NC	4.36	114.56	109.98
24	b	607	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	B	613	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
24	b	604	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
24	c	513	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
36	c	524	HTG	C1'-S1-C1	4.33	109.80	100.45
24	b	612	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
24	b	619	CLA	C1D-CHD-C4C	-4.33	116.82	126.02
24	C	509	CLA	CMD-C2D-C1D	4.32	132.34	124.73
24	C	509	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
24	B	617	CLA	CHD-C4C-C3C	-4.32	118.48	124.77
24	b	615	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
24	A	407	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
24	B	605	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
40	F	101	HEM	CBD-CAD-C3D	-4.30	100.63	112.53
24	C	507	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	c	506	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	a	408	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	C	505	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	B	606	CLA	CHD-C4C-C3C	-4.30	118.50	124.77
39	D	407	DGD	O6D-C5D-C4D	4.30	117.45	109.70
24	C	507	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
24	C	507	CLA	C2C-C1C-NC	4.29	114.49	109.98
24	b	611	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
24	B	606	CLA	C3D-C4D-ND	4.29	116.96	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	C2C-C1C-NC	4.29	114.49	109.98
26	d	406	BCR	C33-C5-C6	-4.29	119.81	124.48
24	a	410	CLA	CHD-C4C-C3C	-4.28	118.53	124.77
24	c	503	CLA	C1C-C2C-C3C	-4.28	102.48	106.98
24	a	409	CLA	O2D-CGD-CBD	4.27	118.70	111.23
24	B	613	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
24	b	615	CLA	C3D-C4D-ND	4.27	116.93	109.99
24	C	503	CLA	O2D-CGD-O1D	-4.27	115.54	123.85
24	C	511	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
24	B	615	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
24	c	515	CLA	C3D-C4D-ND	4.27	116.92	109.99
24	A	409	CLA	CHD-C4C-C3C	-4.26	118.56	124.77
24	C	504	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	A	409	CLA	C3D-C4D-ND	4.26	116.91	109.99
24	A	406	CLA	O2D-CGD-CBD	4.25	118.67	111.23
24	B	613	CLA	C3D-C4D-ND	4.25	116.90	109.99
24	b	612	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	b	608	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
24	C	510	CLA	C1-C2-C3	-4.25	119.24	126.20
24	b	613	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
24	B	614	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
24	B	606	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
36	C	523	HTG	C1-O5-C5	4.24	120.17	112.56
24	b	608	CLA	O2D-CGD-CBD	4.24	118.63	111.23
24	B	607	CLA	C2C-C1C-NC	4.23	114.42	109.98
43	v	1603	HEC	CBB-CAB-C3B	-4.23	118.99	127.43
24	a	409	CLA	C3D-C4D-ND	4.23	116.86	109.99
24	c	512	CLA	C3D-C4D-ND	4.22	116.85	109.99
26	T	102	BCR	C33-C5-C6	-4.22	119.88	124.48
24	D	403	CLA	C3D-C4D-ND	4.22	116.85	109.99
24	c	504	CLA	CHD-C4C-C3C	-4.22	118.63	124.77
27	a	414	SQD	C1-O5-C5	-4.22	105.49	113.72
24	b	618	CLA	C3B-C2B-C1B	-4.21	102.20	107.17
24	C	507	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
24	A	409	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
24	C	502	CLA	C3D-C4D-ND	4.20	116.82	109.99
24	B	609	CLA	CMA-C3A-C4A	-4.20	100.47	111.77
24	a	409	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	b	613	CLA	O2D-CGD-CBD	4.20	118.58	111.23
24	C	512	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	B	614	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	b	611	CLA	O2D-CGD-CBD	4.20	118.57	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	C3B-C4B-NB	4.20	114.28	110.53
24	B	617	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	d	405	CLA	O2D-CGD-CBD	4.19	118.56	111.23
24	C	513	CLA	C3D-C4D-ND	4.19	116.80	109.99
24	a	412	CLA	C1-C2-C3	-4.19	119.33	126.20
24	B	608	CLA	CBC-CAC-C3C	-4.19	101.06	112.42
24	C	513	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
24	A	406	CLA	C2C-C1C-NC	4.19	114.38	109.98
24	c	511	CLA	C1-C2-C3	-4.19	119.34	126.20
24	b	605	CLA	C3D-C4D-ND	4.18	116.79	109.99
24	B	602	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
24	b	617	CLA	C3D-C4D-ND	4.18	116.78	109.99
24	d	405	CLA	C3D-C4D-ND	4.17	116.77	109.99
27	D	408	SQD	O47-C7-C8	4.17	120.51	111.48
24	B	613	CLA	CHD-C4C-C3C	-4.17	118.69	124.77
24	B	604	CLA	CHD-C4C-C3C	-4.17	118.70	124.77
24	b	614	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
24	C	513	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	B	605	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
24	C	503	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
24	b	615	CLA	CHD-C4C-C3C	-4.16	118.71	124.77
24	B	607	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
24	b	619	CLA	CHD-C4C-C3C	-4.16	118.71	124.77
24	b	611	CLA	C3D-C4D-ND	4.15	116.74	109.99
24	C	512	CLA	C2C-C1C-NC	4.15	114.34	109.98
24	D	404	CLA	C3D-C4D-ND	4.15	116.73	109.99
39	D	407	DGD	C3D-C4D-C5D	4.15	117.75	110.23
39	C	518	DGD	O2G-C1B-C2B	4.15	120.45	111.48
24	B	604	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
24	B	612	CLA	CHD-C4C-C3C	-4.15	118.73	124.77
24	c	515	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
24	a	410	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
33	D	406	PL9	C7-C8-C9	-4.14	119.70	126.83
24	C	506	CLA	O2D-CGD-CBD	4.14	118.47	111.23
24	b	608	CLA	C3D-C4D-ND	4.14	116.71	109.99
36	B	625	HTG	C1'-S1-C1	4.13	109.38	100.45
24	C	509	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
26	B	641	BCR	C15-C16-C17	-4.13	115.06	123.52
24	C	502	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
24	B	613	CLA	C1-C2-C3	-4.13	119.43	126.20
24	B	610	CLA	C3D-C4D-ND	4.13	116.70	109.99
24	B	617	CLA	C3D-C4D-ND	4.13	116.69	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	C3D-C4D-ND	4.12	116.68	109.99
24	A	409	CLA	C2C-C1C-NC	4.12	114.31	109.98
26	B	618	BCR	C33-C5-C6	-4.11	120.00	124.48
24	b	615	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
24	c	514	CLA	O2D-CGD-O1D	-4.11	115.84	123.85
24	b	612	CLA	C3D-C4D-ND	4.11	116.67	109.99
24	b	613	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
24	D	403	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	d	405	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	C	511	CLA	C3D-C4D-ND	4.11	116.66	109.99
24	C	510	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
24	C	503	CLA	C3D-C4D-ND	4.10	116.65	109.99
33	A	422[B]	PL9	C7-C8-C9	-4.10	119.77	126.83
24	B	602	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
24	c	514	CLA	CBA-CAA-C2A	-4.09	101.62	113.79
24	C	514	CLA	C3D-C4D-ND	4.08	116.62	109.99
24	C	505	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	B	609	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
28	B	621	LMG	O7-C10-C11	4.08	120.30	111.48
24	a	412	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
24	d	404	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
24	c	511	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
24	b	604	CLA	C3D-C4D-ND	4.07	116.60	109.99
25	D	401	PHO	C1A-C2A-C3A	-4.07	98.97	102.84
24	c	506	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
24	c	512	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
24	B	610	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
24	c	511	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
24	C	511	CLA	CHD-C4C-C3C	-4.05	118.87	124.77
26	b	620	BCR	C33-C5-C6	-4.05	120.07	124.48
24	c	512	CLA	C3B-C2B-C1B	-4.04	102.40	107.17
24	c	504	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
24	B	603	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
24	D	404	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
24	B	603	CLA	C3D-C4D-ND	4.04	116.55	109.99
24	c	503	CLA	C3D-C4D-ND	4.03	116.54	109.99
26	c	516	BCR	C33-C5-C6	-4.03	120.08	124.48
28	C	520	LMG	O7-C10-C11	4.03	120.20	111.48
24	A	405	CLA	C3B-C2B-C1B	-4.03	102.42	107.17
24	B	612	CLA	O2D-CGD-CBD	4.02	118.27	111.23
24	A	405	CLA	C3D-C4D-ND	4.02	116.53	109.99
24	B	611	CLA	C4C-C3C-C2C	-4.02	101.04	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
26	C	516	BCR	C7-C8-C9	-4.02	120.29	126.23
24	B	608	CLA	C3D-C4D-ND	4.02	116.52	109.99
24	c	513	CLA	O2D-CGD-CBD	4.01	118.25	111.23
24	C	510	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
24	c	503	CLA	CHD-C4C-C3C	-4.01	118.92	124.77
24	A	406	CLA	C2B-C1B-NB	4.01	114.49	110.33
24	A	407	CLA	C2B-C1B-NB	4.01	114.49	110.33
24	B	607	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
24	b	607	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
24	b	605	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
24	c	508	CLA	C3D-C4D-ND	4.01	116.50	109.99
24	b	618	CLA	CHD-C4C-C3C	-4.01	118.93	124.77
28	C	532	LMG	C3-C4-C5	4.01	117.49	110.23
24	a	408	CLA	C2B-C1B-NB	4.00	114.48	110.33
24	B	605	CLA	C3D-C4D-ND	4.00	116.50	109.99
24	D	403	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
24	b	616	CLA	C3D-C4D-ND	4.00	116.49	109.99
24	B	614	CLA	CHD-C4C-C3C	-4.00	118.94	124.77
24	B	609	CLA	C1-C2-C3	-4.00	119.64	126.20
24	D	403	CLA	C1-C2-C3	-4.00	119.64	126.20
33	a	425[B]	PL9	C25-C24-C26	4.00	122.16	115.23
24	d	404	CLA	C2C-C1C-NC	3.99	114.18	109.98
24	C	508	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
24	d	404	CLA	C1-C2-C3	-3.99	119.66	126.20
36	V	203	HTG	C2-C1-S1	3.99	117.31	111.30
24	c	503	CLA	C3B-C2B-C1B	-3.99	102.47	107.17
24	B	612	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	b	609	CLA	C3D-C2D-C1D	-3.98	100.39	105.83
24	b	616	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
26	d	406	BCR	C7-C8-C9	-3.98	120.35	126.23
24	b	611	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
33	a	425[B]	PL9	C32-C33-C34	-3.97	118.53	127.62
26	T	102	BCR	C15-C16-C17	-3.97	115.41	123.52
24	c	515	CLA	C2B-C1B-NB	3.96	114.43	110.33
24	b	606	CLA	C3D-C4D-ND	3.96	116.42	109.99
24	C	512	CLA	C4A-NA-C1A	3.96	108.48	106.68
24	b	606	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
24	B	605	CLA	C2C-C1C-NC	3.96	114.14	109.98
24	B	612	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
24	b	612	CLA	CHD-C4C-C3C	-3.95	119.01	124.77
39	c	518	DGD	O2G-C1B-C2B	3.95	120.03	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	510	CLA	C2C-C1C-NC	3.95	114.13	109.98
24	C	511	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
24	b	614	CLA	CHD-C4C-C3C	-3.95	119.02	124.77
24	B	610	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
24	A	409	CLA	C2B-C1B-NB	3.94	114.41	110.33
24	C	513	CLA	CHD-C4C-C3C	-3.94	119.03	124.77
24	c	514	CLA	C3D-C4D-ND	3.94	116.38	109.99
24	b	610	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
24	C	502	CLA	C3B-C2B-C1B	-3.93	102.53	107.17
24	b	606	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
27	a	401	SQD	O47-C7-C8	3.93	119.98	111.48
24	b	616	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
24	B	602	CLA	C3D-C4D-ND	3.93	116.37	109.99
24	C	506	CLA	CHD-C4C-C3C	-3.93	119.05	124.77
24	D	403	CLA	O2D-CGD-CBD	3.92	118.09	111.23
24	b	608	CLA	C1C-C2C-C3C	-3.92	102.85	106.98
24	c	514	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
37	e	101	LHG	O7-C7-C8	3.91	119.95	111.48
24	c	515	CLA	O2D-CGD-CBD	3.91	118.07	111.23
24	B	604	CLA	C2B-C1B-NB	3.91	114.38	110.33
24	b	610	CLA	C3B-C2B-C1B	-3.90	102.57	107.17
24	C	502	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
24	B	611	CLA	CHD-C4C-C3C	-3.90	119.08	124.77
24	a	412	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
24	C	505	CLA	C3B-C2B-C1B	-3.89	102.58	107.17
24	A	405	CLA	C1C-C2C-C3C	-3.89	102.88	106.98
33	A	422[B]	PL9	C32-C33-C34	-3.89	118.72	127.62
24	b	606	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
24	B	614	CLA	C3D-C4D-ND	3.89	116.30	109.99
26	C	515	BCR	C33-C5-C6	-3.88	120.25	124.48
24	C	507	CLA	O2D-CGD-CBD	3.88	118.01	111.23
24	b	617	CLA	O2D-CGD-O1D	-3.88	116.31	123.85
24	B	614	CLA	C2C-C1C-NC	3.88	114.05	109.98
24	B	607	CLA	CHD-C4C-C3C	-3.87	119.13	124.77
24	c	514	CLA	C2B-C1B-NB	3.87	114.34	110.33
36	d	414	HTG	C1-O5-C5	3.87	119.50	112.56
26	c	516	BCR	C15-C14-C13	-3.87	121.85	127.28
24	C	514	CLA	CHD-C4C-C3C	-3.87	119.14	124.77
24	B	605	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
24	B	609	CLA	C2C-C1C-NC	3.86	114.04	109.98
24	C	503	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
24	c	510	CLA	C2B-C1B-NB	3.86	114.33	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
24	b	607	CLA	C2C-C1C-NC	3.86	114.03	109.98
39	C	517	DGD	O2G-C1B-C2B	3.86	119.82	111.48
24	b	615	CLA	C1-C2-C3	-3.85	119.89	126.20
24	b	606	CLA	C4-C3-C5	3.85	121.92	115.23
24	c	503	CLA	CBC-CAC-C3C	-3.85	101.98	112.42
36	b	602	HTG	C1'-S1-C1	3.85	108.77	100.45
24	C	506	CLA	C3D-C2D-C1D	-3.85	100.58	105.83
24	B	616	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
24	B	602	CLA	CHD-C4C-C3C	-3.84	119.18	124.77
24	c	511	CLA	CHD-C4C-C3C	-3.84	119.18	124.77
24	b	610	CLA	C3D-C4D-ND	3.84	116.22	109.99
24	C	510	CLA	C3D-C4D-ND	3.84	116.22	109.99
24	c	507	CLA	C3D-C4D-ND	3.83	116.22	109.99
24	c	509	CLA	C3D-C4D-ND	3.83	116.21	109.99
24	b	606	CLA	C3B-C2B-C1B	-3.82	102.67	107.17
24	d	404	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
24	B	605	CLA	C1-C2-C3	-3.82	119.94	126.20
33	D	406	PL9	C40-C39-C41	3.82	121.86	115.23
24	B	610	CLA	C3B-C2B-C1B	-3.82	102.67	107.17
28	C	520	LMG	O8-C28-C29	3.82	123.48	111.83
24	B	617	CLA	C4-C3-C5	3.82	121.86	115.23
27	A	411	SQD	C45-O47-C7	-3.82	108.66	117.80
24	b	616	CLA	C2C-C1C-NC	3.81	113.99	109.98
24	c	507	CLA	C2C-C1C-NC	3.81	113.99	109.98
24	C	513	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
24	c	506	CLA	CBC-CAC-C3C	-3.81	102.10	112.42
24	B	609	CLA	C3D-C4D-ND	3.80	116.17	109.99
24	A	407	CLA	CHD-C4C-C3C	-3.80	119.23	124.77
24	C	512	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
39	C	519	DGD	O2G-C1B-C2B	3.79	119.68	111.48
24	a	408	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
24	C	503	CLA	CBC-CAC-C3C	-3.78	102.17	112.42
24	b	617	CLA	C2B-C1B-NB	3.78	114.25	110.33
24	a	408	CLA	CAC-C3C-C4C	3.78	129.71	124.79
24	B	611	CLA	C3B-C2B-C1B	-3.78	102.72	107.17
26	Y	302	BCR	C38-C26-C25	-3.77	120.37	124.48
24	C	512	CLA	C3B-C4B-NB	3.77	113.90	110.53
26	D	405	BCR	C29-C30-C25	3.77	115.92	110.44
24	B	611	CLA	C3C-C4C-NC	3.77	115.26	110.43
24	B	616	CLA	C3D-C4D-ND	3.77	116.11	109.99
24	c	510	CLA	O2D-CGD-O1D	-3.76	116.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C1-O2A-CGA	3.76	125.75	116.65
37	D	409	LHG	O8-C23-O10	-3.75	114.25	123.63
24	B	605	CLA	CHD-C4C-C3C	-3.75	119.31	124.77
26	c	517	BCR	C38-C26-C25	-3.75	120.39	124.48
24	b	616	CLA	C3B-C4B-NB	3.75	113.88	110.53
24	A	405	CLA	C2C-C1C-NC	3.75	113.92	109.98
39	c	519	DGD	O2G-C1B-C2B	3.74	119.58	111.48
24	B	615	CLA	C3D-C4D-ND	3.74	116.07	109.99
24	b	604	CLA	C2B-C1B-NB	3.74	114.21	110.33
24	c	508	CLA	C3B-C2B-C1B	-3.74	102.76	107.17
24	A	406	CLA	CHD-C4C-C3C	-3.74	119.33	124.77
37	d	408	LHG	O8-C23-C24	3.73	123.22	111.83
24	B	615	CLA	C2B-C1B-NB	3.73	114.19	110.33
24	b	614	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	B	616	CLA	C11-C10-C8	-3.73	103.57	115.97
24	a	410	CLA	C2B-C1B-NB	3.73	114.19	110.33
24	a	409	CLA	CBC-CAC-C3C	-3.73	102.32	112.42
24	a	409	CLA	C3C-C4C-NC	3.73	115.20	110.43
24	C	508	CLA	C1-C2-C3	-3.73	120.09	126.20
24	C	504	CLA	C2B-C1B-NB	3.72	114.19	110.33
24	B	616	CLA	C11-C12-C13	-3.72	103.60	115.97
24	B	609	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
24	a	412	CLA	C2C-C1C-NC	3.72	113.89	109.98
24	C	509	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
26	k	302	BCR	C15-C14-C13	-3.72	122.06	127.28
24	c	507	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
24	d	405	CLA	C2C-C1C-NC	3.72	113.89	109.98
24	b	618	CLA	C3D-C4D-ND	3.71	116.02	109.99
24	B	610	CLA	CBC-CAC-C3C	-3.71	102.36	112.42
24	B	604	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
24	a	408	CLA	C2C-C1C-NC	3.71	113.88	109.98
24	c	510	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
27	a	414	SQD	C45-O47-C7	-3.71	108.93	117.80
24	d	404	CLA	C3B-C2B-C1B	-3.71	102.80	107.17
24	B	617	CLA	C3B-C4B-NB	3.71	113.84	110.53
24	b	608	CLA	CHD-C1D-ND	-3.70	119.59	124.80
24	A	405	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
24	c	512	CLA	CHD-C4C-C3C	-3.70	119.38	124.77
24	b	609	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	A	405	CLA	CAA-C2A-C3A	-3.70	103.00	113.00
27	A	413	SQD	O47-C7-C8	3.70	119.48	111.48
24	D	403	CLA	C3B-C4B-NB	3.69	113.83	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
24	C	504	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
24	B	611	CLA	C3D-C4D-ND	3.69	115.99	109.99
24	B	603	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
24	b	608	CLA	C2B-C1B-NB	3.69	114.15	110.33
24	b	610	CLA	C2C-C1C-NC	3.69	113.86	109.98
24	C	502	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
24	c	513	CLA	C3D-C4D-ND	3.69	115.98	109.99
24	C	506	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
24	b	619	CLA	O2A-CGA-CBA	3.69	123.08	111.83
24	C	507	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
24	B	605	CLA	C3B-C2B-C1B	-3.68	102.83	107.17
24	b	605	CLA	C2B-C1B-NB	3.68	114.14	110.33
32	A	421[A]	K3C	C6-C5-C4	3.68	122.16	119.32
24	b	609	CLA	CHD-C4C-C3C	-3.68	119.41	124.77
26	C	515	BCR	C7-C8-C9	-3.67	120.80	126.23
24	c	505	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
24	b	607	CLA	C2B-C1B-NB	3.67	114.13	110.33
24	b	609	CLA	C3D-C4D-ND	3.67	115.95	109.99
24	A	409	CLA	CMA-C3A-C4A	-3.67	101.92	111.77
24	c	514	CLA	C2C-C1C-NC	3.67	113.83	109.98
24	c	509	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
24	b	606	CLA	CAA-C2A-C3A	-3.66	103.10	113.00
24	a	408	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
24	b	617	CLA	CHD-C4C-C3C	-3.66	119.44	124.77
29	B	622	LMT	C1-O1'-C1'	-3.66	107.43	113.68
24	b	618	CLA	C2C-C1C-NC	3.66	113.82	109.98
37	B	640	LHG	O7-C7-C8	3.66	119.39	111.48
24	c	509	CLA	CHD-C4C-C3C	-3.65	119.45	124.77
24	A	405	CLA	CAA-C2A-C1A	-3.65	100.01	111.97
24	A	407	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
24	c	503	CLA	C2C-C1C-NC	3.65	113.82	109.98
24	b	608	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
24	A	406	CLA	C3B-C4B-NB	3.65	113.79	110.53
24	a	412	CLA	C2B-C1B-NB	3.65	114.11	110.33
24	B	609	CLA	O2D-CGD-CBD	3.65	117.61	111.23
24	c	515	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
25	d	401	PHO	C4-C3-C5	3.65	121.56	115.23
24	B	607	CLA	C3D-C4D-ND	3.64	115.91	109.99
24	C	506	CLA	C3D-C4D-ND	3.64	115.90	109.99
24	B	617	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
24	B	606	CLA	O2D-CGD-O1D	-3.64	116.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	514	CLA	C1-C2-C3	-3.64	120.24	126.20
24	b	619	CLA	C3B-C4B-NB	3.63	113.77	110.53
24	C	506	CLA	C2C-C1C-NC	3.63	113.79	109.98
27	L	101	SQD	O48-C23-C24	3.63	122.89	111.83
24	c	506	CLA	C2C-C1C-NC	3.62	113.79	109.98
24	c	514	CLA	CBC-CAC-C3C	-3.62	102.60	112.42
37	d	410	LHG	O7-C7-C8	3.62	119.31	111.48
26	C	515	BCR	C38-C26-C25	-3.62	120.54	124.48
32	a	424[A]	K3C	C6-C5-C4	3.62	122.11	119.32
33	a	425[B]	PL9	C7-C8-C9	-3.62	120.60	126.83
24	c	513	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
24	b	606	CLA	C2C-C1C-NC	3.61	113.78	109.98
24	C	508	CLA	C2C-C1C-NC	3.61	113.77	109.98
24	A	407	CLA	C2C-C1C-NC	3.61	113.77	109.98
24	A	407	CLA	C4-C3-C5	3.60	121.48	115.23
24	B	603	CLA	C2B-C1B-NB	3.60	114.06	110.33
24	a	410	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	C	512	CLA	CHD-C4C-C3C	-3.60	119.53	124.77
24	b	618	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	D	404	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	d	405	CLA	C2B-C1B-NB	3.60	114.06	110.33
24	b	616	CLA	O2D-CGD-CBD	3.60	117.52	111.23
24	B	613	CLA	C2B-C1B-NB	3.60	114.06	110.33
24	C	508	CLA	CHD-C4C-C3C	-3.59	119.53	124.77
24	d	404	CLA	C3C-C4C-NC	3.59	115.03	110.43
24	b	617	CLA	CAC-C3C-C4C	3.59	129.46	124.79
24	a	409	CLA	C2B-C1B-NB	3.59	114.05	110.33
24	C	511	CLA	C1-O2A-CGA	3.59	125.34	116.65
24	B	610	CLA	CHD-C4C-C3C	-3.59	119.54	124.77
24	B	605	CLA	C3B-C4B-NB	3.59	113.73	110.53
24	C	502	CLA	CHD-C4C-C3C	-3.58	119.55	124.77
24	D	404	CLA	CHD-C4C-C3C	-3.58	119.55	124.77
24	B	604	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
24	C	503	CLA	C2B-C1B-NB	3.58	114.04	110.33
24	b	615	CLA	C3C-C4C-NC	3.58	115.01	110.43
24	b	619	CLA	C3D-C4D-ND	3.57	115.80	109.99
41	H	101	RRX	C38-C26-C25	-3.57	120.58	124.48
24	B	616	CLA	C2B-C1B-NB	3.57	114.03	110.33
24	B	610	CLA	C2C-C1C-NC	3.57	113.73	109.98
24	b	612	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
24	b	605	CLA	CHD-C4C-C3C	-3.57	119.57	124.77
24	C	502	CLA	CBC-CAC-C3C	-3.57	102.75	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	O2D-CGD-O1D	-3.57	116.91	123.85
24	B	609	CLA	C2B-C1B-NB	3.56	114.02	110.33
28	b	623	LMG	O7-C10-C11	3.56	119.19	111.48
24	A	405	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
24	b	614	CLA	CBC-CAC-C3C	-3.56	102.77	112.42
24	b	613	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
24	c	504	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
24	b	607	CLA	C3D-C4D-ND	3.55	115.76	109.99
24	B	603	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
43	V	202	HEC	C4D-ND-C1D	3.55	111.61	105.82
24	C	504	CLA	C3D-C4D-ND	3.55	115.75	109.99
24	C	511	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
24	c	512	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
36	B	626	HTG	C1-O5-C5	3.54	118.92	112.56
24	B	615	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
24	C	506	CLA	C3C-C4C-NC	3.54	114.97	110.43
24	C	514	CLA	C2B-C1B-NB	3.54	114.00	110.33
26	d	406	BCR	C29-C30-C25	3.54	115.58	110.44
24	B	604	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
24	c	508	CLA	CBC-CAC-C3C	-3.53	102.84	112.42
24	c	507	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
28	C	532	LMG	O6-C5-C4	3.53	116.06	109.70
24	c	513	CLA	C1-O2A-CGA	3.53	125.19	116.65
27	a	414	SQD	C1-C2-C3	-3.52	102.59	110.01
24	c	515	CLA	CMC-C2C-C1C	3.52	130.54	125.03
24	A	406	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
24	B	608	CLA	C4B-C3B-C2B	-3.52	102.93	107.30
24	A	409	CLA	O2D-CGD-CBD	3.52	117.38	111.23
24	C	505	CLA	CHD-C4C-C3C	-3.51	119.65	124.77
27	D	408	SQD	O7-S-C6	3.51	112.00	106.76
24	B	603	CLA	CHD-C4C-C3C	-3.51	119.66	124.77
24	c	514	CLA	CHD-C4C-C3C	-3.51	119.66	124.77
33	a	425[B]	PL9	C42-C43-C44	-3.51	119.59	127.62
24	a	409	CLA	CMA-C3A-C2A	-3.51	100.42	113.98
37	d	408	LHG	O8-C23-O10	-3.50	114.86	123.63
24	b	613	CLA	C1D-CHD-C4C	-3.50	118.57	126.02
24	C	511	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
24	b	614	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
24	B	611	CLA	O2A-CGA-CBA	3.50	122.51	111.83
24	b	611	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
24	c	506	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
26	k	303	BCR	C24-C23-C22	-3.50	121.06	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	CBC-CAC-C3C	-3.50	102.94	112.42
24	B	608	CLA	C3B-C2B-C1B	-3.50	103.05	107.17
24	B	616	CLA	CAC-C3C-C4C	3.50	129.34	124.79
24	c	506	CLA	C2B-C1B-NB	3.50	113.95	110.33
24	B	608	CLA	C3B-C4B-NB	3.50	113.65	110.53
27	A	411	SQD	C1-C2-C3	-3.49	102.67	110.01
24	b	604	CLA	C2C-C1C-NC	3.49	113.65	109.98
24	b	616	CLA	C2B-C1B-NB	3.49	113.94	110.33
26	k	302	BCR	C33-C5-C6	-3.49	120.68	124.48
24	C	508	CLA	C1D-CHD-C4C	-3.48	118.61	126.02
24	b	605	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
24	a	410	CLA	C4-C3-C5	3.48	121.27	115.23
24	C	506	CLA	C4C-C3C-C2C	-3.48	101.83	106.89
24	a	410	CLA	CHD-C1D-ND	-3.48	119.91	124.80
24	B	608	CLA	CHD-C4C-C3C	-3.48	119.71	124.77
24	a	410	CLA	O2D-CGD-CBD	3.47	117.30	111.23
24	a	408	CLA	CAA-C2A-C3A	-3.47	103.61	113.00
24	A	406	CLA	CMA-C3A-C2A	-3.47	100.56	113.98
24	a	412	CLA	CMA-C3A-C4A	-3.47	102.45	111.77
24	c	514	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
24	d	405	CLA	CAC-C3C-C4C	3.47	129.30	124.79
24	c	513	CLA	C4A-NA-C1A	3.47	108.26	106.68
24	b	610	CLA	C3B-C4B-NB	3.47	113.62	110.53
24	C	510	CLA	C2B-C1B-NB	3.47	113.92	110.33
24	C	504	CLA	C2C-C1C-NC	3.46	113.62	109.98
24	b	609	CLA	C1D-CHD-C4C	-3.46	118.66	126.02
24	c	510	CLA	CHD-C4C-C3C	-3.46	119.73	124.77
36	C	522	HTG	C1'-S1-C1	3.46	107.92	100.45
24	B	604	CLA	C3C-C4C-NC	3.46	114.86	110.43
26	b	620	BCR	C15-C14-C13	-3.46	122.43	127.28
36	B	623[A]	HTG	C1'-S1-C1	3.46	107.92	100.45
24	b	613	CLA	O2A-CGA-CBA	3.46	122.37	111.83
24	b	609	CLA	C2B-C1B-NB	3.46	113.91	110.33
26	Y	302	BCR	C16-C17-C18	-3.45	122.44	127.28
24	B	616	CLA	C2C-C1C-NC	3.45	113.61	109.98
24	b	619	CLA	C2B-C1B-NB	3.45	113.91	110.33
26	B	619	BCR	C11-C10-C9	-3.45	122.44	127.28
24	B	608	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
24	B	611	CLA	CAA-CBA-CGA	-3.45	103.42	113.21
24	c	505	CLA	O2D-CGD-CBD	3.45	117.26	111.23
24	B	605	CLA	C3C-C4C-NC	3.45	114.84	110.43
24	b	613	CLA	CHD-C4C-C3C	-3.45	119.75	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	O2D-CGD-CBD	3.44	117.25	111.23
24	B	605	CLA	O2A-CGA-O1A	-3.44	115.02	123.63
24	c	515	CLA	CHD-C4C-C3C	-3.44	119.75	124.77
24	c	511	CLA	C2C-C1C-NC	3.44	113.60	109.98
24	B	613	CLA	CMC-C2C-C1C	3.44	130.41	125.03
24	c	508	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
24	b	606	CLA	CHD-C4C-C3C	-3.44	119.76	124.77
24	C	507	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
28	c	521	LMG	O7-C10-C11	3.44	118.92	111.48
24	C	505	CLA	C2C-C1C-NC	3.44	113.59	109.98
43	v	1603	HEC	CBC-CAC-C3C	-3.44	120.57	127.43
24	C	509	CLA	C2C-C1C-NC	3.44	113.59	109.98
24	b	615	CLA	C4C-C3C-C2C	-3.43	101.89	106.89
24	B	603	CLA	C2C-C1C-NC	3.43	113.59	109.98
24	D	404	CLA	C2B-C1B-NB	3.43	113.89	110.33
24	c	511	CLA	CBC-CAC-C3C	-3.42	103.14	112.42
24	B	610	CLA	C1D-CHD-C4C	-3.42	118.74	126.02
24	b	610	CLA	CHD-C4C-C3C	-3.42	119.78	124.77
24	c	505	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
24	B	617	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
24	B	602	CLA	C2B-C1B-NB	3.42	113.87	110.33
24	b	616	CLA	CHD-C4C-C3C	-3.42	119.79	124.77
24	c	510	CLA	C2C-C1C-NC	3.42	113.57	109.98
24	C	507	CLA	CHD-C4C-C3C	-3.42	119.79	124.77
24	B	611	CLA	CAC-C3C-C4C	3.42	129.24	124.79
24	B	614	CLA	C4-C3-C5	3.42	121.16	115.23
24	b	612	CLA	C2C-C1C-NC	3.41	113.57	109.98
24	b	613	CLA	C2C-C1C-NC	3.41	113.57	109.98
24	b	607	CLA	C4A-NA-C1A	3.41	108.23	106.68
26	k	303	BCR	C20-C21-C22	-3.41	122.50	127.28
24	c	508	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
24	c	507	CLA	C1D-CHD-C4C	-3.41	118.77	126.02
24	B	613	CLA	C6-C5-C3	-3.41	105.16	113.47
24	b	608	CLA	CBC-CAC-C3C	-3.41	103.18	112.42
24	B	615	CLA	CHD-C1D-ND	-3.41	120.01	124.80
24	d	404	CLA	C4-C3-C5	3.41	121.14	115.23
24	b	618	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
24	B	606	CLA	C2C-C1C-NC	3.40	113.55	109.98
24	C	513	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
24	b	605	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
24	b	617	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
24	c	504	CLA	CMB-C2B-C1B	3.39	130.59	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	511	CLA	C4A-NA-C1A	3.39	108.23	106.68
24	C	510	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
24	b	615	CLA	C3B-C4B-NB	3.39	113.56	110.53
24	C	512	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
24	C	513	CLA	CBA-CAA-C2A	-3.39	103.71	113.79
40	f	101	HEM	CBD-CAD-C3D	-3.39	103.17	112.53
24	C	505	CLA	CHD-C1D-ND	-3.39	120.04	124.80
26	Y	302	BCR	C15-C14-C13	-3.38	122.53	127.28
24	C	506	CLA	C2B-C1B-NB	3.38	113.83	110.33
24	c	509	CLA	C2B-C1B-NB	3.38	113.83	110.33
26	B	618	BCR	C7-C8-C9	-3.38	121.24	126.23
26	c	516	BCR	C20-C21-C22	-3.38	122.54	127.28
33	a	425[B]	PL9	C37-C38-C39	-3.38	119.90	127.62
24	C	506	CLA	C1C-C2C-C3C	-3.37	103.43	106.98
24	b	614	CLA	C1-C2-C3	-3.37	120.67	126.20
24	C	507	CLA	O2A-CGA-CBA	3.37	122.11	111.83
24	c	505	CLA	C2C-C1C-NC	3.37	113.52	109.98
24	A	405	CLA	CHD-C4C-C3C	-3.37	119.86	124.77
24	C	509	CLA	CHD-C4C-C3C	-3.37	119.86	124.77
24	C	511	CLA	C2C-C1C-NC	3.37	113.52	109.98
24	D	403	CLA	C3C-C4C-NC	3.37	114.74	110.43
24	B	613	CLA	C3C-C4C-NC	3.37	114.74	110.43
27	a	401	SQD	C3-C4-C5	3.36	116.33	110.23
41	H	101	RRX	C10-C11-C12	-3.36	113.45	123.20
24	C	507	CLA	C3B-C4B-NB	3.36	113.53	110.53
24	b	619	CLA	C2C-C1C-NC	3.36	113.51	109.98
24	c	511	CLA	C3D-C4D-ND	3.36	115.45	109.99
24	b	619	CLA	C4C-C3C-C2C	-3.36	102.00	106.89
24	c	508	CLA	C2B-C1B-NB	3.36	113.81	110.33
24	C	502	CLA	CMB-C2B-C1B	3.36	130.53	125.42
24	c	509	CLA	C2C-C1C-NC	3.36	113.51	109.98
24	B	606	CLA	C1C-C2C-C3C	-3.35	103.45	106.98
24	b	605	CLA	CAA-C2A-C3A	-3.35	103.94	113.00
24	c	504	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
26	D	405	BCR	C33-C5-C6	-3.35	120.83	124.48
24	c	515	CLA	C1D-CHD-C4C	-3.35	118.91	126.02
24	B	616	CLA	C3C-C4C-NC	3.34	114.72	110.43
24	B	613	CLA	C1C-C2C-C3C	-3.34	103.46	106.98
24	c	511	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
24	B	616	CLA	C3B-C4B-NB	3.34	113.51	110.53
39	D	407	DGD	O1G-C1A-C2A	3.34	122.01	111.83
24	b	606	CLA	C4B-C3B-C2B	-3.34	103.15	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	CBC-CAC-C3C	-3.34	103.37	112.42
24	C	512	CLA	CAC-C3C-C4C	3.34	129.13	124.79
24	B	602	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
29	z	101	LMT	C1-O1'-C1'	3.33	118.33	113.26
24	a	412	CLA	C3B-C4B-NB	3.33	113.50	110.53
24	B	617	CLA	C2C-C1C-NC	3.33	113.48	109.98
24	C	512	CLA	C3D-C4D-ND	3.33	115.40	109.99
24	B	609	CLA	CHD-C4C-C3C	-3.33	119.92	124.77
24	B	607	CLA	CHD-C1D-ND	-3.33	120.11	124.80
24	d	404	CLA	C2B-C1B-NB	3.33	113.78	110.33
24	C	502	CLA	CHD-C1D-ND	-3.32	120.12	124.80
27	D	408	SQD	C1-O5-C5	-3.32	107.23	113.72
36	B	624	HTG	O5-C1-C2	3.32	114.90	110.32
24	c	506	CLA	C3B-C4B-NB	3.32	113.50	110.53
24	B	606	CLA	C2B-C1B-NB	3.32	113.77	110.33
24	c	512	CLA	C2C-C1C-NC	3.32	113.47	109.98
43	V	202	HEC	CBC-CAC-C3C	-3.32	120.81	127.43
24	C	503	CLA	C1D-CHD-C4C	-3.31	118.98	126.02
24	b	614	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
26	k	302	BCR	C38-C26-C25	-3.31	120.87	124.48
24	a	410	CLA	CBC-CAC-C3C	-3.31	103.44	112.42
24	B	617	CLA	C3C-C4C-NC	3.31	114.67	110.43
26	k	303	BCR	C33-C5-C6	-3.31	120.87	124.48
24	B	609	CLA	C1D-CHD-C4C	-3.31	118.99	126.02
24	b	606	CLA	O2A-CGA-O1A	-3.31	115.35	123.63
24	A	407	CLA	C1D-CHD-C4C	-3.30	119.00	126.02
26	b	622	BCR	C24-C23-C22	-3.30	121.35	126.23
24	B	617	CLA	C2B-C1B-NB	3.30	113.75	110.33
39	h	1205	DGD	O2G-C1B-C2B	3.30	118.62	111.48
24	b	609	CLA	C4-C3-C5	3.30	120.95	115.23
25	D	401	PHO	C4-C3-C5	3.30	120.95	115.23
24	c	503	CLA	C4A-NA-C1A	3.30	108.18	106.68
24	A	409	CLA	CAA-C2A-C3A	-3.30	104.09	113.00
24	c	506	CLA	CHD-C1D-ND	-3.29	120.17	124.80
24	c	512	CLA	C4-C3-C5	3.29	120.93	115.23
24	B	604	CLA	CAA-C2A-C3A	-3.29	104.12	113.00
29	C	521	LMT	C1B-O5B-C5B	3.29	120.14	113.72
41	h	1204	RRX	C11-C10-C9	-3.28	122.67	127.28
27	D	408	SQD	C1-C2-C3	-3.28	103.11	110.01
24	a	412	CLA	CMA-C3A-C2A	-3.28	101.30	113.98
27	a	401	SQD	O48-C23-C24	3.28	121.84	111.83
24	B	602	CLA	O2A-CGA-CBA	3.28	121.83	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
24	C	504	CLA	C1D-CHD-C4C	-3.27	119.06	126.02
26	C	516	BCR	C15-C14-C13	-3.27	122.69	127.28
24	B	602	CLA	C1D-CHD-C4C	-3.27	119.07	126.02
24	C	503	CLA	CHD-C4C-C3C	-3.27	120.01	124.77
37	D	411	LHG	O7-C7-C8	3.27	118.55	111.48
24	C	513	CLA	CBC-CAC-C3C	-3.27	103.56	112.42
24	B	610	CLA	CMB-C2B-C1B	3.27	130.39	125.42
24	B	607	CLA	C4-C3-C5	3.27	120.90	115.23
24	B	613	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
24	C	512	CLA	C1-O2A-CGA	3.26	124.55	116.65
24	b	608	CLA	C2C-C1C-NC	3.26	113.41	109.98
24	c	515	CLA	C2C-C1C-NC	3.26	113.41	109.98
29	C	521	LMT	O1B-C4'-C3'	3.26	115.52	107.23
26	B	620	BCR	C38-C26-C25	-3.26	120.93	124.48
24	B	615	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
24	b	608	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
41	h	1204	RRX	C24-C23-C22	-3.26	121.41	126.23
24	c	509	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
24	a	412	CLA	C1D-CHD-C4C	-3.25	119.12	126.02
24	c	503	CLA	C3B-C4B-NB	3.25	113.43	110.53
24	C	512	CLA	C1D-CHD-C4C	-3.24	119.13	126.02
24	b	607	CLA	CHD-C4C-C3C	-3.24	120.05	124.77
24	c	512	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
24	A	409	CLA	C1-C2-C3	-3.24	120.89	126.20
24	c	504	CLA	O2A-CGA-O1A	-3.24	115.53	123.63
24	A	407	CLA	CAC-C3C-C4C	3.24	129.00	124.79
24	B	603	CLA	C3C-C4C-NC	3.23	114.57	110.43
28	c	522	LMG	O6-C5-C4	3.23	115.52	109.70
24	b	606	CLA	C2B-C1B-NB	3.23	113.68	110.33
24	b	610	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
24	B	607	CLA	C3B-C4B-NB	3.23	113.41	110.53
24	A	405	CLA	CMA-C3A-C4A	-3.23	103.10	111.77
24	a	409	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
24	b	610	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
24	C	508	CLA	C2B-C1B-NB	3.23	113.67	110.33
24	C	511	CLA	C2B-C1B-NB	3.23	113.67	110.33
24	B	603	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
24	D	404	CLA	C4-C3-C5	3.22	120.82	115.23
33	A	422[B]	PL9	C15-C14-C16	3.22	120.82	115.23
24	c	510	CLA	C1D-CHD-C4C	-3.22	119.17	126.02
24	c	506	CLA	C1-O2A-CGA	3.22	124.45	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	410	CLA	C1D-CHD-C4C	-3.22	119.17	126.02
24	B	607	CLA	C2B-C1B-NB	3.22	113.67	110.33
24	B	603	CLA	CAC-C3C-C4C	3.22	128.98	124.79
24	b	616	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
26	C	515	BCR	C16-C17-C18	-3.22	122.76	127.28
24	D	404	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
24	a	412	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
24	c	513	CLA	C1C-C2C-C3C	-3.22	103.60	106.98
24	C	510	CLA	CHD-C4C-C3C	-3.22	120.08	124.77
24	C	510	CLA	C3B-C4B-NB	3.21	113.40	110.53
24	d	404	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
24	A	406	CLA	CMA-C3A-C4A	-3.21	103.15	111.77
24	c	513	CLA	C4-C3-C5	3.21	120.80	115.23
24	A	406	CLA	CHD-C1D-ND	-3.21	120.29	124.80
24	C	502	CLA	C2C-C1C-NC	3.21	113.35	109.98
36	B	626	HTG	O5-C5-C4	3.21	115.48	109.70
24	b	604	CLA	CHD-C4C-C3C	-3.21	120.10	124.77
24	c	505	CLA	C4A-NA-C1A	3.20	108.14	106.68
24	b	612	CLA	C2B-C1B-NB	3.20	113.65	110.33
24	b	618	CLA	O2D-CGD-CBD	3.20	116.83	111.23
24	b	616	CLA	C3C-C4C-NC	3.20	114.53	110.43
33	A	422[B]	PL9	C25-C24-C26	3.20	120.79	115.23
24	b	612	CLA	O2D-CGD-CBD	3.20	116.83	111.23
24	c	512	CLA	CMA-C3A-C4A	-3.20	103.17	111.77
26	b	622	BCR	C38-C26-C25	-3.20	120.99	124.48
24	A	407	CLA	CBC-CAC-C3C	-3.20	103.75	112.42
24	A	407	CLA	C3B-C4B-NB	3.20	113.39	110.53
25	D	401	PHO	O2D-CGD-O1D	-3.20	117.62	123.85
24	C	511	CLA	C4-C3-C5	3.20	120.78	115.23
33	A	422[B]	PL9	C53-C6-C1	3.20	121.82	115.28
24	c	510	CLA	C1-C2-C3	-3.20	120.96	126.20
24	B	606	CLA	C1D-CHD-C4C	-3.19	119.23	126.02
24	B	606	CLA	CMB-C2B-C1B	3.19	130.28	125.42
24	A	409	CLA	C3C-C4C-NC	3.19	114.52	110.43
24	b	606	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
24	a	408	CLA	O2A-CGA-CBA	3.19	121.57	111.83
24	B	602	CLA	C1C-C2C-C3C	-3.19	103.62	106.98
37	D	409	LHG	O8-C23-C24	3.19	121.56	111.83
36	o	301	HTG	C1'-S1-C1	3.19	107.34	100.45
24	b	615	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
24	a	410	CLA	C2C-C1C-NC	3.18	113.33	109.98
24	D	403	CLA	CHD-C1D-ND	-3.18	120.32	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	B	616	CLA	CBC-CAC-C3C	-3.18	103.80	112.42
24	C	511	CLA	C1-C2-C3	-3.18	120.99	126.20
24	C	514	CLA	C1C-C2C-C3C	-3.18	103.64	106.98
26	K	101	BCR	C11-C10-C9	-3.18	122.82	127.28
24	c	505	CLA	C1-C2-C3	-3.18	121.00	126.20
24	B	604	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
24	c	507	CLA	C3C-C4C-NC	3.17	114.49	110.43
24	c	505	CLA	C3D-C4D-ND	3.17	115.14	109.99
24	C	508	CLA	CMB-C2B-C1B	3.17	130.24	125.42
43	v	1603	HEC	C4D-ND-C1D	3.17	110.98	105.82
24	b	609	CLA	C2C-C1C-NC	3.17	113.31	109.98
24	b	614	CLA	CAC-C3C-C4C	3.17	128.91	124.79
24	B	609	CLA	O2A-CGA-CBA	3.16	121.48	111.83
26	b	620	BCR	C7-C8-C9	-3.16	121.56	126.23
26	c	516	BCR	C38-C26-C25	-3.16	121.03	124.48
27	A	413	SQD	O6-C1-C2	3.16	113.08	108.27
24	B	603	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
24	b	615	CLA	C2C-C1C-NC	3.16	113.30	109.98
24	c	504	CLA	C2C-C1C-NC	3.16	113.30	109.98
24	b	608	CLA	CMB-C2B-C1B	3.16	130.23	125.42
29	B	622	LMT	O1B-C4'-C5'	-3.16	101.18	109.48
24	c	508	CLA	CHD-C4C-C3C	-3.16	120.17	124.77
24	B	613	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
24	b	618	CLA	C2B-C1B-NB	3.16	113.60	110.33
24	b	618	CLA	C3B-C4B-NB	3.16	113.35	110.53
24	A	407	CLA	CMC-C2C-C1C	3.16	129.97	125.03
24	c	505	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
24	A	409	CLA	C1D-CHD-C4C	-3.16	119.31	126.02
24	D	403	CLA	O2A-CGA-CBA	3.16	121.46	111.83
24	c	503	CLA	CMB-C2B-C1B	3.16	130.23	125.42
24	B	615	CLA	O2A-CGA-CBA	3.15	121.45	111.83
33	D	406	PL9	C25-C24-C26	3.15	120.70	115.23
24	B	614	CLA	C3C-C4C-NC	3.15	114.47	110.43
24	b	605	CLA	C2C-C1C-NC	3.15	113.29	109.98
27	L	102	SQD	C1-O5-C5	-3.15	107.57	113.72
24	C	502	CLA	C2B-C1B-NB	3.15	113.59	110.33
24	a	412	CLA	CBC-CAC-C3C	-3.15	103.89	112.42
24	B	612	CLA	CHD-C1D-ND	-3.14	120.38	124.80
24	B	613	CLA	C2C-C1C-NC	3.14	113.28	109.98
24	B	604	CLA	C2C-C1C-NC	3.14	113.28	109.98
24	b	613	CLA	C2B-C1B-NB	3.14	113.58	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
24	B	616	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
24	b	614	CLA	C3C-C4C-NC	3.14	114.45	110.43
24	B	607	CLA	C1D-CHD-C4C	-3.14	119.34	126.02
24	B	615	CLA	C3B-C4B-NB	3.14	113.33	110.53
24	C	503	CLA	C2C-C1C-NC	3.13	113.27	109.98
24	c	511	CLA	C3B-C4B-NB	3.13	113.33	110.53
24	c	510	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
24	c	512	CLA	C3C-C4C-NC	3.13	114.44	110.43
24	c	508	CLA	CAA-C2A-C3A	-3.13	104.54	113.00
24	c	513	CLA	C2C-C1C-NC	3.13	113.27	109.98
24	c	513	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
24	b	615	CLA	C4-C3-C5	3.13	120.65	115.23
24	d	404	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
24	C	511	CLA	C3C-C4C-NC	3.12	114.43	110.43
24	b	615	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
26	C	516	BCR	C33-C5-C6	-3.12	121.08	124.48
24	C	514	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
24	C	505	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
24	B	615	CLA	C4-C3-C5	3.12	120.65	115.23
24	c	511	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
24	B	612	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
24	d	404	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
24	c	508	CLA	C2C-C1C-NC	3.12	113.26	109.98
33	a	425[B]	PL9	C17-C18-C19	-3.12	120.48	127.62
24	D	403	CLA	C1D-CHD-C4C	-3.12	119.39	126.02
24	a	408	CLA	CHD-C4C-C3C	-3.12	120.23	124.77
24	c	512	CLA	C3B-C4B-NB	3.11	113.31	110.53
24	C	510	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
24	a	408	CLA	CAA-C2A-C1A	-3.11	101.78	111.97
24	A	407	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
29	J	102	LMT	C1'-O5'-C5'	3.11	119.79	113.72
27	L	101	SQD	O7-S-C6	3.11	111.40	106.76
24	C	507	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
24	C	512	CLA	C2B-C1B-NB	3.11	113.55	110.33
24	b	604	CLA	C1D-CHD-C4C	-3.11	119.41	126.02
24	B	609	CLA	C3B-C4B-NB	3.11	113.30	110.53
24	C	505	CLA	C3B-C4B-NB	3.11	113.30	110.53
24	c	505	CLA	C2B-C1B-NB	3.11	113.55	110.33
24	c	507	CLA	CAC-C3C-C4C	3.10	128.83	124.79
24	B	611	CLA	CMA-C3A-C4A	-3.10	103.43	111.77
26	d	406	BCR	C15-C14-C13	-3.10	122.93	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	413	SQD	O48-C23-C24	3.10	121.30	111.83
24	c	503	CLA	C1D-CHD-C4C	-3.10	119.43	126.02
24	c	504	CLA	C3C-C4C-NC	3.10	114.40	110.43
24	b	613	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
24	c	507	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
24	c	507	CLA	CHA-C1A-NA	-3.10	119.38	126.39
24	B	617	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
24	b	615	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
24	c	512	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
24	a	408	CLA	C3B-C4B-NB	3.09	113.29	110.53
25	A	408	PHO	C1A-C2A-C3A	-3.09	99.90	102.84
24	C	506	CLA	C3B-C4B-NB	3.08	113.28	110.53
24	b	619	CLA	C3C-C4C-NC	3.08	114.38	110.43
24	D	403	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
24	b	606	CLA	C3B-C4B-NB	3.08	113.28	110.53
24	b	611	CLA	C2B-C1B-NB	3.08	113.52	110.33
24	d	405	CLA	C1-C2-C3	-3.08	121.15	126.20
24	C	509	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
24	B	606	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
24	b	619	CLA	CAC-C3C-C4C	3.08	128.79	124.79
24	C	514	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
24	C	506	CLA	C1-C2-C3	-3.08	121.16	126.20
27	L	102	SQD	C44-O6-C1	-3.07	107.21	113.80
24	B	612	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
24	b	611	CLA	C2C-C1C-NC	3.07	113.21	109.98
24	B	617	CLA	CAC-C3C-C4C	3.07	128.78	124.79
24	b	606	CLA	O2A-CGA-CBA	3.07	121.19	111.83
24	b	608	CLA	C3C-C4C-NC	3.07	114.36	110.43
26	K	101	BCR	C24-C23-C22	-3.07	121.69	126.23
24	B	605	CLA	C4B-C3B-C2B	-3.07	103.49	107.30
24	B	609	CLA	CAC-C3C-C4C	3.07	128.78	124.79
24	b	617	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
24	B	610	CLA	O2D-CGD-CBD	3.06	116.59	111.23
24	c	511	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
25	a	411	PHO	C4A-C3A-C2A	-3.06	99.93	102.84
24	c	504	CLA	C2B-C1B-NB	3.06	113.50	110.33
24	B	616	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
24	c	507	CLA	CMB-C2B-C1B	3.06	130.08	125.42
24	c	504	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
24	B	610	CLA	C3B-C4B-NB	3.06	113.26	110.53
25	D	401	PHO	CMA-C3A-C4A	-3.06	108.02	114.61
24	A	405	CLA	O2D-CGD-CBD	3.06	116.58	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	BCR	C33-C5-C6	-3.06	121.15	124.48
24	d	404	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
26	c	517	BCR	C33-C5-C6	-3.05	121.15	124.48
24	D	403	CLA	C2B-C1B-NB	3.05	113.49	110.33
39	C	518	DGD	O2G-C1B-O1B	-3.05	116.57	123.70
24	b	607	CLA	C1D-CHD-C4C	-3.05	119.53	126.02
28	c	521	LMG	O8-C28-C29	3.05	121.14	111.83
24	b	613	CLA	CAA-CBA-CGA	-3.05	104.55	113.21
24	c	514	CLA	C3B-C4B-NB	3.05	113.25	110.53
24	B	609	CLA	CMC-C2C-C1C	3.05	129.79	125.03
24	c	505	CLA	CAC-C3C-C4C	3.05	128.75	124.79
24	b	611	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
27	D	408	SQD	C44-O6-C1	-3.05	107.27	113.80
24	B	603	CLA	C1C-C2C-C3C	-3.05	103.78	106.98
24	B	604	CLA	O2A-CGA-CBA	3.04	121.12	111.83
24	b	609	CLA	CBC-CAC-C3C	-3.04	104.17	112.42
24	B	604	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
24	b	611	CLA	O2A-CGA-CBA	3.04	121.11	111.83
24	B	602	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
33	a	425[B]	PL9	C27-C28-C29	-3.04	120.67	127.62
24	c	508	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
24	C	508	CLA	C3D-C4D-ND	3.04	114.92	109.99
33	A	422[B]	PL9	C17-C18-C19	3.04	134.57	127.62
24	b	615	CLA	C2B-C1B-NB	3.03	113.47	110.33
24	D	403	CLA	CMC-C2C-C1C	3.03	129.77	125.03
33	a	425[B]	PL9	C7-C3-C2	-3.03	119.82	123.39
24	A	406	CLA	CAA-C2A-C3A	-3.03	104.81	113.00
24	c	507	CLA	CHD-C4C-C3C	-3.03	120.36	124.77
26	C	516	BCR	C38-C26-C25	-3.03	121.18	124.48
28	b	623	LMG	O8-C28-C29	3.03	121.07	111.83
24	c	505	CLA	CHD-C4C-C3C	-3.03	120.36	124.77
24	B	615	CLA	O2A-CGA-O1A	-3.03	116.05	123.63
24	b	616	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
26	B	620	BCR	C24-C23-C22	-3.03	121.76	126.23
24	c	507	CLA	C1-O2A-CGA	3.02	123.97	116.65
24	B	614	CLA	C3B-C4B-NB	3.02	113.23	110.53
24	c	509	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
33	a	425[B]	PL9	C12-C13-C14	-3.02	120.70	127.62
24	c	512	CLA	C2B-C1B-NB	3.02	113.46	110.33
24	D	403	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
24	C	508	CLA	CHA-C1A-NA	-3.02	119.55	126.39
33	a	425[B]	PL9	C22-C23-C24	-3.02	120.71	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	410	LHG	O8-C23-C24	3.02	121.05	111.83
24	b	614	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	B	606	CLA	C4-C3-C5	3.02	120.47	115.23
25	d	401	PHO	C1A-C2A-C3A	-3.02	99.97	102.84
24	B	607	CLA	C3C-C4C-NC	3.01	114.29	110.43
41	H	101	RRX	C24-C23-C22	-3.01	121.78	126.23
24	A	405	CLA	C3C-C4C-NC	3.01	114.29	110.43
26	B	641	BCR	C21-C20-C19	-3.01	114.48	123.20
24	C	514	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
33	d	407	PL9	C40-C39-C41	3.01	120.45	115.23
24	C	508	CLA	CBC-CAC-C3C	-3.01	104.27	112.42
24	C	506	CLA	CHA-C1A-NA	-3.00	119.59	126.39
24	c	510	CLA	C3B-C4B-NB	3.00	113.21	110.53
24	d	404	CLA	C4A-NA-C1A	-3.00	105.31	106.68
24	A	409	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
27	f	102	SQD	O7-S-C6	3.00	111.26	106.73
24	B	612	CLA	C2B-C1B-NB	3.00	113.44	110.33
27	L	102	SQD	O48-C23-C24	3.00	120.97	111.83
24	c	509	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
24	A	406	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
24	c	505	CLA	C4-C3-C5	2.99	120.42	115.23
24	c	513	CLA	C2B-C1B-NB	2.99	113.43	110.33
28	c	522	LMG	C3-C4-C5	2.99	115.65	110.23
24	B	606	CLA	C3C-C4C-NC	2.99	114.25	110.43
28	B	621	LMG	O8-C28-C29	2.99	120.94	111.83
24	B	608	CLA	CHD-C1D-ND	-2.99	120.60	124.80
24	B	609	CLA	C3C-C4C-NC	2.98	114.25	110.43
24	B	614	CLA	C2B-C1B-NB	2.98	113.42	110.33
24	b	612	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
24	b	605	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
24	A	409	CLA	C4-C3-C5	2.98	120.40	115.23
24	b	606	CLA	CBC-CAC-C3C	-2.98	104.34	112.42
24	d	405	CLA	CHD-C4C-C3C	-2.98	120.43	124.77
24	B	617	CLA	CBC-CAC-C3C	-2.98	104.35	112.42
24	b	609	CLA	O2A-CGA-O1A	-2.98	116.18	123.63
24	B	612	CLA	C3C-C4C-NC	2.98	114.24	110.43
24	c	510	CLA	C3C-C4C-NC	2.98	114.24	110.43
24	c	511	CLA	CMC-C2C-C1C	2.98	129.68	125.03
24	b	619	CLA	C4B-C3B-C2B	-2.97	103.60	107.30
24	b	619	CLA	CBC-CAC-C3C	-2.97	104.36	112.42
24	c	504	CLA	O2A-CGA-CBA	2.97	120.90	111.83
24	B	615	CLA	CHC-C1C-C2C	-2.97	118.50	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C4-C3-C5	2.97	120.39	115.23
24	C	511	CLA	C3B-C4B-NB	2.97	113.18	110.53
25	a	411	PHO	CBA-CAA-C2A	-2.97	105.03	113.78
27	D	408	SQD	O48-C23-C24	2.97	120.89	111.83
24	C	513	CLA	C3C-C4C-NC	2.97	114.23	110.43
24	b	611	CLA	CMA-C3A-C2A	-2.97	102.51	113.98
24	C	503	CLA	C1-O2A-CGA	2.97	123.83	116.65
24	a	408	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
24	C	507	CLA	C3C-C4C-NC	2.97	114.23	110.43
24	C	504	CLA	C4C-C3C-C2C	-2.97	102.58	106.89
24	C	509	CLA	C2B-C1B-NB	2.96	113.40	110.33
24	c	507	CLA	C2B-C1B-NB	2.96	113.40	110.33
24	c	509	CLA	CAC-C3C-C4C	2.96	128.65	124.79
24	B	608	CLA	C2B-C1B-NB	2.96	113.40	110.33
24	A	407	CLA	C1-C2-C3	-2.96	121.35	126.20
24	a	410	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
26	D	405	BCR	C3-C4-C5	-2.96	108.78	114.06
41	h	1204	RRX	C38-C26-C25	-2.96	121.26	124.48
24	b	611	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	b	614	CLA	C2B-C1B-NB	2.96	113.39	110.33
24	b	604	CLA	CBC-CAC-C3C	-2.96	104.41	112.42
24	a	412	CLA	CHD-C1D-ND	-2.95	120.64	124.80
41	h	1204	RRX	C10-C11-C12	-2.95	114.65	123.20
24	d	404	CLA	C3B-C4B-NB	2.95	113.16	110.53
24	B	607	CLA	CAC-C3C-C4C	2.95	128.63	124.79
24	b	615	CLA	C4A-NA-C1A	2.95	108.02	106.68
24	b	604	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	B	604	CLA	C3B-C4B-NB	2.95	113.16	110.53
24	B	607	CLA	CMC-C2C-C1C	2.95	129.64	125.03
24	B	612	CLA	C1C-C2C-C3C	-2.94	103.88	106.98
24	C	505	CLA	C1D-CHD-C4C	-2.94	119.76	126.02
24	B	613	CLA	C1D-CHD-C4C	-2.94	119.76	126.02
24	c	513	CLA	CHD-C1D-ND	-2.94	120.66	124.80
24	B	611	CLA	C1D-CHD-C4C	-2.94	119.77	126.02
24	b	615	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
24	d	404	CLA	O2A-CGA-CBA	2.94	120.79	111.83
33	D	406	PL9	C42-C43-C44	-2.94	120.90	127.62
41	H	101	RRX	C7-C8-C9	-2.94	121.89	126.23
24	b	617	CLA	C2C-C1C-NC	2.93	113.06	109.98
24	c	505	CLA	CHA-C1A-NA	-2.93	119.75	126.39
24	C	512	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	b	607	CLA	C3C-C4C-NC	2.93	114.19	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	CAC-C3C-C4C	2.93	128.60	124.79
24	C	514	CLA	CAC-C3C-C4C	2.93	128.60	124.79
24	b	613	CLA	C3C-C4C-NC	2.93	114.18	110.43
24	B	612	CLA	C2C-C1C-NC	2.93	113.06	109.98
24	d	404	CLA	CHD-C1D-ND	-2.93	120.68	124.80
24	c	505	CLA	C3C-C4C-NC	2.93	114.18	110.43
24	D	404	CLA	C1D-CHD-C4C	-2.93	119.80	126.02
24	c	509	CLA	C4A-NA-C1A	2.93	108.01	106.68
24	c	503	CLA	CMC-C2C-C1C	2.92	129.60	125.03
24	C	511	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
24	A	407	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
24	c	506	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
33	d	407	PL9	C42-C43-C44	-2.92	120.93	127.62
24	b	612	CLA	C1D-CHD-C4C	-2.92	119.81	126.02
24	A	407	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
24	B	612	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
28	a	415	LMG	C8-O7-C10	-2.92	110.81	117.80
24	B	612	CLA	CMC-C2C-C1C	2.92	129.60	125.03
24	A	407	CLA	C3C-C4C-NC	2.92	114.17	110.43
26	K	101	BCR	C10-C11-C12	-2.92	114.74	123.20
24	B	615	CLA	CBC-CAC-C3C	-2.92	104.51	112.42
24	b	611	CLA	C3C-C4C-NC	2.92	114.17	110.43
24	c	508	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
24	b	617	CLA	C3C-C4C-NC	2.92	114.17	110.43
24	B	617	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	c	515	CLA	CHD-C1D-ND	-2.92	120.70	124.80
24	c	508	CLA	C7-C6-C5	-2.91	105.50	113.26
24	C	511	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
26	C	515	BCR	C11-C10-C9	-2.91	123.19	127.28
24	A	409	CLA	C3B-C4B-NB	2.91	113.13	110.53
24	a	410	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
24	b	610	CLA	O2D-CGD-CBD	2.91	116.32	111.23
37	E	101	LHG	C5-O7-C7	-2.91	110.84	117.80
24	b	615	CLA	CAC-C3C-C4C	2.91	128.57	124.79
24	C	507	CLA	C2B-C1B-NB	2.90	113.34	110.33
25	A	408	PHO	O1D-CGD-CBD	-2.90	120.32	124.72
26	A	410	BCR	C33-C5-C6	-2.90	121.32	124.48
24	b	616	CLA	CMA-C3A-C4A	-2.90	103.98	111.77
24	b	613	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
24	b	618	CLA	CBC-CAC-C3C	-2.90	104.56	112.42
24	d	405	CLA	CBC-CAC-C3C	-2.90	104.56	112.42
24	c	508	CLA	C4C-C3C-C2C	-2.90	102.67	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	C3B-C4B-NB	2.90	113.12	110.53
24	b	611	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
24	B	614	CLA	CBC-CAC-C3C	-2.90	104.57	112.42
33	a	425[B]	PL9	C20-C19-C21	2.89	120.25	115.23
24	b	609	CLA	CMC-C2C-C1C	2.89	129.56	125.03
24	a	412	CLA	CAA-C2A-C3A	-2.89	105.19	113.00
24	c	513	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
24	b	613	CLA	CAA-C2A-C3A	-2.89	105.19	113.00
27	D	408	SQD	O9-S-C6	2.89	111.07	106.76
24	B	607	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
43	v	1603	HEC	CBD-CAD-C3D	-2.89	104.55	112.53
24	A	405	CLA	C2B-C1B-NB	2.89	113.32	110.33
24	C	507	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
39	H	102	DGD	O1G-C1A-O1A	-2.89	116.41	123.63
24	c	510	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
36	c	525	HTG	C1-O5-C5	2.88	117.73	112.56
24	c	509	CLA	O1D-CGD-CBD	-2.88	118.83	124.52
24	b	618	CLA	CHD-C1D-ND	-2.88	120.75	124.80
24	C	509	CLA	C3C-C4C-NC	2.88	114.12	110.43
24	B	610	CLA	C3C-C4C-NC	2.88	114.12	110.43
24	b	618	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
24	B	611	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
24	B	609	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
24	a	410	CLA	C3C-C4C-NC	2.88	114.12	110.43
24	B	611	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
26	b	620	BCR	C16-C17-C18	-2.88	123.25	127.28
24	b	611	CLA	CHD-C4C-C3C	-2.88	120.58	124.77
24	b	612	CLA	C3C-C4C-NC	2.87	114.11	110.43
24	B	611	CLA	C2B-C1B-NB	2.87	113.31	110.33
39	c	520	DGD	O1G-C1A-C2A	2.87	120.60	111.83
24	C	508	CLA	C3C-C4C-NC	2.87	114.11	110.43
39	C	518	DGD	O1G-C1A-O1A	-2.87	116.45	123.63
24	C	505	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
24	b	610	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
24	a	409	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
24	c	514	CLA	C3C-C4C-NC	2.87	114.11	110.43
39	H	102	DGD	O1G-C1A-C2A	2.87	120.58	111.83
24	C	508	CLA	C4A-NA-C1A	2.87	107.99	106.68
24	b	612	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
24	B	602	CLA	C4-C3-C5	2.87	120.20	115.23
24	b	616	CLA	C1D-CHD-C4C	-2.87	119.93	126.02
41	h	1204	RRX	C7-C8-C9	-2.87	122.00	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C1-C2-C3	-2.86	121.50	126.20
24	C	513	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
24	C	511	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
24	b	607	CLA	C3B-C4B-NB	2.86	113.08	110.53
24	b	607	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
26	B	641	BCR	C1-C6-C7	2.86	123.40	115.65
24	c	514	CLA	C1-C2-C3	-2.86	121.52	126.20
24	B	613	CLA	C4-C3-C5	2.86	120.18	115.23
24	C	514	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	B	612	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	c	504	CLA	CAC-C3C-C4C	2.85	128.50	124.79
43	V	202	HEC	CBD-CAD-C3D	-2.85	104.65	112.53
24	A	405	CLA	O2A-CGA-CBA	2.85	120.52	111.83
24	C	504	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	A	409	CLA	CMA-C3A-C2A	-2.85	102.97	113.98
41	H	101	RRX	C16-C17-C18	-2.85	123.28	127.28
24	b	613	CLA	C1-C2-C3	-2.85	121.53	126.20
24	B	607	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
24	B	610	CLA	CED-O2D-CGD	2.85	122.37	115.92
24	b	605	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
24	a	412	CLA	C4-C3-C5	2.85	120.17	115.23
24	D	403	CLA	CMA-C3A-C4A	-2.85	104.12	111.77
24	C	505	CLA	CBC-CAC-C3C	-2.85	104.71	112.42
24	B	602	CLA	CHD-C1D-ND	-2.84	120.80	124.80
24	c	508	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
28	C	532	LMG	O8-C28-C29	2.84	120.50	111.83
24	b	607	CLA	CHA-C1A-NA	-2.84	119.95	126.39
24	c	510	CLA	C4-C3-C5	2.84	120.16	115.23
24	C	512	CLA	C3C-C4C-NC	2.84	114.07	110.43
24	B	608	CLA	C4-C3-C5	2.84	120.16	115.23
24	b	619	CLA	C1-C2-C3	-2.84	121.54	126.20
39	C	519	DGD	O1G-C1A-C2A	2.84	120.50	111.83
24	B	611	CLA	CHA-C1A-NA	-2.84	119.96	126.39
24	B	615	CLA	C3C-C4C-NC	2.84	114.07	110.43
24	D	404	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
24	c	505	CLA	CMB-C2B-C1B	2.84	129.74	125.42
24	B	616	CLA	C1-C2-C3	-2.84	121.55	126.20
24	c	511	CLA	C2B-C1B-NB	2.83	113.27	110.33
24	c	515	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
26	b	622	BCR	C15-C14-C13	-2.83	123.31	127.28
26	B	641	BCR	C7-C6-C5	-2.83	115.03	121.56
24	a	410	CLA	CMB-C2B-C1B	2.83	129.73	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	512	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
27	L	102	SQD	O7-S-C6	2.83	110.98	106.76
24	C	509	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
24	B	608	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
24	C	509	CLA	C1D-CHD-C4C	-2.82	120.02	126.02
24	C	507	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
24	c	510	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
24	B	610	CLA	CHA-C1A-NA	-2.82	120.00	126.39
24	b	615	CLA	O2A-CGA-CBA	2.82	120.44	111.83
24	c	503	CLA	CHD-C1D-ND	-2.82	120.83	124.80
26	C	515	BCR	C15-C14-C13	-2.82	123.32	127.28
29	J	102	LMT	C3'-C4'-C5'	2.82	115.34	110.23
24	c	512	CLA	CBC-CAC-C3C	-2.82	104.78	112.42
33	a	425[B]	PL9	C7-C3-C4	2.82	119.23	116.91
26	K	101	BCR	C7-C8-C9	-2.82	122.07	126.23
24	b	615	CLA	CMB-C2B-C1B	2.81	129.71	125.42
24	B	603	CLA	C1-C2-C3	-2.81	121.59	126.20
27	a	414	SQD	O47-C7-O49	-2.81	117.13	123.70
24	B	605	CLA	O2A-CGA-CBA	2.81	120.41	111.83
24	B	605	CLA	C2B-C1B-NB	2.81	113.24	110.33
37	d	409	LHG	O7-C7-C8	2.81	117.56	111.48
24	c	509	CLA	O2A-CGA-O1A	-2.81	116.61	123.63
24	B	614	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
24	b	618	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
24	C	512	CLA	CBC-CAC-C3C	-2.81	104.81	112.42
24	b	619	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
24	b	610	CLA	C3C-C4C-NC	2.80	114.02	110.43
24	d	405	CLA	C1D-CHD-C4C	-2.80	120.07	126.02
24	b	607	CLA	O1D-CGD-CBD	-2.80	119.00	124.52
24	B	611	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
37	d	409	LHG	O8-C23-O10	-2.80	116.63	123.63
24	d	405	CLA	C3B-C4B-NB	2.79	113.03	110.53
24	b	610	CLA	C1-C2-C3	-2.79	121.62	126.20
24	b	611	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
24	b	616	CLA	CMB-C2B-C1B	2.79	129.67	125.42
24	c	513	CLA	C3C-C4C-NC	2.79	114.01	110.43
36	O	302	HTG	C1'-S1-C1	2.79	106.48	100.45
24	C	514	CLA	C4-C3-C5	2.79	120.07	115.23
24	C	513	CLA	C2C-C1C-NC	2.79	112.91	109.98
24	A	407	CLA	O2A-CGA-O1A	-2.79	116.66	123.63
24	B	603	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
24	b	618	CLA	C3C-C4C-NC	2.79	114.00	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	422[B]	PL9	C12-C13-C14	-2.79	121.25	127.62
24	B	617	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
37	D	411	LHG	O8-C23-O10	-2.78	116.67	123.63
24	c	507	CLA	C3B-C4B-NB	2.78	113.01	110.53
24	c	515	CLA	O2A-CGA-CBA	2.78	120.32	111.83
24	C	508	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
24	a	409	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
24	a	412	CLA	CMB-C2B-C1B	2.78	129.65	125.42
24	b	607	CLA	O2A-CGA-CBA	2.78	120.30	111.83
24	C	514	CLA	CBC-CAC-C3C	-2.78	104.89	112.42
24	C	508	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
24	C	510	CLA	C1D-CHD-C4C	-2.78	120.12	126.02
27	f	102	SQD	O48-C23-C24	2.77	120.30	111.83
27	A	411	SQD	O48-C23-C24	2.77	120.29	111.83
24	a	410	CLA	O2A-CGA-CBA	2.77	120.29	111.83
24	B	615	CLA	CAC-C3C-C4C	2.77	128.40	124.79
24	b	604	CLA	CHD-C1D-ND	-2.77	120.90	124.80
24	B	613	CLA	CAC-C3C-C4C	2.77	128.40	124.79
24	C	505	CLA	C4-C3-C5	2.77	120.04	115.23
24	b	604	CLA	C4-C3-C5	2.77	120.04	115.23
24	B	608	CLA	C1D-CHD-C4C	-2.77	120.13	126.02
33	a	425[B]	PL9	C53-C6-C1	2.77	120.94	115.28
24	c	509	CLA	C3C-C4C-NC	2.77	113.97	110.43
24	A	405	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
24	a	409	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
24	d	404	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
24	a	408	CLA	CHD-C1D-ND	-2.76	120.92	124.80
24	c	503	CLA	C1-C2-C3	-2.76	121.67	126.20
24	b	609	CLA	O2A-CGA-CBA	2.76	120.24	111.83
24	B	602	CLA	C2C-C1C-NC	2.76	112.88	109.98
24	c	511	CLA	O2A-CGA-CBA	2.76	120.24	111.83
24	c	511	CLA	C3C-C4C-NC	2.75	113.96	110.43
37	B	640	LHG	O8-C23-C24	2.75	120.23	111.83
24	b	614	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
24	B	605	CLA	CMB-C2B-C1B	2.75	129.61	125.42
40	f	101	HEM	CHC-C1C-NC	2.75	127.45	124.45
24	C	505	CLA	CMC-C2C-C1C	2.75	129.33	125.03
24	B	603	CLA	C4-C3-C5	2.75	120.00	115.23
26	T	102	BCR	C2-C1-C6	2.75	114.43	110.44
24	c	508	CLA	C3C-C4C-NC	2.74	113.95	110.43
24	B	605	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
24	b	605	CLA	C3C-C4C-NC	2.74	113.94	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	b	612	CLA	CHD-C1D-ND	-2.74	120.94	124.80
24	B	603	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
24	c	508	CLA	CHA-C1A-NA	-2.74	120.18	126.39
24	c	514	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
24	A	406	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
24	C	509	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
24	D	404	CLA	C2C-C1C-NC	2.74	112.86	109.98
24	c	511	CLA	C11-C12-C13	-2.74	106.87	115.97
37	D	411	LHG	O8-C23-C24	2.74	120.18	111.83
24	C	512	CLA	CHA-C1A-NA	-2.74	120.20	126.39
24	b	612	CLA	C3B-C4B-NB	2.74	112.97	110.53
24	C	507	CLA	C4-C3-C5	2.73	119.97	115.23
24	C	507	CLA	CAA-C2A-C3A	-2.73	105.61	113.00
24	a	412	CLA	O2A-CGA-CBA	2.73	120.17	111.83
24	b	618	CLA	C1-C2-C3	-2.73	121.72	126.20
24	C	513	CLA	C4C-C3C-C2C	-2.73	102.91	106.89
36	I	102	HTG	O5-C5-C4	2.73	114.62	109.70
24	c	503	CLA	C3C-C4C-NC	2.73	113.93	110.43
29	C	521	LMT	C1'-O5'-C5'	2.73	119.05	113.72
24	b	606	CLA	CMA-C3A-C2A	-2.73	103.43	113.98
24	C	509	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
24	b	614	CLA	C2C-C1C-NC	2.73	112.85	109.98
26	Y	302	BCR	C24-C23-C22	-2.73	122.20	126.23
25	a	411	PHO	O2D-CGD-O1D	-2.72	118.55	123.85
24	b	606	CLA	C3C-C4C-NC	2.72	113.92	110.43
24	A	409	CLA	CHD-C1D-ND	-2.72	120.97	124.80
24	c	503	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
24	b	613	CLA	CMA-C3A-C4A	-2.72	104.46	111.77
24	d	405	CLA	CMC-C2C-C1C	2.72	129.29	125.03
24	B	607	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
24	b	607	CLA	CAC-C3C-C4C	2.72	128.33	124.79
24	b	606	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
24	c	509	CLA	C3B-C4B-NB	2.72	112.96	110.53
24	b	610	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
24	b	610	CLA	C1D-CHD-C4C	-2.72	120.24	126.02
24	b	608	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
24	b	608	CLA	CHD-C4C-NC	2.72	128.44	124.23
24	C	510	CLA	CHD-C1D-ND	-2.72	120.98	124.80
24	c	509	CLA	O2A-CGA-CBA	2.72	120.12	111.83
24	C	514	CLA	CMC-C2C-C1C	2.71	129.27	125.03
24	c	508	CLA	C4-C3-C5	2.71	119.93	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	412	LMG	O8-C28-O10	-2.71	116.85	123.63
24	C	505	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
33	A	422[B]	PL9	C27-C28-C29	-2.71	121.42	127.62
24	B	616	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
24	B	607	CLA	C1-C2-C3	-2.71	121.76	126.20
24	B	603	CLA	CHA-C1A-NA	-2.71	120.26	126.39
26	k	303	BCR	C38-C26-C25	-2.71	121.53	124.48
25	d	401	PHO	CMB-C2B-C3B	2.71	130.09	124.68
24	b	609	CLA	C1-C2-C3	-2.70	121.77	126.20
24	B	616	CLA	CMC-C2C-C1C	2.70	129.26	125.03
24	a	412	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
24	b	618	CLA	C4-C3-C5	2.70	119.92	115.23
24	a	412	CLA	C3C-C4C-NC	2.70	113.89	110.43
24	C	504	CLA	CHA-C1A-NA	-2.70	120.28	126.39
24	a	410	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
24	B	602	CLA	C3C-C4C-NC	2.70	113.89	110.43
24	C	512	CLA	CHD-C1D-ND	-2.70	121.01	124.80
33	a	425[B]	PL9	C10-C9-C11	2.70	119.91	115.23
24	B	610	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
24	C	507	CLA	O2A-CGA-O1A	-2.70	116.89	123.63
24	D	403	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
24	b	619	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	C	502	CLA	C1D-CHD-C4C	-2.69	120.30	126.02
24	b	615	CLA	CMC-C2C-C1C	2.69	129.24	125.03
24	C	505	CLA	C2B-C1B-NB	2.69	113.12	110.33
24	B	606	CLA	CHD-C1D-ND	-2.69	121.02	124.80
33	A	422[B]	PL9	C7-C3-C2	-2.69	120.22	123.39
37	d	408	LHG	O7-C7-C8	2.69	117.30	111.48
24	D	404	CLA	C3C-C4C-NC	2.69	113.87	110.43
40	F	101	HEM	C2A-C1A-NA	-2.69	107.17	110.15
24	B	612	CLA	C7-C6-C5	-2.69	106.10	113.26
24	a	410	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
36	D	413	HTG	C1'-S1-C1	2.68	106.24	100.45
24	a	412	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
24	B	611	CLA	C2C-C1C-NC	2.68	112.80	109.98
24	C	506	CLA	CAC-C3C-C4C	2.68	128.28	124.79
39	h	1205	DGD	O1G-C1A-C2A	2.68	120.00	111.83
24	b	608	CLA	C4-C3-C5	2.68	119.88	115.23
24	c	503	CLA	C2B-C1B-NB	2.68	113.10	110.33
24	B	614	CLA	CMC-C2C-C1C	2.68	129.22	125.03
24	B	609	CLA	CHA-C1A-NA	-2.68	120.33	126.39
24	B	604	CLA	O2A-CGA-O1A	-2.68	116.93	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	513	CLA	C3B-C4B-NB	2.68	112.92	110.53
24	a	408	CLA	O2D-CGD-CBD	2.67	115.90	111.23
26	d	406	BCR	C29-C28-C27	2.67	117.15	111.28
37	D	409	LHG	O7-C7-C8	2.67	117.26	111.48
24	b	608	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
24	b	610	CLA	C2B-C1B-NB	2.67	113.09	110.33
24	B	614	CLA	CMB-C2B-C1B	2.67	129.48	125.42
24	B	604	CLA	CAA-C2A-C1A	-2.67	103.24	111.97
24	C	510	CLA	C4B-C3B-C2B	-2.67	103.99	107.30
24	b	614	CLA	C4B-C3B-C2B	-2.67	103.99	107.30
36	b	625	HTG	C1-C2-C3	2.67	115.76	110.55
36	B	626	HTG	C4-C3-C2	-2.66	106.15	110.83
24	b	604	CLA	CMB-C2B-C1B	2.66	129.47	125.42
26	b	620	BCR	C21-C20-C19	-2.66	115.48	123.20
24	B	611	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
24	b	617	CLA	CMC-C2C-C1C	2.66	129.19	125.03
24	B	609	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
24	b	616	CLA	CHA-C1A-NA	-2.66	120.37	126.39
24	B	616	CLA	C6-C7-C8	-2.66	107.12	115.97
24	b	609	CLA	CAC-C3C-C4C	2.66	128.25	124.79
24	B	607	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
24	d	405	CLA	CHD-C1D-ND	-2.66	121.06	124.80
24	c	514	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
27	L	101	SQD	O47-C7-O49	-2.66	117.49	123.70
24	b	604	CLA	C4C-C3C-C2C	-2.66	103.03	106.89
33	A	422[B]	PL9	C45-C44-C46	2.66	119.84	115.23
24	B	615	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
24	A	405	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
24	a	409	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
24	C	509	CLA	O2A-CGA-CBA	2.65	119.92	111.83
24	b	609	CLA	C3B-C4B-NB	2.65	112.90	110.53
24	C	508	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
37	D	410	LHG	O7-C7-C8	2.65	117.22	111.48
24	C	510	CLA	C4C-C3C-C2C	-2.65	103.03	106.89
24	c	509	CLA	CMB-C2B-C1B	2.65	129.45	125.42
39	C	517	DGD	O3G-C3G-C2G	-2.65	104.38	110.82
24	d	405	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
24	B	613	CLA	C1-O2A-CGA	2.65	123.06	116.65
24	A	405	CLA	CMA-C3A-C2A	-2.65	103.75	113.98
24	B	607	CLA	CBC-CAC-C3C	-2.65	105.25	112.42
26	k	302	BCR	C37-C22-C23	2.65	122.13	118.09
24	a	409	CLA	CHD-C1D-ND	-2.65	121.08	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	101	SQD	O48-C23-O10	-2.64	117.01	123.63
26	B	618	BCR	C24-C23-C22	-2.64	122.32	126.23
24	B	613	CLA	C4B-C3B-C2B	-2.64	104.01	107.30
26	c	517	BCR	C21-C20-C19	-2.64	115.54	123.20
24	b	619	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
24	C	506	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
24	c	508	CLA	CGD-CBD-CAD	-2.64	102.30	110.85
24	c	509	CLA	C1D-CHD-C4C	-2.64	120.41	126.02
24	C	502	CLA	C1-C2-C3	-2.64	121.88	126.20
24	c	515	CLA	C4-C3-C5	2.64	119.80	115.23
24	C	502	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
29	T	104	LMT	O5'-C5'-C4'	2.63	114.45	109.70
24	B	614	CLA	C1D-CHD-C4C	-2.63	120.42	126.02
27	a	414	SQD	C44-O6-C1	-2.63	108.15	113.80
24	a	408	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
26	K	101	BCR	C20-C21-C22	-2.63	123.59	127.28
24	b	611	CLA	CAC-C3C-C4C	2.63	128.21	124.79
33	D	406	PL9	C37-C38-C39	-2.63	121.61	127.62
28	c	522	LMG	O8-C28-C29	2.63	119.85	111.83
24	d	405	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
24	c	513	CLA	CHD-C4C-NC	2.63	128.30	124.23
39	C	517	DGD	O1G-C1A-O1A	-2.63	117.06	123.63
26	d	406	BCR	C21-C20-C19	-2.62	115.60	123.20
24	C	509	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
24	B	612	CLA	C4-C3-C5	2.62	119.78	115.23
33	a	425[B]	PL9	C30-C29-C31	2.62	119.78	115.23
33	a	425[B]	PL9	C45-C44-C46	2.62	119.78	115.23
26	B	619	BCR	C38-C26-C25	-2.62	121.62	124.48
26	b	622	BCR	C21-C20-C19	-2.62	115.61	123.20
24	B	610	CLA	O2A-CGA-CBA	2.62	119.83	111.83
24	C	506	CLA	CMB-C2B-C1B	2.62	129.41	125.42
24	C	506	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
33	d	407	PL9	C10-C9-C11	2.62	119.77	115.23
33	a	425[B]	PL9	C15-C14-C16	2.62	119.77	115.23
24	D	403	CLA	C4-C3-C5	2.62	119.77	115.23
39	c	518	DGD	C2G-O2G-C1B	-2.61	111.54	117.80
24	c	515	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
37	D	409	LHG	C5-O7-C7	-2.61	111.54	117.80
24	a	408	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
24	c	515	CLA	C3C-C4C-NC	2.61	113.78	110.43
24	A	409	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
29	c	523	LMT	O5'-C5'-C4'	2.61	115.12	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	503	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
24	b	617	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
24	c	512	CLA	C1-O2A-CGA	2.61	122.96	116.65
27	A	411	SQD	O47-C7-O49	-2.61	117.61	123.70
24	C	502	CLA	C3C-C4C-NC	2.61	113.77	110.43
24	B	616	CLA	CHA-C1A-NA	-2.61	120.49	126.39
24	c	506	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
33	A	422[B]	PL9	C42-C43-C44	-2.60	121.67	127.62
24	b	611	CLA	CMA-C3A-C4A	-2.60	104.78	111.77
26	B	641	BCR	C29-C28-C27	-2.60	105.56	111.28
28	A	412	LMG	C8-O7-C10	-2.60	111.58	117.80
24	b	617	CLA	O2A-CGA-CBA	2.60	119.76	111.83
24	b	609	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
27	a	401	SQD	O8-S-C6	2.60	110.98	105.97
24	c	506	CLA	C3C-C4C-NC	2.60	113.75	110.43
24	A	409	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
24	b	605	CLA	CMA-C3A-C4A	-2.60	104.80	111.77
24	c	509	CLA	CHD-C1D-ND	-2.59	121.15	124.80
26	b	620	BCR	C24-C23-C22	-2.59	122.40	126.23
24	b	606	CLA	CAC-C3C-C4C	2.59	128.16	124.79
24	B	610	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
27	a	401	SQD	O5-C5-C4	2.59	114.37	109.70
24	B	614	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
24	B	616	CLA	O2D-CGD-CBD	2.59	115.75	111.23
24	c	506	CLA	C4-C3-C5	2.59	119.72	115.23
24	B	616	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
24	A	409	CLA	O2A-CGA-CBA	2.58	119.71	111.83
28	a	415	LMG	C7-O1-C1	-2.58	108.26	113.80
24	b	610	CLA	CAA-CBA-CGA	2.58	120.54	113.21
24	B	608	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	b	618	CLA	CHA-C1A-NA	-2.58	120.55	126.39
24	C	504	CLA	CHD-C1D-ND	-2.58	121.17	124.80
24	B	610	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
24	b	605	CLA	C4B-C3B-C2B	-2.57	104.10	107.30
33	D	406	PL9	C17-C18-C19	-2.57	121.73	127.62
25	a	411	PHO	CMA-C3A-C4A	-2.57	109.07	114.61
24	B	614	CLA	CHD-C1D-ND	-2.57	121.18	124.80
24	b	608	CLA	CMC-C2C-C1C	2.57	129.06	125.03
24	C	503	CLA	C3C-C4C-NC	2.57	113.72	110.43
24	B	612	CLA	C3B-C4B-NB	2.57	112.82	110.53
24	C	512	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
24	C	503	CLA	C4C-C3C-C2C	-2.57	103.15	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k	302	BCR	C10-C11-C12	-2.57	115.76	123.20
24	b	618	CLA	CAC-C3C-C4C	2.57	128.13	124.79
24	d	405	CLA	C11-C10-C8	-2.57	107.44	115.97
39	h	1205	DGD	O1G-C1A-O1A	-2.57	117.21	123.63
24	C	510	CLA	C4A-NA-C1A	2.56	107.85	106.68
24	c	511	CLA	C4C-C3C-C2C	-2.56	103.16	106.89
26	b	621	BCR	C20-C21-C22	-2.56	123.68	127.28
24	b	614	CLA	CMA-C3A-C4A	-2.56	104.88	111.77
24	a	408	CLA	C3C-C4C-NC	2.56	113.71	110.43
24	b	609	CLA	C4C-C3C-C2C	-2.56	103.16	106.89
37	E	101	LHG	O8-C23-C24	2.56	119.65	111.83
24	C	503	CLA	CMB-C2B-C1B	2.56	129.32	125.42
24	C	510	CLA	CAC-C3C-C4C	2.56	128.12	124.79
26	k	302	BCR	C24-C23-C22	-2.56	122.45	126.23
24	d	405	CLA	C6-C7-C8	-2.56	107.46	115.97
24	D	404	CLA	CBC-CAC-C3C	-2.56	105.49	112.42
24	a	410	CLA	CHA-C1A-NA	-2.56	120.60	126.39
24	b	619	CLA	CHA-C1A-NA	-2.56	120.60	126.39
33	D	406	PL9	C22-C23-C24	-2.56	121.78	127.62
25	a	411	PHO	O1D-CGD-CBD	-2.56	120.85	124.72
24	D	403	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
27	A	411	SQD	O48-C23-O10	-2.55	117.24	123.63
26	b	621	BCR	C38-C26-C25	-2.55	121.70	124.48
24	B	603	CLA	C3B-C4B-NB	2.55	112.81	110.53
24	B	609	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
29	c	523	LMT	C1B-O5B-C5B	2.55	118.69	113.72
26	Y	302	BCR	C10-C11-C12	-2.55	115.82	123.20
24	b	605	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
24	C	510	CLA	O2A-CGA-CBA	2.54	119.59	111.83
24	C	513	CLA	CHA-C1A-NA	-2.54	120.63	126.39
24	C	514	CLA	CHD-C1D-ND	-2.54	121.22	124.80
24	b	606	CLA	CMC-C2C-C1C	2.54	129.01	125.03
24	B	611	CLA	CMB-C2B-C1B	2.54	129.29	125.42
39	c	518	DGD	O1G-C1A-O1A	-2.54	117.28	123.63
24	d	405	CLA	C3C-C4C-NC	2.54	113.68	110.43
24	D	404	CLA	CHD-C1D-ND	-2.54	121.23	124.80
24	c	508	CLA	CAC-C3C-C4C	2.54	128.09	124.79
24	B	612	CLA	C1-C2-C3	-2.54	122.04	126.20
24	C	502	CLA	C4B-C3B-C2B	-2.54	104.15	107.30
24	C	514	CLA	C2C-C1C-NC	2.54	112.64	109.98
24	B	604	CLA	CMC-C2C-C1C	2.53	129.00	125.03
37	d	410	LHG	O8-C23-O10	-2.53	117.29	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
37	e	101	LHG	C5-O7-C7	-2.53	111.73	117.80
27	L	101	SQD	C1-O5-C5	2.53	118.67	113.72
25	A	408	PHO	CBC-CAC-C3C	-2.53	109.25	112.87
29	z	101	LMT	O5B-C1B-C2B	-2.53	105.17	110.37
27	L	102	SQD	O47-C7-O49	-2.53	117.79	123.70
24	b	609	CLA	C3C-C4C-NC	2.53	113.67	110.43
24	B	617	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
24	A	407	CLA	CMA-C3A-C2A	-2.53	104.22	113.98
24	a	408	CLA	CHC-C1C-C2C	-2.52	119.77	126.95
24	c	514	CLA	C4-C3-C5	2.52	119.61	115.23
29	B	622	LMT	O1'-C1'-C2'	2.52	112.11	108.27
24	B	613	CLA	CHD-C1D-ND	-2.52	121.25	124.80
24	b	612	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
24	B	612	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
24	b	613	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
26	B	620	BCR	C21-C20-C19	-2.52	115.90	123.20
24	C	512	CLA	CMB-C2B-C1B	2.52	129.25	125.42
24	c	509	CLA	C1-C2-C3	-2.52	122.07	126.20
33	a	425[B]	PL9	C40-C39-C41	2.52	119.60	115.23
24	B	605	CLA	CHA-C1A-NA	-2.52	120.69	126.39
24	c	514	CLA	CHA-C1A-NA	-2.52	120.69	126.39
26	C	515	BCR	C23-C24-C25	-2.52	120.28	127.00
27	a	414	SQD	O48-C23-C24	2.51	119.50	111.83
28	d	411	LMG	O8-C28-O10	-2.51	117.34	123.63
24	B	617	CLA	CMB-C2B-C1B	2.51	129.25	125.42
26	b	622	BCR	C8-C7-C6	-2.51	120.29	127.00
24	c	506	CLA	C4C-C3C-C2C	-2.51	103.24	106.89
26	D	405	BCR	C37-C22-C23	2.51	121.92	118.09
24	C	509	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
24	b	614	CLA	CHA-C1A-NA	-2.51	120.71	126.39
24	b	604	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
24	C	505	CLA	C1-O2A-CGA	2.51	122.72	116.65
24	B	604	CLA	CHD-C1D-ND	-2.51	121.27	124.80
37	D	410	LHG	O8-C23-O10	-2.51	117.36	123.63
29	z	101	LMT	O1B-C4'-C3'	2.51	113.60	107.23
24	C	513	CLA	CMC-C2C-C1C	2.50	128.95	125.03
27	A	413	SQD	C3-C4-C5	2.50	114.77	110.23
26	d	406	BCR	C3-C4-C5	-2.50	109.59	114.06
24	c	508	CLA	CAA-CBA-CGA	2.50	120.32	113.21
24	b	605	CLA	CBC-CAC-C3C	-2.50	105.63	112.42
26	c	517	BCR	C3-C4-C5	-2.50	109.59	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	F	101	HEM	C3B-C2B-C1B	2.50	108.29	106.41
24	a	408	CLA	CMA-C3A-C4A	-2.50	105.05	111.77
33	A	422[B]	PL9	C10-C9-C11	2.50	119.57	115.23
24	b	617	CLA	C4-C3-C5	2.50	119.57	115.23
24	b	611	CLA	C1D-CHD-C4C	-2.50	120.71	126.02
24	C	510	CLA	CMB-C2B-C1B	2.50	129.22	125.42
24	B	604	CLA	CAC-C3C-C4C	2.50	128.04	124.79
24	B	608	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
33	d	407	PL9	C27-C28-C29	-2.50	121.91	127.62
24	b	610	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
29	A	414	LMT	C1B-O1B-C4'	-2.49	112.07	117.98
24	b	619	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
24	b	608	CLA	C1-C2-C3	-2.49	122.11	126.20
24	c	511	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
24	B	614	CLA	CED-O2D-CGD	2.49	121.57	115.92
24	b	615	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
24	A	407	CLA	O2A-CGA-CBA	2.49	119.43	111.83
24	c	509	CLA	C4-C3-C5	2.49	119.55	115.23
24	C	513	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
26	B	641	BCR	C11-C10-C9	-2.49	123.79	127.28
24	B	602	CLA	CMB-C2B-C1B	2.49	129.20	125.42
24	B	606	CLA	C3B-C4B-NB	2.48	112.75	110.53
24	D	404	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
24	C	514	CLA	O2A-CGA-CBA	2.48	119.40	111.83
37	d	409	LHG	O8-C23-C24	2.48	119.40	111.83
25	d	401	PHO	O2D-CGD-O1D	-2.48	119.03	123.85
24	B	603	CLA	CBC-CAC-C3C	-2.48	105.70	112.42
24	C	511	CLA	C6-C7-C8	-2.48	107.74	115.97
24	B	615	CLA	CMB-C2B-C1B	2.48	129.19	125.42
24	B	610	CLA	C7-C6-C5	-2.47	106.67	113.26
24	c	513	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
24	B	612	CLA	CHA-C1A-NA	-2.47	120.79	126.39
24	c	505	CLA	C3B-C4B-NB	2.47	112.74	110.53
24	c	512	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
24	C	511	CLA	CMA-C3A-C4A	-2.47	105.13	111.77
24	C	511	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
24	B	617	CLA	CHA-C1A-NA	-2.47	120.80	126.39
26	T	102	BCR	C21-C20-C19	-2.47	116.05	123.20
24	C	512	CLA	C4-C3-C5	2.47	119.51	115.23
33	d	407	PL9	C20-C19-C21	2.47	119.51	115.23
24	C	504	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
26	C	516	BCR	C23-C24-C25	-2.47	120.41	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	640	LHG	O8-C23-O10	-2.47	117.46	123.63
24	D	404	CLA	CMC-C2C-C1C	2.47	128.89	125.03
26	B	641	BCR	C35-C13-C12	2.46	121.85	118.09
24	C	514	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
25	A	408	PHO	CBA-CAA-C2A	-2.46	106.52	113.78
24	C	508	CLA	O2A-CGA-CBA	2.46	119.35	111.83
24	a	408	CLA	CMA-C3A-C2A	-2.46	104.46	113.98
25	D	401	PHO	CMB-C2B-C3B	2.46	129.60	124.68
29	A	414	LMT	O5'-C5'-C4'	2.46	114.81	109.72
27	A	413	SQD	O5-C5-C4	2.46	114.13	109.70
24	c	506	CLA	CMC-C2C-C1C	2.46	128.88	125.03
24	d	405	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
36	C	523	HTG	O5-C5-C4	2.46	114.13	109.70
24	b	607	CLA	CMB-C2B-C1B	2.46	129.16	125.42
24	B	602	CLA	C4B-C3B-C2B	-2.46	104.25	107.30
24	B	608	CLA	C3C-C4C-NC	2.46	113.58	110.43
24	b	605	CLA	CMA-C3A-C2A	-2.46	104.49	113.98
24	B	604	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
36	B	623[B]	HTG	C1-C2-C3	2.45	115.35	110.55
26	A	410	BCR	C8-C7-C6	-2.45	120.44	127.00
24	C	505	CLA	C4C-C3C-C2C	-2.45	103.33	106.89
25	A	408	PHO	C1-C2-C3	-2.45	122.18	126.20
24	b	610	CLA	CHD-C1D-ND	-2.45	121.36	124.80
24	b	617	CLA	CHD-C1D-ND	-2.45	121.36	124.80
24	b	617	CLA	C3B-C4B-NB	2.45	112.72	110.53
27	a	414	SQD	O8-S-C6	2.45	110.70	105.97
24	b	604	CLA	CAA-C2A-C3A	-2.45	106.39	113.00
24	b	616	CLA	O2A-CGA-CBA	2.45	119.29	111.83
33	A	422[B]	PL9	C30-C29-C31	2.45	119.47	115.23
27	L	102	SQD	C3-C4-C5	2.44	114.66	110.23
26	T	102	BCR	C29-C28-C27	-2.44	105.91	111.28
24	b	617	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	b	619	CLA	C4-C3-C5	2.44	119.47	115.23
24	B	605	CLA	CMC-C2C-C1C	2.44	128.85	125.03
33	a	425[B]	PL9	C51-C49-C50	2.44	120.20	114.59
24	a	409	CLA	CAA-CBA-CGA	2.44	120.14	113.21
29	Z	101	LMT	O1B-C1B-C2B	2.44	114.09	108.09
39	C	517	DGD	O6D-C5D-C6D	2.44	111.53	106.69
26	K	101	BCR	C38-C26-C25	-2.44	121.82	124.48
24	b	605	CLA	O2A-CGA-CBA	2.44	119.27	111.83
24	c	514	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
24	c	511	CLA	CHA-C1A-NA	-2.43	120.88	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
24	c	512	CLA	CHA-C1A-NA	-2.43	120.88	126.39
25	D	401	PHO	C4D-CHA-CBD	2.43	109.62	108.45
24	A	406	CLA	C4-C3-C5	2.43	119.45	115.23
24	b	613	CLA	CMB-C2B-C1B	2.43	129.12	125.42
26	c	517	BCR	C15-C14-C13	-2.43	123.87	127.28
39	D	407	DGD	O6D-C1D-C2D	-2.43	105.38	110.37
24	C	503	CLA	CHA-C1A-NA	-2.43	120.89	126.39
24	A	405	CLA	CAC-C3C-C4C	2.43	127.95	124.79
24	D	403	CLA	CMB-C2B-C1B	2.43	129.11	125.42
24	D	404	CLA	C3B-C4B-NB	2.43	112.70	110.53
26	b	622	BCR	C3-C4-C5	-2.43	109.73	114.06
24	B	615	CLA	CMC-C2C-C1C	2.43	128.82	125.03
24	B	608	CLA	C1-O2A-CGA	2.42	122.52	116.65
24	c	513	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
33	D	406	PL9	C27-C28-C29	-2.42	122.08	127.62
24	d	404	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
24	b	607	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
24	b	609	CLA	C4A-NA-C1A	2.42	107.78	106.68
24	C	503	CLA	C4-C3-C5	2.42	119.43	115.23
24	B	614	CLA	C1-C2-C3	-2.42	122.23	126.20
24	c	514	CLA	CMC-C2C-C1C	2.42	128.81	125.03
24	b	610	CLA	CAC-C3C-C4C	2.42	127.93	124.79
24	b	608	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
24	a	409	CLA	CMB-C2B-C1B	2.41	129.10	125.42
24	B	606	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
24	C	511	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
33	d	407	PL9	C53-C6-C1	2.41	120.22	115.28
24	a	410	CLA	CAA-CBA-CGA	2.41	120.06	113.21
24	C	502	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
25	A	408	PHO	C4-C3-C5	2.41	119.42	115.23
26	T	102	BCR	C16-C17-C18	-2.41	123.90	127.28
24	b	605	CLA	C3B-C4B-NB	2.41	112.68	110.53
24	B	614	CLA	CMA-C3A-C4A	-2.41	105.30	111.77
24	c	513	CLA	CMA-C3A-C4A	2.41	118.25	111.77
24	B	605	CLA	C4A-NA-C1A	2.41	107.78	106.68
24	B	612	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
27	a	401	SQD	O48-C23-O10	-2.41	117.61	123.63
24	b	614	CLA	CMB-C2B-C1B	2.41	129.08	125.42
24	B	614	CLA	CHC-C1C-C2C	-2.40	120.11	126.95
24	B	608	CLA	O2A-CGA-CBA	2.40	119.17	111.83
24	B	605	CLA	O2D-CGD-O1D	-2.40	119.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	CAC-C3C-C4C	2.40	127.92	124.79
26	A	410	BCR	C15-C16-C17	-2.40	118.61	123.52
24	b	609	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
40	f	101	HEM	CBA-CAA-C2A	-2.40	105.89	112.53
24	B	609	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	B	605	CLA	C6-C5-C3	-2.40	107.62	113.47
24	b	618	CLA	CMB-C2B-C1B	2.40	129.07	125.42
24	b	617	CLA	CMB-C2B-C1B	2.40	129.07	125.42
36	B	623[A]	HTG	C1-O5-C5	2.40	116.86	112.56
24	b	604	CLA	C1-C2-C3	-2.40	122.27	126.20
24	B	616	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
24	b	609	CLA	CHA-C1A-NA	-2.40	120.97	126.39
24	a	410	CLA	C1-C2-C3	-2.39	122.27	126.20
24	D	404	CLA	C1-C2-C3	-2.39	122.28	126.20
24	b	612	CLA	C1-C2-C3	-2.39	122.28	126.20
24	C	514	CLA	C3B-C4B-NB	2.39	112.67	110.53
24	C	509	CLA	CHD-C1D-ND	-2.39	121.44	124.80
24	C	503	CLA	CMC-C2C-C1C	2.39	128.77	125.03
39	c	520	DGD	O2G-C1B-C2B	2.39	116.65	111.48
24	B	613	CLA	C7-C6-C5	-2.39	106.89	113.26
24	b	607	CLA	C6-C5-C3	-2.39	107.65	113.47
24	B	603	CLA	CHC-C1C-C2C	-2.39	120.16	126.95
25	d	401	PHO	CMC-C2C-C1C	2.39	129.03	124.73
24	b	604	CLA	C3B-C4B-NB	2.39	112.66	110.53
24	C	502	CLA	CAC-C3C-C4C	2.39	127.89	124.79
24	b	610	CLA	CHC-C1C-C2C	-2.39	120.17	126.95
24	A	409	CLA	CMC-C2C-C1C	2.39	128.76	125.03
24	c	515	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
26	B	618	BCR	C21-C20-C19	-2.39	116.29	123.20
24	c	510	CLA	O2A-CGA-CBA	2.39	119.11	111.83
24	B	603	CLA	CMA-C3A-C2A	-2.38	104.76	113.98
24	b	612	CLA	C4-C3-C5	2.38	119.36	115.23
24	a	412	CLA	CHC-C1C-C2C	-2.38	120.18	126.95
24	B	612	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
26	T	102	BCR	C1-C6-C7	2.38	122.11	115.65
33	D	406	PL9	C51-C49-C50	2.38	120.07	114.59
24	c	506	CLA	CMB-C2B-C1B	2.38	129.04	125.42
24	c	515	CLA	CMB-C2B-C1B	2.38	129.04	125.42
24	c	504	CLA	CMC-C2C-C1C	2.38	128.75	125.03
24	C	507	CLA	CED-O2D-CGD	2.38	121.31	115.92
33	d	407	PL9	C37-C38-C39	-2.38	122.18	127.62
24	B	607	CLA	CMB-C2B-C1B	2.38	129.04	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	CMC-C2C-C1C	2.38	128.75	125.03
24	d	405	CLA	O2A-CGA-CBA	2.38	119.08	111.83
26	Y	302	BCR	C21-C20-C19	-2.38	116.31	123.20
25	d	401	PHO	O2A-CGA-CBA	2.38	119.08	111.83
24	B	606	CLA	CBC-CAC-C3C	-2.38	105.98	112.42
24	C	505	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
25	A	408	PHO	C4A-C3A-C2A	-2.38	100.58	102.84
33	a	425[B]	PL9	C32-C31-C29	-2.37	105.32	113.19
24	b	610	CLA	CMA-C3A-C2A	-2.37	104.80	113.98
28	a	415	LMG	O7-C10-O9	-2.37	118.16	123.70
24	B	616	CLA	CHD-C1D-ND	-2.37	121.46	124.80
24	b	604	CLA	C1-O2A-CGA	2.37	122.39	116.65
24	b	609	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
24	c	513	CLA	C1-C2-C3	-2.37	122.32	126.20
24	B	610	CLA	CMA-C3A-C4A	-2.37	105.41	111.77
24	b	608	CLA	CMA-C3A-C4A	-2.37	105.41	111.77
24	B	610	CLA	C2B-C1B-NB	2.37	112.78	110.33
26	A	410	BCR	C15-C14-C13	-2.36	123.96	127.28
39	H	102	DGD	O2G-C1B-C2B	2.36	116.60	111.48
24	B	610	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	B	616	CLA	CED-O2D-CGD	2.36	121.28	115.92
37	D	410	LHG	O8-C23-C24	2.36	119.04	111.83
29	a	402	LMT	O5'-C5'-C4'	2.36	114.61	109.72
24	b	611	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	c	505	CLA	O2A-CGA-CBA	2.36	119.03	111.83
24	C	502	CLA	CMC-C2C-C1C	2.36	128.72	125.03
37	d	408	LHG	O7-C7-O9	-2.36	118.19	123.70
24	B	612	CLA	CMB-C2B-C1B	2.36	129.01	125.42
29	B	622	LMT	O1B-C4'-C3'	2.36	113.22	107.23
24	b	604	CLA	C3C-C4C-NC	2.36	113.45	110.43
24	c	509	CLA	CHA-C1A-NA	-2.36	121.06	126.39
24	B	616	CLA	CMB-C2B-C1B	2.35	129.00	125.42
24	c	506	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
24	a	410	CLA	C3B-C4B-NB	2.35	112.63	110.53
24	C	510	CLA	C3C-C4C-NC	2.35	113.44	110.43
24	C	507	CLA	CMB-C2B-C1B	2.35	129.00	125.42
24	c	513	CLA	C6-C5-C3	-2.35	107.74	113.47
27	A	411	SQD	O8-S-C6	2.35	110.51	105.97
30	C	524	GOL	C3-C2-C1	-2.35	103.17	111.80
24	c	510	CLA	CHC-C1C-C2C	-2.35	120.27	126.95
33	D	406	PL9	C10-C9-C11	2.35	119.31	115.23
24	C	503	CLA	CAC-C3C-C4C	2.35	127.85	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	CHC-C1C-C2C	-2.35	120.27	126.95
24	C	505	CLA	C3C-C4C-NC	2.35	113.44	110.43
36	D	413	HTG	O5-C1-C2	2.35	113.55	110.32
26	D	405	BCR	C29-C28-C27	2.35	116.44	111.28
24	d	404	CLA	CHA-C1A-NA	-2.35	121.08	126.39
24	c	510	CLA	CHB-C4A-NA	2.34	127.78	124.40
33	a	425[B]	PL9	C35-C34-C36	2.34	119.30	115.23
24	A	405	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
24	c	514	CLA	CMB-C2B-C1B	2.34	128.99	125.42
39	C	519	DGD	O3G-C3G-C2G	-2.34	105.12	110.82
24	b	617	CLA	CBC-CAC-C3C	-2.34	106.07	112.42
24	c	510	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
24	C	513	CLA	O2A-CGA-CBA	2.34	118.97	111.83
26	T	102	BCR	C7-C6-C5	-2.34	116.16	121.56
26	B	641	BCR	C20-C21-C22	-2.34	124.00	127.28
24	b	616	CLA	C1-O2A-CGA	2.34	122.32	116.65
24	D	404	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
26	b	621	BCR	C8-C7-C6	-2.34	120.75	127.00
24	b	618	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	b	619	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
24	c	508	CLA	C3B-C4B-NB	2.34	112.61	110.53
24	a	408	CLA	CMC-C2C-C1C	2.34	128.68	125.03
24	A	405	CLA	C3B-C4B-NB	2.33	112.61	110.53
24	b	618	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
24	A	406	CLA	O2A-CGA-CBA	2.33	118.95	111.83
24	b	605	CLA	CED-O2D-CGD	2.33	121.21	115.92
24	b	607	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
24	C	511	CLA	CHA-C1A-NA	-2.33	121.11	126.39
24	b	612	CLA	CMB-C2B-C1B	2.33	128.97	125.42
24	A	407	CLA	CHD-C1D-ND	-2.33	121.52	124.80
30	M	102	GOL	C3-C2-C1	-2.33	103.25	111.80
28	A	412	LMG	C7-O1-C1	-2.33	108.80	113.80
27	A	413	SQD	O48-C23-O10	-2.33	117.81	123.63
24	c	508	CLA	O2A-CGA-CBA	2.32	118.92	111.83
26	b	622	BCR	C10-C11-C12	-2.32	116.47	123.20
33	A	422[B]	PL9	C7-C3-C4	2.32	118.82	116.91
24	c	510	CLA	C6-C7-C8	-2.32	108.25	115.97
24	C	504	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
28	c	522	LMG	C8-O7-C10	-2.32	112.24	117.80
24	c	515	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
24	c	514	CLA	CAC-C3C-C4C	2.32	127.81	124.79
24	c	505	CLA	O2A-CGA-O1A	-2.32	117.83	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	O2A-CGA-CBA	2.32	118.90	111.83
37	e	101	LHG	O8-C23-C24	2.32	118.90	111.83
24	B	615	CLA	C4C-C3C-C2C	-2.32	103.52	106.89
24	C	510	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
24	C	505	CLA	C4A-NA-C1A	2.32	107.74	106.68
24	C	510	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
24	B	614	CLA	C4A-NA-C1A	2.31	107.73	106.68
26	T	102	BCR	C15-C14-C13	2.31	130.52	127.28
24	b	617	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
26	k	303	BCR	C10-C11-C12	-2.31	116.50	123.20
26	B	619	BCR	C29-C28-C27	-2.31	106.20	111.28
26	T	102	BCR	C23-C24-C25	-2.31	120.83	127.00
36	b	601	HTG	O5-C5-C4	2.31	113.85	109.70
24	C	508	CLA	C3B-C4B-NB	2.31	112.59	110.53
24	C	511	CLA	CHD-C1D-ND	-2.30	121.56	124.80
36	d	414	HTG	O5-C5-C4	2.30	113.85	109.70
26	b	621	BCR	C28-C27-C26	-2.30	109.95	114.06
24	c	511	CLA	C17-C16-C15	-2.30	102.96	113.28
24	B	603	CLA	O2A-CGA-CBA	2.30	118.85	111.83
24	B	610	CLA	C1-O2A-CGA	2.30	122.22	116.65
25	A	408	PHO	CMB-C2B-C3B	2.30	129.28	124.68
24	c	504	CLA	C4-C3-C5	2.30	119.22	115.23
24	c	509	CLA	CMC-C2C-C1C	2.30	128.63	125.03
39	D	407	DGD	O2G-C1B-O1B	-2.30	118.33	123.70
24	B	615	CLA	CHD-C4C-NC	2.30	127.80	124.23
27	L	102	SQD	C1-C2-C3	-2.30	105.17	110.01
24	c	509	CLA	CHC-C4B-NB	2.30	127.50	124.05
39	C	518	DGD	O1G-C1A-C2A	2.30	118.84	111.83
39	c	519	DGD	O2G-C1B-O1B	-2.30	118.33	123.70
24	c	506	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	B	603	CLA	CAA-CBA-CGA	-2.30	106.69	113.21
24	d	405	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
24	C	510	CLA	C1-O2A-CGA	2.30	122.21	116.65
24	c	506	CLA	CAA-C2A-C3A	-2.29	106.80	113.00
36	V	203	HTG	C1-O5-C5	-2.29	108.44	112.56
24	B	610	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
24	B	603	CLA	CHD-C1D-ND	-2.29	121.58	124.80
39	c	520	DGD	O3G-C3G-C2G	-2.29	105.25	110.82
28	C	520	LMG	O8-C28-O10	-2.29	117.90	123.63
24	B	614	CLA	C1-O2A-CGA	2.29	122.19	116.65
26	B	641	BCR	C23-C24-C25	-2.29	120.88	127.00
39	h	1205	DGD	C6D-C5D-C4D	2.29	116.87	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	518	DGD	O3G-C1D-C2D	-2.28	104.80	108.27
27	A	411	SQD	O9-S-C6	2.28	110.17	106.76
24	b	616	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
33	d	407	PL9	C22-C23-C24	-2.28	122.40	127.62
24	C	503	CLA	C4B-C3B-C2B	-2.28	104.46	107.30
24	b	605	CLA	CHA-C1A-NA	-2.28	121.22	126.39
30	C	530	GOL	C3-C2-C1	-2.28	103.42	111.80
28	D	412	LMG	O7-C10-C11	2.28	116.42	111.48
24	C	507	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
24	b	605	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	b	612	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
27	D	408	SQD	O48-C23-O10	-2.28	117.92	123.63
39	c	520	DGD	O1G-C1A-O1A	-2.28	117.93	123.63
24	b	618	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
24	B	604	CLA	CHB-C1B-C2B	-2.28	120.81	127.43
24	C	506	CLA	CMA-C3A-C4A	-2.28	105.66	111.77
24	b	607	CLA	CMC-C2C-C1C	2.28	128.59	125.03
26	k	302	BCR	C1-C6-C7	2.28	121.82	115.65
24	B	611	CLA	C1C-C2C-C3C	-2.28	104.59	106.98
24	C	507	CLA	CAC-C3C-C4C	2.28	127.75	124.79
24	A	406	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	B	607	CLA	CHA-C1A-NA	-2.27	121.24	126.39
24	b	611	CLA	C3B-C4B-NB	2.27	112.56	110.53
24	B	609	CLA	C11-C10-C8	-2.27	108.41	115.97
24	A	409	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
24	b	612	CLA	C1-O2A-CGA	2.27	122.15	116.65
24	b	615	CLA	CHD-C1D-ND	-2.27	121.61	124.80
24	B	615	CLA	C7-C6-C5	-2.27	107.22	113.26
24	c	503	CLA	C4-C3-C5	2.27	119.16	115.23
24	c	513	CLA	CMC-C2C-C1C	2.27	128.58	125.03
24	C	508	CLA	CMC-C2C-C1C	2.27	128.58	125.03
24	D	403	CLA	CAA-C2A-C3A	-2.27	106.88	113.00
24	b	611	CLA	CBC-CAC-C3C	-2.27	106.28	112.42
24	C	511	CLA	CAC-C3C-C4C	2.27	127.74	124.79
28	a	415	LMG	O6-C5-C4	2.27	113.78	109.70
26	Y	302	BCR	C37-C22-C23	2.26	121.54	118.09
24	b	614	CLA	CMC-C2C-C1C	2.26	128.57	125.03
24	B	615	CLA	C1-O2A-CGA	2.26	122.12	116.65
25	d	401	PHO	O1D-CGD-CBD	-2.26	121.30	124.72
24	c	503	CLA	O2A-CGA-CBA	2.26	118.72	111.83
24	C	513	CLA	C4B-C3B-C2B	-2.26	104.49	107.30
26	A	410	BCR	C20-C21-C22	-2.26	124.11	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	602	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
26	D	405	BCR	C21-C20-C19	-2.26	116.66	123.20
24	D	403	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
24	B	605	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
24	B	612	CLA	CAA-C2A-C3A	-2.26	106.91	113.00
24	b	610	CLA	C4A-NA-C1A	2.25	107.71	106.68
27	D	408	SQD	O47-C7-O49	-2.25	118.44	123.70
24	a	410	CLA	CMA-C3A-C2A	-2.25	105.28	113.98
24	A	406	CLA	CAA-CBA-CGA	2.25	119.60	113.21
24	c	513	CLA	CHA-C1A-NA	-2.25	121.30	126.39
25	a	411	PHO	CMC-C2C-C1C	2.25	128.78	124.73
24	C	507	CLA	CGD-CBD-CAD	-2.25	103.57	110.85
24	c	511	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	A	405	CLA	CMC-C2C-C1C	2.25	128.54	125.03
24	c	504	CLA	CHD-C1D-ND	-2.24	121.64	124.80
24	C	509	CLA	CAC-C3C-C4C	2.24	127.71	124.79
24	A	409	CLA	CMB-C2B-C1B	2.24	128.84	125.42
43	v	1603	HEC	C1D-C2D-C3D	-2.24	104.25	106.82
24	B	614	CLA	CAC-C3C-C4C	2.24	127.71	124.79
27	L	101	SQD	O6-C1-C2	2.24	111.68	108.27
40	F	101	HEM	CHC-C4B-NB	2.24	126.84	124.42
24	c	504	CLA	C3B-C4B-NB	2.24	112.53	110.53
24	B	615	CLA	CHA-C1A-NA	-2.24	121.32	126.39
24	c	507	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	C	507	CLA	CHD-C1D-ND	-2.24	121.65	124.80
24	b	614	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
24	a	412	CLA	CHD-C4C-NC	2.24	127.70	124.23
26	d	406	BCR	C16-C17-C18	-2.24	124.14	127.28
24	A	405	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
41	H	101	RRX	C20-C21-C22	-2.24	124.14	127.28
24	B	616	CLA	C4-C3-C5	2.24	119.11	115.23
24	a	410	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
24	A	406	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
24	d	405	CLA	CHA-C1A-NA	-2.23	121.33	126.39
24	c	515	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
39	C	518	DGD	O6E-C5E-C6E	2.23	111.97	106.44
24	a	408	CLA	C4-C3-C5	2.23	119.10	115.23
24	A	409	CLA	CHB-C4A-NA	2.23	127.62	124.40
24	b	612	CLA	CHA-C1A-NA	-2.23	121.34	126.39
24	b	619	CLA	OBD-CAD-C3D	-2.23	123.21	128.42
29	T	104	LMT	C3'-C4'-C5'	2.22	114.26	110.23
26	a	413	BCR	C7-C8-C9	-2.22	122.95	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	413	SQD	C1-C2-C3	-2.22	105.33	110.01
24	a	410	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
24	b	613	CLA	C4-C3-C5	2.22	119.08	115.23
24	c	508	CLA	CED-O2D-CGD	2.22	120.95	115.92
24	b	608	CLA	O2A-CGA-CBA	2.22	118.61	111.83
28	D	412	LMG	O8-C28-C29	2.22	118.61	111.83
24	a	409	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	c	515	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	c	507	CLA	C4-C3-C5	2.22	119.08	115.23
27	A	413	SQD	C1-O5-C5	-2.22	109.39	113.72
28	a	415	LMG	C30-C29-C28	-2.22	105.57	113.69
24	b	606	CLA	C5-C3-C2	-2.22	116.19	121.17
27	L	102	SQD	O9-S-C6	2.22	110.07	106.76
43	V	202	HEC	CAD-CBD-CGD	-2.22	107.79	113.67
24	b	608	CLA	C1-O2A-CGA	2.22	122.01	116.65
24	a	412	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
26	B	620	BCR	C7-C8-C9	-2.22	122.96	126.23
24	B	614	CLA	CHA-C1A-NA	-2.22	121.38	126.39
29	J	102	LMT	O5'-C5'-C4'	2.21	113.69	109.70
29	c	523	LMT	O1B-C1B-C2B	2.21	113.54	108.09
30	a	416	GOL	C3-C2-C1	-2.21	103.67	111.80
24	C	506	CLA	C4-C3-C5	2.21	119.07	115.23
24	b	614	CLA	C4A-NA-C1A	2.21	107.69	106.68
24	c	504	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
24	B	602	CLA	CHA-C1A-NA	-2.21	121.38	126.39
24	C	509	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
26	k	302	BCR	C35-C13-C12	2.21	121.46	118.09
26	C	516	BCR	C21-C20-C19	-2.21	116.80	123.20
26	K	101	BCR	C8-C7-C6	-2.21	121.10	127.00
24	a	409	CLA	CHA-C1A-NA	-2.21	121.39	126.39
24	b	616	CLA	CHD-C1D-ND	-2.21	121.69	124.80
26	B	641	BCR	C16-C15-C14	2.21	128.04	123.52
24	B	613	CLA	CBC-CAC-C3C	-2.21	106.44	112.42
36	I	102	HTG	O5-C1-C2	2.21	113.36	110.32
24	C	505	CLA	CAC-C3C-C4C	2.21	127.66	124.79
24	A	405	CLA	CAA-CBA-CGA	-2.20	106.95	113.21
24	D	403	CLA	C4A-NA-C1A	-2.20	105.67	106.68
25	d	401	PHO	C4A-C3A-C2A	-2.20	100.74	102.84
28	b	623	LMG	O7-C10-O9	-2.20	118.56	123.70
24	c	513	CLA	O2A-CGA-CBA	2.20	118.55	111.83
24	c	505	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
40	F	101	HEM	CMD-C2D-C1D	2.20	128.47	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	CLA	CAC-C3C-C4C	2.20	127.65	124.79
24	c	512	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
24	c	503	CLA	CAC-C3C-C4C	2.20	127.65	124.79
24	C	511	CLA	CMC-C2C-C1C	2.20	128.47	125.03
28	A	412	LMG	O7-C10-O9	-2.20	118.56	123.70
24	C	504	CLA	CMB-C2B-C1B	2.20	128.77	125.42
24	C	508	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
24	A	406	CLA	CMC-C2C-C1C	2.20	128.47	125.03
24	c	507	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
24	d	405	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
24	C	503	CLA	C16-C15-C13	-2.20	108.67	115.97
26	T	102	BCR	C16-C15-C14	2.20	128.01	123.52
39	C	519	DGD	C9B-C8B-C7B	-2.20	103.27	114.37
26	c	517	BCR	C23-C24-C25	-2.19	121.14	127.00
24	c	506	CLA	CHD-C4C-NC	2.19	127.63	124.23
39	c	519	DGD	C3B-C2B-C1B	-2.19	105.66	113.69
41	h	1204	RRX	C16-C15-C14	-2.19	119.03	123.52
30	A	415	GOL	C3-C2-C1	-2.19	103.76	111.80
26	c	516	BCR	C8-C7-C6	-2.19	121.15	127.00
27	A	411	SQD	C44-O6-C1	-2.19	109.10	113.80
24	B	612	CLA	C1-O2A-CGA	2.19	121.95	116.65
24	b	604	CLA	CHA-C1A-NA	-2.19	121.44	126.39
24	c	503	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
26	b	622	BCR	C16-C15-C14	-2.19	119.05	123.52
24	b	615	CLA	CMA-C3A-C2A	-2.19	105.53	113.98
24	C	506	CLA	CMC-C2C-C1C	2.18	128.44	125.03
24	C	512	CLA	CMC-C2C-C1C	2.18	128.44	125.03
24	c	512	CLA	C1-C2-C3	-2.18	122.63	126.20
24	c	513	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
24	d	405	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
30	C	528	GOL	C3-C2-C1	-2.18	103.82	111.80
26	Y	302	BCR	C1-C6-C7	2.18	121.55	115.65
24	C	504	CLA	C1-O2A-CGA	2.18	121.92	116.65
26	a	413	BCR	C24-C23-C22	-2.17	123.02	126.23
24	c	511	CLA	CAC-C3C-C4C	2.17	127.62	124.79
24	c	506	CLA	CAC-C3C-C4C	2.17	127.62	124.79
24	C	504	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
24	B	614	CLA	O2D-CGD-CBD	2.17	115.03	111.23
24	C	509	CLA	CMB-C2B-C1B	2.17	128.73	125.42
39	c	518	DGD	O2G-C1B-O1B	-2.17	118.63	123.70
39	C	517	DGD	O1G-C1A-C2A	2.17	118.45	111.83
39	C	517	DGD	C3G-C2G-C1G	-2.17	106.72	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	641	BCR	C12-C13-C14	-2.17	115.60	119.01
24	C	513	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	B	606	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
24	b	614	CLA	C7-C6-C5	-2.17	107.48	113.26
28	A	412	LMG	O6-C5-C4	2.17	113.61	109.70
24	c	507	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
28	A	412	LMG	O8-C28-C29	2.17	118.44	111.83
24	D	404	CLA	CHA-C1A-NA	-2.17	121.49	126.39
26	T	102	BCR	C35-C13-C12	2.16	121.39	118.09
24	b	605	CLA	CHB-C1B-C2B	-2.16	121.14	127.43
24	A	409	CLA	C7-C6-C5	-2.16	107.50	113.26
26	D	405	BCR	C30-C25-C24	2.16	121.51	115.65
24	C	508	CLA	CHC-C4B-NB	2.16	127.29	124.05
39	c	518	DGD	O1G-C1A-C2A	2.16	118.42	111.83
26	T	102	BCR	C12-C13-C14	-2.16	115.61	119.01
24	d	404	CLA	CMA-C3A-C2A	-2.16	105.64	113.98
24	a	409	CLA	O2A-CGA-CBA	2.16	118.41	111.83
24	B	614	CLA	OBD-CAD-C3D	-2.15	123.39	128.42
24	B	607	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
24	D	403	CLA	CMA-C3A-C2A	-2.15	105.66	113.98
24	D	403	CLA	CED-O2D-CGD	2.15	120.80	115.92
29	C	521	LMT	C3B-C4B-C5B	-2.15	106.33	110.23
24	b	608	CLA	CED-O2D-CGD	2.15	120.79	115.92
24	b	613	CLA	CHA-C1A-NA	-2.15	121.53	126.39
24	B	609	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
24	A	406	CLA	CAC-C3C-C4C	2.15	127.58	124.79
24	c	507	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
39	c	519	DGD	O6E-C5E-C6E	2.14	111.75	106.44
24	c	503	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
28	C	520	LMG	O7-C10-O9	-2.14	118.69	123.70
24	B	617	CLA	CHD-C1D-ND	-2.14	121.79	124.80
43	V	202	HEC	C2A-C1A-NA	-2.14	108.26	110.32
24	b	616	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
40	F	101	HEM	O2A-CGA-CBA	2.14	120.77	114.00
24	C	508	CLA	CBA-CAA-C2A	-2.14	107.42	113.79
24	C	514	CLA	C11-C10-C8	-2.14	108.85	115.97
24	c	508	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
24	C	508	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
24	A	406	CLA	CHD-C4C-NC	2.14	127.55	124.23
29	T	104	LMT	C1'-O5'-C5'	2.14	117.90	113.72
26	k	303	BCR	C21-C20-C19	-2.14	117.00	123.20
24	a	409	CLA	C1-C2-C3	-2.14	122.69	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C4-C3-C5	2.14	118.94	115.23
26	k	302	BCR	C28-C27-C26	-2.14	110.24	114.06
24	d	405	CLA	CMB-C2B-C1B	2.14	128.67	125.42
24	D	404	CLA	CHB-C4A-NA	2.14	127.48	124.40
24	C	502	CLA	O2A-CGA-CBA	2.14	118.35	111.83
24	c	508	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
26	b	622	BCR	C2-C1-C6	2.14	113.54	110.44
28	d	411	LMG	O8-C28-C29	2.13	118.34	111.83
24	c	505	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
36	C	523	HTG	O5-C1-C2	2.13	113.26	110.32
24	C	504	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
26	A	410	BCR	C23-C24-C25	-2.13	121.30	127.00
26	B	641	BCR	C15-C14-C13	2.13	130.27	127.28
27	D	408	SQD	C3-C4-C5	2.13	114.10	110.23
24	b	618	CLA	O2A-CGA-CBA	2.13	118.33	111.83
24	B	605	CLA	C6-C7-C8	-2.13	108.89	115.97
24	c	504	CLA	CHA-C1A-NA	-2.13	121.57	126.39
24	D	404	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	c	512	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
26	b	622	BCR	C11-C10-C9	-2.13	124.30	127.28
26	D	405	BCR	C10-C11-C12	-2.13	117.04	123.20
24	b	617	CLA	CHC-C1C-C2C	-2.12	120.91	126.95
24	b	604	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
29	c	523	LMT	C1B-C2B-C3B	2.12	114.48	110.01
26	B	618	BCR	C15-C14-C13	-2.12	124.30	127.28
24	c	513	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
24	B	611	CLA	CMA-C3A-C2A	-2.12	105.78	113.98
27	A	411	SQD	C3-C4-C5	2.12	114.08	110.23
26	k	302	BCR	C21-C20-C19	-2.12	117.06	123.20
24	B	608	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
24	B	610	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
24	b	608	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
24	c	514	CLA	OBD-CAD-C3D	-2.12	123.47	128.42
24	B	617	CLA	C1-O2A-CGA	2.12	121.77	116.65
24	B	609	CLA	CAA-C2A-C3A	-2.11	107.28	113.00
24	B	610	CLA	CGD-CBD-CAD	-2.11	104.00	110.85
28	c	521	LMG	O8-C28-O10	-2.11	118.34	123.63
24	c	507	CLA	CBC-CAC-C3C	-2.11	106.69	112.42
24	b	616	CLA	C4A-NA-C1A	2.11	107.64	106.68
24	d	404	CLA	CMC-C2C-C1C	2.11	128.33	125.03
24	c	514	CLA	CHB-C4A-NA	2.11	127.44	124.40
24	C	504	CLA	CHB-C1B-C2B	-2.11	121.31	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	509	CLA	C1-O2A-CGA	2.11	121.75	116.65
36	c	525	HTG	O5-C5-C4	2.11	113.50	109.70
25	A	408	PHO	CMC-C2C-C1C	2.11	128.52	124.73
24	B	613	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
39	H	102	DGD	O6E-C5E-C6E	2.10	111.66	106.44
24	c	504	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
39	C	517	DGD	C2G-O2G-C1B	-2.10	112.76	117.80
28	c	521	LMG	C8-O7-C10	-2.10	112.76	117.80
26	k	302	BCR	C1-C6-C5	-2.10	119.76	122.64
24	B	616	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
36	V	203	HTG	O2-C2-C1	2.10	114.03	110.30
24	D	403	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
24	D	404	CLA	CMA-C3A-C4A	-2.10	106.13	111.77
24	C	504	CLA	C4-C3-C5	2.10	118.87	115.23
24	b	610	CLA	CED-O2D-CGD	2.10	120.68	115.92
24	B	612	CLA	O2A-CGA-CBA	2.10	118.23	111.83
24	C	503	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	b	611	CLA	CMC-C2C-C1C	2.10	128.31	125.03
26	K	101	BCR	C16-C17-C18	-2.10	124.34	127.28
24	B	608	CLA	CMB-C2B-C1B	2.10	128.61	125.42
24	b	612	CLA	CED-O2D-CGD	2.10	120.67	115.92
24	B	614	CLA	O2A-CGA-CBA	2.10	118.23	111.83
24	B	602	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
24	B	615	CLA	CMA-C3A-C2A	-2.09	105.88	113.98
24	b	612	CLA	CMC-C2C-C1C	2.09	128.31	125.03
24	c	515	CLA	C3B-C4B-NB	2.09	112.40	110.53
24	b	604	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
24	A	406	CLA	CMB-C2B-C1B	2.09	128.61	125.42
26	K	101	BCR	C15-C14-C13	-2.09	124.34	127.28
24	d	404	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
24	c	510	CLA	CMB-C2B-C1B	2.09	128.60	125.42
37	D	409	LHG	O7-C7-O9	-2.09	118.82	123.70
39	c	520	DGD	C6B-C5B-C4B	-2.09	103.81	114.37
24	A	406	CLA	C3C-C4C-NC	2.09	113.11	110.43
26	Y	302	BCR	C23-C24-C25	-2.09	121.42	127.00
37	l	302	LHG	O4-P-O5	2.09	122.16	112.44
26	k	302	BCR	C23-C24-C25	-2.09	121.43	127.00
28	B	621	LMG	O8-C28-O10	-2.09	118.41	123.63
24	B	603	CLA	C1-O2A-CGA	2.09	121.70	116.65
24	c	512	CLA	O2A-CGA-CBA	2.08	118.19	111.83
24	C	507	CLA	CMC-C2C-C1C	2.08	128.29	125.03
24	C	514	CLA	CAA-C2A-C3A	-2.08	107.37	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
28	a	415	LMG	O1-C1-C2	2.08	111.44	108.27
26	k	302	BCR	C35-C13-C14	-2.08	119.44	122.82
24	b	616	CLA	CED-O2D-CGD	2.08	120.64	115.92
24	D	403	CLA	CHA-C1A-NA	-2.08	121.68	126.39
24	c	513	CLA	CAC-C3C-C4C	2.08	127.50	124.79
26	b	621	BCR	C11-C10-C9	-2.08	124.36	127.28
24	B	607	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
39	H	102	DGD	C6D-C5D-C4D	2.08	116.43	112.07
26	k	303	BCR	C11-C10-C9	-2.08	124.36	127.28
26	d	406	BCR	C35-C13-C12	2.08	121.26	118.09
25	d	401	PHO	CBA-CAA-C2A	-2.08	107.66	113.78
26	b	620	BCR	C10-C11-C12	-2.08	117.18	123.20
43	v	1603	HEC	C2A-C1A-NA	-2.08	108.32	110.32
24	D	403	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
24	a	409	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
24	C	505	CLA	C16-C17-C18	-2.08	106.67	115.94
24	C	505	CLA	C7-C6-C5	-2.07	107.73	113.26
24	B	606	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
24	b	611	CLA	OBD-CAD-C3D	-2.07	123.57	128.42
24	a	412	CLA	CHB-C4A-NA	2.07	127.39	124.40
26	d	406	BCR	C40-C30-C25	-2.07	106.99	110.24
24	C	507	CLA	CAA-CBA-CGA	2.07	119.09	113.21
24	C	504	CLA	O2A-CGA-CBA	2.07	118.15	111.83
24	B	602	CLA	CAC-C3C-C4C	2.07	127.49	124.79
24	b	611	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
24	B	603	CLA	CED-O2D-CGD	2.07	120.61	115.92
24	B	607	CLA	O2A-CGA-CBA	2.07	118.15	111.83
26	d	406	BCR	C16-C15-C14	-2.07	119.28	123.52
24	B	602	CLA	C4-C3-C2	-2.07	118.31	123.63
24	B	609	CLA	CMA-C3A-C2A	-2.07	105.98	113.98
33	d	407	PL9	C47-C48-C49	-2.07	120.75	127.64
24	b	614	CLA	C3B-C4B-NB	2.07	112.38	110.53
26	T	102	BCR	C31-C1-C6	-2.07	107.00	110.24
30	v	1606	GOL	C3-C2-C1	-2.07	104.22	111.80
24	b	614	CLA	O2A-CGA-CBA	2.06	118.13	111.83
26	b	622	BCR	C2-C3-C4	-2.06	106.74	111.28
24	A	409	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	a	414	SQD	O9-S-C6	2.06	109.83	106.76
28	a	415	LMG	O8-C28-C29	2.06	118.11	111.83
26	B	620	BCR	C10-C11-C12	-2.06	117.24	123.20
26	d	406	BCR	C10-C11-C12	-2.05	117.25	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	517	DGD	O1G-C1G-C2G	-2.05	102.48	108.40
24	B	606	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	d	401	PHO	CBC-CAC-C3C	-2.05	109.94	112.87
25	D	401	PHO	O2A-CGA-CBA	2.05	118.08	111.83
24	a	408	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
28	B	621	LMG	O7-C10-O9	-2.05	118.92	123.70
32	a	424[A]	K3C	C5-C12-C1	-2.05	120.97	122.58
33	d	407	PL9	C25-C24-C26	2.04	118.78	115.23
24	b	612	CLA	O2A-CGA-CBA	2.04	118.07	111.83
24	c	510	CLA	C1-O2A-CGA	2.04	121.60	116.65
25	a	411	PHO	CMB-C2B-C3B	2.04	128.77	124.68
24	C	510	CLA	C4-C3-C5	2.04	118.77	115.23
24	a	412	CLA	CMC-C2C-C1C	2.04	128.23	125.03
24	c	506	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
24	c	508	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
24	c	506	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
24	B	610	CLA	C4-C3-C5	2.04	118.77	115.23
26	c	516	BCR	C7-C8-C9	-2.04	123.22	126.23
24	B	616	CLA	C4A-NA-C1A	2.04	107.61	106.68
24	B	606	CLA	CMC-C2C-C1C	2.04	128.22	125.03
24	c	515	CLA	C1-O2A-CGA	2.04	121.58	116.65
24	B	602	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
32	A	421[A]	K3C	C5-C12-C1	-2.03	120.98	122.58
24	C	504	CLA	C3B-C4B-NB	2.03	112.34	110.53
24	B	612	CLA	C4A-NA-C1A	2.03	107.61	106.68
33	D	406	PL9	C53-C6-C1	2.03	119.44	115.28
24	C	503	CLA	O2A-CGA-CBA	2.03	118.02	111.83
24	B	609	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
33	D	406	PL9	C40-C39-C38	-2.03	118.42	123.63
24	C	513	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
36	b	601	HTG	C1-O5-C5	2.03	116.20	112.56
24	D	404	CLA	O2A-CGA-CBA	2.03	118.02	111.83
39	c	519	DGD	O1G-C1A-C2A	2.03	118.02	111.83
24	C	503	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
24	C	511	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
24	b	613	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
24	C	507	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
26	B	619	BCR	C33-C5-C6	-2.02	122.28	124.48
24	a	412	CLA	CAC-C3C-C4C	2.02	127.42	124.79
24	B	614	CLA	CMA-C3A-C2A	-2.02	106.16	113.98
40	F	101	HEM	CBA-CAA-C2A	-2.02	106.94	112.53
27	A	413	SQD	C44-O6-C1	-2.02	109.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	C4-C3-C5	2.02	118.74	115.23
40	f	101	HEM	C3B-C2B-C1B	2.02	107.93	106.41
26	a	413	BCR	C11-C10-C9	-2.02	124.44	127.28
39	C	519	DGD	C2G-O2G-C1B	-2.02	112.97	117.80
24	c	512	CLA	C11-C10-C8	-2.02	109.26	115.97
24	b	616	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
24	b	605	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	A	410	BCR	C24-C23-C22	-2.02	123.25	126.23
24	b	609	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
36	B	626	HTG	C6-C5-C4	-2.02	108.07	113.02
24	D	404	CLA	C16-C15-C13	-2.01	109.27	115.97
24	b	618	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
24	d	405	CLA	C4-C3-C5	2.01	118.72	115.23
26	A	410	BCR	C38-C26-C25	-2.01	122.29	124.48
24	c	512	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
24	B	607	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	d	401	PHO	O2A-CGA-O1A	-2.01	118.60	123.63
26	T	102	BCR	C28-C27-C26	-2.01	110.47	114.06
24	c	509	CLA	C4B-C3B-C2B	-2.01	104.80	107.30
24	c	511	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
24	B	610	CLA	CMC-C2C-C1C	2.01	128.18	125.03
24	C	508	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	C	507	CLA	CMA-C3A-C2A	-2.01	106.22	113.98
24	b	606	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
24	B	606	CLA	CHC-C1C-C2C	-2.01	121.25	126.95
24	c	514	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
24	a	410	CLA	CHD-C4C-NC	2.01	127.34	124.23
37	d	410	LHG	O7-C7-O9	-2.01	119.02	123.70
24	b	607	CLA	C6-C7-C8	-2.00	109.30	115.97
24	C	511	CLA	C4-C3-C2	-2.00	118.48	123.63
24	a	410	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
24	d	404	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
26	k	302	BCR	C16-C17-C18	-2.00	124.47	127.28
24	c	511	CLA	C4-C3-C5	2.00	118.70	115.23
25	a	411	PHO	C1-O2A-CGA	2.00	121.49	116.65

All (59) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	502	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	403	CLA	ND
24	D	404	CLA	ND
24	a	408	CLA	ND
24	a	409	CLA	ND
24	a	412	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	619	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	d	404	CLA	ND

All (1123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	606	CLA	C2-C3-C5-C6
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	604	CLA	C2-C1-O2A-CGA
24	b	608	CLA	C2-C3-C5-C6
24	b	617	CLA	CAD-CBD-CGD-O1D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	515	CLA	CBD-CGD-O2D-CED
26	D	405	BCR	C21-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	Y	302	BCR	C21-C22-C23-C24
26	d	406	BCR	C21-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
26	k	302	BCR	C21-C22-C23-C24
27	A	413	SQD	O6-C44-C45-O47
27	D	408	SQD	C8-C7-O47-C45
27	L	101	SQD	O5-C1-O6-C44
27	L	101	SQD	O49-C7-O47-C45
27	L	101	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
27	L	101	SQD	C5-C6-S-O8
27	L	101	SQD	C5-C6-S-O9
27	L	102	SQD	O49-C7-O47-C45
27	a	401	SQD	O6-C44-C45-O47
27	a	401	SQD	O5-C5-C6-S
27	f	102	SQD	O49-C7-O47-C45
28	C	532	LMG	O9-C10-O7-C8
29	B	642	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
29	c	523	LMT	C2'-C1'-O1'-C1
29	c	523	LMT	O5'-C1'-O1'-C1
29	f	104	LMT	O5'-C1'-O1'-C1
29	z	101	LMT	C2'-C1'-O1'-C1
30	T	101	GOL	O1-C1-C2-C3
30	a	416	GOL	C1-C2-C3-O3
30	a	417	GOL	O1-C1-C2-O2
30	a	417	GOL	O1-C1-C2-C3
30	a	418	GOL	O1-C1-C2-C3
30	a	421	GOL	O1-C1-C2-C3
30	b	630	GOL	O1-C1-C2-O2
30	k	304	GOL	O1-C1-C2-O2
30	o	305	GOL	C1-C2-C3-O3
30	u	202	GOL	C1-C2-C3-O3
30	v	1606	GOL	O1-C1-C2-C3
30	v	1607	GOL	O1-C1-C2-O2
33	A	422[B]	PL9	C16-C17-C18-C19
33	A	422[B]	PL9	C24-C26-C27-C28
33	a	425[B]	PL9	C19-C21-C22-C23
36	B	623[B]	HTG	C2'-C1'-S1-C1
36	B	624	HTG	O5-C1-S1-C1'
36	I	102	HTG	O5-C1-S1-C1'
36	V	203	HTG	O5-C1-S1-C1'
36	b	626	HTG	O5-C1-S1-C1'
37	B	640	LHG	C4-O6-P-O3
37	B	640	LHG	C4-O6-P-O4
37	B	640	LHG	C4-O6-P-O5
37	D	410	LHG	C3-O3-P-O4
37	D	410	LHG	C3-O3-P-O6
37	D	410	LHG	C4-O6-P-O3
37	D	410	LHG	C4-O6-P-O4
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	O6-C4-C5-O7
37	d	409	LHG	C3-O3-P-O4
37	d	409	LHG	C3-O3-P-O5
37	d	409	LHG	C3-O3-P-O6
37	d	409	LHG	C4-O6-P-O4
37	e	101	LHG	C1-C2-C3-O3
37	e	101	LHG	C3-O3-P-O5
37	e	101	LHG	C4-O6-P-O3
37	e	101	LHG	C4-O6-P-O4
37	e	101	LHG	O10-C23-O8-C6
37	e	101	LHG	C24-C23-O8-C6
37	l	302	LHG	C4-O6-P-O3
37	l	302	LHG	C4-O6-P-O4
37	l	302	LHG	C4-O6-P-O5
39	D	407	DGD	C2B-C1B-O2G-C2G
39	D	407	DGD	O1B-C1B-O2G-C2G
43	V	202	HEC	C2B-C3B-CAB-CBB
43	V	202	HEC	C4B-C3B-CAB-CBB
43	V	202	HEC	C2C-C3C-CAC-CBC
43	V	202	HEC	C4C-C3C-CAC-CBC
43	v	1603	HEC	C2B-C3B-CAB-CBB
43	v	1603	HEC	C4B-C3B-CAB-CBB
43	v	1603	HEC	C2C-C3C-CAC-CBC
43	v	1603	HEC	C4C-C3C-CAC-CBC
29	C	521	LMT	C3'-C4'-O1B-C1B
24	C	514	CLA	CBD-CGD-O2D-CED
24	c	514	CLA	CBD-CGD-O2D-CED
27	D	408	SQD	O10-C23-O48-C46
39	D	407	DGD	O1A-C1A-O1G-C1G
29	Z	101	LMT	O5B-C1B-O1B-C4'
39	D	407	DGD	C2A-C1A-O1G-C1G
29	Z	101	LMT	C2B-C1B-O1B-C4'
27	D	408	SQD	O49-C7-O47-C45
29	z	101	LMT	O5B-C1B-O1B-C4'
24	c	515	CLA	O1D-CGD-O2D-CED
27	D	408	SQD	C24-C23-O48-C46
24	c	503	CLA	CBD-CGD-O2D-CED
27	L	101	SQD	C8-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
28	C	532	LMG	C11-C10-O7-C8
24	C	514	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	C4-C3-C5-C6
24	b	608	CLA	C4-C3-C5-C6
33	a	425[B]	PL9	C30-C29-C31-C32
33	a	425[B]	PL9	C28-C29-C31-C32
29	z	101	LMT	O5'-C1'-O1'-C1
29	B	622	LMT	O5B-C5B-C6B-O6B
26	B	641	BCR	C13-C14-C15-C16
26	T	102	BCR	C13-C14-C15-C16
29	f	104	LMT	C4B-C5B-C6B-O6B
36	I	102	HTG	C4-C5-C6-O6
37	D	410	LHG	O2-C2-C3-O3
37	E	101	LHG	O2-C2-C3-O3
37	d	409	LHG	O2-C2-C3-O3
37	e	101	LHG	O2-C2-C3-O3
36	I	102	HTG	O5-C5-C6-O6
29	C	521	LMT	C4'-C5'-C6'-O6'
29	T	104	LMT	O5'-C5'-C6'-O6'
24	C	504	CLA	CBD-CGD-O2D-CED
29	C	521	LMT	O5'-C5'-C6'-O6'
36	b	625	HTG	S1-C1'-C2'-C3'
24	b	617	CLA	C4-C3-C5-C6
33	A	422[B]	PL9	C40-C39-C41-C42
24	b	617	CLA	C2-C3-C5-C6
33	A	422[B]	PL9	C34-C36-C37-C38
33	a	425[B]	PL9	C14-C16-C17-C18
36	h	1202	HTG	C4-C5-C6-O6
24	C	503	CLA	CBD-CGD-O2D-CED
24	b	604	CLA	O1A-CGA-O2A-C1
29	B	642	LMT	O5'-C1'-O1'-C1
29	Z	101	LMT	O5'-C1'-O1'-C1
29	b	624	LMT	O5'-C1'-O1'-C1
39	D	407	DGD	O6D-C1D-O3G-C3G
29	f	104	LMT	O5B-C5B-C6B-O6B
29	B	622	LMT	C4B-C5B-C6B-O6B
29	Z	101	LMT	C4'-C5'-C6'-O6'
29	z	101	LMT	C2B-C1B-O1B-C4'
24	b	604	CLA	CBA-CGA-O2A-C1
24	C	502	CLA	CBD-CGD-O2D-CED
29	a	402	LMT	O5B-C5B-C6B-O6B
36	C	523	HTG	O5-C5-C6-O6
36	h	1202	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
28	c	522	LMG	O6-C5-C6-O5
29	m	103	LMT	O5'-C5'-C6'-O6'
29	T	104	LMT	C4'-C5'-C6'-O6'
24	C	512	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	C3-C5-C6-C7
32	A	421[A]	K3C	C4-C5-C6-C7
32	A	421[A]	K3C	C4-C5-C6-C11
27	L	102	SQD	C13-C14-C15-C16
24	A	409	CLA	C14-C13-C15-C16
24	B	602	CLA	C11-C10-C8-C9
24	b	613	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C12-C13-C14
24	c	511	CLA	C6-C7-C8-C9
29	Z	101	LMT	C2'-C1'-O1'-C1
29	b	624	LMT	C2'-C1'-O1'-C1
29	f	104	LMT	C2'-C1'-O1'-C1
39	D	407	DGD	C2D-C1D-O3G-C3G
29	m	103	LMT	C4'-C5'-C6'-O6'
26	Y	302	BCR	C37-C22-C23-C24
26	k	302	BCR	C37-C22-C23-C24
24	b	604	CLA	C3-C5-C6-C7
29	a	402	LMT	C4B-C5B-C6B-O6B
24	c	503	CLA	O1D-CGD-O2D-CED
28	C	532	LMG	O6-C5-C6-O5
24	b	619	CLA	C15-C16-C17-C18
24	c	511	CLA	C8-C10-C11-C12
29	Z	101	LMT	O5'-C5'-C6'-O6'
30	B	629	GOL	O1-C1-C2-O2
30	T	101	GOL	O1-C1-C2-O2
30	v	1606	GOL	O1-C1-C2-O2
30	v	1607	GOL	O2-C2-C3-O3
28	c	522	LMG	C4-C5-C6-O5
29	C	521	LMT	O5B-C5B-C6B-O6B
24	A	407	CLA	C13-C15-C16-C17
27	f	102	SQD	C23-C24-C25-C26
33	A	422[B]	PL9	C14-C16-C17-C18
33	D	406	PL9	C39-C41-C42-C43
33	d	407	PL9	C39-C41-C42-C43
24	b	619	CLA	C10-C11-C12-C13
36	B	626	HTG	C4-C5-C6-O6
24	a	408	CLA	C15-C16-C17-C18
24	b	607	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C2A-CAA-CBA-CGA
29	Z	101	LMT	O1'-C1-C2-C3
37	E	101	LHG	C7-C8-C9-C10
39	c	520	DGD	C1A-C2A-C3A-C4A
36	C	523	HTG	S1-C1'-C2'-C3'
27	L	101	SQD	C31-C32-C33-C34
37	D	411	LHG	C10-C11-C12-C13
37	D	411	LHG	C16-C17-C18-C19
24	B	602	CLA	C10-C11-C12-C13
24	C	511	CLA	C8-C10-C11-C12
24	a	412	CLA	C5-C6-C7-C8
24	C	508	CLA	CBD-CGD-O2D-CED
28	B	621	LMG	C28-C29-C30-C31
37	d	408	LHG	C23-C24-C25-C26
24	B	615	CLA	C8-C10-C11-C12
33	A	422[B]	PL9	C38-C39-C41-C42
24	C	503	CLA	O1D-CGD-O2D-CED
39	C	518	DGD	C6B-C7B-C8B-C9B
24	a	412	CLA	C10-C11-C12-C13
24	b	609	CLA	C10-C11-C12-C13
24	B	602	CLA	CBA-CGA-O2A-C1
36	U	201	HTG	S1-C1'-C2'-C3'
36	h	1202	HTG	S1-C1'-C2'-C3'
36	u	201	HTG	S1-C1'-C2'-C3'
29	B	622	LMT	C5'-C4'-O1B-C1B
27	A	413	SQD	C16-C17-C18-C19
39	h	1205	DGD	CCA-CDA-CEA-CFA
32	a	424[A]	K3C	C4-C5-C6-C7
32	a	424[A]	K3C	C4-C5-C6-C11
24	b	606	CLA	C5-C6-C7-C8
24	A	409	CLA	C8-C10-C11-C12
24	C	507	CLA	C5-C6-C7-C8
24	c	511	CLA	C13-C15-C16-C17
24	d	405	CLA	C8-C10-C11-C12
24	B	605	CLA	C3-C5-C6-C7
28	C	520	LMG	C11-C10-O7-C8
28	C	520	LMG	O9-C10-O7-C8
27	L	101	SQD	C2-C1-O6-C44
29	C	521	LMT	C2'-C1'-O1'-C1
28	C	520	LMG	C10-C11-C12-C13
39	C	518	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
36	B	623[A]	HTG	C1'-C2'-C3'-C4'
29	T	104	LMT	O1'-C1-C2-C3
26	D	405	BCR	C7-C8-C9-C34
27	L	102	SQD	C31-C32-C33-C34
24	c	508	CLA	C15-C16-C17-C18
39	H	102	DGD	CCA-CDA-CEA-CFA
39	c	519	DGD	CBB-CCB-CDB-CEB
30	B	627	GOL	C1-C2-C3-O3
30	B	629	GOL	O1-C1-C2-C3
30	V	204	GOL	O1-C1-C2-C3
30	a	417	GOL	C1-C2-C3-O3
30	a	421	GOL	C1-C2-C3-O3
30	b	630	GOL	O1-C1-C2-C3
30	k	304	GOL	O1-C1-C2-C3
30	k	304	GOL	C1-C2-C3-O3
30	o	302	GOL	O1-C1-C2-C3
30	o	302	GOL	C1-C2-C3-O3
30	v	1602	GOL	C1-C2-C3-O3
30	v	1605	GOL	O1-C1-C2-C3
30	v	1607	GOL	O1-C1-C2-C3
30	v	1607	GOL	C1-C2-C3-O3
37	e	101	LHG	O1-C1-C2-C3
24	B	616	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C19
24	B	602	CLA	O1A-CGA-O2A-C1
28	A	412	LMG	O9-C10-O7-C8
29	C	521	LMT	O5'-C1'-O1'-C1
28	A	412	LMG	C11-C10-O7-C8
29	a	402	LMT	C1-C2-C3-C4
24	B	614	CLA	C15-C16-C17-C18
29	A	414	LMT	O5B-C5B-C6B-O6B
24	C	510	CLA	C2-C1-O2A-CGA
24	C	507	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C19
24	D	404	CLA	C8-C10-C11-C12
39	c	520	DGD	C6A-C7A-C8A-C9A
29	A	414	LMT	C7-C8-C9-C10
29	C	521	LMT	C5-C6-C7-C8
37	D	411	LHG	C12-C13-C14-C15
37	d	410	LHG	C28-C29-C30-C31
39	C	517	DGD	O6D-C5D-C6D-O5D
29	B	622	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
27	D	408	SQD	C24-C25-C26-C27
27	L	101	SQD	C27-C28-C29-C30
28	A	412	LMG	C13-C14-C15-C16
37	E	101	LHG	C28-C29-C30-C31
37	E	101	LHG	C29-C30-C31-C32
29	B	622	LMT	C2-C1-O1'-C1'
29	C	521	LMT	C2-C1-O1'-C1'
30	a	418	GOL	O1-C1-C2-O2
30	a	421	GOL	O1-C1-C2-O2
29	B	622	LMT	C3'-C4'-O1B-C1B
28	b	623	LMG	C20-C21-C22-C23
24	B	606	CLA	C4B-C3B-CAB-CBB
24	C	504	CLA	C4B-C3B-CAB-CBB
24	c	515	CLA	C4B-C3B-CAB-CBB
28	a	415	LMG	C11-C12-C13-C14
28	a	415	LMG	C15-C16-C17-C18
24	B	616	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C20
24	C	512	CLA	O1D-CGD-O2D-CED
37	d	408	LHG	C32-C33-C34-C35
24	c	512	CLA	CBD-CGD-O2D-CED
36	B	626	HTG	S1-C1'-C2'-C3'
29	c	523	LMT	C4-C5-C6-C7
39	C	517	DGD	C5B-C6B-C7B-C8B
39	c	518	DGD	C7A-C8A-C9A-CAA
24	C	510	CLA	C13-C15-C16-C17
27	a	401	SQD	C30-C31-C32-C33
39	C	517	DGD	C4B-C5B-C6B-C7B
39	C	518	DGD	C7A-C8A-C9A-CAA
39	c	520	DGD	CBA-CCA-CDA-CEA
28	D	412	LMG	C12-C13-C14-C15
24	b	618	CLA	C5-C6-C7-C8
24	C	502	CLA	O1D-CGD-O2D-CED
27	f	102	SQD	O6-C1-O5-C5
27	A	411	SQD	C15-C16-C17-C18
37	d	408	LHG	C27-C28-C29-C30
24	c	512	CLA	O1D-CGD-O2D-CED
27	L	102	SQD	C24-C23-O48-C46
36	B	625	HTG	C2'-C3'-C4'-C5'
39	C	519	DGD	CBA-CCA-CDA-CEA
24	B	615	CLA	C3-C5-C6-C7
27	A	411	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	C	532	LMG	C12-C13-C14-C15
28	c	521	LMG	C15-C16-C17-C18
29	m	101	LMT	C11-C10-C9-C8
36	O	302	HTG	C3'-C4'-C5'-C6'
37	e	101	LHG	C17-C18-C19-C20
39	D	407	DGD	C8A-C9A-CAA-CBA
39	c	519	DGD	C4B-C5B-C6B-C7B
28	d	411	LMG	O6-C5-C6-O5
29	B	622	LMT	O1'-C1-C2-C3
29	m	101	LMT	C4'-C5'-C6'-O6'
28	D	412	LMG	C35-C36-C37-C38
28	a	415	LMG	C36-C37-C38-C39
37	B	640	LHG	C33-C34-C35-C36
28	d	411	LMG	C21-C22-C23-C24
29	f	104	LMT	C4'-C5'-C6'-O6'
28	A	412	LMG	C36-C37-C38-C39
24	C	504	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	Y	302	BCR	C1-C6-C7-C8
26	Y	302	BCR	C5-C6-C7-C8
26	k	302	BCR	C1-C6-C7-C8
26	k	302	BCR	C5-C6-C7-C8
28	C	520	LMG	C19-C20-C21-C22
28	C	520	LMG	C31-C32-C33-C34
29	T	104	LMT	C11-C10-C9-C8
37	l	302	LHG	C33-C34-C35-C36
24	d	405	CLA	CBD-CGD-O2D-CED
28	A	412	LMG	C21-C22-C23-C24
39	c	519	DGD	CBA-CCA-CDA-CEA
24	a	409	CLA	C2C-C3C-CAC-CBC
37	D	411	LHG	C27-C28-C29-C30
39	c	519	DGD	C1B-C2B-C3B-C4B
24	C	508	CLA	C15-C16-C17-C18
33	a	425[B]	PL9	C4-C3-C7-C8
37	D	409	LHG	C32-C33-C34-C35
27	A	413	SQD	C28-C29-C30-C31
28	D	412	LMG	C20-C21-C22-C23
37	D	411	LHG	C11-C12-C13-C14
39	C	518	DGD	C4B-C5B-C6B-C7B
36	b	626	HTG	O5-C5-C6-O6
27	L	102	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	a	414	SQD	C9-C10-C11-C12
28	b	623	LMG	C39-C40-C41-C42
37	E	101	LHG	C17-C18-C19-C20
28	C	532	LMG	C10-C11-C12-C13
24	C	504	CLA	O1D-CGD-O2D-CED
29	B	642	LMT	C9-C10-C11-C12
24	C	510	CLA	C11-C10-C8-C9
27	L	102	SQD	C27-C28-C29-C30
29	T	104	LMT	C4-C5-C6-C7
27	L	102	SQD	C11-C10-C9-C8
27	L	102	SQD	C17-C18-C19-C20
39	C	518	DGD	C9A-CAA-CBA-CCA
28	d	411	LMG	C20-C21-C22-C23
39	c	518	DGD	C4B-C5B-C6B-C7B
39	c	518	DGD	C8A-C9A-CAA-CBA
36	U	201	HTG	C4'-C5'-C6'-C7'
24	c	504	CLA	C16-C17-C18-C20
39	C	517	DGD	C2A-C3A-C4A-C5A
24	c	515	CLA	C10-C11-C12-C13
29	B	622	LMT	C6-C7-C8-C9
29	T	104	LMT	C6-C7-C8-C9
39	c	519	DGD	CAA-CBA-CCA-CDA
39	h	1205	DGD	C7A-C8A-C9A-CAA
36	I	102	HTG	C1'-C2'-C3'-C4'
36	b	626	HTG	C1'-C2'-C3'-C4'
36	h	1202	HTG	C1'-C2'-C3'-C4'
26	d	406	BCR	C7-C8-C9-C34
37	l	302	LHG	C7-C8-C9-C10
28	C	532	LMG	C33-C34-C35-C36
37	e	101	LHG	C11-C10-C9-C8
24	C	507	CLA	C16-C17-C18-C19
28	A	412	LMG	C19-C20-C21-C22
33	A	422[B]	PL9	C15-C14-C16-C17
33	A	422[B]	PL9	C13-C14-C16-C17
27	a	414	SQD	C34-C35-C36-C37
37	D	410	LHG	C32-C33-C34-C35
24	c	509	CLA	C5-C6-C7-C8
24	b	614	CLA	C13-C15-C16-C17
32	A	421[A]	K3C	C12-C5-C6-C7
24	b	617	CLA	C10-C11-C12-C13
24	b	617	CLA	C13-C15-C16-C17
27	a	414	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
39	c	519	DGD	C9B-CAB-CBB-CCB
28	D	412	LMG	O6-C5-C6-O5
29	B	642	LMT	C6-C7-C8-C9
37	D	411	LHG	C18-C19-C20-C21
39	H	102	DGD	C7A-C8A-C9A-CAA
27	L	102	SQD	C29-C30-C31-C32
24	A	409	CLA	C15-C16-C17-C18
37	D	410	LHG	C1-C2-C3-O3
37	E	101	LHG	C1-C2-C3-O3
37	d	409	LHG	C1-C2-C3-O3
39	D	407	DGD	C6A-C7A-C8A-C9A
24	a	412	CLA	CBA-CGA-O2A-C1
27	L	101	SQD	C30-C31-C32-C33
39	C	517	DGD	O6E-C5E-C6E-O5E
30	a	421	GOL	O2-C2-C3-O3
30	k	304	GOL	O2-C2-C3-O3
30	o	305	GOL	O2-C2-C3-O3
30	u	202	GOL	O2-C2-C3-O3
27	L	102	SQD	O10-C23-O48-C46
24	B	617	CLA	C3-C5-C6-C7
29	Z	101	LMT	C1-C2-C3-C4
24	C	512	CLA	C1A-C2A-CAA-CBA
24	c	510	CLA	C1A-C2A-CAA-CBA
37	e	101	LHG	C13-C14-C15-C16
27	A	413	SQD	C24-C25-C26-C27
29	T	104	LMT	C7-C8-C9-C10
37	E	101	LHG	O6-C4-C5-C6
24	A	409	CLA	C11-C12-C13-C15
24	B	611	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	D	404	CLA	C11-C10-C8-C7
24	b	604	CLA	C6-C7-C8-C10
24	c	507	CLA	C11-C12-C13-C15
28	a	415	LMG	C16-C17-C18-C19
39	c	518	DGD	O6E-C5E-C6E-O5E
39	D	407	DGD	C5B-C6B-C7B-C8B
27	A	411	SQD	C13-C14-C15-C16
29	C	521	LMT	C3-C4-C5-C6
39	C	519	DGD	C8B-C9B-CAB-CBB
24	b	619	CLA	C4-C3-C5-C6
24	B	616	CLA	C2-C3-C5-C6
24	b	612	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	C2-C3-C5-C6
24	a	412	CLA	O1A-CGA-O2A-C1
24	a	410	CLA	C15-C16-C17-C18
24	c	512	CLA	C8-C10-C11-C12
24	C	505	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C14
24	C	514	CLA	C11-C10-C8-C9
24	D	404	CLA	C11-C10-C8-C9
24	b	604	CLA	C6-C7-C8-C9
28	C	520	LMG	C16-C17-C18-C19
28	b	623	LMG	C19-C20-C21-C22
28	b	623	LMG	C21-C22-C23-C24
24	b	604	CLA	C16-C17-C18-C19
29	Z	101	LMT	C4-C5-C6-C7
24	c	515	CLA	CBA-CGA-O2A-C1
28	b	623	LMG	C34-C35-C36-C37
37	E	101	LHG	C27-C28-C29-C30
36	B	625	HTG	C4-C5-C6-O6
28	A	412	LMG	C10-C11-C12-C13
28	C	520	LMG	O1-C7-C8-C9
28	a	415	LMG	C7-C8-C9-O8
28	B	621	LMG	C36-C37-C38-C39
37	D	409	LHG	C29-C30-C31-C32
39	C	518	DGD	CBB-CCB-CDB-CEB
28	A	412	LMG	C29-C30-C31-C32
39	C	519	DGD	C9B-CAB-CBB-CCB
39	c	520	DGD	CCB-CDB-CEB-CFB
29	c	523	LMT	O5B-C5B-C6B-O6B
27	f	102	SQD	C32-C33-C34-C35
24	d	405	CLA	O1D-CGD-O2D-CED
32	A	421[A]	K3C	C12-C5-C6-C11
24	c	515	CLA	O1A-CGA-O2A-C1
24	B	616	CLA	C4-C3-C5-C6
24	B	617	CLA	C4-C3-C5-C6
24	B	617	CLA	C2-C3-C5-C6
36	d	414	HTG	O5-C5-C6-O6
29	c	523	LMT	O5'-C5'-C6'-O6'
24	a	412	CLA	C8-C10-C11-C12
28	C	520	LMG	C37-C38-C39-C40
28	A	412	LMG	C12-C13-C14-C15
39	C	518	DGD	C3A-C4A-C5A-C6A
24	b	604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C16-C17-C18-C19
29	E	104	LMT	C4-C5-C6-C7
37	E	101	LHG	C15-C16-C17-C18
37	E	101	LHG	C24-C23-O8-C6
39	h	1205	DGD	C5B-C6B-C7B-C8B
39	H	102	DGD	C5B-C6B-C7B-C8B
29	m	101	LMT	O5'-C5'-C6'-O6'
28	d	411	LMG	C12-C13-C14-C15
24	B	608	CLA	C16-C17-C18-C19
28	c	521	LMG	C18-C19-C20-C21
37	e	101	LHG	C25-C26-C27-C28
39	c	520	DGD	C3B-C4B-C5B-C6B
27	L	102	SQD	O47-C45-C46-O48
27	f	102	SQD	O6-C44-C45-O47
28	c	521	LMG	C32-C33-C34-C35
37	l	302	LHG	C27-C28-C29-C30
28	C	532	LMG	C40-C41-C42-C43
24	B	602	CLA	CAA-CBA-CGA-O2A
39	C	517	DGD	C4D-C5D-C6D-O5D
37	D	409	LHG	C25-C26-C27-C28
37	E	101	LHG	C11-C12-C13-C14
39	c	520	DGD	C2A-C1A-O1G-C1G
37	B	640	LHG	C27-C28-C29-C30
39	c	519	DGD	C5B-C6B-C7B-C8B
24	C	507	CLA	O1D-CGD-O2D-CED
27	D	408	SQD	C23-C24-C25-C26
24	D	404	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	C16-C17-C18-C20
28	C	520	LMG	C34-C35-C36-C37
28	C	520	LMG	C40-C41-C42-C43
28	C	520	LMG	C30-C31-C32-C33
29	Z	101	LMT	C2-C1-O1'-C1'
30	b	629	GOL	O2-C2-C3-O3
30	o	302	GOL	O1-C1-C2-O2
30	o	302	GOL	O2-C2-C3-O3
37	e	101	LHG	O1-C1-C2-O2
24	B	611	CLA	C11-C12-C13-C14
24	B	611	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C12-C13-C14
24	b	618	CLA	C11-C10-C8-C9
32	a	424[A]	K3C	C12-C5-C6-C7
29	Z	101	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	E	104	LMT	C2'-C1'-O1'-C1
27	L	102	SQD	C28-C29-C30-C31
24	c	515	CLA	C3-C5-C6-C7
39	C	517	DGD	C5A-C6A-C7A-C8A
39	C	519	DGD	CDA-CEA-CFA-CGA
24	A	409	CLA	C11-C10-C8-C7
24	B	617	CLA	C11-C12-C13-C15
24	C	505	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C7
24	a	410	CLA	C11-C10-C8-C7
24	b	618	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	514	CLA	C11-C10-C8-C7
24	B	609	CLA	C13-C15-C16-C17
24	c	514	CLA	C15-C16-C17-C18
27	a	401	SQD	C29-C30-C31-C32
28	A	412	LMG	C14-C15-C16-C17
36	b	601	HTG	C4'-C5'-C6'-C7'
37	E	101	LHG	C19-C20-C21-C22
27	D	408	SQD	C31-C32-C33-C34
28	c	521	LMG	C16-C17-C18-C19
24	b	604	CLA	C4-C3-C5-C6
24	b	612	CLA	C4-C3-C5-C6
37	E	101	LHG	O10-C23-O8-C6
24	B	615	CLA	C5-C6-C7-C8
29	C	521	LMT	C9-C10-C11-C12
41	H	101	RRX	C9-C10-C11-C12
41	h	1204	RRX	C9-C10-C11-C12
27	A	413	SQD	C9-C10-C11-C12
39	D	407	DGD	C4B-C5B-C6B-C7B
24	c	504	CLA	O1D-CGD-O2D-CED
29	a	402	LMT	C3-C4-C5-C6
27	A	413	SQD	O6-C44-C45-C46
28	A	412	LMG	C7-C8-C9-O8
28	C	520	LMG	C7-C8-C9-O8
28	c	521	LMG	C7-C8-C9-O8
39	D	407	DGD	O1G-C1G-C2G-C3G
24	B	608	CLA	C16-C17-C18-C20
29	Z	101	LMT	C3-C4-C5-C6
29	b	624	LMT	O1'-C1-C2-C3
27	A	413	SQD	C14-C15-C16-C17
29	J	102	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
39	H	102	DGD	C9B-CAB-CBB-CCB
24	C	504	CLA	C10-C11-C12-C13
27	a	401	SQD	C26-C27-C28-C29
37	e	101	LHG	C23-C24-C25-C26
24	b	604	CLA	C2-C3-C5-C6
33	a	425[B]	PL9	C13-C14-C16-C17
39	h	1205	DGD	C9B-CAB-CBB-CCB
28	b	623	LMG	C36-C37-C38-C39
29	B	642	LMT	C3-C4-C5-C6
28	b	623	LMG	C31-C32-C33-C34
26	D	405	BCR	C23-C24-C25-C30
26	b	620	BCR	C1-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C30
39	C	518	DGD	C8B-C9B-CAB-CBB
32	a	424[A]	K3C	C12-C5-C6-C11
27	a	401	SQD	C31-C32-C33-C34
27	A	413	SQD	C15-C16-C17-C18
29	A	414	LMT	C6-C7-C8-C9
27	L	101	SQD	C28-C29-C30-C31
27	L	101	SQD	O47-C45-C46-O48
28	A	412	LMG	O1-C7-C8-O7
39	D	407	DGD	O1G-C1G-C2G-O2G
39	c	519	DGD	C1A-C2A-C3A-C4A
33	a	425[B]	PL9	C15-C14-C16-C17
39	C	517	DGD	C4A-C5A-C6A-C7A
28	C	532	LMG	C38-C39-C40-C41
27	a	414	SQD	C10-C11-C12-C13
28	C	520	LMG	C39-C40-C41-C42
28	c	521	LMG	C11-C12-C13-C14
28	C	532	LMG	C28-C29-C30-C31
37	E	101	LHG	C13-C14-C15-C16
24	c	514	CLA	C11-C10-C8-C9
28	a	415	LMG	C22-C23-C24-C25
36	B	626	HTG	O5-C5-C6-O6
37	d	410	LHG	C29-C30-C31-C32
28	a	415	LMG	C40-C41-C42-C43
24	c	511	CLA	C16-C17-C18-C20
39	C	517	DGD	CCA-CDA-CEA-CFA
37	d	408	LHG	C29-C30-C31-C32
37	e	101	LHG	C19-C20-C21-C22
36	B	624	HTG	C4-C5-C6-O6
30	a	416	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	c	526	GOL	O2-C2-C3-O3
30	v	1602	GOL	O2-C2-C3-O3
28	B	621	LMG	C40-C41-C42-C43
39	c	520	DGD	C1B-C2B-C3B-C4B
28	C	532	LMG	C34-C35-C36-C37
37	E	101	LHG	C24-C25-C26-C27
24	B	617	CLA	C12-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C10
28	A	412	LMG	C16-C17-C18-C19
29	a	402	LMT	C2-C3-C4-C5
26	D	405	BCR	C7-C8-C9-C10
28	c	522	LMG	C8-C7-O1-C1
39	C	518	DGD	C2G-C3G-O3G-C1D
39	C	518	DGD	C5D-C6D-O5D-C1E
39	c	519	DGD	C2G-C3G-O3G-C1D
39	c	519	DGD	C5D-C6D-O5D-C1E
37	e	101	LHG	C8-C7-O7-C5
37	d	408	LHG	C33-C34-C35-C36
27	A	413	SQD	C35-C36-C37-C38
39	h	1205	DGD	O2G-C1B-C2B-C3B
39	c	520	DGD	O1A-C1A-O1G-C1G
24	b	618	CLA	C10-C11-C12-C13
29	E	104	LMT	O1'-C1-C2-C3
27	L	101	SQD	C46-C45-O47-C7
28	b	623	LMG	C30-C31-C32-C33
24	C	511	CLA	C13-C15-C16-C17
29	E	104	LMT	O5'-C1'-O1'-C1
27	L	101	SQD	C44-C45-C46-O48
27	L	102	SQD	C44-C45-C46-O48
28	A	412	LMG	O1-C7-C8-C9
33	A	422[B]	PL9	C39-C41-C42-C43
24	C	507	CLA	C15-C16-C17-C18
40	f	101	HEM	C4C-C3C-CAC-CBC
27	A	411	SQD	C10-C11-C12-C13
27	L	102	SQD	C15-C16-C17-C18
27	L	102	SQD	C34-C35-C36-C37
25	a	411	PHO	C8-C10-C11-C12
28	C	520	LMG	C32-C33-C34-C35
39	c	518	DGD	C2A-C3A-C4A-C5A
27	D	408	SQD	O47-C45-C46-O48
28	A	412	LMG	O7-C8-C9-O8
28	a	415	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
28	c	521	LMG	O7-C8-C9-O8
24	C	505	CLA	C11-C12-C13-C14
24	C	507	CLA	C6-C7-C8-C9
27	L	102	SQD	C14-C15-C16-C17
28	d	411	LMG	C29-C30-C31-C32
37	B	640	LHG	C11-C10-C9-C8
39	c	518	DGD	C5B-C6B-C7B-C8B
39	c	520	DGD	C8B-C9B-CAB-CBB
28	C	520	LMG	C11-C12-C13-C14
28	D	412	LMG	C15-C16-C17-C18
29	E	104	LMT	C5-C6-C7-C8
39	c	518	DGD	O6D-C5D-C6D-O5D
39	H	102	DGD	CDB-CEB-CFB-CGB
24	c	511	CLA	C16-C17-C18-C19
27	L	102	SQD	C9-C10-C11-C12
39	h	1205	DGD	CDB-CEB-CFB-CGB
24	C	513	CLA	C1A-C2A-CAA-CBA
24	a	410	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	C4B-C3B-CAB-CBB
39	C	517	DGD	C3B-C4B-C5B-C6B
29	f	104	LMT	O5'-C5'-C6'-O6'
24	a	409	CLA	C4C-C3C-CAC-CBC
26	d	406	BCR	C7-C8-C9-C10
29	A	414	LMT	O1'-C1-C2-C3
39	c	518	DGD	C4D-C5D-C6D-O5D
24	B	603	CLA	C13-C15-C16-C17
27	a	401	SQD	C27-C28-C29-C30
28	b	623	LMG	O9-C10-O7-C8
27	L	101	SQD	C32-C33-C34-C35
37	E	101	LHG	C30-C31-C32-C33
37	D	411	LHG	C15-C16-C17-C18
24	C	505	CLA	C6-C7-C8-C10
24	C	508	CLA	C12-C13-C15-C16
24	a	410	CLA	C11-C12-C13-C15
24	b	609	CLA	C12-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C15
24	c	511	CLA	C6-C7-C8-C10
39	C	518	DGD	C5B-C6B-C7B-C8B
39	H	102	DGD	C9A-CAA-CBA-CCA
24	b	605	CLA	C16-C17-C18-C19
24	d	405	CLA	C16-C17-C18-C20
37	l	302	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
39	c	519	DGD	C8B-C9B-CAB-CBB
27	L	101	SQD	C24-C25-C26-C27
39	C	518	DGD	C8A-C9A-CAA-CBA
37	D	411	LHG	C2-C3-O3-P
37	d	410	LHG	C2-C3-O3-P
28	b	623	LMG	C29-C30-C31-C32
24	C	513	CLA	C3A-C2A-CAA-CBA
39	c	518	DGD	C6B-C7B-C8B-C9B
37	e	101	LHG	O9-C7-O7-C5
37	l	302	LHG	O6-C4-C5-O7
28	b	623	LMG	C11-C10-O7-C8
24	C	507	CLA	C11-C10-C8-C9
24	b	609	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C10-C8-C9
24	B	617	CLA	C13-C15-C16-C17
36	b	625	HTG	C1'-C2'-C3'-C4'
24	b	613	CLA	C15-C16-C17-C18
37	B	640	LHG	C16-C17-C18-C19
28	C	520	LMG	O1-C7-C8-O7
28	C	520	LMG	O7-C8-C9-O8
24	b	619	CLA	C13-C15-C16-C17
28	a	415	LMG	C12-C13-C14-C15
36	U	201	HTG	C2'-C3'-C4'-C5'
27	a	401	SQD	O6-C44-C45-C46
29	C	521	LMT	O1'-C1-C2-C3
37	B	640	LHG	C25-C26-C27-C28
24	B	603	CLA	C15-C16-C17-C18
24	b	611	CLA	C13-C15-C16-C17
27	A	411	SQD	C16-C17-C18-C19
24	D	404	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	608	CLA	CAD-CBD-CGD-O2D
24	b	604	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	C8-C10-C11-C12
39	D	407	DGD	C7A-C8A-C9A-CAA
28	D	412	LMG	C19-C20-C21-C22
39	H	102	DGD	O2G-C1B-C2B-C3B
27	a	414	SQD	C14-C15-C16-C17
37	E	101	LHG	C14-C15-C16-C17
24	B	602	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	b	604	CLA	CAD-CBD-CGD-O1D
24	b	608	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
37	D	410	LHG	C4-O6-P-O5
37	d	409	LHG	C4-O6-P-O3
37	e	101	LHG	C3-O3-P-O6
24	B	606	CLA	C2B-C3B-CAB-CBB
24	c	515	CLA	C2B-C3B-CAB-CBB
28	D	412	LMG	C18-C19-C20-C21
27	L	101	SQD	C7-C8-C9-C10
28	d	411	LMG	C10-C11-C12-C13
29	B	642	LMT	C11-C10-C9-C8
24	c	511	CLA	C10-C11-C12-C13
39	C	519	DGD	CDB-CEB-CFB-CGB
27	a	414	SQD	C30-C31-C32-C33
30	B	627	GOL	O2-C2-C3-O3
30	V	204	GOL	O1-C1-C2-O2
30	v	1605	GOL	O1-C1-C2-O2
37	d	410	LHG	O1-C1-C2-C3
28	b	623	LMG	C10-C11-C12-C13
28	A	412	LMG	C15-C16-C17-C18
27	D	408	SQD	C46-C45-O47-C7
27	L	102	SQD	C46-C45-O47-C7
28	B	621	LMG	C17-C18-C19-C20
36	u	201	HTG	C2'-C3'-C4'-C5'
39	D	407	DGD	C4A-C5A-C6A-C7A
27	A	411	SQD	C7-C8-C9-C10
39	c	520	DGD	C7A-C8A-C9A-CAA
28	A	412	LMG	O6-C5-C6-O5
29	m	102	LMT	O5'-C5'-C6'-O6'
37	l	302	LHG	O6-C4-C5-C6
24	B	617	CLA	C5-C6-C7-C8
24	A	409	CLA	C11-C10-C8-C9
24	B	617	CLA	C11-C12-C13-C14
24	a	410	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	C	521	LMT	C4-C5-C6-C7
37	D	409	LHG	C17-C18-C19-C20
37	D	411	LHG	C14-C15-C16-C17
24	a	408	CLA	C2C-C3C-CAC-CBC
28	A	412	LMG	C2-C1-O1-C7
37	l	302	LHG	C16-C17-C18-C19
24	d	405	CLA	C16-C17-C18-C19
36	I	102	HTG	S1-C1'-C2'-C3'
28	c	521	LMG	C36-C37-C38-C39
27	A	411	SQD	O6-C44-C45-O47
28	b	623	LMG	C28-C29-C30-C31
24	B	611	CLA	C16-C17-C18-C20
29	B	642	LMT	C4-C5-C6-C7
39	C	519	DGD	C6B-C7B-C8B-C9B
27	f	102	SQD	O6-C44-C45-C46
39	D	407	DGD	CBB-CCB-CDB-CEB
28	c	521	LMG	C14-C15-C16-C17
24	b	614	CLA	C16-C17-C18-C20
36	b	625	HTG	C2'-C1'-S1-C1
27	L	102	SQD	C30-C31-C32-C33
24	b	604	CLA	CAA-CBA-CGA-O2A
39	C	517	DGD	C5D-C6D-O5D-C1E
24	B	602	CLA	C8-C10-C11-C12
39	c	519	DGD	C6B-C7B-C8B-C9B
24	B	611	CLA	C2A-CAA-CBA-CGA
39	c	518	DGD	C9A-CAA-CBA-CCA
33	a	425[B]	PL9	C25-C24-C26-C27
24	b	613	CLA	C13-C15-C16-C17
28	c	521	LMG	C17-C18-C19-C20
39	C	518	DGD	C3B-C4B-C5B-C6B
24	A	405	CLA	C2C-C3C-CAC-CBC
28	B	621	LMG	C16-C17-C18-C19
28	a	415	LMG	C30-C31-C32-C33
27	a	414	SQD	C11-C12-C13-C14
24	C	505	CLA	C6-C7-C8-C9
24	a	410	CLA	C11-C12-C13-C14
28	c	521	LMG	C29-C28-O8-C9
24	b	618	CLA	C4B-C3B-CAB-CBB
28	d	411	LMG	C36-C37-C38-C39
29	M	101	LMT	O5'-C5'-C6'-O6'
39	H	102	DGD	CBA-CCA-CDA-CEA
24	a	408	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C16-C17-C18-C20
27	a	414	SQD	C32-C33-C34-C35
28	c	521	LMG	O10-C28-O8-C9
33	A	422[B]	PL9	C20-C19-C21-C22
29	a	402	LMT	C7-C8-C9-C10
37	d	410	LHG	C25-C26-C27-C28
33	a	425[B]	PL9	C24-C26-C27-C28
25	D	401	PHO	C2C-C3C-CAC-CBC
27	a	401	SQD	C17-C18-C19-C20
24	C	508	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	O1D-CGD-O2D-CED
37	B	640	LHG	C31-C32-C33-C34
24	A	409	CLA	C12-C13-C15-C16
24	a	412	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	b	609	CLA	C11-C12-C13-C15
24	B	606	CLA	C8-C10-C11-C12
28	d	411	LMG	C34-C35-C36-C37
28	D	412	LMG	C21-C22-C23-C24
28	b	623	LMG	C17-C18-C19-C20
24	C	507	CLA	C3A-C2A-CAA-CBA
24	c	509	CLA	C2A-CAA-CBA-CGA
27	L	102	SQD	C7-C8-C9-C10
28	A	412	LMG	C30-C31-C32-C33
28	c	522	LMG	C38-C39-C40-C41
37	d	409	LHG	C11-C10-C9-C8
24	c	504	CLA	C2-C1-O2A-CGA
24	b	609	CLA	C3-C5-C6-C7
37	E	101	LHG	C10-C11-C12-C13
36	B	624	HTG	O5-C5-C6-O6
37	l	302	LHG	C31-C32-C33-C34
28	B	621	LMG	C37-C38-C39-C40
24	c	509	CLA	C4-C3-C5-C6
24	B	602	CLA	CAA-CBA-CGA-O1A
39	C	518	DGD	CAA-CBA-CCA-CDA
24	B	615	CLA	C14-C13-C15-C16
24	C	508	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C9
24	b	619	CLA	C14-C13-C15-C16
30	c	526	GOL	O1-C1-C2-C3
37	D	409	LHG	O1-C1-C2-C3
24	B	611	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	L	101	SQD	C12-C13-C14-C15
29	f	104	LMT	C1-C2-C3-C4
28	a	415	LMG	O8-C28-C29-C30
37	E	101	LHG	O1-C1-C2-O2
39	C	518	DGD	C2E-C1E-O5D-C6D
24	b	607	CLA	C1A-C2A-CAA-CBA
24	A	406	CLA	C2C-C3C-CAC-CBC
37	D	409	LHG	C7-C8-C9-C10
37	e	101	LHG	O6-C4-C5-O7
24	a	410	CLA	C2B-C3B-CAB-CBB
24	b	604	CLA	C2B-C3B-CAB-CBB
24	b	618	CLA	C2B-C3B-CAB-CBB
24	c	504	CLA	C2B-C3B-CAB-CBB
24	d	404	CLA	C2B-C3B-CAB-CBB
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C23-C24-C25-C30
26	D	405	BCR	C23-C24-C25-C26
26	b	620	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
39	c	520	DGD	C8A-C9A-CAA-CBA
27	a	401	SQD	C13-C14-C15-C16
24	a	412	CLA	C4-C3-C5-C6
37	B	640	LHG	O6-C4-C5-C6
24	A	407	CLA	C12-C13-C15-C16
24	B	602	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C10-C8-C7
24	B	605	CLA	C6-C7-C8-C10
24	B	615	CLA	C12-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C7
24	c	507	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
27	L	101	SQD	O6-C44-C45-O47
27	a	414	SQD	O6-C44-C45-O47
37	d	408	LHG	C11-C10-C9-C8
33	A	422[B]	PL9	C4-C3-C7-C8
33	d	407	PL9	C4-C3-C7-C8
36	b	602	HTG	O5-C1-S1-C1'
43	V	202	HEC	CAD-CBD-CGD-O2D
33	A	422[B]	PL9	C18-C19-C21-C22
28	D	412	LMG	C36-C37-C38-C39
37	d	409	LHG	C32-C33-C34-C35
24	b	618	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
43	v	1603	HEC	CAD-CBD-CGD-O2D
24	c	508	CLA	C13-C15-C16-C17
24	b	609	CLA	C11-C12-C13-C14
24	b	609	CLA	C8-C10-C11-C12
24	b	611	CLA	C5-C6-C7-C8
27	L	102	SQD	C10-C11-C12-C13
29	c	523	LMT	C5-C6-C7-C8
37	d	409	LHG	C26-C27-C28-C29
28	A	412	LMG	O6-C1-O1-C7
29	b	624	LMT	C6-C7-C8-C9
29	m	101	LMT	C7-C8-C9-C10
24	b	611	CLA	C4-C3-C5-C6
24	b	618	CLA	C4-C3-C5-C6
43	v	1603	HEC	CAD-CBD-CGD-O1D
24	a	412	CLA	C2-C3-C5-C6
24	c	509	CLA	C2-C3-C5-C6
33	a	425[B]	PL9	C23-C24-C26-C27
28	c	521	LMG	C20-C21-C22-C23
27	D	408	SQD	C44-C45-C46-O48
27	a	414	SQD	O6-C44-C45-C46
37	D	409	LHG	C11-C12-C13-C14
43	V	202	HEC	CAD-CBD-CGD-O1D
29	J	102	LMT	C9-C10-C11-C12
24	b	613	CLA	C2A-CAA-CBA-CGA
27	f	102	SQD	C29-C30-C31-C32
24	b	606	CLA	C13-C15-C16-C17
24	b	613	CLA	C16-C17-C18-C19
36	O	302	HTG	C2'-C3'-C4'-C5'
39	D	407	DGD	CBA-CCA-CDA-CEA
24	c	505	CLA	C10-C11-C12-C13
30	T	101	GOL	O2-C2-C3-O3
33	A	422[B]	PL9	C30-C29-C31-C32
24	B	614	CLA	C13-C15-C16-C17
36	b	625	HTG	C4'-C5'-C6'-C7'
24	c	504	CLA	C4B-C3B-CAB-CBB
24	d	404	CLA	C4B-C3B-CAB-CBB
28	c	521	LMG	C10-C11-C12-C13
36	b	625	HTG	C2'-C3'-C4'-C5'
24	A	407	CLA	C16-C17-C18-C20
39	h	1205	DGD	C9A-CAA-CBA-CCA
25	A	408	PHO	CHA-CBD-CGD-O1D
40	F	101	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
37	e	101	LHG	O6-C4-C5-C6
37	E	101	LHG	O7-C5-C6-O8
24	B	607	CLA	C15-C16-C17-C18
28	A	412	LMG	C38-C39-C40-C41
39	C	517	DGD	O6E-C1E-O5D-C6D
39	C	518	DGD	O6E-C1E-O5D-C6D
39	D	407	DGD	CAA-CBA-CCA-CDA
39	c	518	DGD	CAA-CBA-CCA-CDA
27	a	414	SQD	C15-C16-C17-C18
24	A	405	CLA	C4C-C3C-CAC-CBC
39	C	519	DGD	C4B-C5B-C6B-C7B
24	C	509	CLA	C11-C10-C8-C9
24	b	606	CLA	C6-C7-C8-C9
29	A	414	LMT	C1-C2-C3-C4
39	c	518	DGD	C5D-C6D-O5D-C1E
24	B	602	CLA	C2-C1-O2A-CGA
24	b	613	CLA	C16-C17-C18-C20
37	D	409	LHG	C30-C31-C32-C33
27	D	408	SQD	C29-C30-C31-C32
24	C	513	CLA	O1A-CGA-O2A-C1
24	b	619	CLA	CBA-CGA-O2A-C1
24	C	507	CLA	CBD-CGD-O2D-CED
24	B	617	CLA	C16-C17-C18-C19
24	C	503	CLA	C16-C17-C18-C20
28	c	522	LMG	C37-C38-C39-C40
37	D	411	LHG	C19-C20-C21-C22
29	E	104	LMT	C2-C3-C4-C5
27	A	413	SQD	C19-C20-C21-C22
24	a	408	CLA	C4C-C3C-CAC-CBC
37	e	101	LHG	C4-C5-C6-O8
24	b	619	CLA	O1A-CGA-O2A-C1
24	c	505	CLA	C5-C6-C7-C8
27	f	102	SQD	C31-C32-C33-C34
30	C	527	GOL	O2-C2-C3-O3
27	a	414	SQD	C28-C29-C30-C31
28	b	623	LMG	C18-C19-C20-C21
36	D	413	HTG	C4'-C5'-C6'-C7'
24	C	508	CLA	C16-C17-C18-C19
39	c	519	DGD	CCA-CDA-CEA-CFA
36	B	625	HTG	O5-C5-C6-O6
37	e	101	LHG	O7-C5-C6-O8
24	B	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C14-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C9
24	c	508	CLA	C16-C17-C18-C19
26	b	622	BCR	C21-C22-C23-C24
33	d	407	PL9	C15-C14-C16-C17
27	D	408	SQD	C33-C34-C35-C36
27	L	101	SQD	C29-C30-C31-C32
24	C	509	CLA	C11-C10-C8-C7
24	b	606	CLA	C6-C7-C8-C10
24	D	403	CLA	C2B-C3B-CAB-CBB
26	C	515	BCR	C5-C6-C7-C8
26	Y	302	BCR	C23-C24-C25-C30
41	H	101	RRX	C23-C24-C25-C30
28	d	411	LMG	C13-C14-C15-C16
24	B	609	CLA	C2-C1-O2A-CGA
24	C	507	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
27	A	411	SQD	O47-C7-C8-C9
27	D	408	SQD	O48-C23-C24-C25
37	B	640	LHG	C17-C18-C19-C20
39	c	518	DGD	C2B-C3B-C4B-C5B
24	b	618	CLA	C13-C15-C16-C17
25	a	411	PHO	C4-C3-C5-C6
27	f	102	SQD	O48-C23-C24-C25
37	D	409	LHG	O8-C23-C24-C25
24	B	612	CLA	C2-C3-C5-C6
33	D	406	PL9	C13-C14-C16-C17
33	d	407	PL9	C13-C14-C16-C17
28	a	415	LMG	O9-C10-O7-C8
24	b	614	CLA	C8-C10-C11-C12
36	C	522	HTG	C2'-C1'-S1-C1
24	c	508	CLA	C3-C5-C6-C7
28	B	621	LMG	C15-C16-C17-C18
28	b	623	LMG	C16-C17-C18-C19
27	L	101	SQD	C33-C34-C35-C36
39	C	518	DGD	O2G-C1B-C2B-C3B
24	B	613	CLA	C13-C15-C16-C17
24	b	614	CLA	C2-C3-C5-C6
25	a	411	PHO	C2-C3-C5-C6
40	f	101	HEM	CAD-CBD-CGD-O1D
29	a	402	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	B	613	CLA	O1A-CGA-O2A-C1
27	L	101	SQD	C11-C10-C9-C8
37	d	410	LHG	O8-C23-C24-C25
27	D	408	SQD	C26-C27-C28-C29
30	c	526	GOL	O1-C1-C2-O2
29	z	101	LMT	C3-C4-C5-C6
24	B	602	CLA	C6-C7-C8-C9
24	B	615	CLA	C11-C10-C8-C9
24	B	616	CLA	C14-C13-C15-C16
27	L	101	SQD	C16-C17-C18-C19
36	C	523	HTG	C4-C5-C6-O6
27	L	101	SQD	O6-C44-C45-C46
39	C	518	DGD	C6A-C7A-C8A-C9A
24	C	502	CLA	C4B-C3B-CAB-CBB
24	D	403	CLA	C4B-C3B-CAB-CBB
40	F	101	HEM	CAD-CBD-CGD-O2D
27	L	102	SQD	O48-C23-C24-C25
28	c	522	LMG	O7-C8-C9-O8
24	C	507	CLA	C10-C11-C12-C13
27	a	401	SQD	O10-C23-O48-C46
39	C	519	DGD	C4A-C5A-C6A-C7A
28	b	623	LMG	O8-C28-C29-C30
28	d	411	LMG	C35-C36-C37-C38
39	c	518	DGD	O2G-C1B-C2B-C3B
39	c	519	DGD	O2G-C1B-C2B-C3B
39	c	520	DGD	O1G-C1A-C2A-C3A
30	B	631	GOL	O1-C1-C2-C3
30	E	105	GOL	C1-C2-C3-O3
24	B	604	CLA	C6-C7-C8-C10
24	B	616	CLA	C12-C13-C15-C16
24	a	412	CLA	C11-C10-C8-C7
24	b	610	CLA	C12-C13-C15-C16
24	c	510	CLA	C12-C13-C15-C16
37	l	302	LHG	C17-C18-C19-C20
24	B	605	CLA	C16-C17-C18-C20
24	C	502	CLA	C2A-CAA-CBA-CGA
28	C	520	LMG	C21-C22-C23-C24
37	B	640	LHG	C13-C14-C15-C16
24	c	505	CLA	C15-C16-C17-C18
24	B	607	CLA	C10-C11-C12-C13
28	B	621	LMG	C10-C11-C12-C13
28	c	521	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	C8-C10-C11-C12
39	h	1205	DGD	CBB-CCB-CDB-CEB
27	f	102	SQD	O10-C23-C24-C25
37	D	409	LHG	O10-C23-C24-C25
28	a	415	LMG	C29-C30-C31-C32
28	a	415	LMG	C20-C21-C22-C23
37	d	410	LHG	C11-C12-C13-C14
24	B	611	CLA	C15-C16-C17-C18
24	C	513	CLA	CBA-CGA-O2A-C1
24	A	407	CLA	C14-C13-C15-C16
24	B	617	CLA	C14-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C9
25	d	401	PHO	C8-C10-C11-C12
40	f	101	HEM	CAD-CBD-CGD-O2D
29	a	402	LMT	C4-C5-C6-C7
33	d	407	PL9	C45-C44-C46-C47
37	l	302	LHG	C11-C12-C13-C14
27	a	401	SQD	C24-C23-O48-C46
39	C	519	DGD	O1G-C1A-C2A-C3A
37	E	101	LHG	C11-C10-C9-C8
39	C	518	DGD	O1B-C1B-C2B-C3B
28	c	521	LMG	C37-C38-C39-C40
30	d	413	GOL	O2-C2-C3-O3
28	b	623	LMG	C22-C23-C24-C25
39	C	519	DGD	CCA-CDA-CEA-CFA
27	A	411	SQD	O49-C7-C8-C9
39	c	520	DGD	O1A-C1A-C2A-C3A
39	D	407	DGD	C2G-C3G-O3G-C1D
39	c	519	DGD	C2E-C1E-O5D-C6D
24	C	508	CLA	C2A-CAA-CBA-CGA
37	D	411	LHG	C30-C31-C32-C33
27	D	408	SQD	O10-C23-C24-C25
39	c	518	DGD	O1B-C1B-C2B-C3B
24	C	509	CLA	C5-C6-C7-C8
28	B	621	LMG	O8-C28-C29-C30
24	c	506	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
25	a	411	PHO	CAD-CBD-CGD-O2D
24	C	511	CLA	CAA-CBA-CGA-O2A
27	L	102	SQD	O10-C23-C24-C25
37	d	410	LHG	O10-C23-C24-C25
39	D	407	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
39	c	518	DGD	O6E-C1E-O5D-C6D
39	c	519	DGD	O6E-C1E-O5D-C6D
24	B	614	CLA	CAA-CBA-CGA-O2A
36	C	523	HTG	C1'-C2'-C3'-C4'
24	c	503	CLA	CAA-CBA-CGA-O2A
28	D	412	LMG	O7-C10-C11-C12
24	b	617	CLA	C8-C10-C11-C12

There are no ring outliers.

151 monomers are involved in 262 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	616	CLA	8	0
29	a	402	LMT	1	0
26	c	516	BCR	2	0
38	o	308	DMS	1	0
29	m	102	LMT	1	0
24	C	503	CLA	4	0
26	d	406	BCR	1	0
24	C	512	CLA	3	0
25	d	401	PHO	2	0
26	C	515	BCR	2	0
39	c	520	DGD	2	0
36	O	302	HTG	1	0
39	D	407	DGD	6	0
26	a	413	BCR	3	0
24	C	510	CLA	1	0
24	c	511	CLA	2	0
28	C	532	LMG	1	0
24	B	617	CLA	4	0
29	C	521	LMT	4	0
26	Y	302	BCR	1	0
28	c	521	LMG	1	0
27	L	101	SQD	1	0
26	B	619	BCR	4	0
28	C	520	LMG	1	0
36	h	1202	HTG	2	0
24	A	405	CLA	2	0
24	D	403	CLA	1	0
24	b	605	CLA	2	0
39	H	102	DGD	1	0
26	A	410	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	507	CLA	2	0
24	b	607	CLA	2	0
30	d	402	GOL	2	0
36	b	602	HTG	1	0
24	c	505	CLA	4	0
29	M	101	LMT	1	0
26	b	622	BCR	3	0
36	B	625	HTG	1	0
24	d	404	CLA	2	0
24	c	503	CLA	3	0
24	B	606	CLA	5	0
39	h	1205	DGD	1	0
28	B	621	LMG	1	0
24	b	615	CLA	1	0
27	L	102	SQD	2	0
25	D	401	PHO	2	0
24	c	514	CLA	3	0
37	e	101	LHG	1	0
24	a	410	CLA	1	0
24	b	617	CLA	1	0
26	B	618	BCR	1	0
26	b	620	BCR	2	0
29	z	101	LMT	2	0
37	D	411	LHG	5	0
24	B	602	CLA	1	0
24	b	606	CLA	3	0
39	C	518	DGD	2	0
24	B	603	CLA	2	0
24	c	508	CLA	1	0
30	a	418	GOL	1	0
24	A	409	CLA	2	0
24	b	610	CLA	1	0
39	c	518	DGD	1	0
26	B	620	BCR	2	0
24	A	407	CLA	1	0
39	C	517	DGD	2	0
27	a	414	SQD	1	0
24	c	506	CLA	1	0
36	b	626	HTG	1	0
24	b	604	CLA	4	0
26	b	621	BCR	3	0
24	b	609	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	618	CLA	4	0
30	v	1606	GOL	1	0
26	k	303	BCR	1	0
27	A	411	SQD	3	0
24	c	512	CLA	1	0
36	B	626	HTG	1	0
37	E	101	LHG	1	0
24	B	611	CLA	3	0
24	C	502	CLA	5	0
24	C	504	CLA	2	0
24	C	506	CLA	2	0
24	c	510	CLA	3	0
38	c	536	DMS	1	0
38	B	643	DMS	1	0
29	B	622	LMT	1	0
36	D	413	HTG	3	0
37	D	409	LHG	3	0
24	B	610	CLA	3	0
24	B	614	CLA	1	0
24	B	607	CLA	2	0
37	B	640	LHG	1	0
27	D	408	SQD	2	0
24	D	404	CLA	1	0
24	C	511	CLA	3	0
26	K	101	BCR	2	0
24	c	504	CLA	2	0
26	B	641	BCR	4	0
27	f	102	SQD	1	0
37	l	302	LHG	1	0
26	c	517	BCR	2	0
24	B	605	CLA	3	0
24	b	608	CLA	4	0
28	b	623	LMG	2	0
41	H	101	RRX	3	0
41	h	1204	RRX	5	0
24	A	406	CLA	4	0
33	a	425[B]	PL9	6	0
40	F	101	HEM	1	0
40	f	101	HEM	3	0
36	B	623[A]	HTG	3	0
24	c	515	CLA	3	0
29	A	414	LMT	1	0

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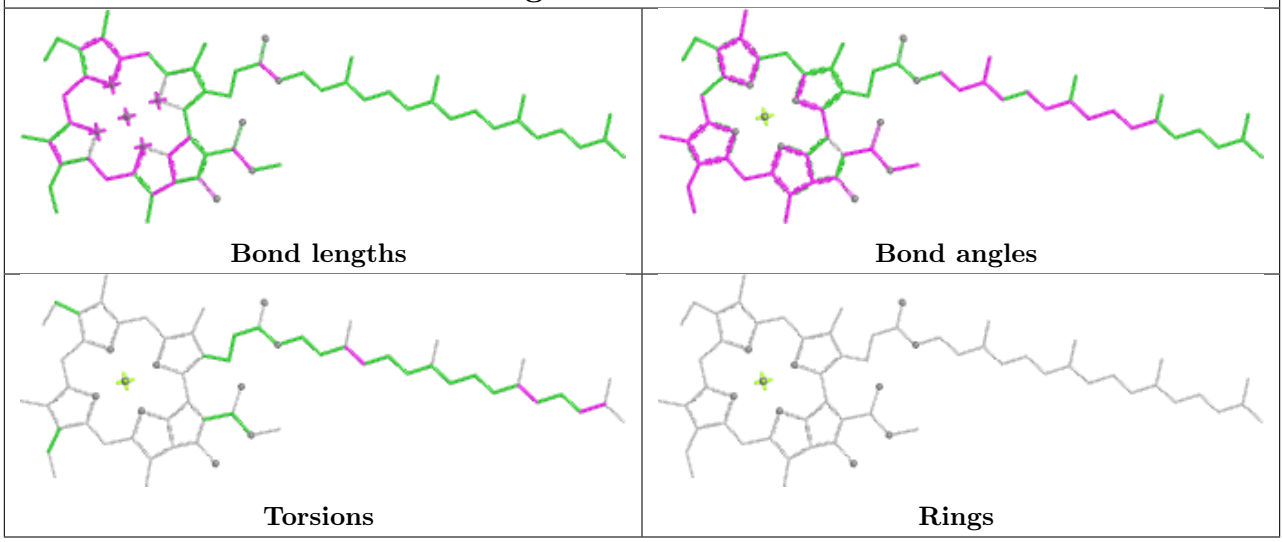
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	T	101	GOL	1	0
29	f	104	LMT	1	0
24	C	509	CLA	4	0
24	C	505	CLA	1	0
38	b	638	DMS	3	0
26	C	516	BCR	1	0
24	C	513	CLA	2	0
24	b	616	CLA	3	0
24	B	604	CLA	1	0
26	k	302	BCR	4	0
38	c	533	DMS	1	0
36	b	625	HTG	4	0
26	D	405	BCR	3	0
24	C	514	CLA	1	0
24	d	405	CLA	1	0
24	b	612	CLA	4	0
26	T	102	BCR	3	0
29	J	102	LMT	1	0
30	a	417	GOL	2	0
29	b	624	LMT	1	0
29	c	523	LMT	2	0
39	c	519	DGD	3	0
24	c	507	CLA	2	0
24	C	508	CLA	1	0
24	a	408	CLA	3	0
28	d	411	LMG	1	0
28	a	415	LMG	2	0
36	b	601	HTG	1	0
24	b	619	CLA	2	0
30	c	527	GOL	1	0
33	A	422[B]	PL9	6	0
30	C	530	GOL	2	0
30	o	305	GOL	1	0
24	b	613	CLA	3	0
24	c	513	CLA	3	0
28	D	412	LMG	2	0
24	a	409	CLA	1	0

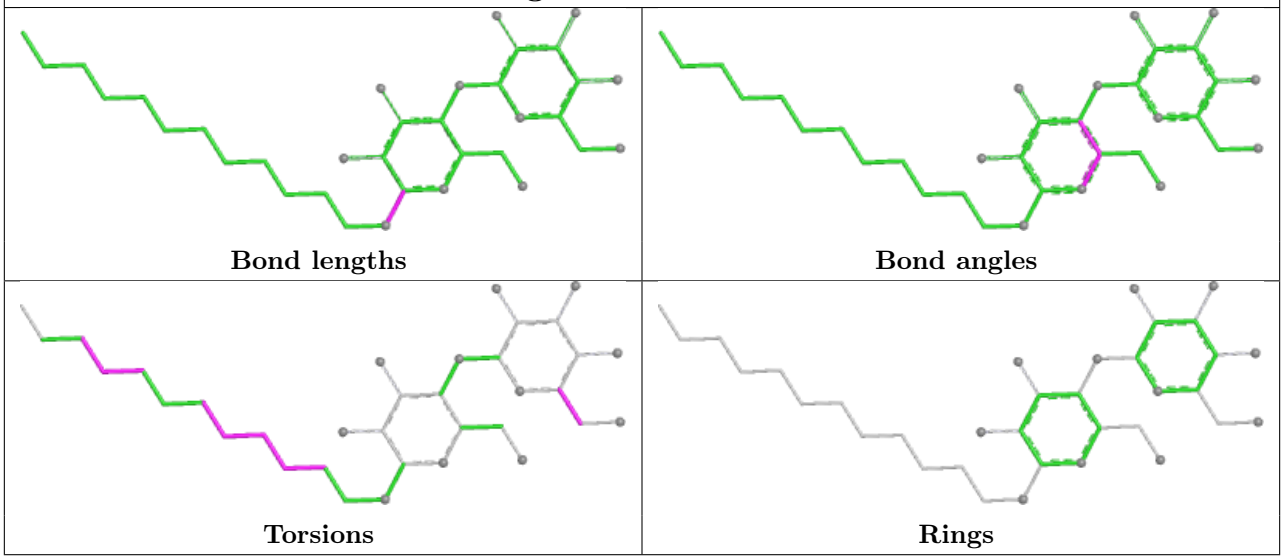
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

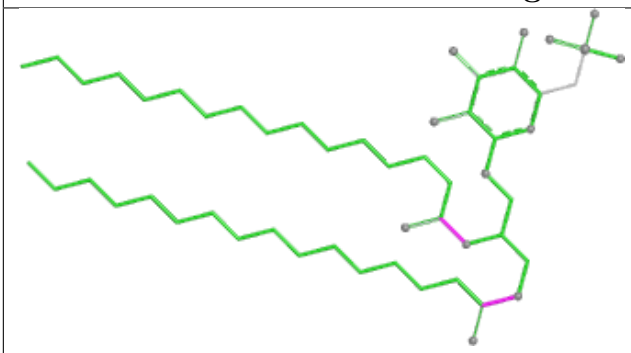
Ligand CLA B 616



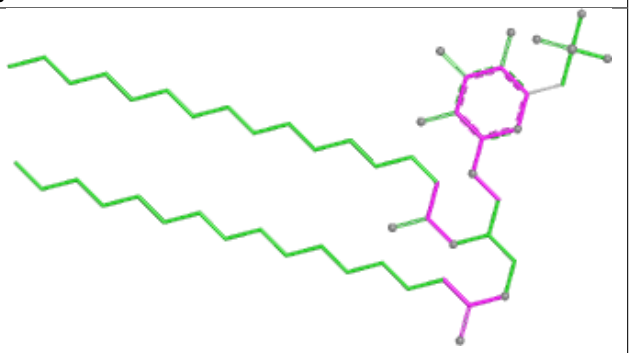
Ligand LMT a 402



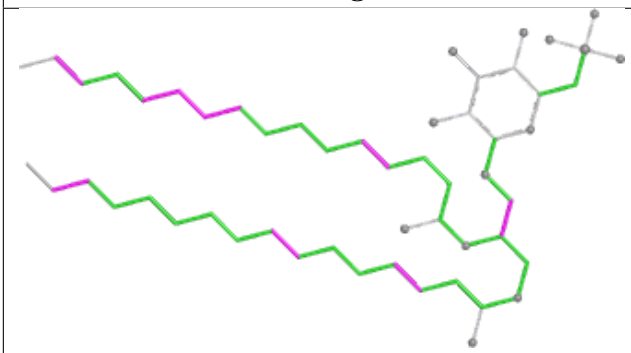
Ligand SQD A 413



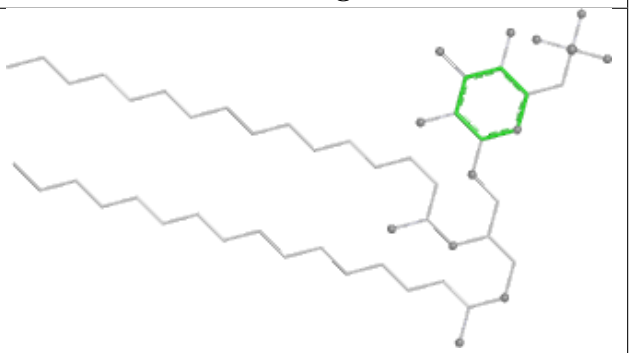
Bond lengths



Bond angles

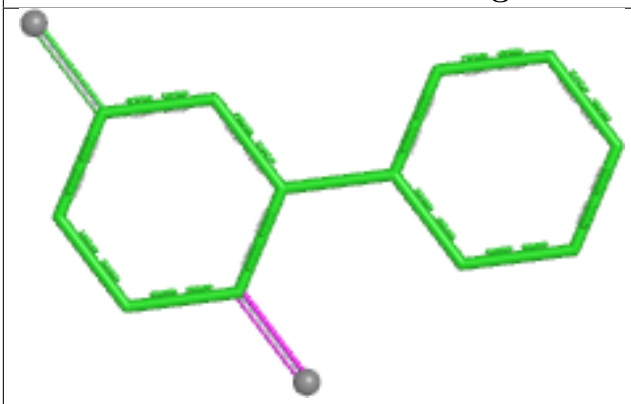


Torsions

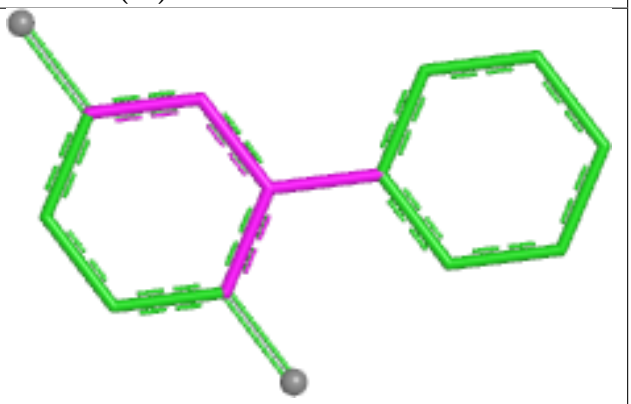


Rings

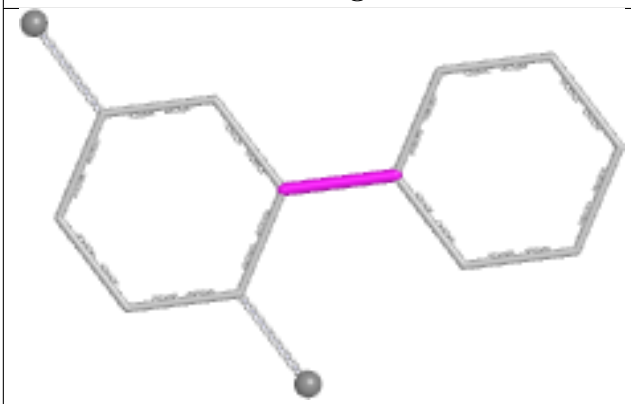
Ligand K3C A 421 (A)



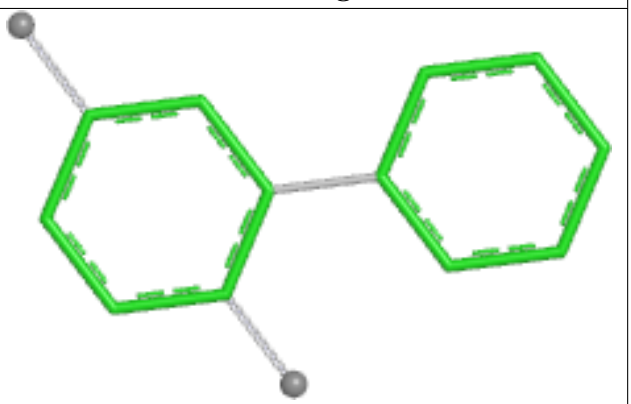
Bond lengths



Bond angles

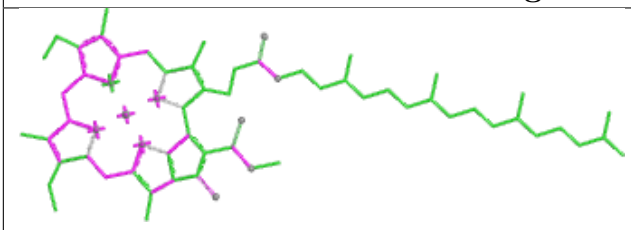


Torsions

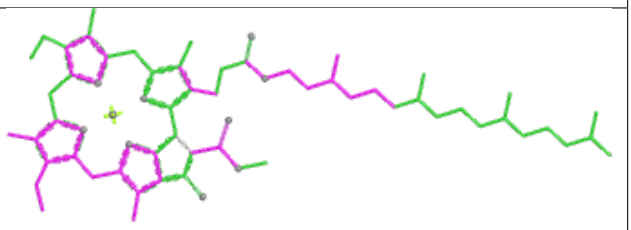


Rings

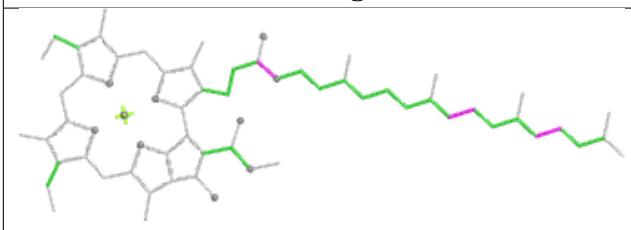
Ligand CLA B 613



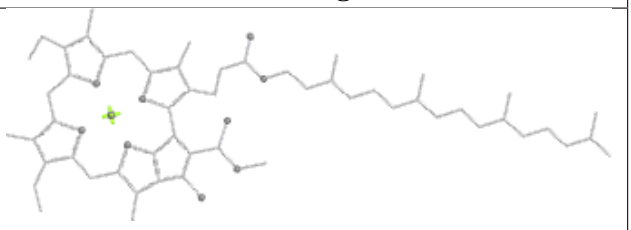
Bond lengths



Bond angles

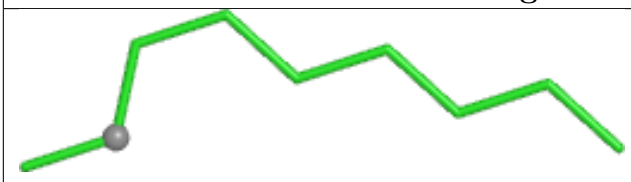


Torsions

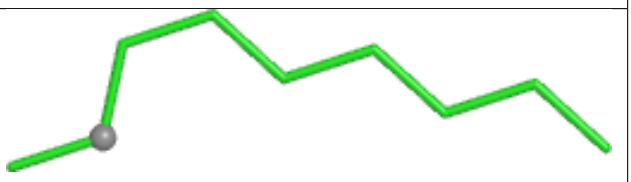


Rings

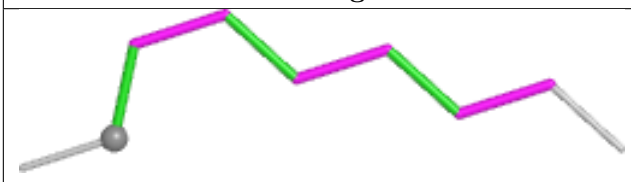
Ligand HTG U 201



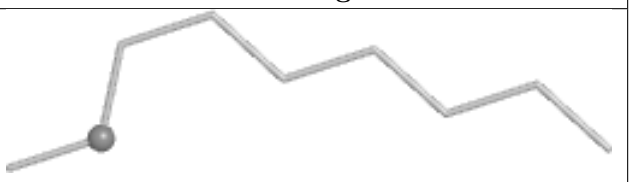
Bond lengths



Bond angles

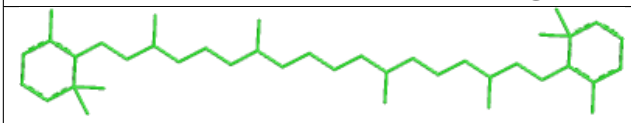


Torsions



Rings

Ligand BCR c 516



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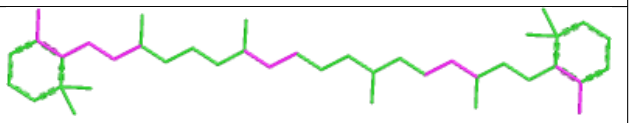
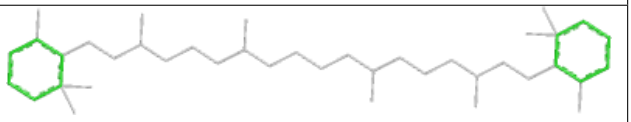


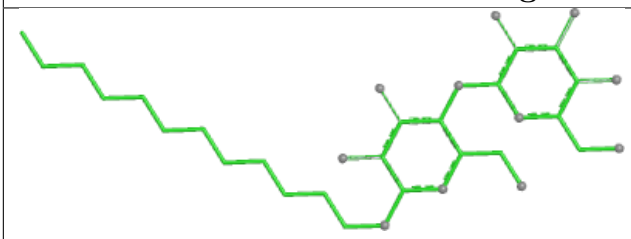
Bond angles

Torsions



Rings

Ligand LMT m 102



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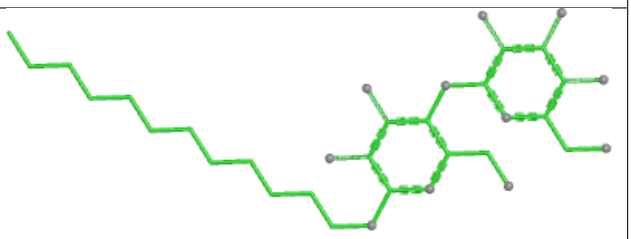
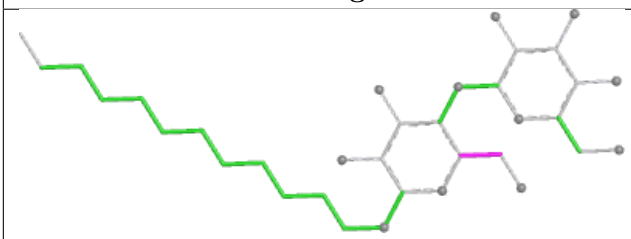
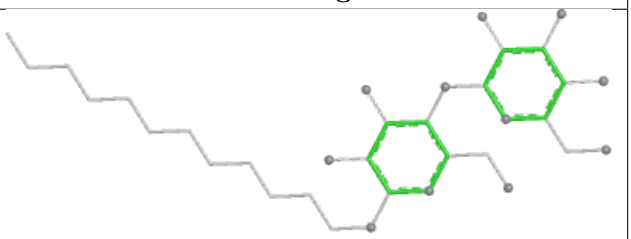


Bond angles

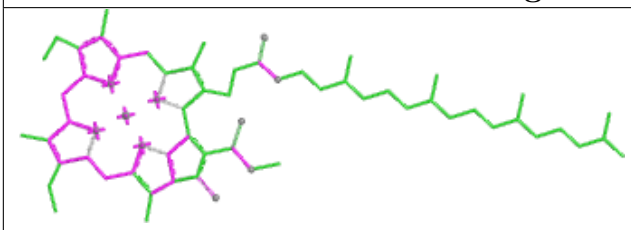


Torsions



Rings

Ligand CLA C 503



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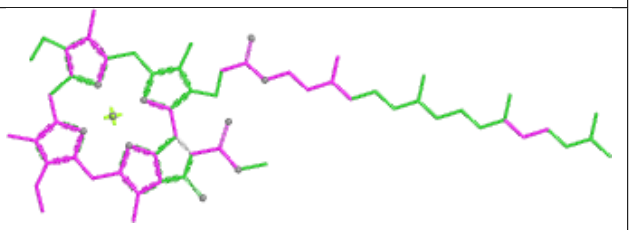
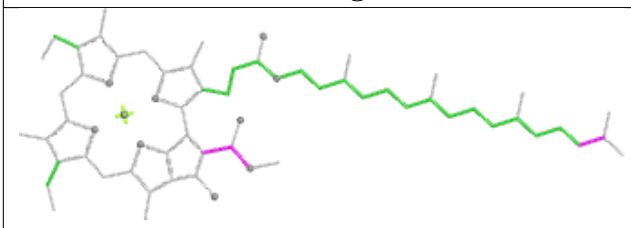


Bond angles



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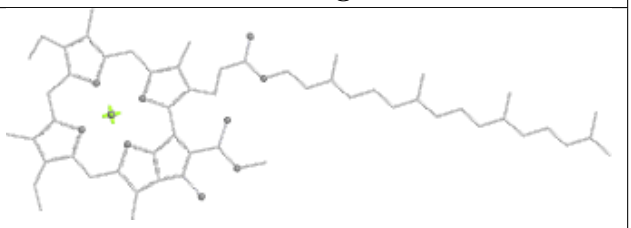
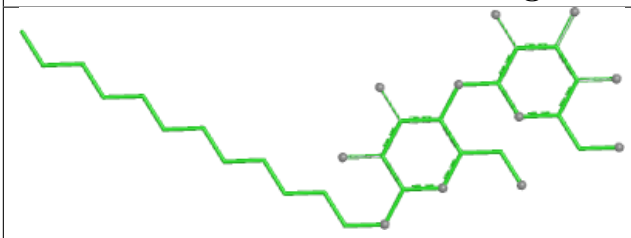
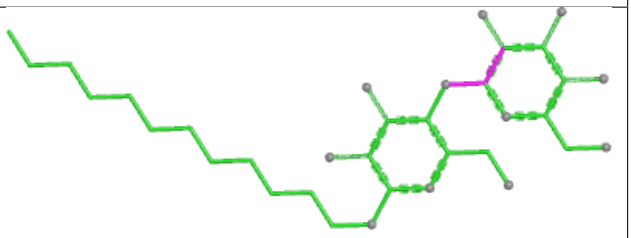


Rings

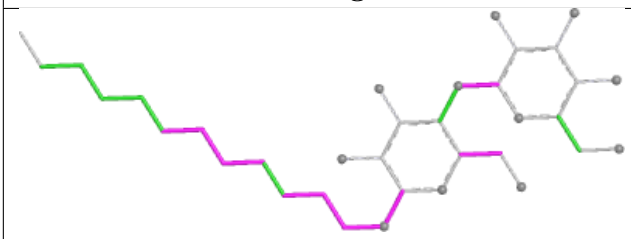
Ligand LMT Z 101



Bond lengths



Bond angles



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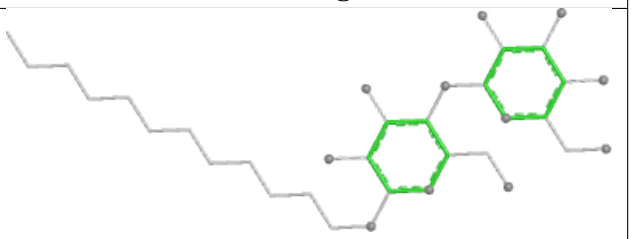
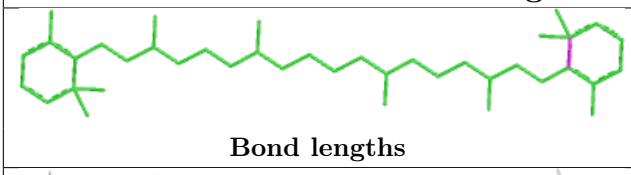


Rings

Ligand BCR d 406



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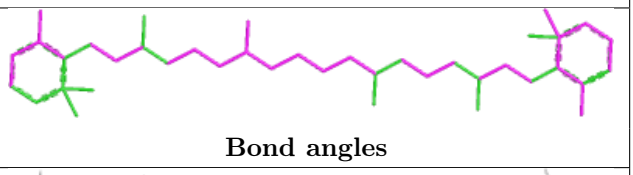
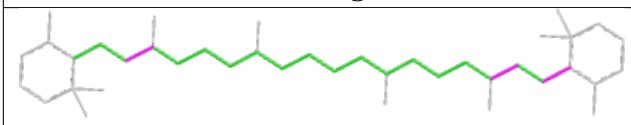


Bond angles



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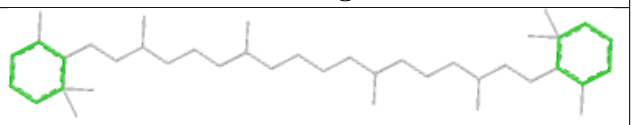
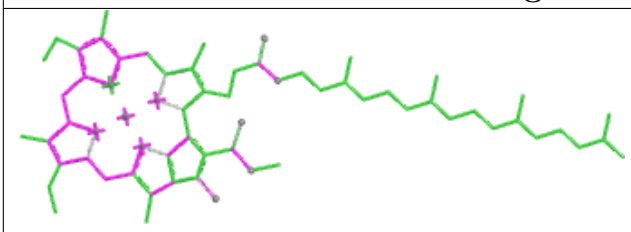


Rings

Ligand CLA C 512



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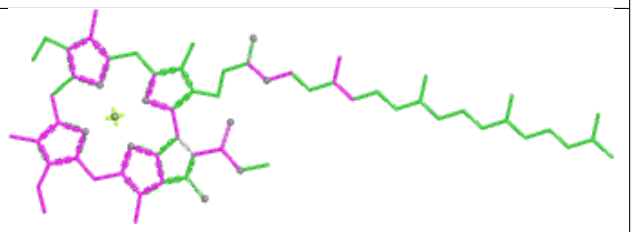
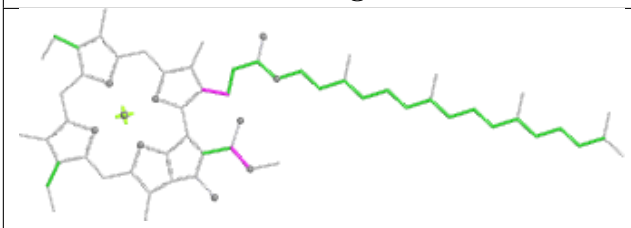


Bond angles



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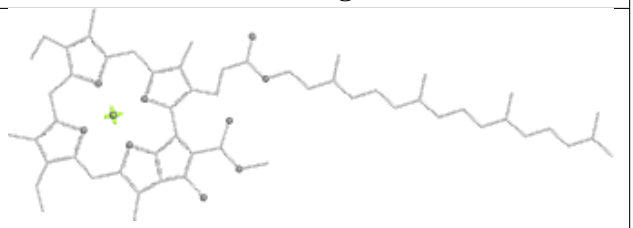
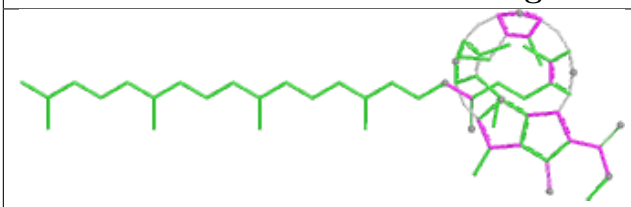


Rings

Ligand PHO d 401



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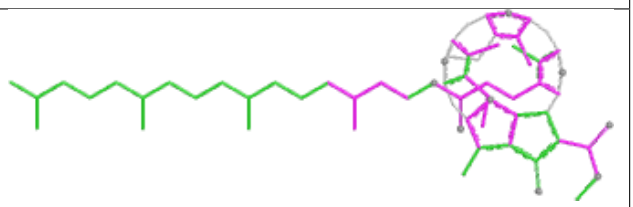
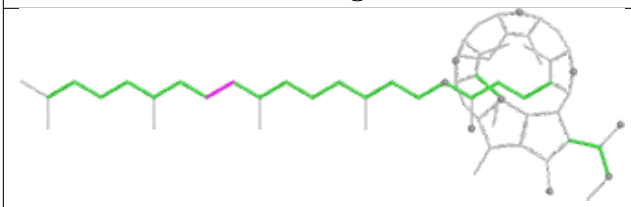
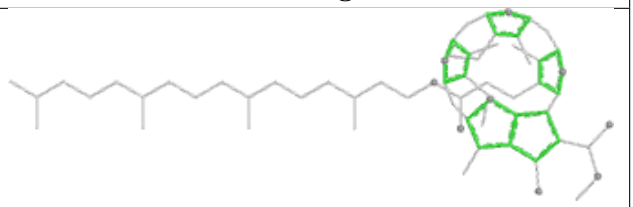


Bond angles

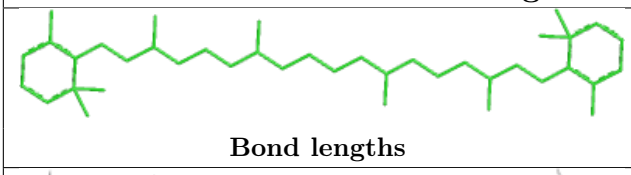


Torsions

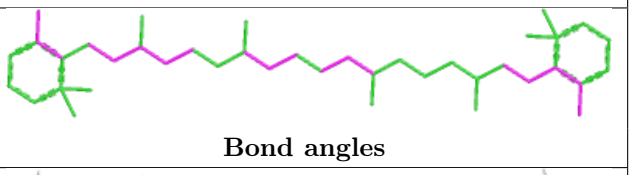


Rings

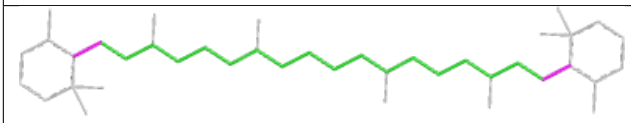
Ligand BCR C 515



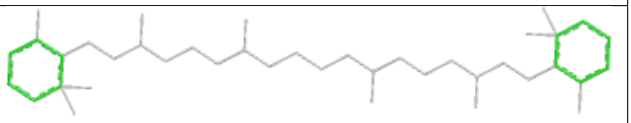
Bond lengths



Bond angles

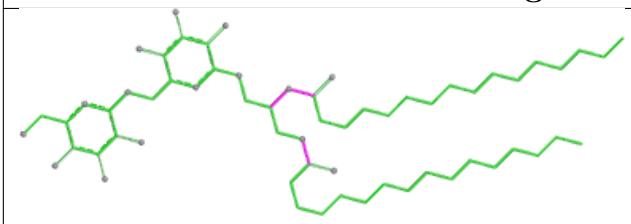


Torsions



Rings

Ligand DGD c 520



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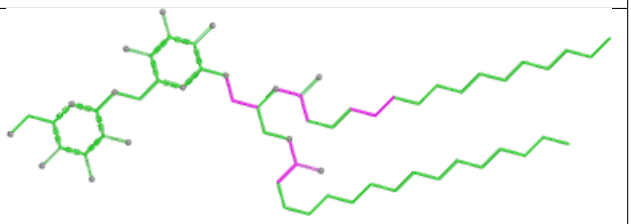
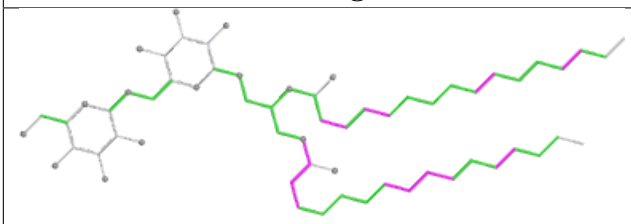
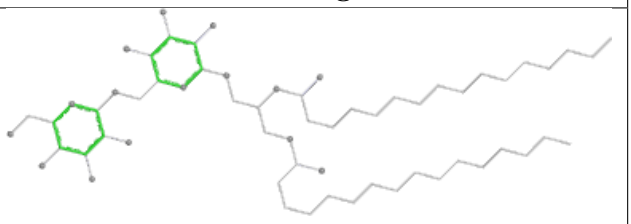


Bond angles

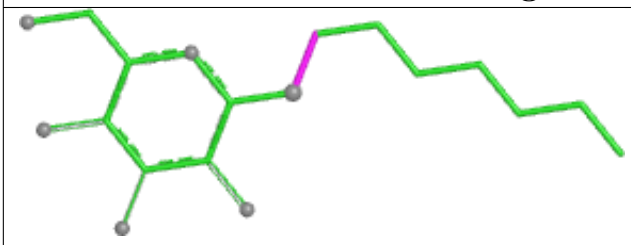


Torsions



Rings

Ligand HTG O 302



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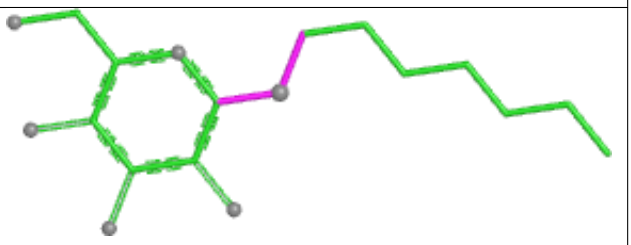
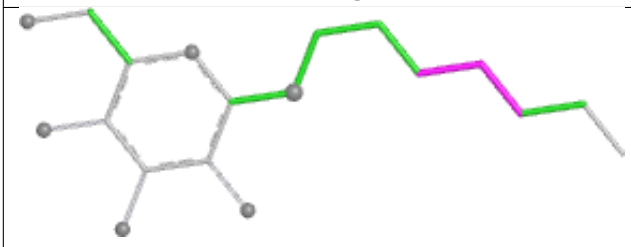
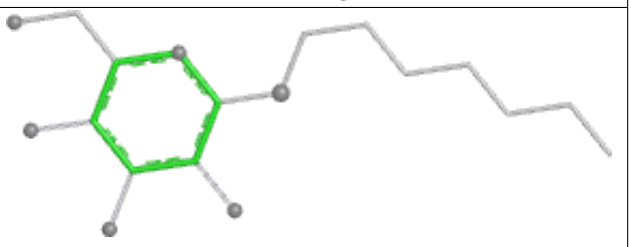


Bond angles

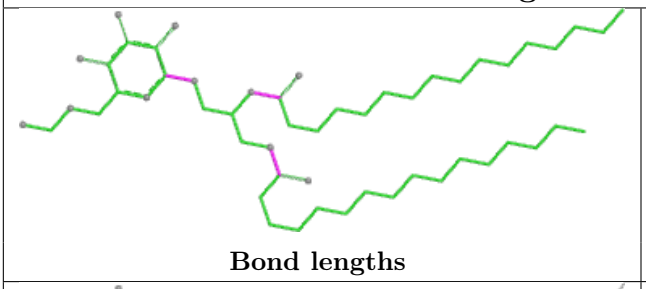


Torsions

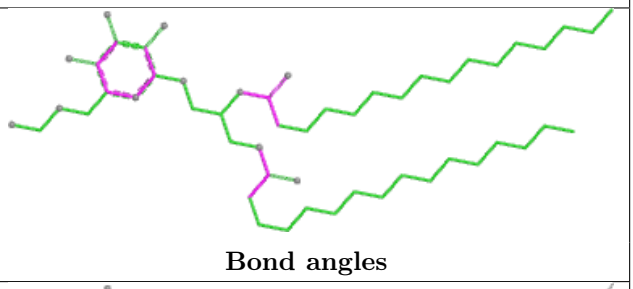


Rings

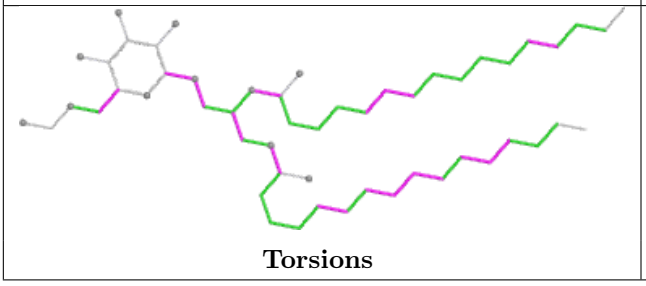
Ligand DGD D 407



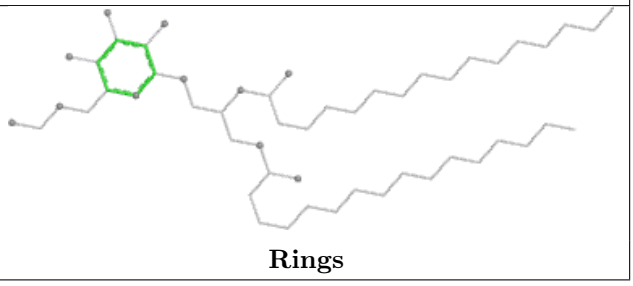
Bond lengths



Bond angles



Torsions



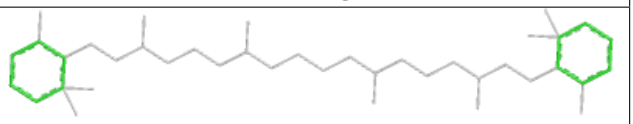
Rings

Ligand BCR a 413

Bond lengths

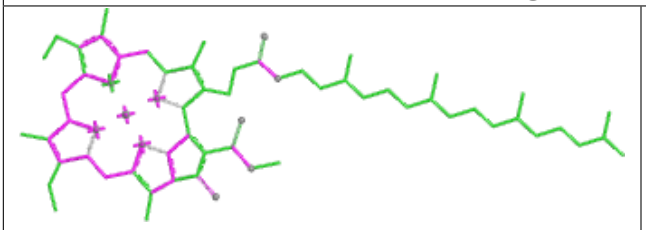
Bond angles

Torsions

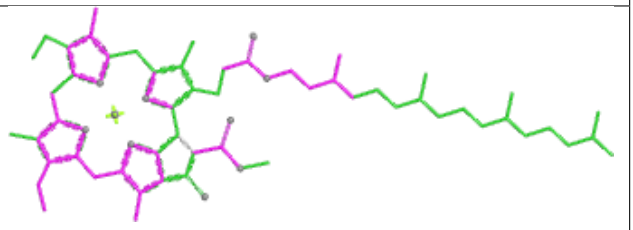


Rings

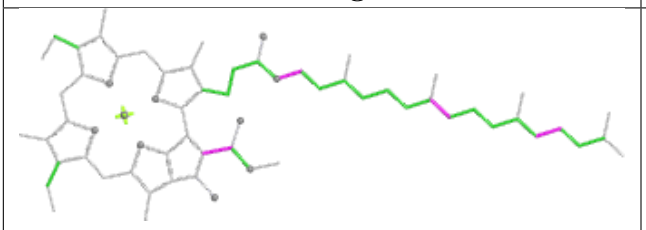
Ligand CLA C 510



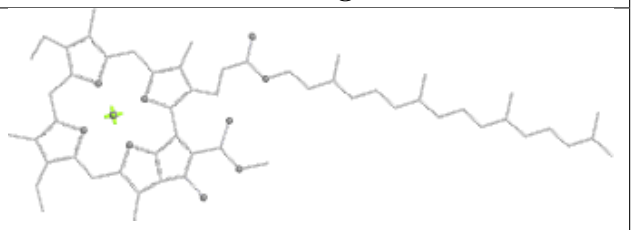
Bond lengths



Bond angles

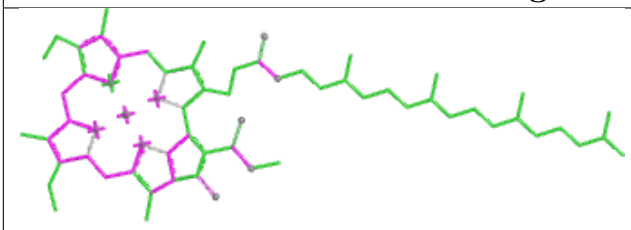


Torsions

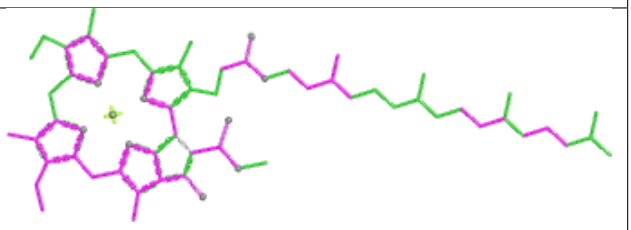


Rings

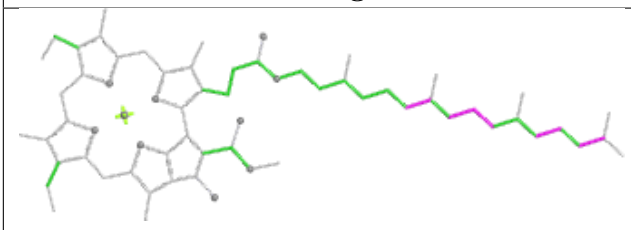
Ligand CLA c 511



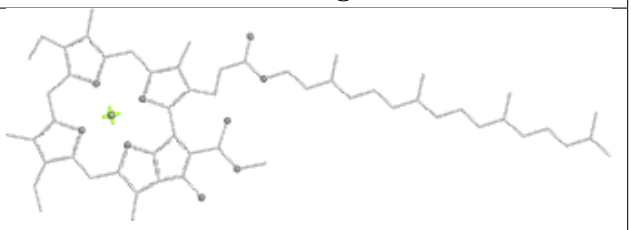
Bond lengths



Bond angles

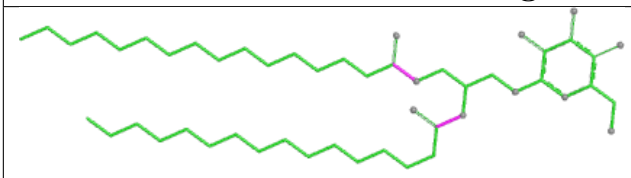


Torsions

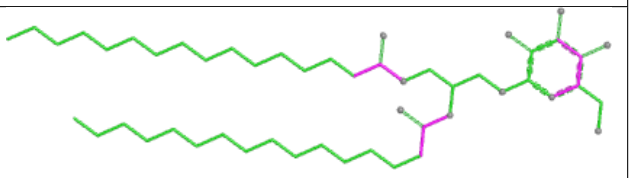


Rings

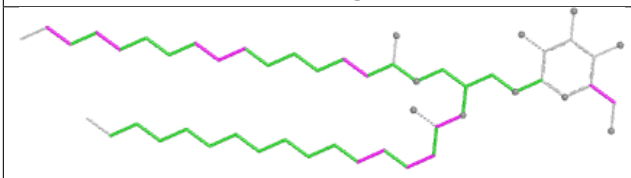
Ligand LMG C 532



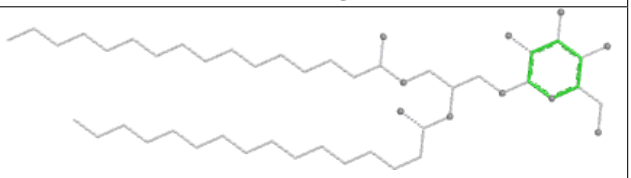
Bond lengths



Bond angles

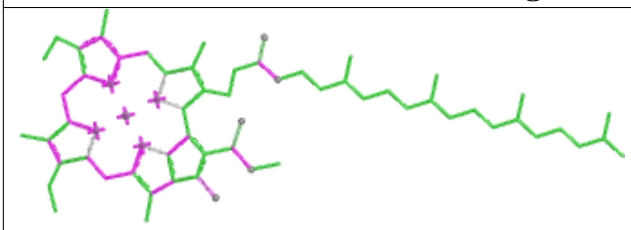


Torsions

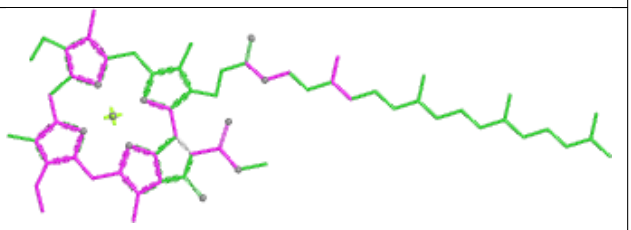


Rings

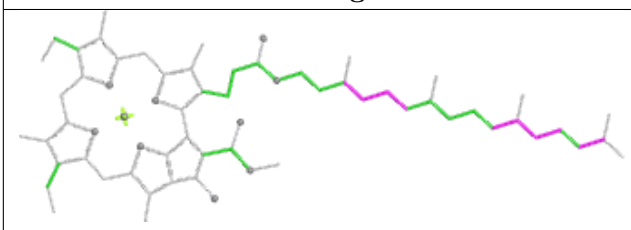
Ligand CLA B 617



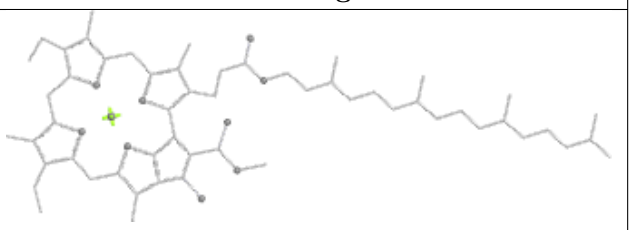
Bond lengths



Bond angles

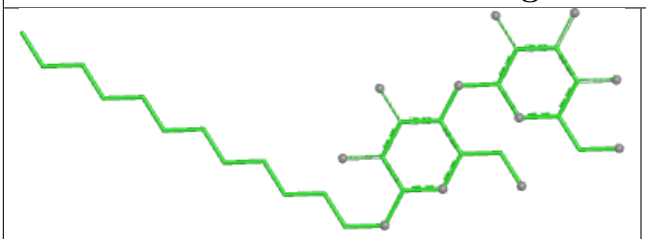


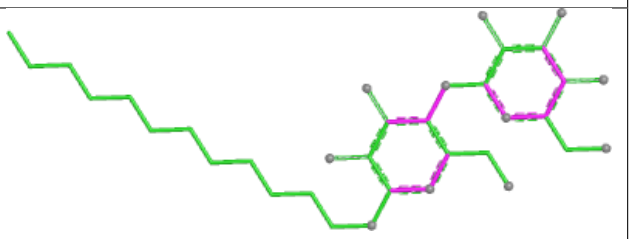
Torsions

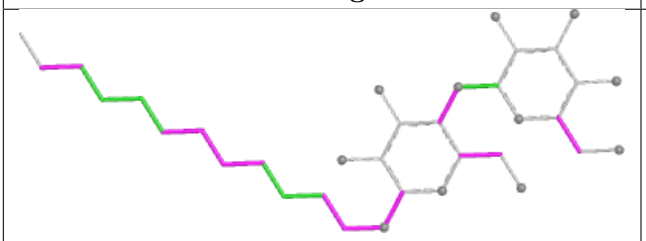


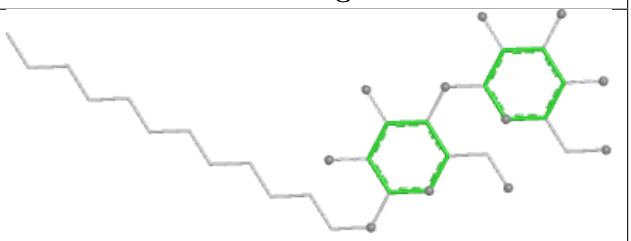
Rings

Ligand LMT C 521

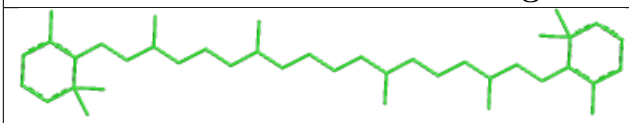

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR Y 302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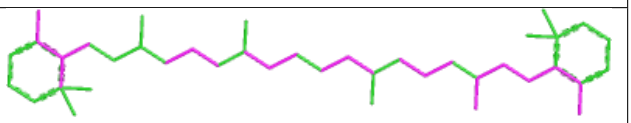
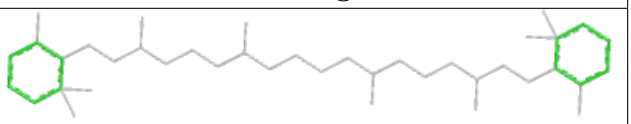
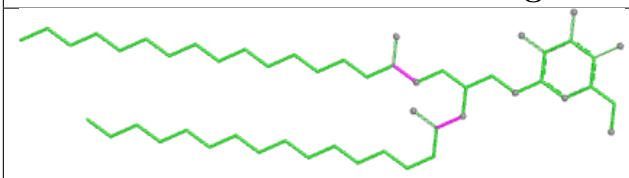

Bond angles

Torsions


Rings

Ligand LMG c 521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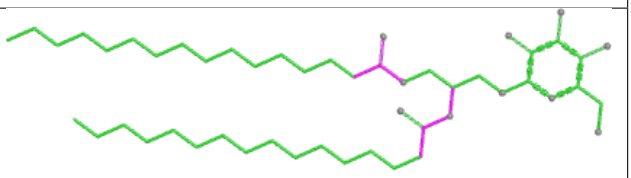
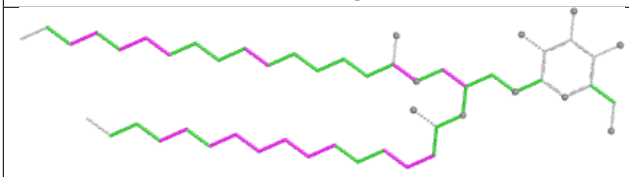
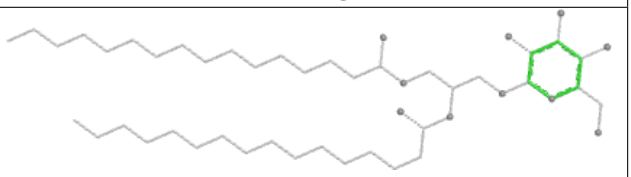
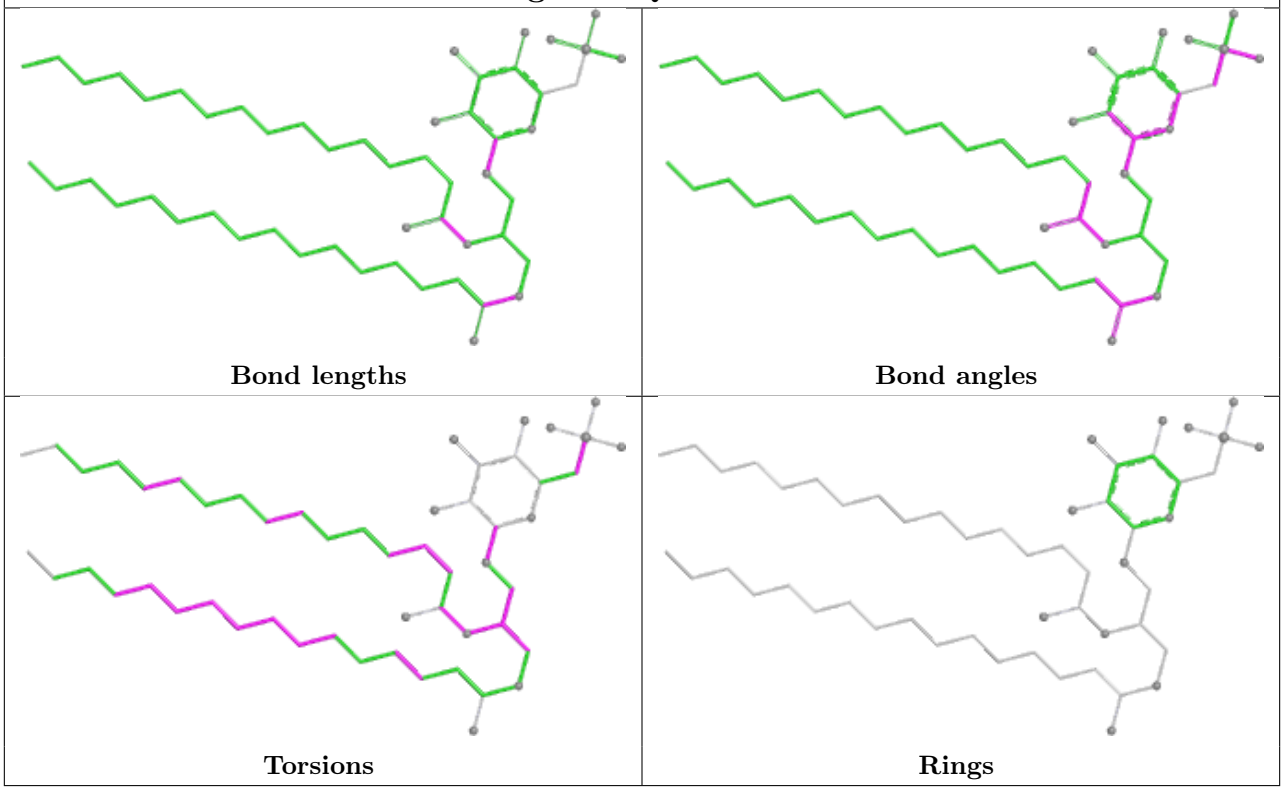

Bond angles

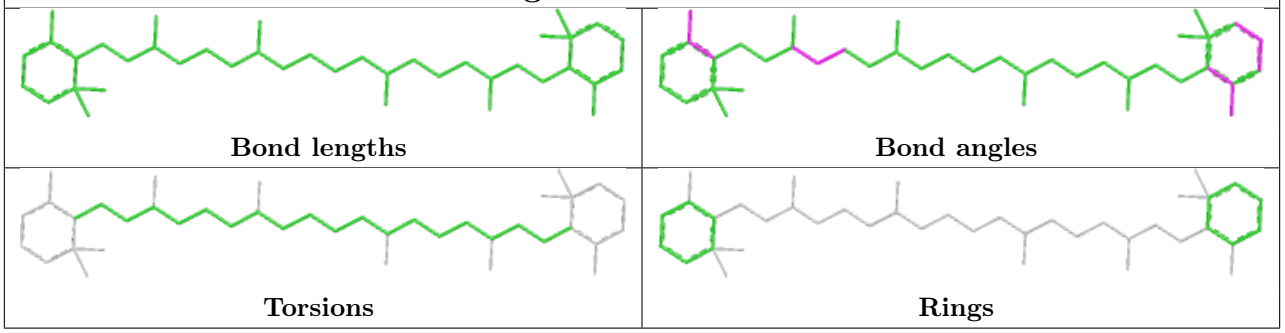

Torsions


Rings

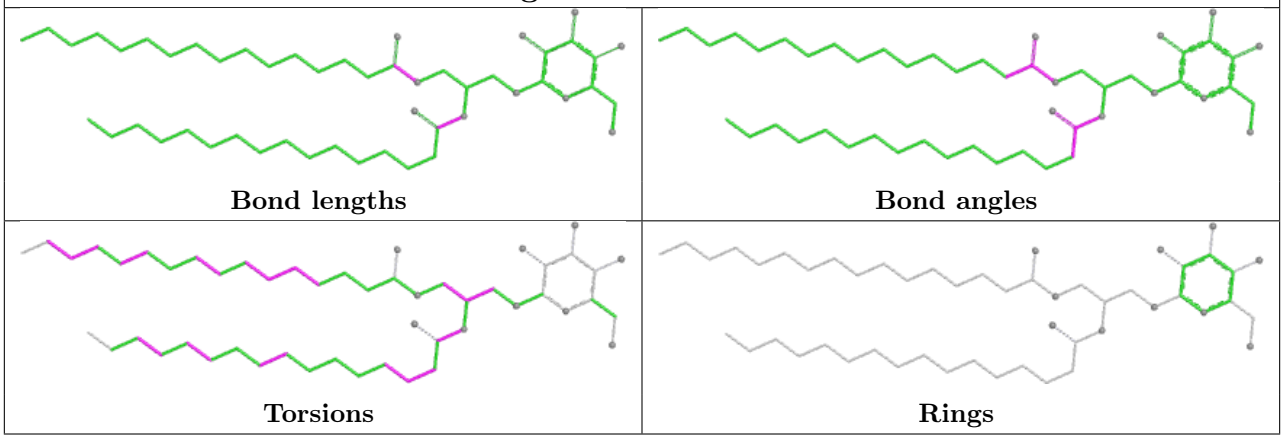
Ligand SQD L 101



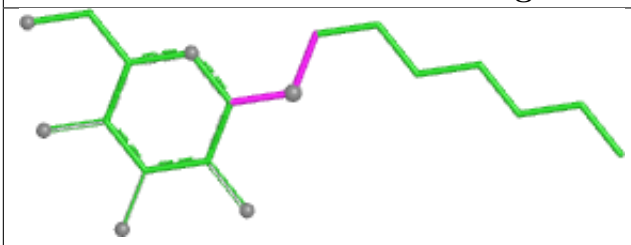
Ligand BCR B 619



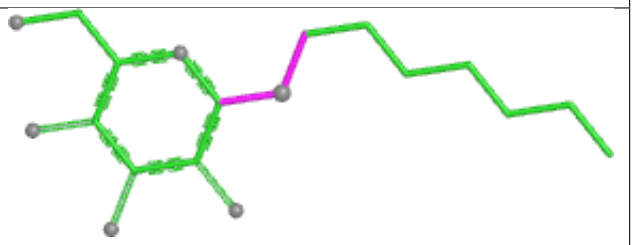
Ligand LMG C 520



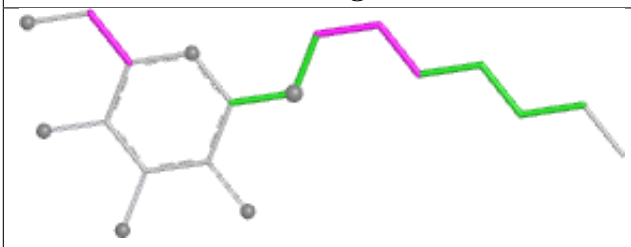
Ligand HTG h 1202



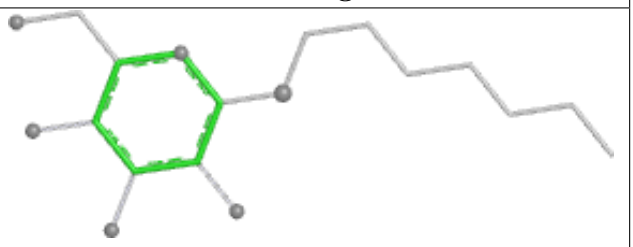
Bond lengths



Bond angles

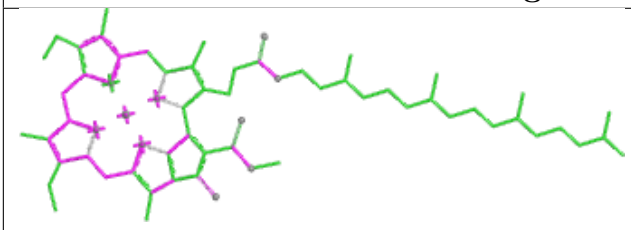


Torsions



Rings

Ligand CLA A 405



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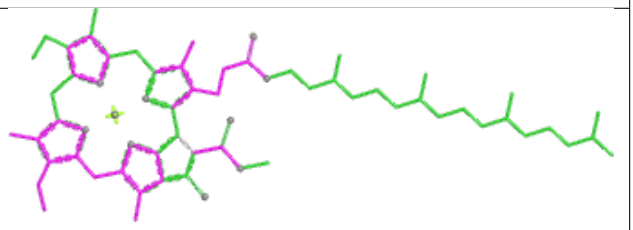
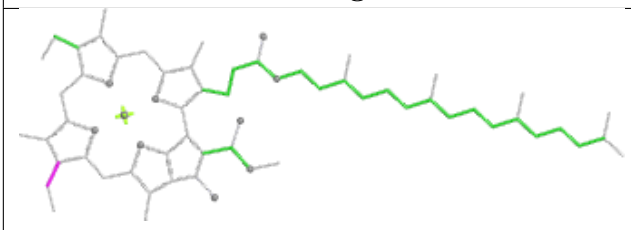
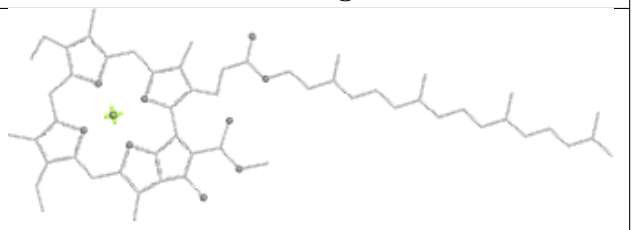


Bond angles

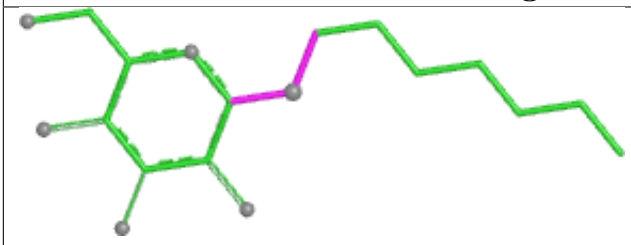


Torsions



Rings

Ligand HTG C 522



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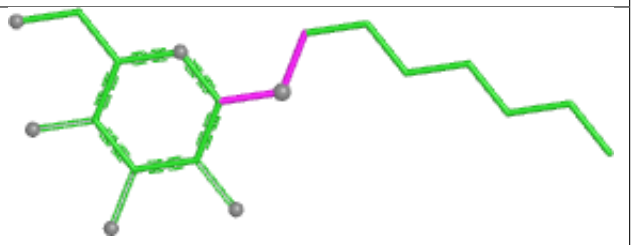
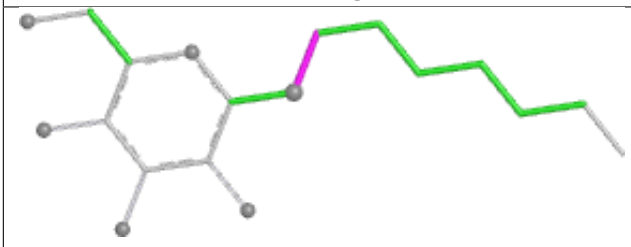
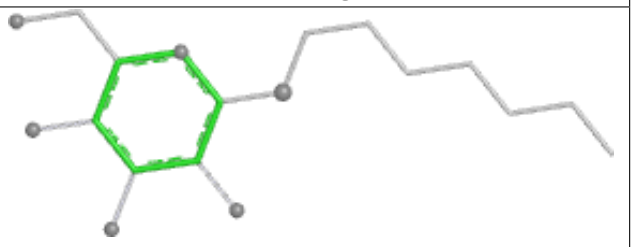


Bond angles

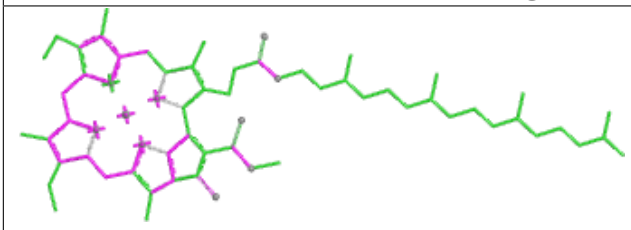


Torsions



Rings

Ligand CLA D 403



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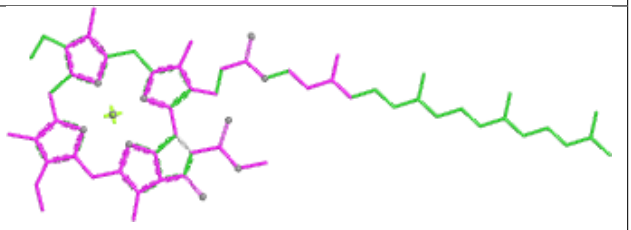
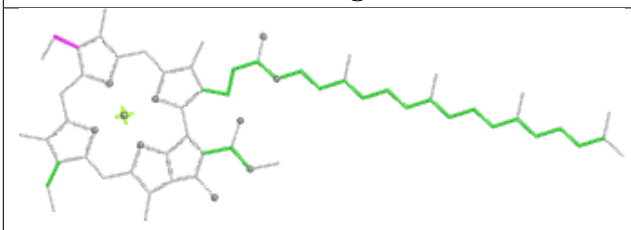
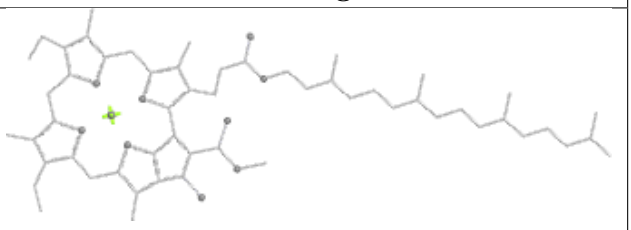


Bond angles

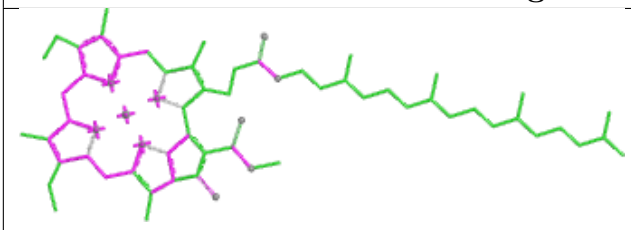


Torsions



Rings

Ligand CLA b 611



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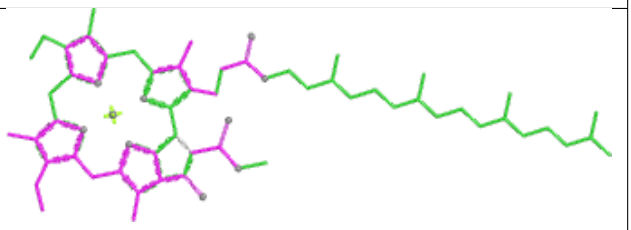
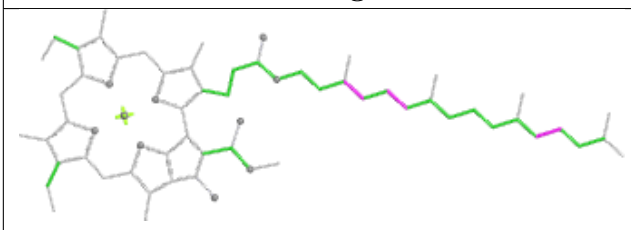
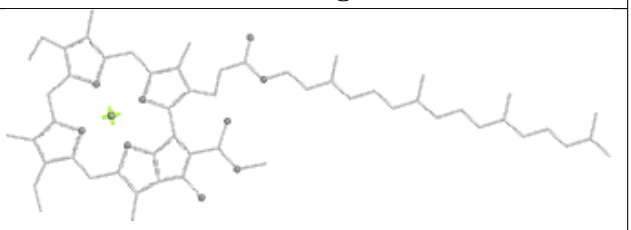


Bond angles

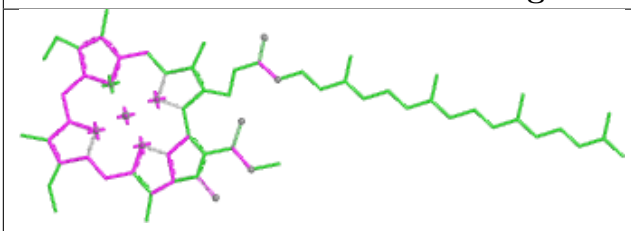


Torsions



Rings

Ligand CLA b 605



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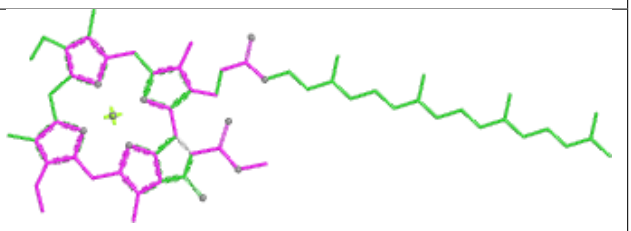
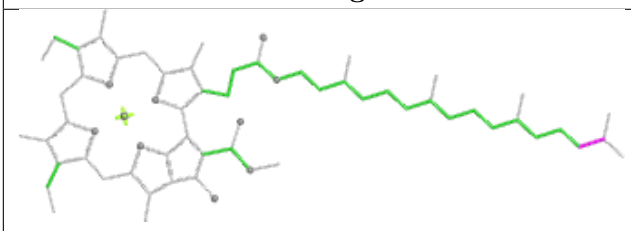
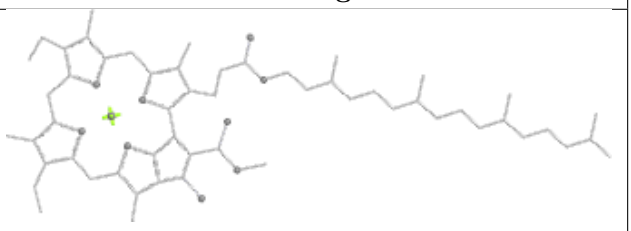


Bond angles

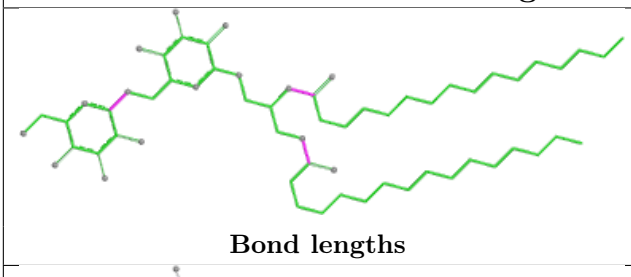


Torsions

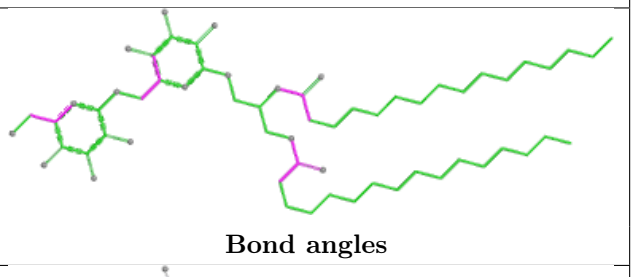


Rings

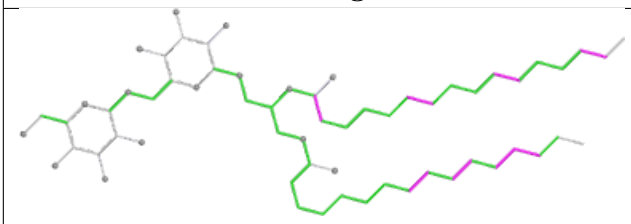
Ligand DGD H 102



Bond lengths



Bond angles



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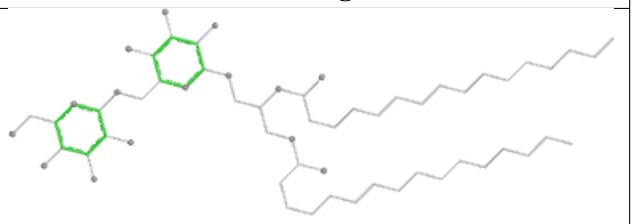
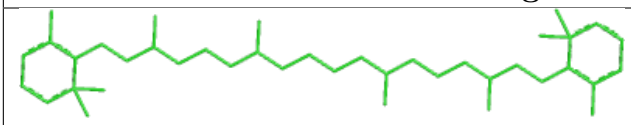
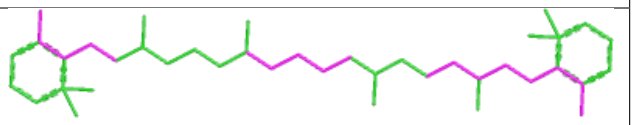


Rings

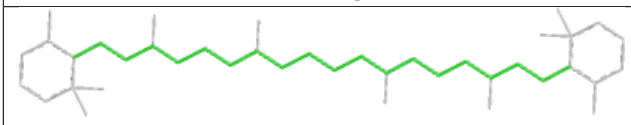
Ligand BCR A 410



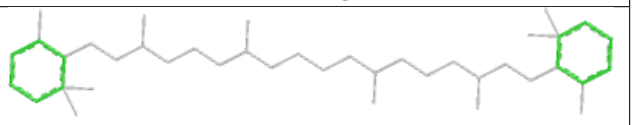
Bond lengths



Bond angles

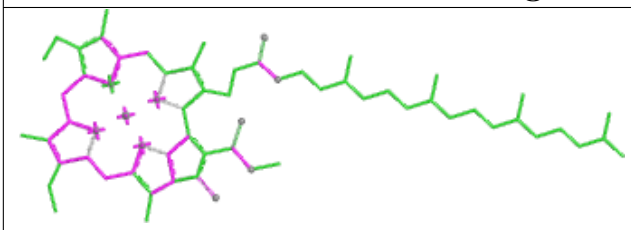


Torsions

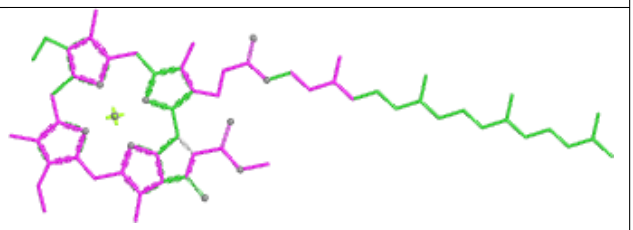


Rings

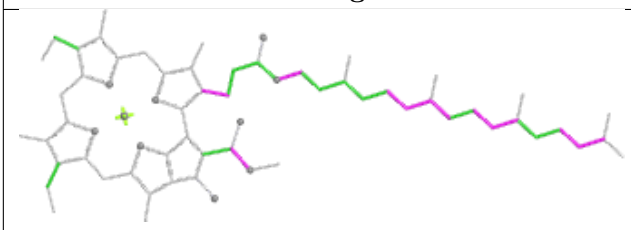
Ligand CLA C 507



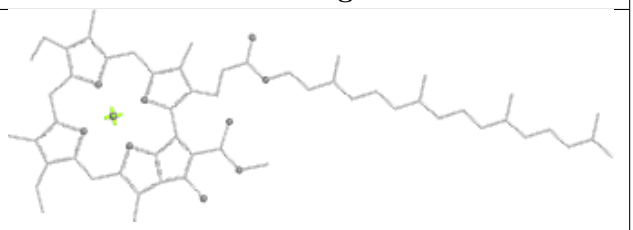
Bond lengths



Bond angles

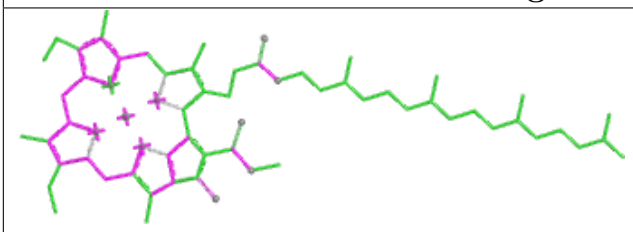


Torsions



Rings

Ligand CLA b 607



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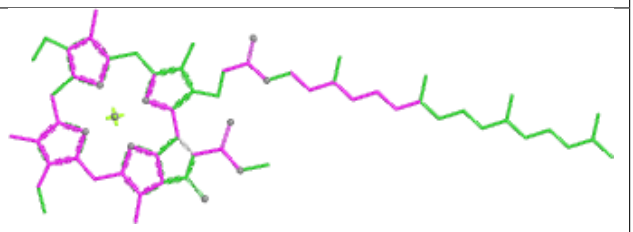
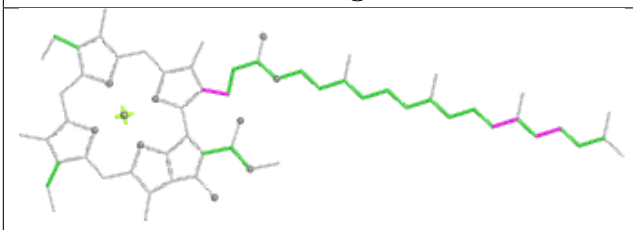


Bond angles



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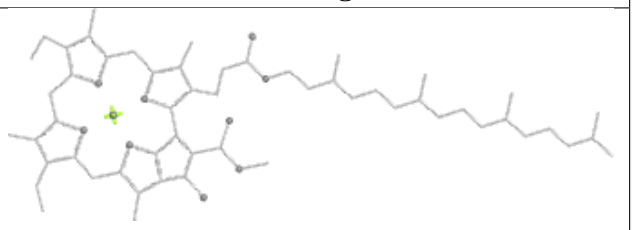
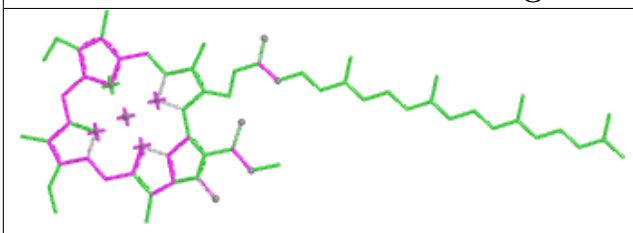
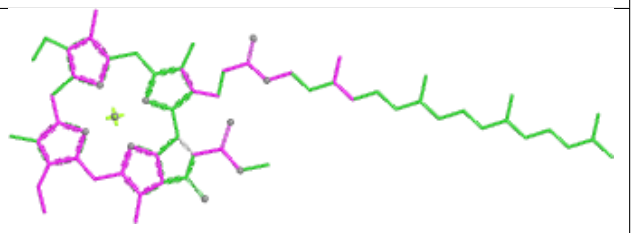


Rings

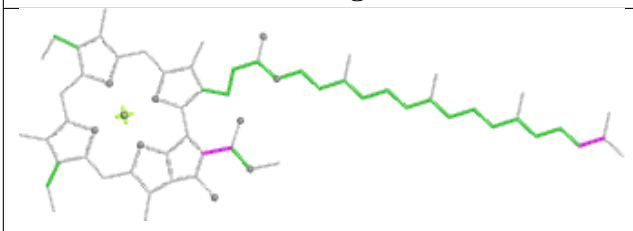
Ligand CLA B 608



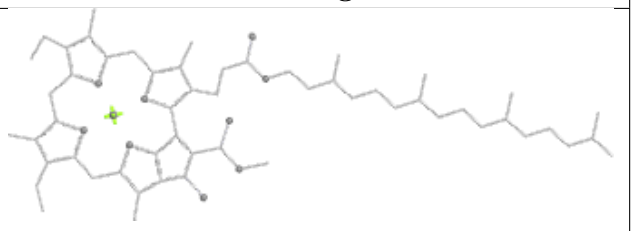
Bond lengths



Bond angles

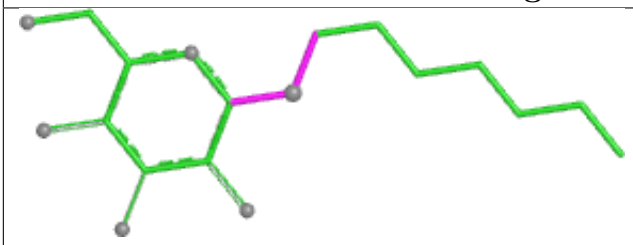


Torsions



Rings

Ligand HTG b 602



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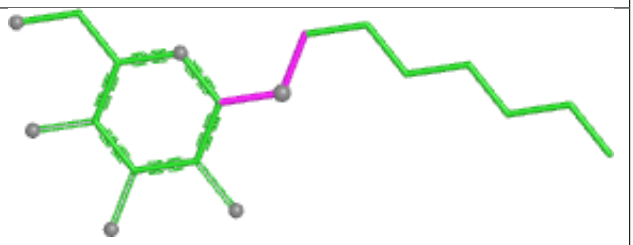
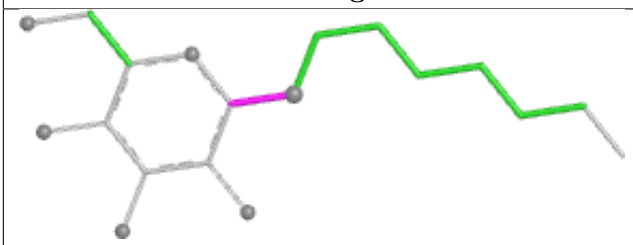
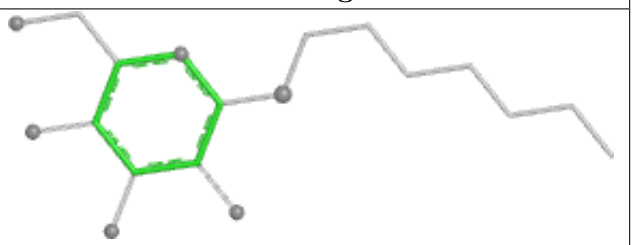


Bond angles

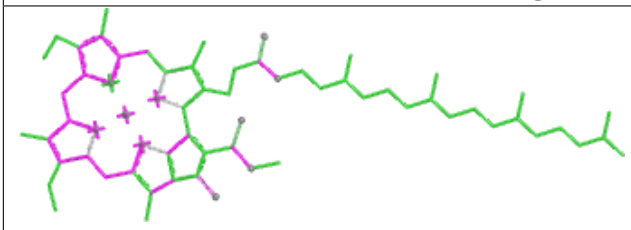


Torsions



Rings

Ligand CLA c 505



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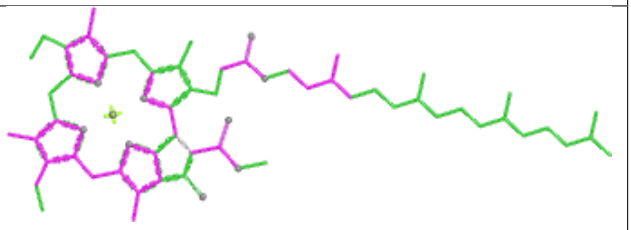
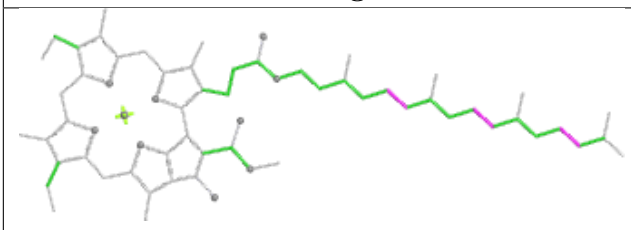


Bond angles



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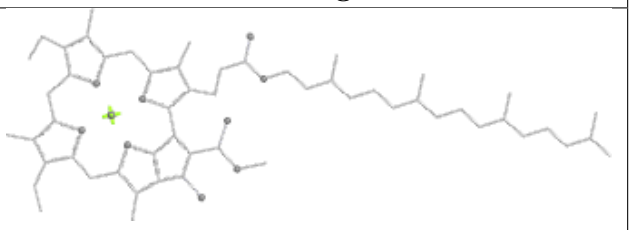
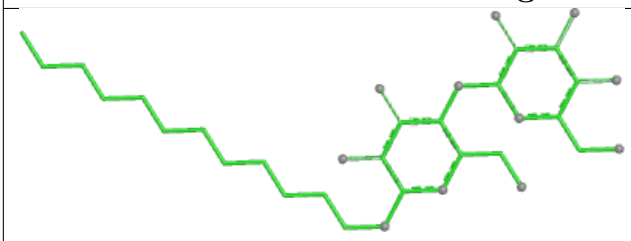
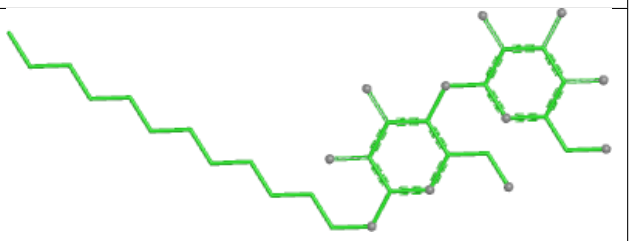


Rings

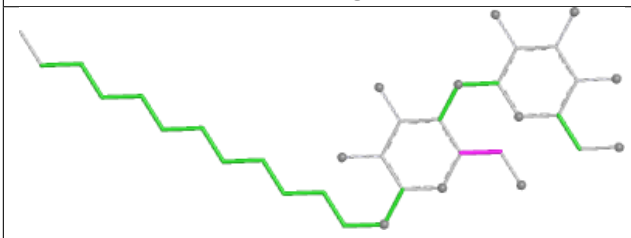
Ligand LMT M 101



Bond lengths



Bond angles



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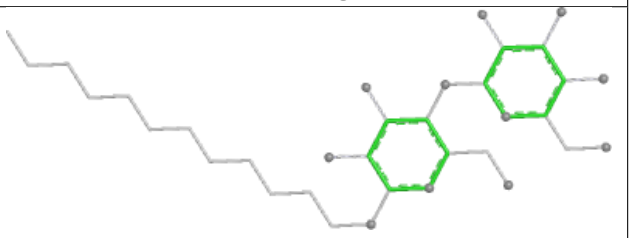
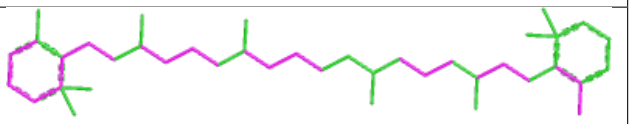


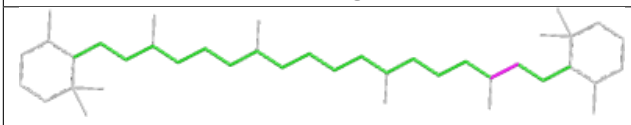
Rings

Ligand BCR b 622

Bond lengths



Bond angles



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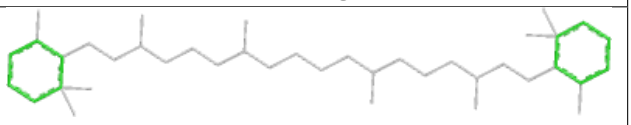
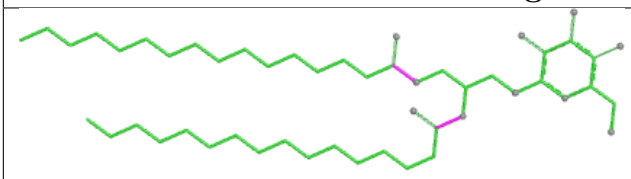
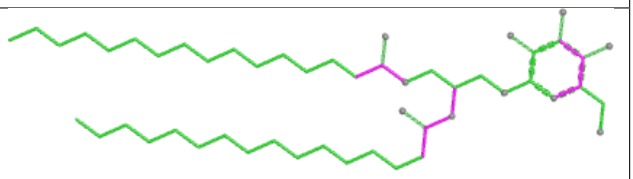


Rings

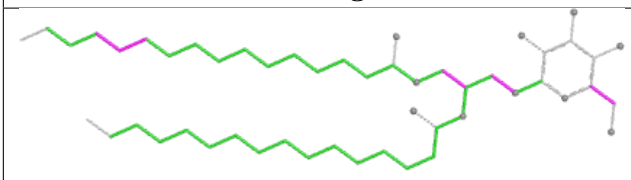
Ligand LMG c 522



Bond lengths



Bond angles



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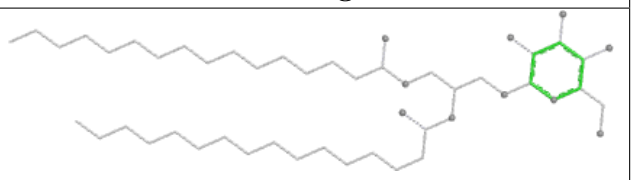
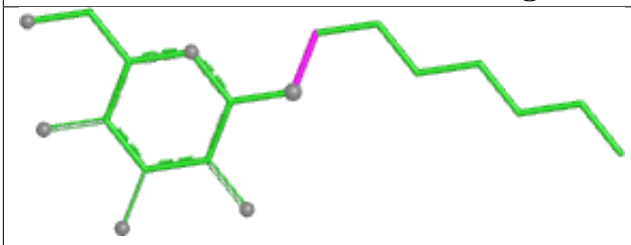


Rings

Ligand HTG B 625



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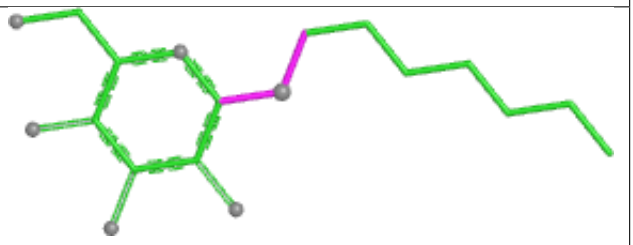
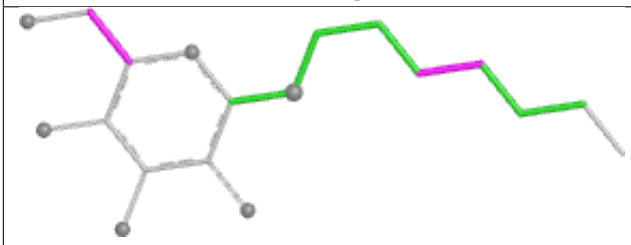


Bond angles



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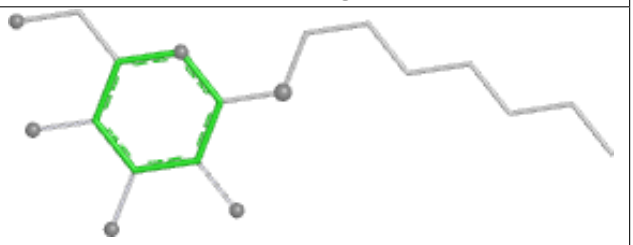
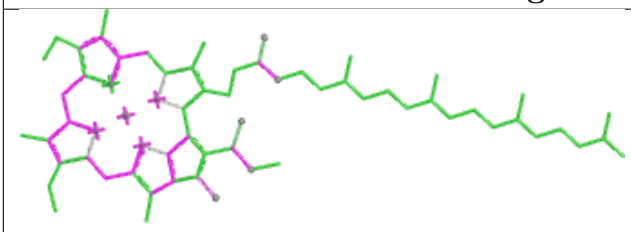


Rings

Ligand CLA d 404



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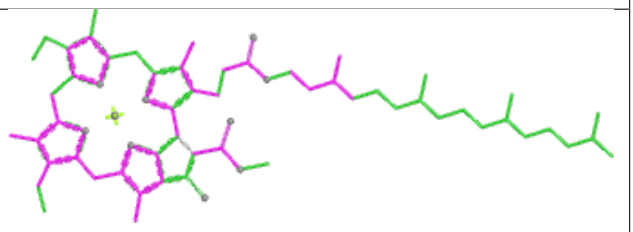
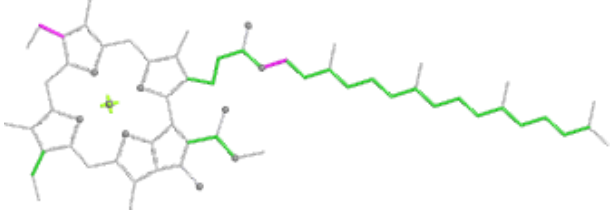


Bond angles



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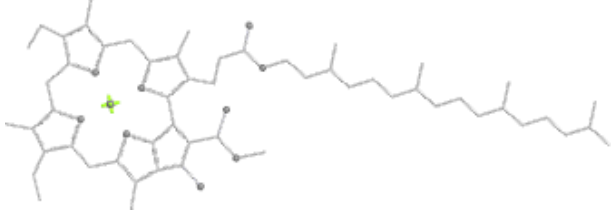
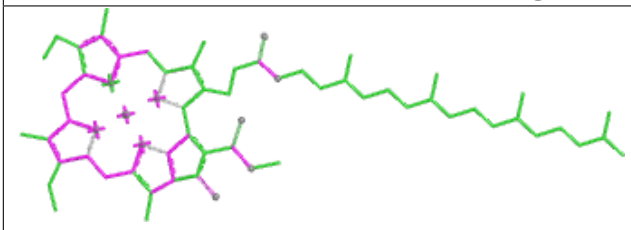


Rings

Ligand CLA c 503



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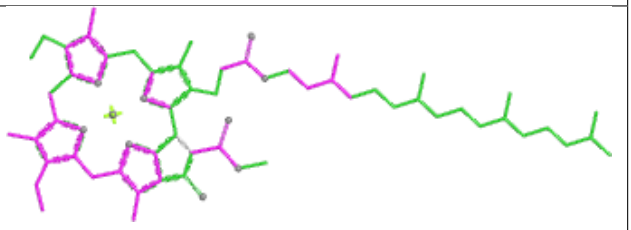
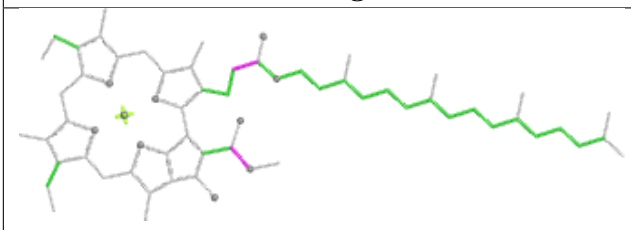
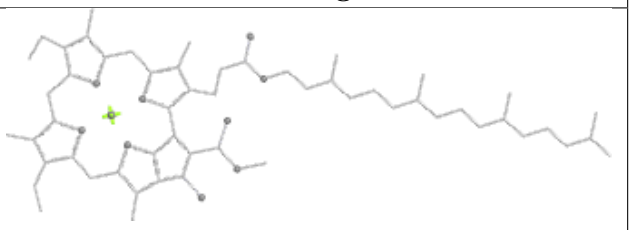


Bond angles

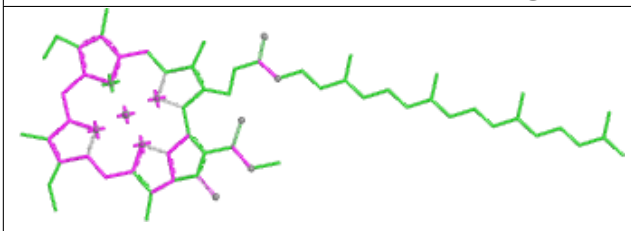


Torsions



Rings

Ligand CLA B 606



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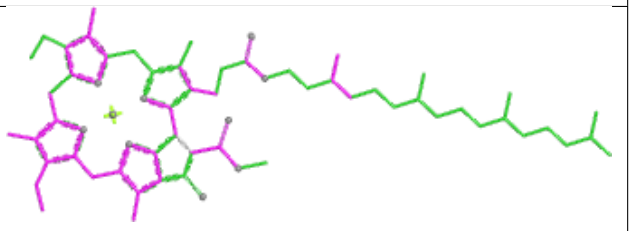
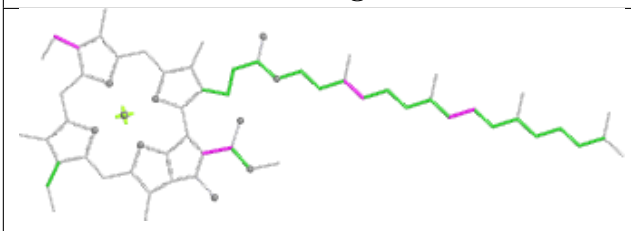
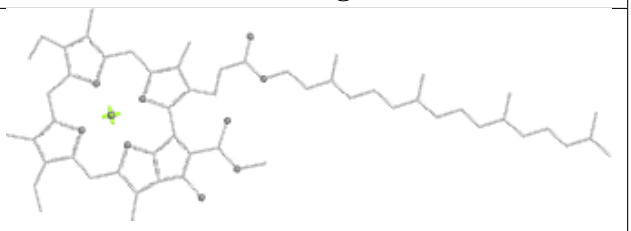


Bond angles

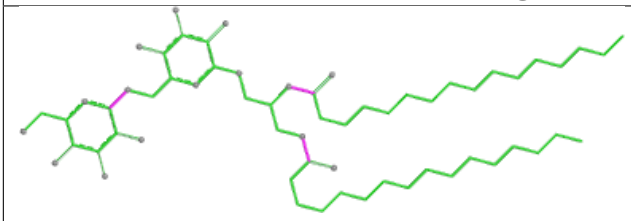


Torsions

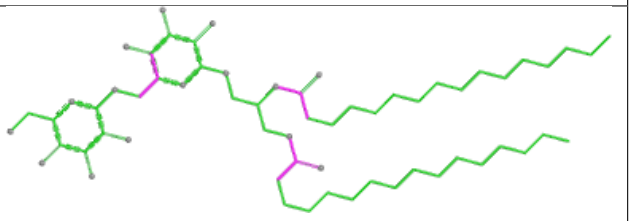


Rings

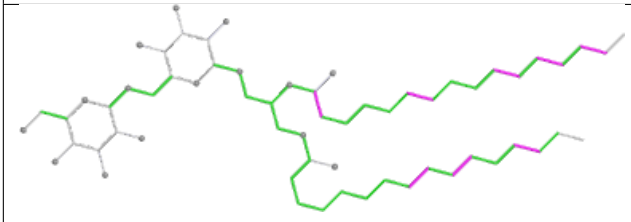
Ligand DGD h 1205



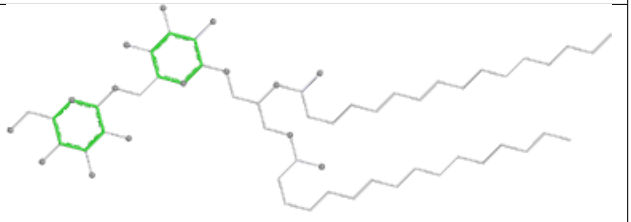
Bond lengths



Bond angles

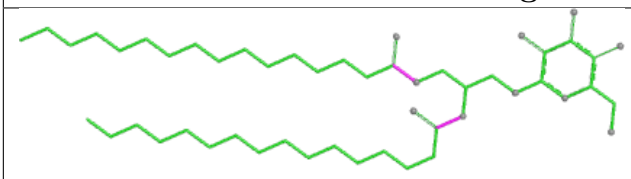


Torsions

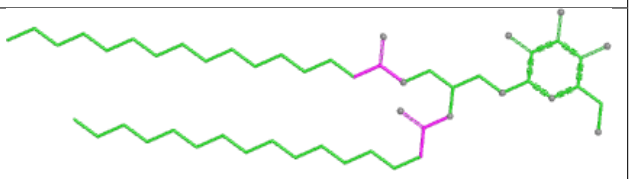


Rings

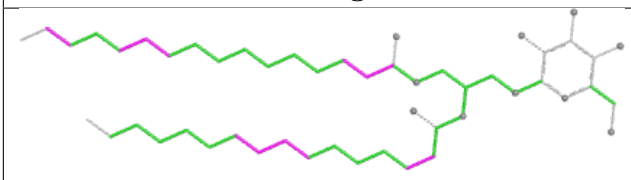
Ligand LMG B 621



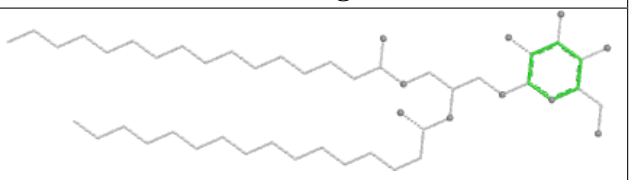
Bond lengths



Bond angles

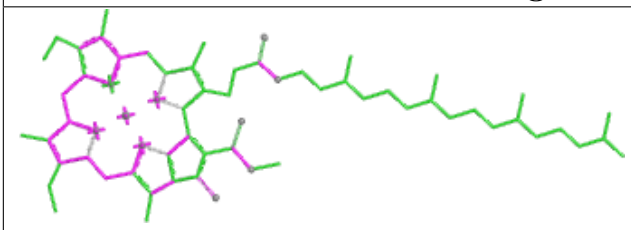


Torsions



Rings

Ligand CLA b 615



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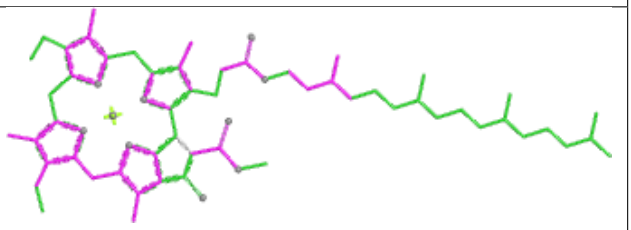
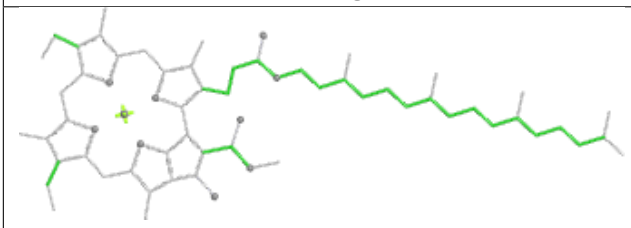


Bond angles



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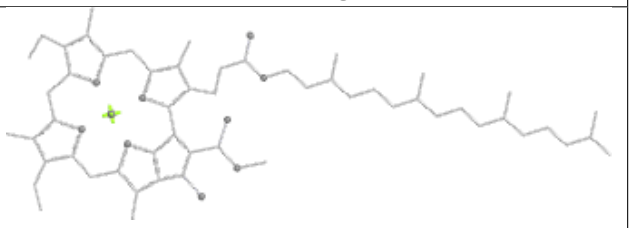
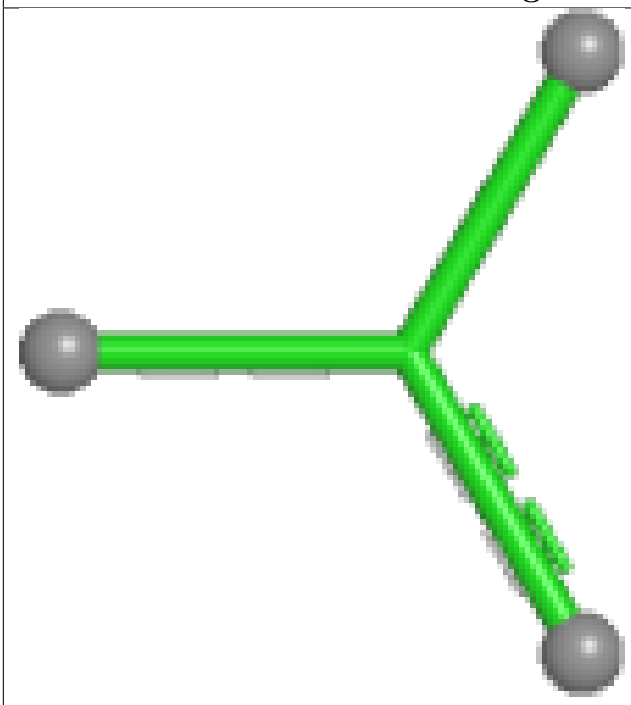


Rings

Ligand BCT A 423



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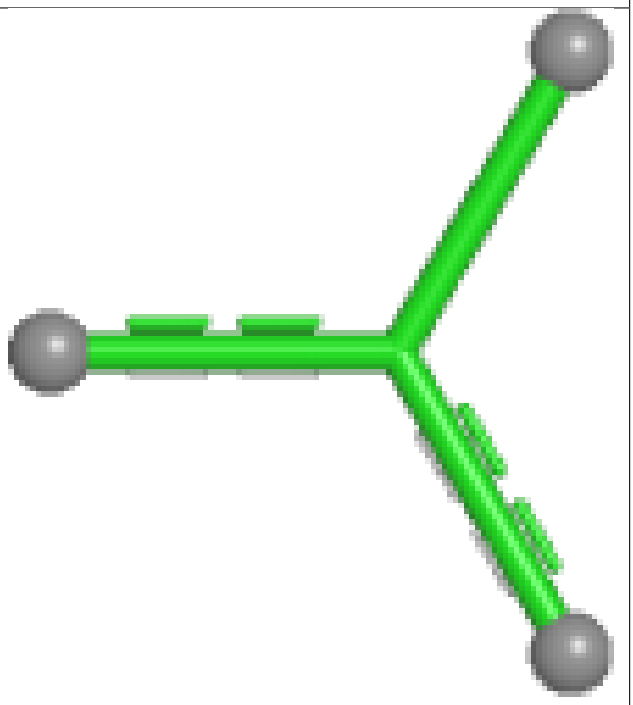
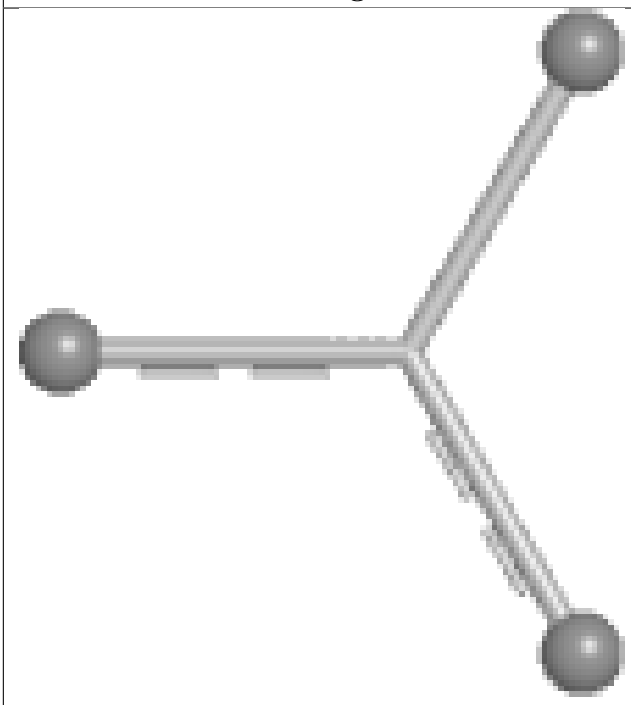


Bond angles



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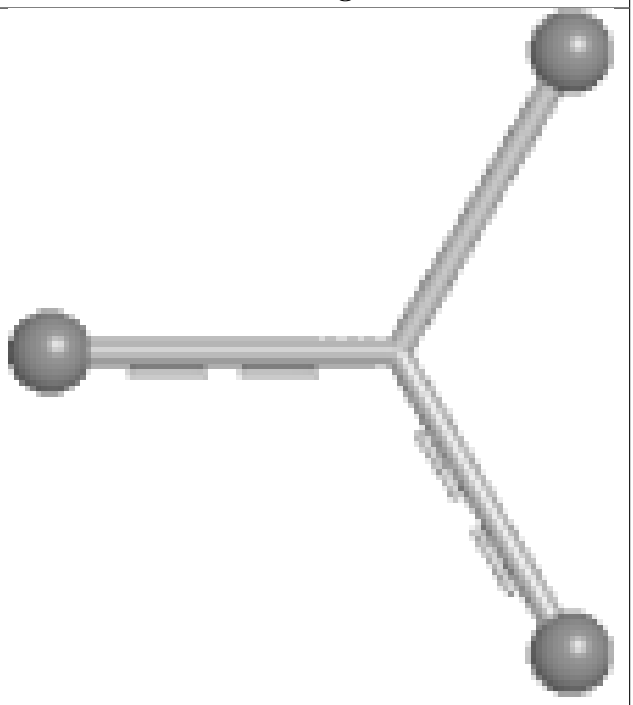
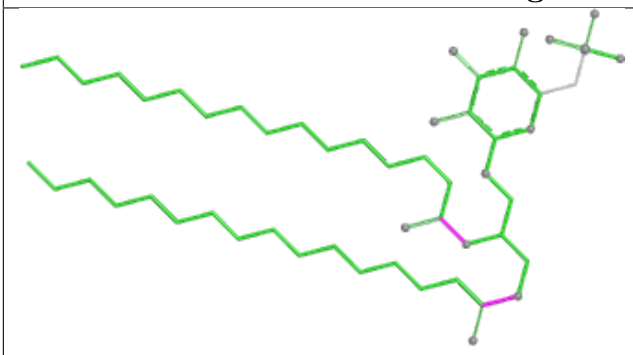


Rings

Ligand SQD L 102



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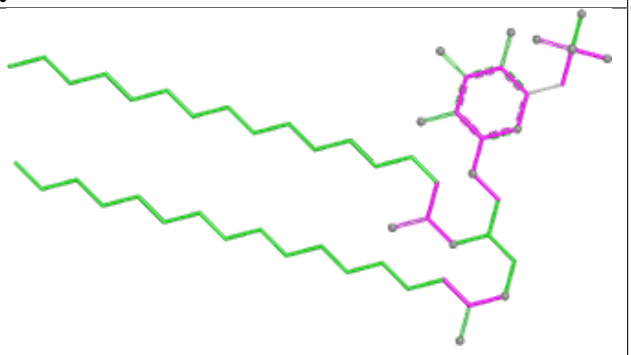
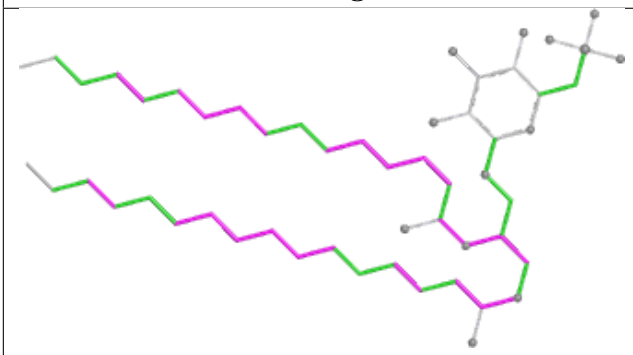


Bond angles



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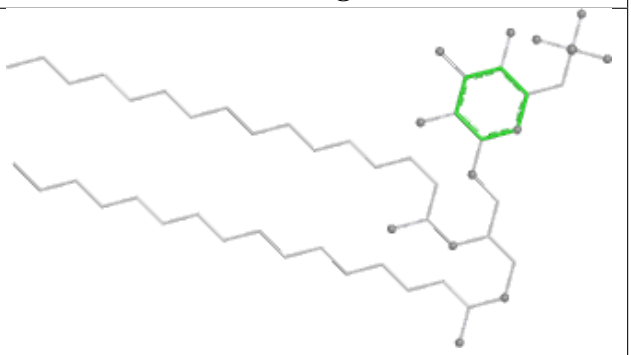
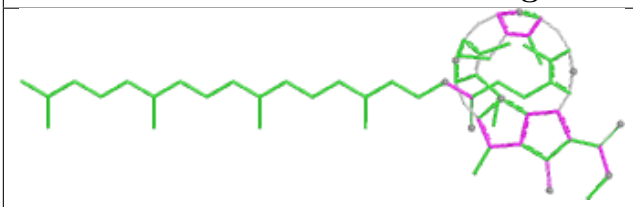


Rings

Ligand PHO D 401



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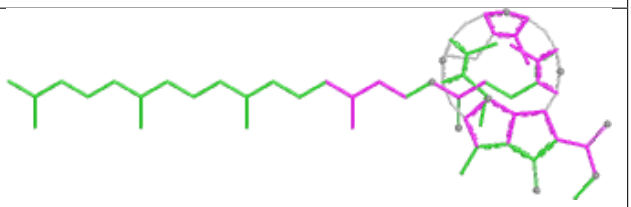
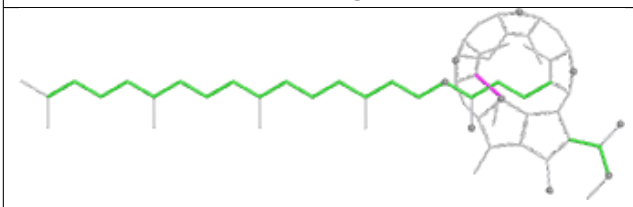


Bond angles



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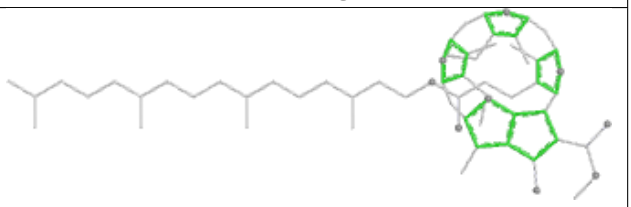
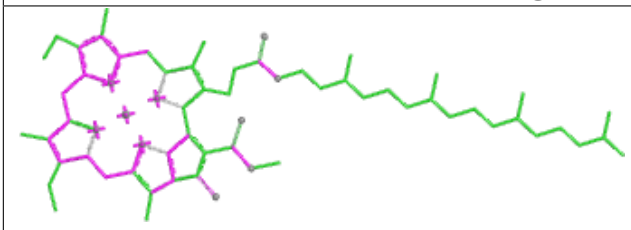


Rings

Ligand CLA c 514



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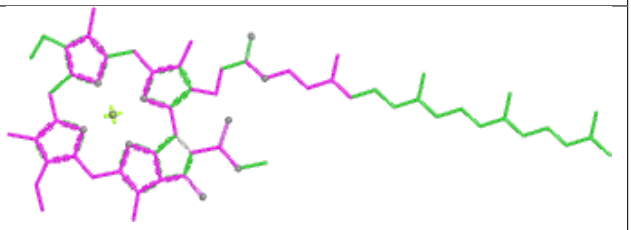
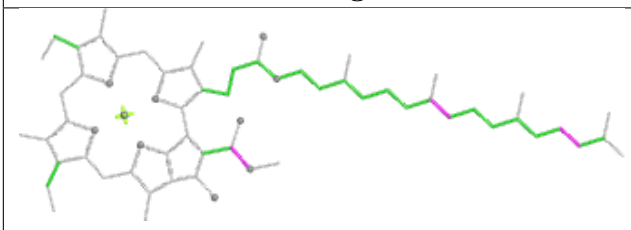


Bond angles



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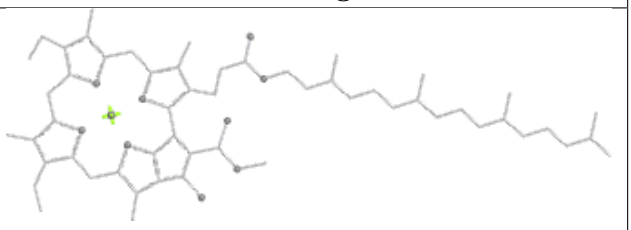
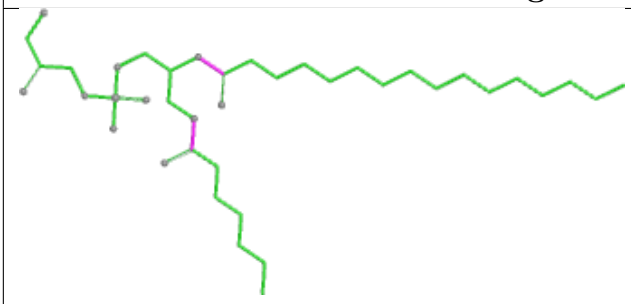


Rings

Ligand LHG e 101



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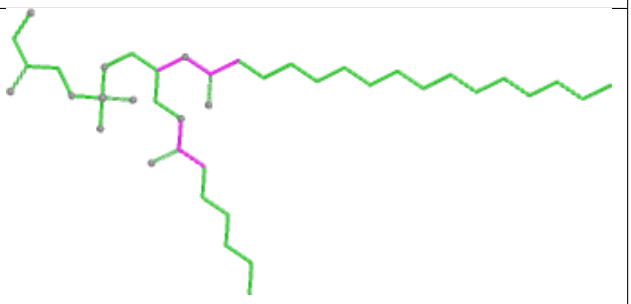
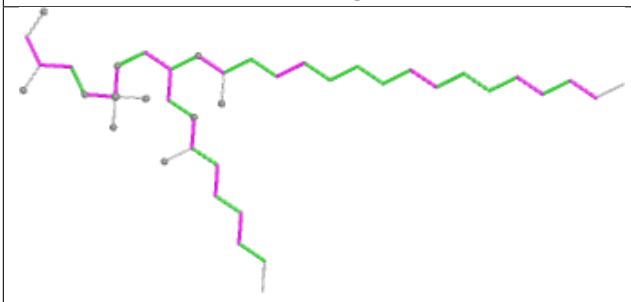


Bond angles



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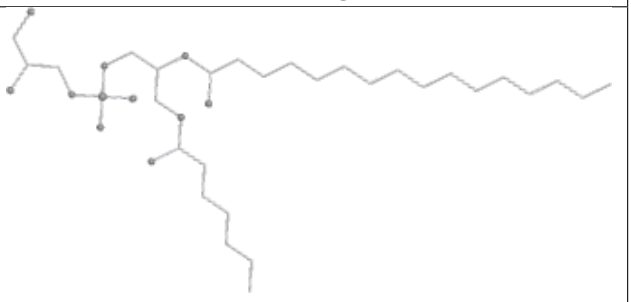
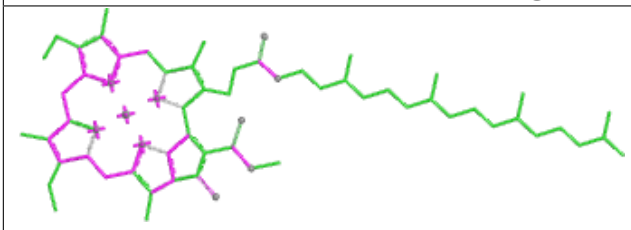


Rings

Ligand CLA a 410



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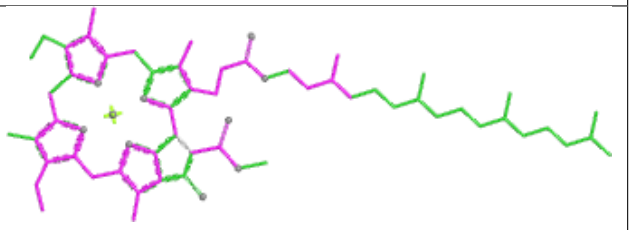
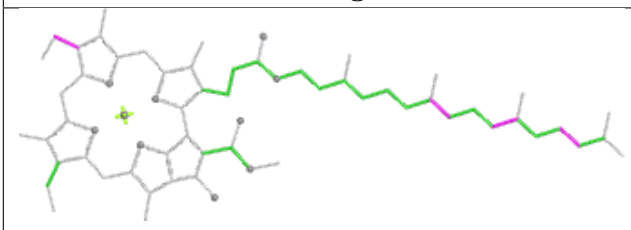


Bond angles



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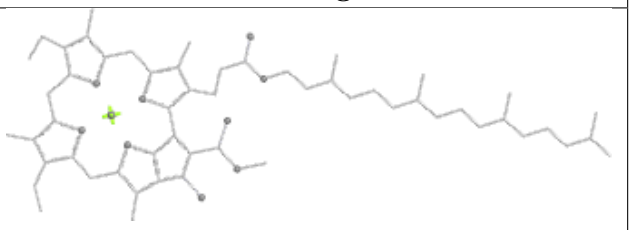
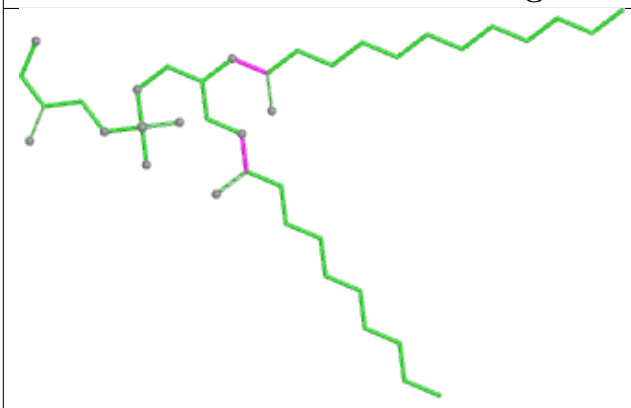


Rings

Ligand LHG d 410



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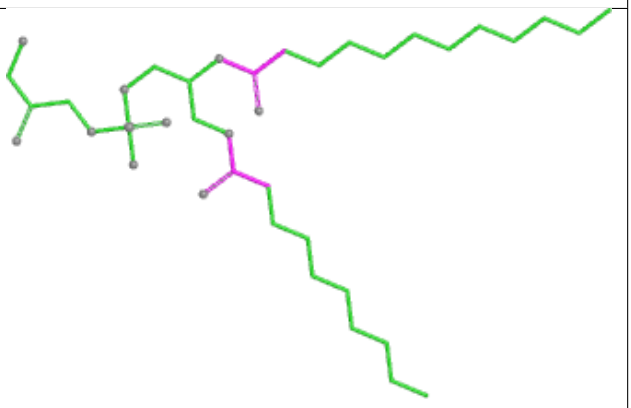
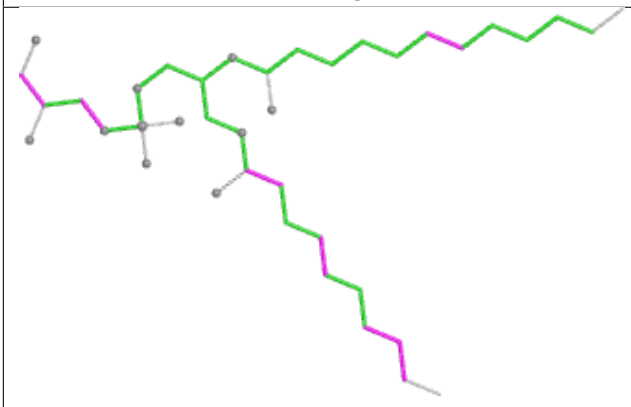
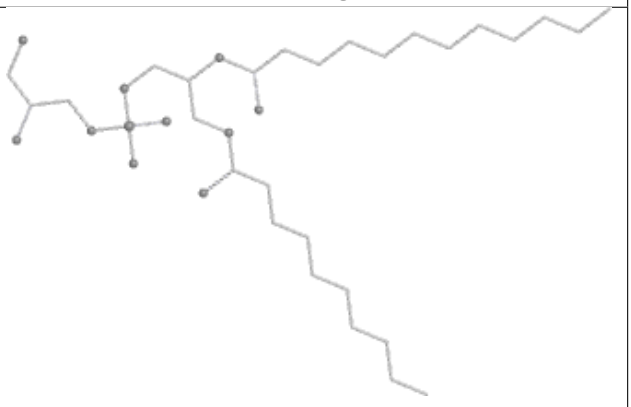


Bond angles

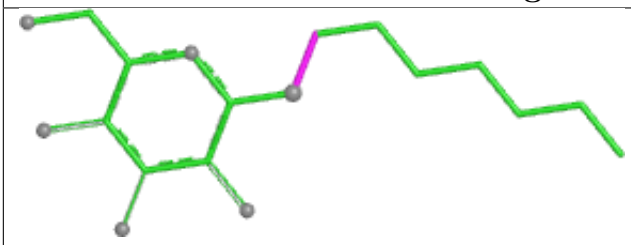


Torsions



Rings

Ligand HTG d 414



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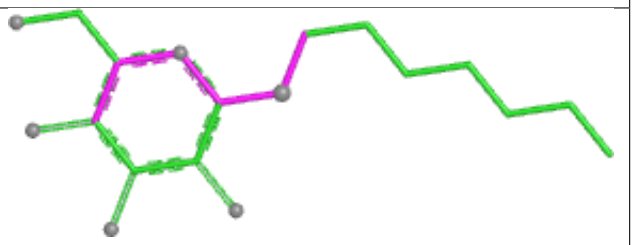

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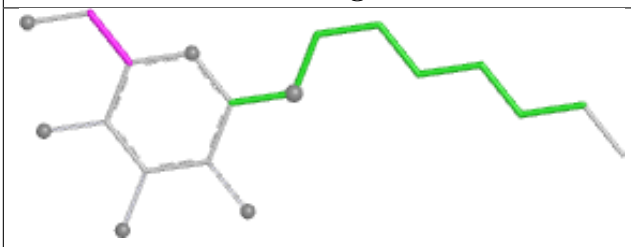

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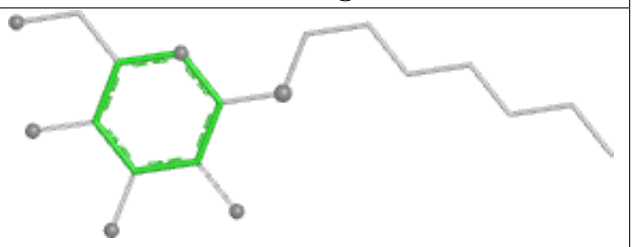
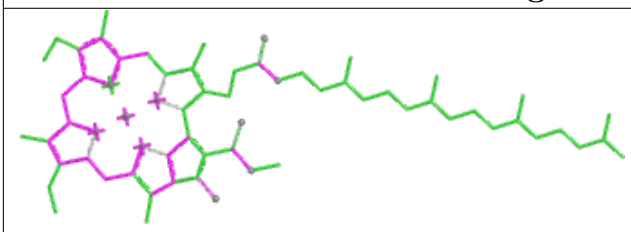


Rings

Ligand CLA b 617



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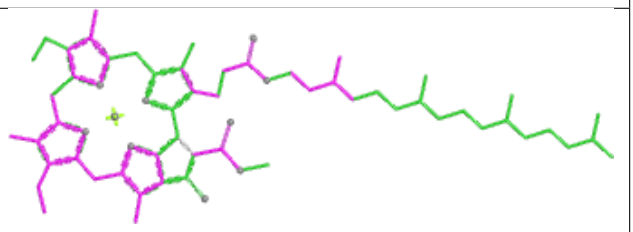
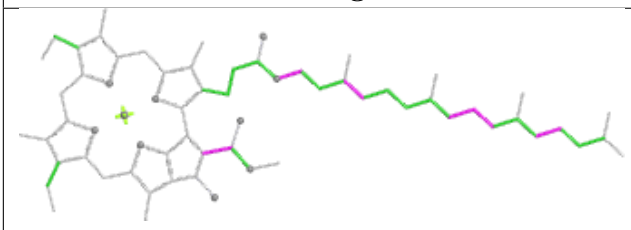


Bond angles



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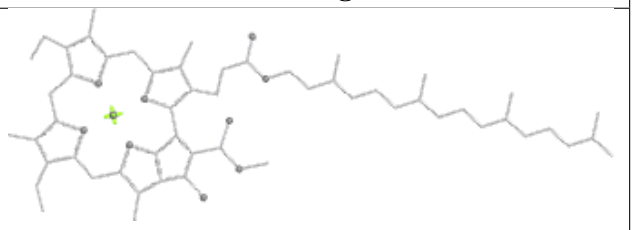
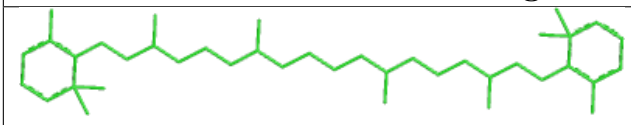


Rings

Ligand BCR B 618



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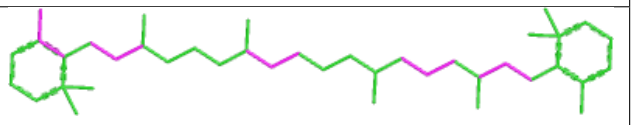
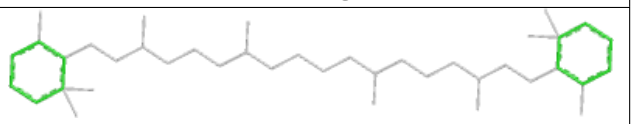


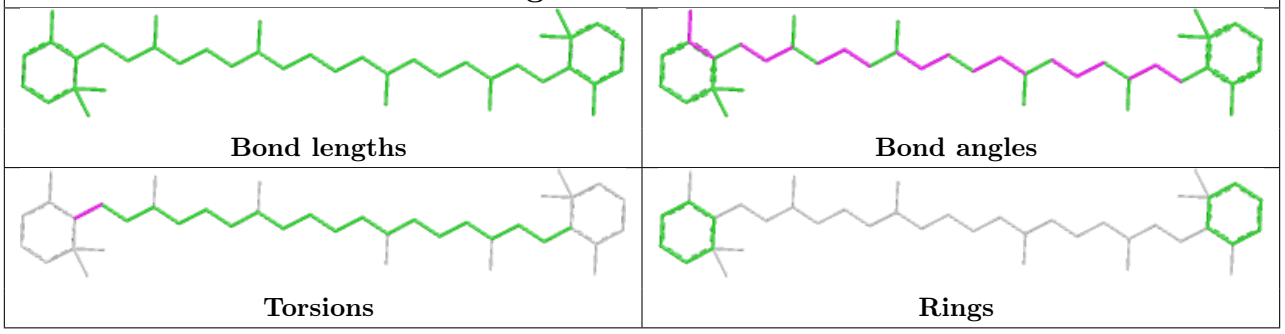
Bond angles

Torsions

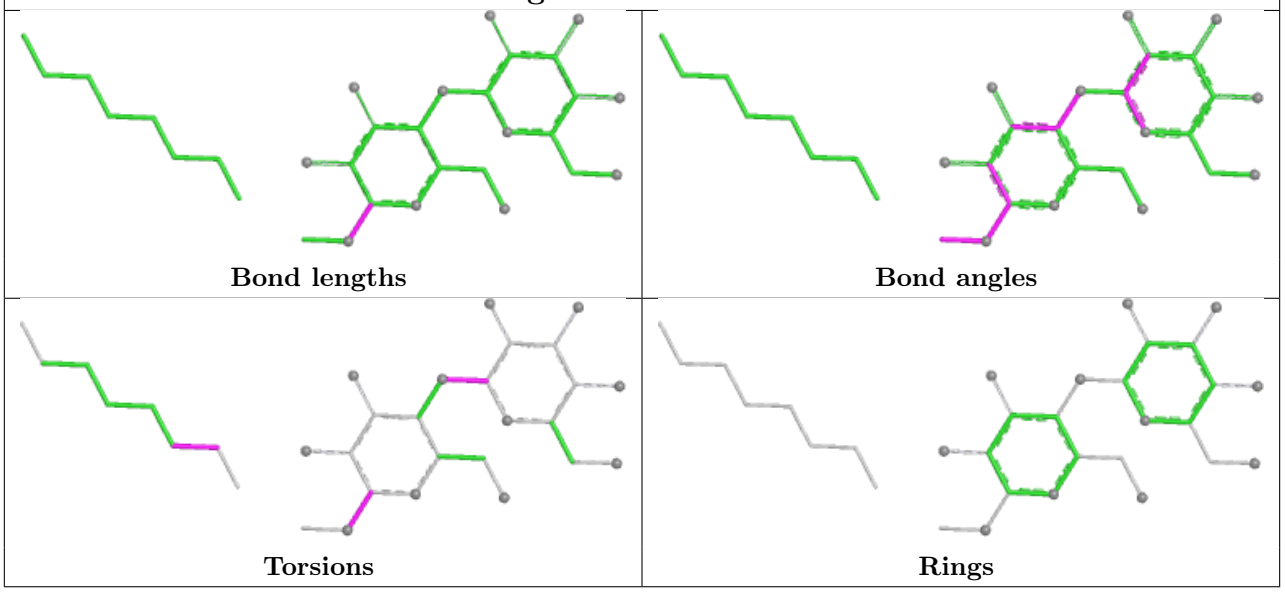


Rings

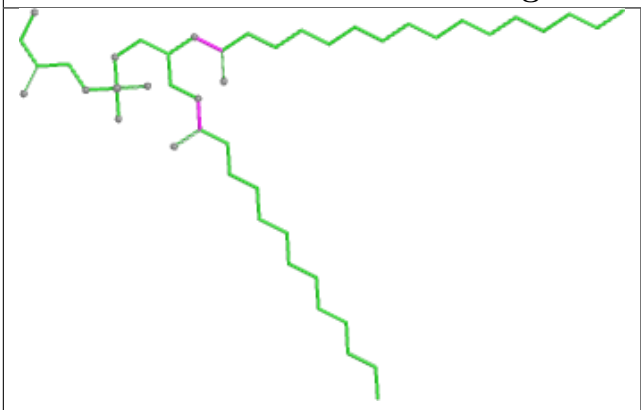
Ligand BCR b 620



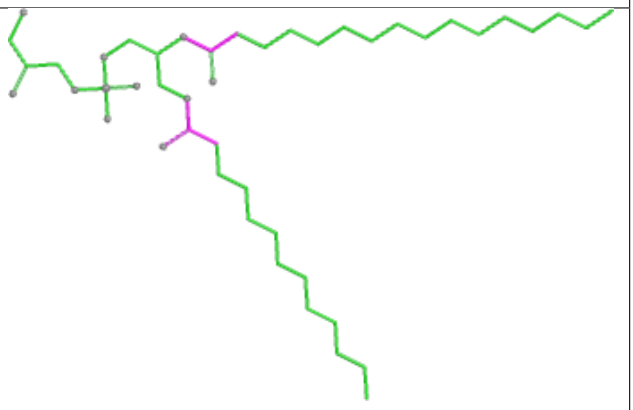
Ligand LMT z 101



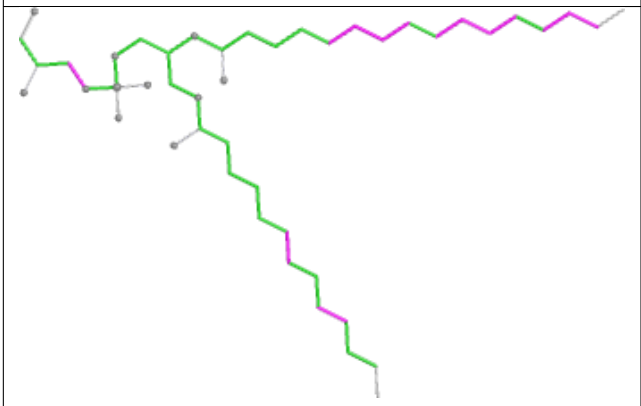
Ligand LHG D 411



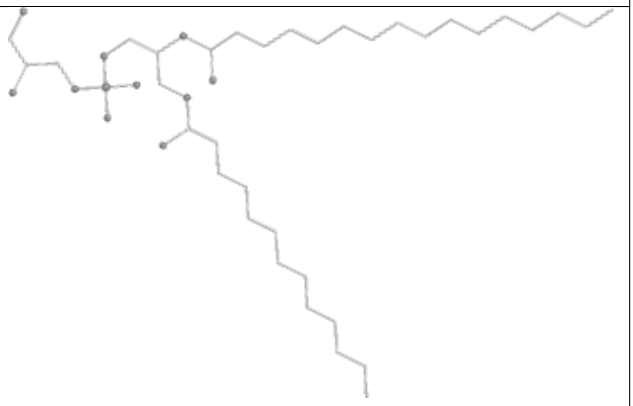
Bond lengths



Bond angles

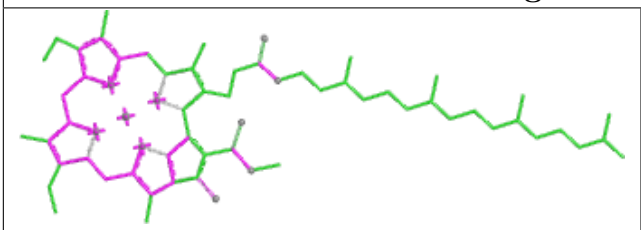


Torsions

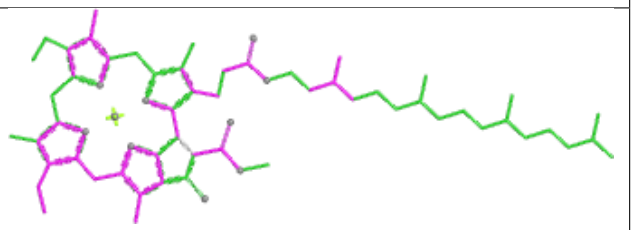


Rings

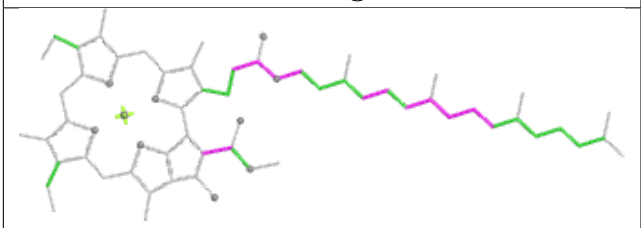
Ligand CLA B 602



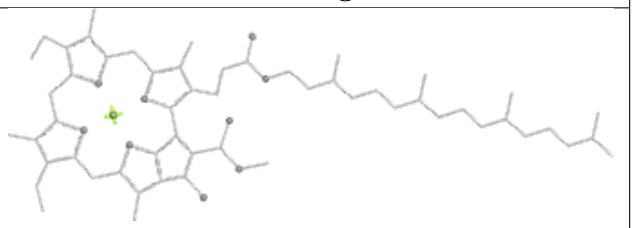
Bond lengths



Bond angles

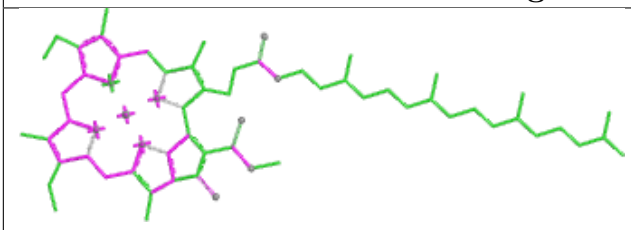


Torsions

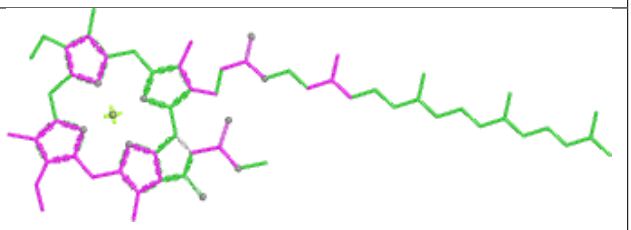


Rings

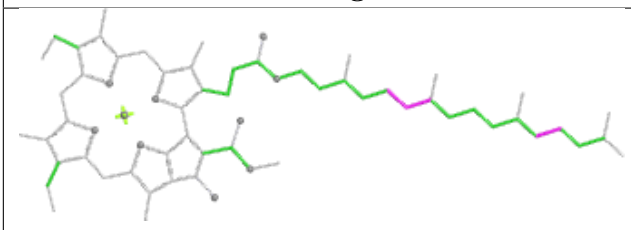
Ligand CLA b 606



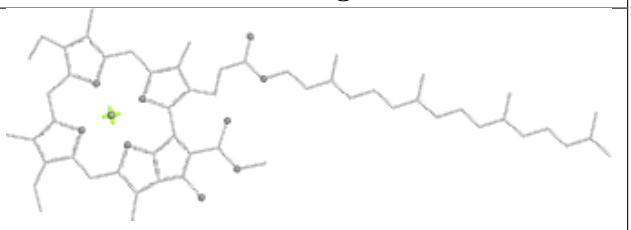
Bond lengths



Bond angles

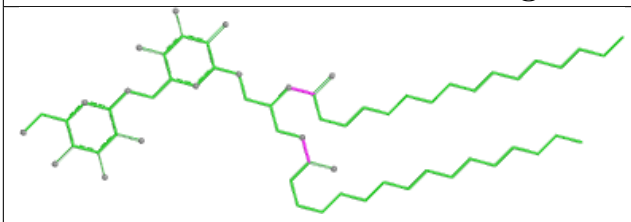


Torsions



Rings

Ligand DGD C 518



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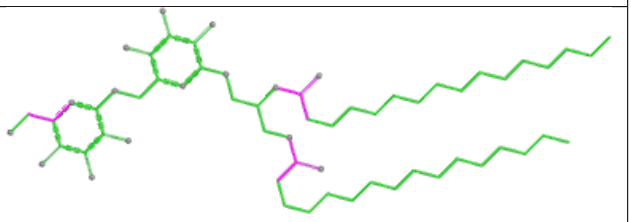
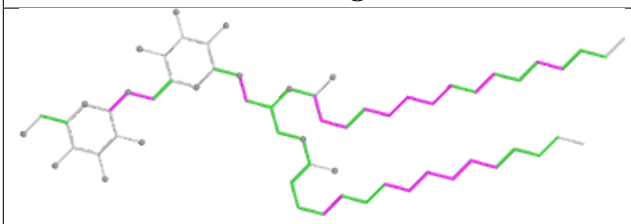
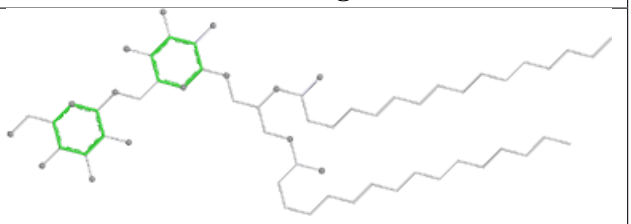


Bond angles

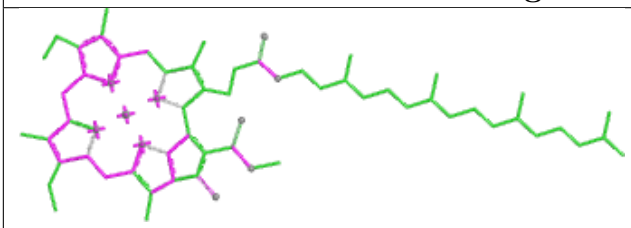


Torsions



Rings

Ligand CLA B 603



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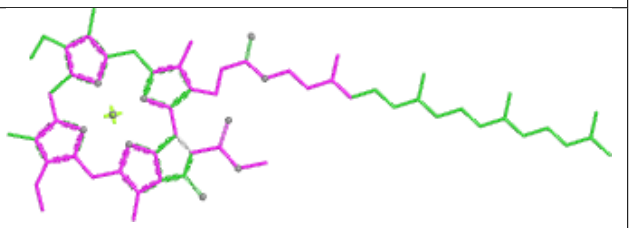
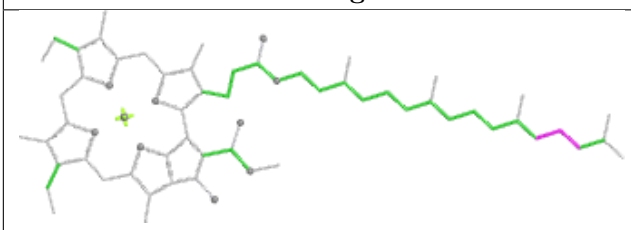


Bond angles



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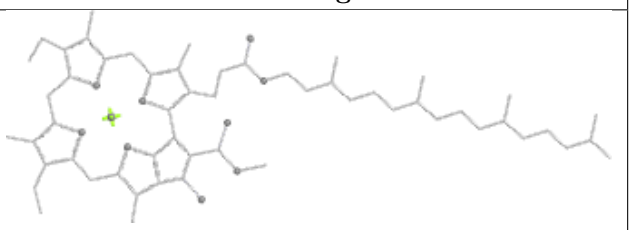
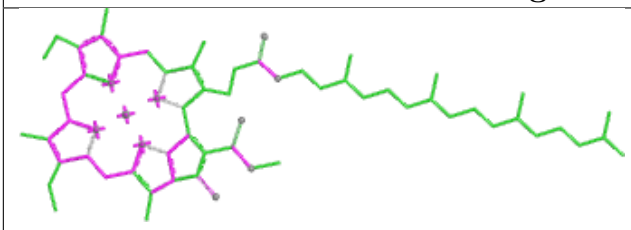
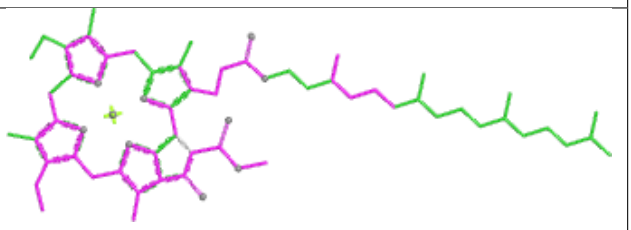


Rings

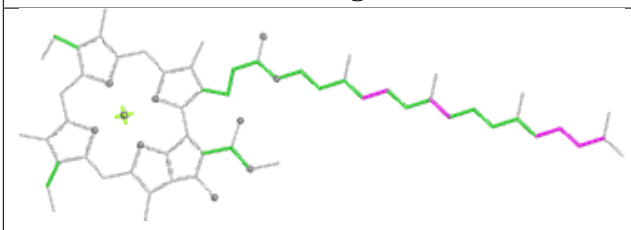
Ligand CLA c 508



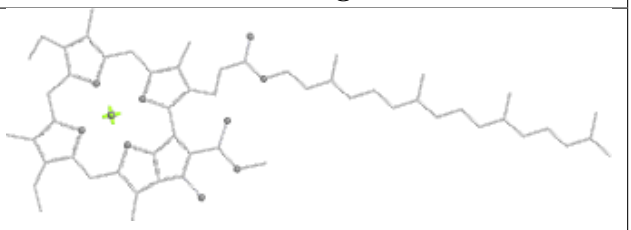
Bond lengths



Bond angles

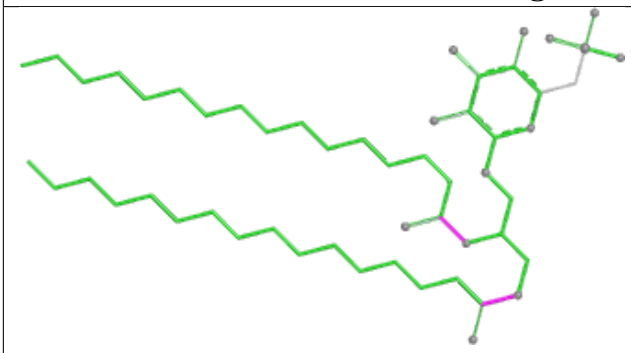


Torsions



Rings

Ligand SQD a 401



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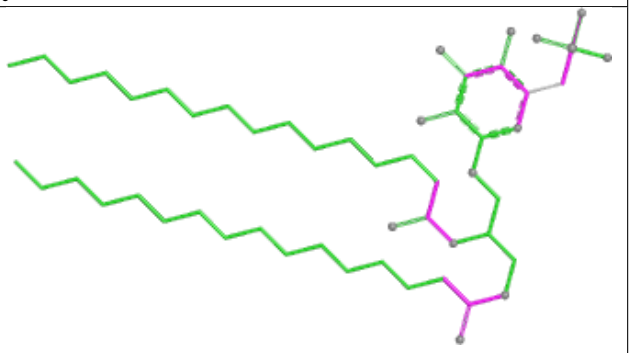
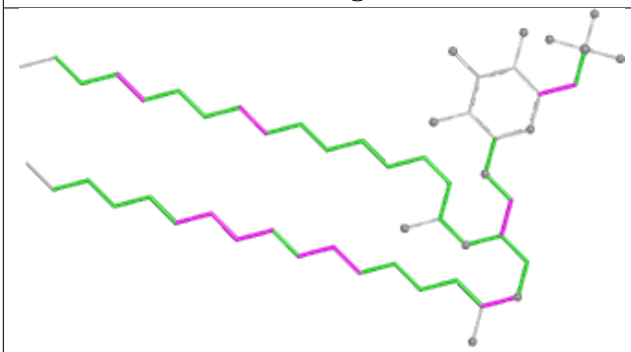


Bond angles



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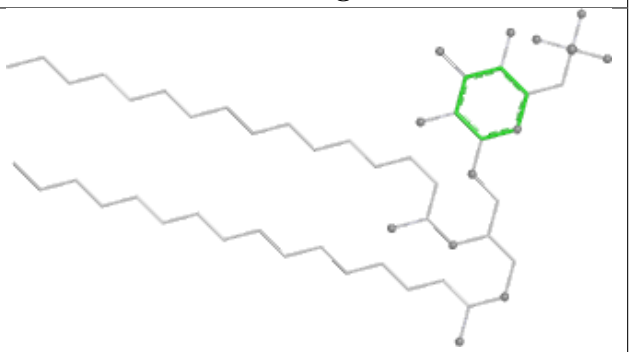
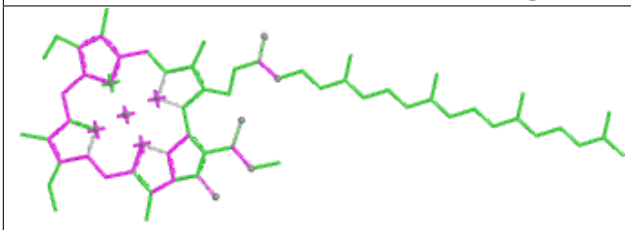


Rings

Ligand CLA A 409



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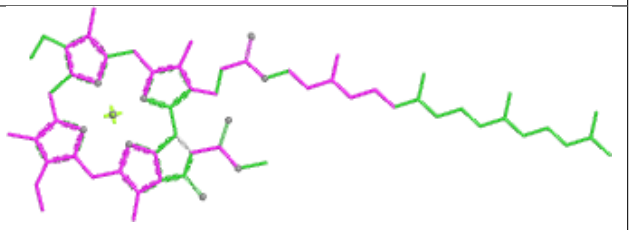
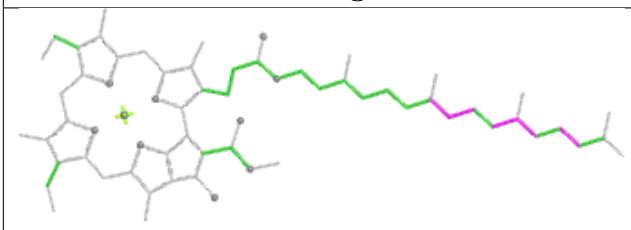


Bond angles



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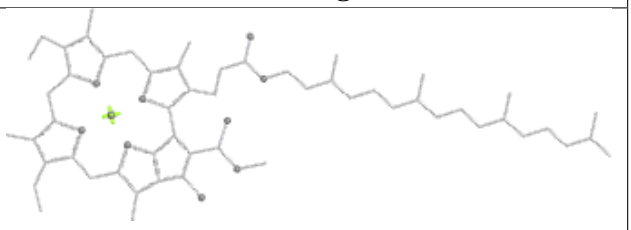
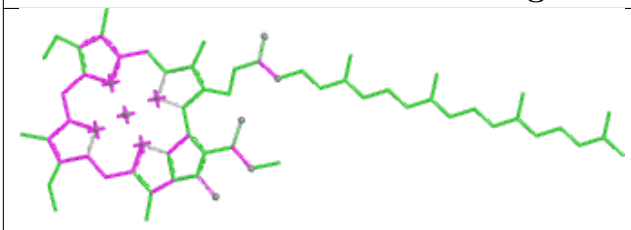


Rings

Ligand CLA b 610



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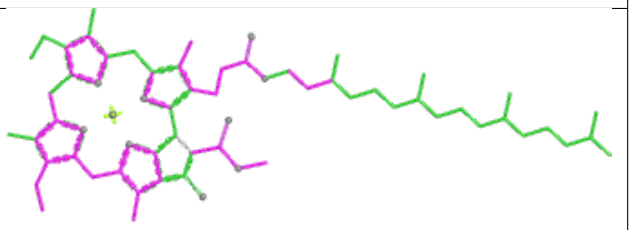
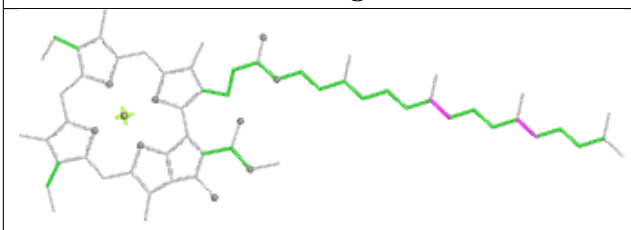


Bond angles



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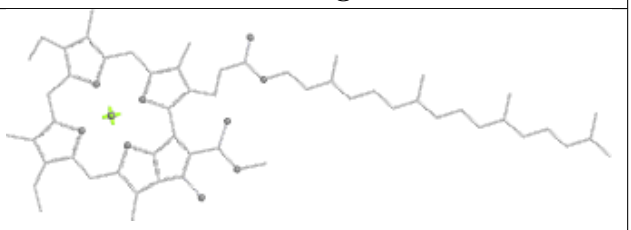
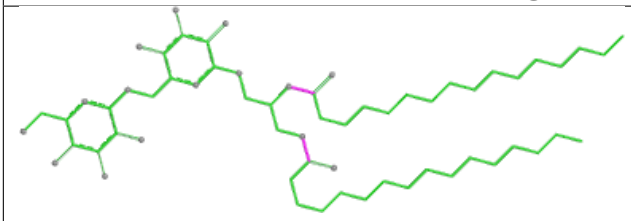


Rings

Ligand DGD c 518



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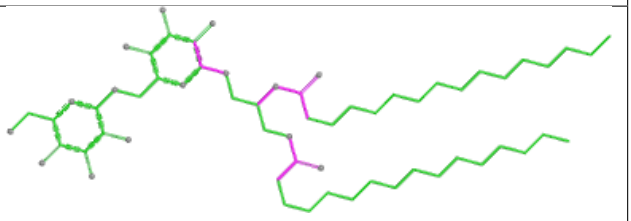
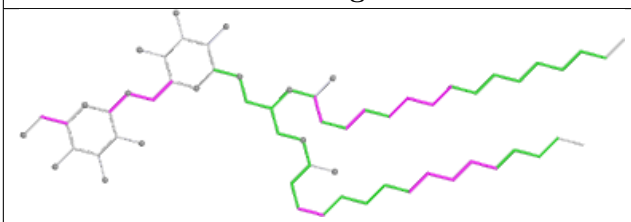
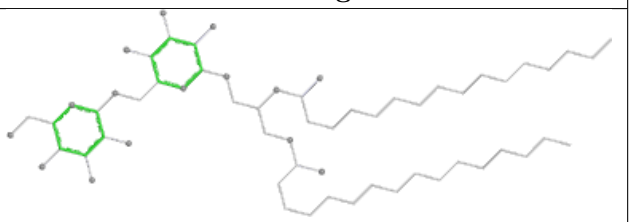


Bond angles

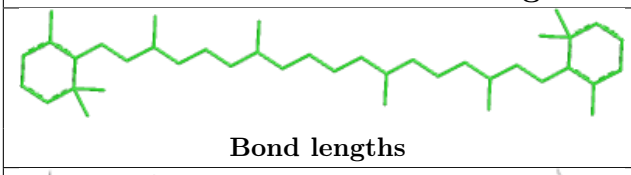


Torsions



Rings

Ligand BCR B 620



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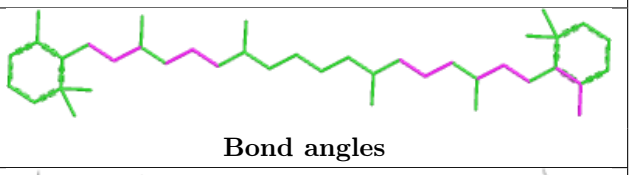
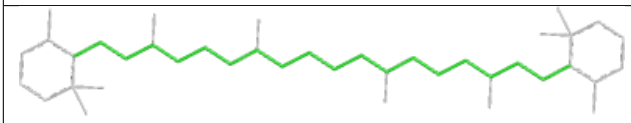
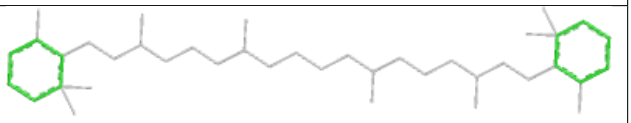


Bond angles

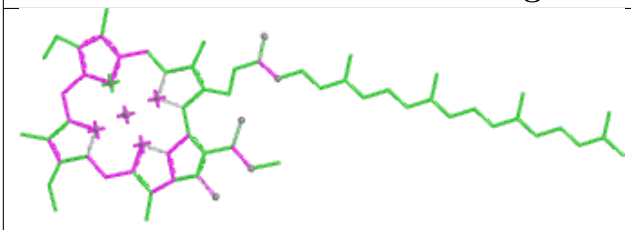


Torsions



Rings

Ligand CLA A 407



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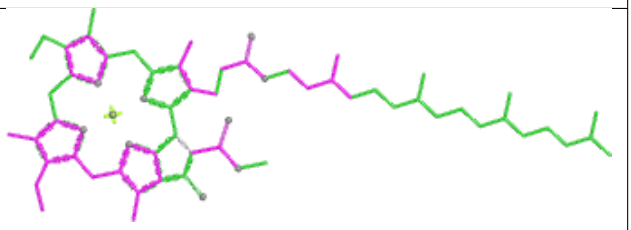
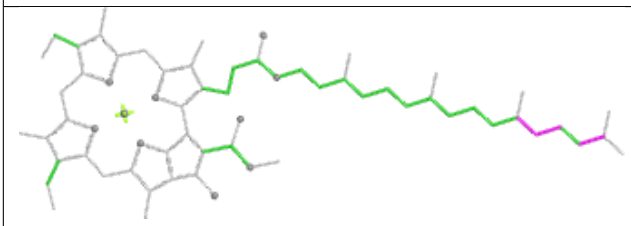
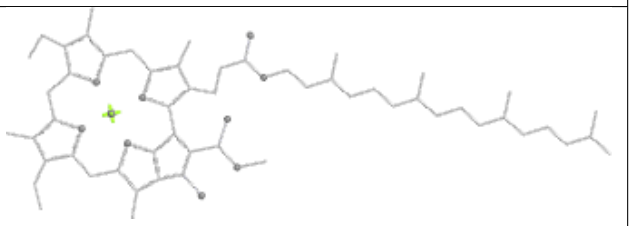


Bond angles

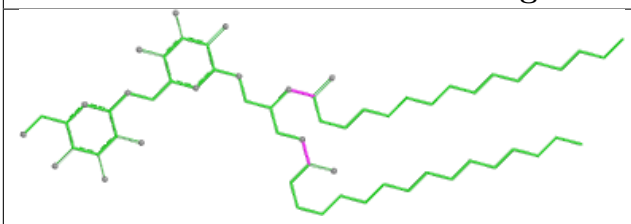


Torsions

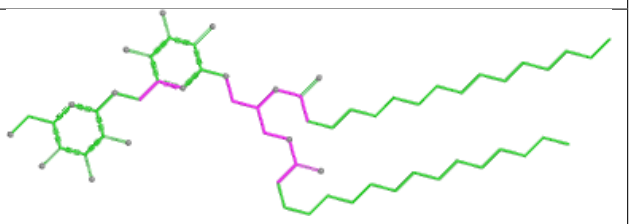


Rings

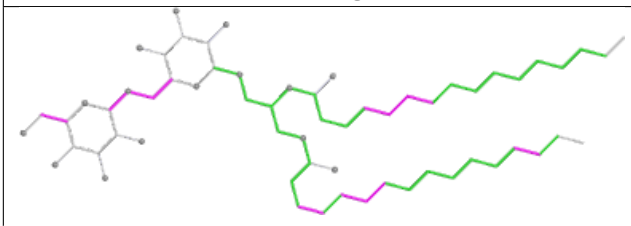
Ligand DGD C 517



Bond lengths



Bond angles



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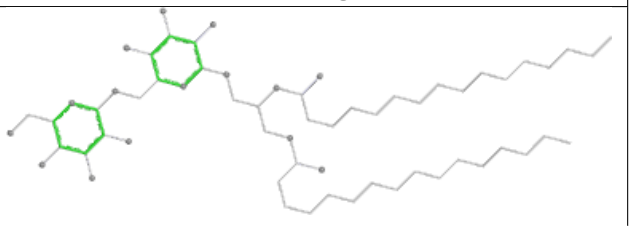
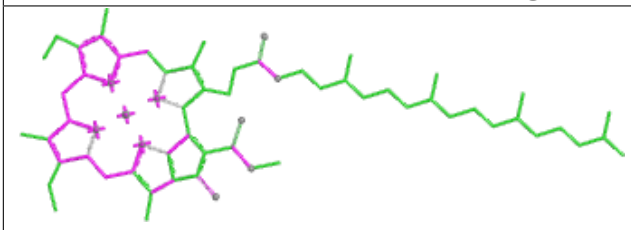


Rings

Ligand CLA B 612



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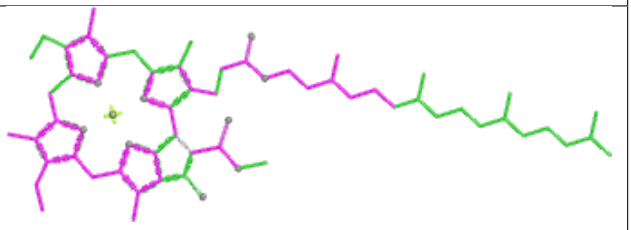
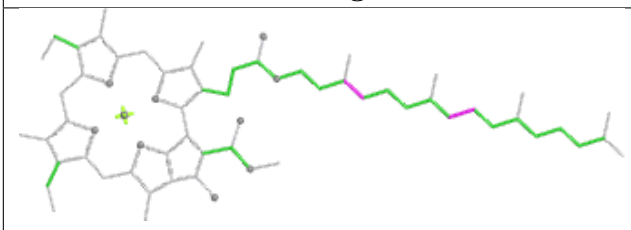
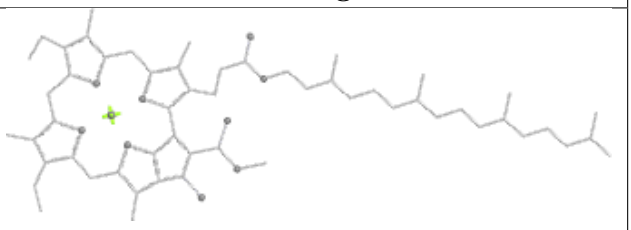


Bond angles

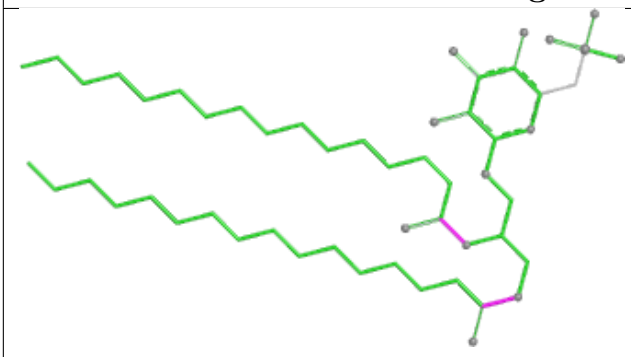


Torsions

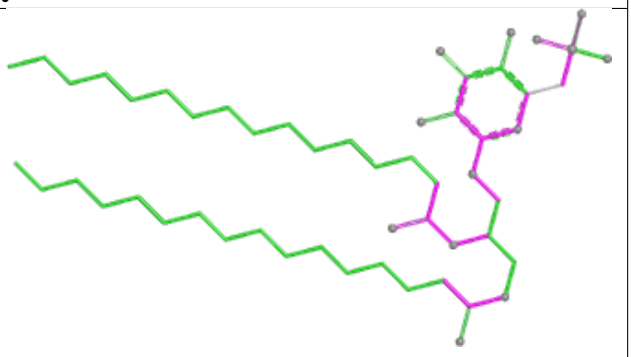


Rings

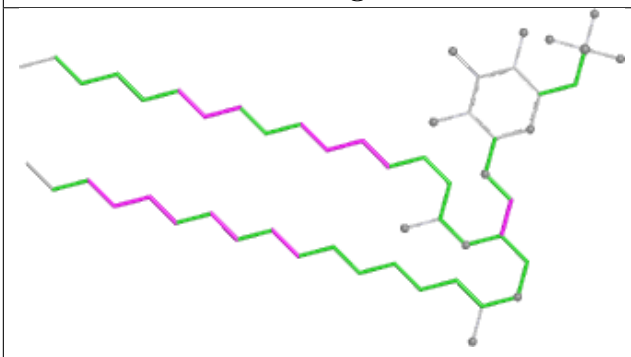
Ligand SQD a 414



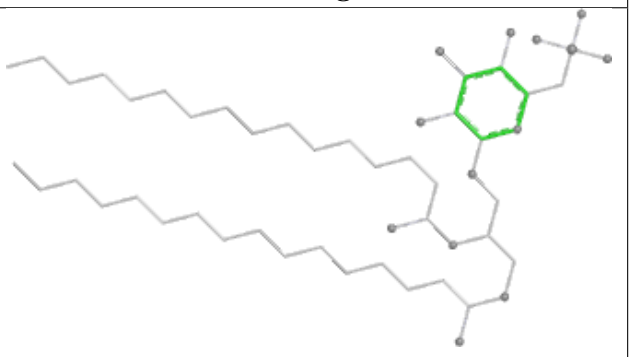
Bond lengths



Bond angles

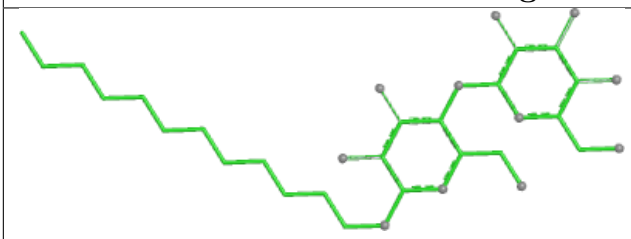


Torsions

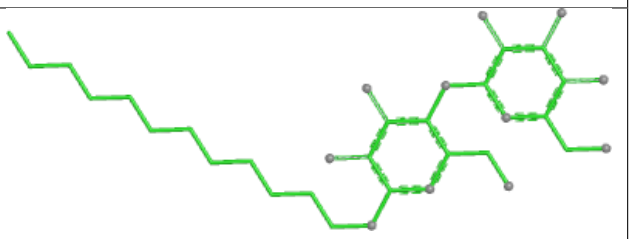


Rings

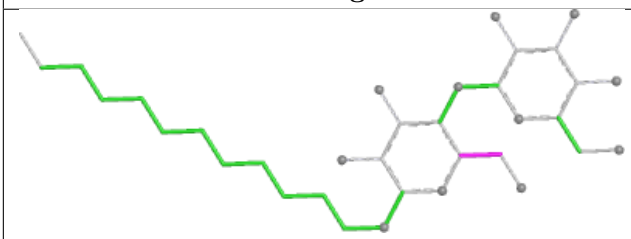
Ligand LMT m 103



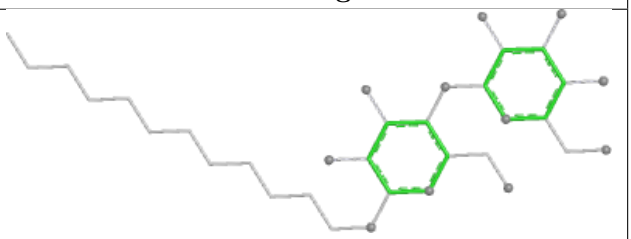
Bond lengths



Bond angles

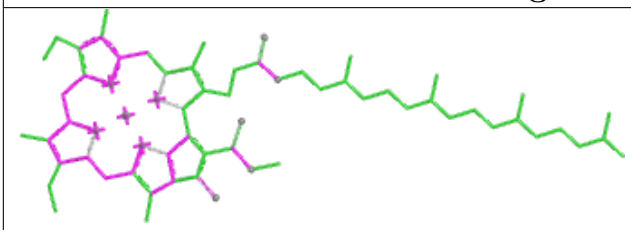


Torsions



Rings

Ligand CLA c 506



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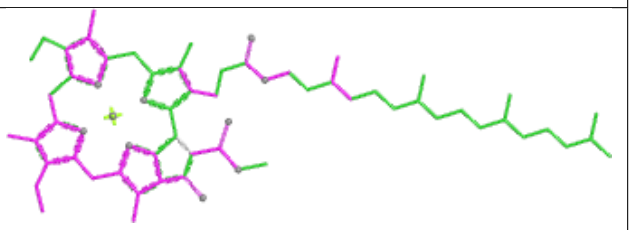

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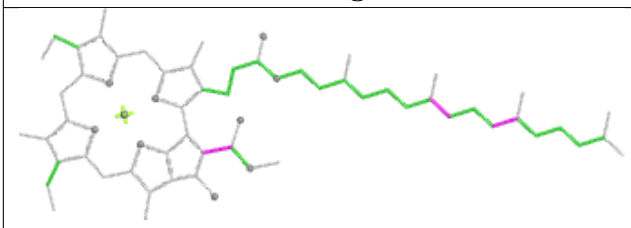

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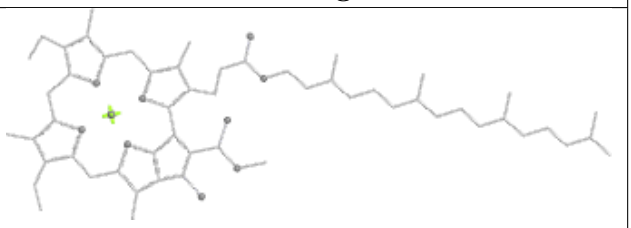
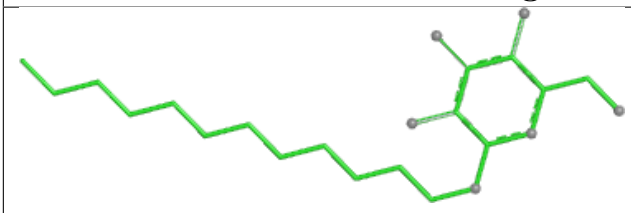


Rings

Ligand LMT T 104



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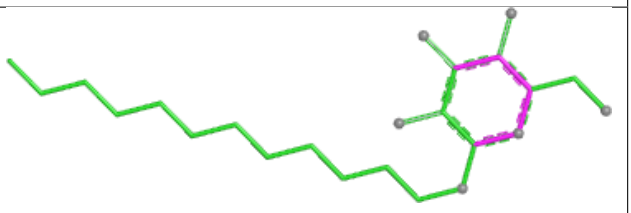

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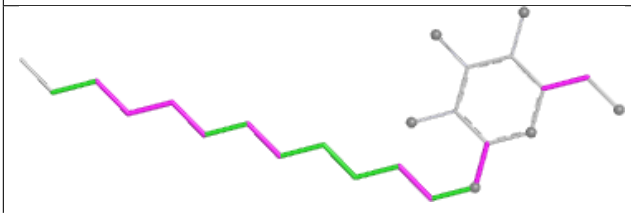

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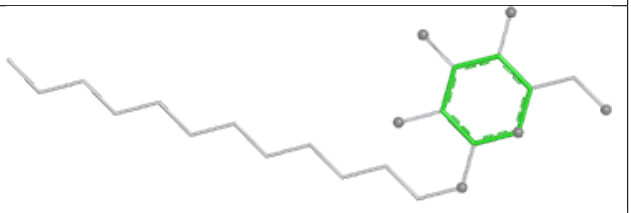
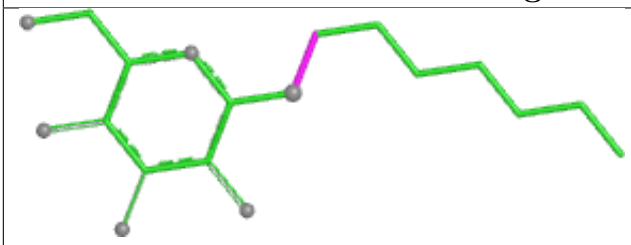


Rings

Ligand HTG b 626



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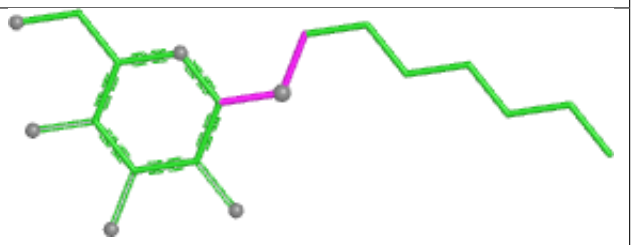

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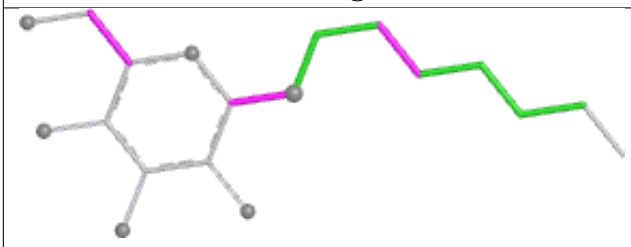

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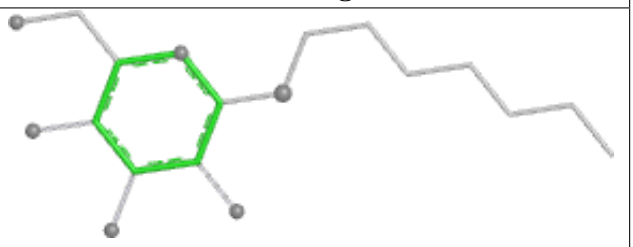
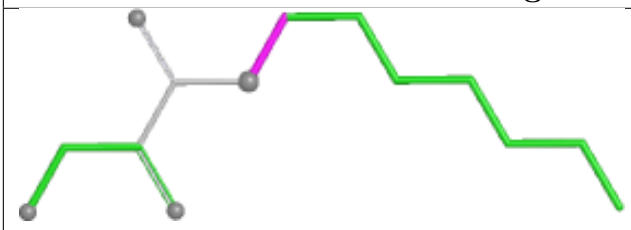


Rings

Ligand HTG u 201



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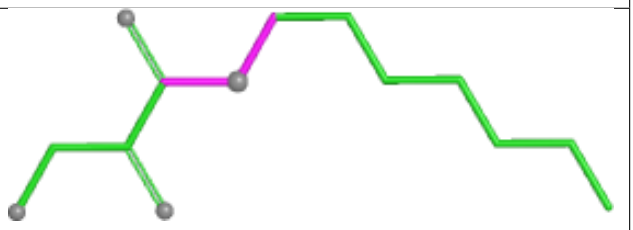
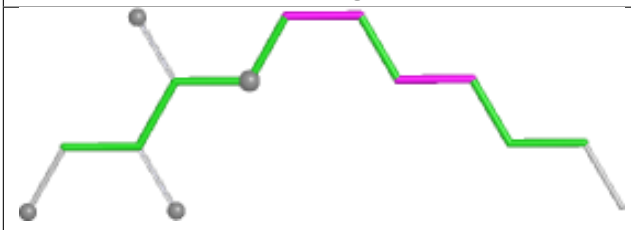


Bond angles



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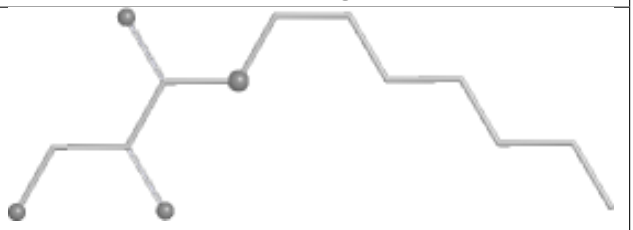
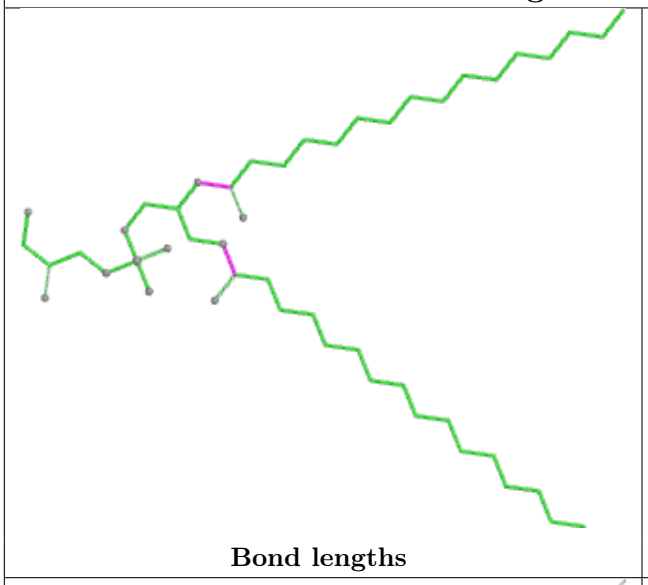


Rings

Ligand LHG d 408



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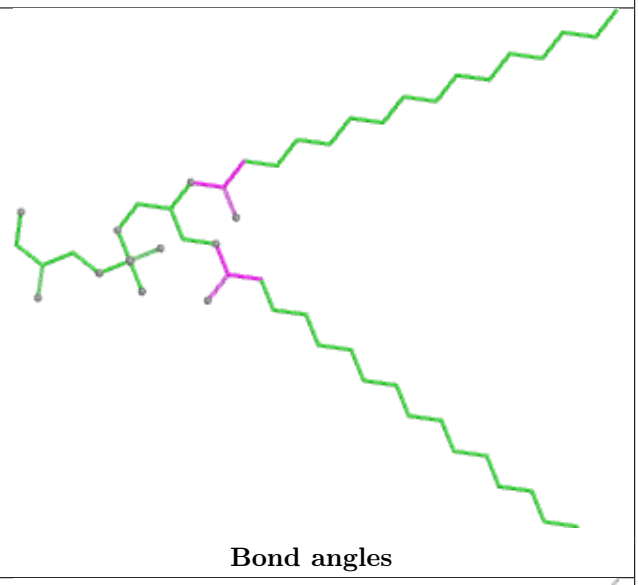

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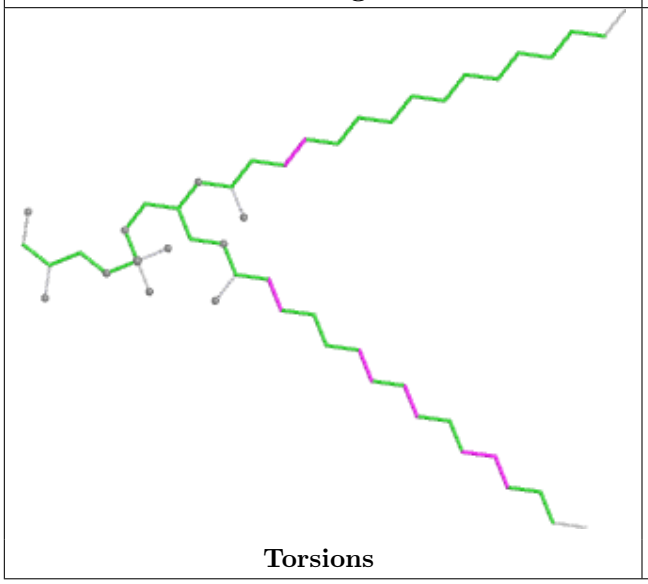

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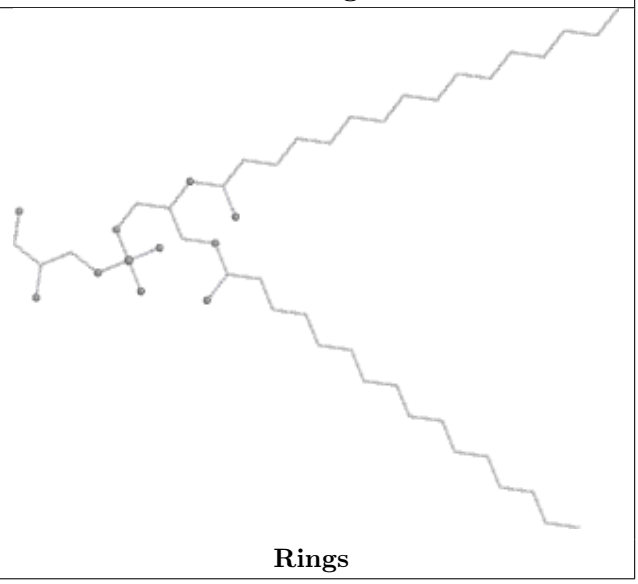
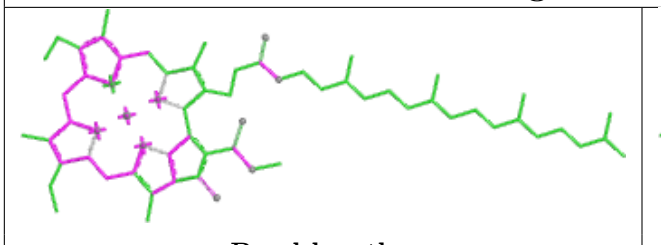


Rings

Ligand CLA b 604



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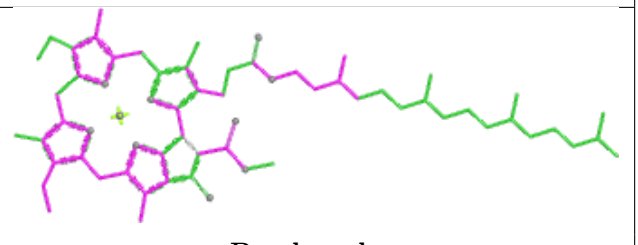
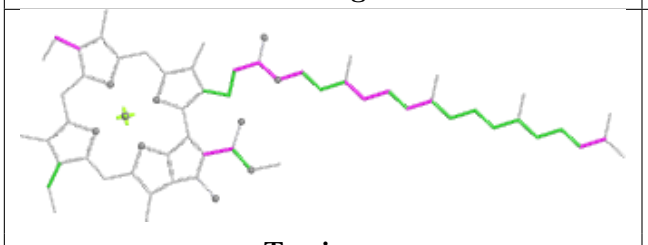


Bond angles



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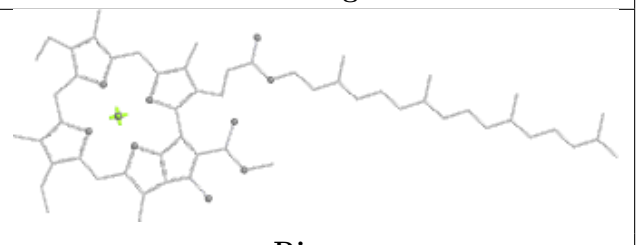
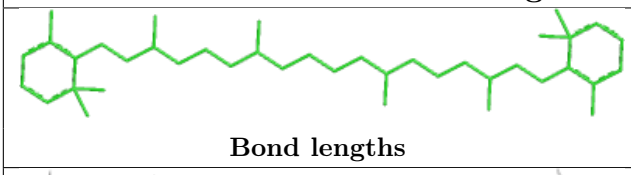


Rings

Ligand BCR b 621



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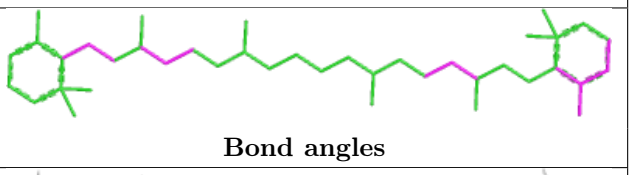
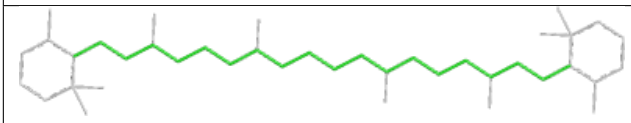


Bond angles



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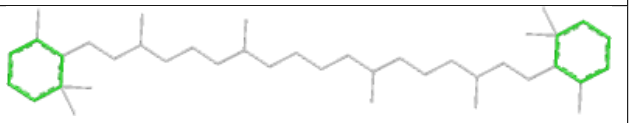
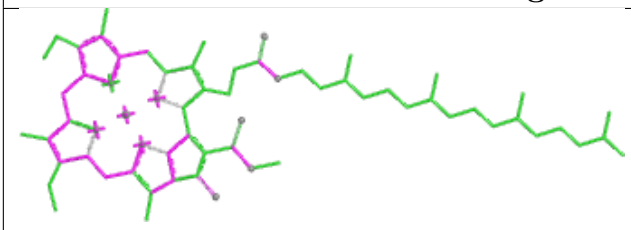


Rings

Ligand CLA b 609



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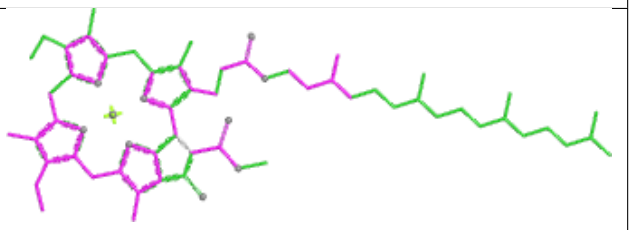
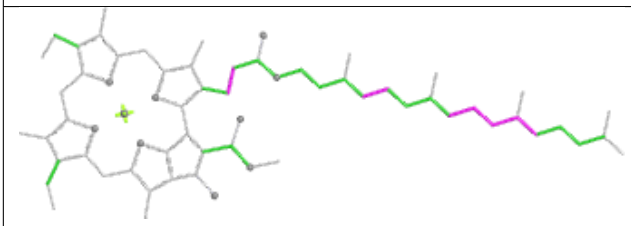


Bond angles



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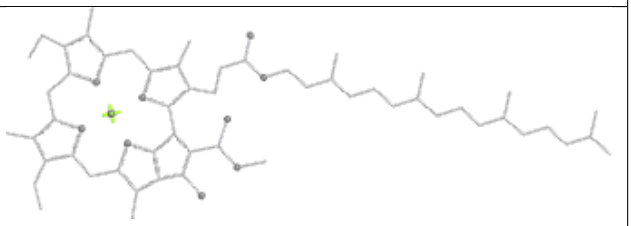
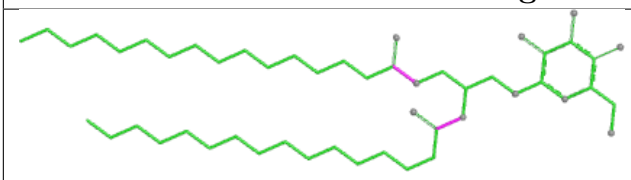


Rings

Ligand LMG A 412



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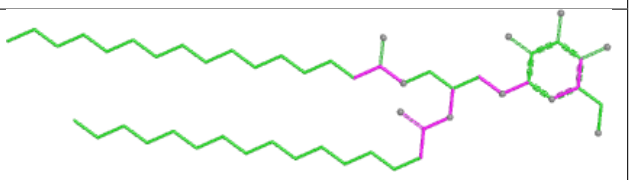
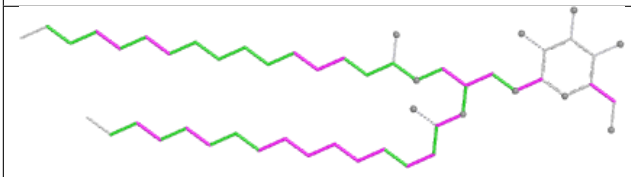


Bond angles



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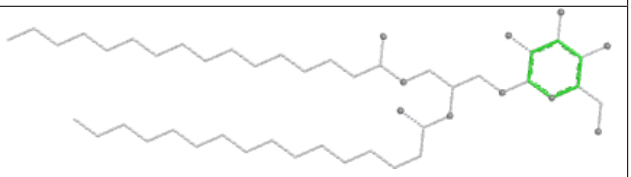
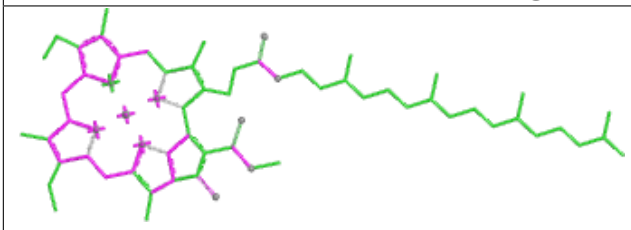


Rings

Ligand CLA b 618



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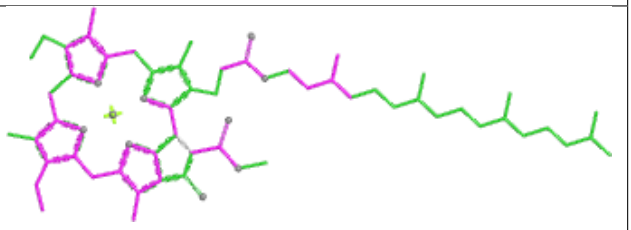
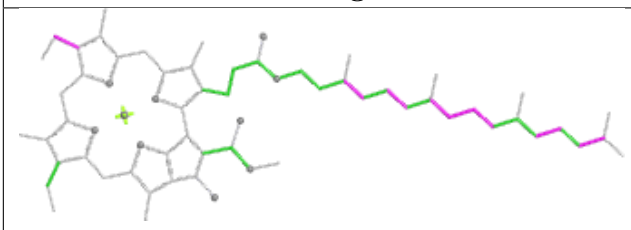


Bond angles



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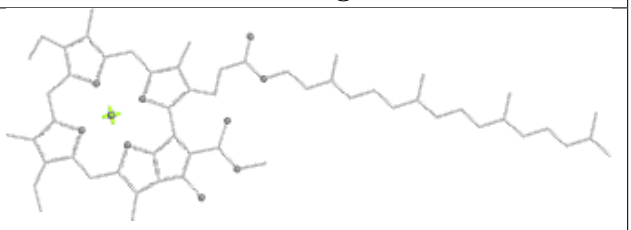
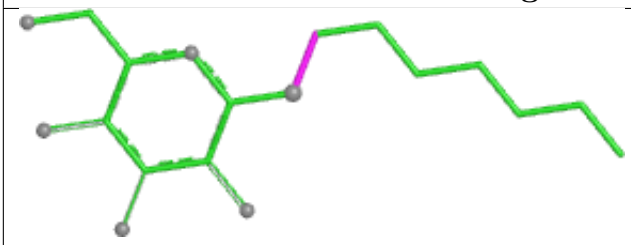


Rings

Ligand HTG C 523



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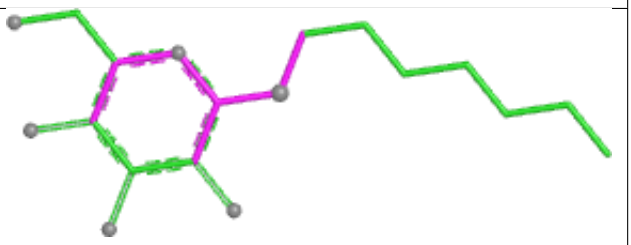
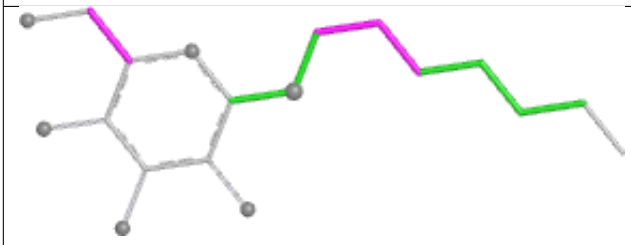


Bond angles



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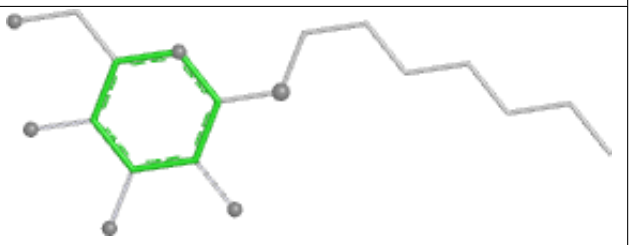
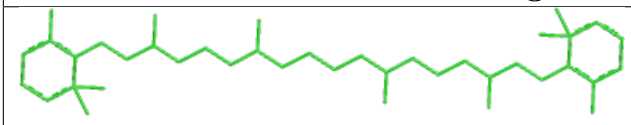


Rings

Ligand BCR k 303



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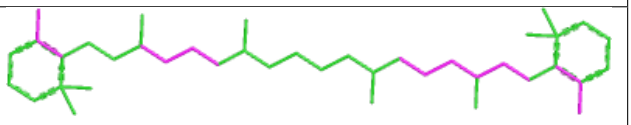
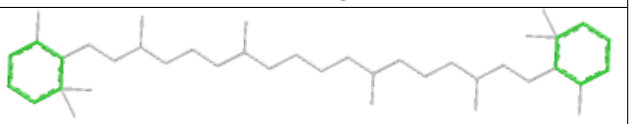


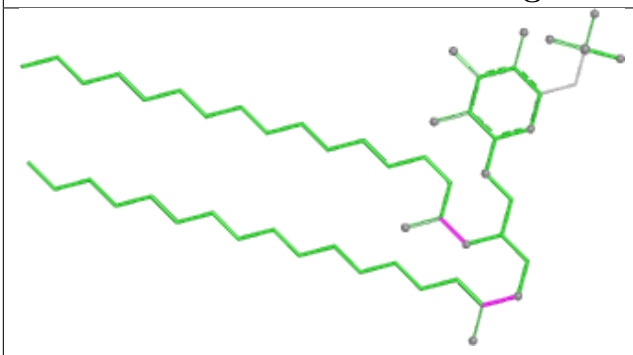
Bond angles

Torsions



Rings

Ligand SQD A 411



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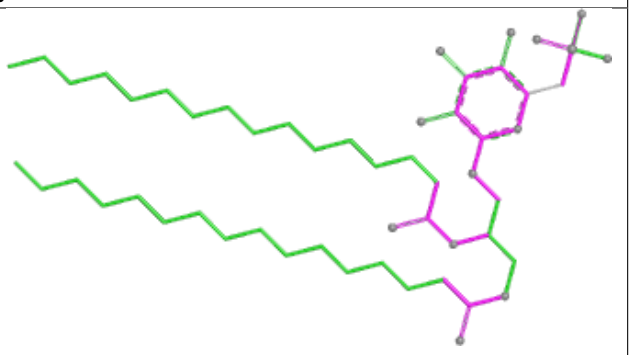
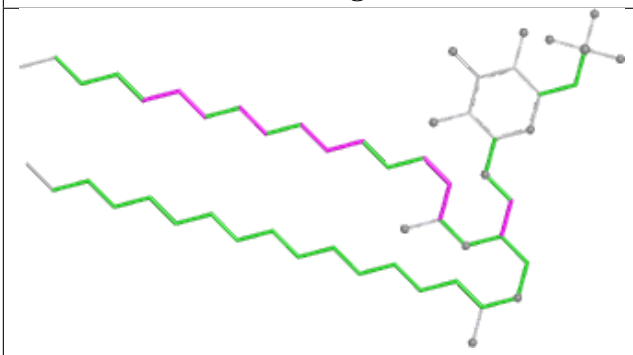
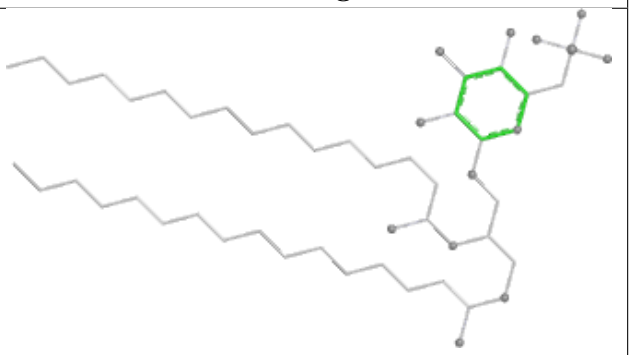


Bond angles

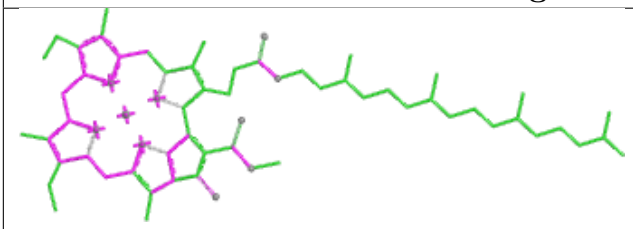


Torsions

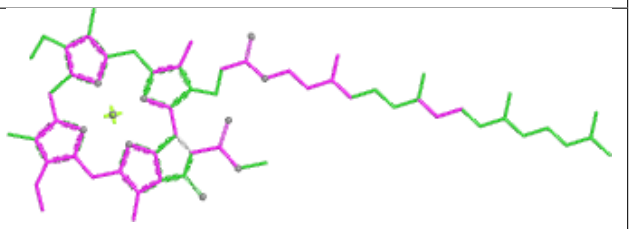


Rings

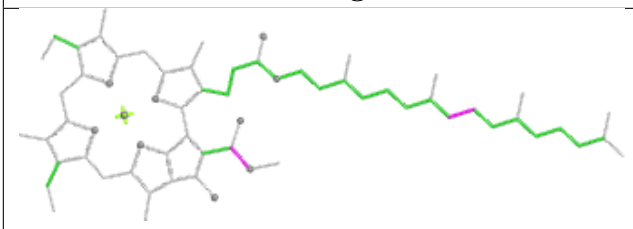
Ligand CLA c 512



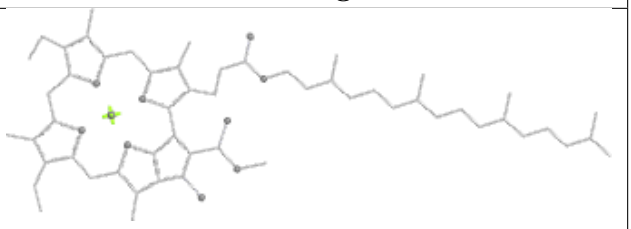
Bond lengths



Bond angles

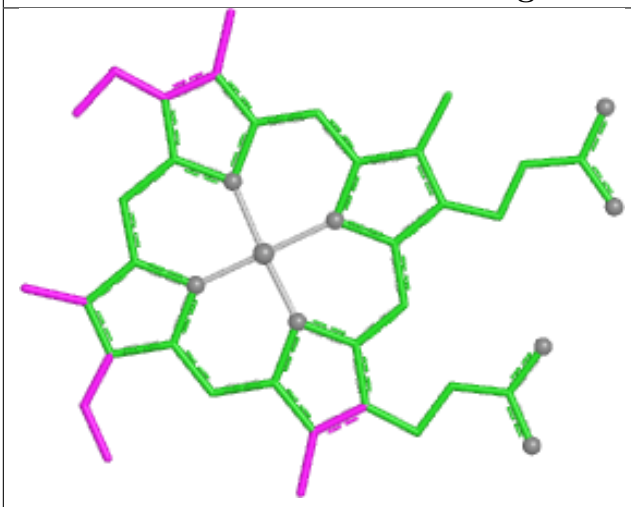


Torsions



Rings

Ligand HEC v 1603



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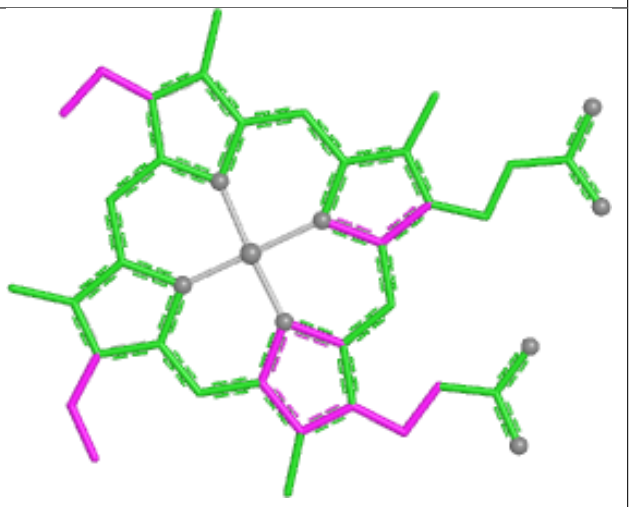
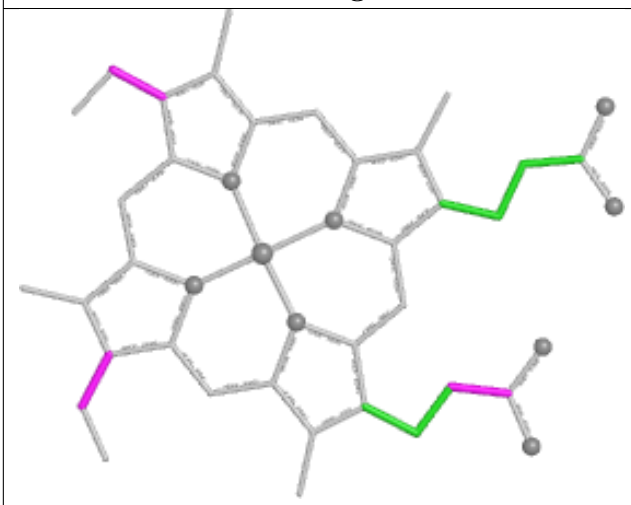
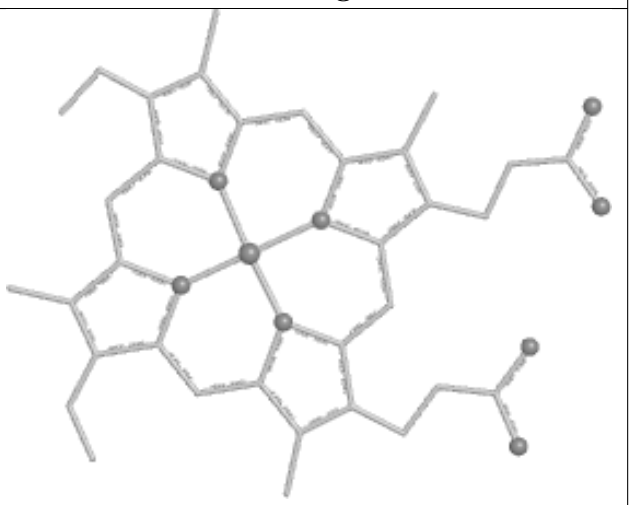


Bond angles

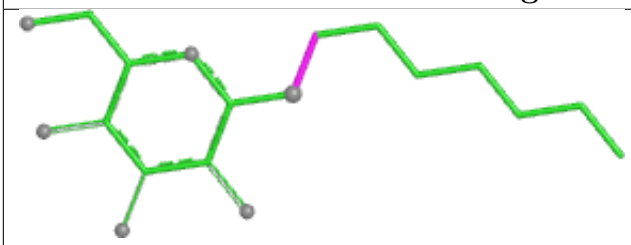


Torsions



Rings

Ligand HTG B 626



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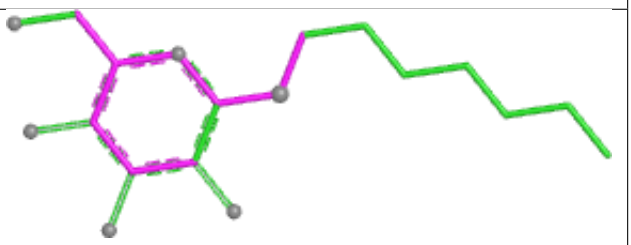
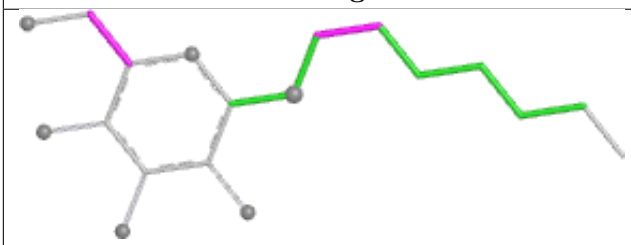


Bond angles



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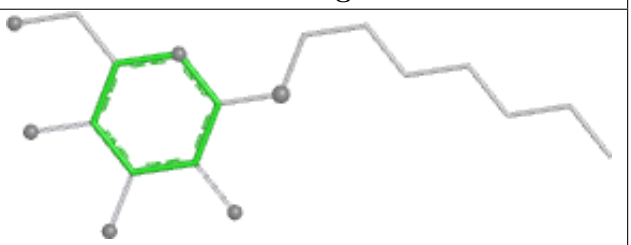
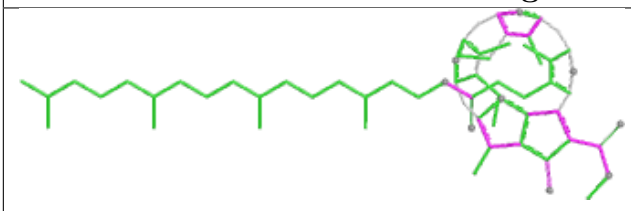


Rings

Ligand PHO A 408



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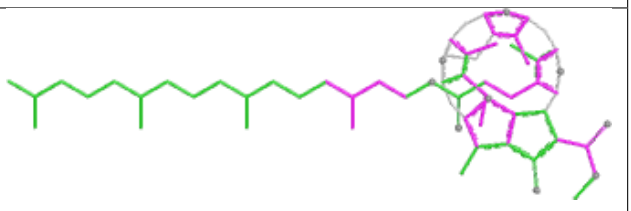
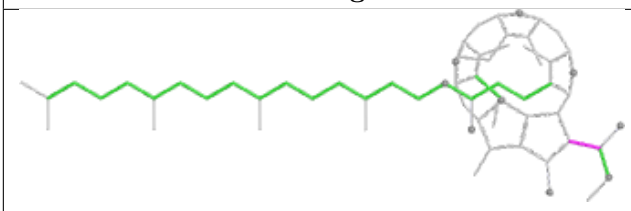


Bond angles



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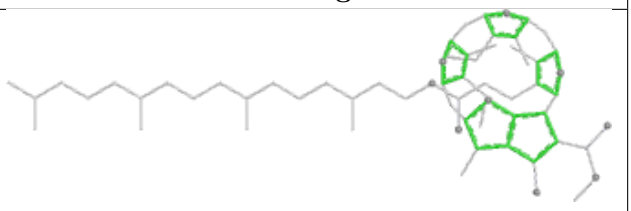
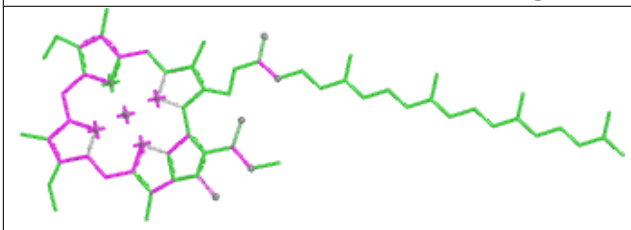


Rings

Ligand CLA c 509



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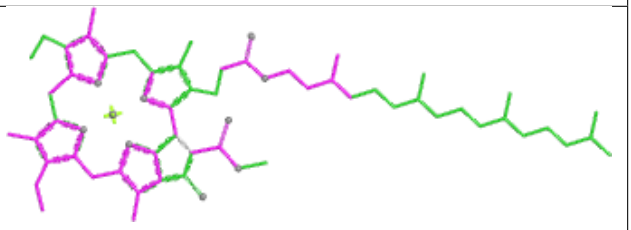
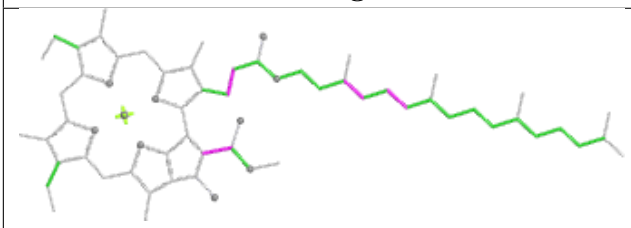


Bond angles



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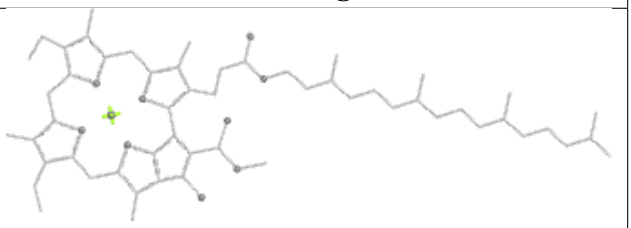
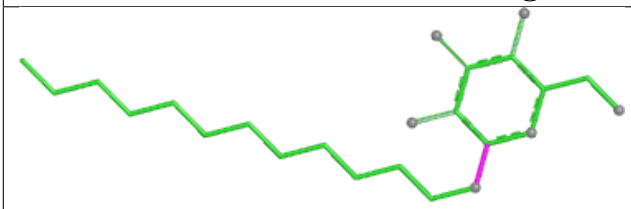


Rings

Ligand LMT B 642



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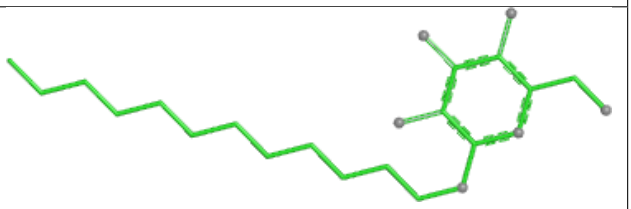
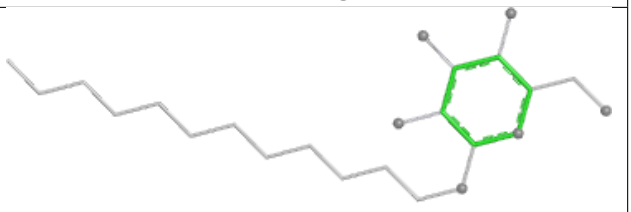


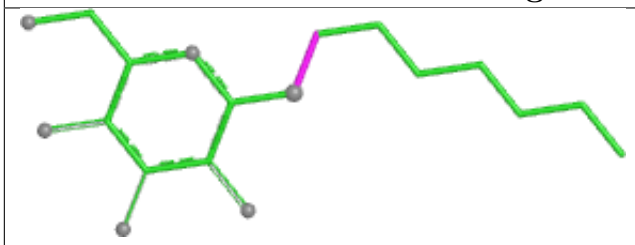
Bond angles

Torsions



Rings

Ligand HTG o 301



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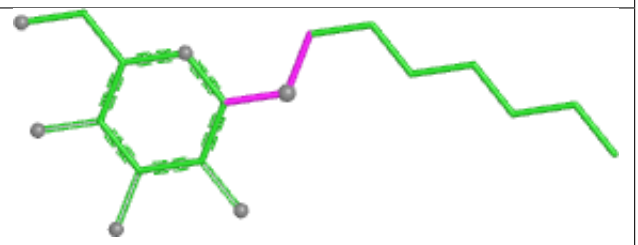
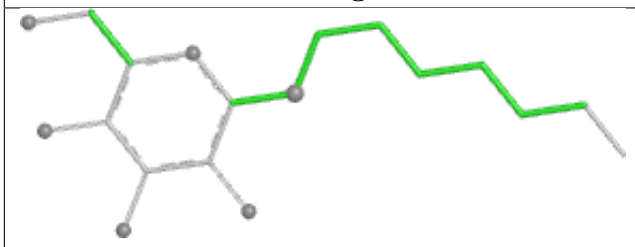


Bond angles



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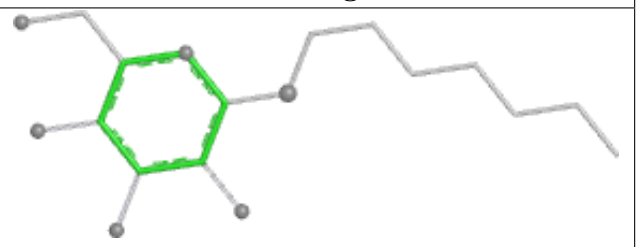
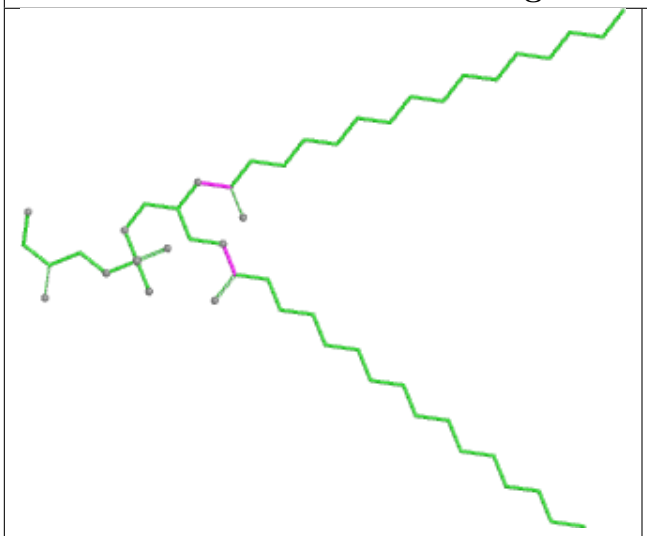


Rings

Ligand LHG E 101



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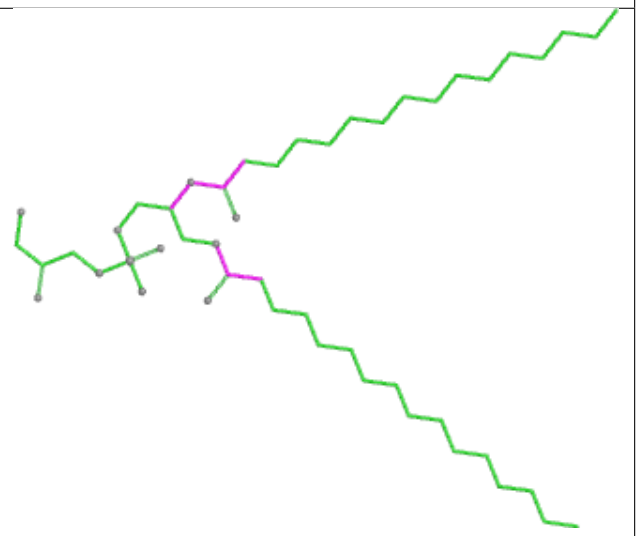
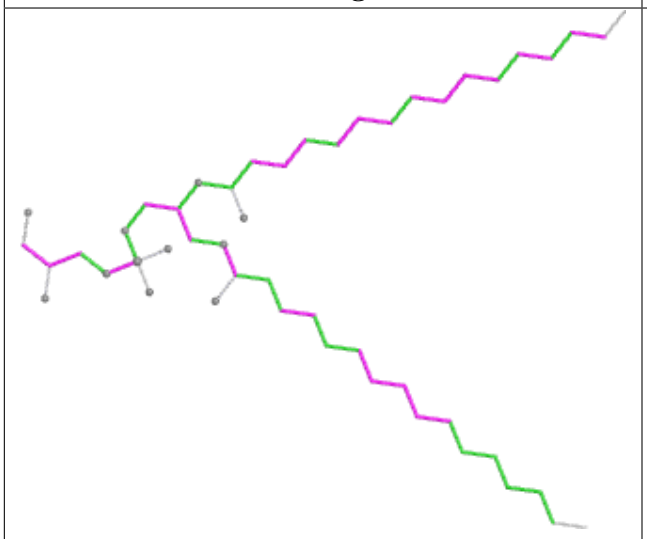
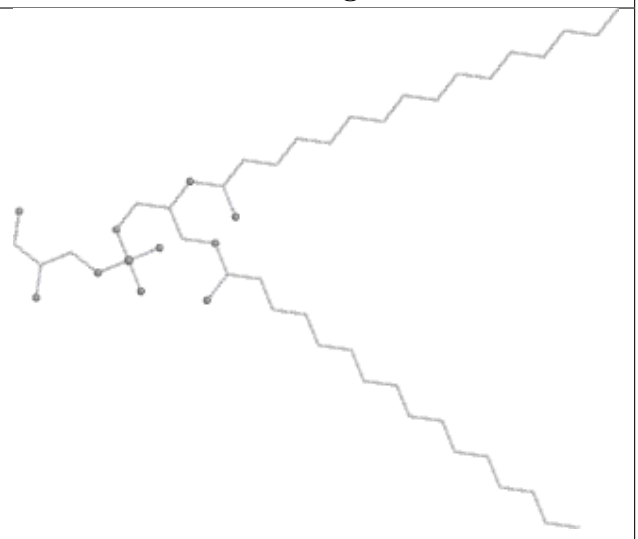


Bond angles

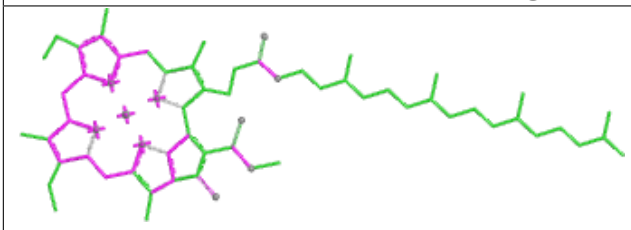


Torsions



Rings

Ligand CLA B 611



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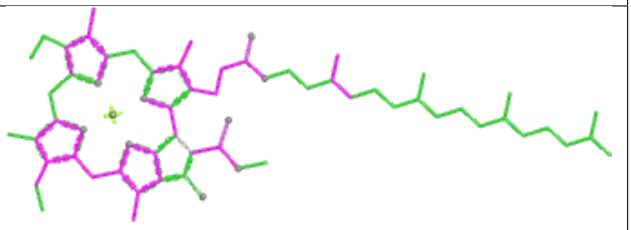
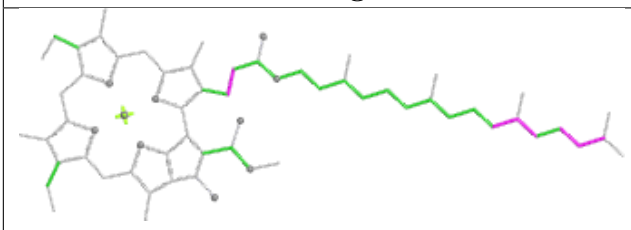


Bond angles



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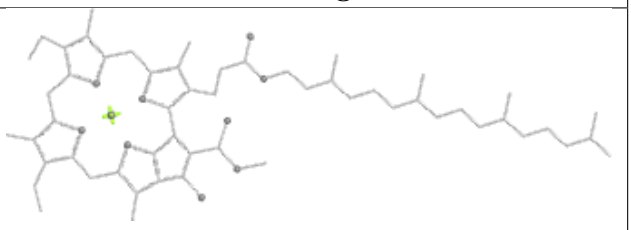
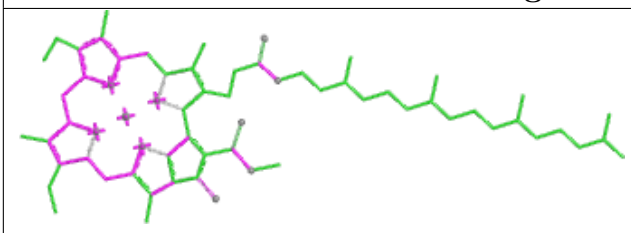


Rings

Ligand CLA C 502



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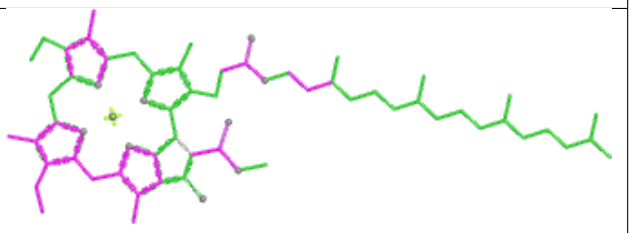
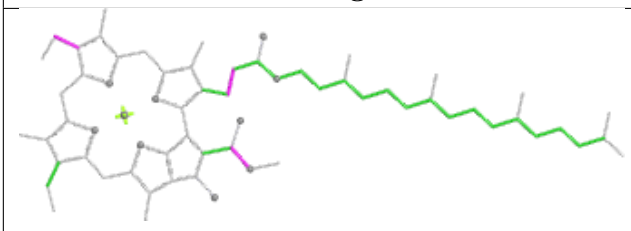
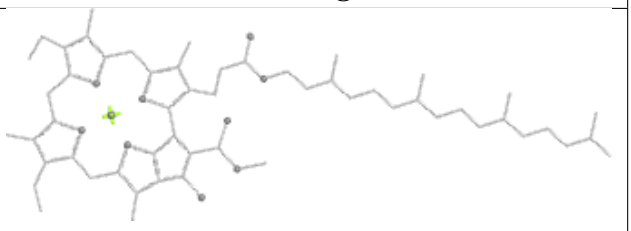


Bond angles

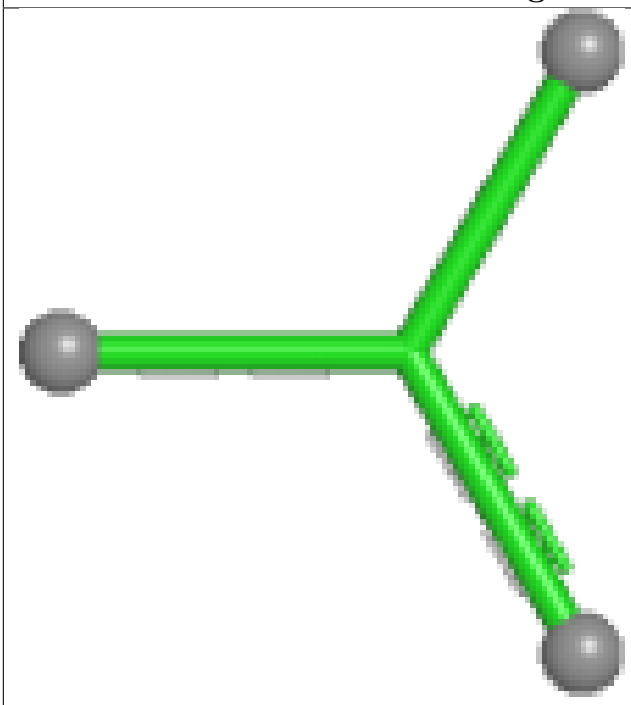


Torsions



Rings

Ligand BCT a 407



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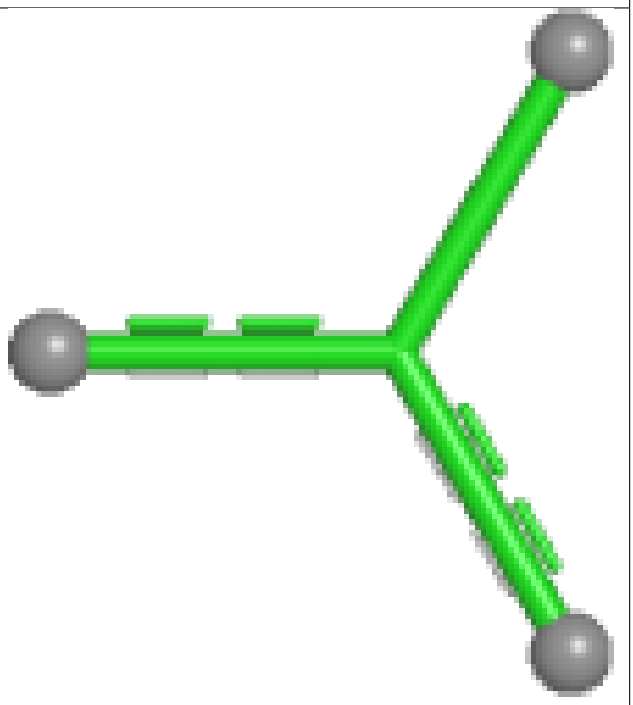
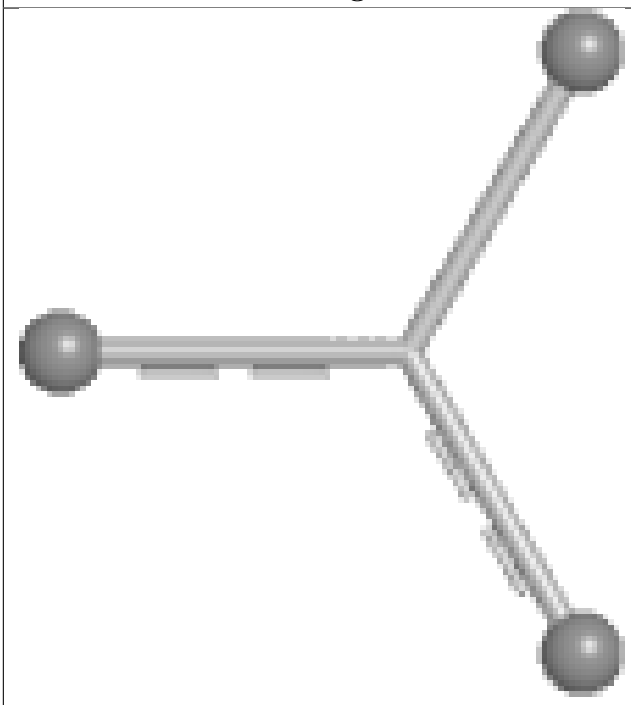
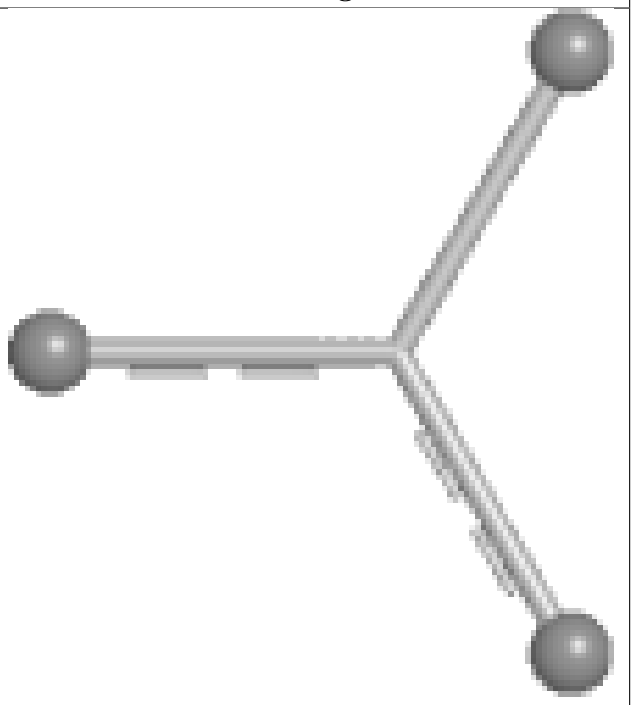


Bond angles

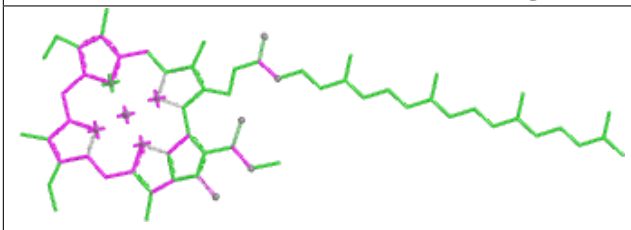


Torsions



Rings

Ligand CLA C 504



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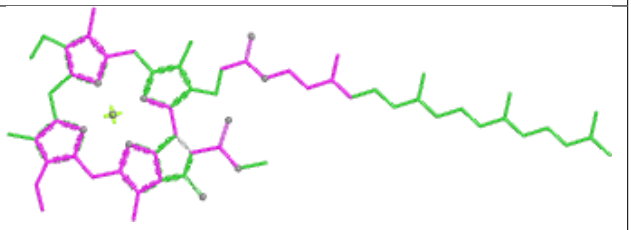
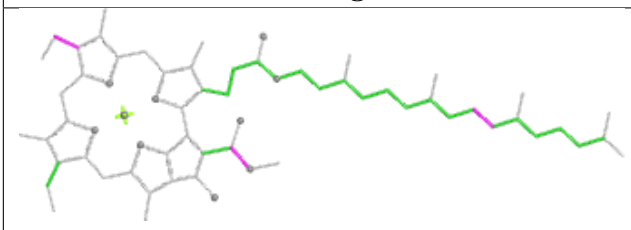
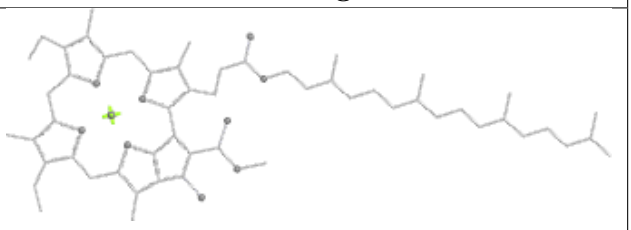


Bond angles

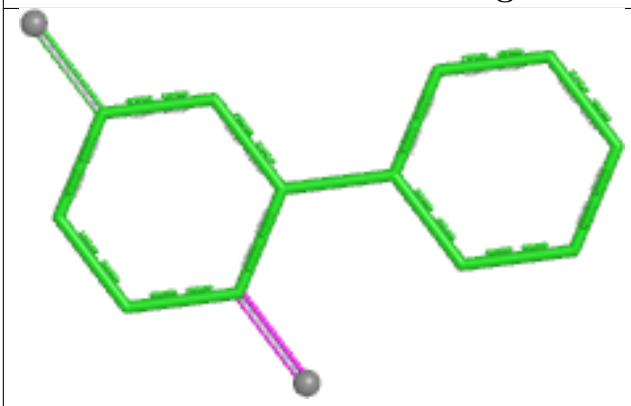


Torsions



Rings

Ligand K3C a 424 (A)



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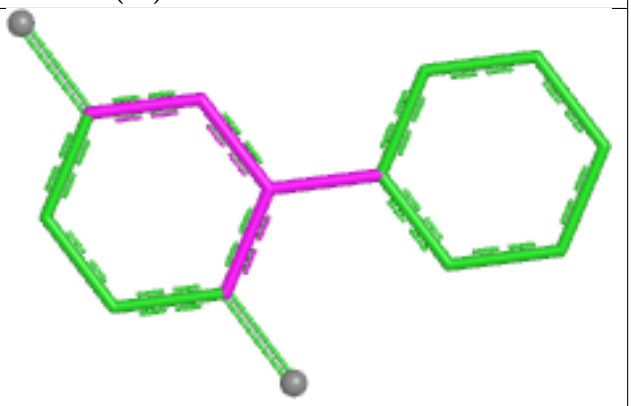
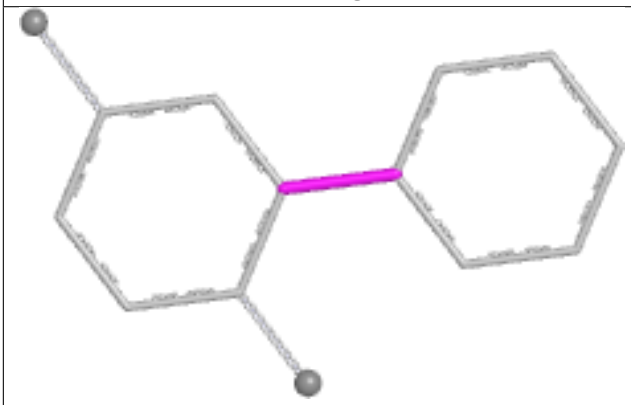
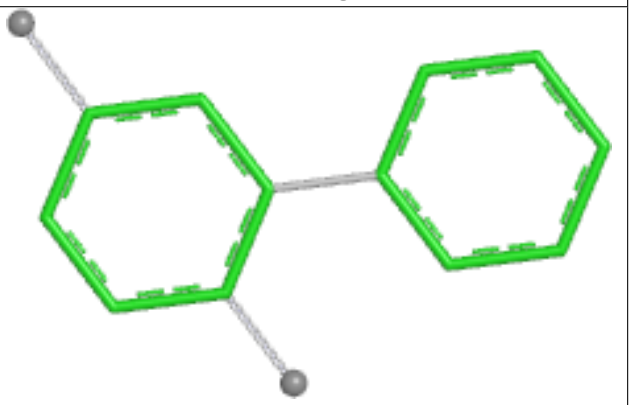


Bond angles

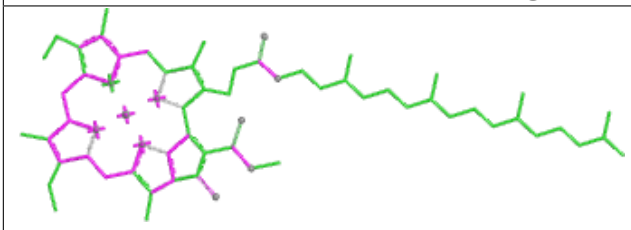


Torsions



Rings

Ligand CLA C 506



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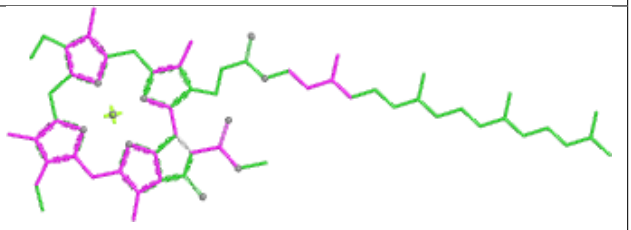
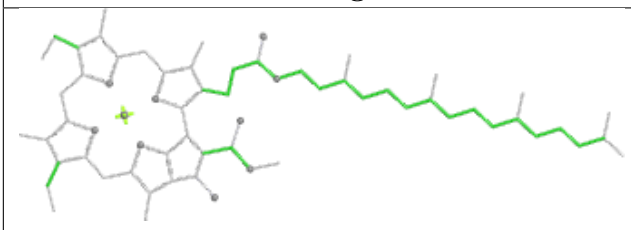
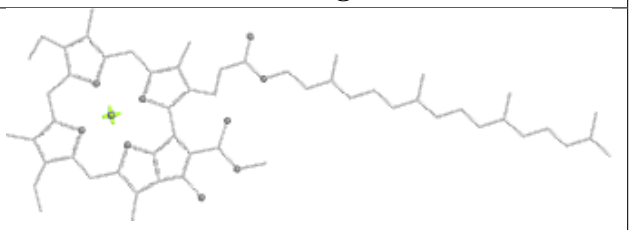


Bond angles

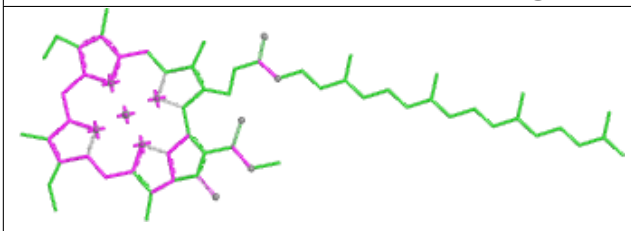


Torsions

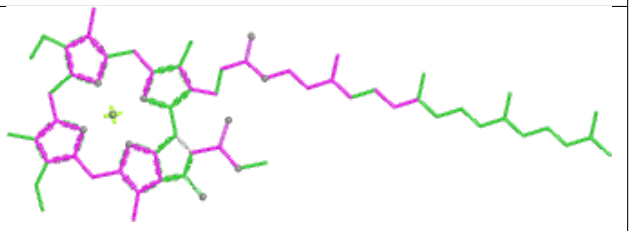


Rings

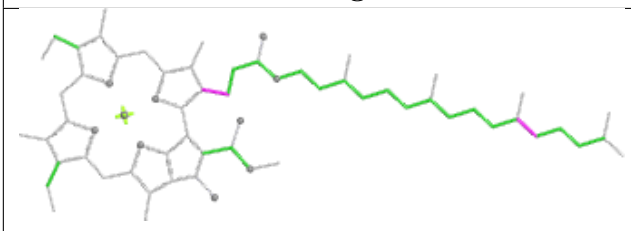
Ligand CLA c 510



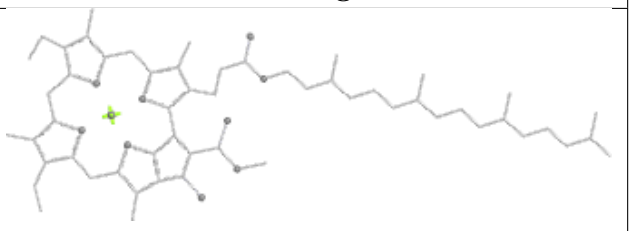
Bond lengths



Bond angles

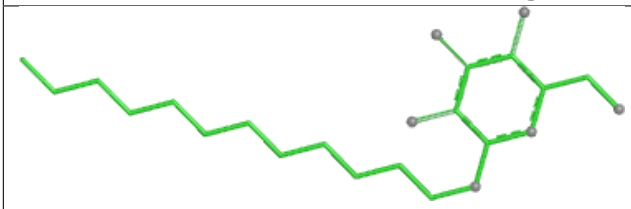


Torsions

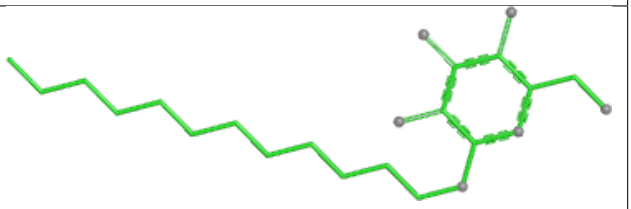


Rings

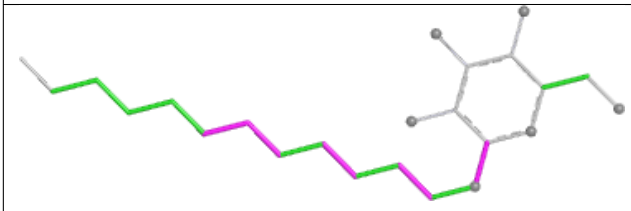
Ligand LMT E 104



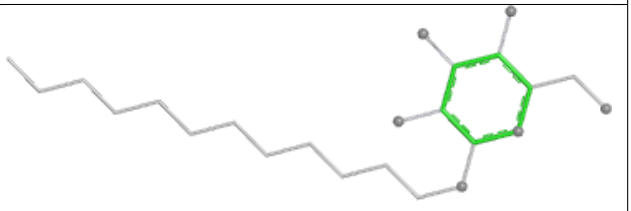
Bond lengths



Bond angles

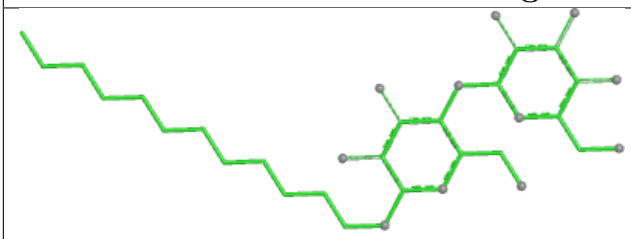


Torsions

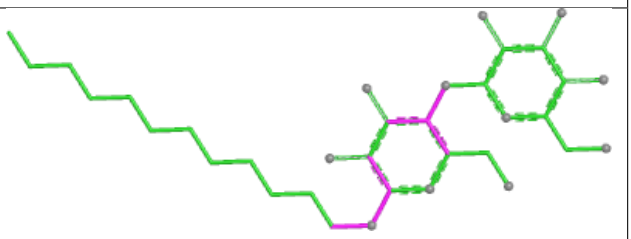


Rings

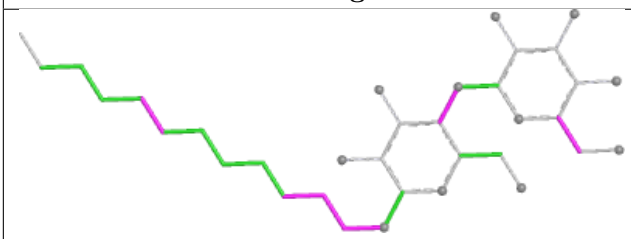
Ligand LMT B 622



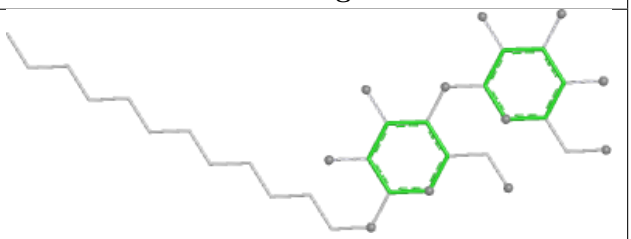
Bond lengths



Bond angles

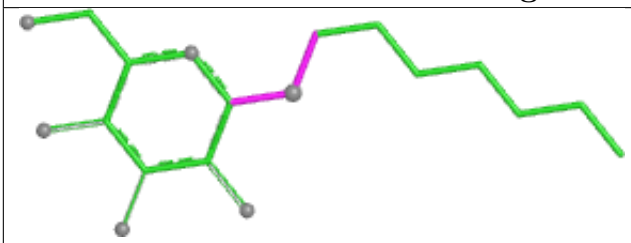


Torsions



Rings

Ligand HTG D 413



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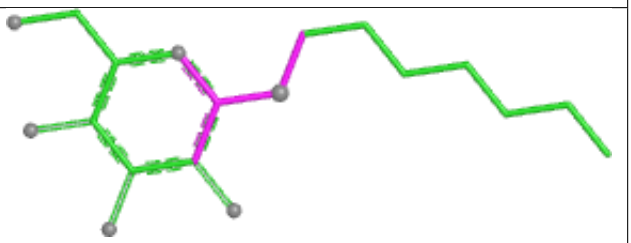
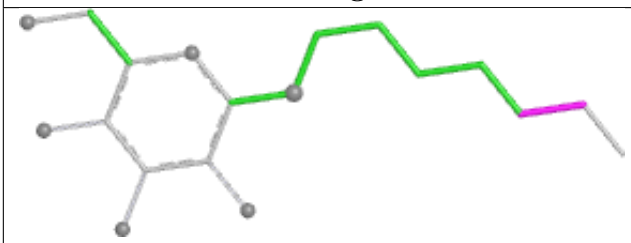
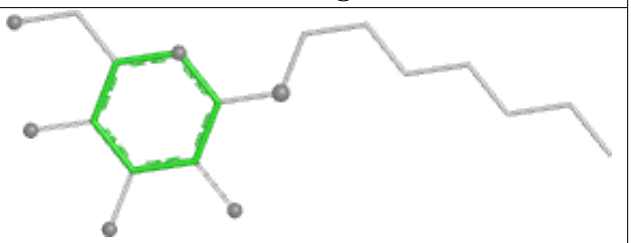


Bond angles

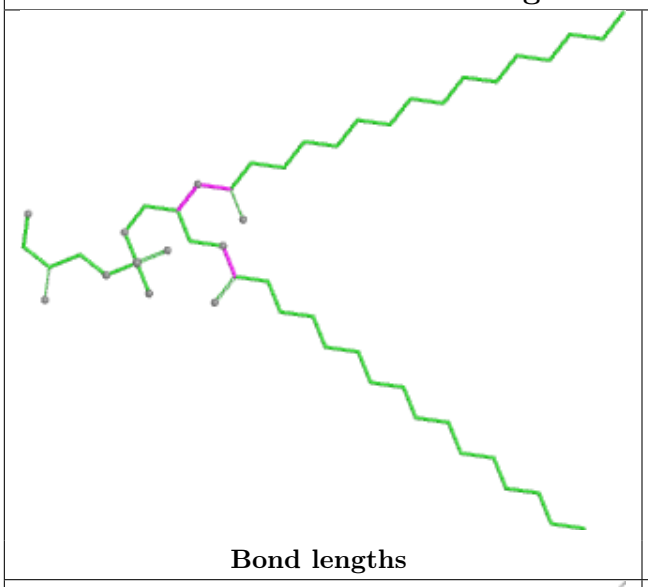


Torsions



Rings

Ligand LHG D 409



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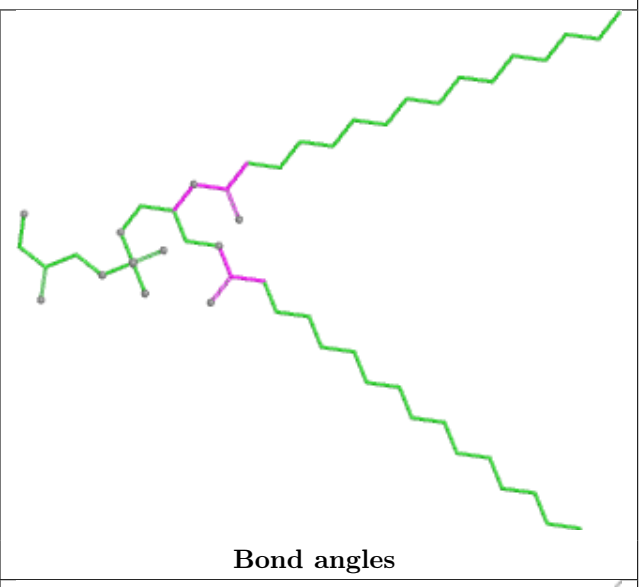
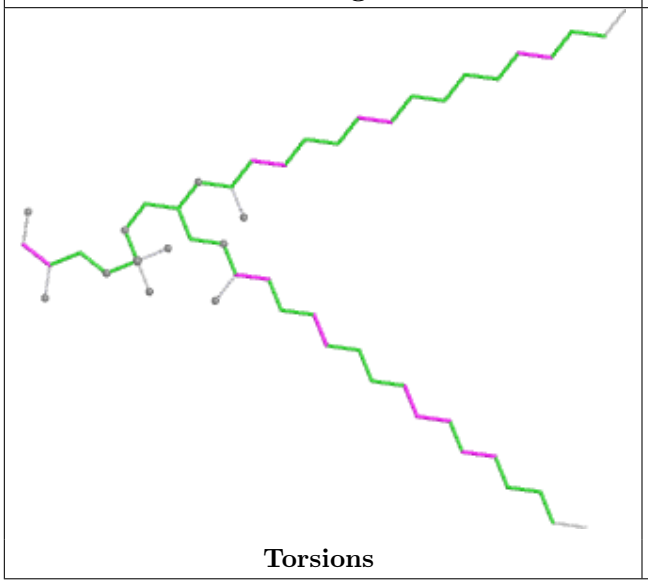
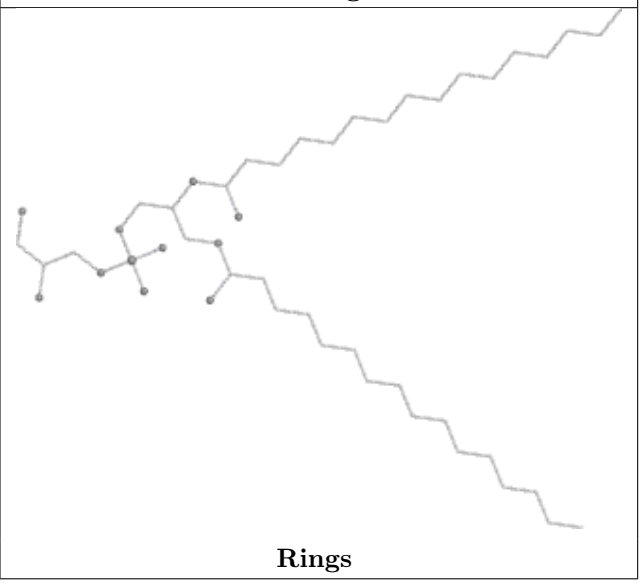


Bond angles

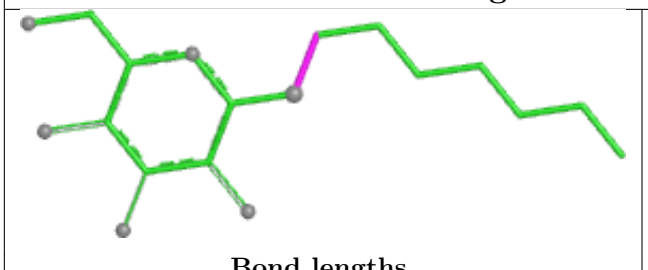


Torsions



Rings

Ligand HTG B 623 (B)



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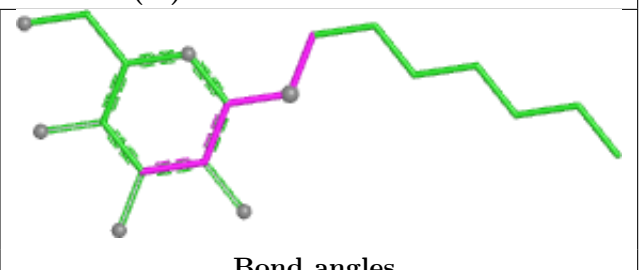
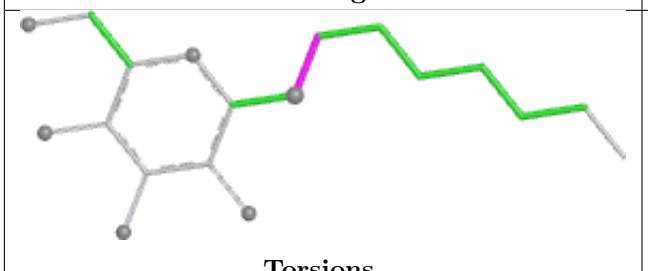


Bond angles



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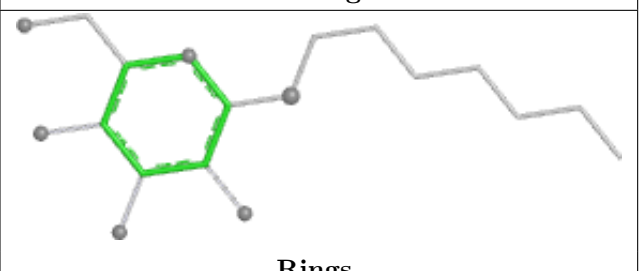
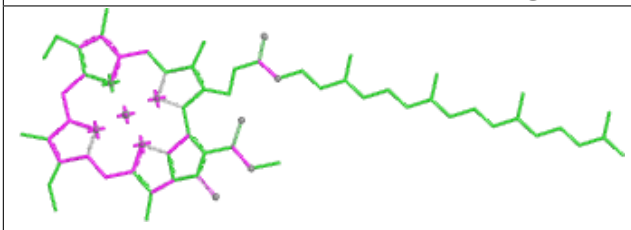
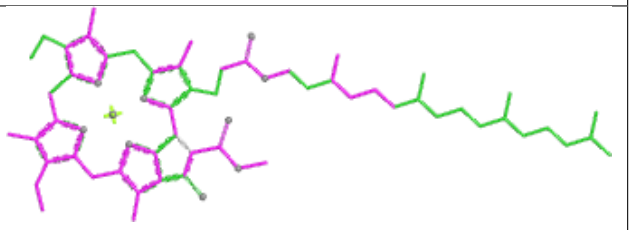


Rings

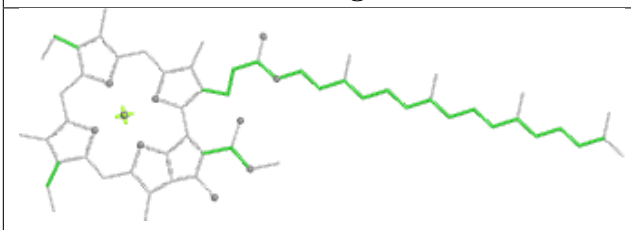
Ligand CLA B 610



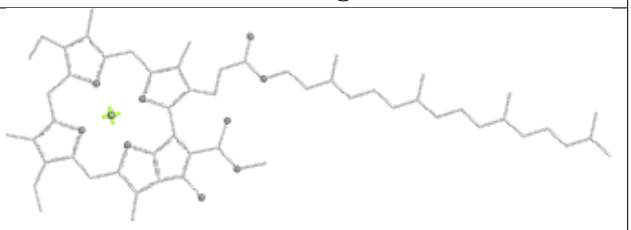
Bond lengths



Bond angles

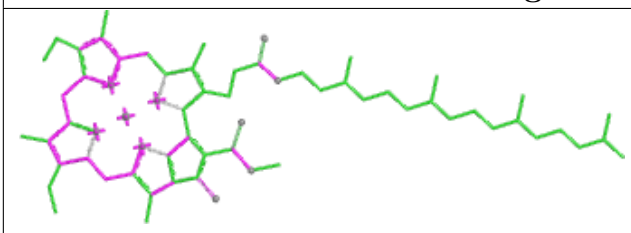


Torsions



Rings

Ligand CLA B 614



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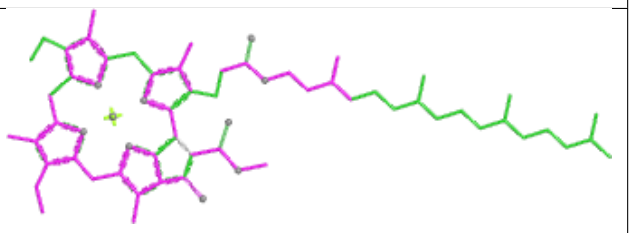
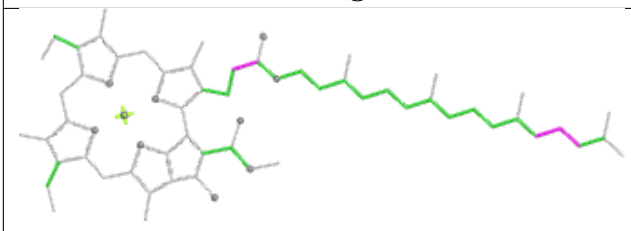
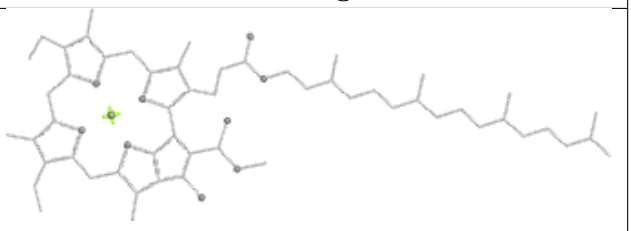


Bond angles

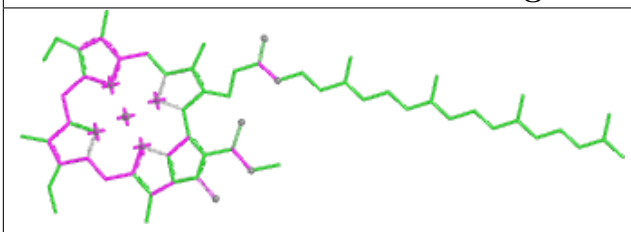


Torsions



Rings

Ligand CLA B 607



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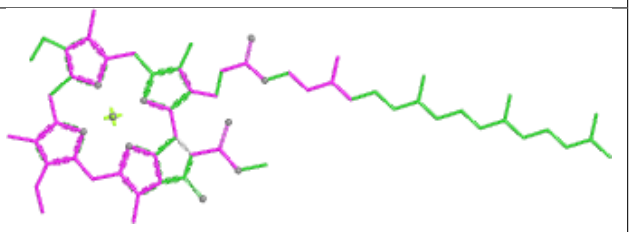
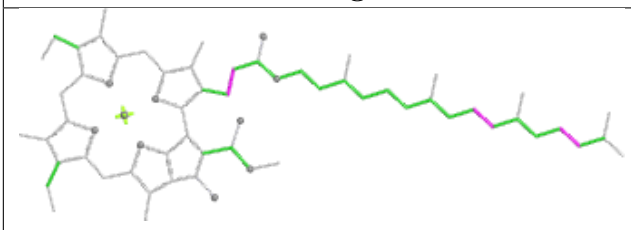
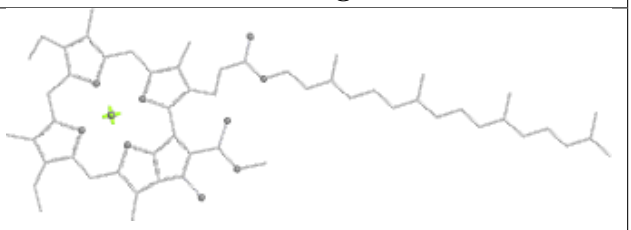


Bond angles

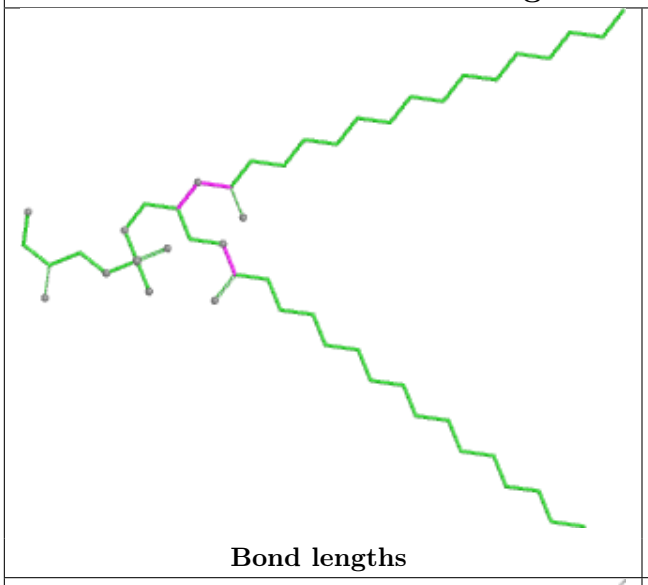


Torsions



Rings

Ligand LHG B 640



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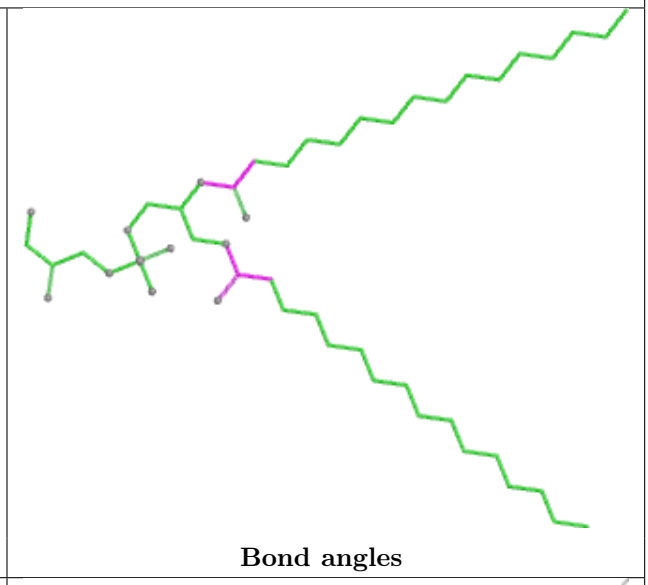
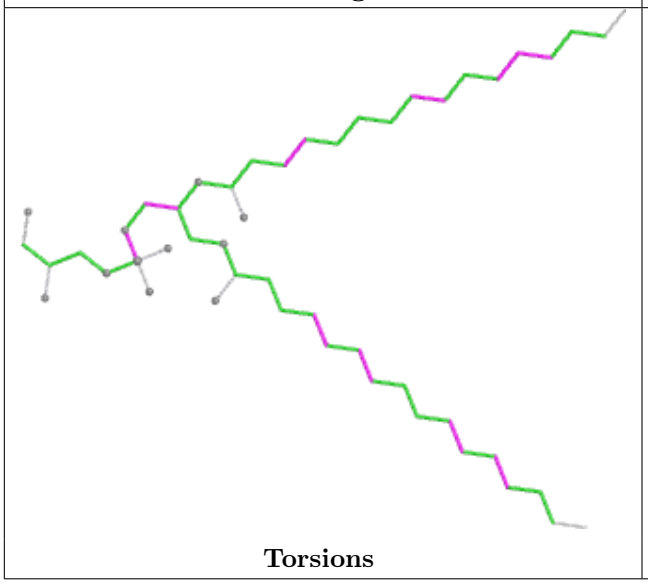


Bond angles



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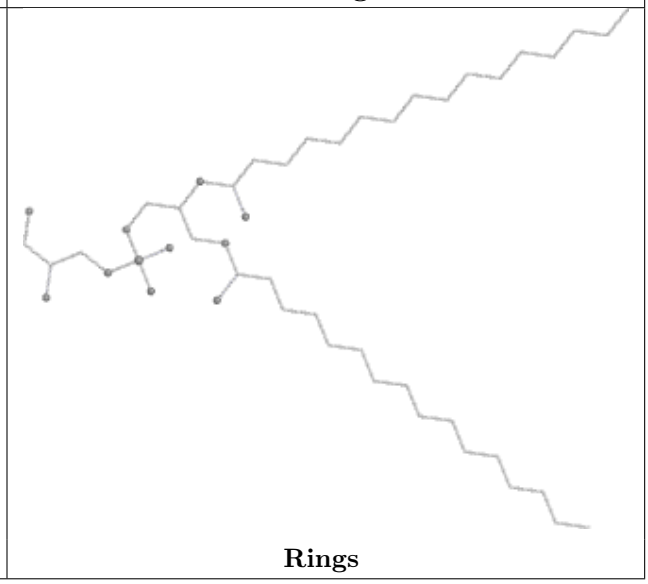
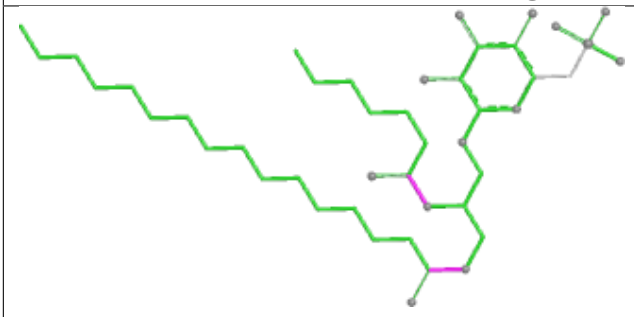


Rings

Ligand SQD D 408



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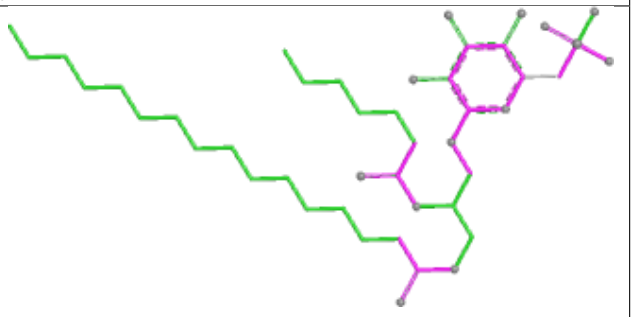
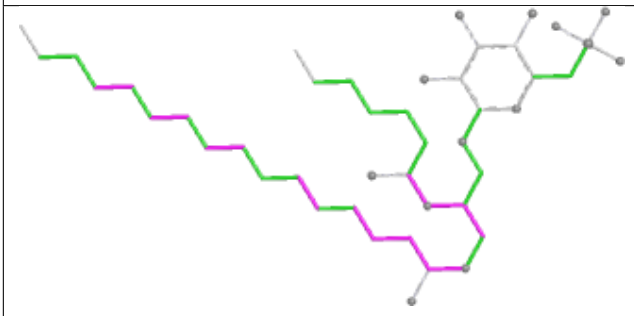
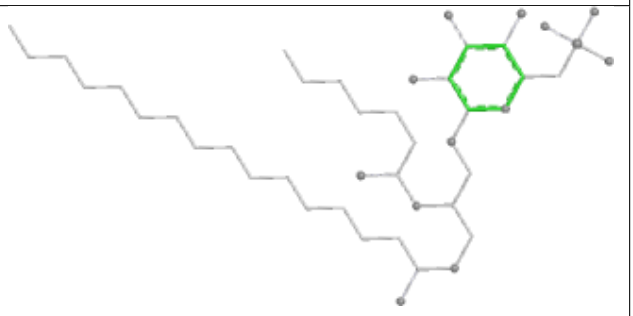


Bond angles

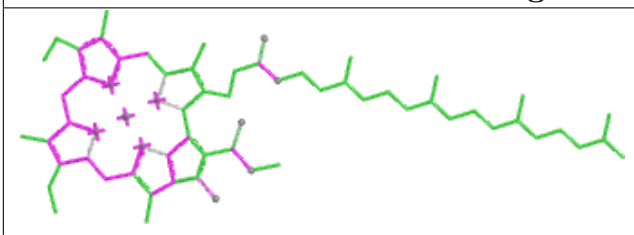


Torsions



Rings

Ligand CLA b 614



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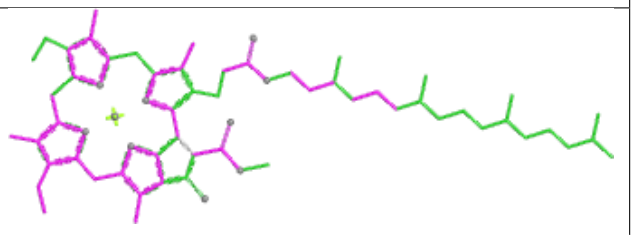
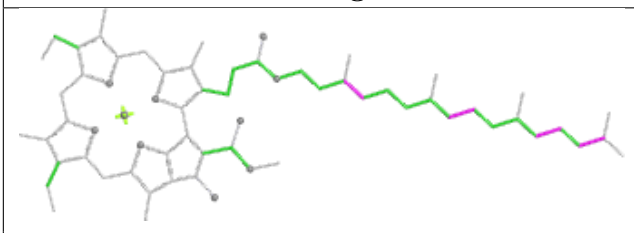
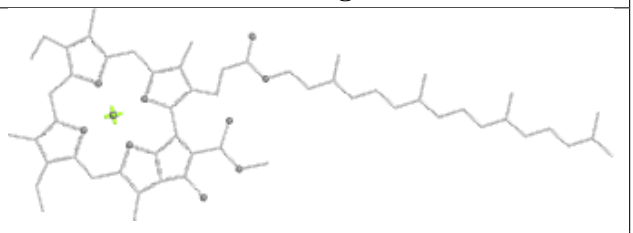


Bond angles

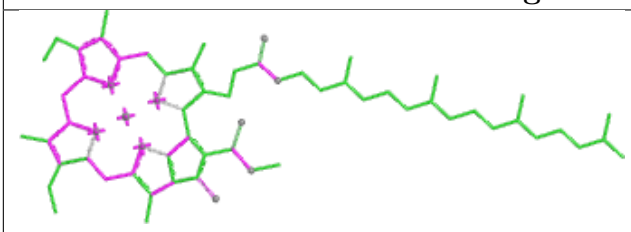


Torsions



Rings

Ligand CLA D 404



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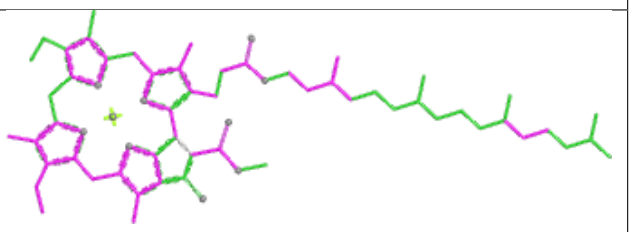
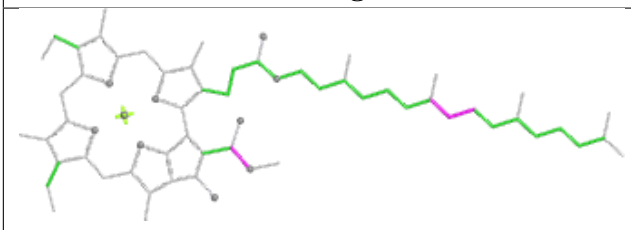
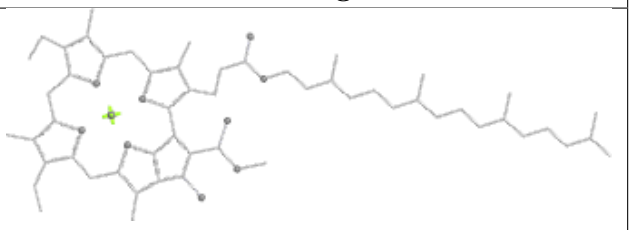


Bond angles

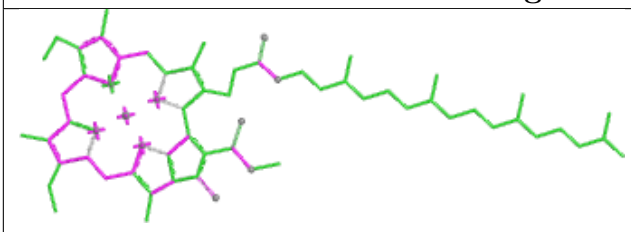


Torsions

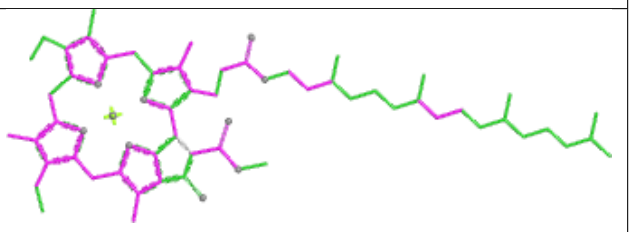


Rings

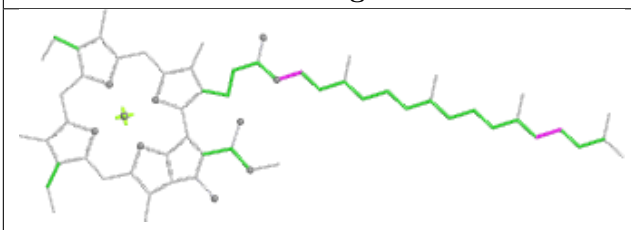
Ligand CLA B 609



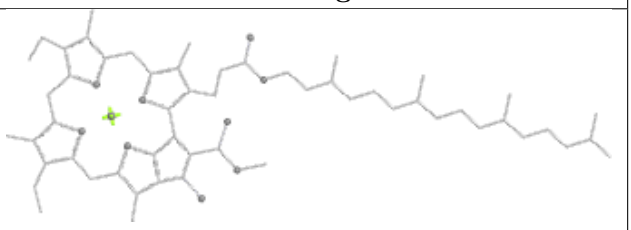
Bond lengths



Bond angles

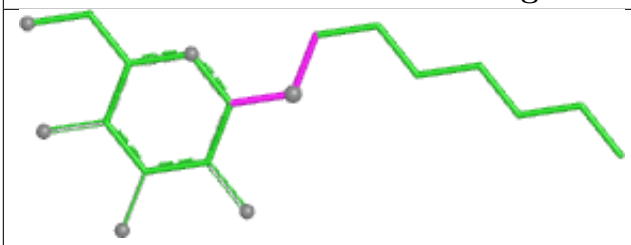


Torsions

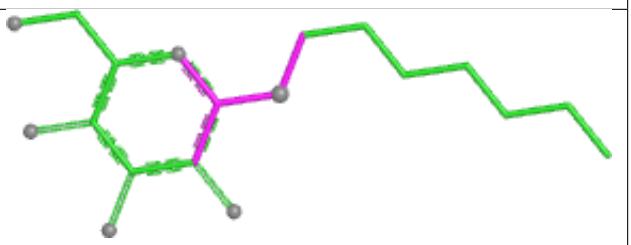


Rings

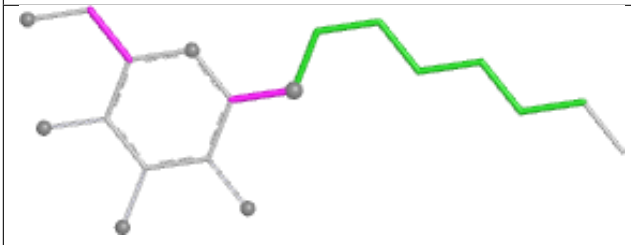
Ligand HTG B 624



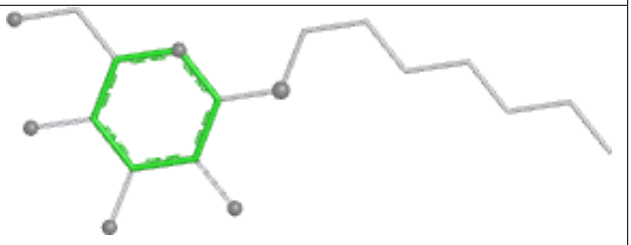
Bond lengths



Bond angles

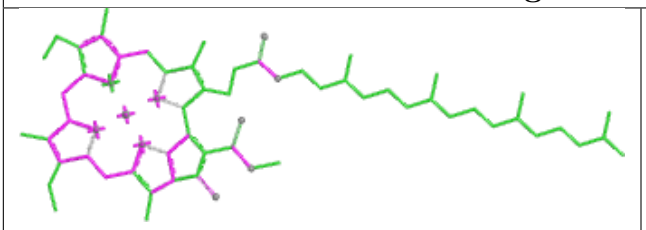


Torsions

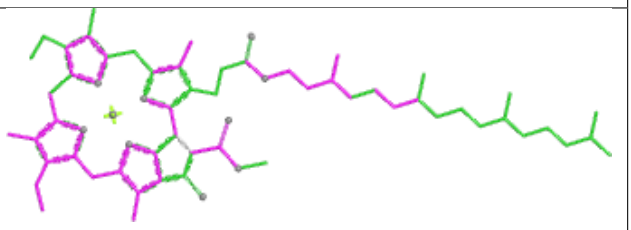


Rings

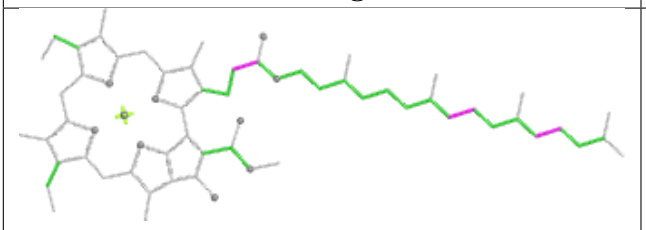
Ligand CLA C 511



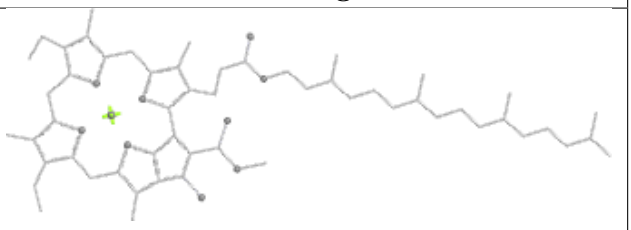
Bond lengths



Bond angles

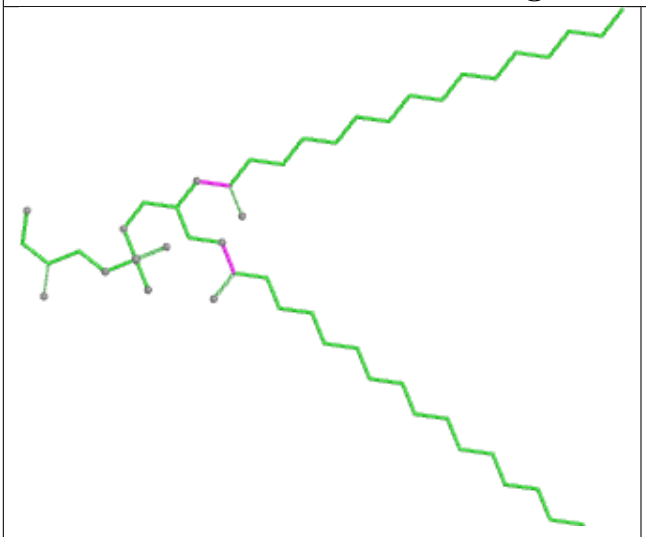


Torsions

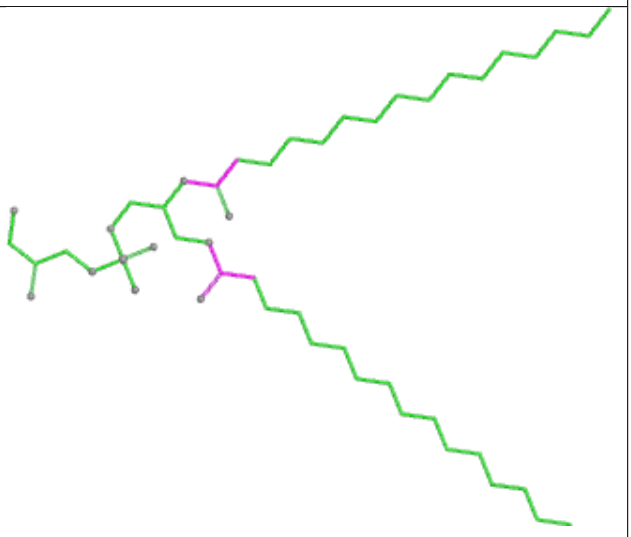


Rings

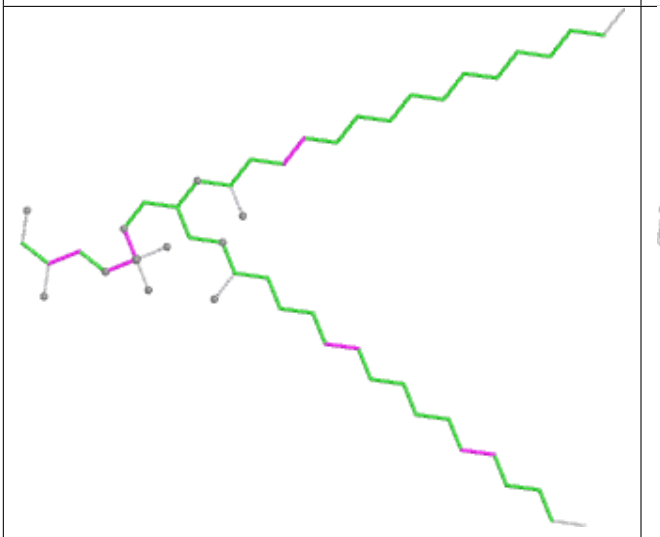
Ligand LHG d 409



Bond lengths



Bond angles



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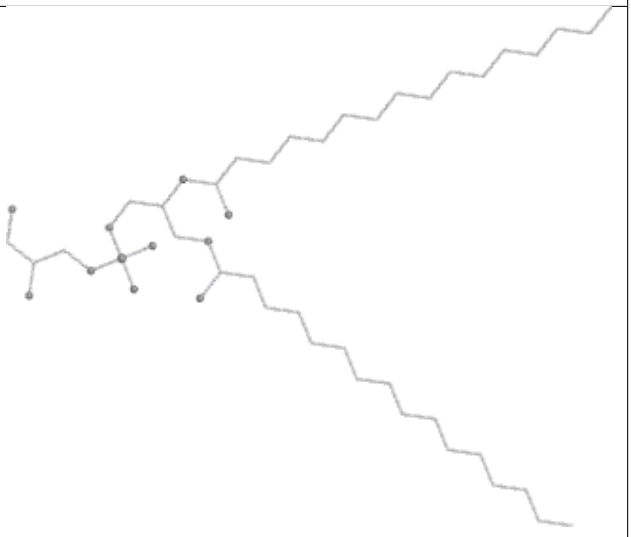
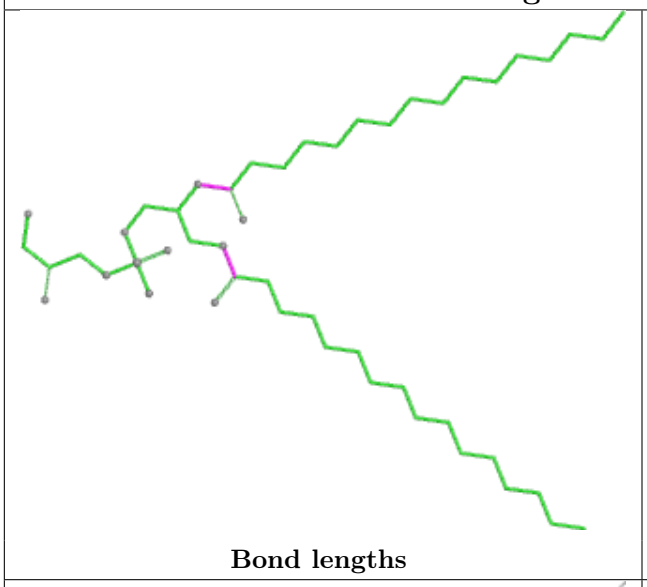
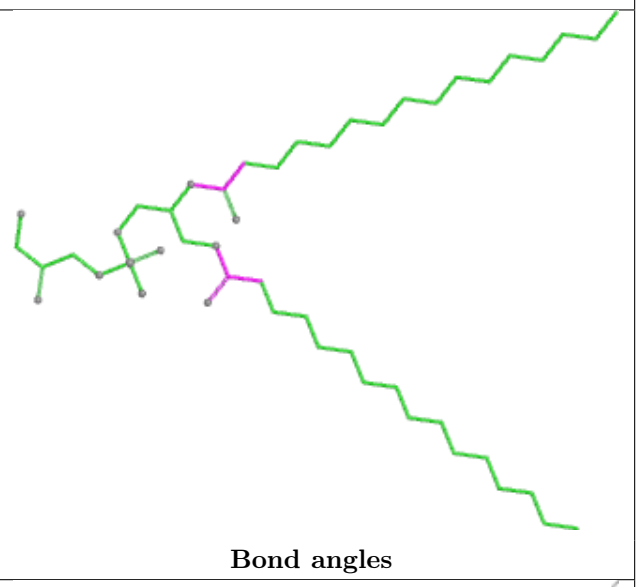


Rings

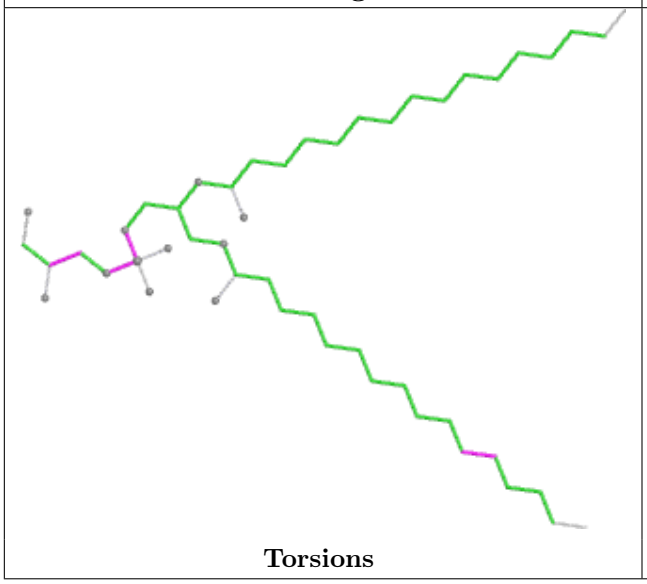
Ligand LHG D 410



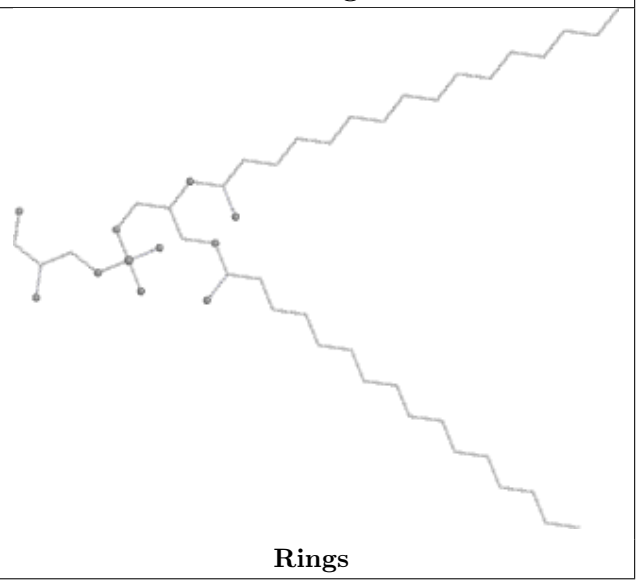
Bond lengths



Bond angles



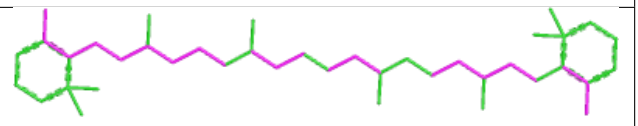
Torsions



Rings

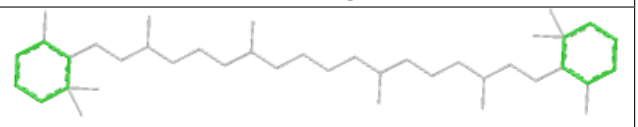
Ligand BCR K 101

Bond lengths



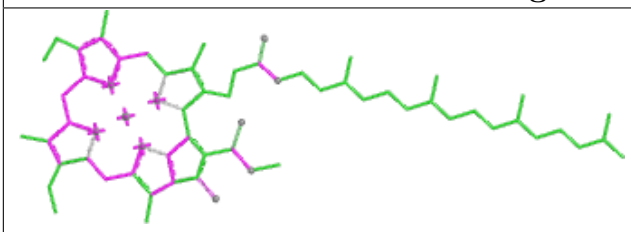
Bond angles

Torsions

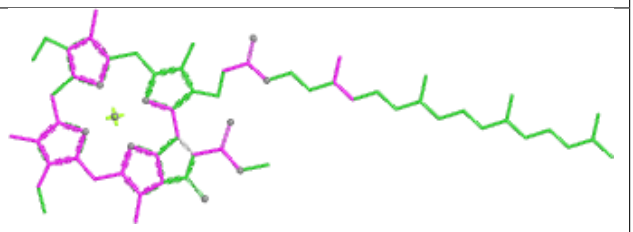


Rings

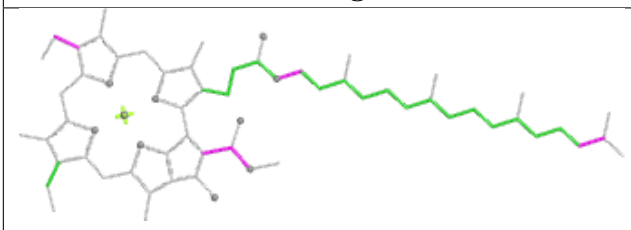
Ligand CLA c 504



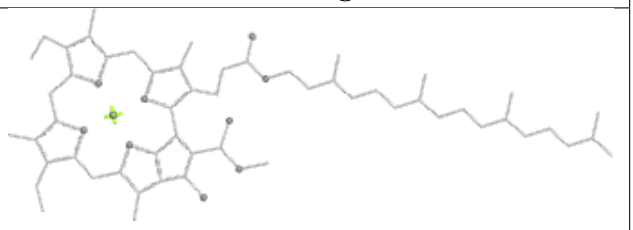
Bond lengths



Bond angles



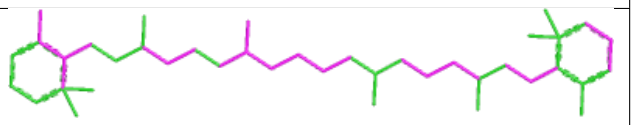
Torsions



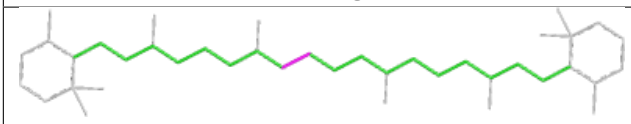
Rings

Ligand BCR B 641

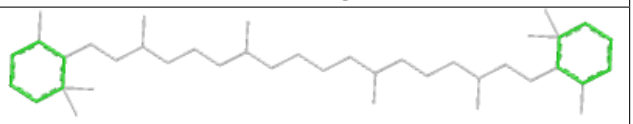
Bond lengths



Bond angles

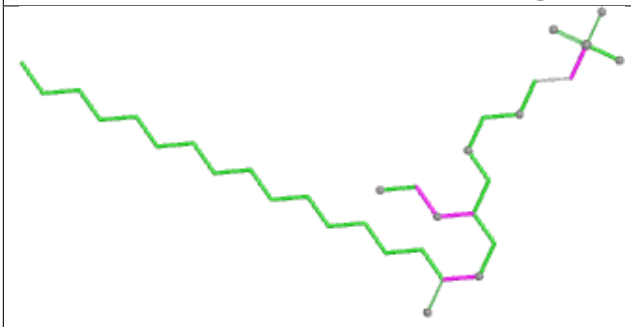


Torsions



Rings

Ligand SQD f 102



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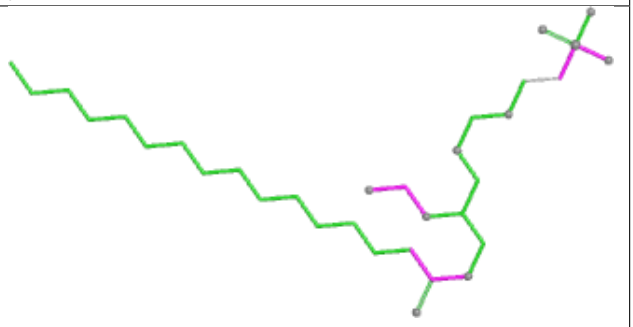
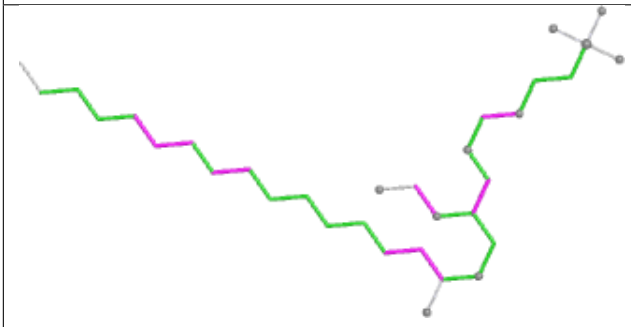
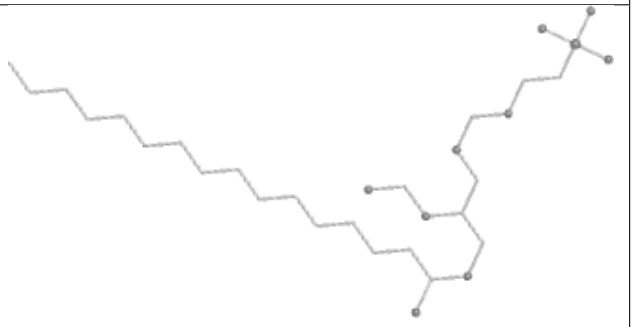


Bond angles

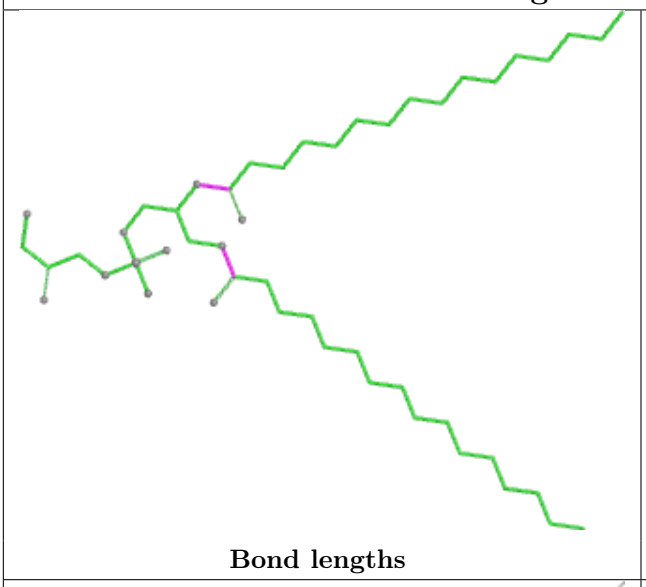


Torsions



Rings

Ligand LHG l 302



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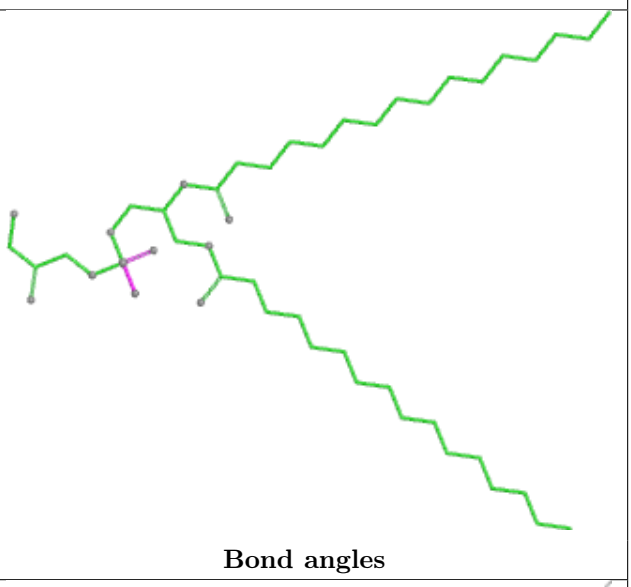
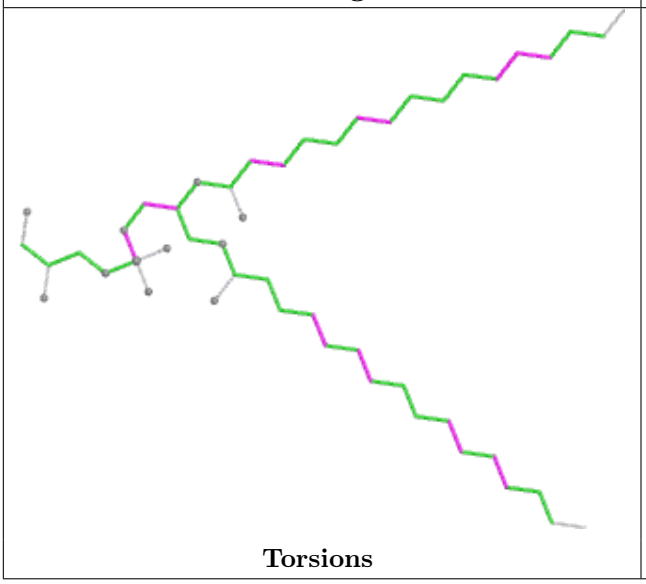


Bond angles



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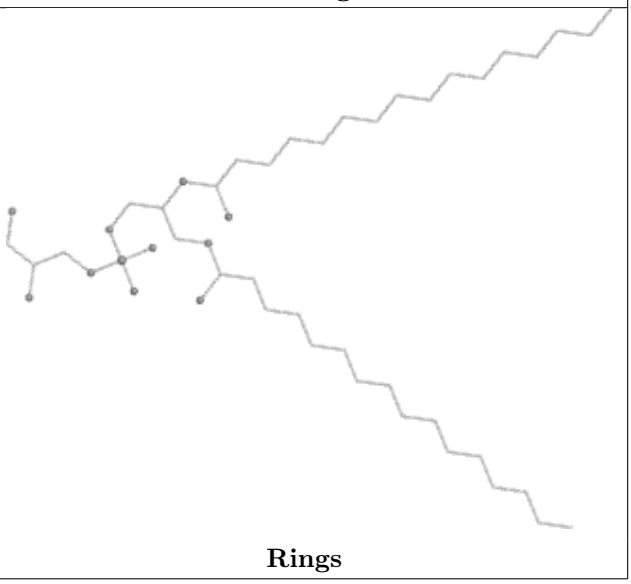
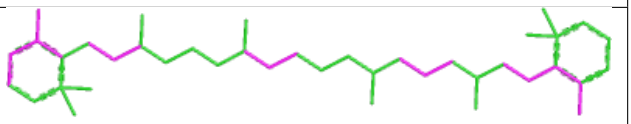


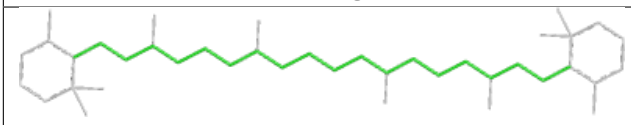
Rings

Ligand BCR c 517

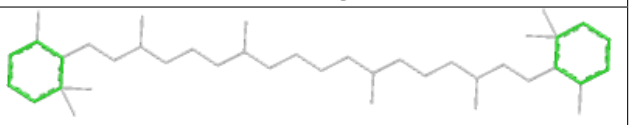
Bond lengths



Bond angles

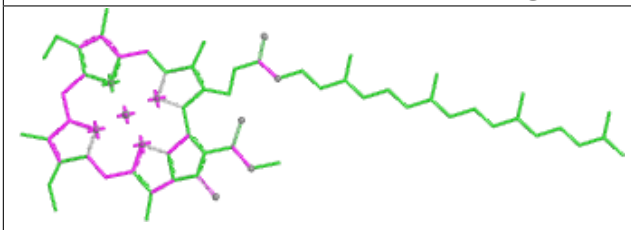


Torsions



Rings

Ligand CLA B 605



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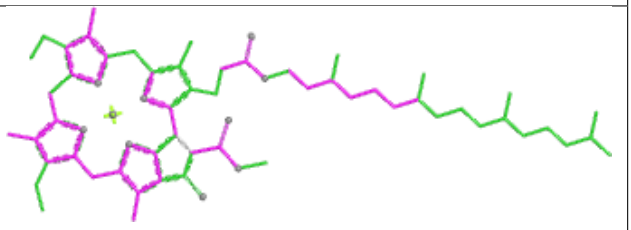
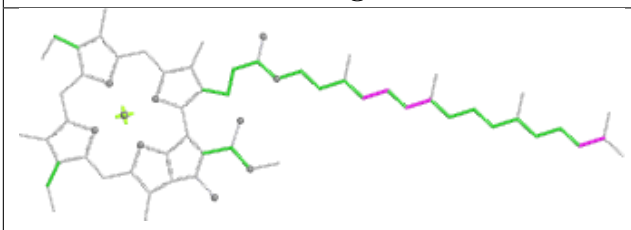


Bond angles



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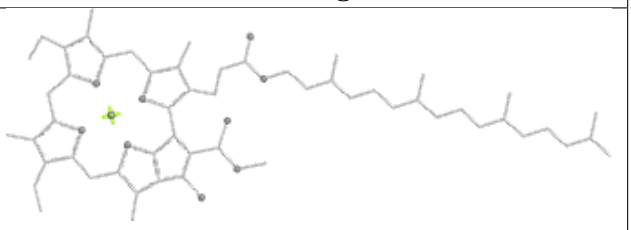
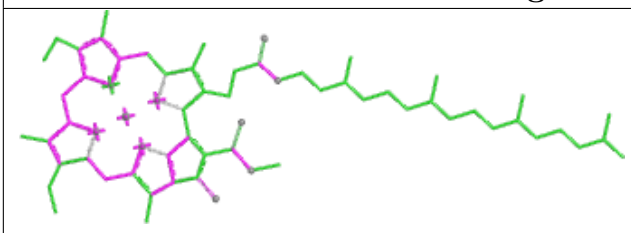


Rings

Ligand CLA b 608



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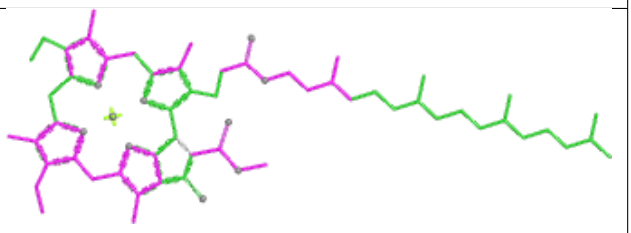
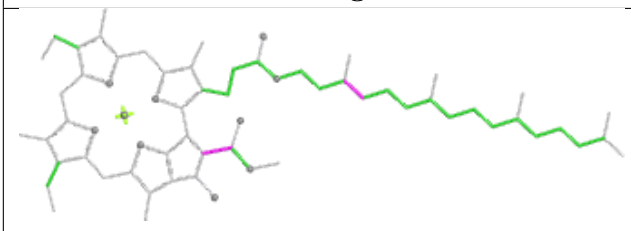
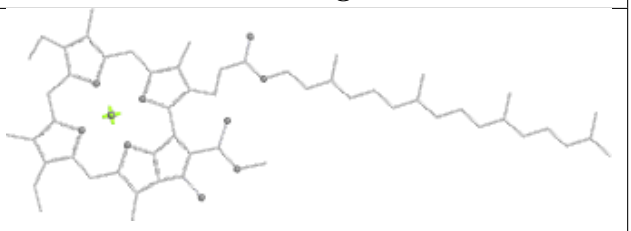


Bond angles

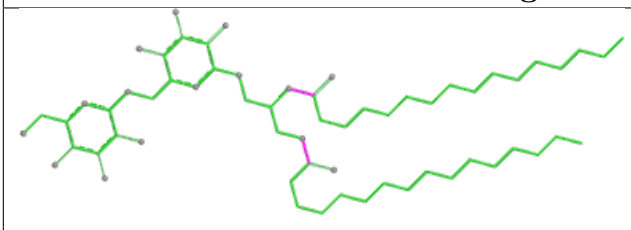


Torsions

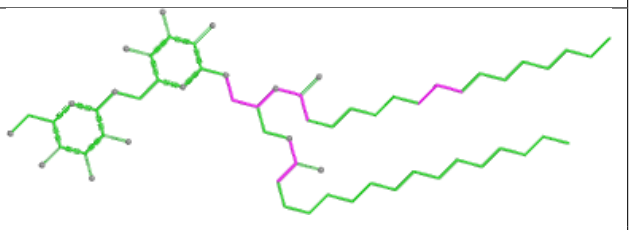


Rings

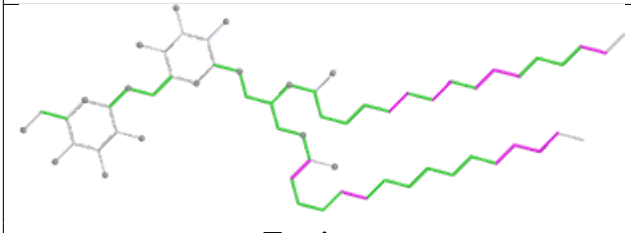
Ligand DGD C 519



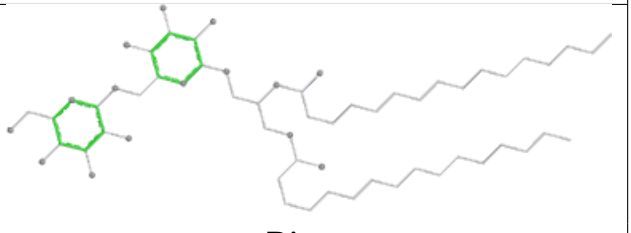
Bond lengths



Bond angles

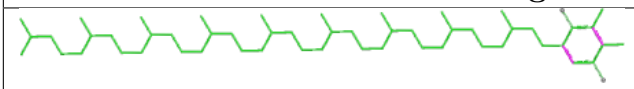


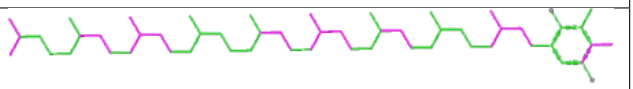
Torsions

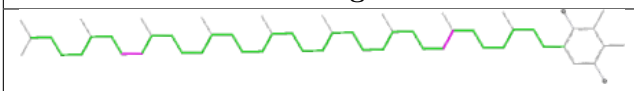


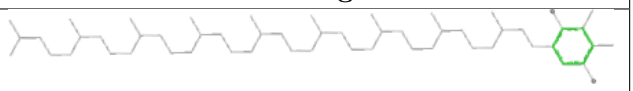
Rings

Ligand PL9 D 406

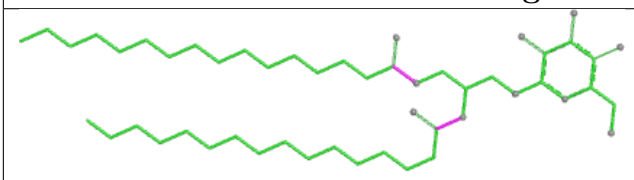

Bond lengths

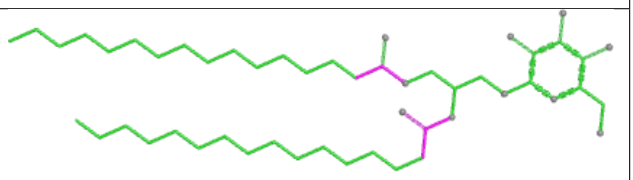

Bond angles

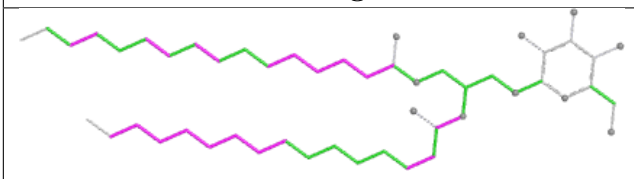

Torsions

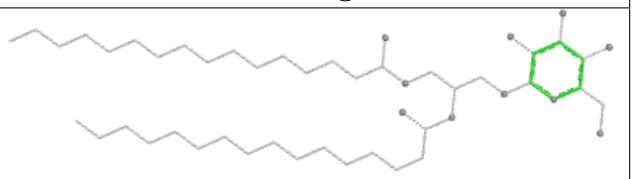

Rings

Ligand LMG b 623

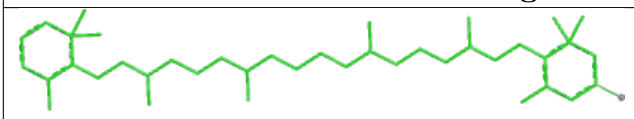

Bond lengths


Bond angles


Torsions


Rings

Ligand RRX H 101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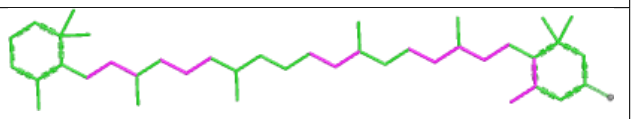
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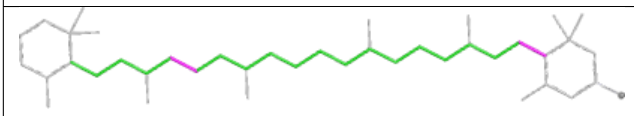
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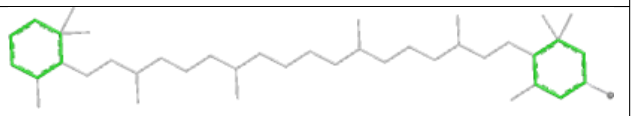
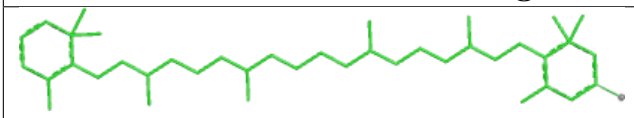

Rings

Ligand RRX h 1204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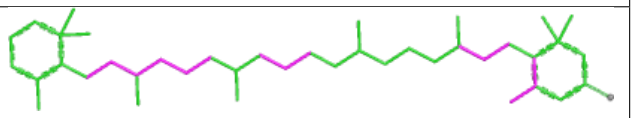
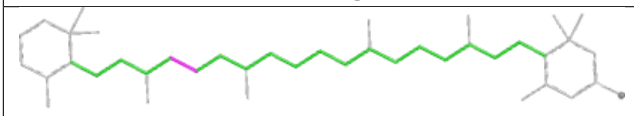
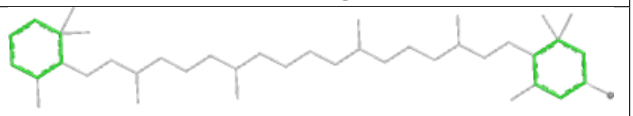
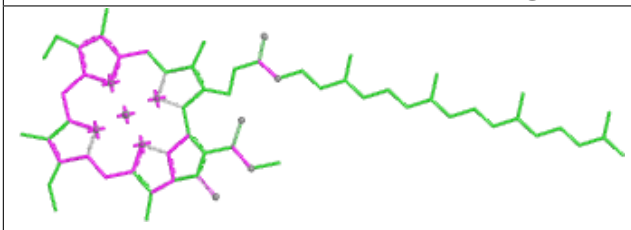

Bond angles


Torsions


Rings

Ligand CLA A 406



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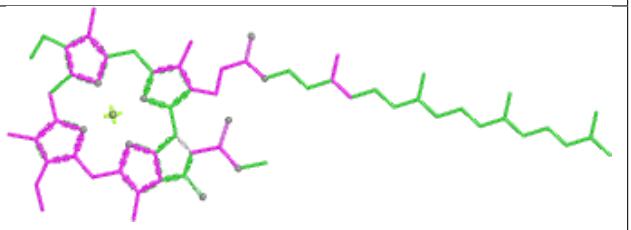
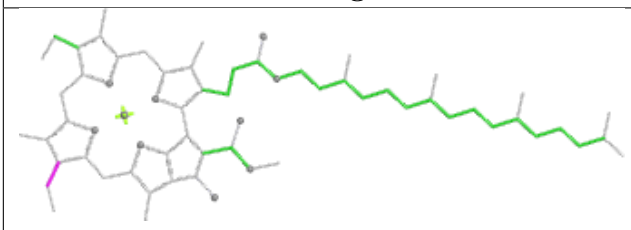


Bond angles



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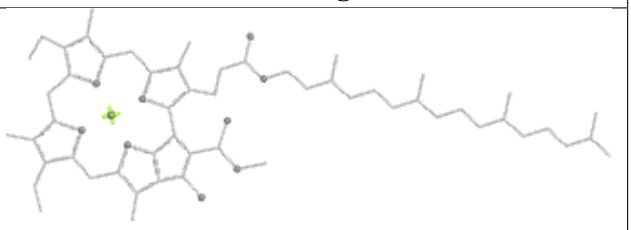
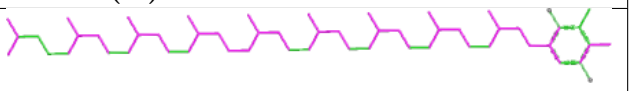


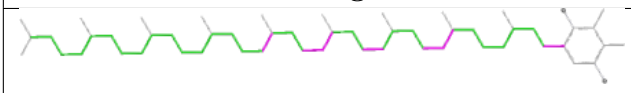
Rings

Ligand PL9 a 425 (B)

Bond lengths



Bond angles



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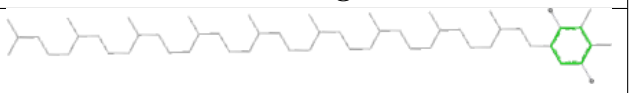
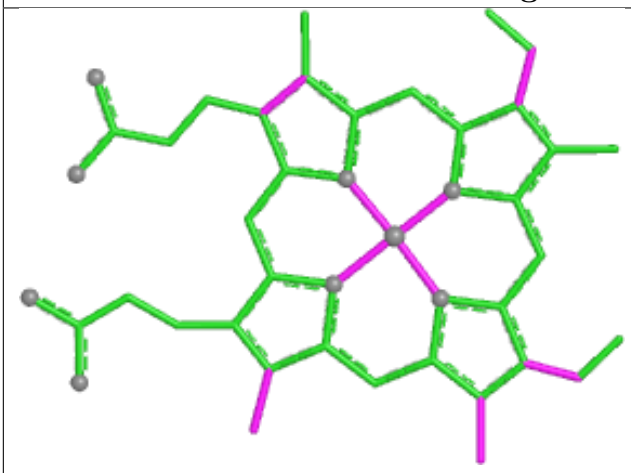


Rings

Ligand HEM F 101



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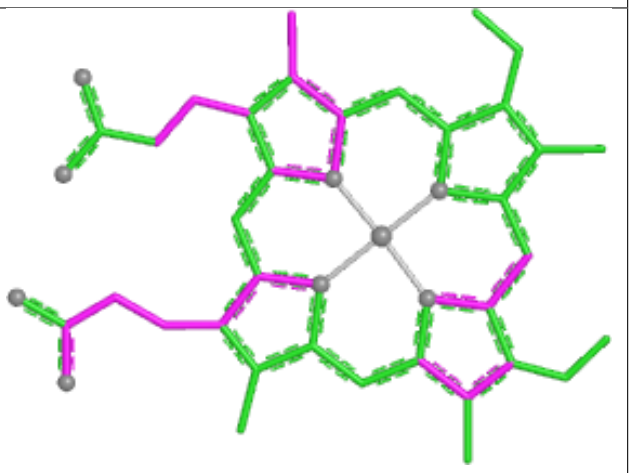
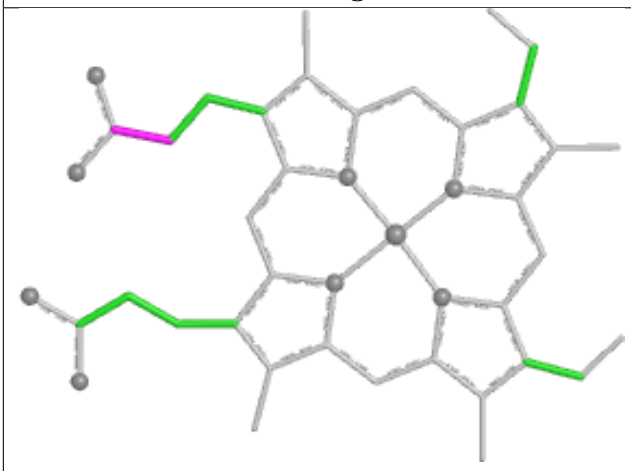
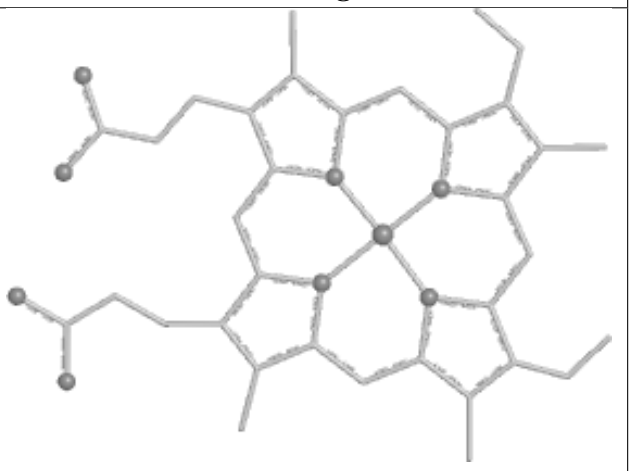


Bond angles

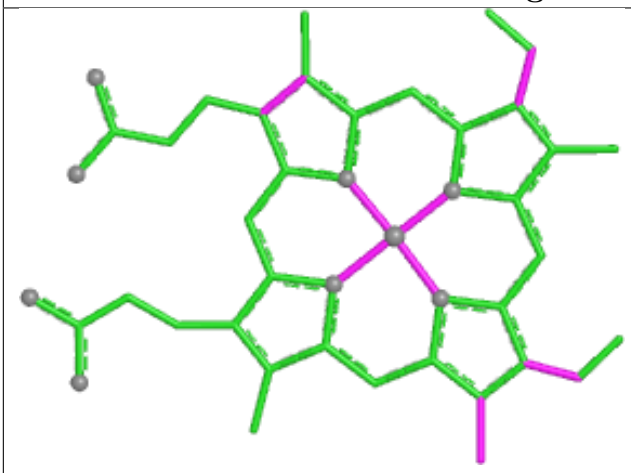


Torsions



Rings

Ligand HEM f 101



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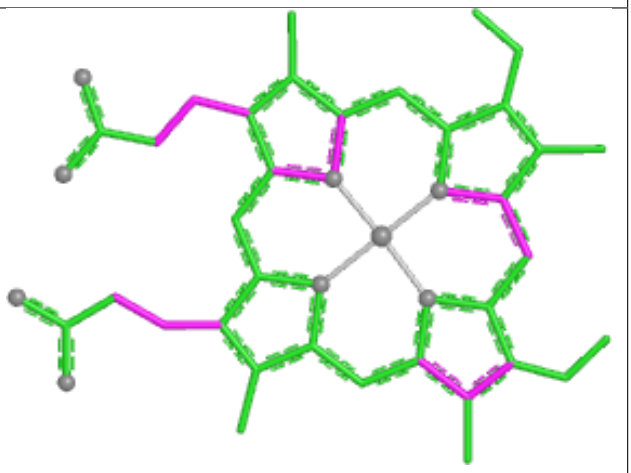
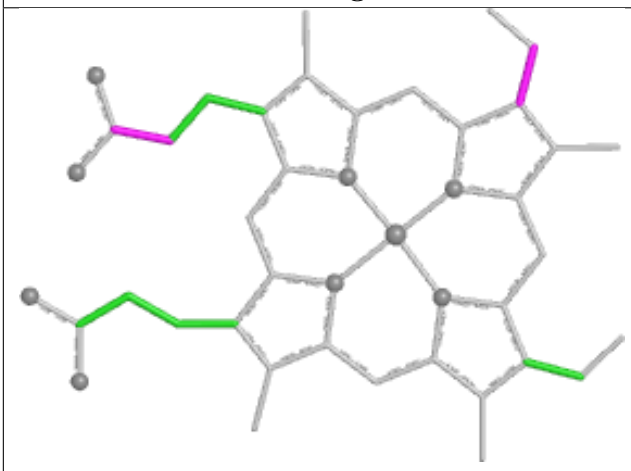


Bond angles



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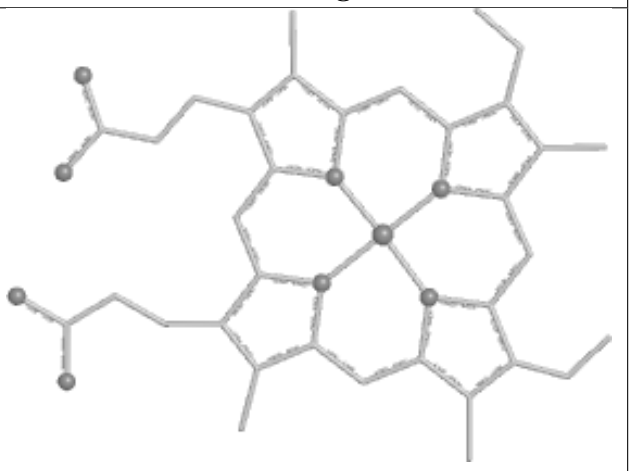
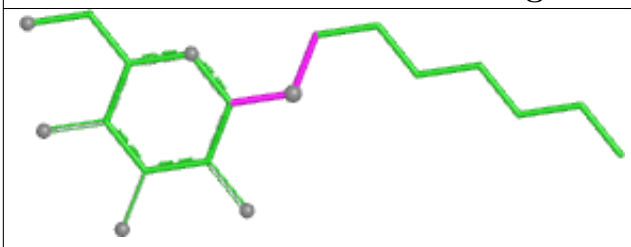


Rings

Ligand HTG c 524



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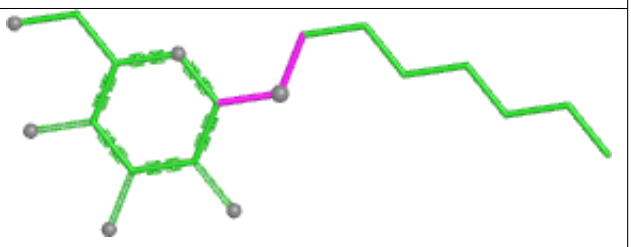
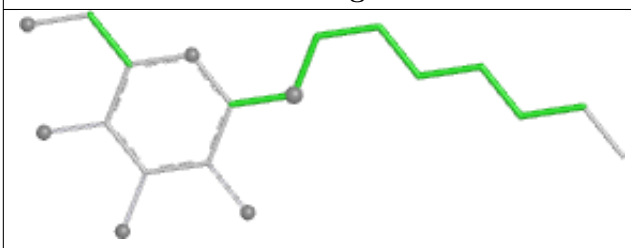


Bond angles



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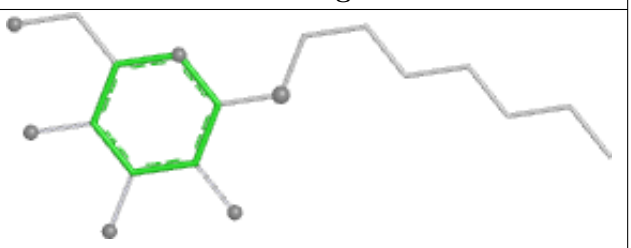
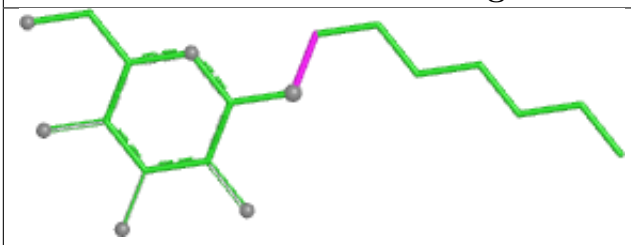


Rings

Ligand HTG B 623 (A)



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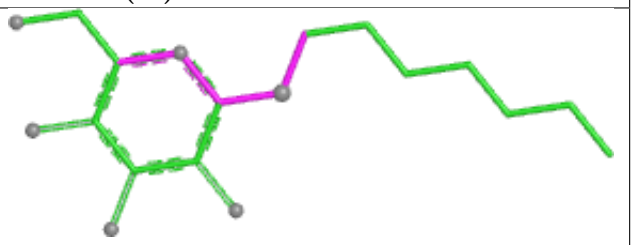
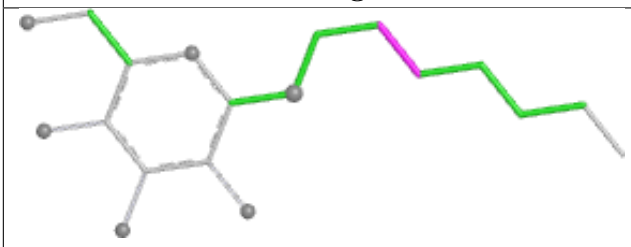


Bond angles



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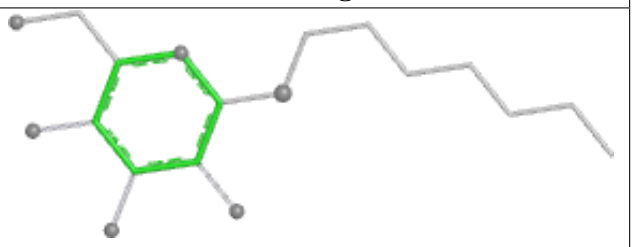
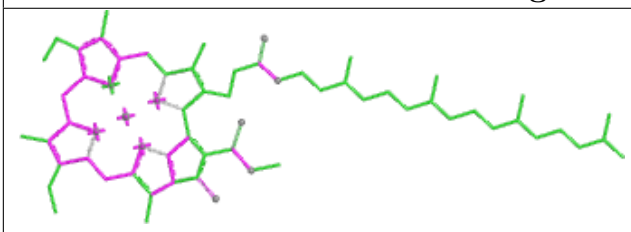
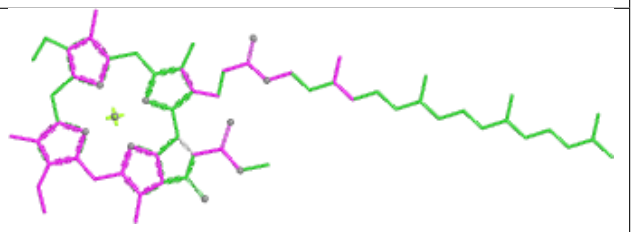


Rings

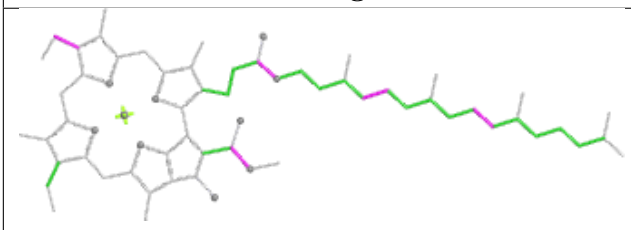
Ligand CLA c 515



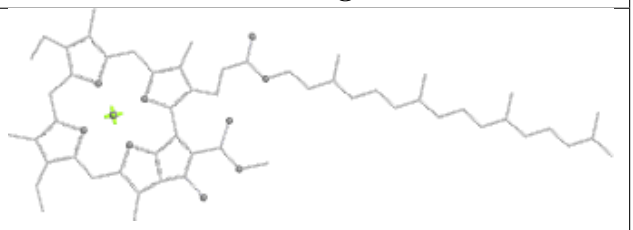
Bond lengths



Bond angles

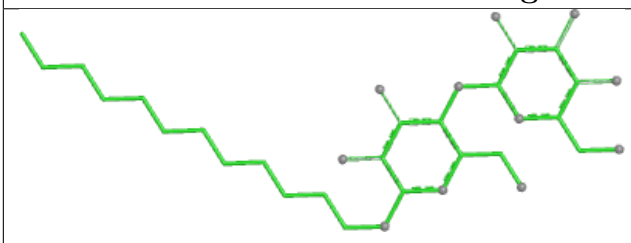


Torsions



Rings

Ligand LMT A 414



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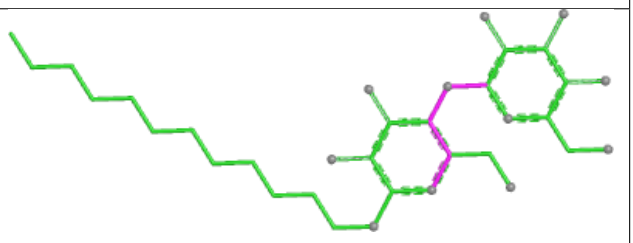
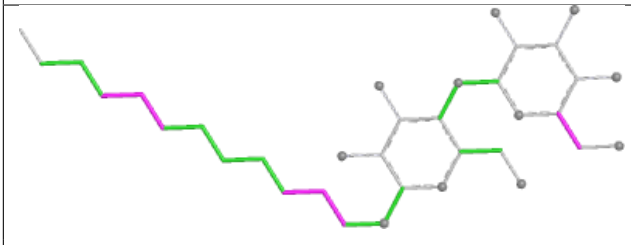


Bond angles



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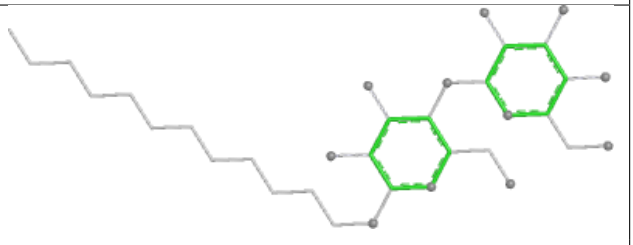
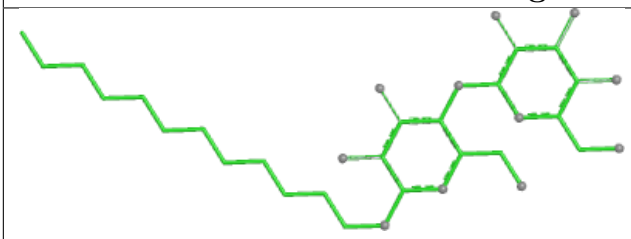


Rings

Ligand LMT f 104



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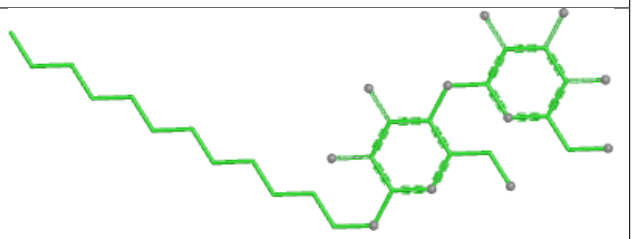
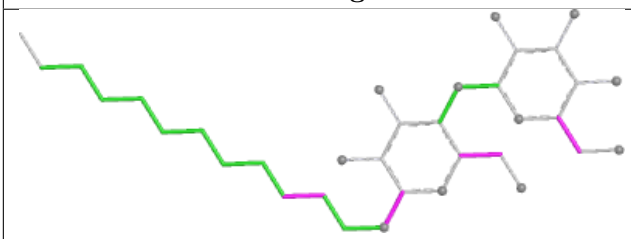
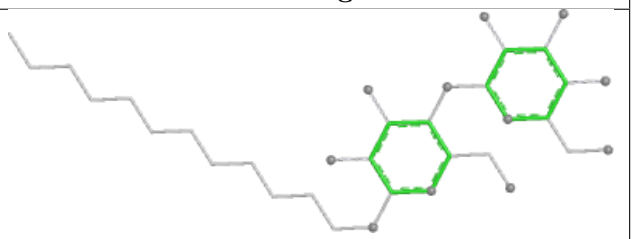


Bond angles

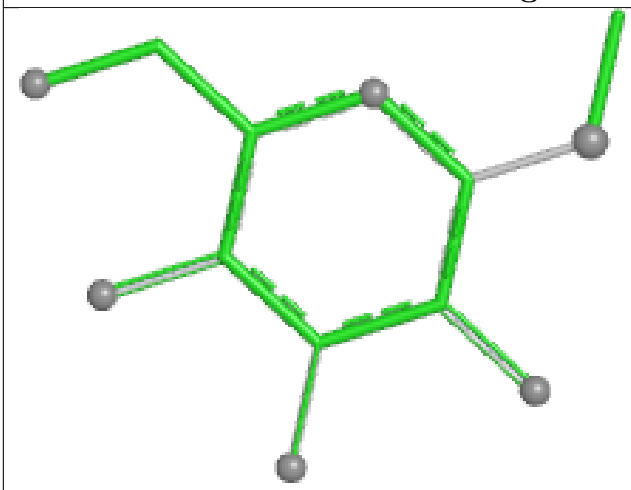


Torsions

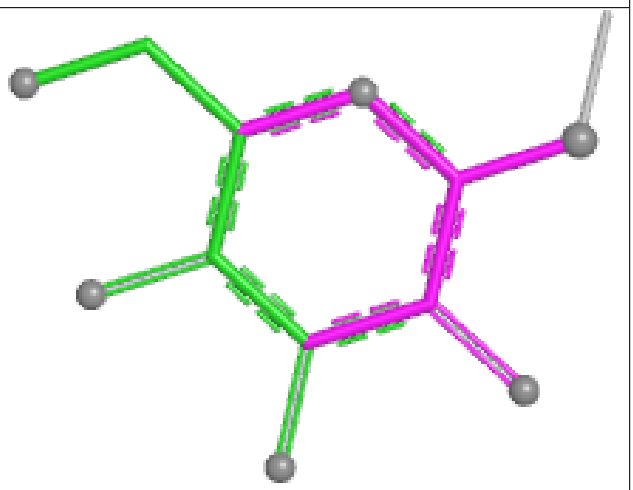


Rings

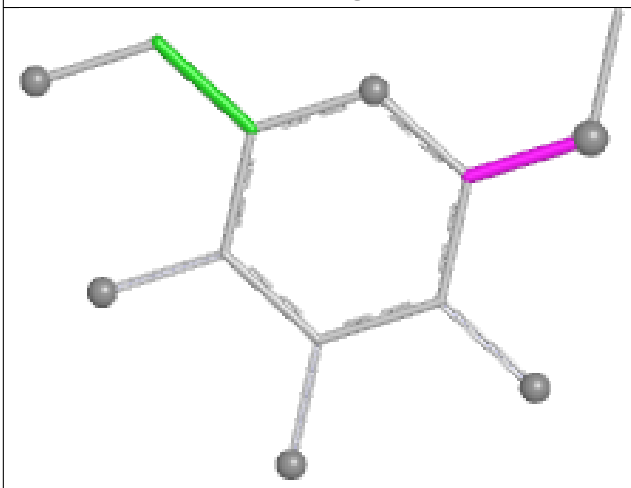
Ligand HTG V 203



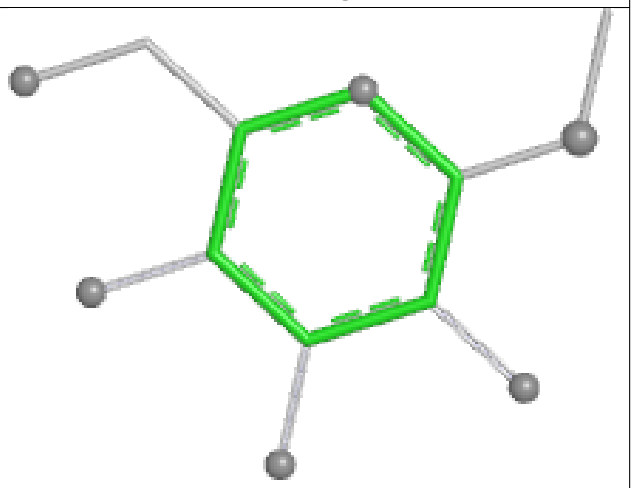
Bond lengths



Bond angles

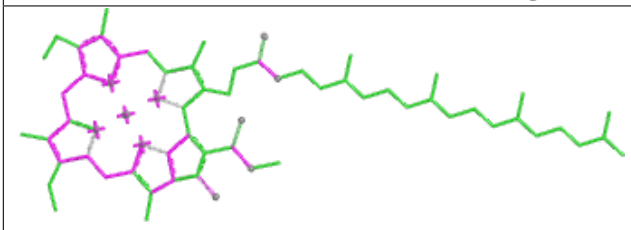


Torsions

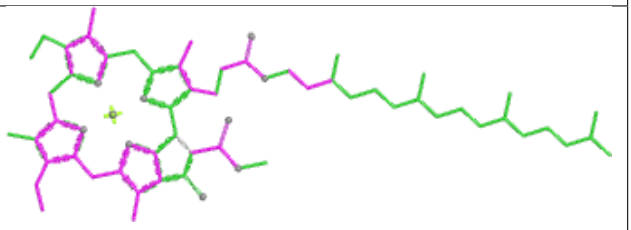


Rings

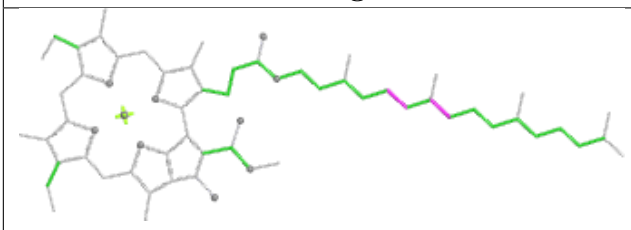
Ligand CLA C 509



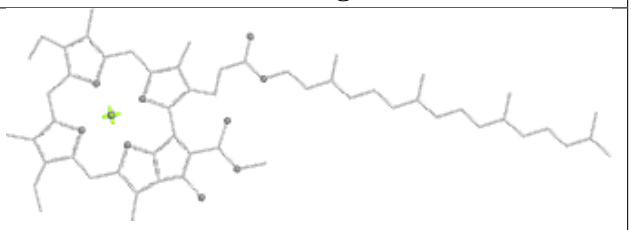
Bond lengths



Bond angles

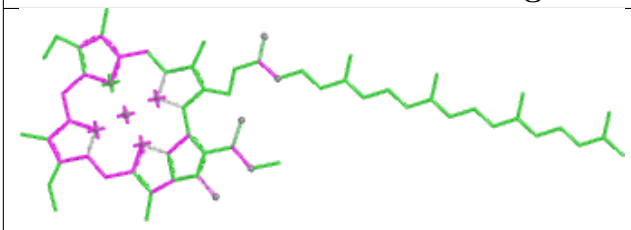


Torsions

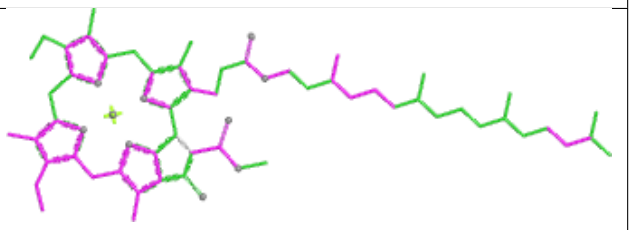


Rings

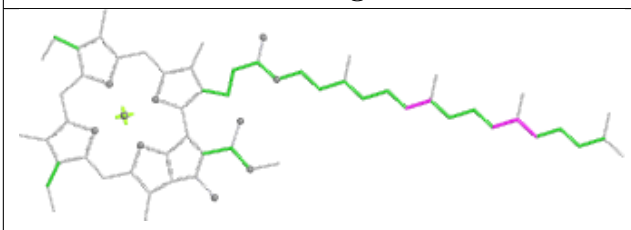
Ligand CLA C 505



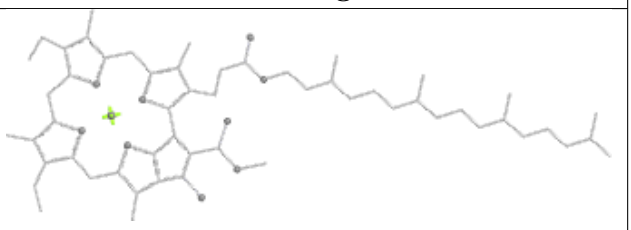
Bond lengths



Bond angles



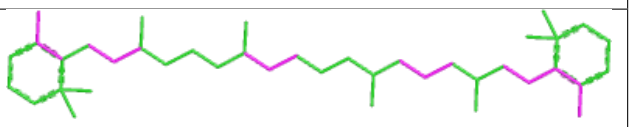
Torsions



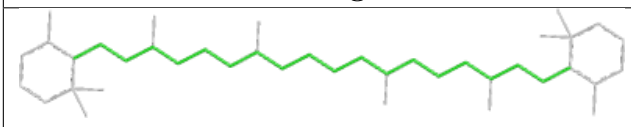
Rings

Ligand BCR C 516

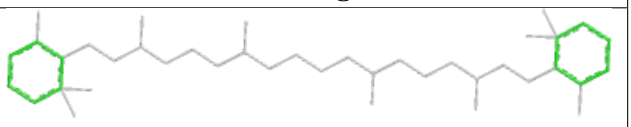
Bond lengths



Bond angles

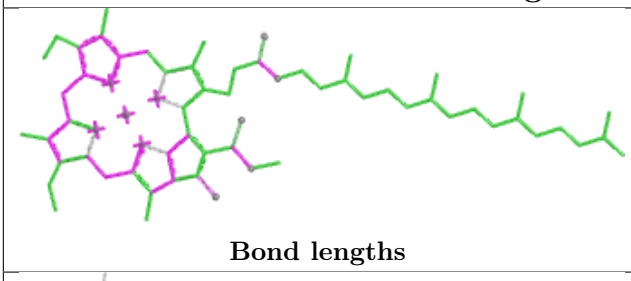


Torsions

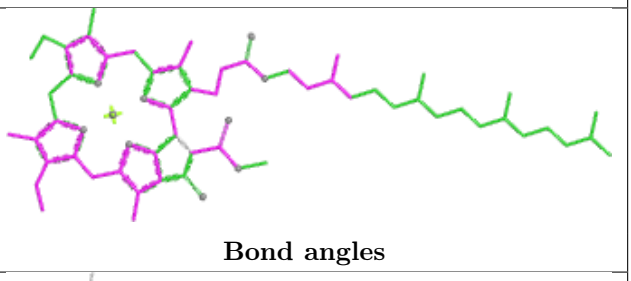


Rings

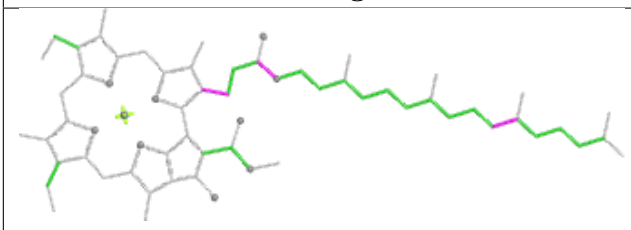
Ligand CLA C 513



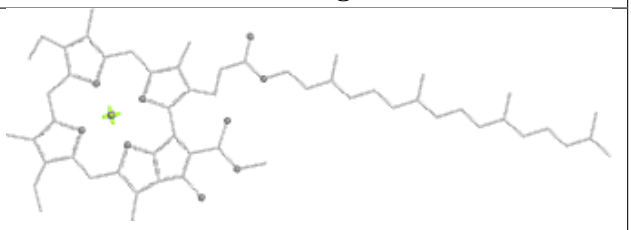
Bond lengths



Bond angles

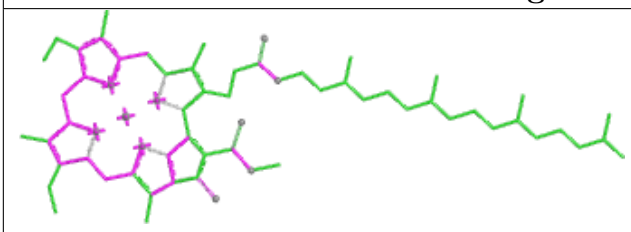


Torsions

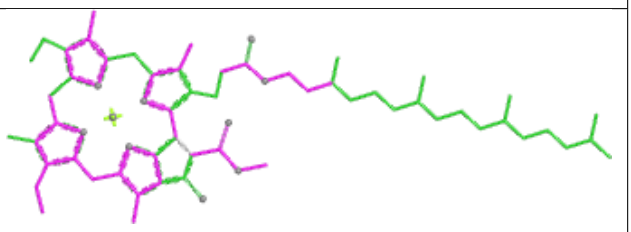


Rings

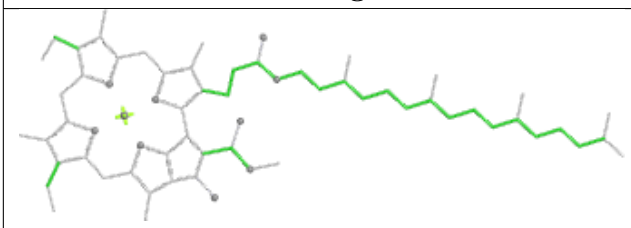
Ligand CLA b 616



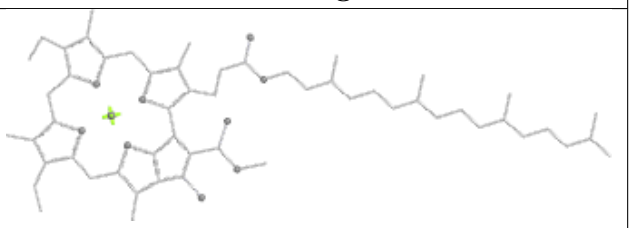
Bond lengths



Bond angles

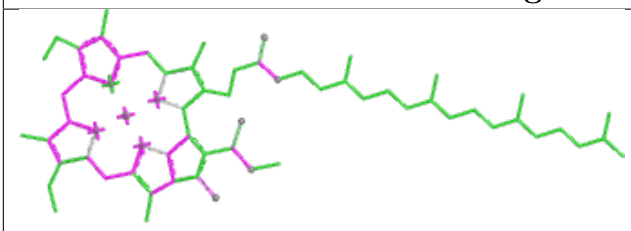


Torsions

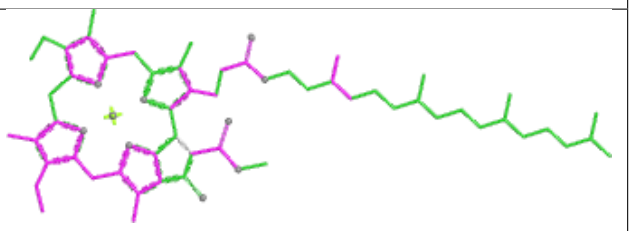


Rings

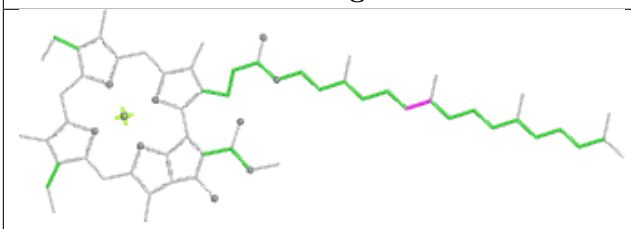
Ligand CLA B 604



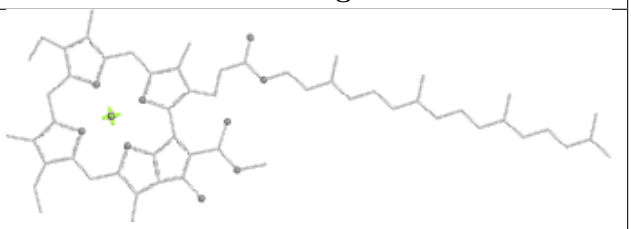
Bond lengths



Bond angles

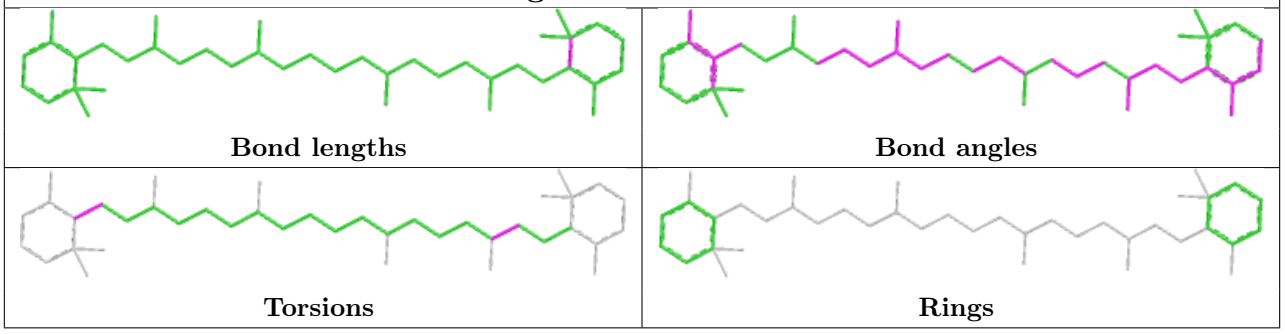


Torsions

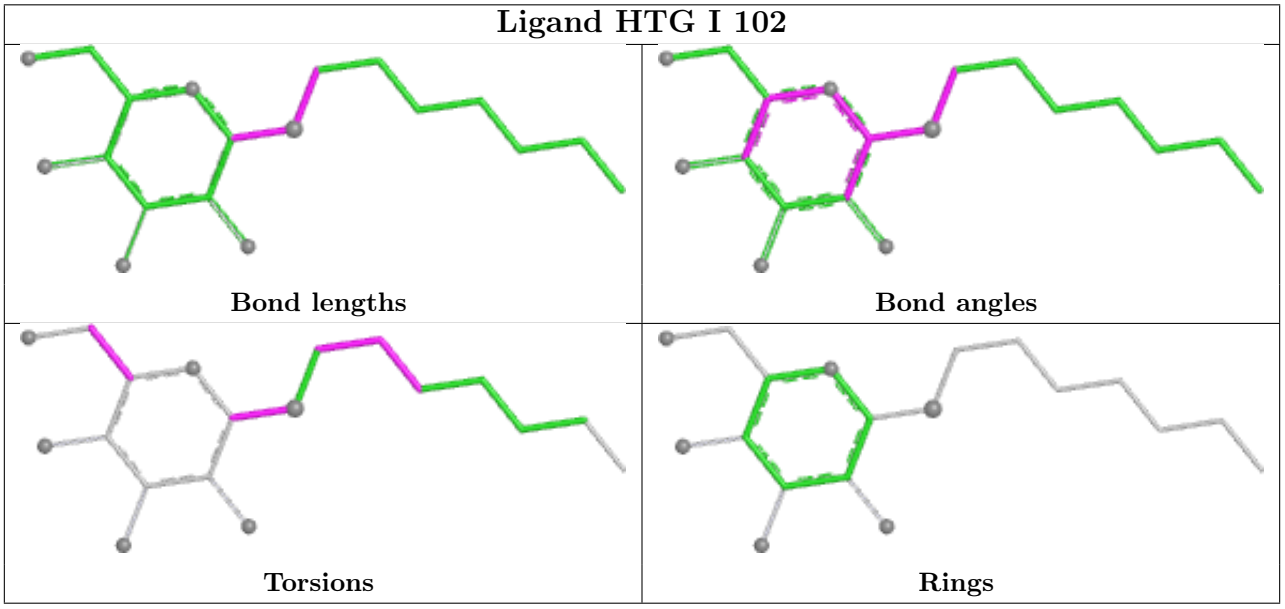


Rings

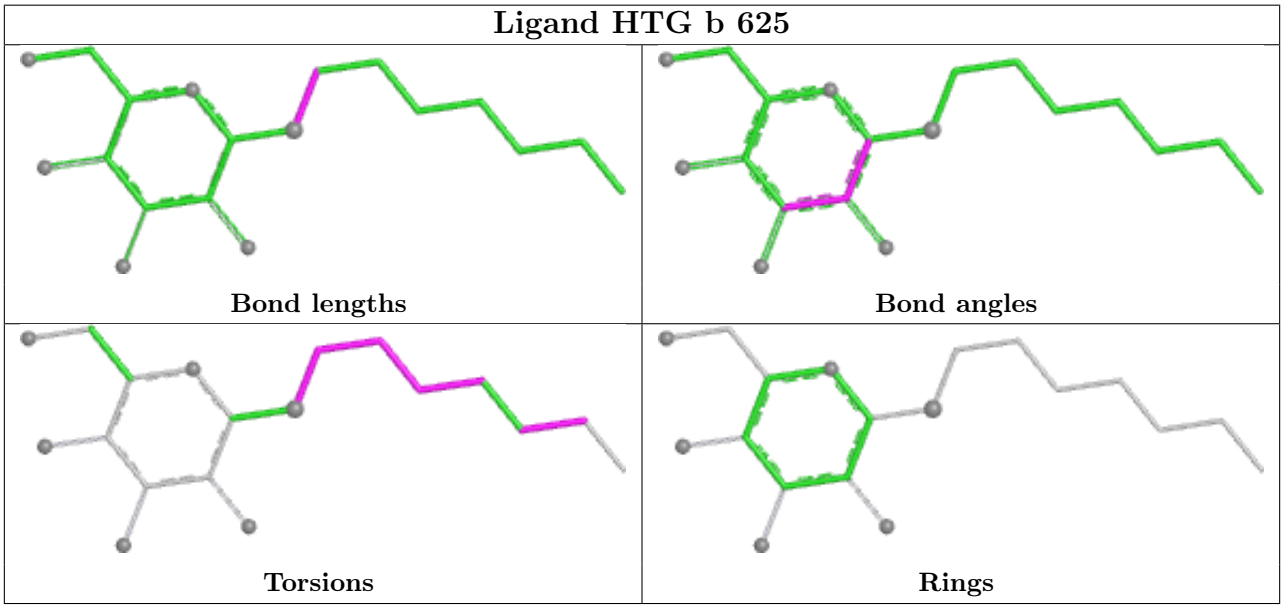
Ligand BCR k 302



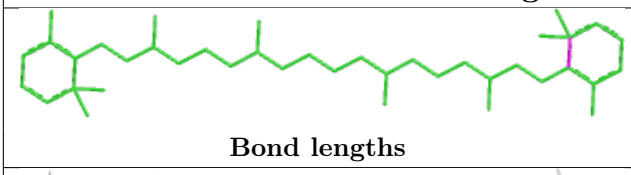
Ligand HTG I 102



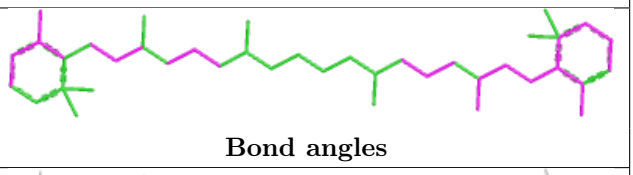
Ligand HTG b 625



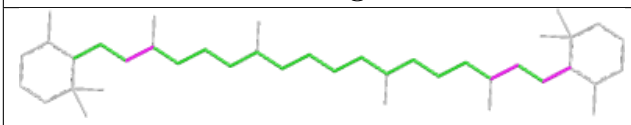
Ligand BCR D 405



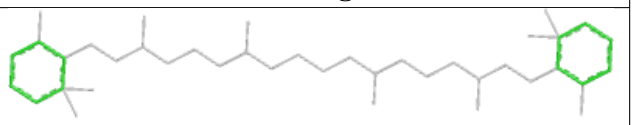
Bond lengths



Bond angles

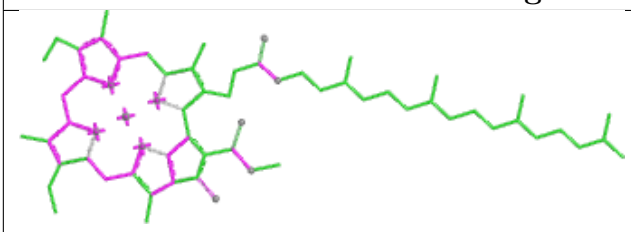


Torsions

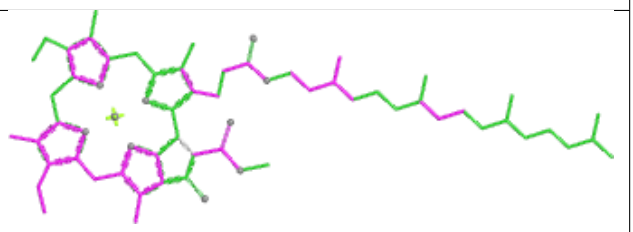


Rings

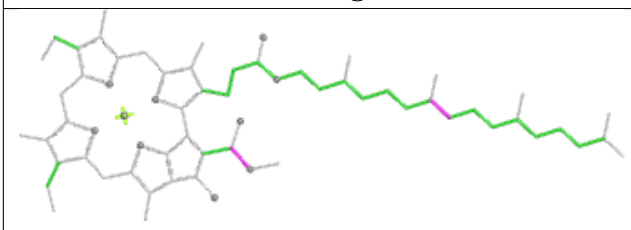
Ligand CLA C 514



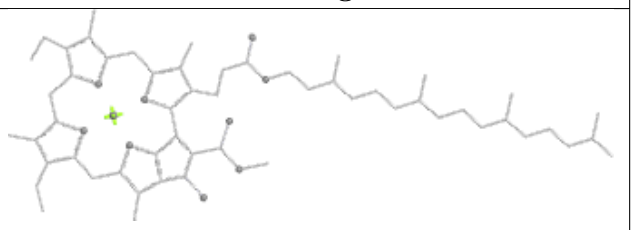
Bond lengths



Bond angles

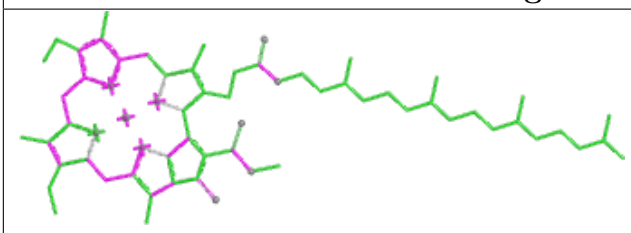


Torsions

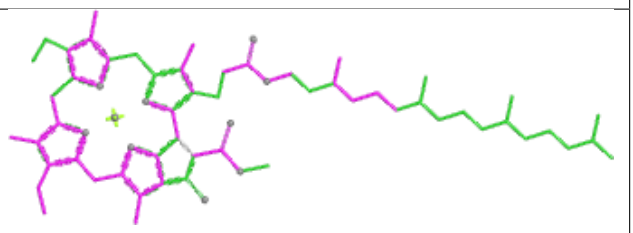


Rings

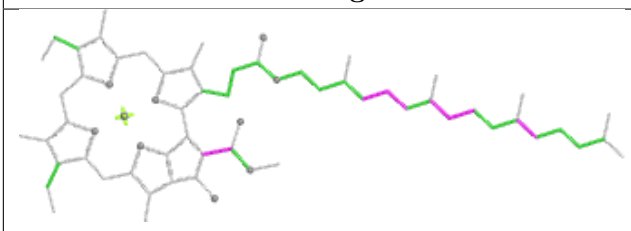
Ligand CLA B 615



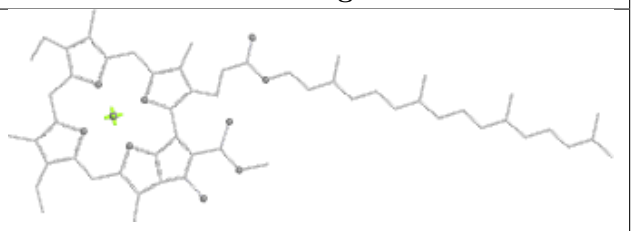
Bond lengths



Bond angles

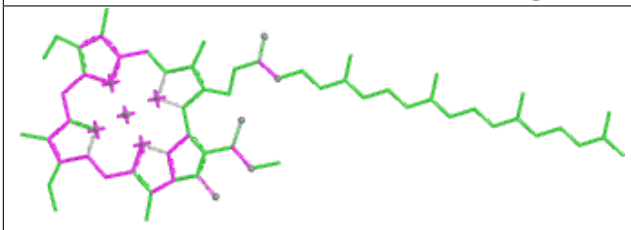


Torsions



Rings

Ligand CLA d 405



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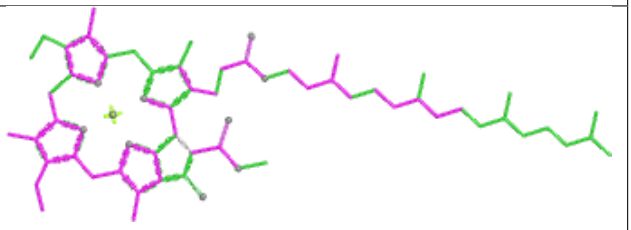
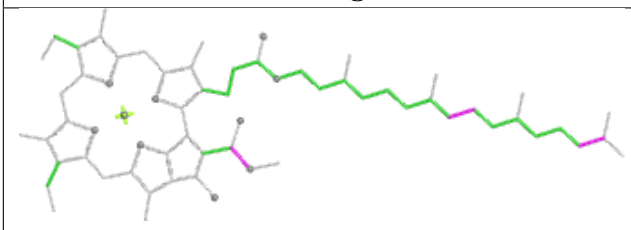
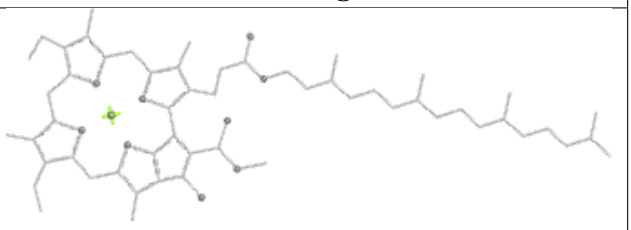


Bond angles

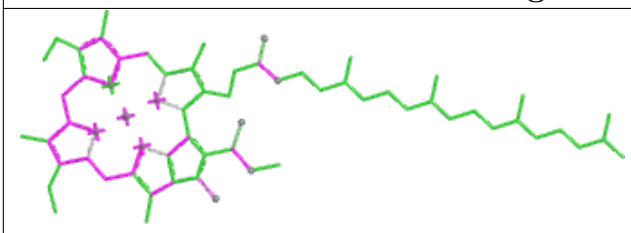


Torsions



Rings

Ligand CLA b 612



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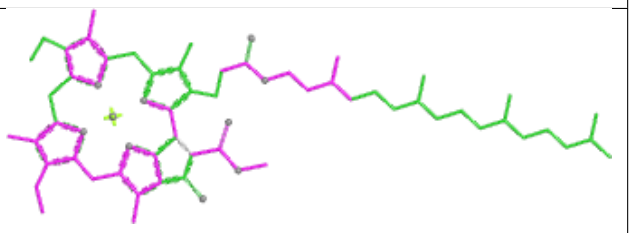
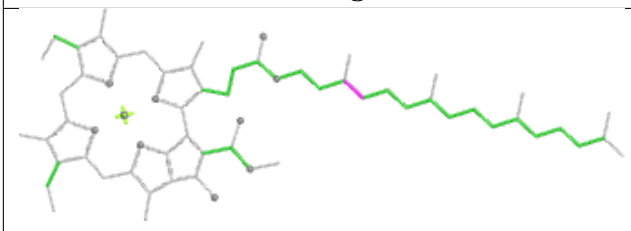
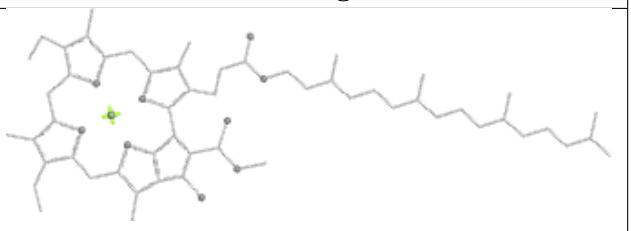


Bond angles

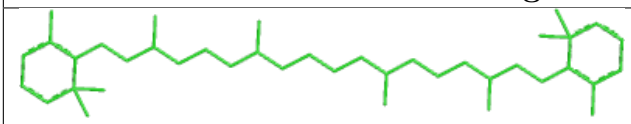


Torsions



Rings

Ligand BCR T 102



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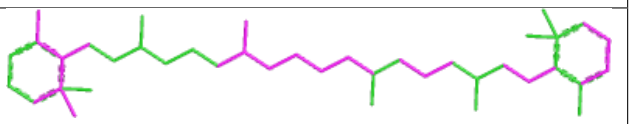
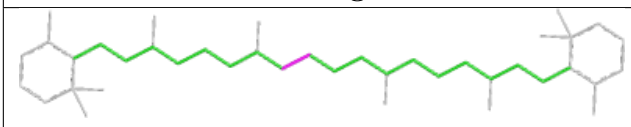
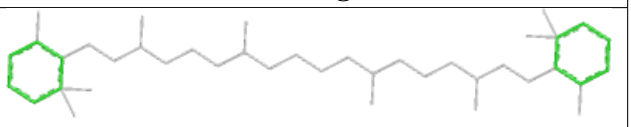


Bond angles

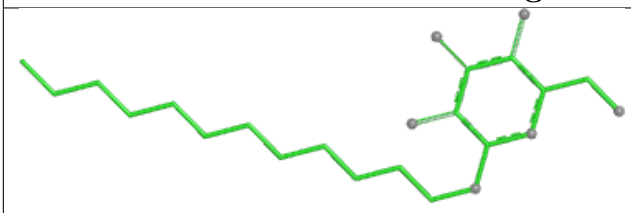


Torsions

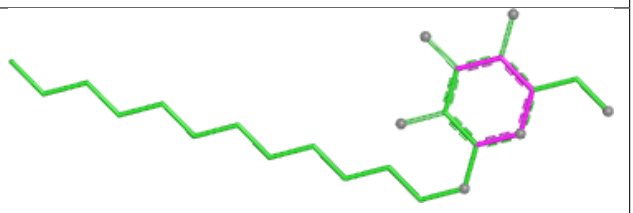


Rings

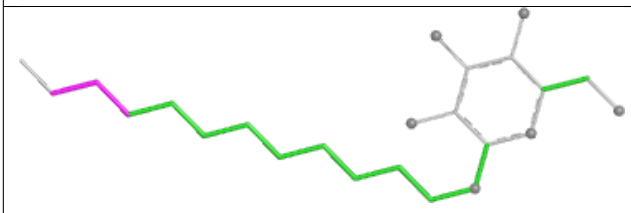
Ligand LMT J 102



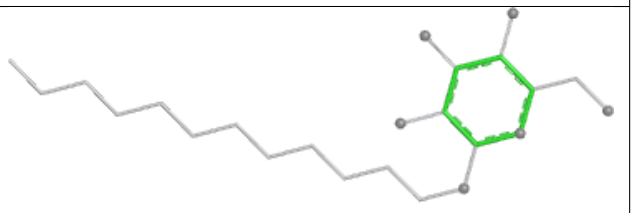
Bond lengths



Bond angles

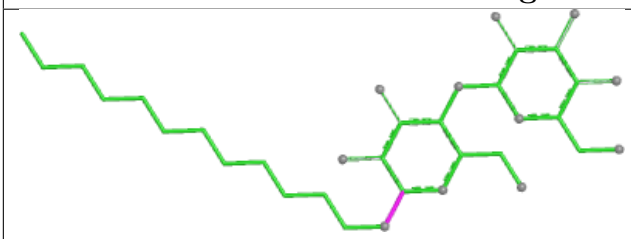


Torsions

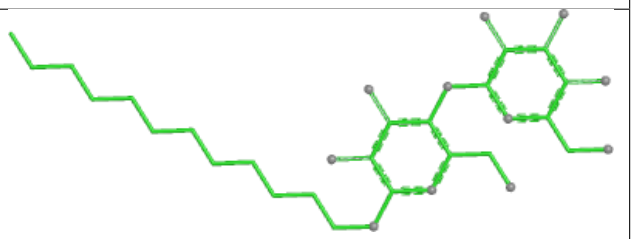


Rings

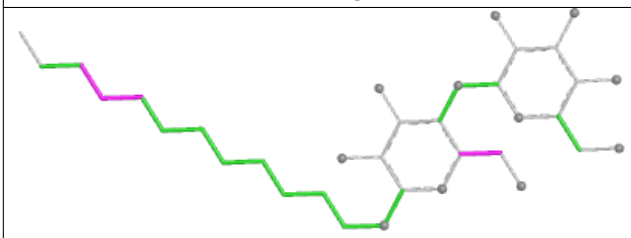
Ligand LMT m 101



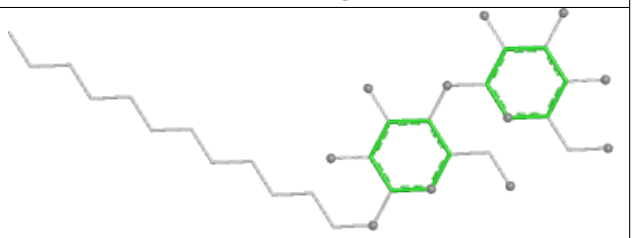
Bond lengths



Bond angles

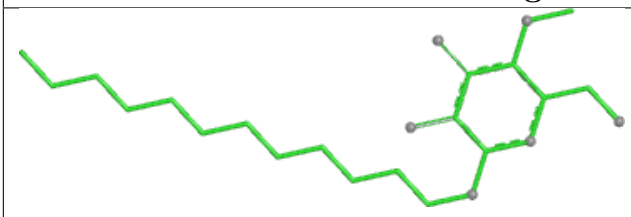


Torsions

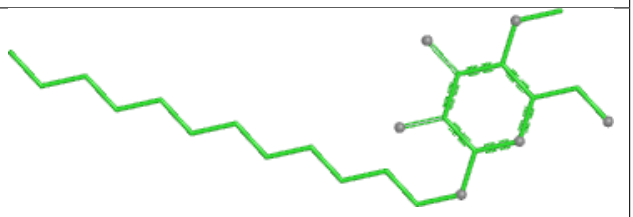


Rings

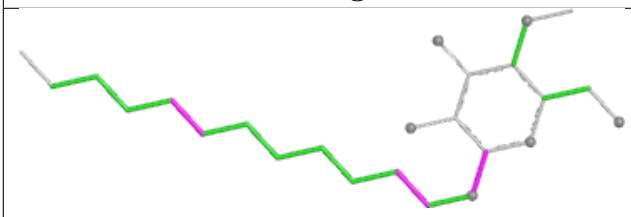
Ligand LMT b 624



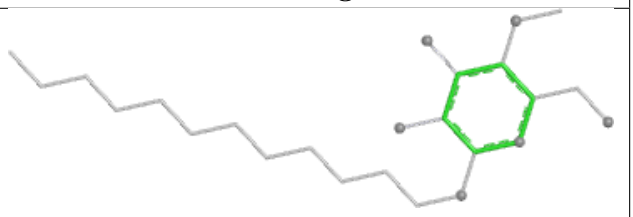
Bond lengths



Bond angles

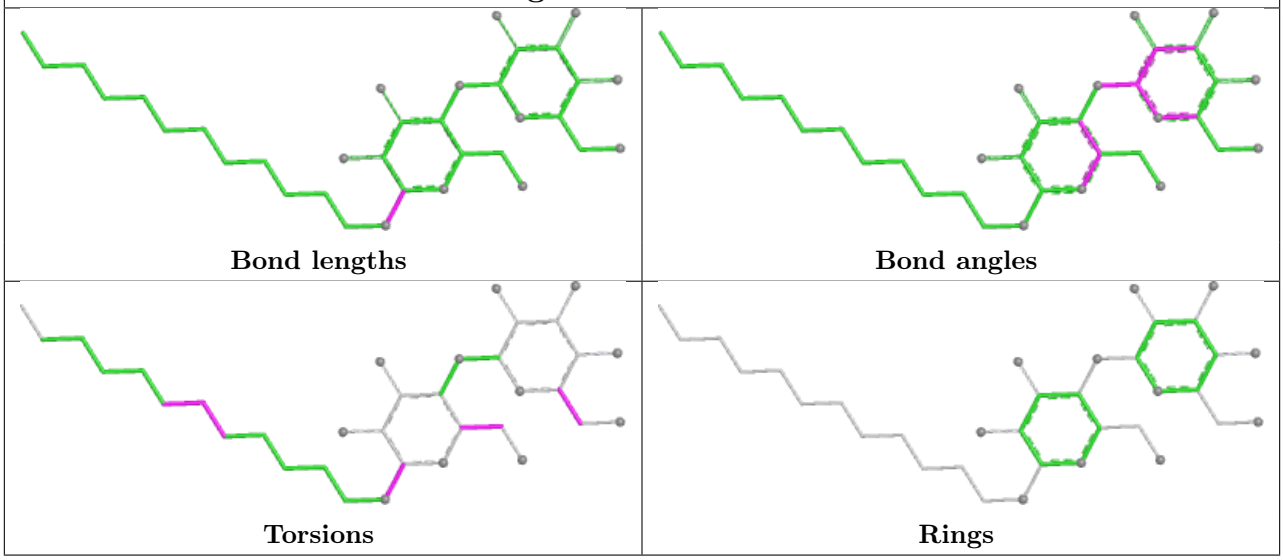


Torsions

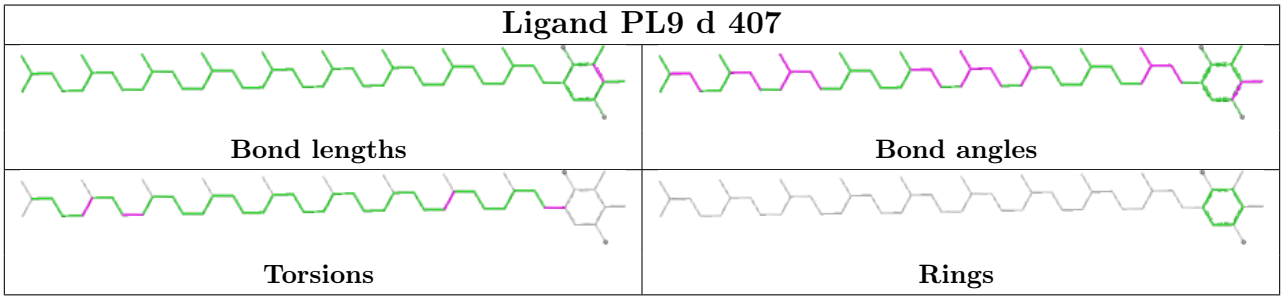


Rings

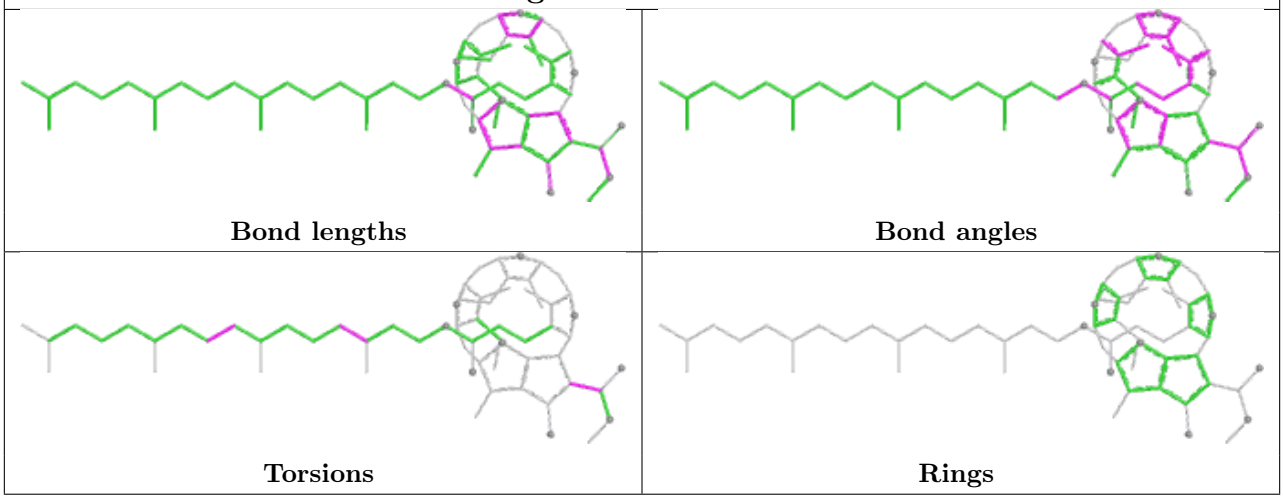
Ligand LMT c 523



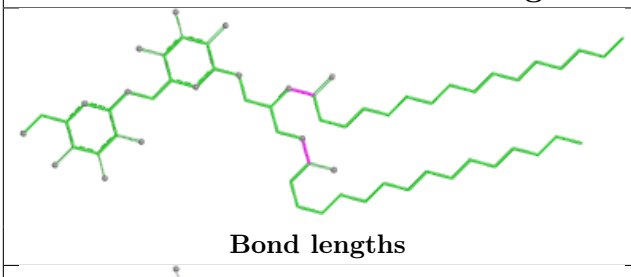
Ligand PL9 d 407



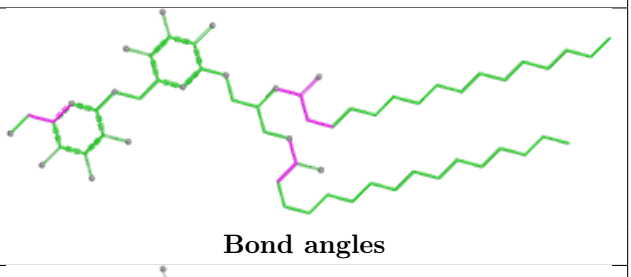
Ligand PHO a 411



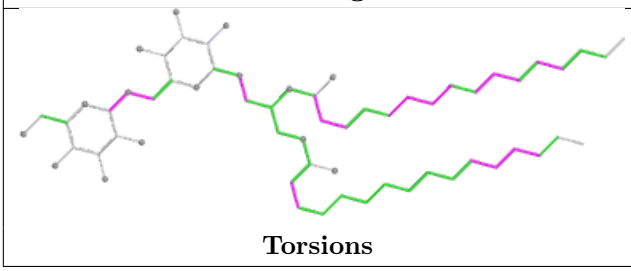
Ligand DGD c 519



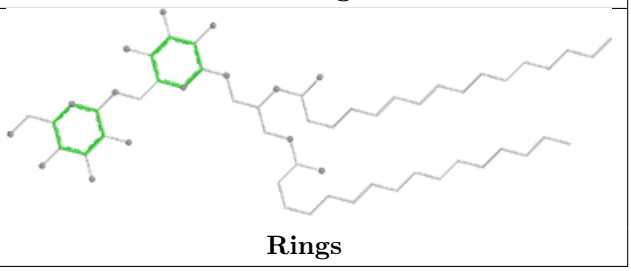
Bond lengths



Bond angles

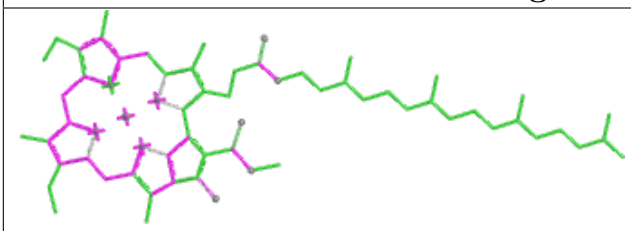


Torsions



Rings

Ligand CLA c 507



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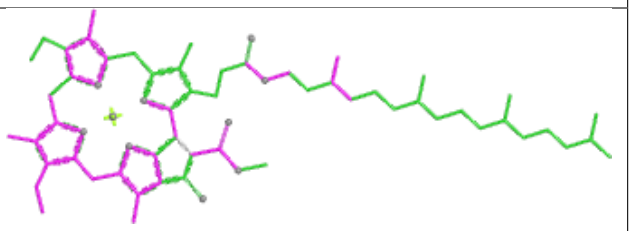
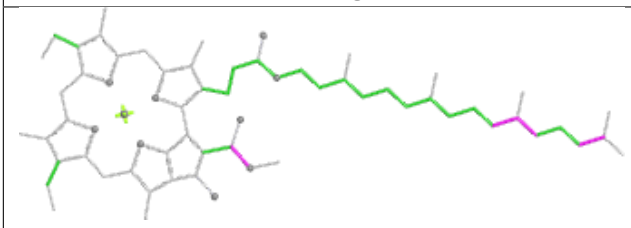
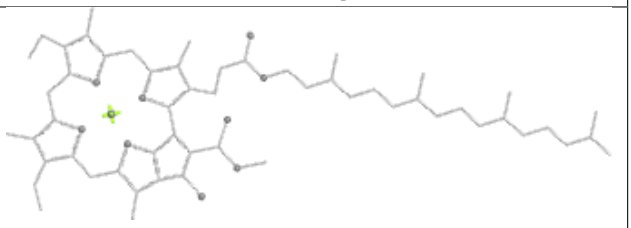


Bond angles

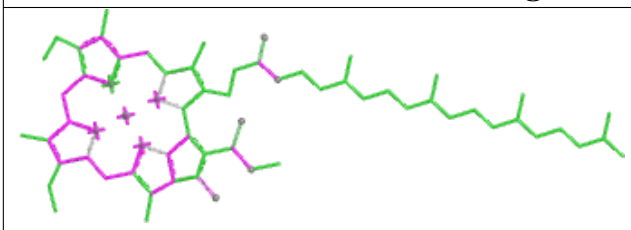


Torsions

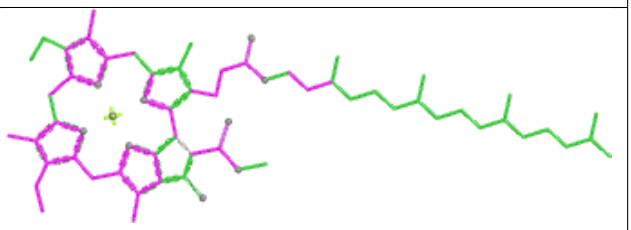


Rings

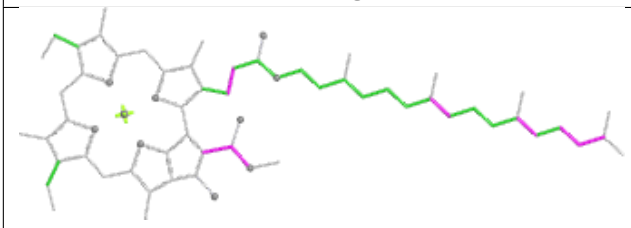
Ligand CLA C 508



Bond lengths



Bond angles



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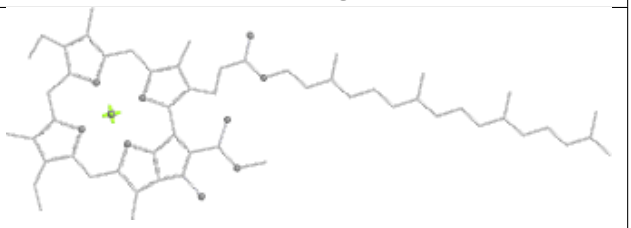
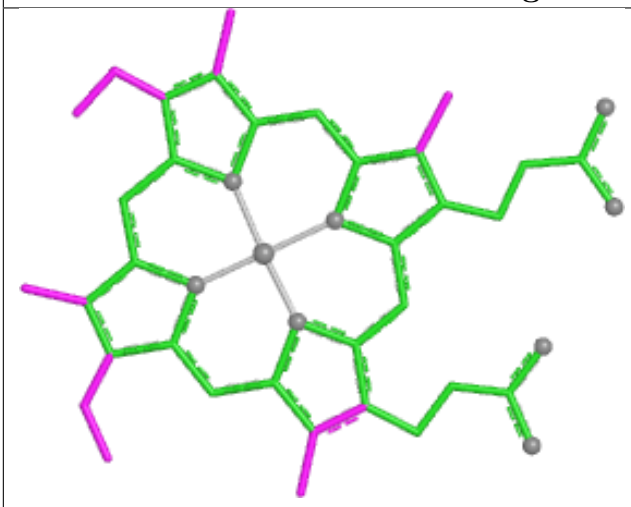


Rings

Ligand HEC V 202



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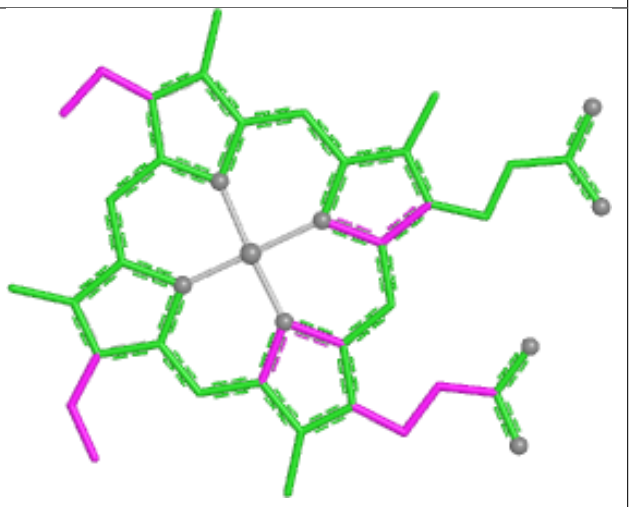
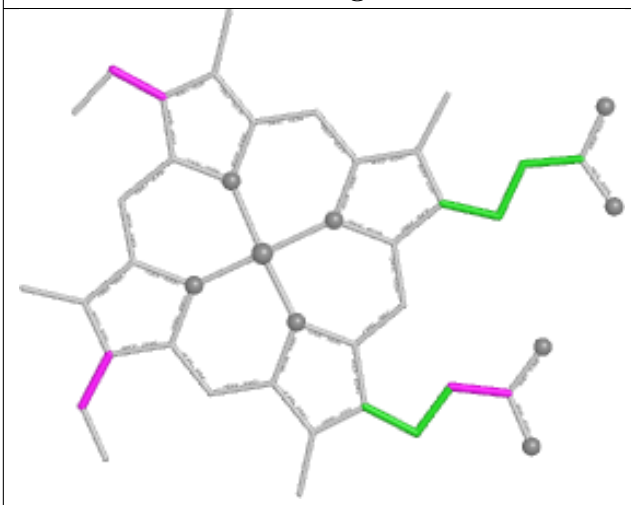
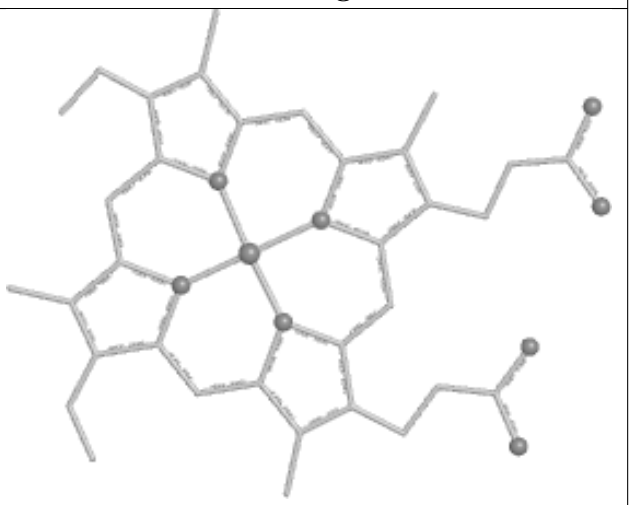


Bond angles

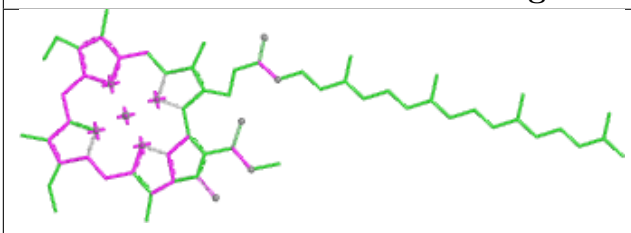


Torsions

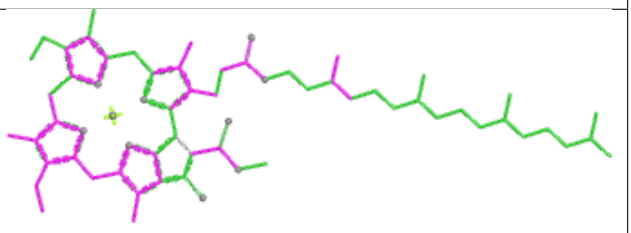


Rings

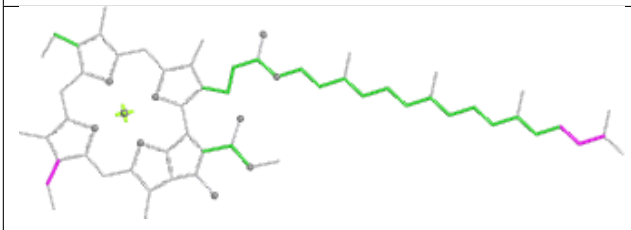
Ligand CLA a 408



Bond lengths



Bond angles



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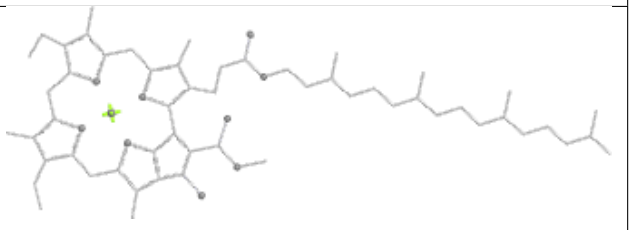
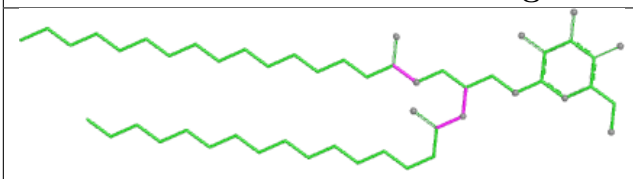


Rings

Ligand LMG d 411



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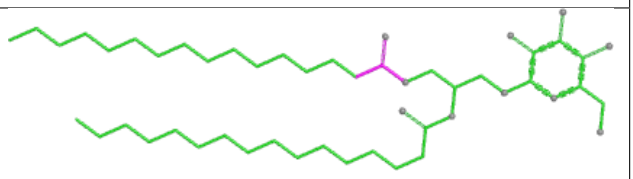
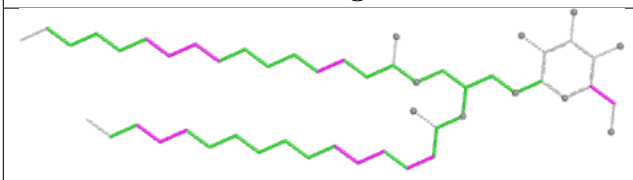


Bond angles



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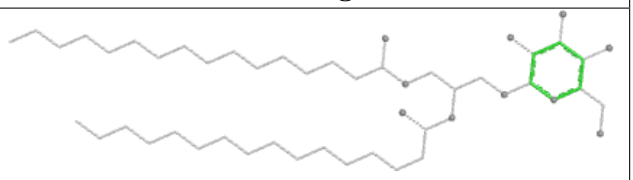
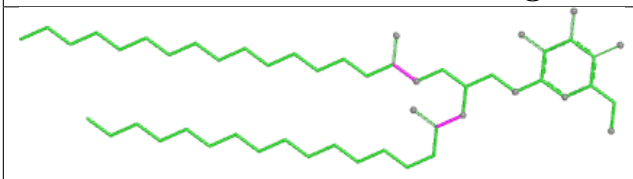
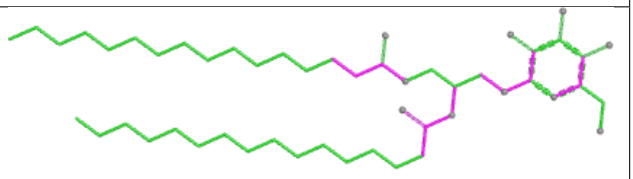


Rings

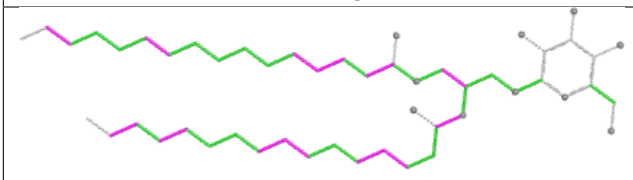
Ligand LMG a 415



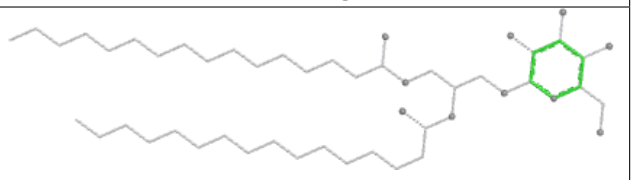
Bond lengths



Bond angles

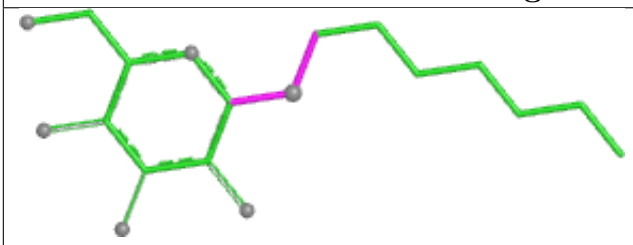


Torsions



Rings

Ligand HTG b 601



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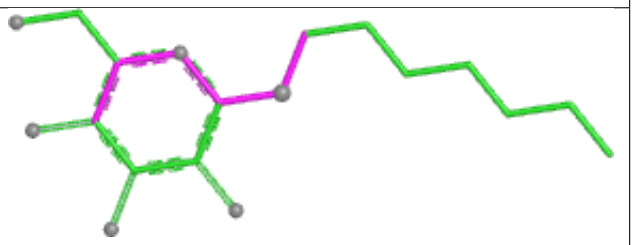
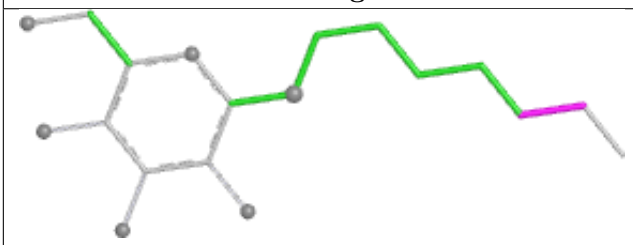
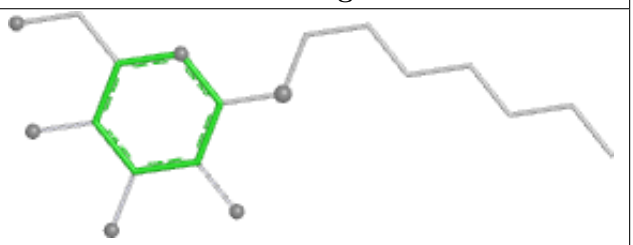


Bond angles

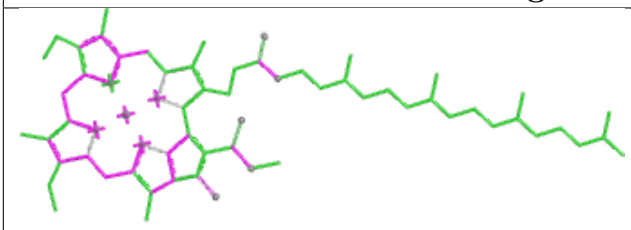


Torsions



Rings

Ligand CLA b 619



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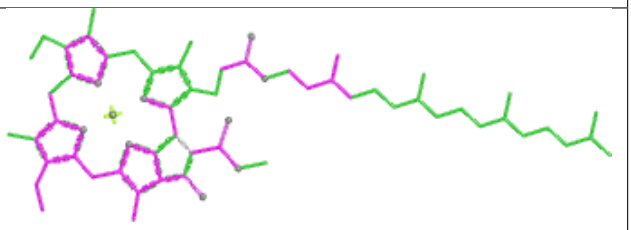
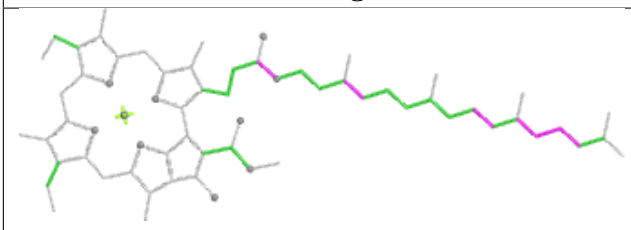
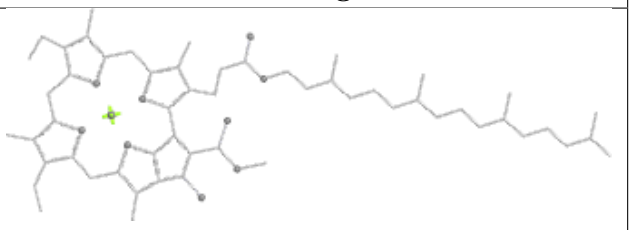


Bond angles

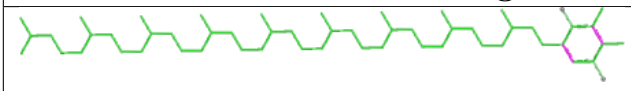


Torsions



Rings

Ligand PL9 A 422 (B)



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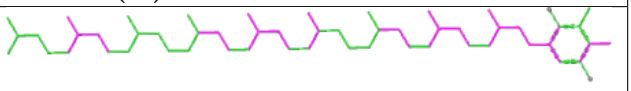
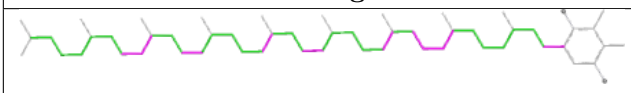
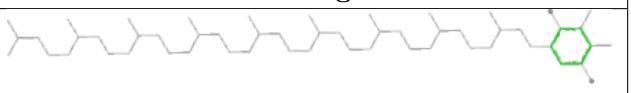


Bond angles

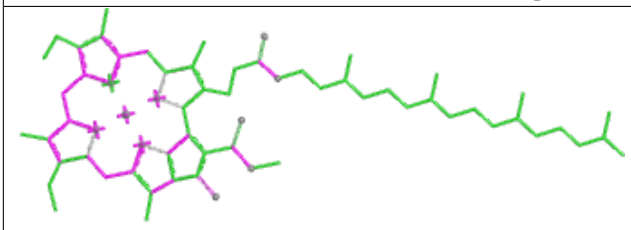


Torsions

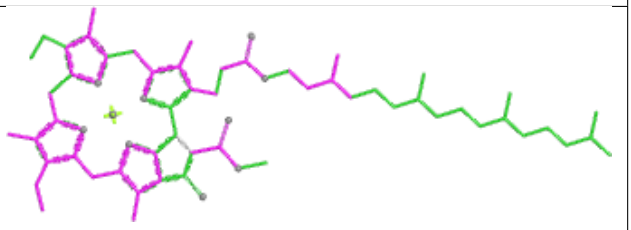


Rings

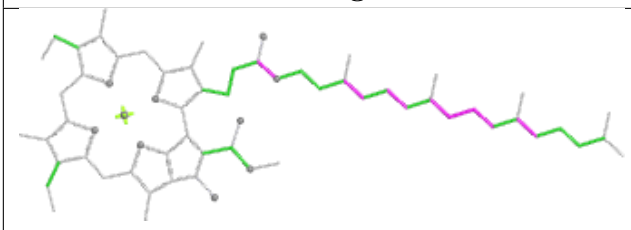
Ligand CLA a 412



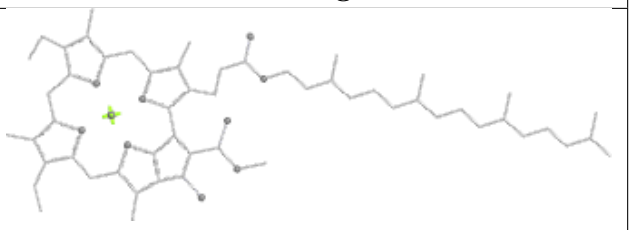
Bond lengths



Bond angles

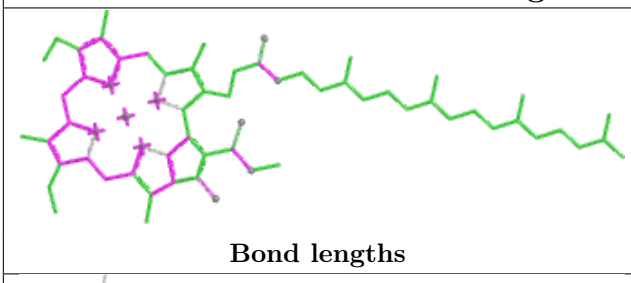


Torsions

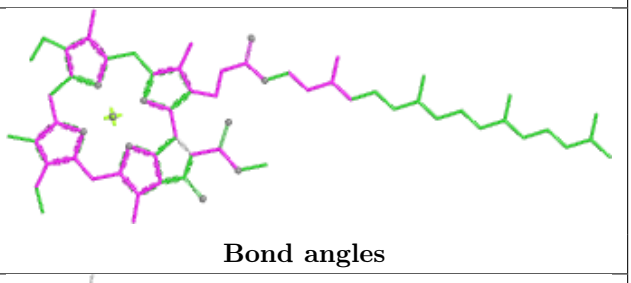


Rings

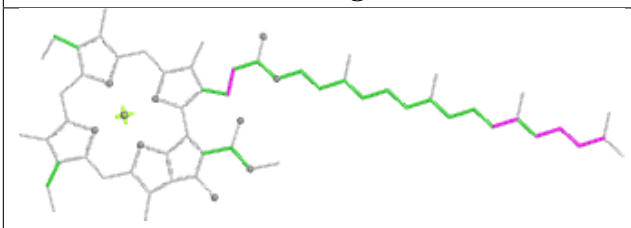
Ligand CLA b 613



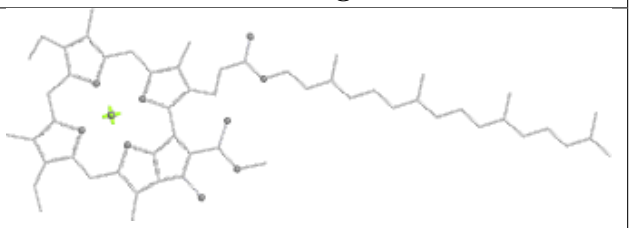
Bond lengths



Bond angles

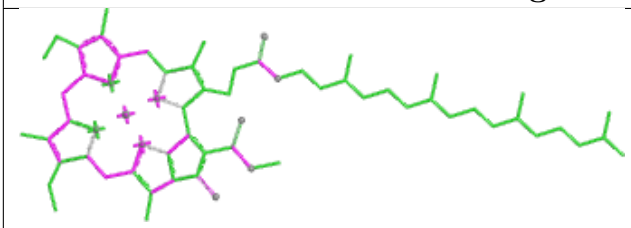


Torsions

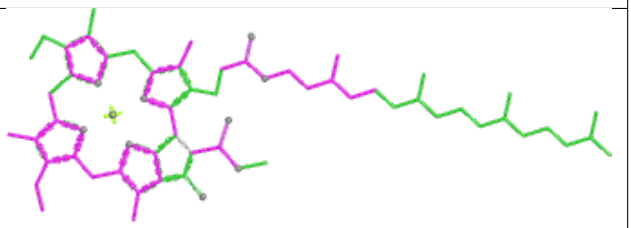


Rings

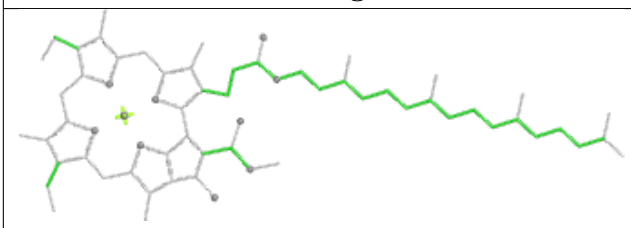
Ligand CLA c 513



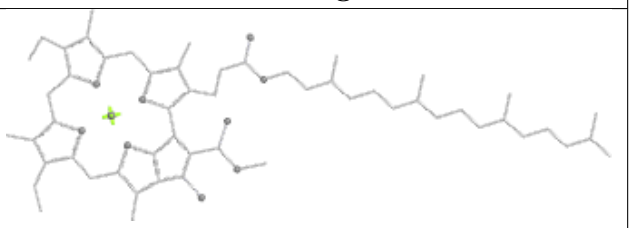
Bond lengths



Bond angles

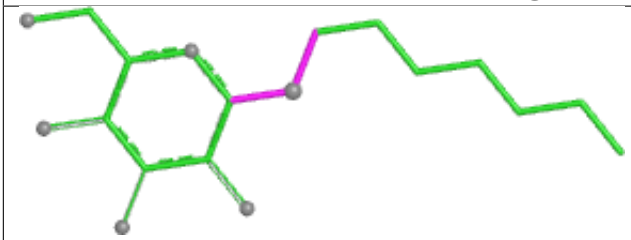


Torsions

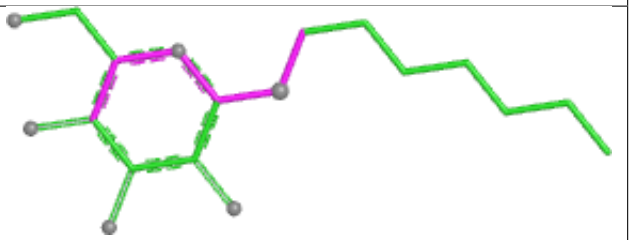


Rings

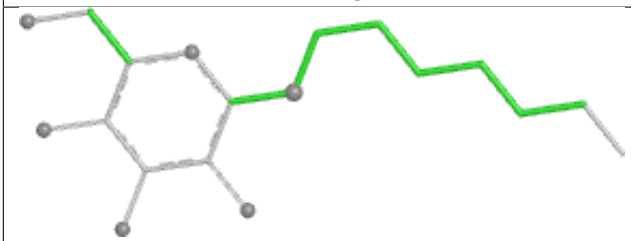
Ligand HTG c 525



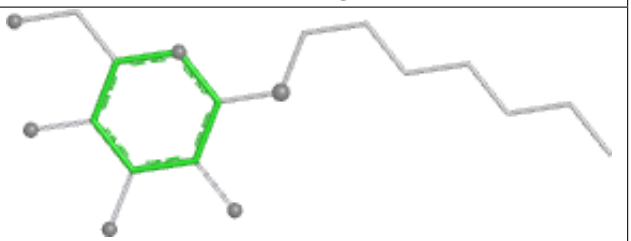
Bond lengths



Bond angles

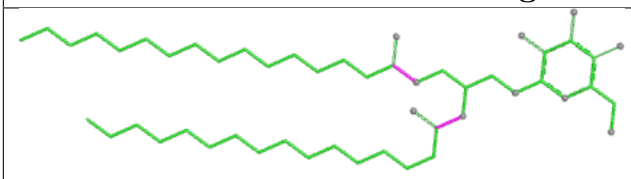


Torsions

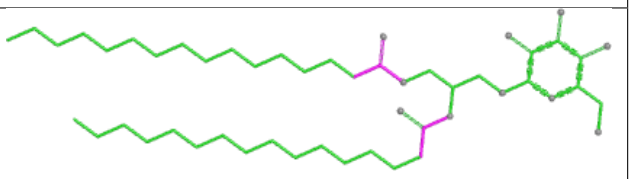


Rings

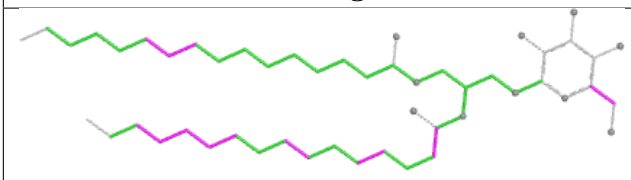
Ligand LMG D 412



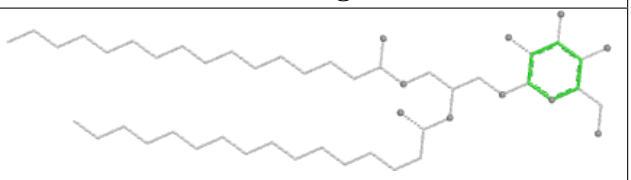
Bond lengths



Bond angles

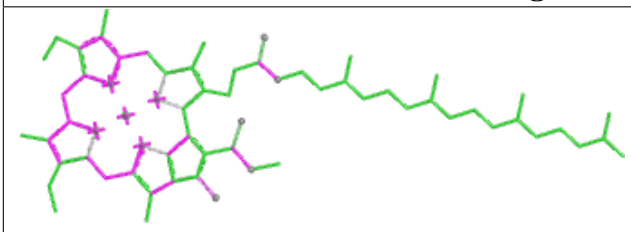


Torsions

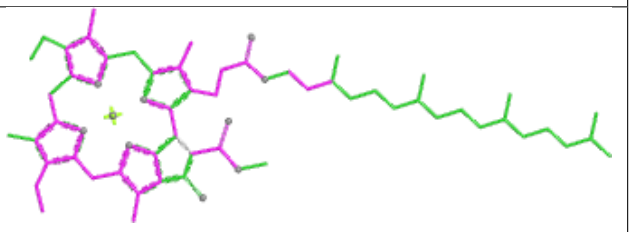


Rings

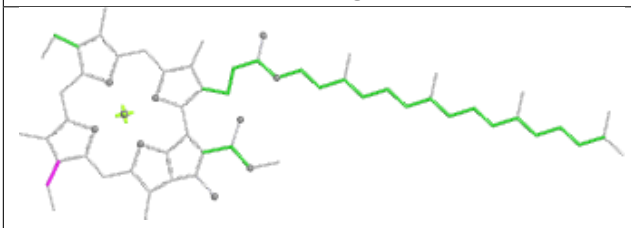
Ligand CLA a 409



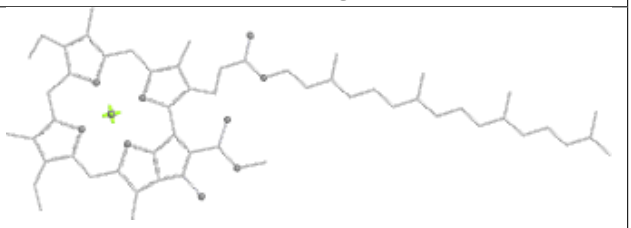
Bond lengths



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%)	-0.08	5 (1%)	72	78	24, 37, 60, 107	3 (0%)
1	a	334/344 (97%)	-0.07	6 (1%)	67	75	26, 39, 72, 113	3 (0%)
2	B	505/505 (100%)	-0.04	11 (2%)	62	69	24, 41, 67, 98	9 (1%)
2	b	503/505 (99%)	0.07	16 (3%)	50	56	27, 45, 79, 146	10 (1%)
3	C	451/455 (99%)	0.02	3 (0%)	84	88	33, 47, 64, 116	2 (0%)
3	c	455/455 (100%)	0.11	7 (1%)	72	78	31, 51, 67, 121	2 (0%)
4	D	341/342 (99%)	-0.14	2 (0%)	85	89	19, 38, 53, 116	1 (0%)
4	d	341/342 (99%)	-0.14	2 (0%)	85	89	22, 42, 63, 115	2 (0%)
5	E	81/83 (97%)	0.36	3 (3%)	45	52	41, 54, 77, 107	0
5	e	79/83 (95%)	0.51	4 (5%)	33	39	49, 63, 102, 131	0
6	F	34/44 (77%)	-0.07	1 (2%)	53	60	41, 46, 66, 88	0
6	f	31/44 (70%)	0.24	2 (6%)	25	28	47, 54, 71, 107	0
7	H	63/63 (100%)	0.20	2 (3%)	50	56	39, 48, 62, 106	0
7	h	63/63 (100%)	0.32	2 (3%)	50	56	43, 54, 69, 103	0
8	I	35/38 (92%)	0.69	3 (8%)	16	19	44, 53, 98, 126	0
8	i	35/38 (92%)	0.21	1 (2%)	53	60	42, 51, 89, 144	0
9	J	36/40 (90%)	0.27	1 (2%)	55	62	39, 51, 83, 101	0
9	j	39/40 (97%)	0.44	1 (2%)	57	64	46, 60, 129, 148	0
10	K	37/37 (100%)	-0.03	0	100	100	34, 52, 68, 82	1 (2%)
10	k	37/37 (100%)	0.30	1 (2%)	56	62	49, 59, 74, 90	0
11	L	37/37 (100%)	-0.05	2 (5%)	31	37	19, 36, 83, 113	1 (2%)
11	l	37/37 (100%)	-0.13	1 (2%)	56	62	21, 36, 85, 112	2 (5%)
12	M	32/36 (88%)	-0.16	0	100	100	22, 37, 54, 85	1 (3%)
12	m	33/36 (91%)	-0.14	0	100	100	22, 37, 59, 88	3 (9%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	0.08	2 (0%) 82 86	28, 50, 90, 139	6 (2%)
13	o	243/244 (99%)	0.20	4 (1%) 70 77	25, 50, 96, 134	5 (2%)
14	T	29/32 (90%)	-0.09	1 (3%) 48 54	32, 37, 71, 108	0
14	t	29/32 (90%)	0.05	1 (3%) 48 54	32, 37, 67, 88	0
15	U	97/104 (93%)	0.00	0 100 100	37, 49, 73, 80	1 (1%)
15	u	97/104 (93%)	0.02	0 100 100	36, 51, 71, 102	1 (1%)
16	V	137/137 (100%)	-0.11	1 (0%) 84 88	25, 46, 62, 85	2 (1%)
16	v	137/137 (100%)	0.05	0 100 100	31, 56, 77, 107	1 (0%)
17	Y	28/30 (93%)	0.85	3 (10%) 11 12	50, 62, 117, 138	0
17	y	28/30 (93%)	0.94	2 (7%) 22 25	59, 75, 110, 127	0
18	X	38/40 (95%)	0.30	0 100 100	46, 56, 69, 91	0
18	x	37/40 (92%)	0.51	3 (8%) 18 21	36, 63, 101, 124	1 (2%)
19	Z	61/62 (98%)	0.46	2 (3%) 49 55	52, 64, 100, 117	0
19	z	60/62 (96%)	1.00	9 (15%) 5 6	61, 74, 107, 118	0
20	R	34/41 (82%)	1.57	10 (29%) 1 1	68, 92, 107, 117	0
All	All	5272/5387 (97%)	0.07	114 (2%) 62 69	19, 46, 80, 148	57 (1%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	37	VAL	5.7
2	b	486	LEU	5.6
2	B	86	ILE	5.3
2	B	479	PHE	4.9
2	b	484	PRO	4.3
2	b	491	VAL	4.3
2	b	479	PHE	4.2
6	f	15	ILE	4.1
7	H	64	ALA	4.0
7	h	64	ALA	3.9
1	A	11	ALA	3.9
1	a	260	PHE	3.8
19	z	3	ILE	3.8
2	B	84	THR	3.7
1	A	230	THR	3.5
2	b	495	PHE	3.5
2	b	85	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
17	Y	22	LEU	3.4
2	b	86	ILE	3.3
17	Y	19	ILE	3.2
14	T	30	THR	3.2
2	b	84	THR	3.2
2	B	85	GLY	3.1
3	C	257	PHE	3.1
4	D	238	THR	3.1
8	I	36	ASP	3.1
20	R	35	LEU	3.1
19	Z	62	VAL	3.0
2	B	487	SER	3.0
2	B	494	GLY	3.0
14	t	30	THR	2.9
8	i	36	ASP	2.9
17	Y	23	THR	2.9
2	B	488	PRO	2.9
1	A	229	GLU	2.9
10	k	18	PHE	2.9
4	D	12	ARG	2.8
20	R	28	VAL	2.8
2	B	495	PHE	2.8
1	a	248	ILE	2.8
19	z	5	PHE	2.7
5	e	61	ARG	2.7
19	z	61	VAL	2.7
20	R	15	ALA	2.6
2	b	497	GLN	2.6
19	z	2	THR	2.6
19	z	60	PHE	2.6
19	z	4	LEU	2.6
19	z	9	LEU	2.6
3	C	255	THR	2.6
19	Z	7	LEU	2.5
2	b	493	TRP	2.5
5	e	17	VAL	2.5
2	b	496	TYR	2.5
13	o	58	ASN	2.5
2	b	488	PRO	2.5
7	h	6	TRP	2.5
7	H	63	LYS	2.4
3	c	20	SER	2.4

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Mol	Chain	Res	Type	RSRZ
11	L	10	VAL	2.4
2	B	486	LEU	2.4
19	z	32	ASP	2.4
1	a	11	ALA	2.4
18	x	38	GLN	2.4
20	R	18	TRP	2.4
4	d	237	PRO	2.3
2	b	500	GLY	2.3
8	I	34	ARG	2.3
9	j	7	ARG	2.3
6	f	16	PHE	2.3
20	R	24	LEU	2.3
13	o	246	ALA	2.3
3	c	21	ILE	2.3
9	J	6	GLY	2.3
2	b	499	VAL	2.3
2	b	502	VAL	2.3
1	A	12	ASN	2.3
5	E	4	THR	2.3
20	R	10	LEU	2.3
2	b	485	GLU	2.2
4	d	240	ALA	2.2
20	R	3	TRP	2.2
3	C	134	ILE	2.2
3	c	143	TYR	2.2
2	B	490	GLN	2.2
5	E	72	ALA	2.2
17	y	20	ALA	2.2
20	R	19	ALA	2.2
17	y	25	ILE	2.1
11	L	8	GLN	2.1
13	o	56	PRO	2.1
1	a	263	ALA	2.1
19	z	11	ALA	2.1
1	a	224	ILE	2.1
1	A	14	TRP	2.1
1	a	14	TRP	2.1
6	F	12	SER	2.1
5	e	84	LYS	2.1
3	c	200	THR	2.1
13	o	62	GLU	2.1
20	R	6	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	61	ARG	2.1
11	l	7	ARG	2.1
8	I	25	SER	2.0
16	V	19	ILE	2.0
13	O	246	ALA	2.0
3	c	281	MET	2.0
3	c	147	PHE	2.0
5	e	63	ILE	2.0
13	O	65	PHE	2.0
18	x	34	ILE	2.0
2	B	2	GLY	2.0
3	c	192	GLY	2.0
20	R	20	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	FME	Z	1	10/11	0.79	0.14	88,100,114,119	0
14	FME	t	1	10/11	0.93	0.10	34,38,57,70	0
14	FME	T	1	10/11	0.94	0.08	37,44,64,68	0
12	FME	m	1	10/11	0.95	0.11	42,50,78,87	0
12	FME	M	1	10/11	0.95	0.09	44,51,79,81	0
4	HSK	d	336[A]	10/12	0.96	0.08	46,49,54,56	7
4	HSK	d	336[B]	11/12	0.96	0.08	46,49,55,57	8
8	FME	i	1	10/11	0.96	0.08	43,48,54,55	0
4	HSK	D	336[B]	11/12	0.96	0.08	40,41,43,45	8
4	HSK	D	336[A]	10/12	0.96	0.08	40,42,44,46	7
8	FME	I	1	10/11	0.98	0.06	44,49,54,54	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, 95^{th} 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
38	DMS	a	426	4/4	0.42	0.16	144,146,147,147	0
38	DMS	Y	303	4/4	0.47	0.19	141,143,145,146	0
38	DMS	o	309	4/4	0.50	0.21	140,142,142,143	0
38	DMS	z	102	4/4	0.58	0.19	141,143,143,144	0
31	UNL	b	635	15/-	0.61	0.23	89,106,109,110	0
38	DMS	b	636	4/4	0.62	0.25	134,135,138,139	0
38	DMS	C	525	4/4	0.65	0.21	111,114,116,117	0
38	DMS	o	307	4/4	0.65	0.23	121,123,123,124	0
31	UNL	D	415	12/-	0.67	0.26	79,86,92,94	0
29	LMT	C	521	35/35	0.67	0.17	76,138,158,160	0
30	GOL	h	1206	6/6	0.67	0.14	95,104,105,109	0
29	LMT	f	104	35/35	0.68	0.16	90,115,143,147	0
31	UNL	B	635	13/-	0.71	0.20	78,94,106,107	0
31	UNL	B	638	9/-	0.72	0.25	67,73,84,86	0
38	DMS	c	536	4/4	0.72	0.18	105,108,109,111	0
30	GOL	k	304	6/6	0.72	0.14	101,105,108,118	0
31	UNL	a	423	10/-	0.72	0.22	94,98,104,104	0
31	UNL	b	632	15/-	0.72	0.21	71,86,107,108	0
38	DMS	c	535	4/4	0.73	0.15	112,112,112,113	0
38	DMS	B	645	4/4	0.73	0.22	129,130,130,130	0
38	DMS	d	415	4/4	0.73	0.21	114,118,118,119	0
30	GOL	u	202	6/6	0.74	0.16	76,100,104,106	0
31	UNL	A	419	10/-	0.74	0.22	79,90,94,95	0
38	DMS	B	644	4/4	0.74	0.27	136,138,138,138	0
29	LMT	c	523	35/35	0.74	0.15	103,134,152,153	0
38	DMS	B	647	4/4	0.74	0.15	122,122,122,123	0
36	HTG	D	413	19/19	0.75	0.20	71,120,132,134	0
31	UNL	A	420	9/-	0.75	0.19	98,100,108,110	0
31	UNL	b	633	15/-	0.76	0.26	80,90,106,106	0
31	UNL	I	103	16/-	0.77	0.18	66,83,91,91	0
36	HTG	b	625	19/19	0.77	0.21	47,59,82,86	0
36	HTG	h	1202	19/19	0.77	0.18	89,109,120,121	0
31	UNL	I	104	15/-	0.77	0.20	87,94,102,103	0
39	DGD	D	407	53/66	0.77	0.17	76,89,137,139	0
31	UNL	B	639	15/-	0.78	0.26	88,95,108,108	0
38	DMS	o	304	4/4	0.78	0.24	101,113,115,116	0
31	UNL	a	422	11/-	0.78	0.15	87,91,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	LHG	e	101	40/49	0.79	0.17	90,135,148,150	0
31	UNL	h	1203	12/-	0.79	0.21	80,88,90,93	0
31	UNL	a	419	40/-	0.79	0.19	78,107,124,132	0
36	HTG	u	201	14/19	0.79	0.17	73,89,104,111	0
30	GOL	E	105	6/6	0.80	0.11	100,107,109,110	0
31	UNL	h	1201	15/-	0.80	0.18	87,104,123,123	0
38	DMS	B	643	4/4	0.80	0.22	87,99,102,103	0
30	GOL	c	532	6/6	0.80	0.16	59,87,90,93	0
31	UNL	h	1207	12/-	0.80	0.19	67,87,101,103	0
31	UNL	i	103	40/-	0.80	0.16	73,93,120,123	0
31	UNL	E	103	15/-	0.80	0.23	76,79,90,95	0
38	DMS	v	1608	4/4	0.80	0.26	118,122,124,126	0
30	GOL	d	413	6/6	0.80	0.13	74,93,98,99	0
31	UNL	A	417	40/-	0.80	0.19	74,94,119,122	0
31	UNL	B	637	10/-	0.81	0.17	89,96,99,100	0
31	UNL	E	102	15/-	0.81	0.23	77,85,99,99	0
29	LMT	m	103	35/35	0.81	0.14	57,74,104,105	0
31	UNL	k	301	16/-	0.81	0.29	82,118,131,131	0
31	UNL	c	501	40/-	0.81	0.19	76,101,136,137	0
38	DMS	o	306	4/4	0.81	0.24	113,116,117,117	0
31	UNL	e	102	15/-	0.81	0.20	76,82,97,98	0
36	HTG	b	626	19/19	0.81	0.15	74,133,142,142	0
38	DMS	C	533	4/4	0.81	0.22	99,102,107,111	0
36	HTG	d	414	19/19	0.81	0.18	71,103,114,118	19
30	GOL	v	1607	6/6	0.81	0.15	56,68,79,84	0
31	UNL	c	531	11/-	0.82	0.20	84,96,105,106	0
38	DMS	b	638	4/4	0.82	0.18	79,91,95,98	0
37	LHG	E	101	49/49	0.82	0.18	53,87,108,115	0
36	HTG	B	626	19/19	0.82	0.14	55,122,127,128	0
38	DMS	c	537	4/4	0.82	0.18	93,100,100,103	0
36	HTG	C	523	19/19	0.82	0.12	72,102,110,111	0
38	DMS	d	416	4/4	0.82	0.25	88,90,90,93	0
31	UNL	J	104	16/-	0.82	0.25	76,87,94,96	0
36	HTG	I	102	19/19	0.82	0.12	73,112,128,132	0
36	HTG	V	203	13/19	0.82	0.12	65,71,107,111	0
31	UNL	C	501	40/-	0.82	0.17	68,92,106,108	0
29	LMT	m	101	35/35	0.82	0.14	49,71,97,101	0
31	UNL	J	103	15/-	0.82	0.23	76,86,98,99	0
31	UNL	c	529	12/-	0.82	0.24	93,97,103,105	0
31	UNL	x	801	12/-	0.83	0.16	77,89,94,95	0
29	LMT	E	104	24/35	0.83	0.15	84,98,107,112	0
30	GOL	L	103	6/6	0.83	0.15	58,69,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
38	DMS	D	416	4/4	0.83	0.16	91,98,102,102	0
31	UNL	A	418	15/-	0.83	0.21	85,88,97,98	0
30	GOL	C	529	6/6	0.83	0.18	93,95,101,107	0
38	DMS	o	308	4/4	0.83	0.24	77,78,84,97	0
30	GOL	d	402	6/6	0.83	0.11	83,103,103,106	0
31	UNL	j	1302	16/-	0.83	0.18	69,82,99,100	0
31	UNL	b	631	16/-	0.83	0.18	58,63,74,76	0
38	DMS	B	646	4/4	0.83	0.20	108,110,113,115	0
31	UNL	b	634	9/-	0.84	0.21	67,85,95,96	0
36	HTG	U	201	9/19	0.84	0.18	71,84,122,126	0
38	DMS	O	304	4/4	0.84	0.19	83,99,100,102	0
31	UNL	i	101	16/-	0.84	0.22	59,67,82,84	0
33	PL9	a	425[B]	55/55	0.84	0.36	41,71,125,126	55
28	LMG	C	532	51/55	0.85	0.18	64,117,127,130	0
31	UNL	Y	301	12/-	0.85	0.23	82,91,97,98	0
35	CA	B	601	1/1	0.85	0.10	110,110,110,110	0
30	GOL	o	305	6/6	0.85	0.13	60,85,88,89	0
30	GOL	b	630	6/6	0.85	0.19	57,75,76,76	0
29	LMT	Z	101	35/35	0.85	0.16	54,108,130,136	0
31	UNL	B	634	18/-	0.85	0.15	73,82,96,99	0
31	UNL	C	531	18/-	0.85	0.17	69,93,106,107	0
38	DMS	E	106	4/4	0.85	0.19	109,113,116,119	0
30	GOL	a	418	6/6	0.86	0.15	69,82,85,86	0
29	LMT	M	101	35/35	0.86	0.13	47,71,83,85	0
30	GOL	c	527	6/6	0.86	0.16	65,68,78,86	0
36	HTG	B	624	19/19	0.86	0.12	62,98,106,108	19
28	LMG	c	522	51/55	0.86	0.16	58,121,129,132	0
29	LMT	z	101	32/35	0.86	0.14	63,112,129,131	0
29	LMT	b	624	25/35	0.86	0.16	69,95,125,130	0
27	SQD	f	102	33/54	0.86	0.15	74,97,122,123	0
27	SQD	L	101	54/54	0.86	0.15	55,83,128,132	0
30	GOL	O	303	6/6	0.86	0.09	73,77,82,88	0
30	GOL	T	101	6/6	0.86	0.15	37,55,59,63	0
30	GOL	v	1601	6/6	0.86	0.22	70,85,94,98	0
36	HTG	c	525	19/19	0.86	0.13	69,92,102,104	19
31	UNL	D	402	40/-	0.86	0.19	55,72,101,107	0
30	GOL	T	103	6/6	0.86	0.18	116,117,119,120	0
36	HTG	b	602	19/19	0.87	0.13	70,114,131,134	0
31	UNL	d	403	40/-	0.87	0.19	57,83,114,117	0
31	UNL	l	301	16/-	0.87	0.21	58,76,110,111	0
36	HTG	c	524	19/19	0.87	0.11	87,102,108,110	0
30	GOL	b	629	6/6	0.87	0.13	58,68,71,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	UNL	H	103	8/-	0.87	0.20	71,78,81,83	0
38	DMS	c	533	4/4	0.87	0.17	100,104,104,105	0
29	LMT	T	104	24/35	0.87	0.17	44,71,113,118	0
36	HTG	B	623[A]	19/19	0.87	0.17	39,52,67,67	19
36	HTG	B	623[B]	19/19	0.87	0.17	31,50,67,70	19
27	SQD	a	401	54/54	0.88	0.14	54,73,95,98	0
27	SQD	A	413	54/54	0.88	0.13	54,72,100,102	0
38	DMS	i	104	4/4	0.88	0.20	107,108,109,109	0
30	GOL	B	627	6/6	0.88	0.16	53,58,67,78	0
30	GOL	B	630	6/6	0.88	0.13	51,60,67,75	0
29	LMT	J	102	24/35	0.88	0.14	65,86,117,122	0
31	UNL	C	526	15/-	0.88	0.18	80,91,111,112	0
29	LMT	A	414	35/35	0.88	0.13	52,73,95,108	0
31	UNL	B	632	16/-	0.88	0.20	59,74,97,97	0
29	LMT	B	622	35/35	0.88	0.13	59,89,115,120	0
31	UNL	a	420	12/-	0.88	0.20	75,89,106,107	0
33	PL9	A	422[B]	55/55	0.89	0.22	54,80,96,98	55
27	SQD	L	102	54/54	0.89	0.14	52,76,113,120	0
38	DMS	V	207	4/4	0.89	0.18	97,105,106,109	0
30	GOL	c	526	6/6	0.89	0.15	58,80,93,98	0
30	GOL	B	631	6/6	0.89	0.15	49,60,67,73	0
31	UNL	c	530	11/-	0.89	0.17	85,92,105,108	0
31	UNL	j	1301	18/-	0.89	0.14	66,81,110,112	0
29	LMT	B	642	24/35	0.89	0.17	51,69,117,121	0
31	UNL	T	105	9/-	0.89	0.19	72,78,85,88	0
30	GOL	A	416	6/6	0.89	0.14	55,78,82,86	0
29	LMT	m	102	35/35	0.89	0.12	39,58,71,73	0
30	GOL	A	415	6/6	0.90	0.12	44,54,55,58	0
30	GOL	a	421	6/6	0.90	0.13	90,97,107,111	0
29	LMT	a	402	35/35	0.90	0.13	49,68,83,93	0
30	GOL	C	528	6/6	0.90	0.14	66,81,86,93	0
27	SQD	D	408	45/54	0.90	0.13	50,85,118,127	0
31	UNL	t	101	8/-	0.90	0.18	70,80,85,86	0
30	GOL	C	530	6/6	0.90	0.13	44,50,54,61	6
30	GOL	a	416	6/6	0.90	0.14	43,53,57,59	0
30	GOL	v	1606	6/6	0.90	0.10	74,86,91,98	0
31	UNL	B	636	18/-	0.90	0.14	56,74,98,108	0
35	CA	b	603	1/1	0.90	0.10	142,142,142,142	0
31	UNL	i	102	15/-	0.90	0.17	70,79,106,106	0
30	GOL	o	302	6/6	0.91	0.11	61,71,78,85	0
30	GOL	C	527	6/6	0.91	0.18	80,86,90,90	0
28	LMG	a	415	51/55	0.91	0.13	58,75,87,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	UNL	X	101	16/-	0.91	0.16	55,63,78,84	0
36	HTG	b	601	19/19	0.91	0.12	57,68,82,86	0
30	GOL	b	627	6/6	0.91	0.14	64,66,69,84	0
28	LMG	C	520	51/55	0.91	0.14	43,80,103,106	0
38	DMS	b	637	4/4	0.91	0.21	89,93,97,99	0
36	HTG	B	625	19/19	0.91	0.12	52,73,95,96	0
24	CLA	B	602	65/65	0.91	0.10	38,58,106,113	0
36	HTG	C	522	19/19	0.91	0.11	82,86,95,97	0
30	GOL	B	633	6/6	0.91	0.12	41,52,57,58	6
26	BCR	T	102	40/40	0.92	0.09	35,47,58,59	0
30	GOL	a	417	6/6	0.92	0.12	54,63,66,70	0
24	CLA	b	604	65/65	0.92	0.11	48,66,112,120	0
30	GOL	v	1602	6/6	0.92	0.10	64,75,79,86	0
28	LMG	c	521	51/55	0.92	0.14	48,80,115,117	0
31	UNL	x	802	18/-	0.92	0.14	60,74,107,110	0
30	GOL	V	204	6/6	0.92	0.12	42,53,56,57	0
31	UNL	d	412	16/-	0.93	0.18	54,71,95,97	0
28	LMG	d	411	51/55	0.93	0.12	45,53,108,114	0
26	BCR	K	101	40/40	0.93	0.10	39,49,56,59	0
27	SQD	a	414	54/54	0.93	0.12	54,73,92,96	0
37	LHG	D	409	49/49	0.93	0.11	40,49,57,62	0
38	DMS	c	534	4/4	0.93	0.13	62,74,78,78	0
24	CLA	C	507	65/65	0.93	0.11	43,58,101,104	0
28	LMG	A	412	51/55	0.93	0.13	51,73,97,101	0
31	UNL	D	414	16/-	0.93	0.16	46,62,78,84	0
28	LMG	B	621	51/55	0.93	0.11	45,52,69,84	0
26	BCR	b	622	40/40	0.93	0.09	41,49,61,68	0
24	CLA	b	619	65/65	0.93	0.10	40,47,113,115	0
24	CLA	c	508	65/65	0.93	0.12	47,57,86,89	0
31	UNL	I	101	16/-	0.93	0.13	50,63,75,76	0
30	GOL	B	629	6/6	0.93	0.14	50,65,76,78	0
30	GOL	V	205	6/6	0.93	0.09	72,87,90,100	0
28	LMG	b	623	51/55	0.93	0.13	45,56,76,79	0
32	K3C	a	424[A]	14/14	0.93	0.23	116,122,125,126	14
24	CLA	c	515	65/65	0.93	0.11	50,64,103,106	0
26	BCR	B	641	40/40	0.93	0.09	35,47,61,62	0
41	RRX	h	1204	41/41	0.93	0.09	41,53,65,73	0
30	GOL	M	102	6/6	0.94	0.08	36,38,61,71	0
24	CLA	b	609	65/65	0.94	0.09	36,46,76,79	0
24	CLA	b	617	65/65	0.94	0.11	32,41,97,106	0
26	BCR	c	516	40/40	0.94	0.11	58,70,74,76	0
30	GOL	V	201	6/6	0.94	0.09	56,73,76,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	GOL	B	628	6/6	0.94	0.09	44,49,50,52	0
37	LHG	d	408	49/49	0.94	0.10	38,52,66,74	0
26	BCR	d	406	40/40	0.94	0.10	42,51,76,82	0
37	LHG	l	302	49/49	0.94	0.10	38,47,66,78	0
30	GOL	V	206	6/6	0.94	0.07	55,56,63,63	0
26	BCR	k	303	40/40	0.94	0.10	49,56,65,67	0
27	SQD	A	411	54/54	0.94	0.12	40,69,91,94	0
30	GOL	v	1605	6/6	0.94	0.12	46,56,63,65	0
24	CLA	B	617	65/65	0.94	0.12	35,45,111,116	0
24	CLA	B	607	65/65	0.94	0.09	33,41,67,79	0
24	CLA	C	513	65/65	0.94	0.10	45,57,86,95	0
24	CLA	d	405	65/65	0.94	0.10	43,49,94,101	0
24	CLA	C	514	65/65	0.94	0.10	46,59,99,100	0
32	K3C	A	421[A]	14/14	0.94	0.21	84,85,87,88	14
26	BCR	D	405	40/40	0.94	0.10	36,45,76,77	0
39	DGD	h	1205	62/66	0.94	0.10	41,49,62,76	0
24	CLA	B	615	65/65	0.94	0.11	28,38,94,99	0
25	PHO	D	401	64/64	0.95	0.07	28,36,44,47	0
35	CA	f	103	1/1	0.95	0.08	86,86,86,86	0
26	BCR	B	618	40/40	0.95	0.07	34,40,47,48	0
26	BCR	B	619	40/40	0.95	0.07	34,41,56,63	0
26	BCR	B	620	40/40	0.95	0.07	38,44,58,60	0
24	CLA	C	504	65/65	0.95	0.08	40,47,56,67	0
26	BCR	C	515	40/40	0.95	0.09	47,62,66,73	0
26	BCR	C	516	40/40	0.95	0.09	42,52,57,59	0
24	CLA	D	404	65/65	0.95	0.09	36,42,98,100	0
24	CLA	c	506	65/65	0.95	0.09	40,48,77,80	0
30	GOL	v	1604	6/6	0.95	0.09	49,57,59,60	0
36	HTG	O	302	19/19	0.95	0.10	42,46,68,71	0
24	CLA	a	412	65/65	0.95	0.10	33,41,113,114	0
26	BCR	Y	302	40/40	0.95	0.08	44,50,58,64	0
28	LMG	D	412	51/55	0.95	0.11	37,51,102,112	0
26	BCR	a	413	40/40	0.95	0.07	29,39,45,46	0
26	BCR	b	620	40/40	0.95	0.08	37,43,49,51	0
26	BCR	b	621	40/40	0.95	0.08	34,46,59,63	0
24	CLA	c	509	65/65	0.95	0.10	41,49,68,77	0
24	CLA	c	510	65/65	0.95	0.09	38,47,105,126	0
30	GOL	b	628	6/6	0.95	0.09	47,58,62,64	0
26	BCR	c	517	40/40	0.95	0.09	45,52,66,72	0
36	HTG	o	301	19/19	0.95	0.10	40,48,64,67	0
24	CLA	c	514	65/65	0.95	0.10	49,60,88,94	0
26	BCR	k	302	40/40	0.95	0.09	48,56,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	LHG	D	411	46/49	0.95	0.11	36,44,100,104	0
24	CLA	B	610	65/65	0.95	0.07	37,42,47,54	0
33	PL9	D	406	55/55	0.95	0.07	31,37,47,49	0
37	LHG	d	409	49/49	0.95	0.09	34,41,59,70	0
37	LHG	d	410	39/49	0.95	0.11	40,46,97,100	0
39	DGD	C	518	62/66	0.95	0.10	36,47,91,102	0
30	GOL	c	528	6/6	0.95	0.08	38,45,47,47	0
39	DGD	H	102	62/66	0.95	0.10	36,46,58,64	0
39	DGD	c	518	62/66	0.95	0.10	38,49,91,96	0
39	DGD	c	519	62/66	0.95	0.11	43,53,110,123	0
33	PL9	d	407	55/55	0.95	0.08	30,39,49,52	0
41	RRX	H	101	41/41	0.95	0.08	40,50,61,71	0
24	CLA	B	611	65/65	0.95	0.09	35,41,52,64	0
34	BCT	a	407	4/4	0.96	0.08	45,48,53,58	0
26	BCR	A	410	40/40	0.96	0.07	32,40,45,47	0
35	CA	F	102	1/1	0.96	0.09	77,77,77,77	0
24	CLA	B	612	65/65	0.96	0.07	28,35,51,61	0
24	CLA	B	606	65/65	0.96	0.07	30,37,51,54	0
24	CLA	a	410	65/65	0.96	0.10	34,40,104,109	0
24	CLA	B	616	65/65	0.96	0.08	36,42,65,71	0
24	CLA	A	409	65/65	0.96	0.10	33,39,118,122	0
24	CLA	b	605	65/65	0.96	0.08	39,46,56,58	0
24	CLA	b	608	65/65	0.96	0.08	33,39,56,62	0
24	CLA	C	502	65/65	0.96	0.07	38,47,64,75	0
24	CLA	b	610	65/65	0.96	0.07	30,38,49,52	0
24	CLA	b	611	65/65	0.96	0.07	37,44,52,58	0
24	CLA	b	612	65/65	0.96	0.07	41,48,55,60	0
24	CLA	b	613	65/65	0.96	0.08	35,46,54,70	0
24	CLA	b	615	65/65	0.96	0.07	34,40,51,58	0
24	CLA	b	616	65/65	0.96	0.07	32,38,68,71	0
24	CLA	C	503	65/65	0.96	0.07	36,42,59,65	0
24	CLA	b	618	65/65	0.96	0.08	34,47,69,75	0
24	CLA	B	608	65/65	0.96	0.07	28,34,48,53	0
24	CLA	c	503	65/65	0.96	0.09	41,50,64,71	0
24	CLA	c	504	65/65	0.96	0.08	38,47,62,70	0
24	CLA	c	505	65/65	0.96	0.07	41,51,59,71	0
24	CLA	C	505	65/65	0.96	0.09	36,43,80,86	0
24	CLA	c	507	65/65	0.96	0.07	35,45,62,67	0
24	CLA	B	603	65/65	0.96	0.07	34,41,47,53	0
24	CLA	C	508	65/65	0.96	0.08	41,49,68,71	0
37	LHG	B	640	49/49	0.96	0.09	37,46,65,67	0
24	CLA	C	509	65/65	0.96	0.08	35,43,95,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	LHG	D	410	49/49	0.96	0.08	32,42,65,78	0
39	DGD	C	517	62/66	0.96	0.10	36,47,90,91	0
24	CLA	c	512	65/65	0.96	0.08	39,48,60,71	0
39	DGD	C	519	62/66	0.96	0.09	34,43,85,94	0
24	CLA	C	510	65/65	0.96	0.08	39,46,70,77	0
24	CLA	C	511	65/65	0.96	0.07	38,44,61,72	0
24	CLA	C	512	65/65	0.96	0.07	39,50,56,58	0
25	PHO	A	408	64/64	0.96	0.06	28,34,38,40	0
39	DGD	c	520	62/66	0.96	0.10	39,50,80,95	0
24	CLA	B	604	65/65	0.96	0.08	32,40,49,53	0
40	HEM	f	101	43/43	0.96	0.09	55,66,96,113	0
25	PHO	a	411	64/64	0.96	0.06	31,37,41,47	0
34	BCT	A	423	4/4	0.96	0.07	38,39,48,52	0
24	CLA	d	404	65/65	0.97	0.07	28,36,58,65	0
24	CLA	B	605	65/65	0.97	0.07	27,35,72,80	0
24	CLA	A	406	65/65	0.97	0.06	26,32,38,53	0
24	CLA	A	407	65/65	0.97	0.08	29,35,98,100	0
24	CLA	b	606	65/65	0.97	0.07	37,44,54,57	0
25	PHO	d	401	64/64	0.97	0.06	33,41,50,54	0
24	CLA	b	607	65/65	0.97	0.08	29,39,83,87	0
24	CLA	B	613	65/65	0.97	0.07	28,37,46,53	0
24	CLA	B	614	65/65	0.97	0.07	30,36,67,81	0
24	CLA	C	506	65/65	0.97	0.08	36,46,65,70	0
24	CLA	D	403	65/65	0.97	0.07	25,32,50,54	0
24	CLA	A	405	65/65	0.97	0.06	27,32,41,63	0
24	CLA	a	408	65/65	0.97	0.06	31,35,43,64	0
24	CLA	c	511	65/65	0.97	0.08	42,50,66,70	0
24	CLA	b	614	65/65	0.97	0.07	32,38,57,65	0
24	CLA	c	513	65/65	0.97	0.07	42,53,62,67	0
24	CLA	a	409	65/65	0.97	0.06	29,34,43,53	0
24	CLA	B	609	65/65	0.97	0.06	31,39,47,50	0
42	MG	J	101	1/1	0.97	0.08	43,43,43,43	0
30	GOL	C	524	6/6	0.98	0.05	36,41,43,44	0
35	CA	o	303	1/1	0.98	0.04	67,67,67,67	0
40	HEM	F	101	43/43	0.98	0.06	42,52,61,65	0
23	CL	a	406	1/1	0.98	0.05	41,41,41,41	0
23	CL	A	403	1/1	0.98	0.06	38,38,38,38	0
23	CL	a	405	1/1	0.98	0.11	44,44,44,44	0
35	CA	c	502	1/1	0.98	0.04	61,61,61,61	0
43	HEC	v	1603	43/43	0.98	0.07	40,49,54,55	0
21	OEX	a	403	10/10	0.99	0.03	38,40,42,42	0
22	FE2	A	402	1/1	0.99	0.02	39,39,39,39	0

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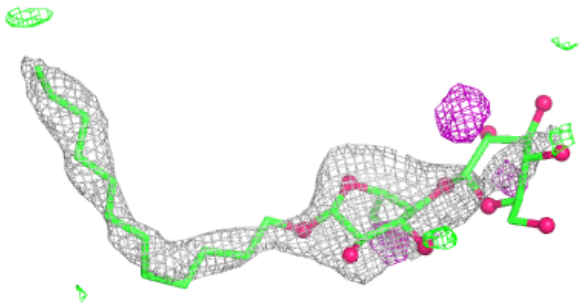
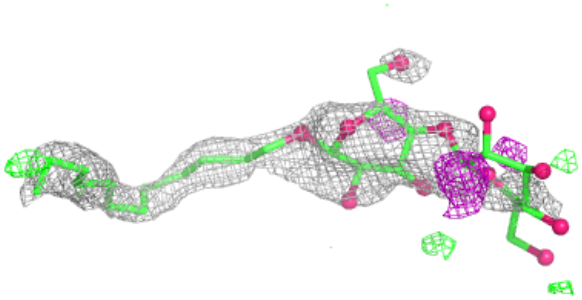
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CA	O	301	1/1	0.99	0.09	70,70,70,70	0
21	OEX	A	401	10/10	0.99	0.03	35,37,41,42	0
42	MG	j	1303	1/1	0.99	0.11	52,52,52,52	0
43	HEC	V	202	43/43	0.99	0.05	36,42,45,49	0
23	CL	A	404	1/1	0.99	0.04	38,38,38,38	0
22	FE2	a	404	1/1	1.00	0.02	42,42,42,42	0

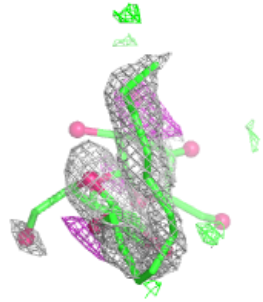
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT C 521:

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

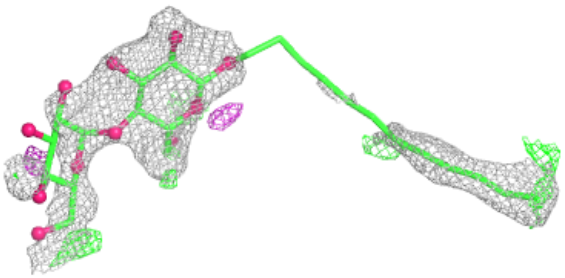


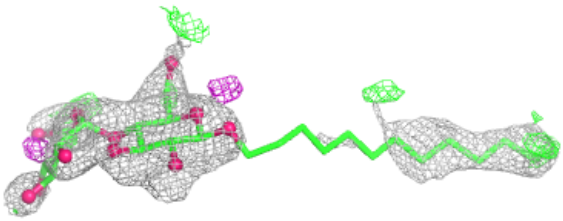


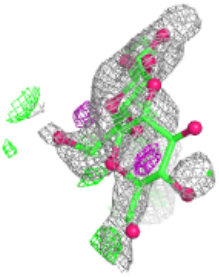


Electron density around LMT f 104:

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

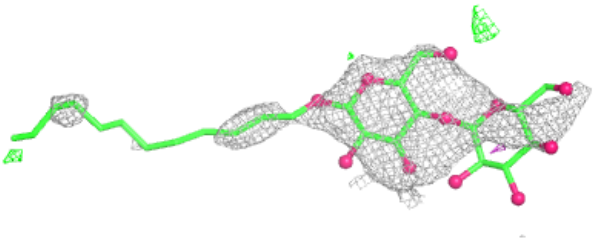


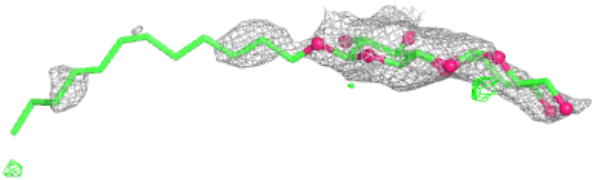


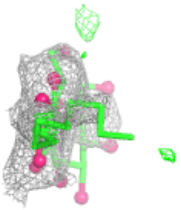


Electron density around LMT c 523:

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

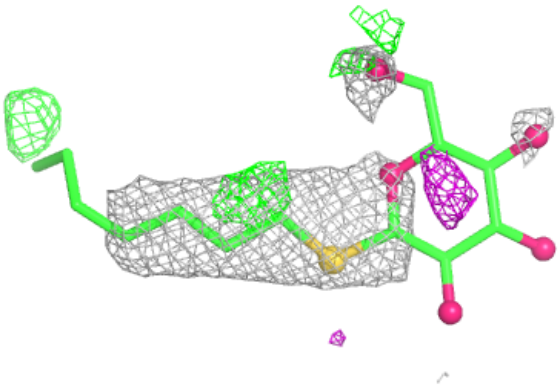


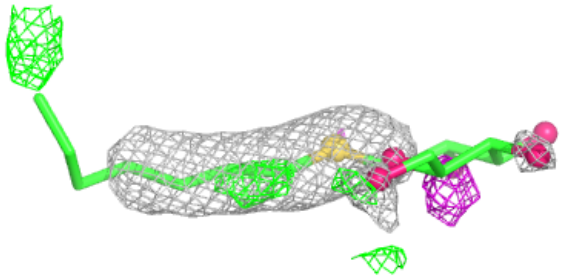


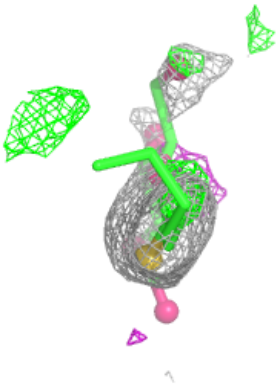


Electron density around HTG D 413:

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

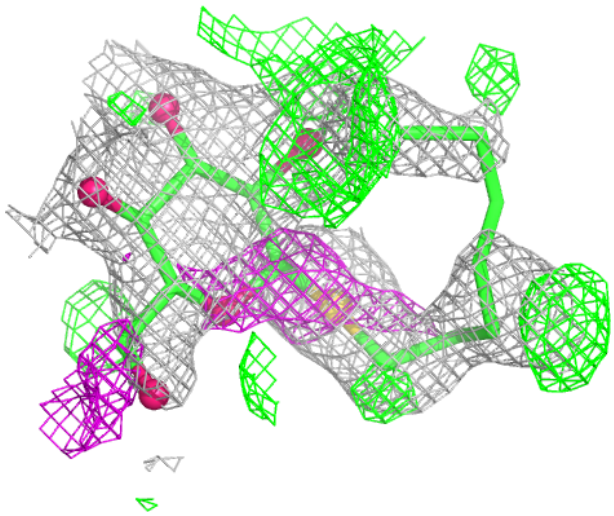


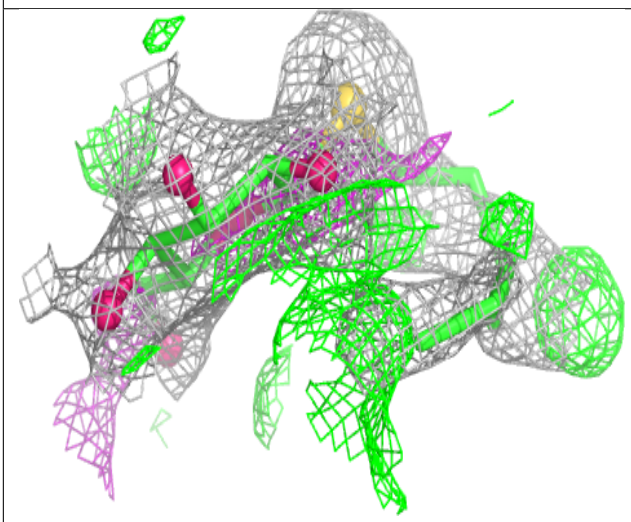


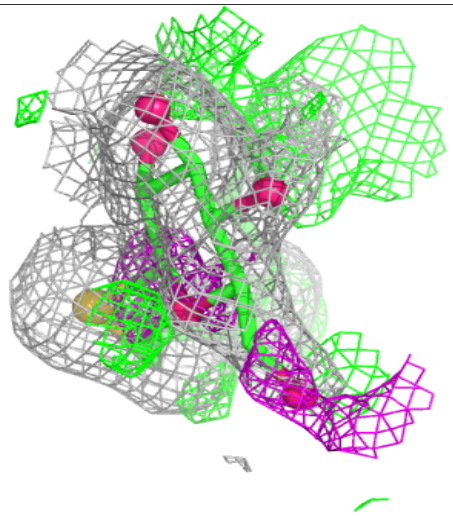


Electron density around HTG b 625:

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

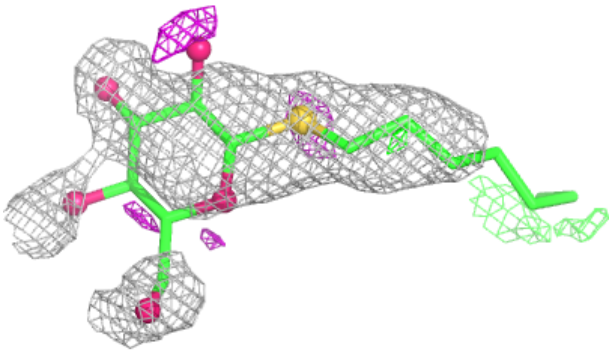


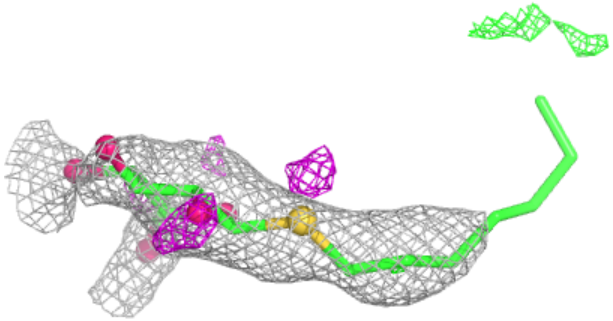


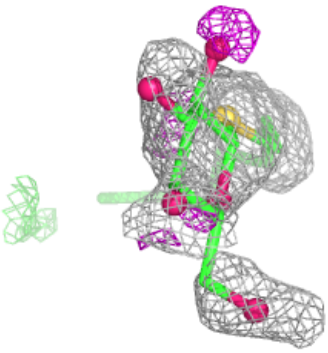


Electron density around HTG h 1202:

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

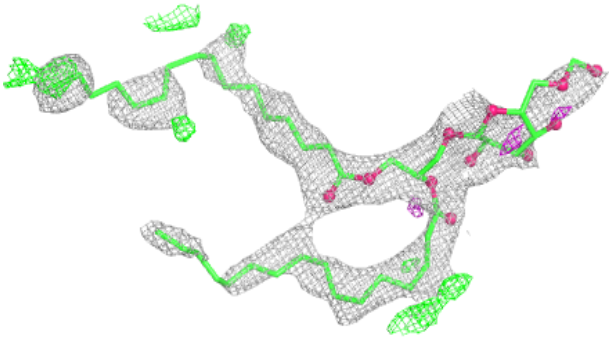


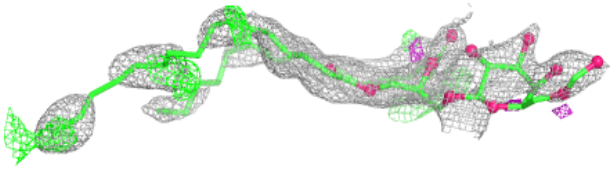


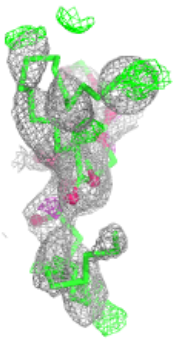


Electron density around DGD D 407:

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

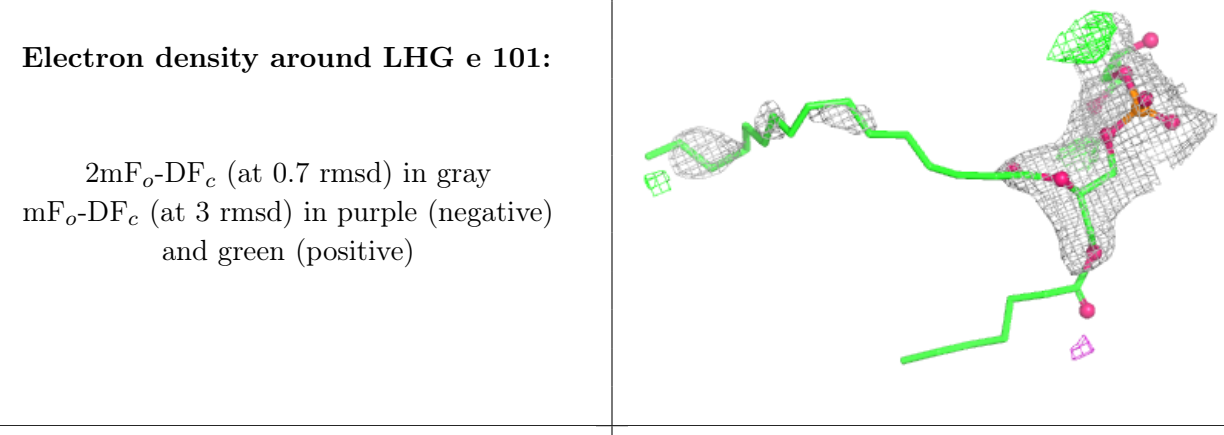






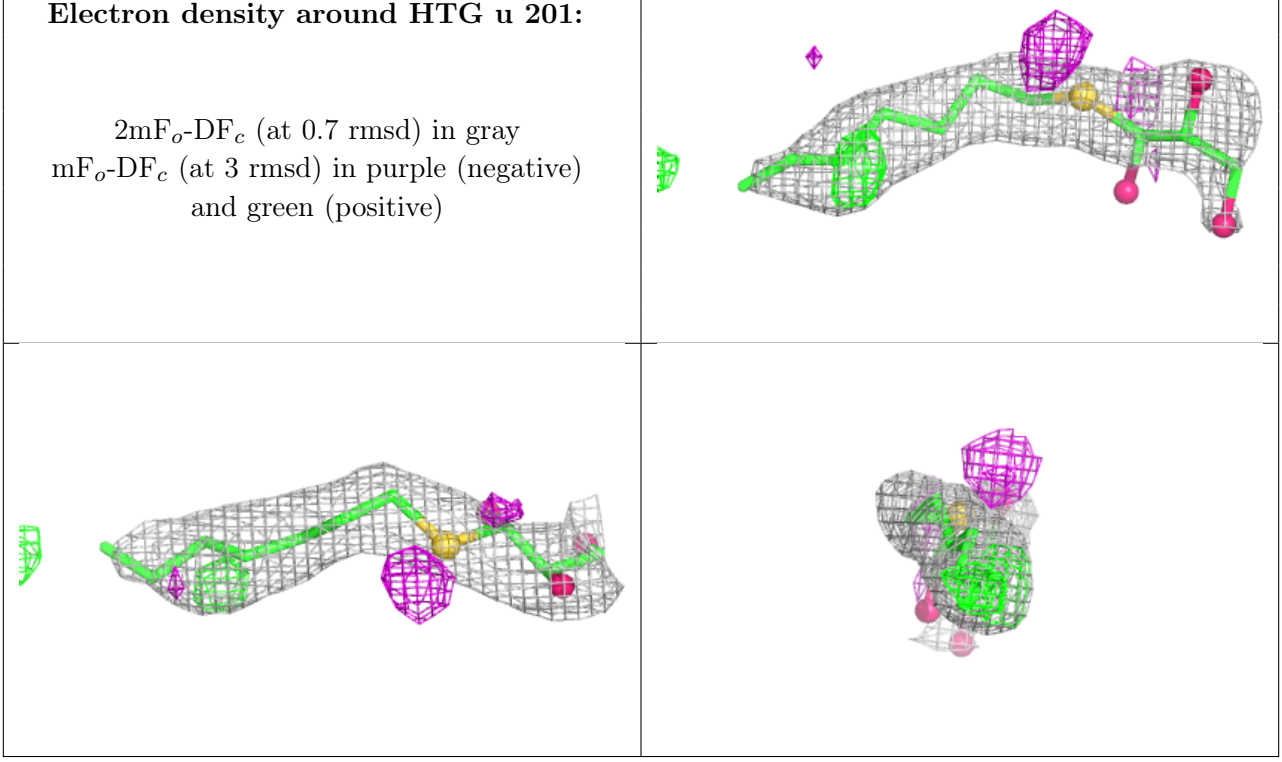
Electron density around LHG e 101:

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



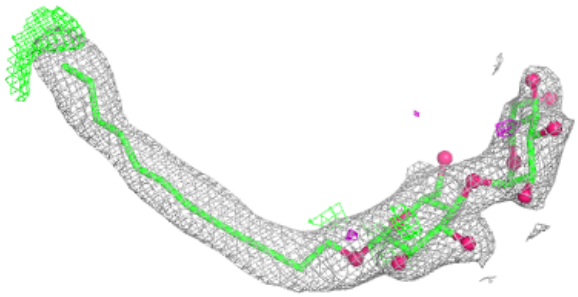
Electron density around HTG u 201:

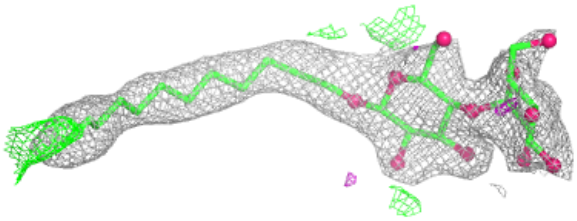
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

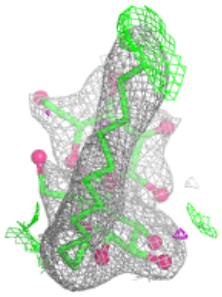


Electron density around LMT m 103:

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

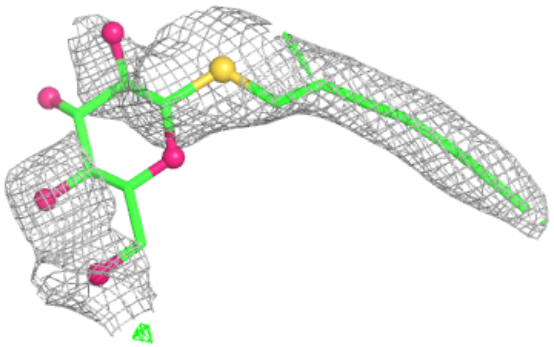


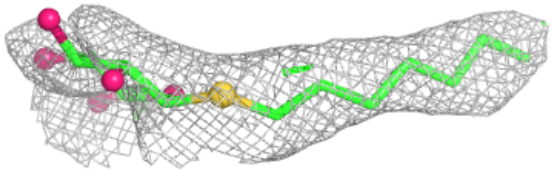


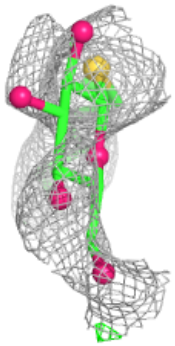


Electron density around HTG b 626:

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

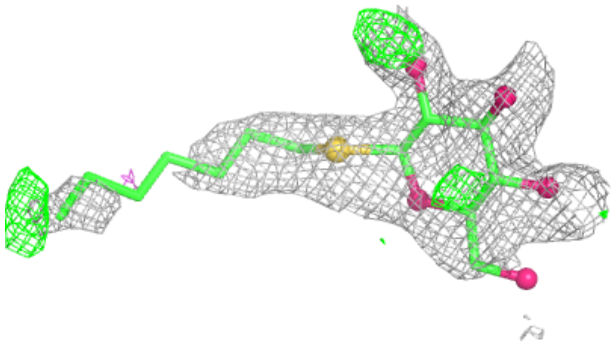


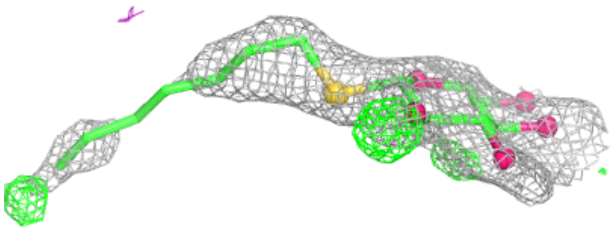


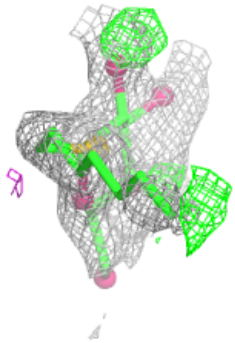


Electron density around HTG d 414:

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

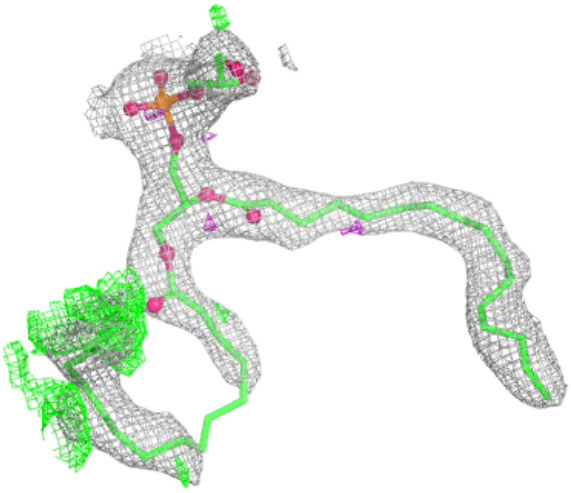


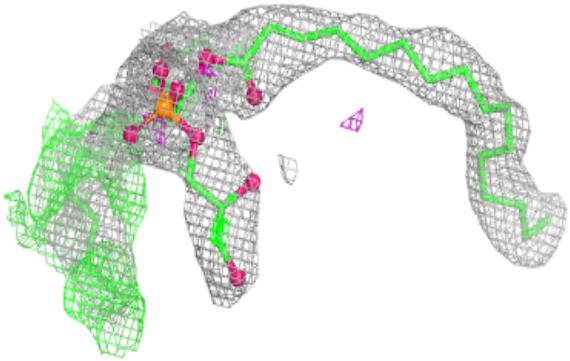


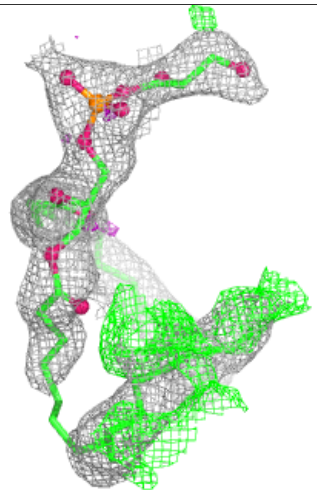


Electron density around LHG E 101:

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

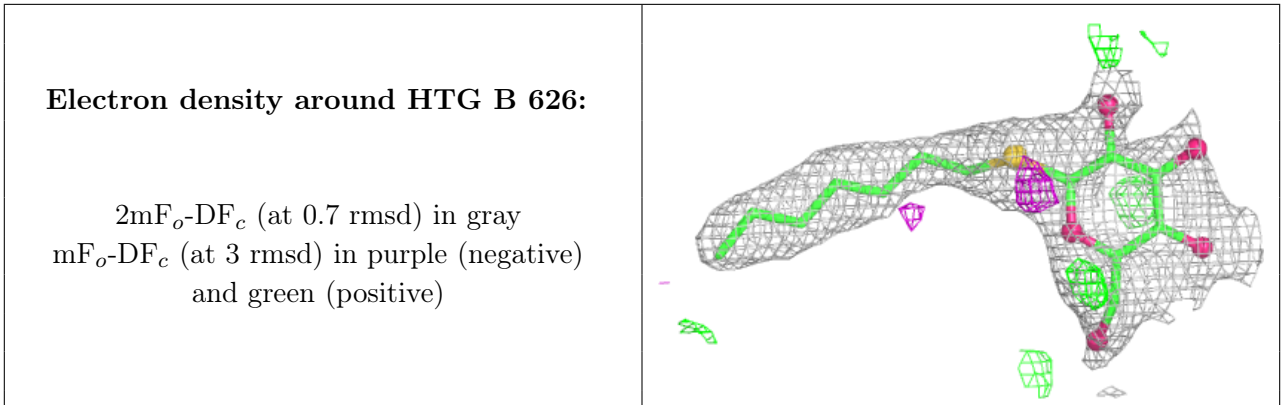


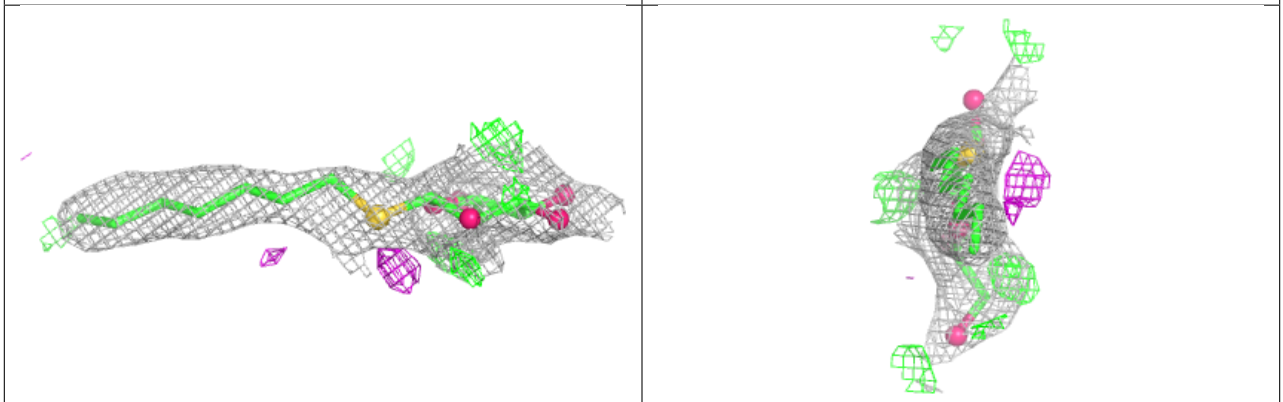




Electron density around HTG B 626:

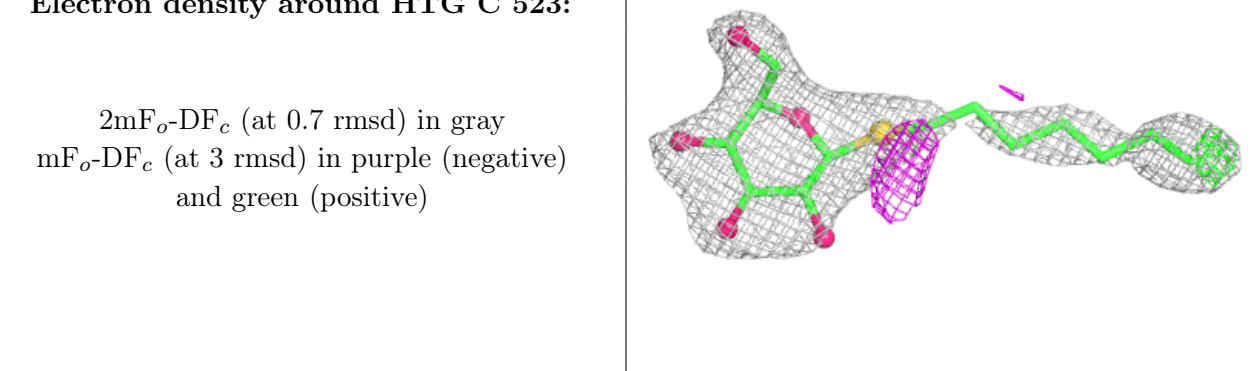
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

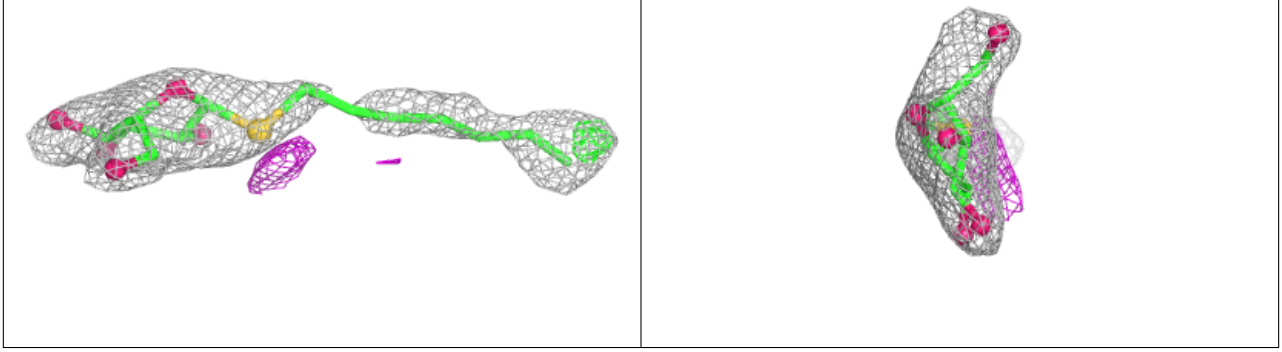




Electron density around HTG C 523:

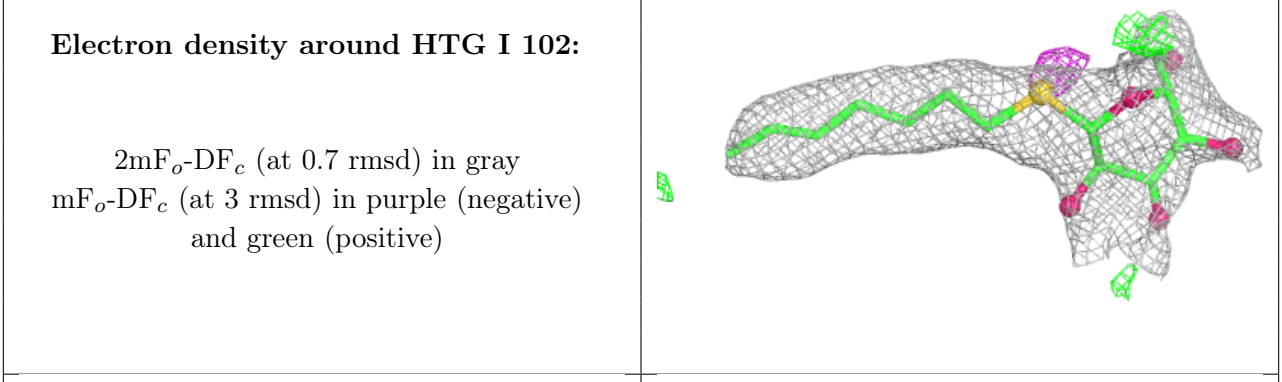
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

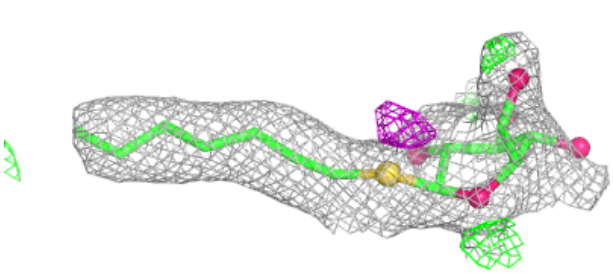


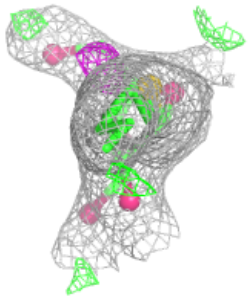


Electron density around HTG I 102:

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

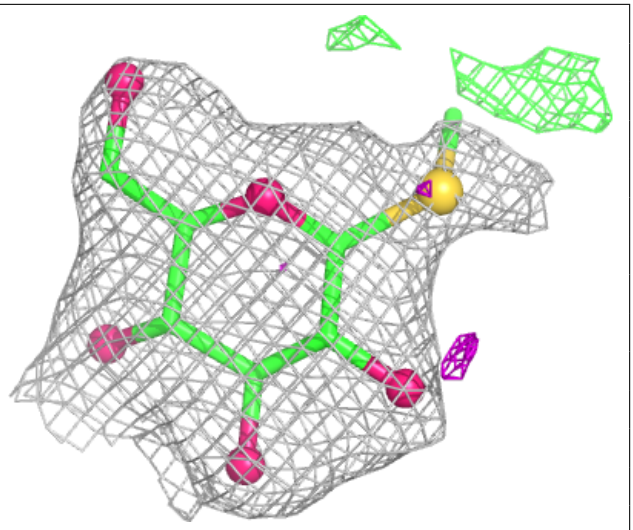


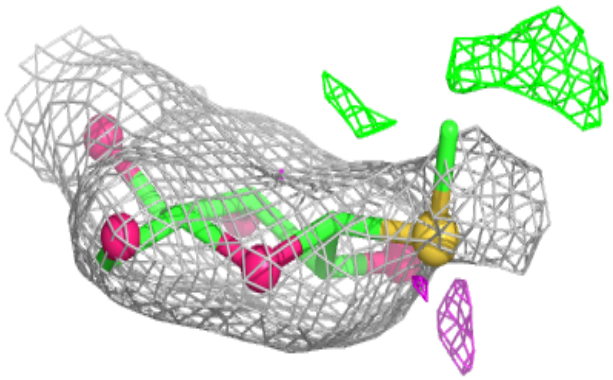


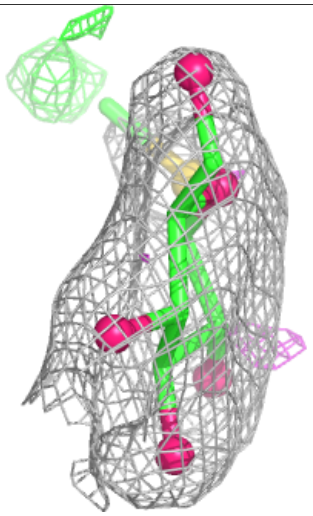


Electron density around HTG V 203:

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

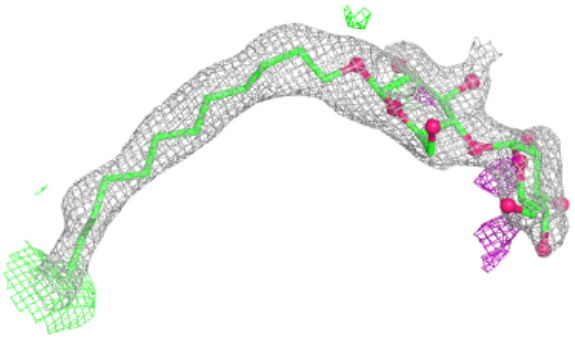


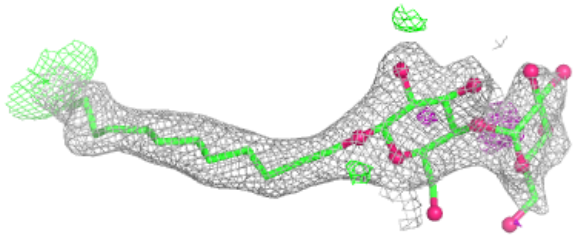


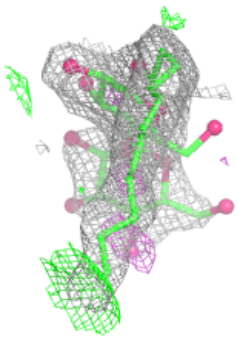


Electron density around LMT m 101:

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

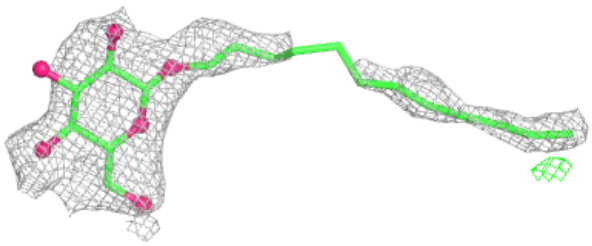


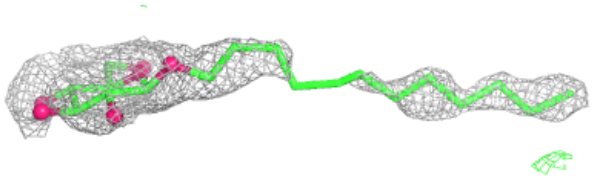


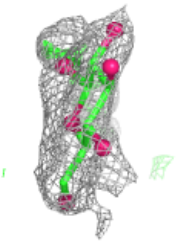


Electron density around LMT E 104:

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

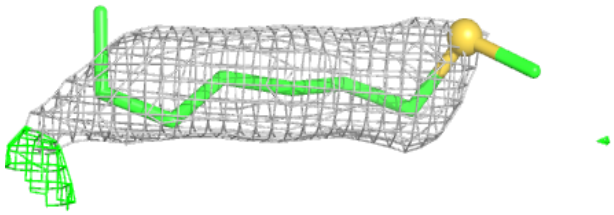


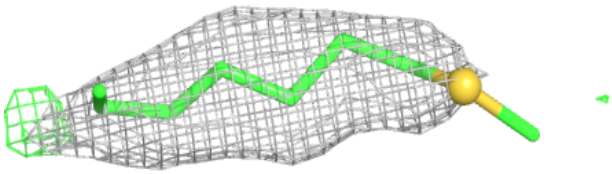


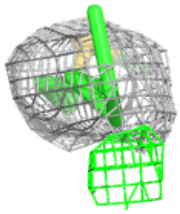


Electron density around HTG U 201:

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

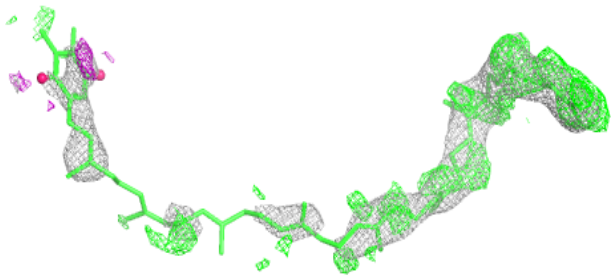


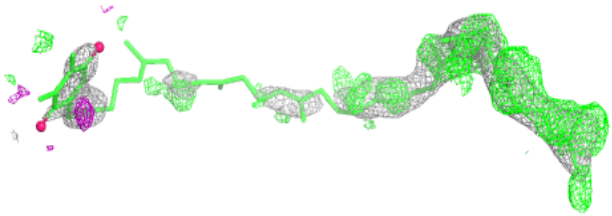


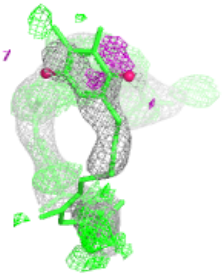


Electron density around PL9 a 425 (B):

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

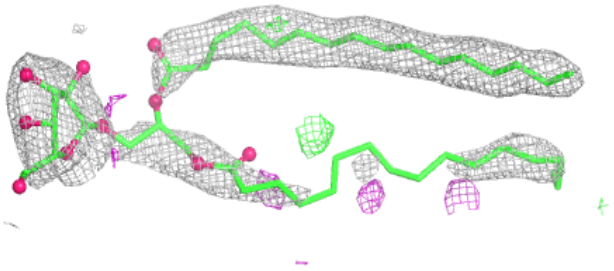


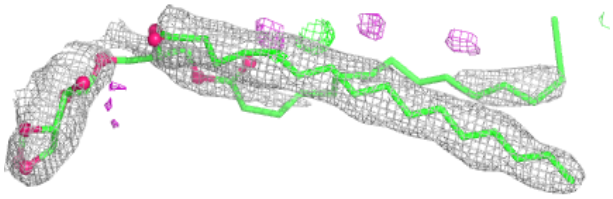


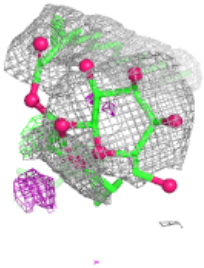


Electron density around LMG C 532:

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

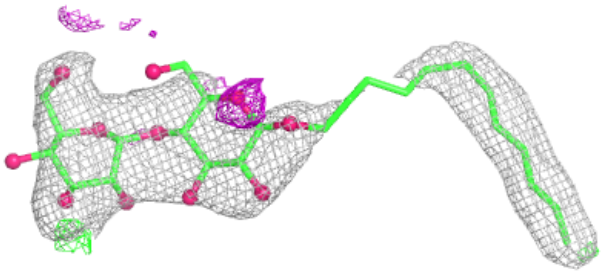


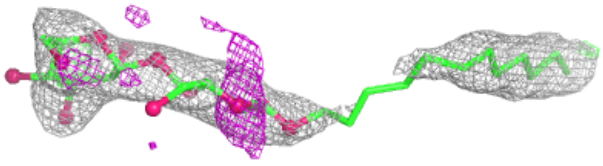


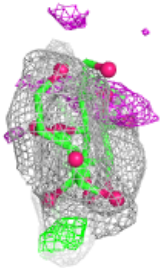


Electron density around LMT Z 101:

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

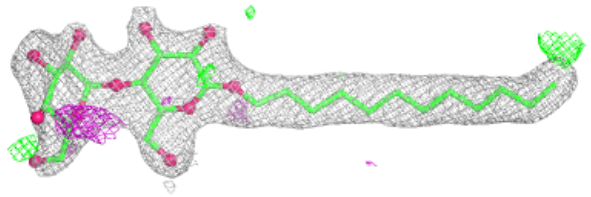


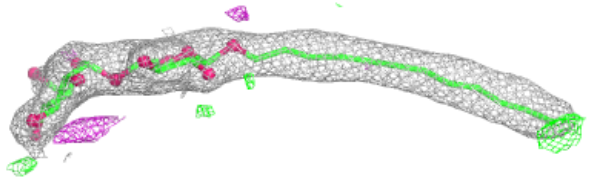


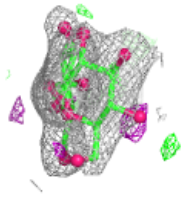


Electron density around LMT M 101:

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

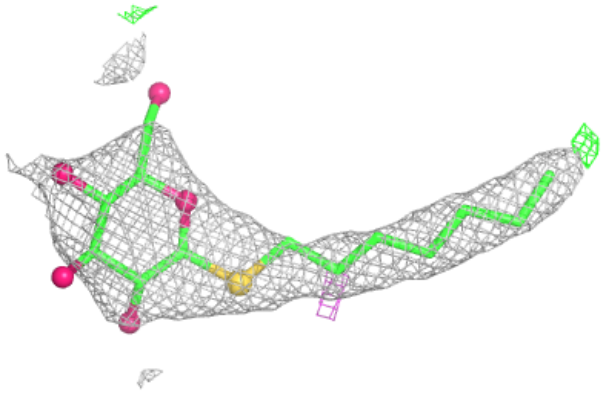


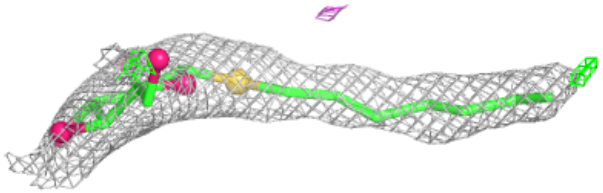


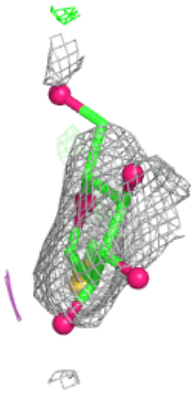


Electron density around HTG B 624:

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

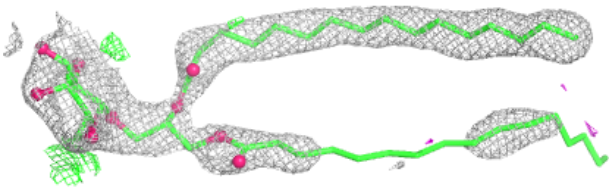


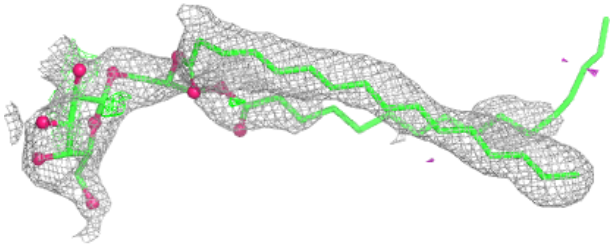


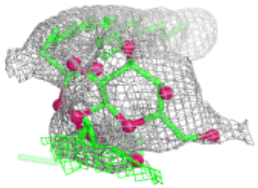


Electron density around LMG c 522:

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

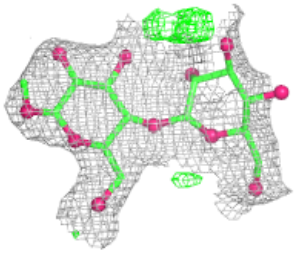


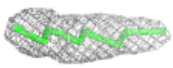


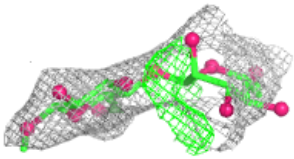


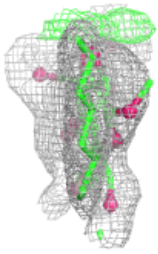
Electron density around LMT z 101:

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



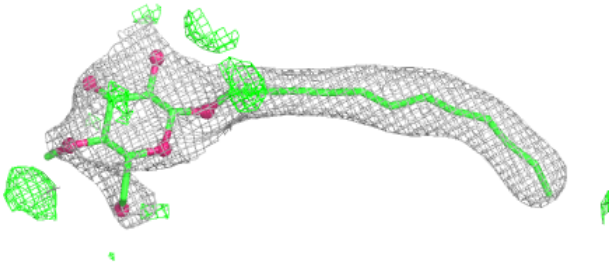


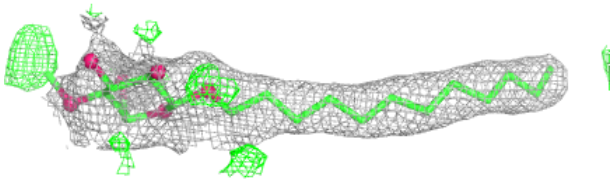


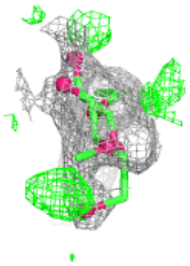


Electron density around LMT b 624:

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

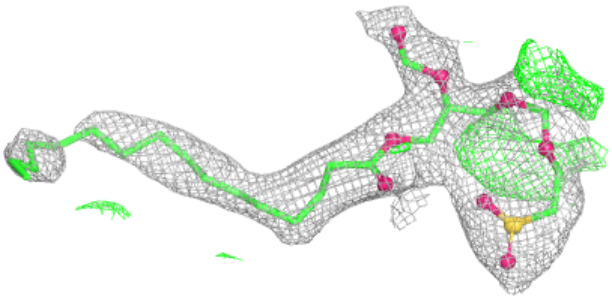


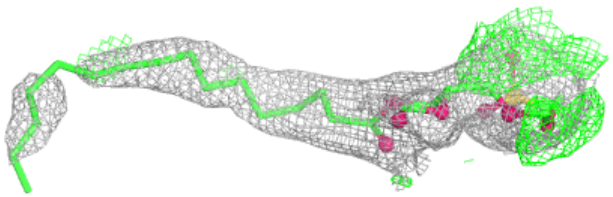


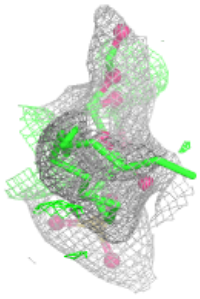


Electron density around SQD f 102:

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

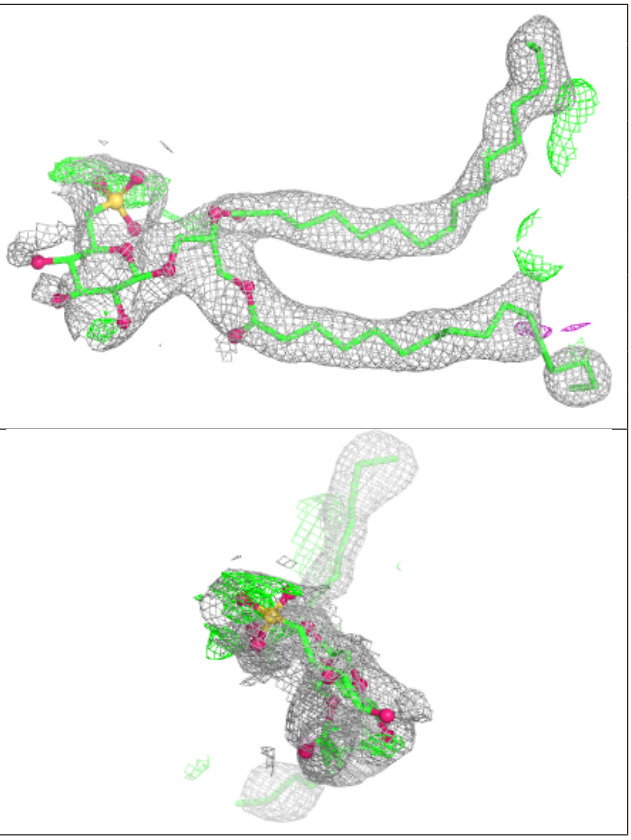






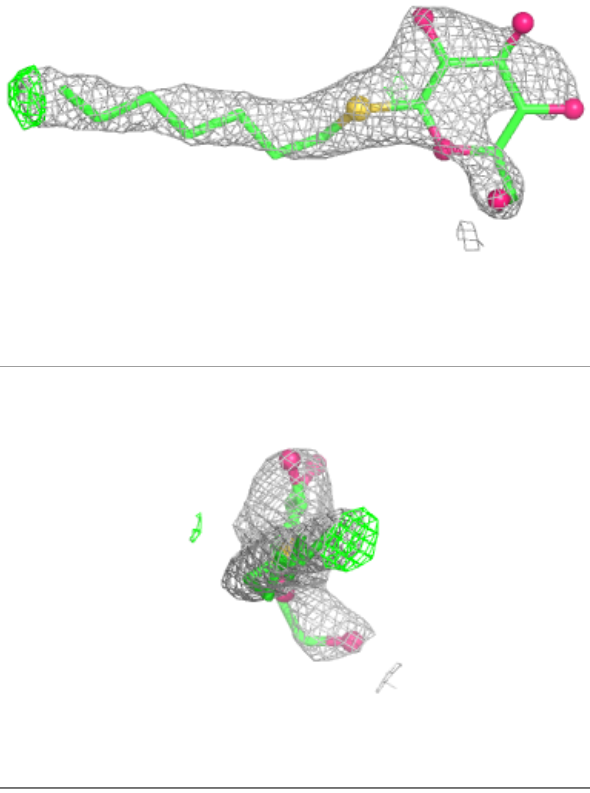
Electron density around SQD L 101:

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



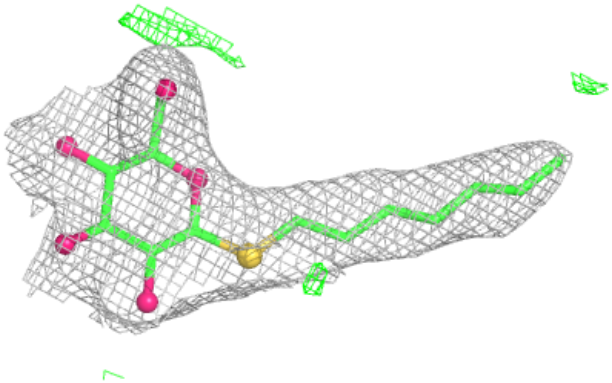
Electron density around HTG c 525:

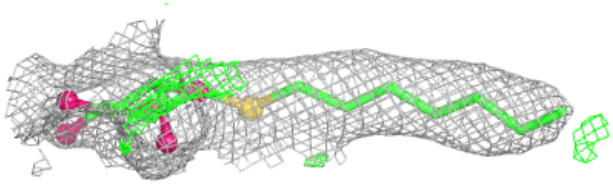
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

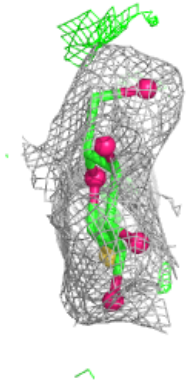


Electron density around HTG b 602:

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

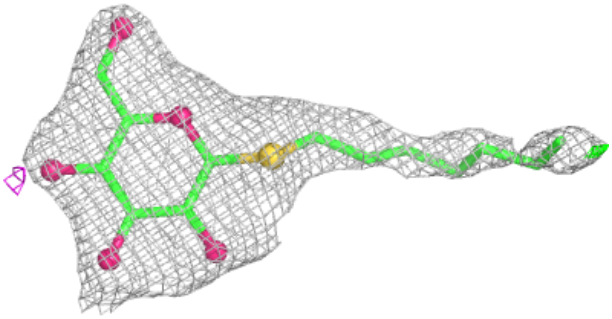


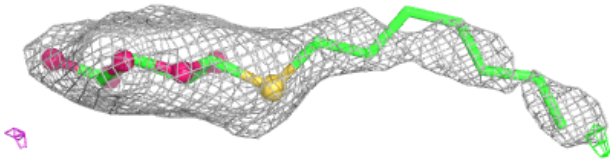


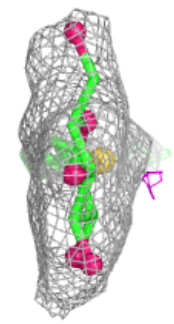


Electron density around HTG c 524:

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

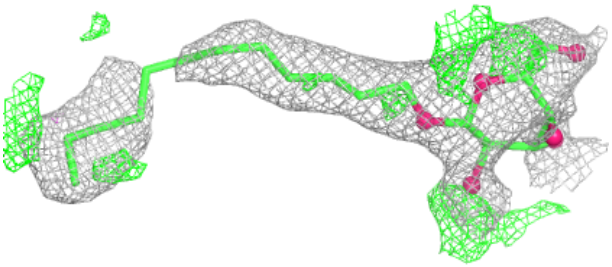


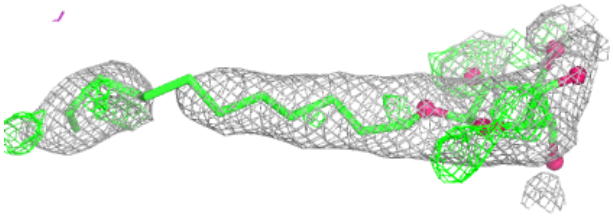


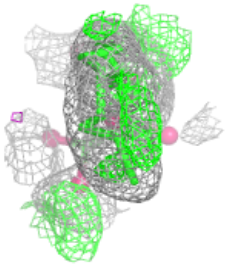


Electron density around LMT T 104:

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

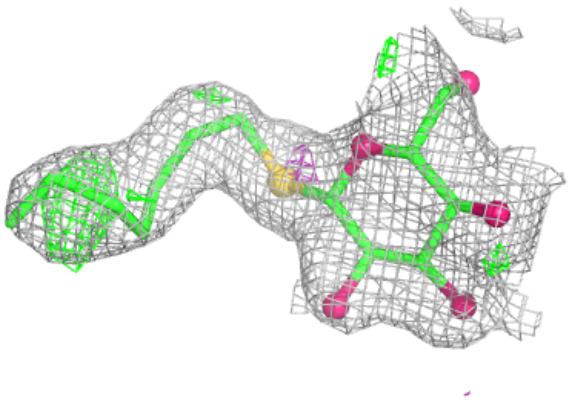


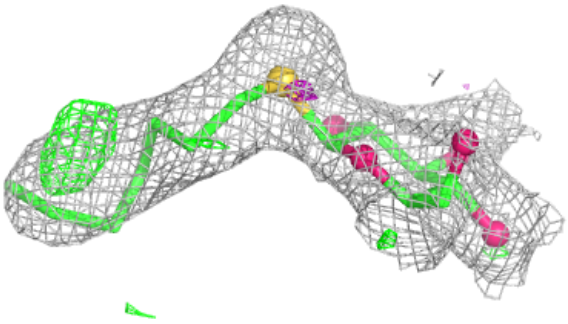


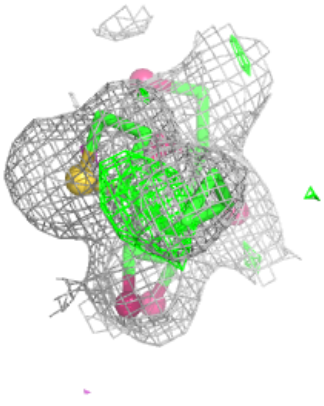


Electron density around HTG B 623 (A):

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

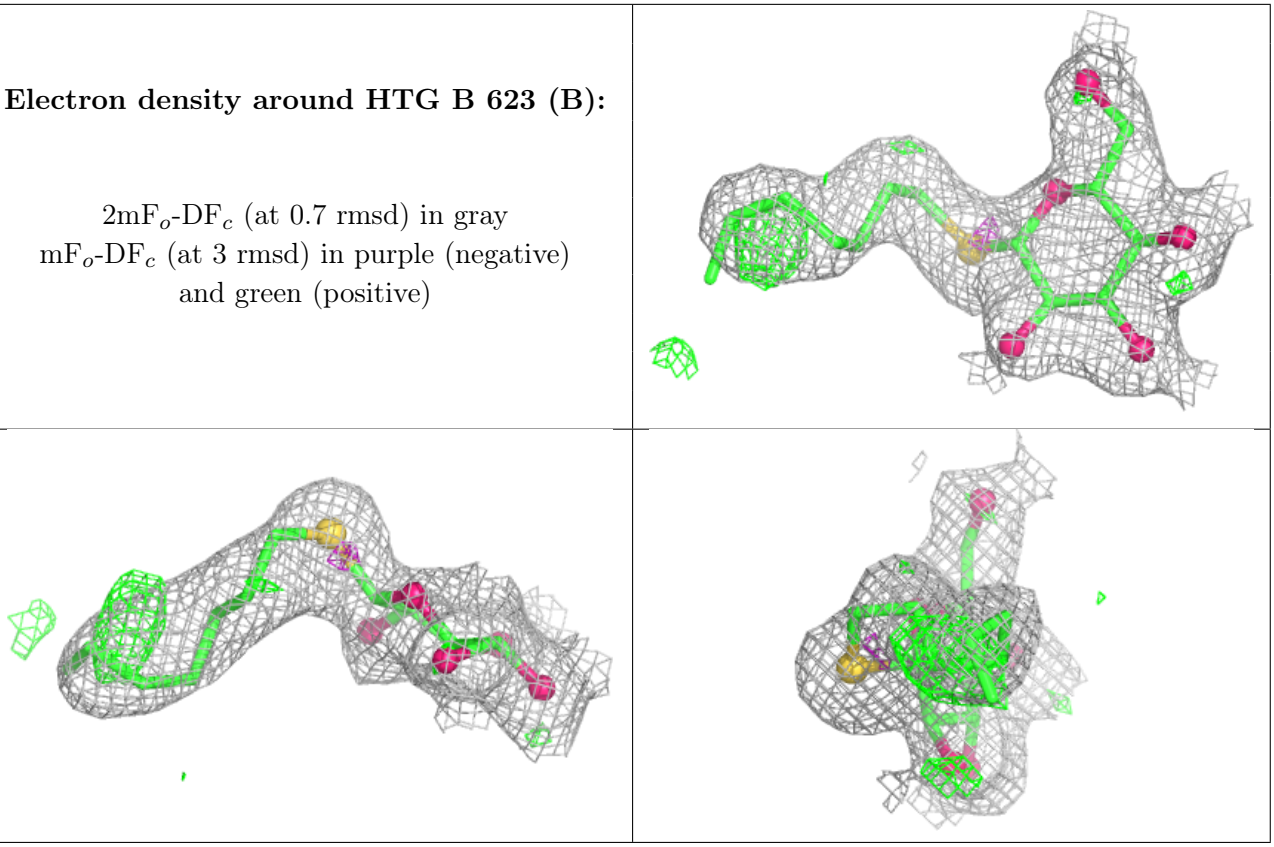






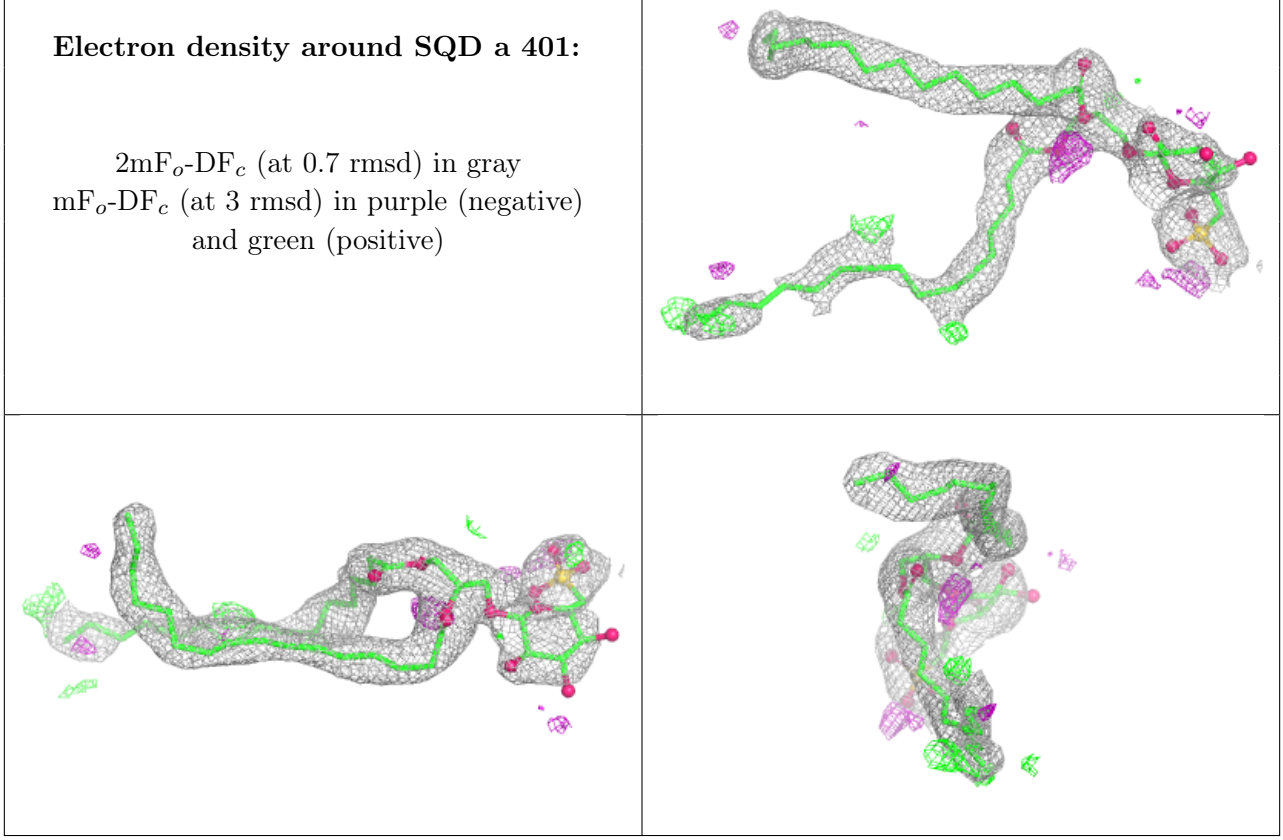
Electron density around HTG B 623 (B):

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



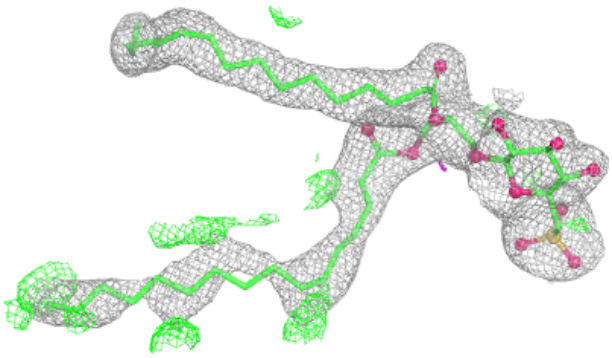
Electron density around SQD a 401:

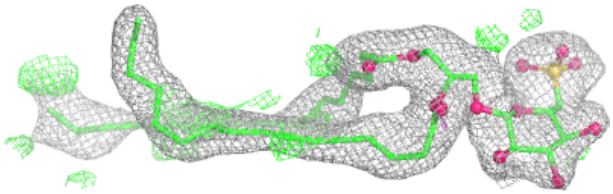
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD A 413:

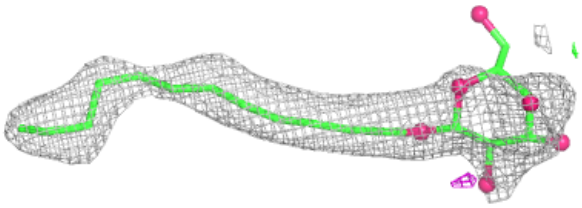
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

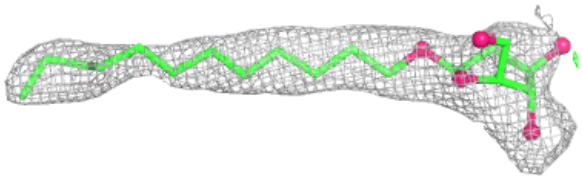


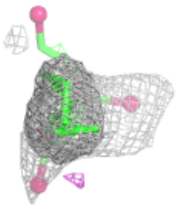


Electron density around LMT J 102:

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

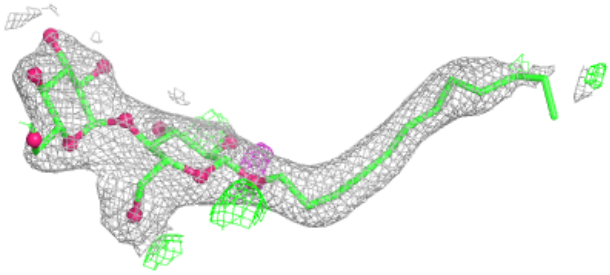


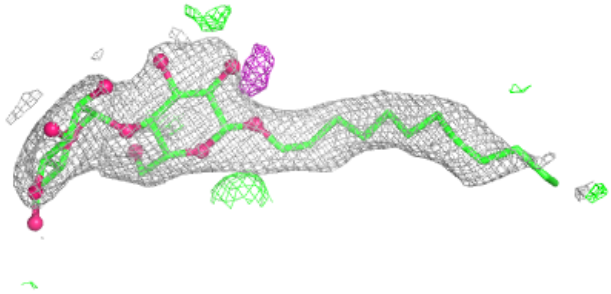


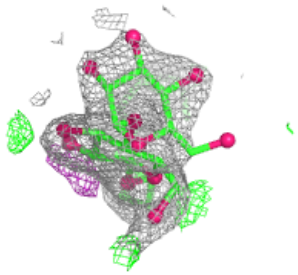


Electron density around LMT A 414:

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

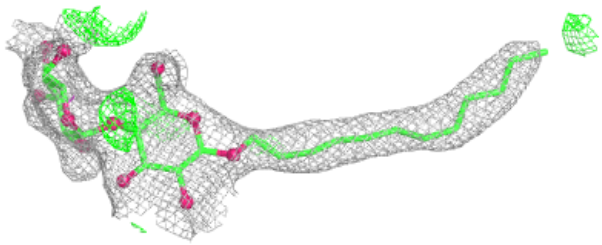


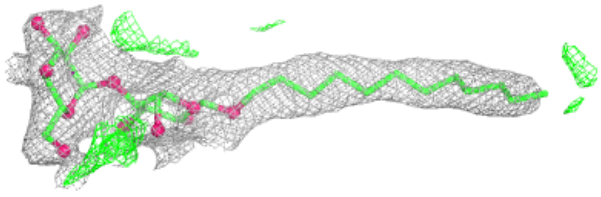


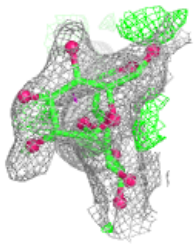


Electron density around LMT B 622:

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

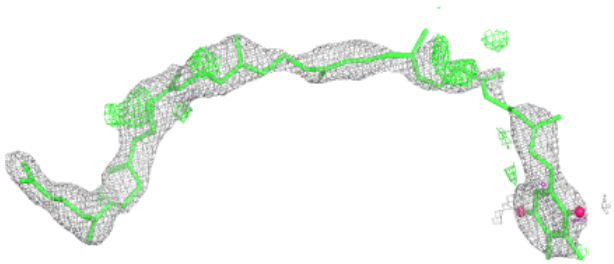


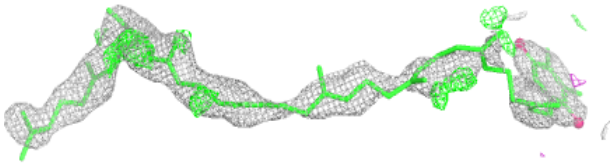


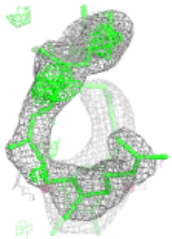


Electron density around PL9 A 422 (B):

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

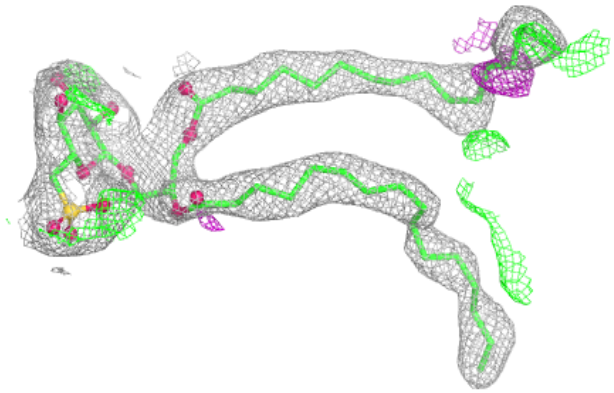


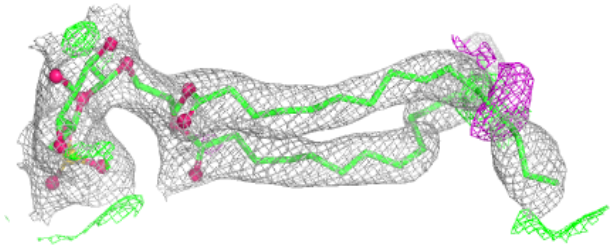


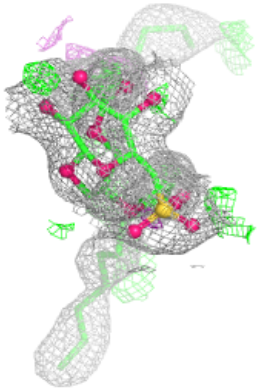


Electron density around SQD L 102:

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

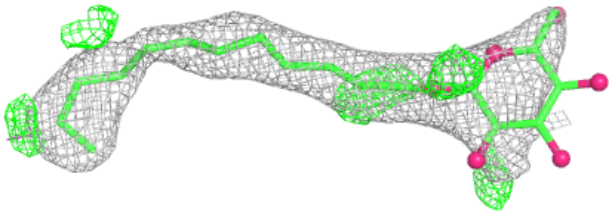


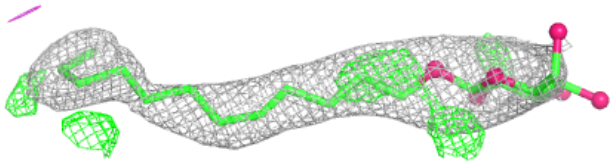


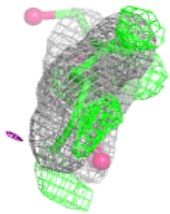


Electron density around LMT B 642:

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

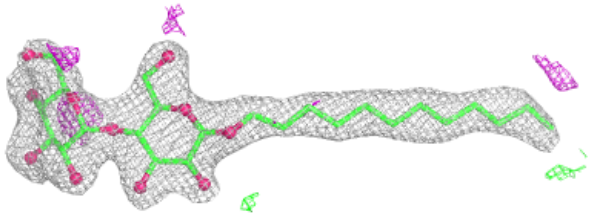


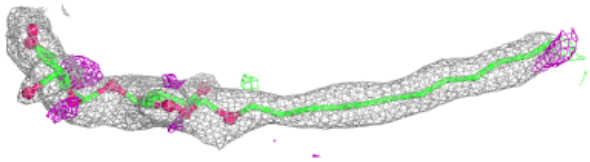


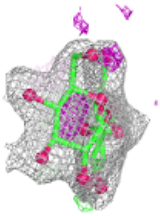


Electron density around LMT m 102:

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

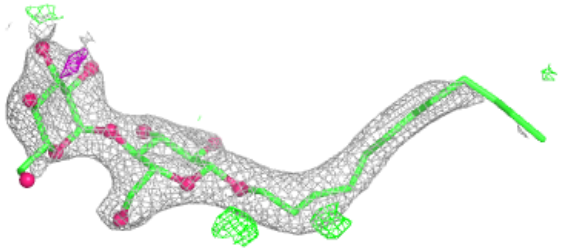


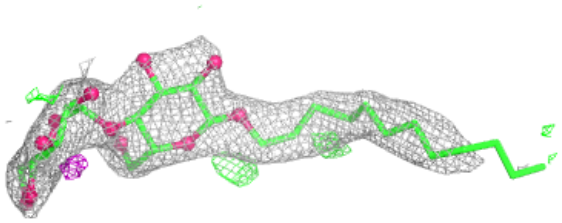


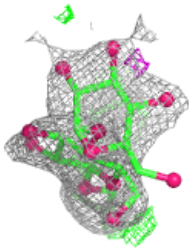


Electron density around LMT a 402:

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

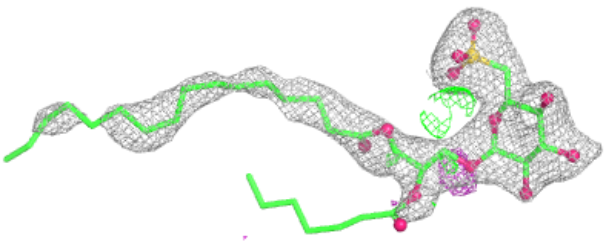


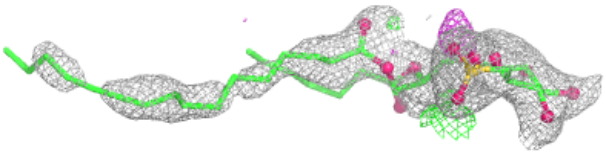


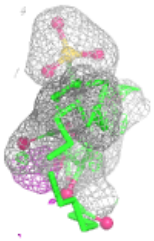


Electron density around SQD D 408:

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

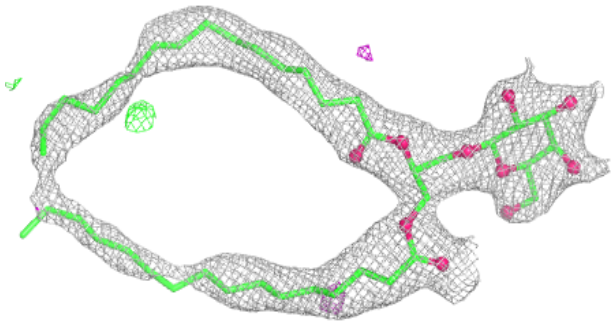


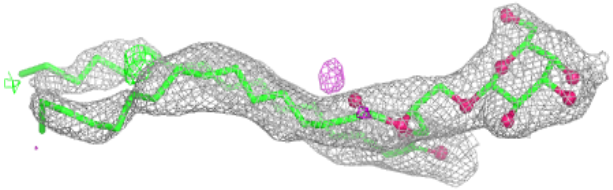


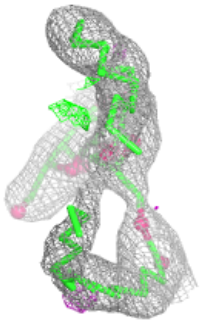


Electron density around LMG a 415:

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

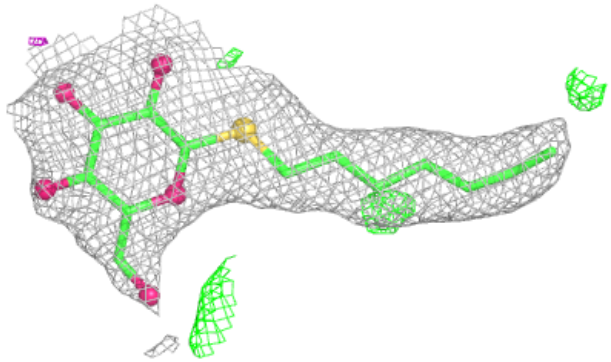


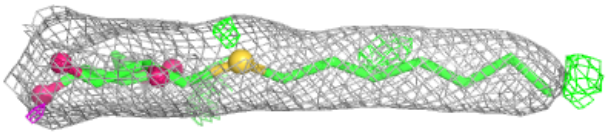


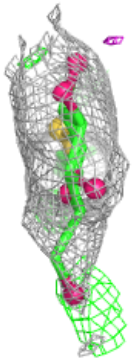


Electron density around HTG b 601:

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

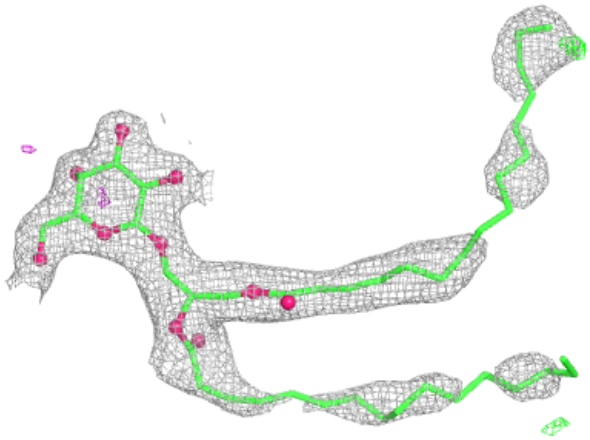


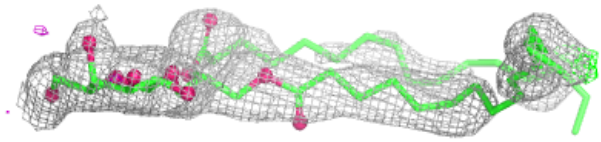


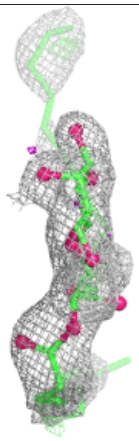


Electron density around LMG C 520:

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

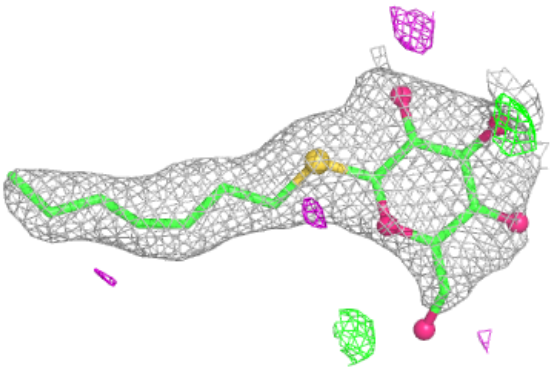


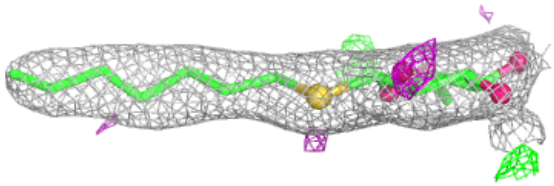


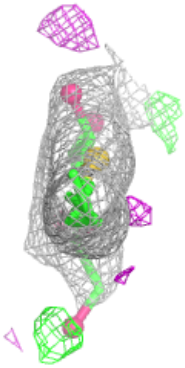


Electron density around HTG B 625:

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

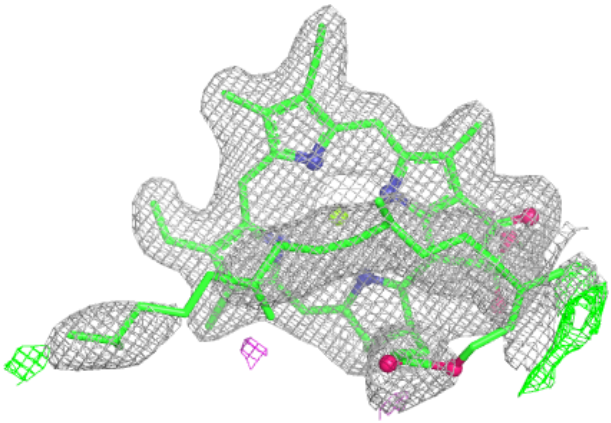


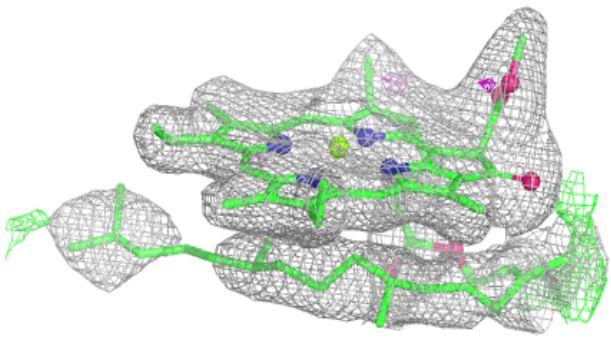


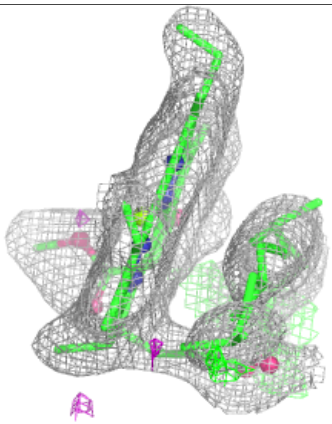


Electron density around CLA B 602:

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

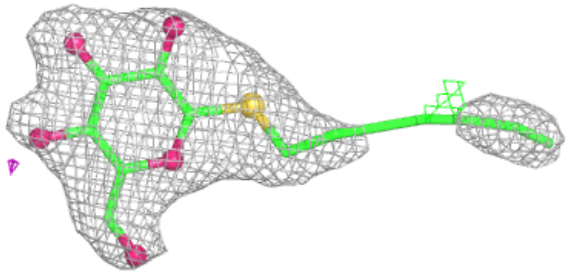


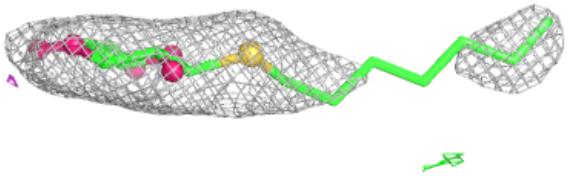


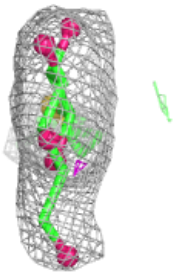


Electron density around HTG C 522:

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

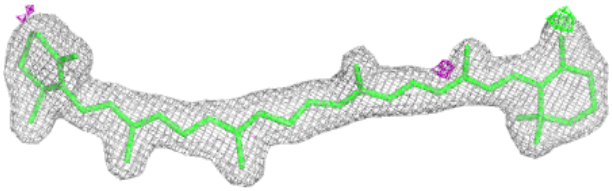


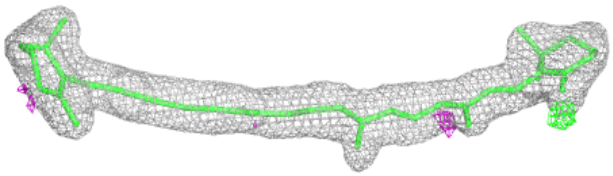


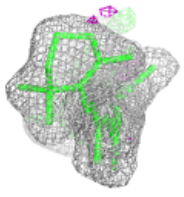


Electron density around BCR T 102:

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

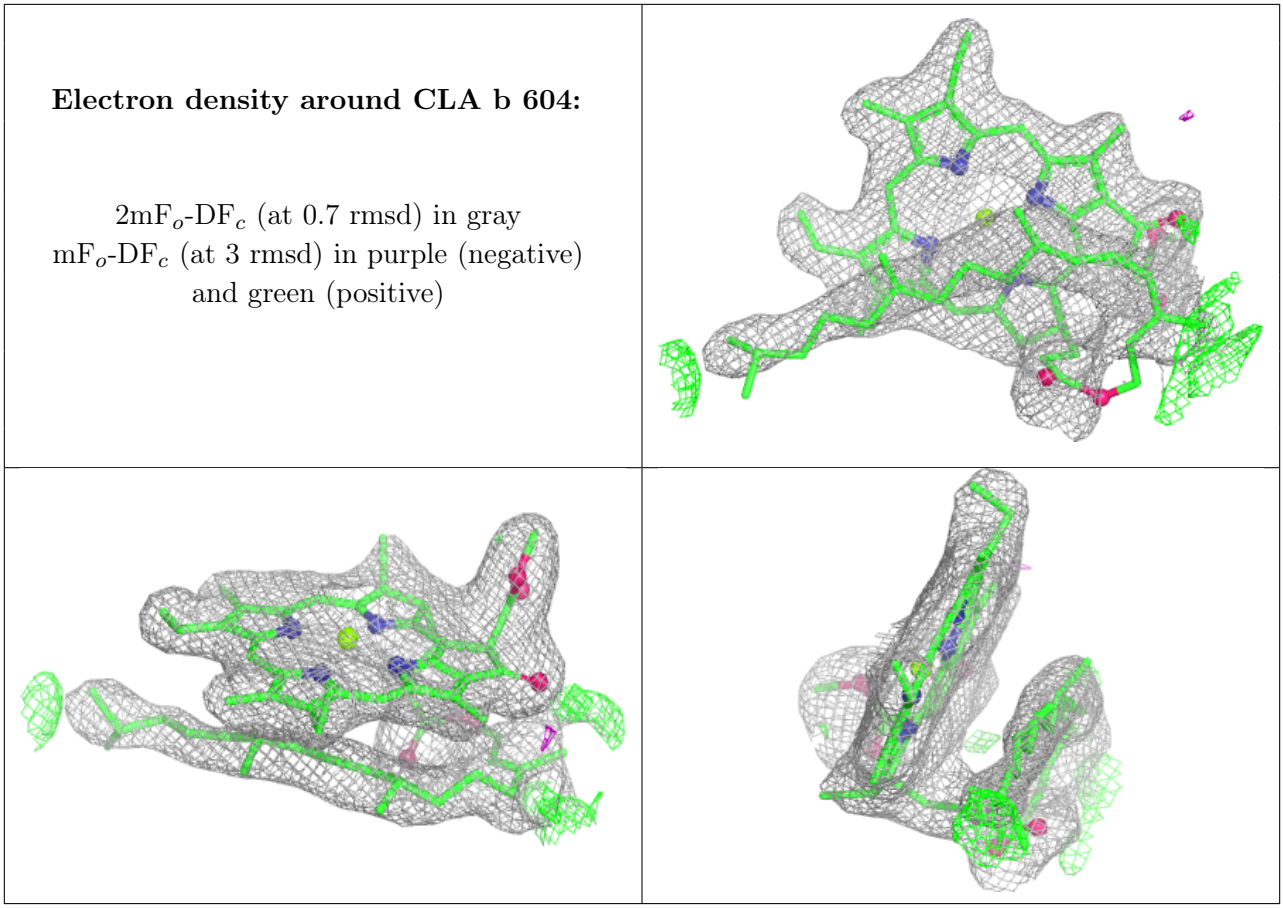






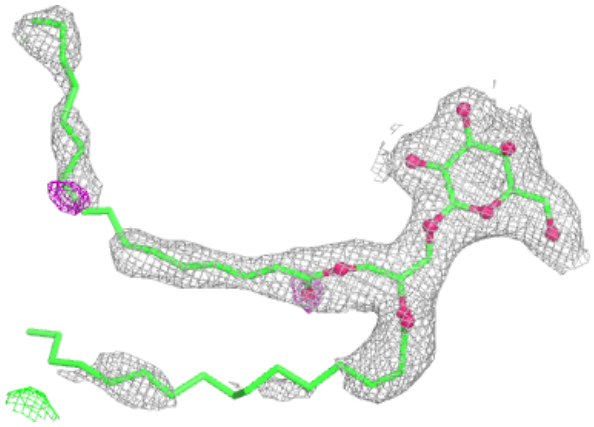
Electron density around CLA b 604:

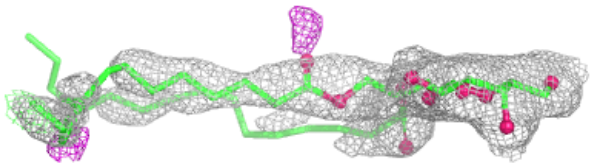
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

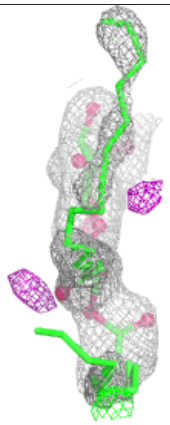


Electron density around LMG c 521:

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

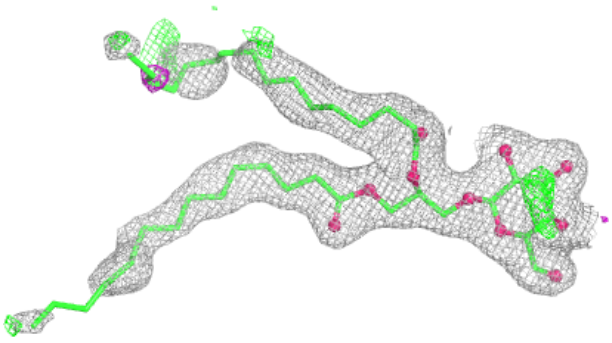


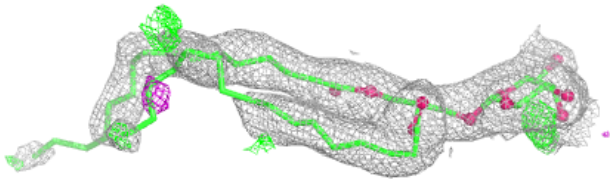


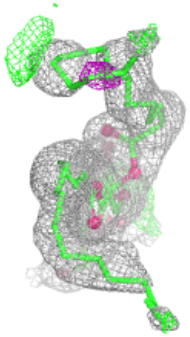


Electron density around LMG d 411:

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

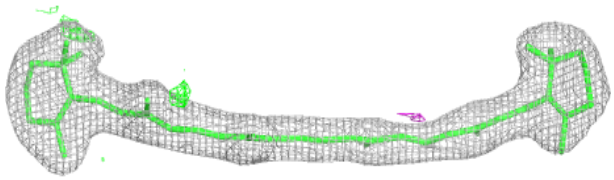


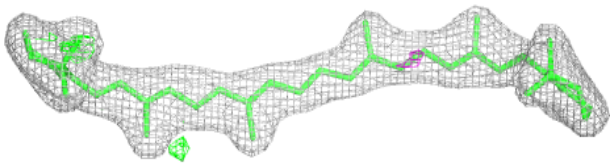


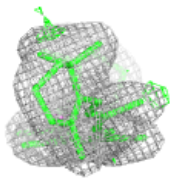


Electron density around BCR K 101:

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

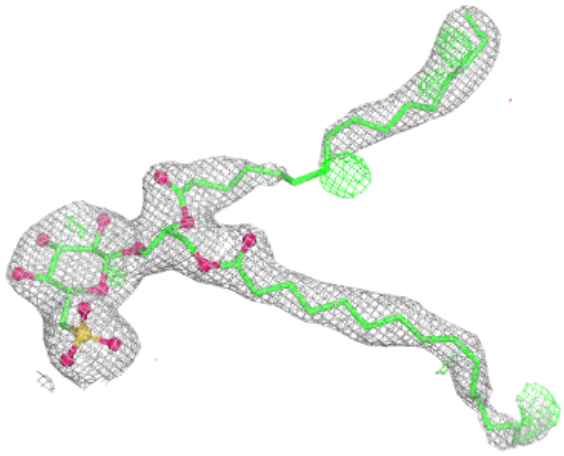


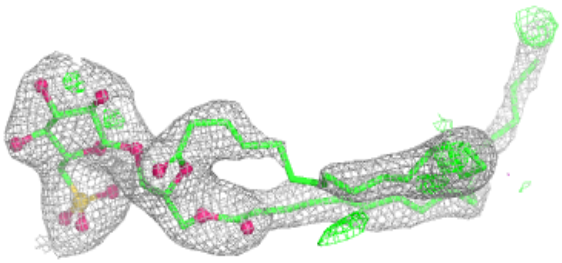


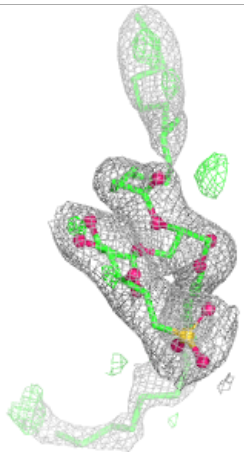


Electron density around SQD a 414:

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

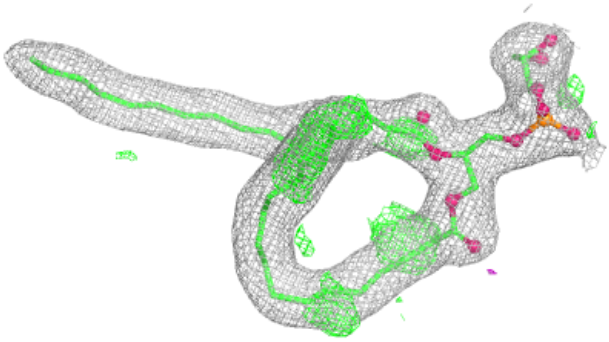


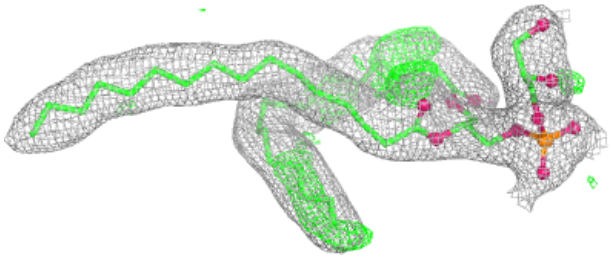


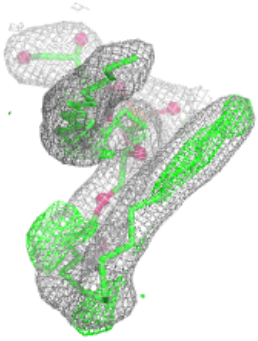


Electron density around LHG D 409:

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

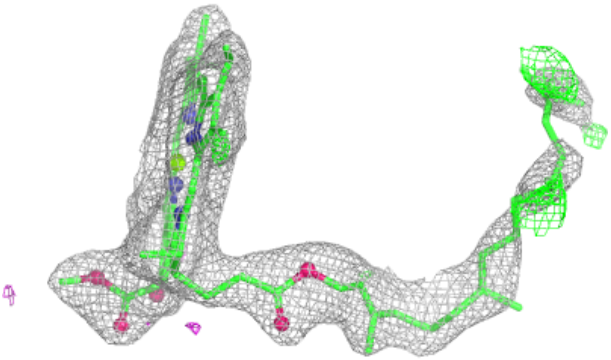


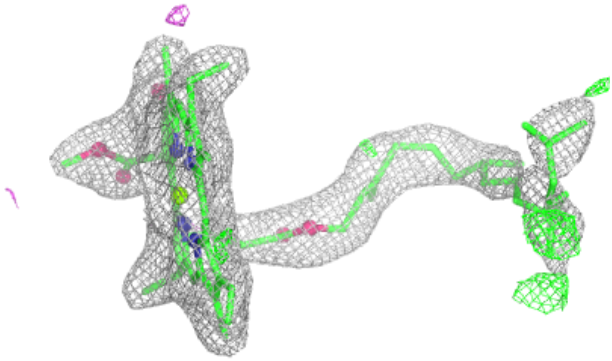


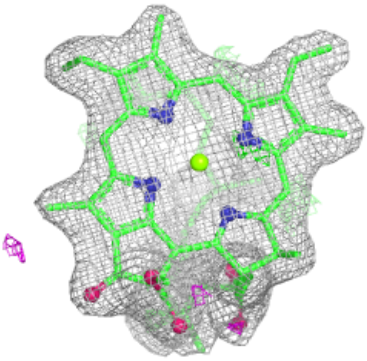


Electron density around CLA C 507:

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

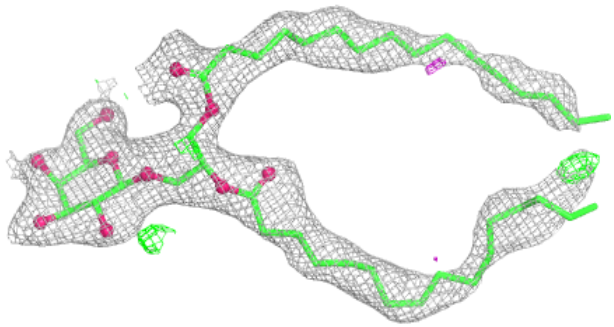


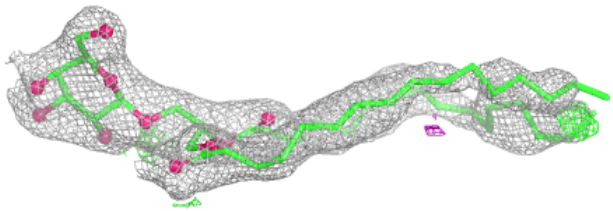


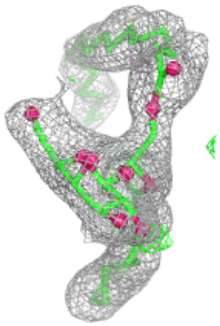


Electron density around LMG A 412:

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

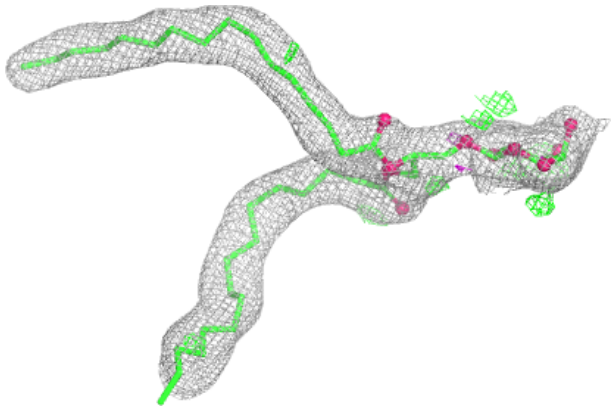


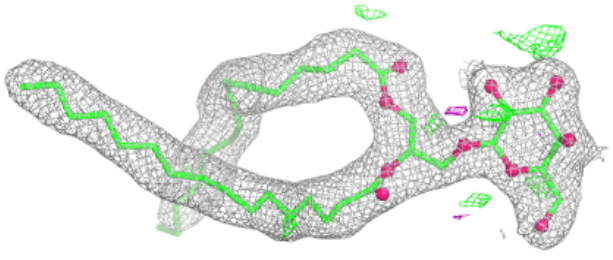


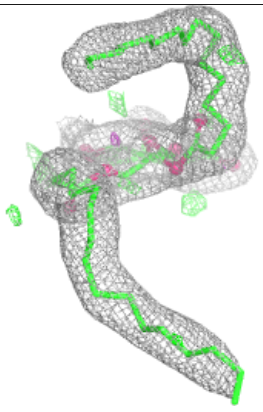


Electron density around LMG B 621:

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

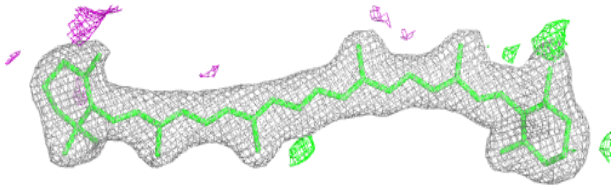


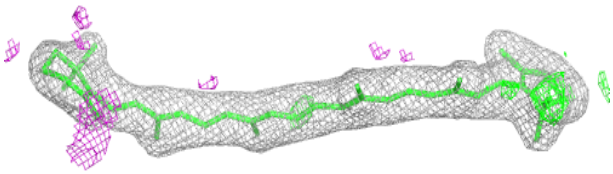


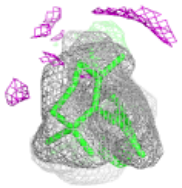


Electron density around BCR b 622:

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

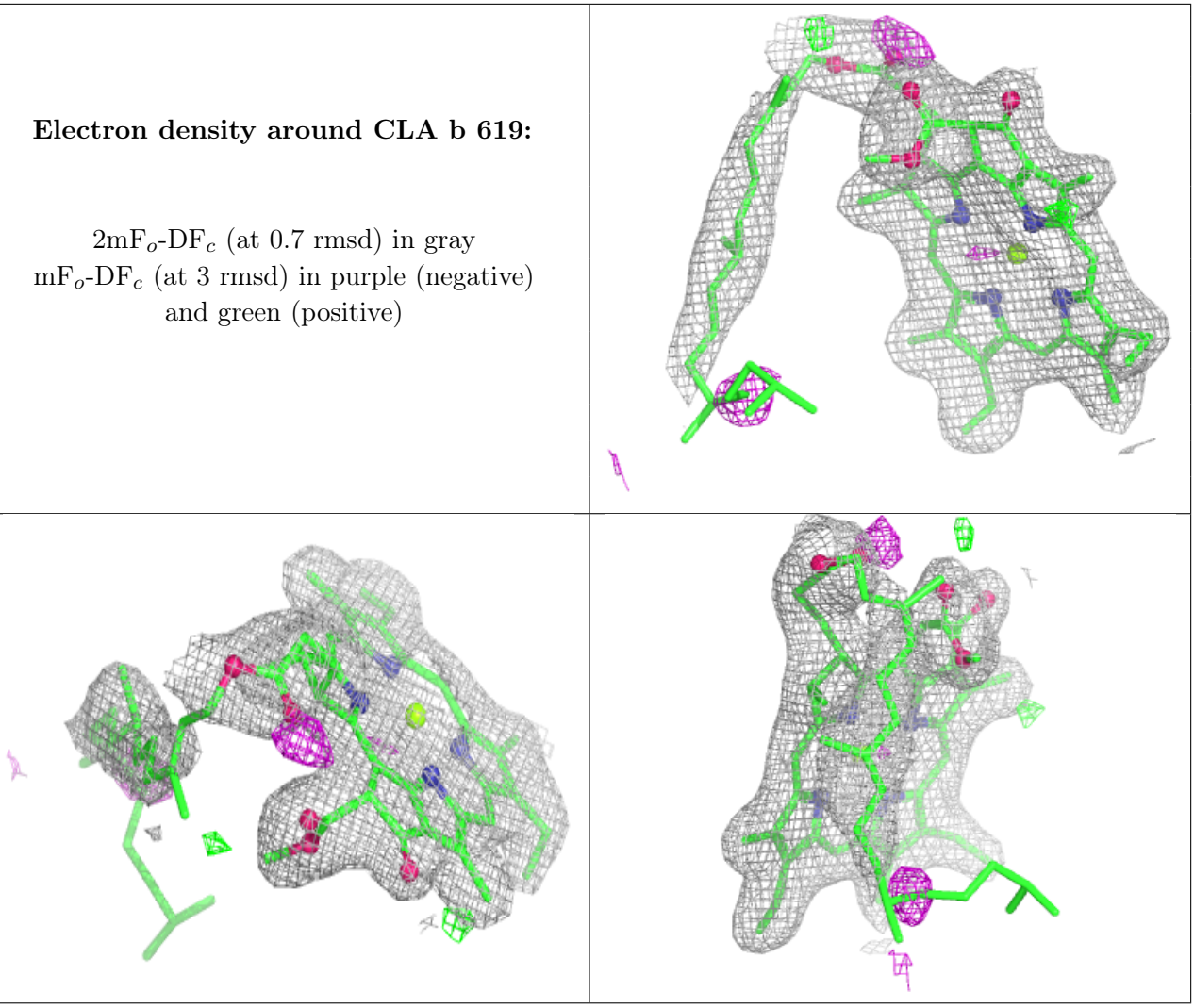






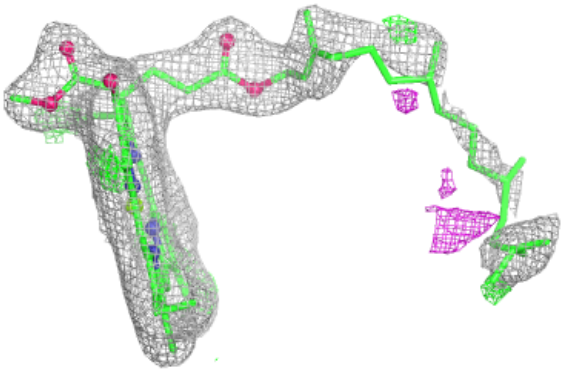
Electron density around CLA b 619:

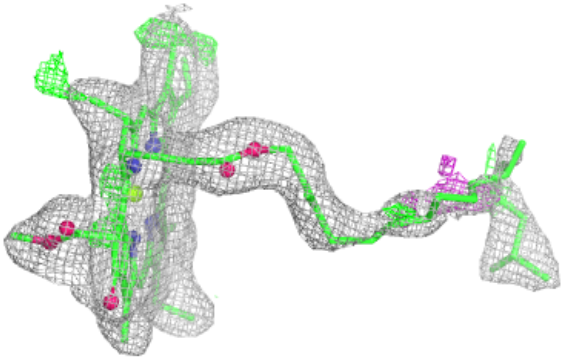
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

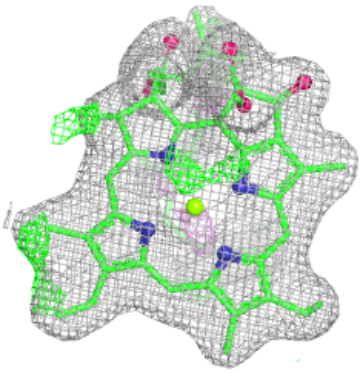


Electron density around CLA c 508:

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

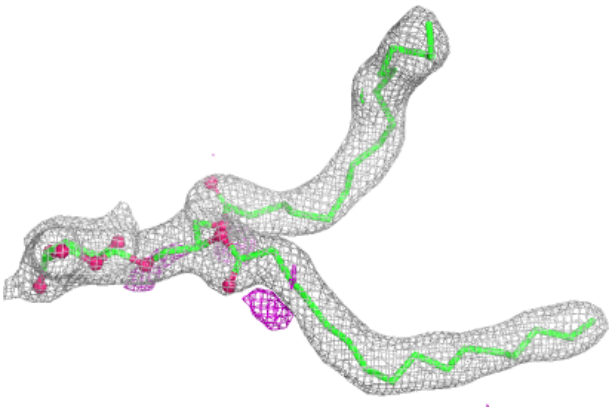


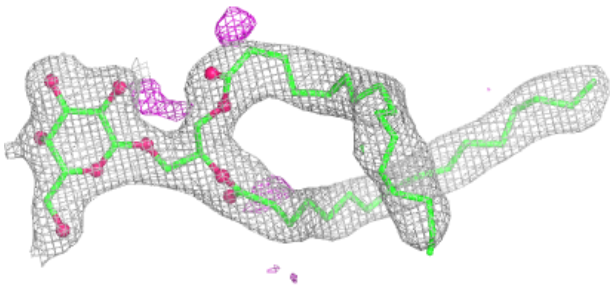


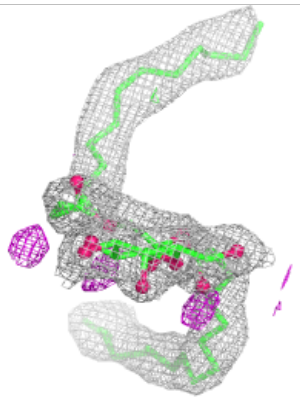


Electron density around LMG b 623:

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

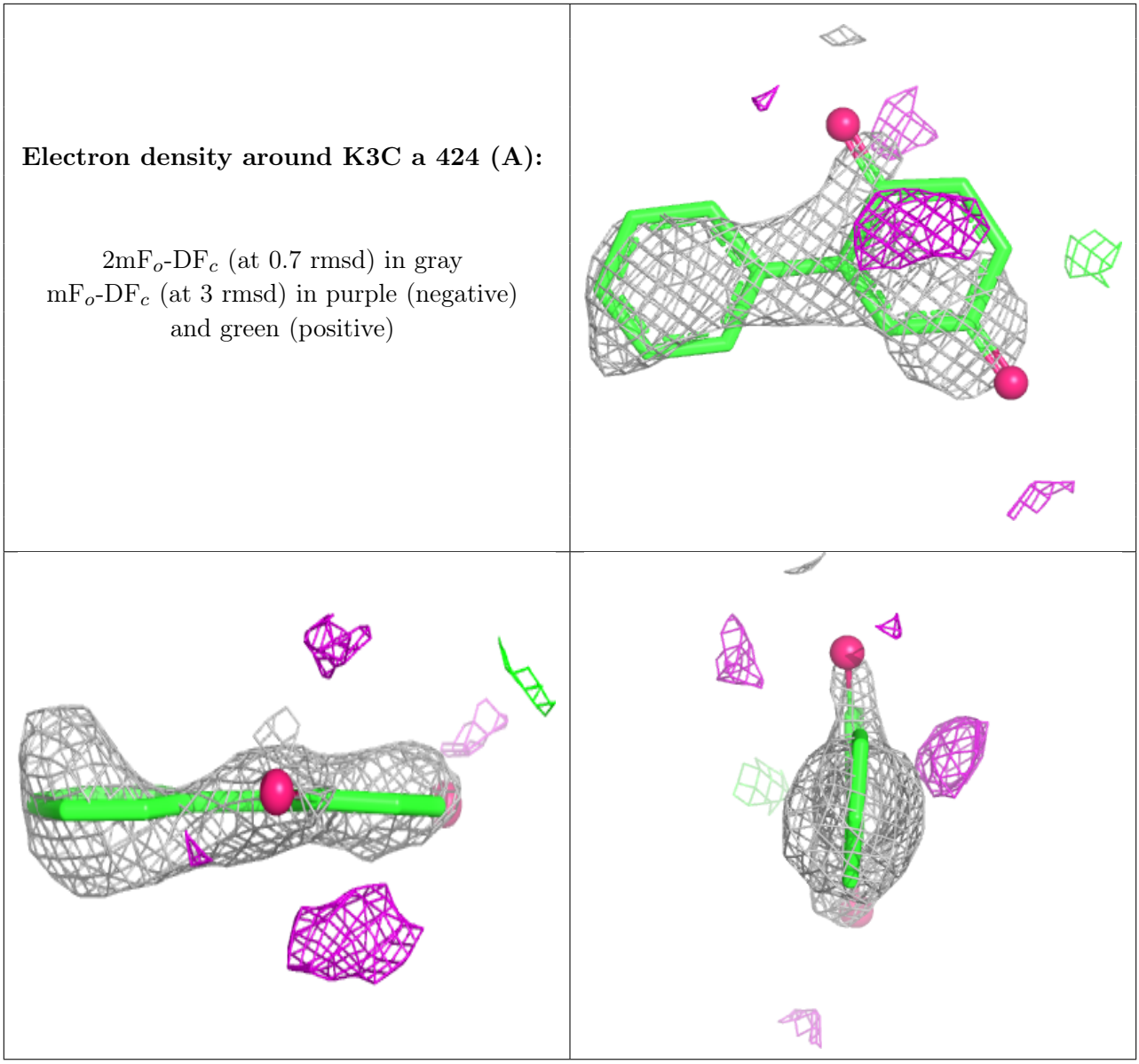






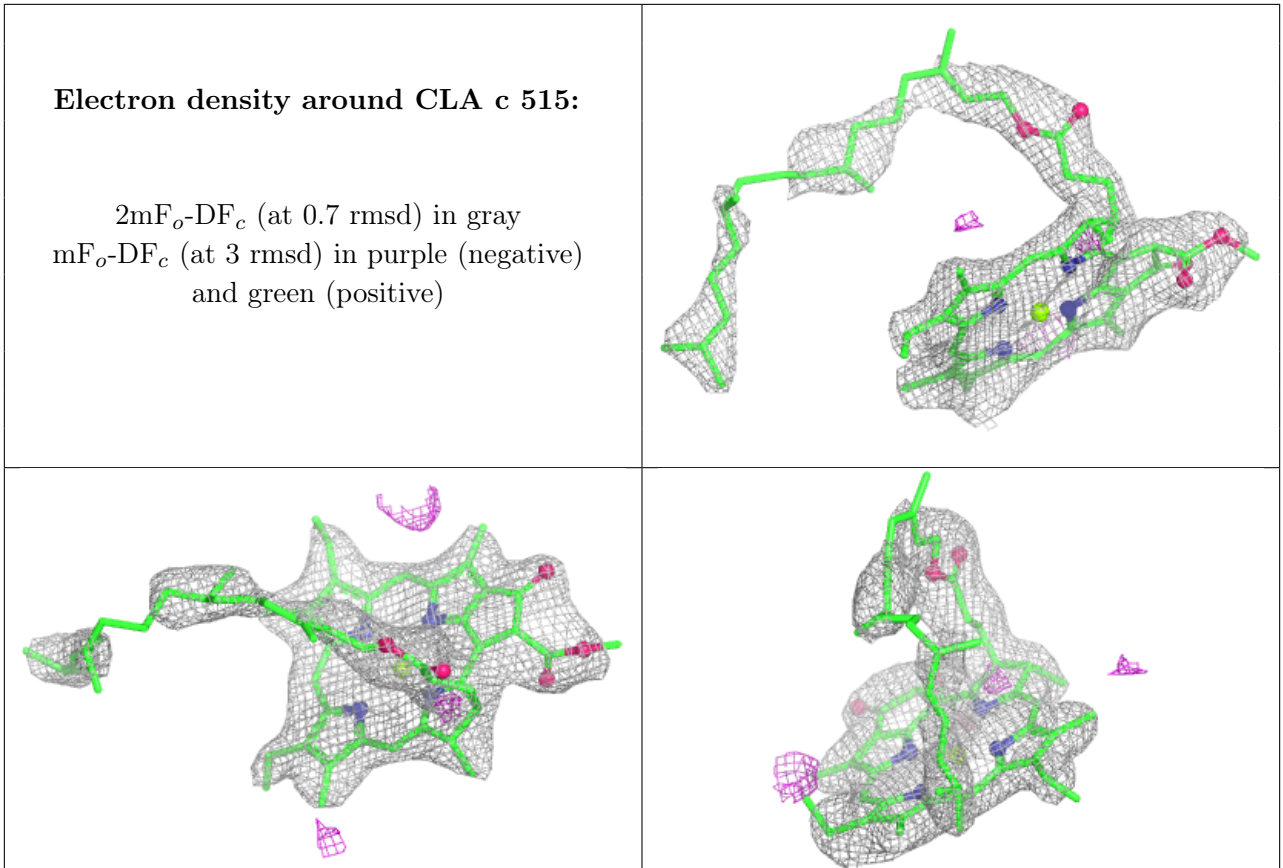
Electron density around K3C a 424 (A):

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



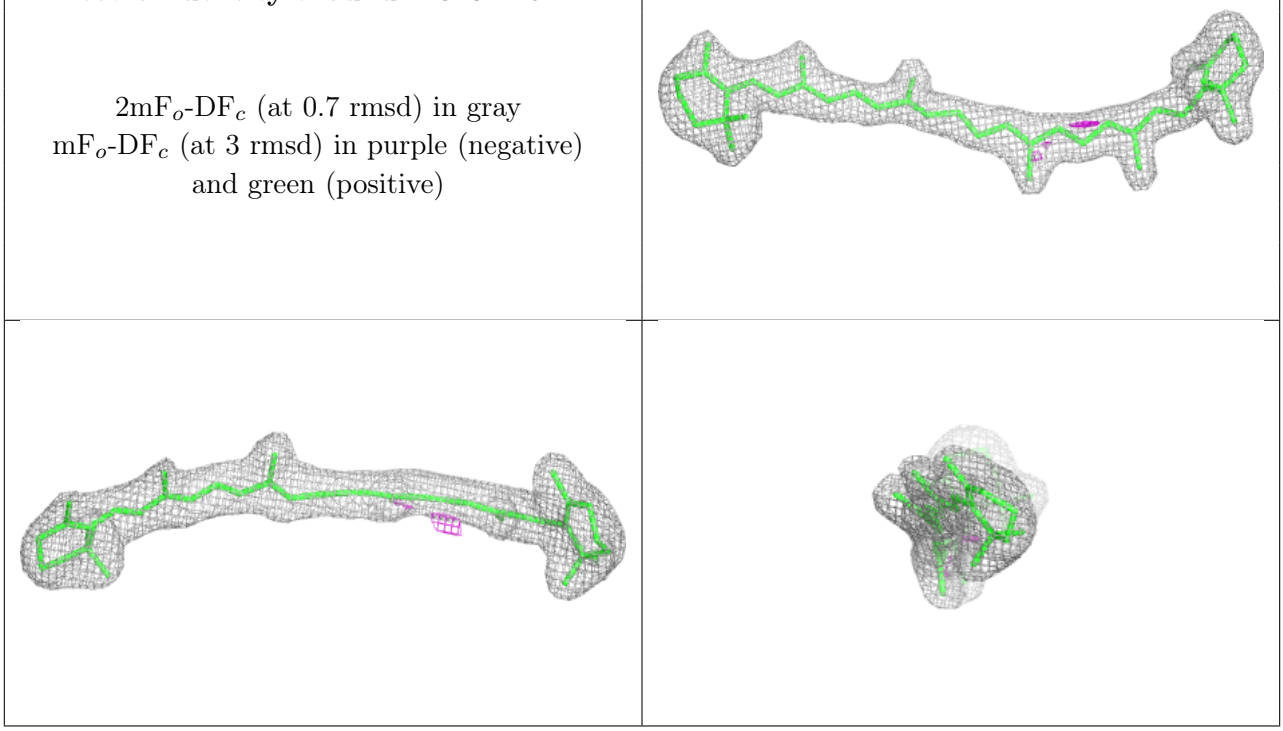
Electron density around CLA c 515:

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



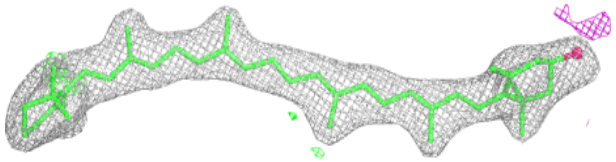
Electron density around BCR B 641:

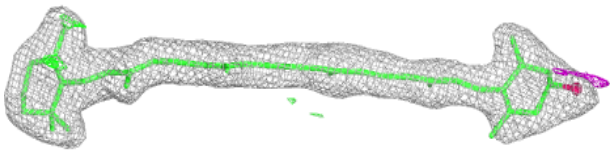
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

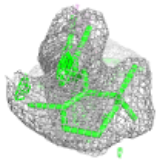


Electron density around RRX h 1204:

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

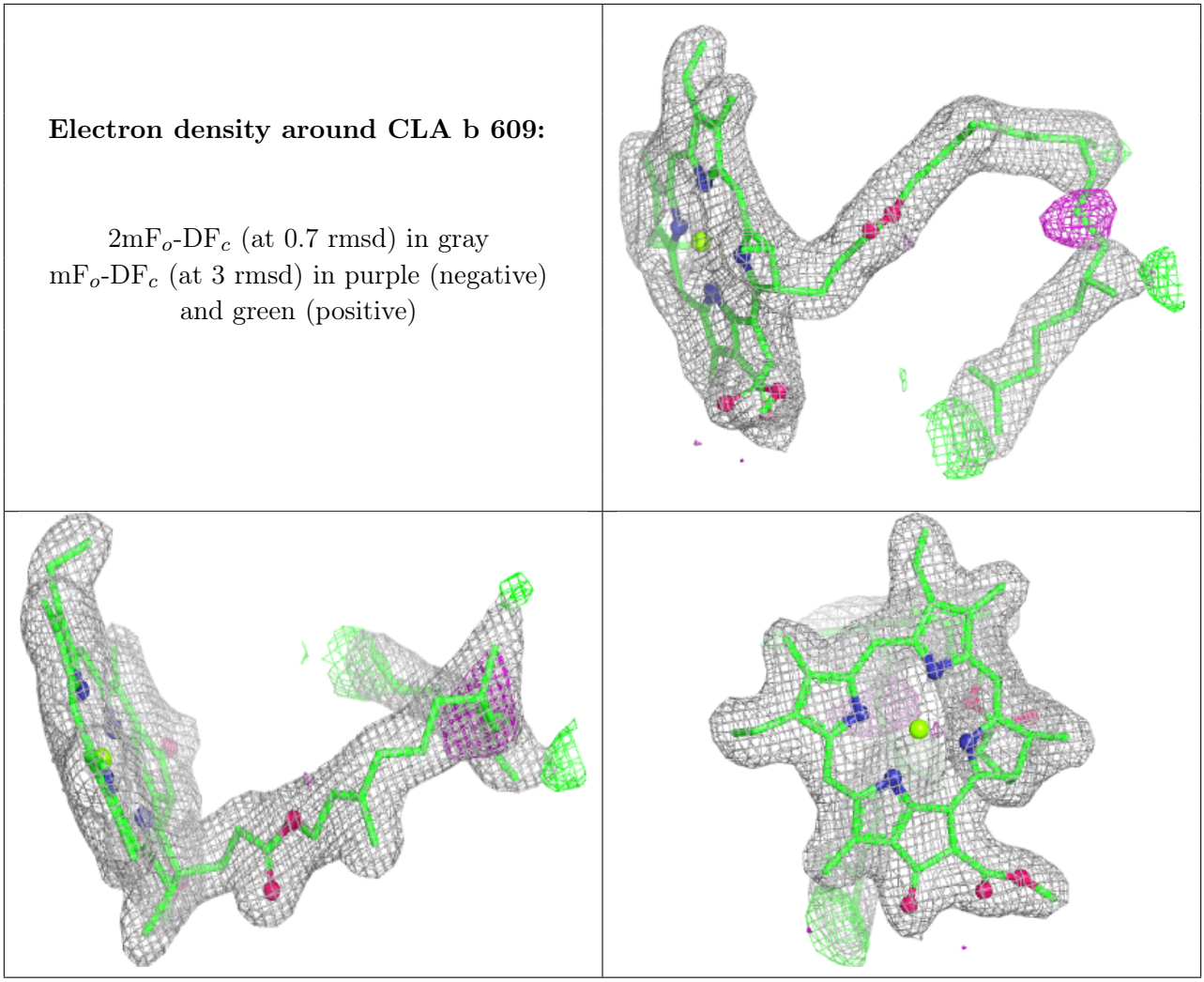






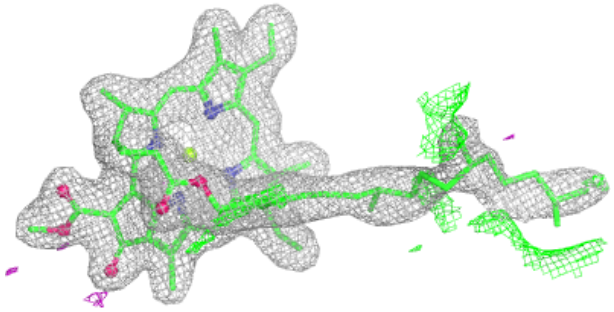
Electron density around CLA b 609:

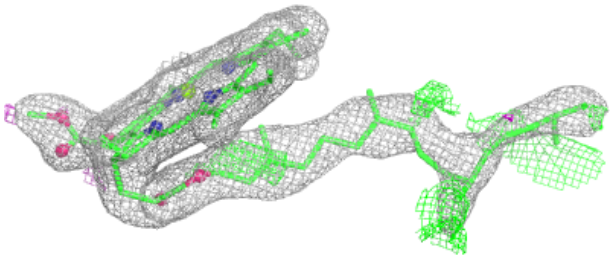
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

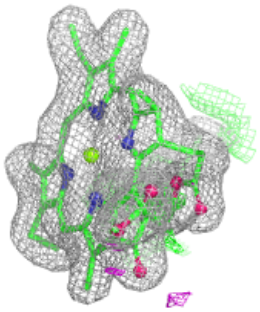


Electron density around CLA b 617:

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

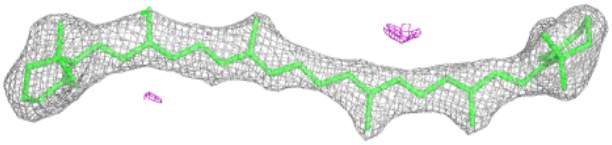


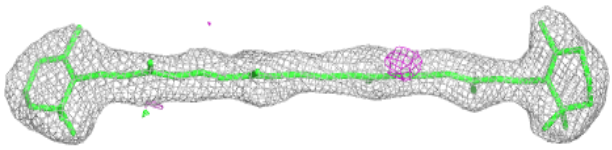


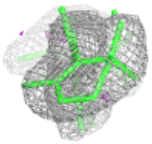


Electron density around BCR c 516:

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

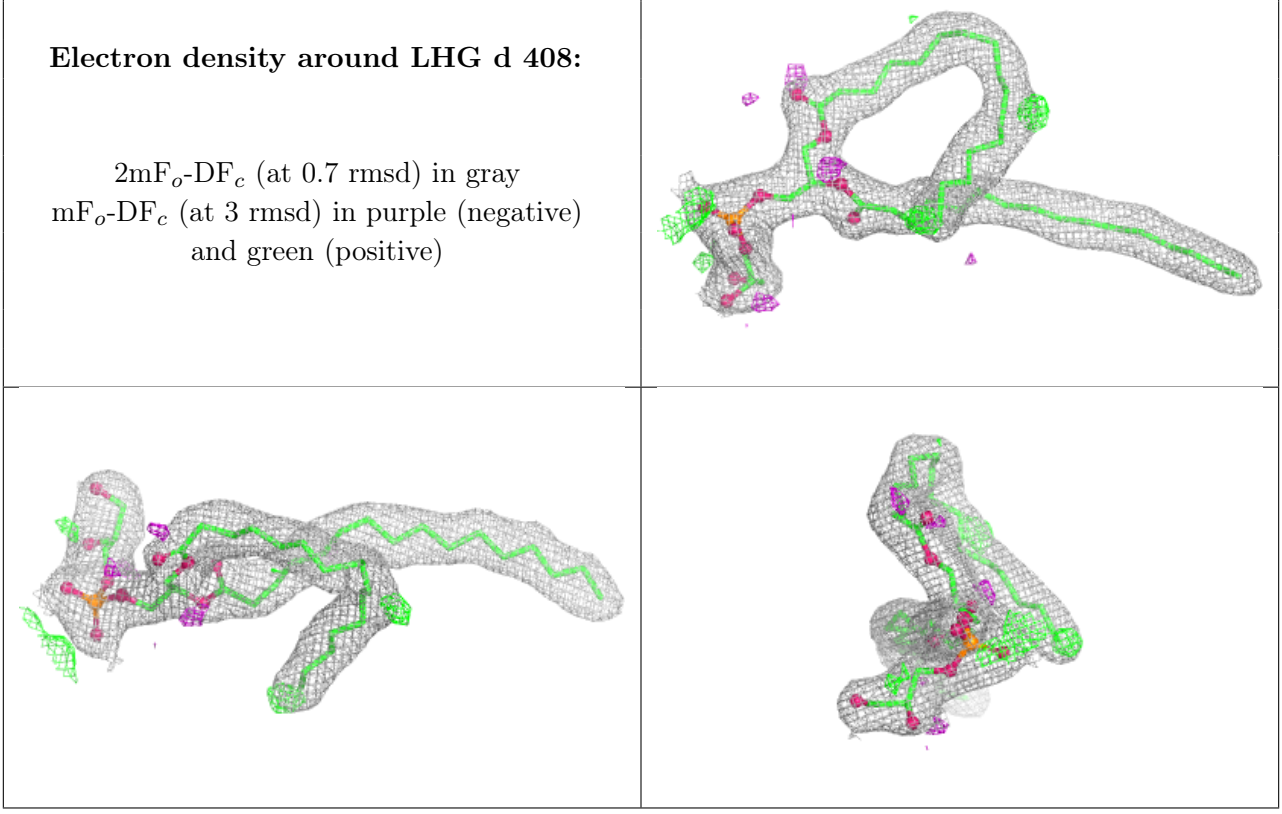






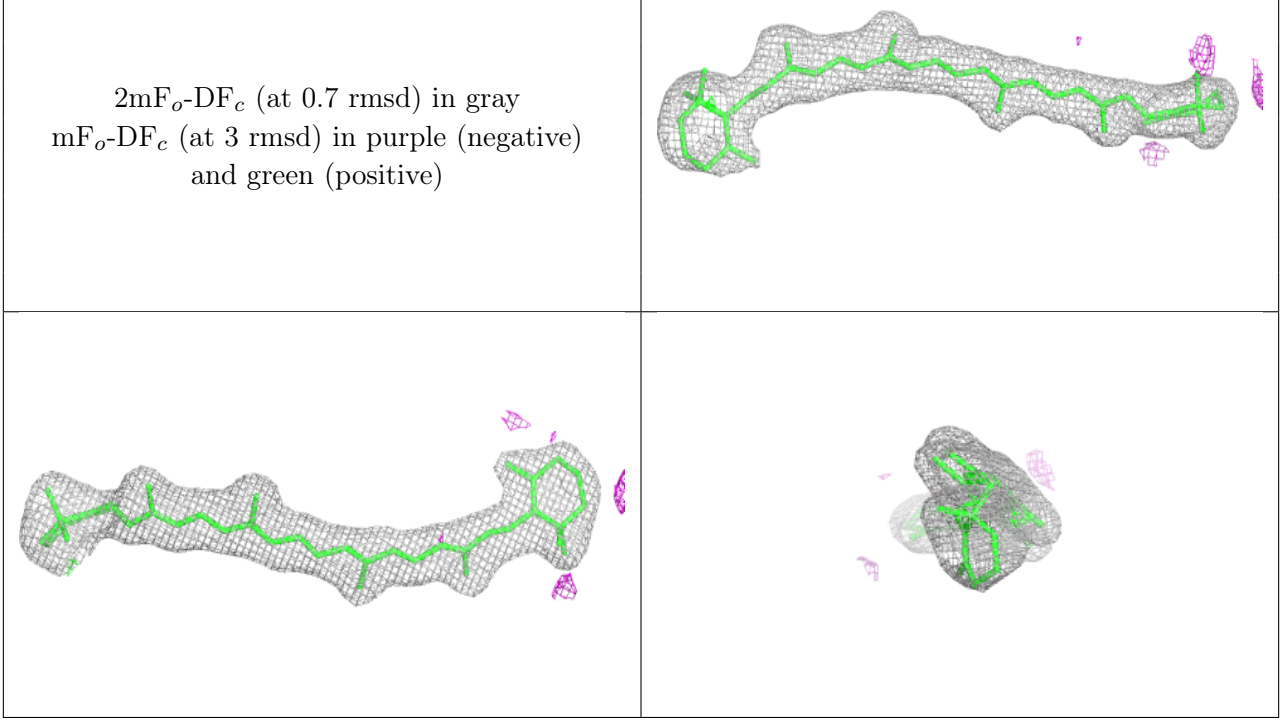
Electron density around LHG d 408:

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



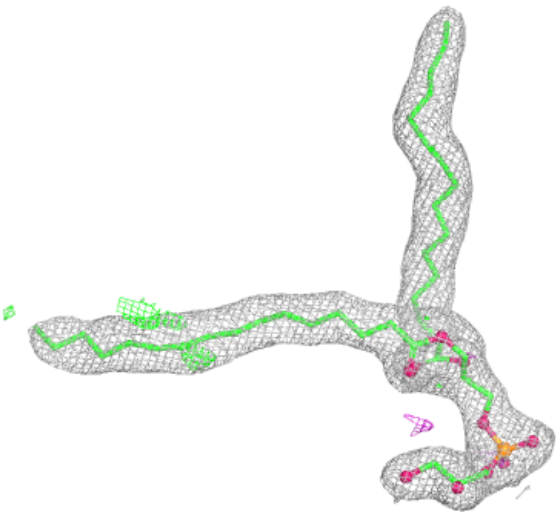
Electron density around BCR d 406:

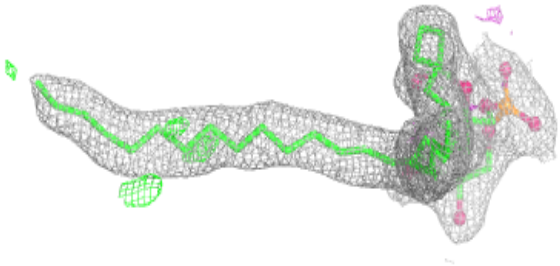
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

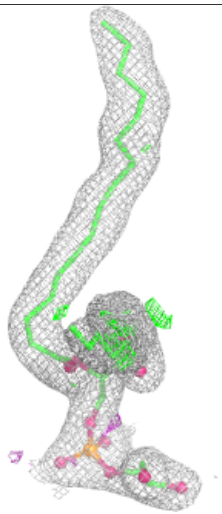


Electron density around LHG l 302:

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

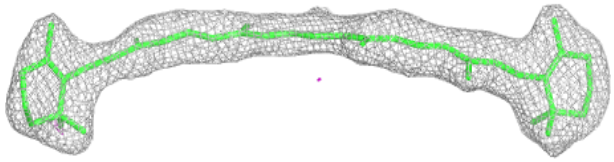


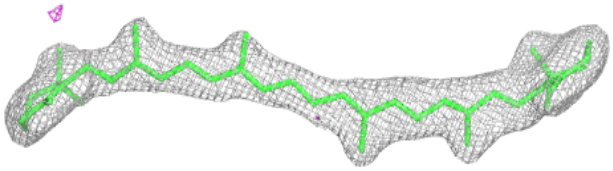


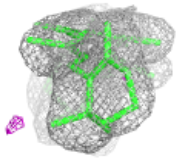


Electron density around BCR k 303:

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

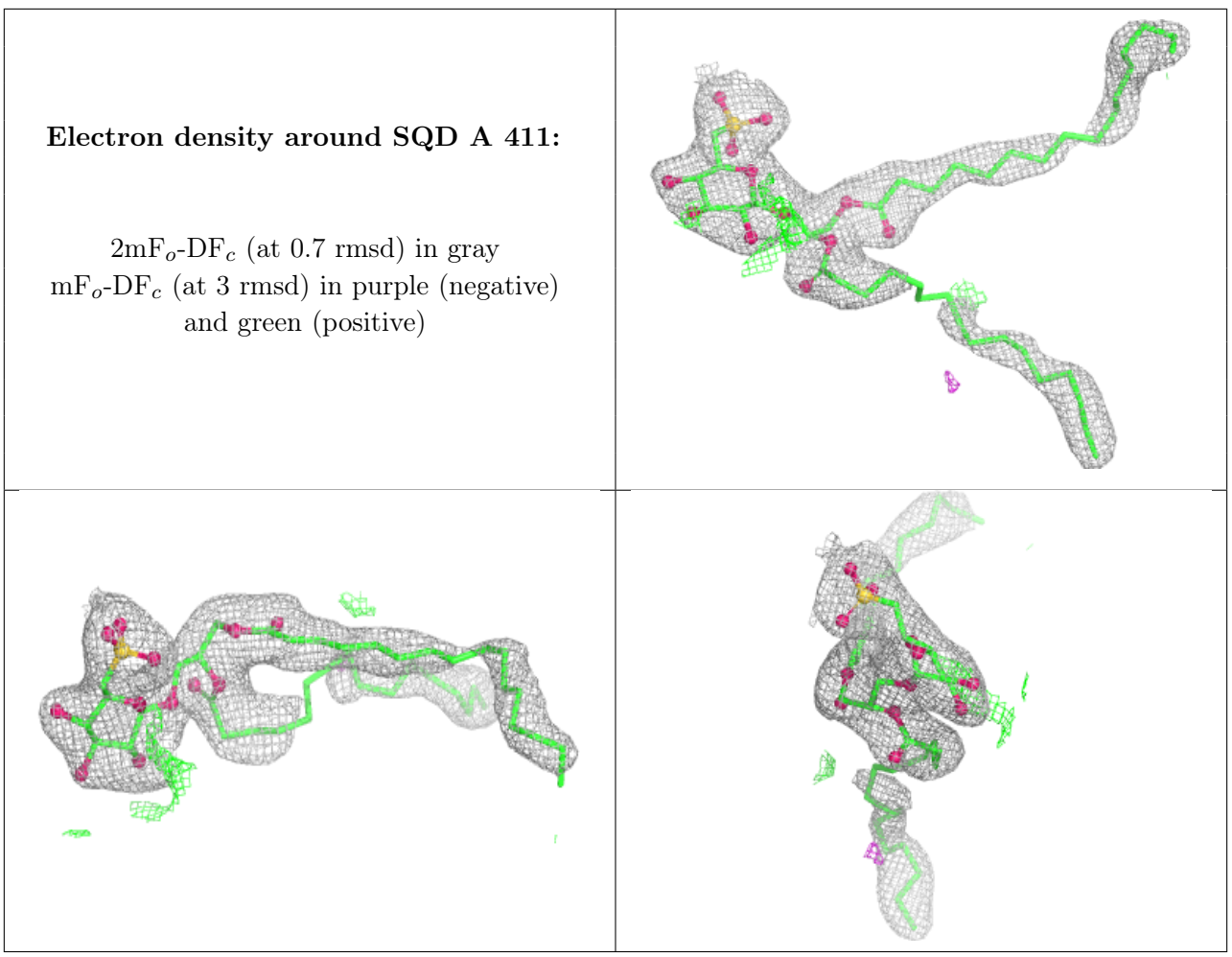






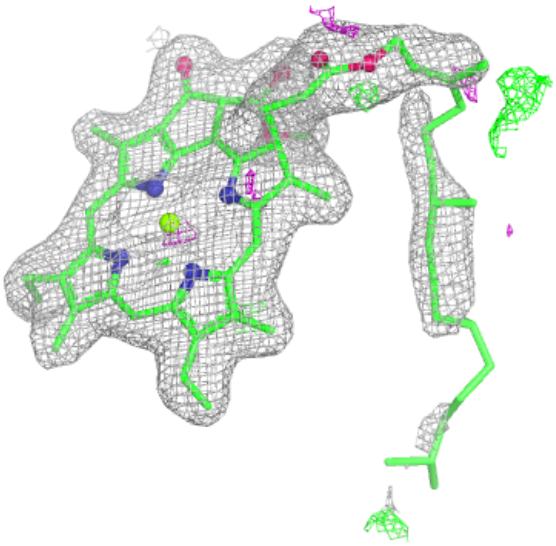
Electron density around SQD A 411:

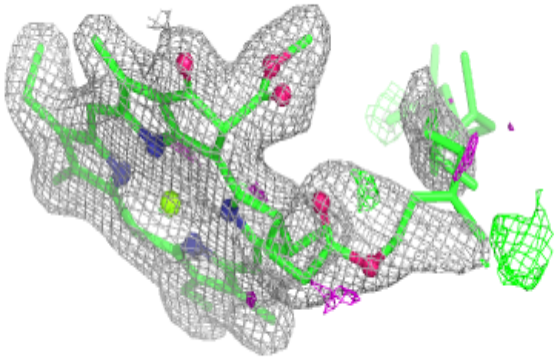
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

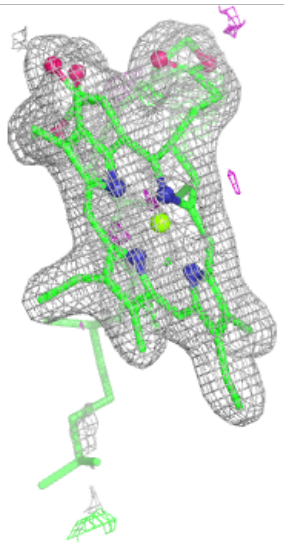


Electron density around CLA B 617:

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

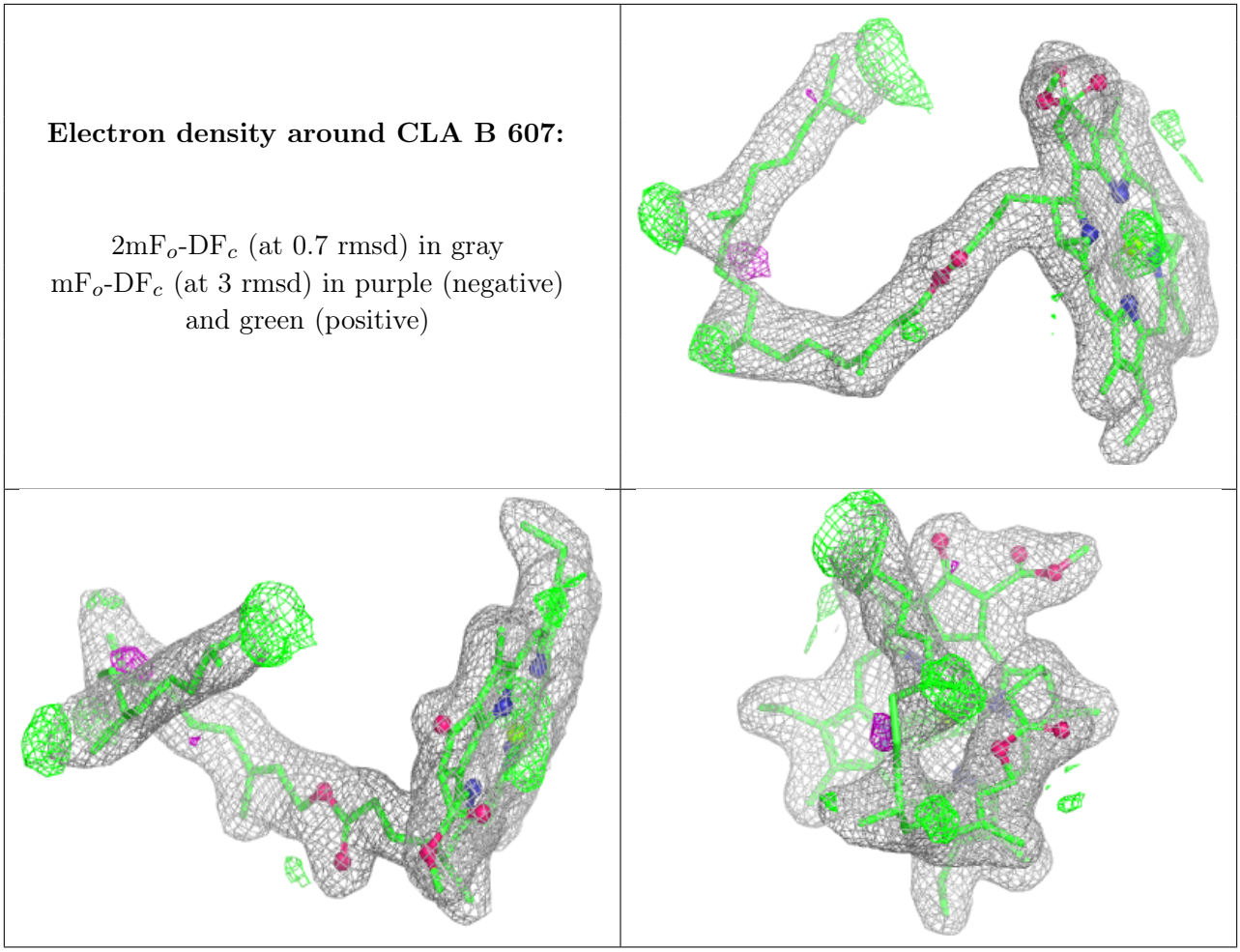






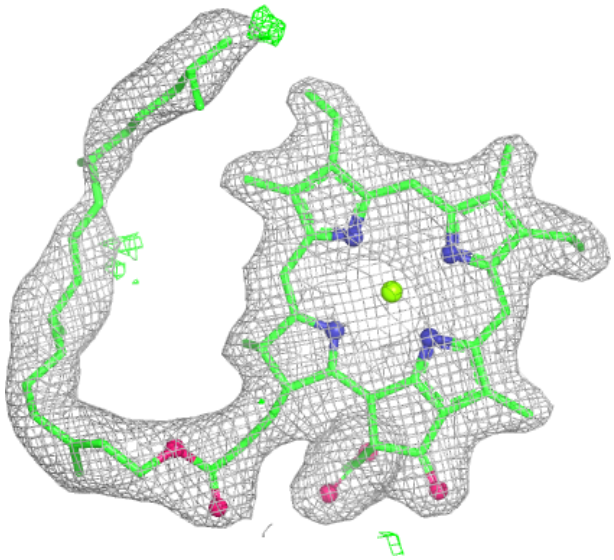
Electron density around CLA B 607:

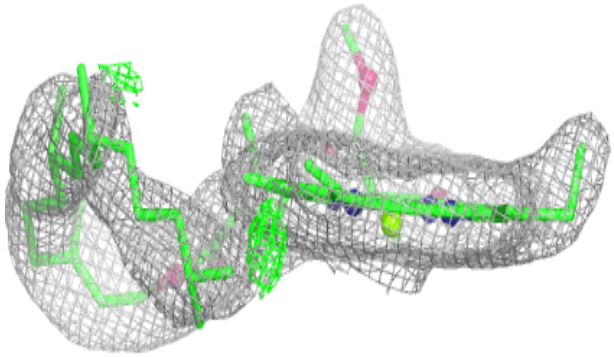
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

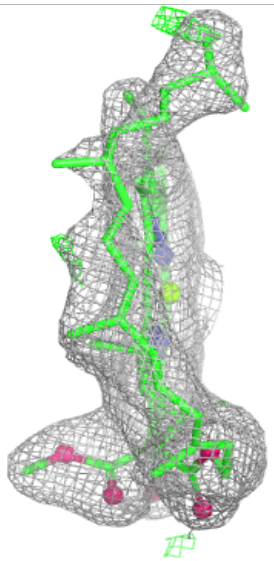


Electron density around CLA C 513:

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

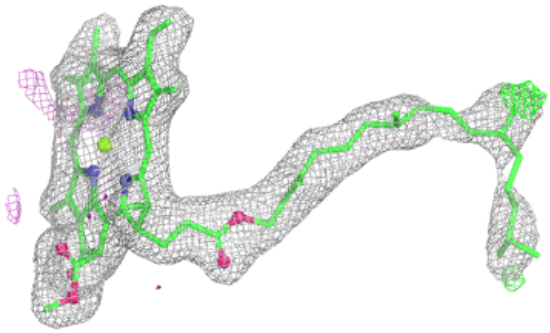


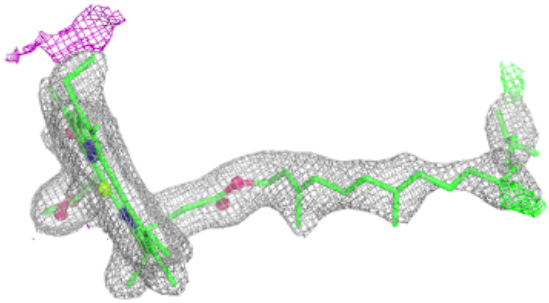


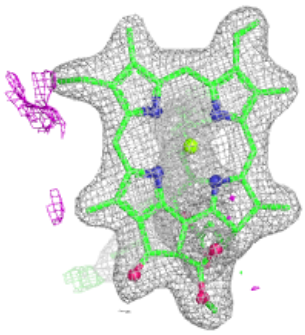


Electron density around CLA d 405:

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

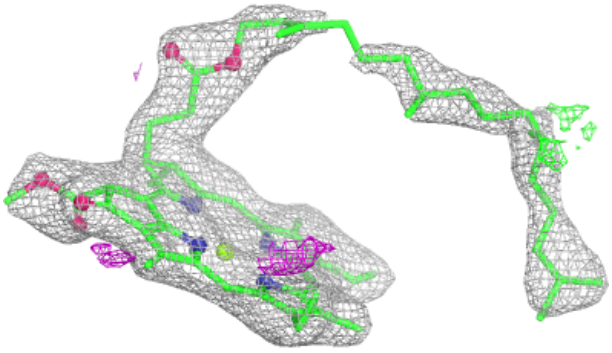


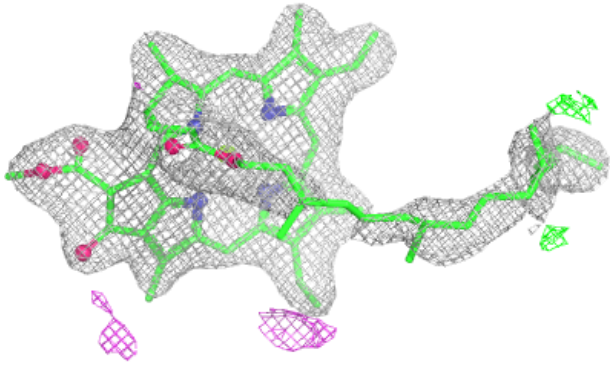


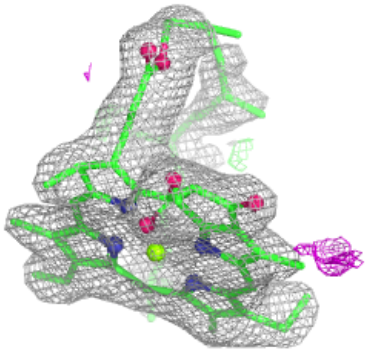


Electron density around CLA C 514:

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

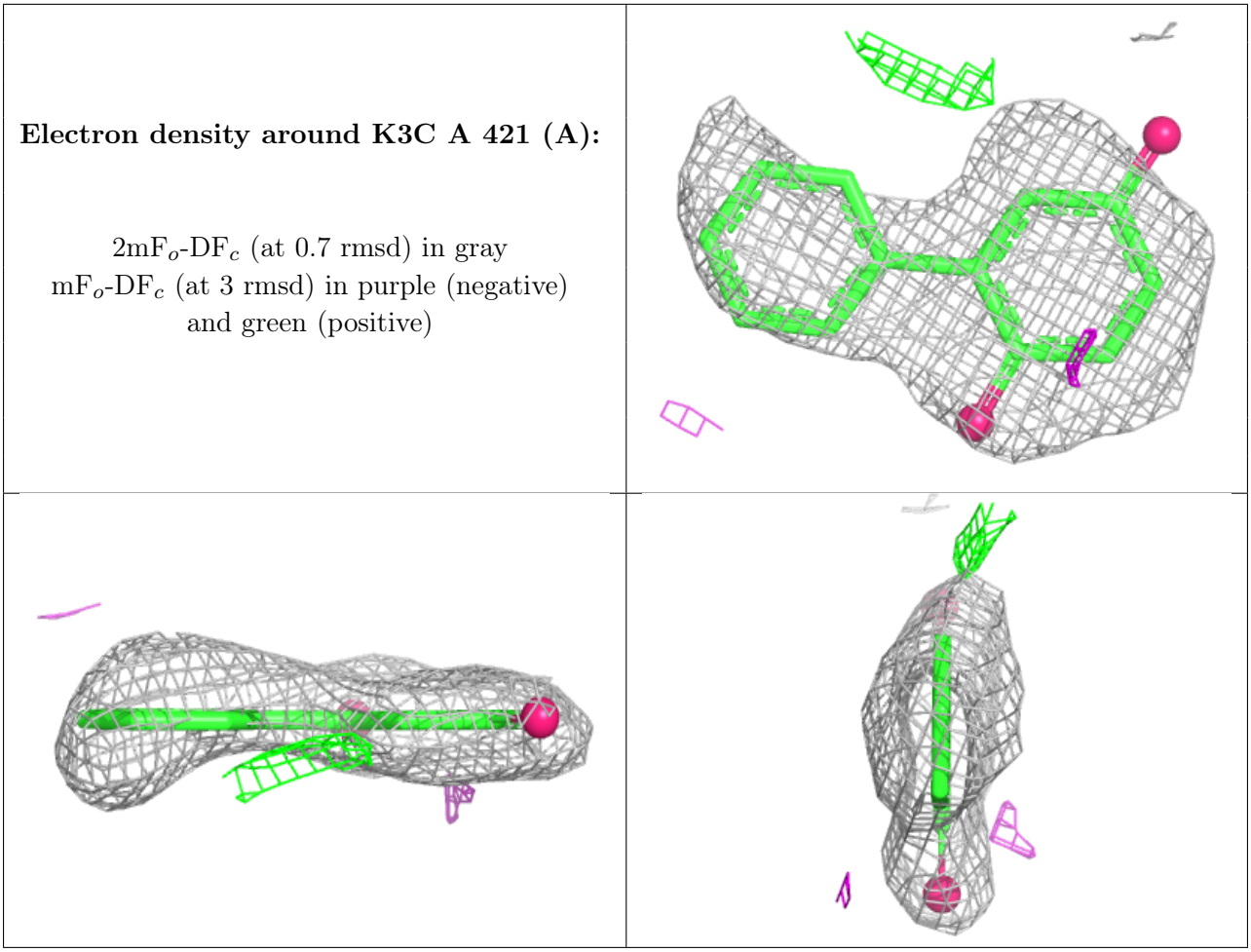






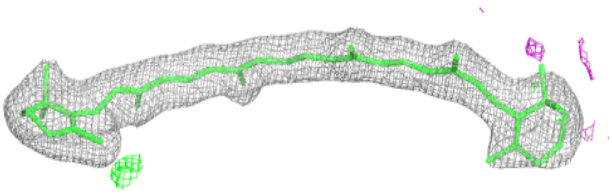
Electron density around K3C A 421 (A):

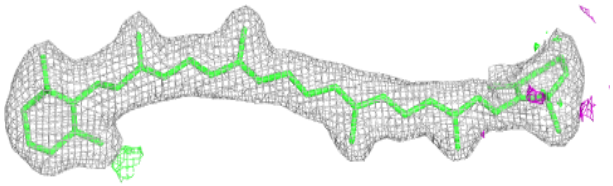
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

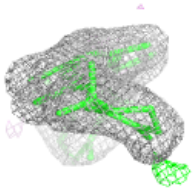


Electron density around BCR D 405:

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

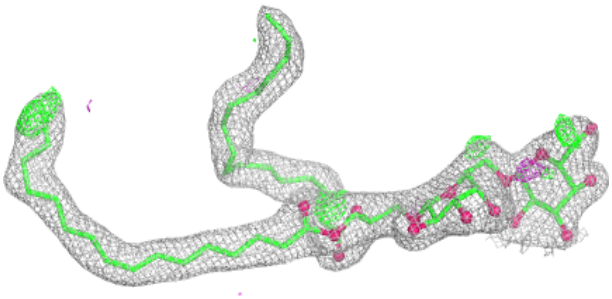


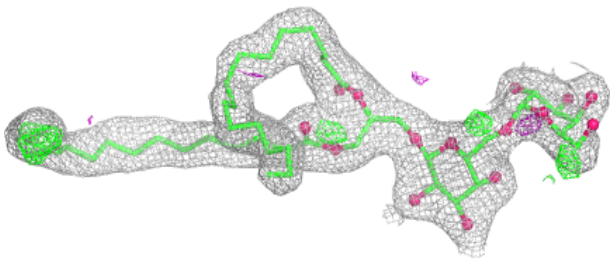


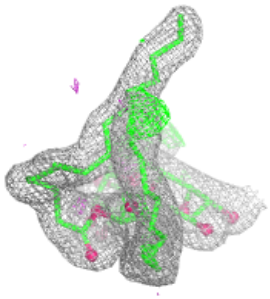


Electron density around DGD h 1205:

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

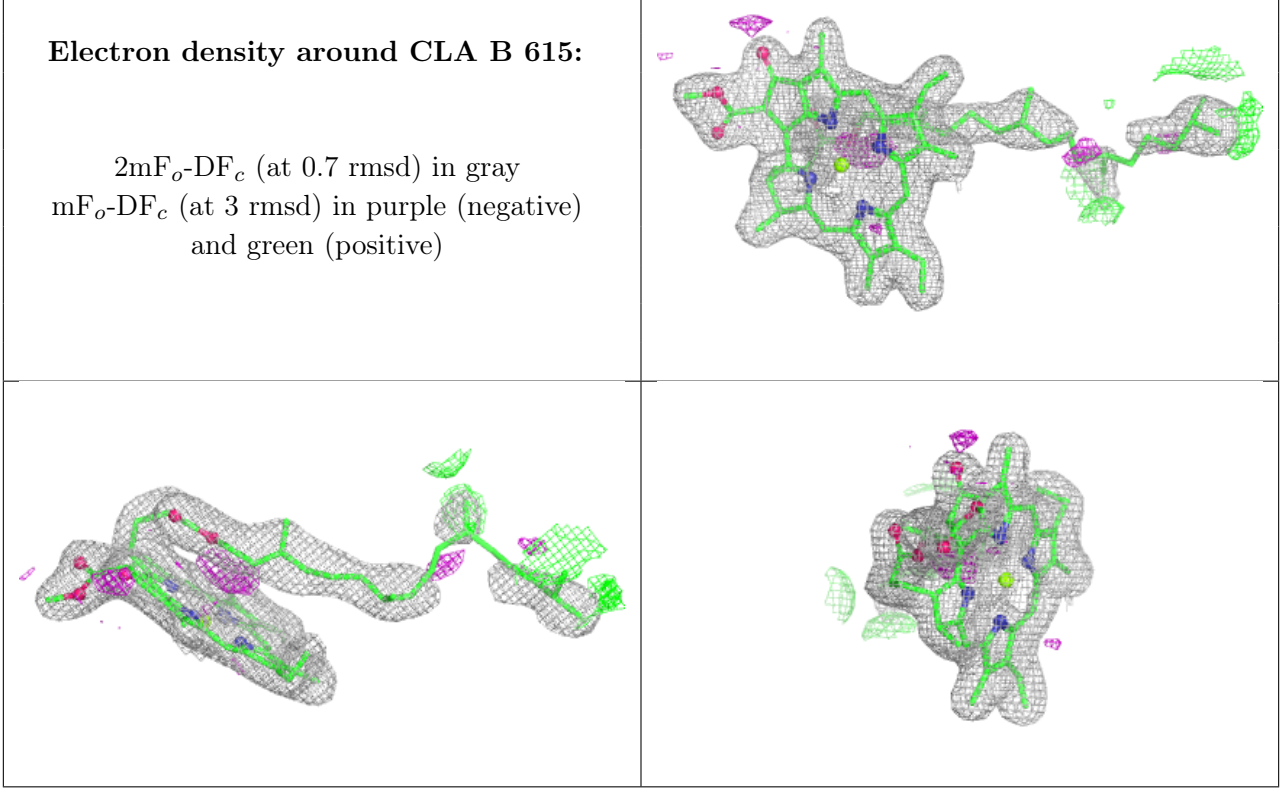






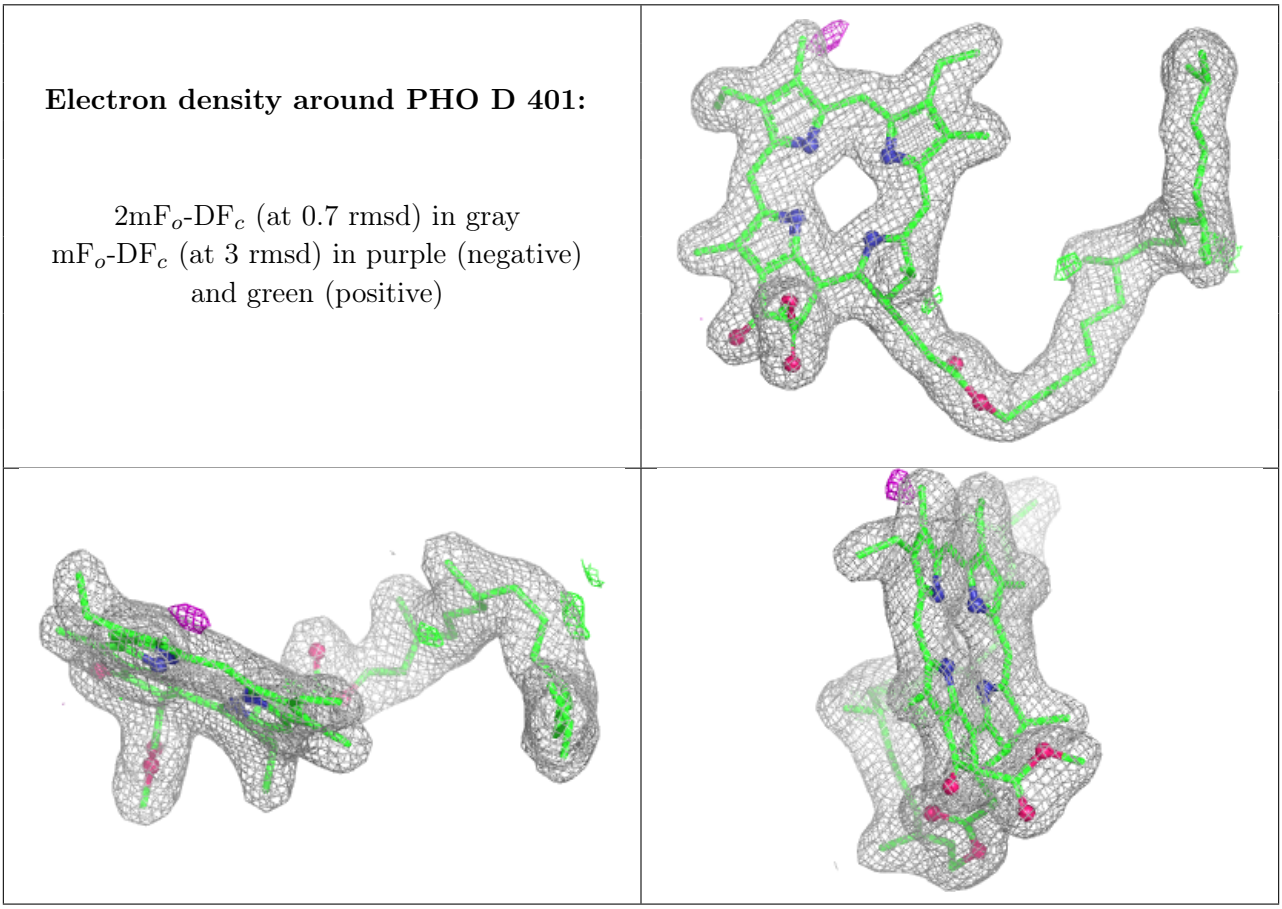
Electron density around CLA B 615:

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



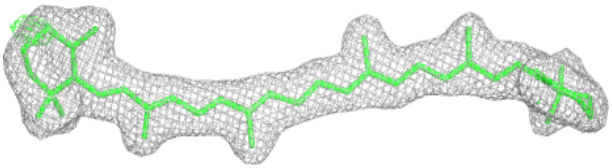
Electron density around PHO D 401:

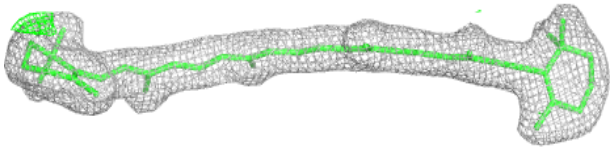
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

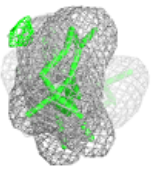


Electron density around BCR B 618:

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

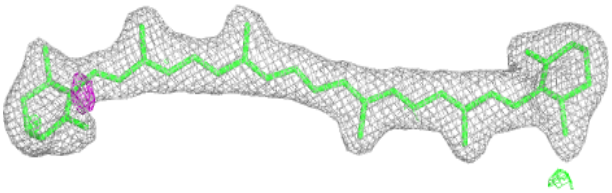


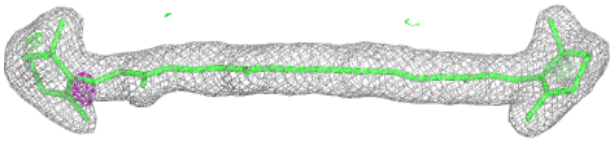


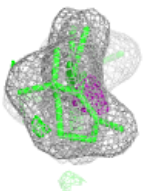


Electron density around BCR B 619:

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

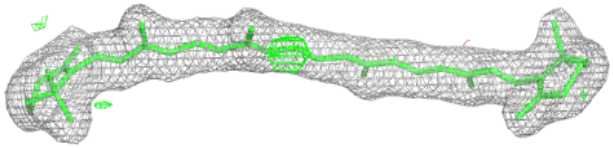


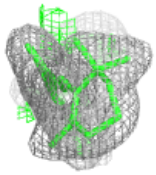




Electron density around BCR B 620:

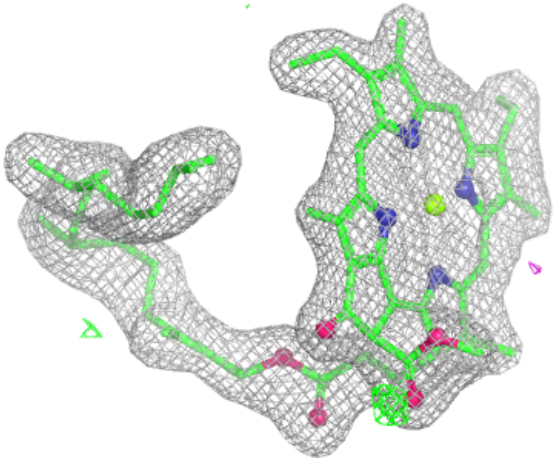
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

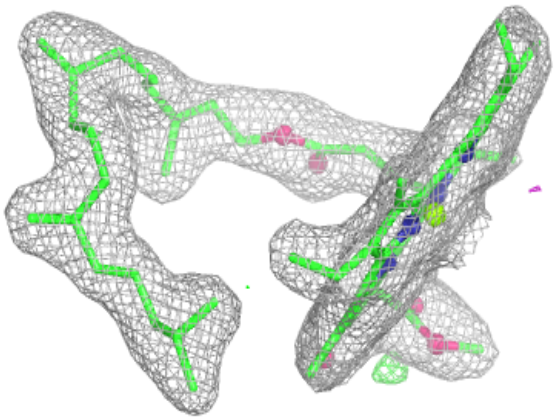


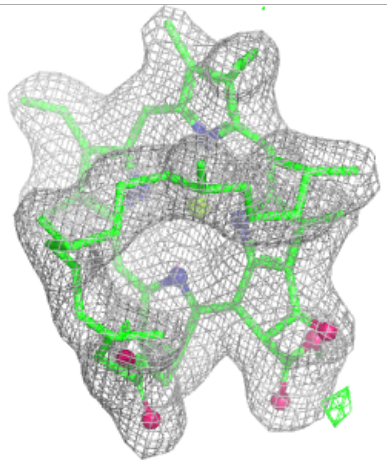


Electron density around CLA C 504:

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

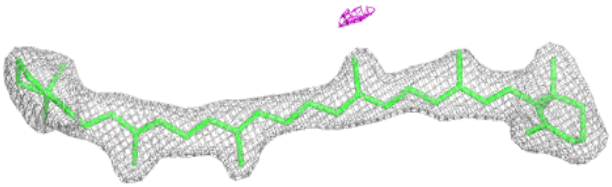


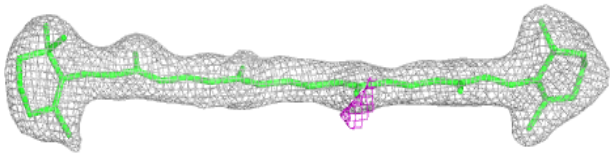


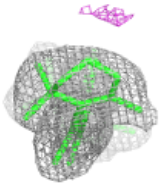


Electron density around BCR C 515:

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

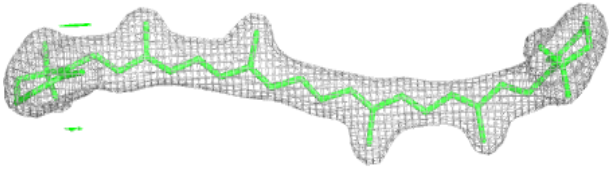


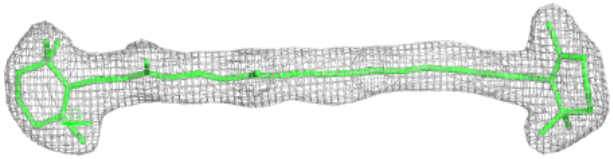


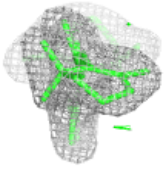


Electron density around BCR C 516:

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

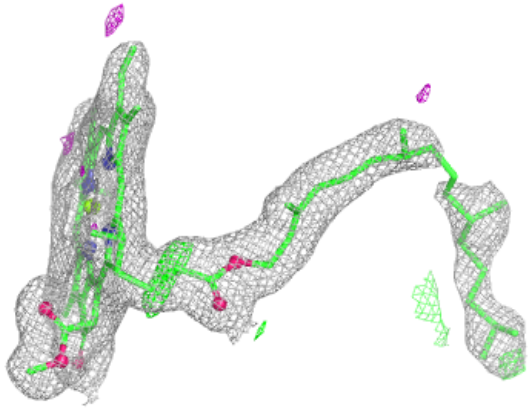


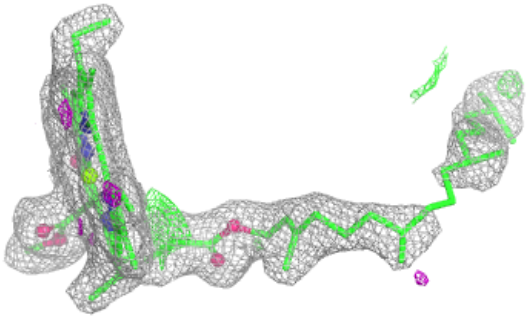


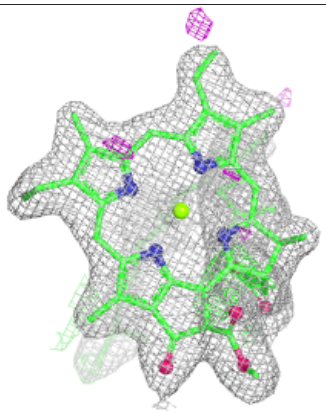


Electron density around CLA D 404:

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

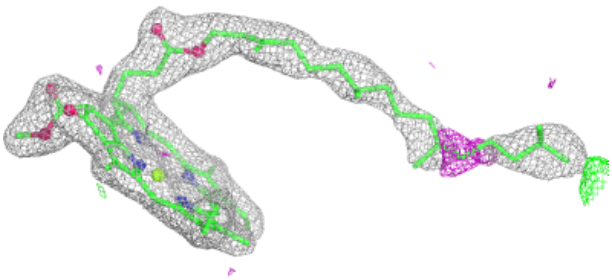


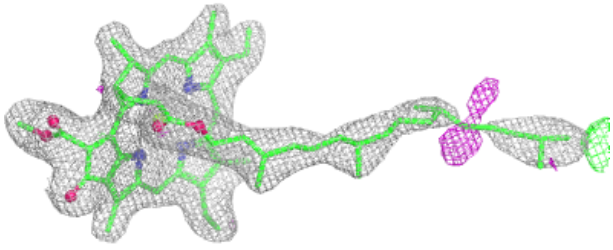


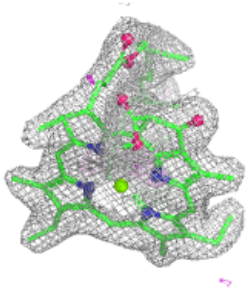


Electron density around CLA c 506:

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

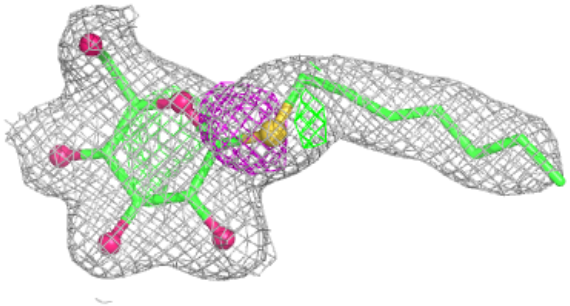


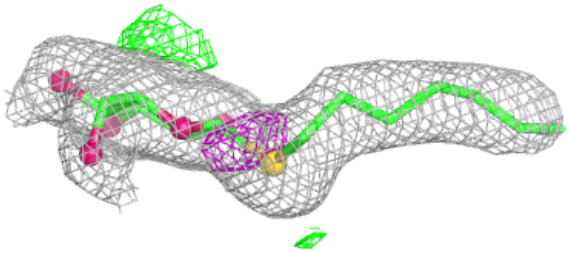


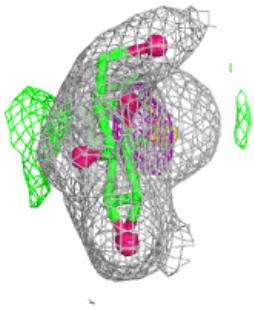


Electron density around HTG O 302:

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

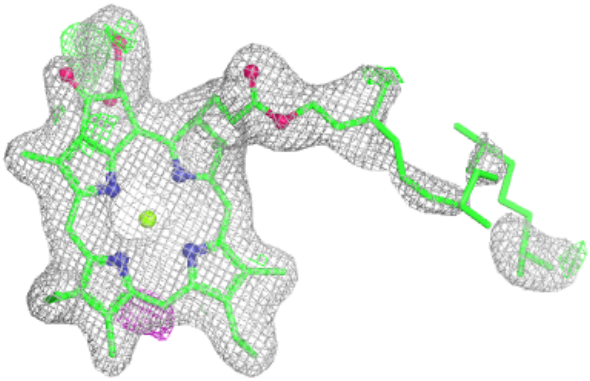


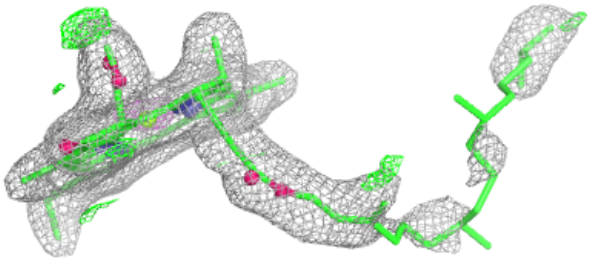


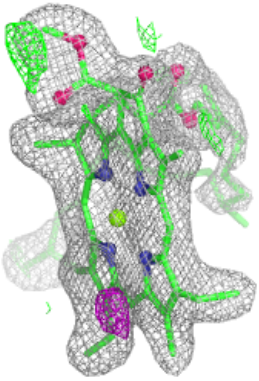


Electron density around CLA a 412:

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

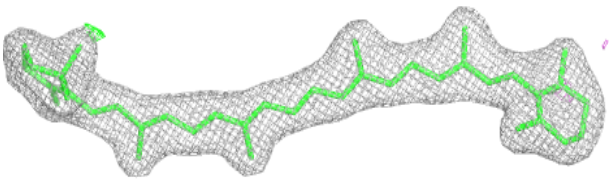


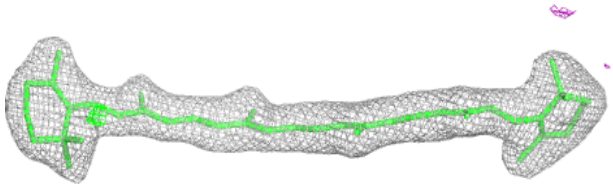


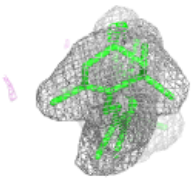


Electron density around BCR Y 302:

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

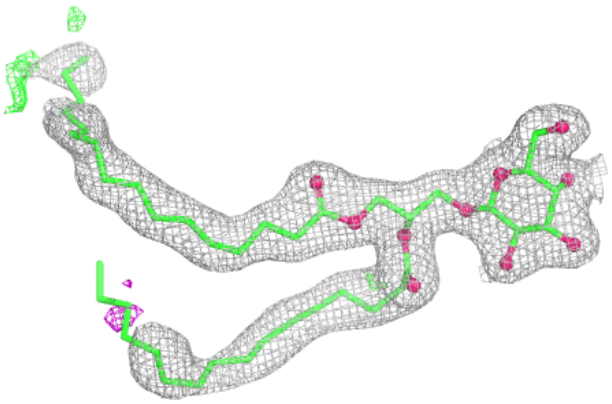


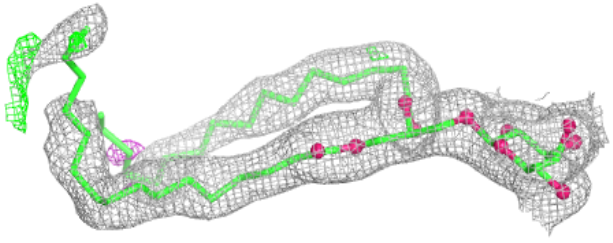


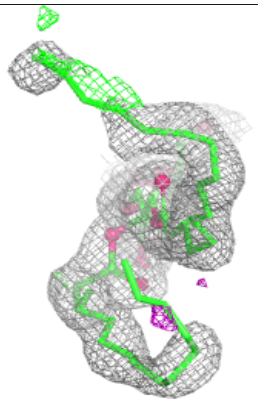


Electron density around LMG D 412:

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

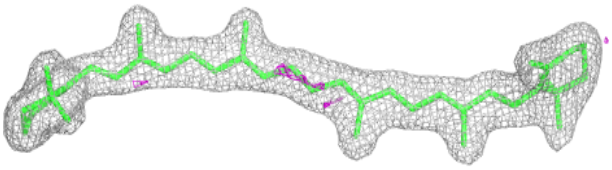


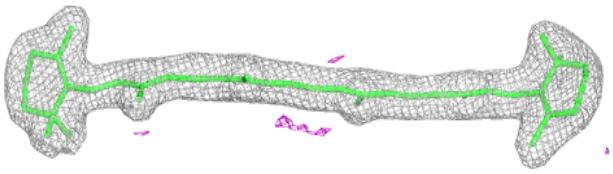


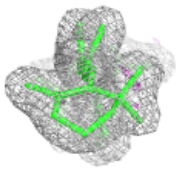


Electron density around BCR a 413:

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

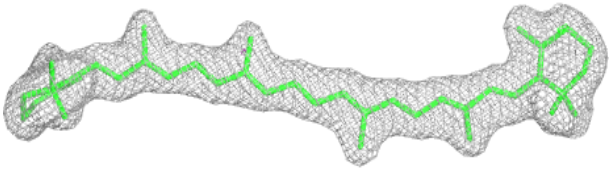


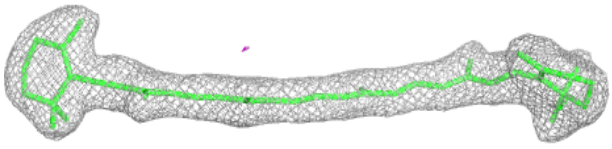


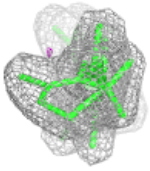


Electron density around BCR b 620:

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

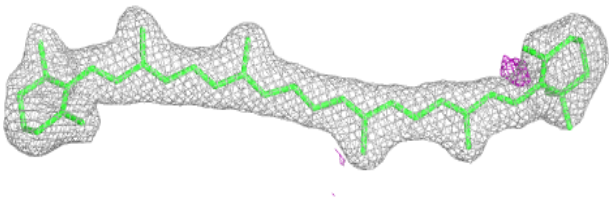


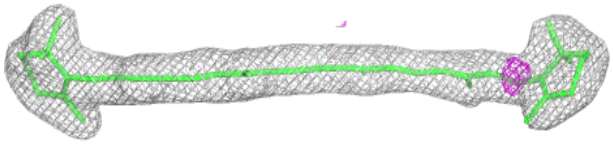


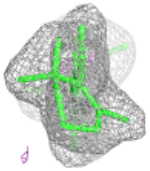


Electron density around BCR b 621:

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

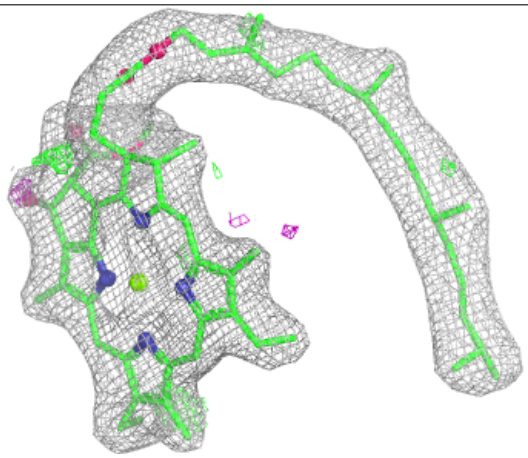


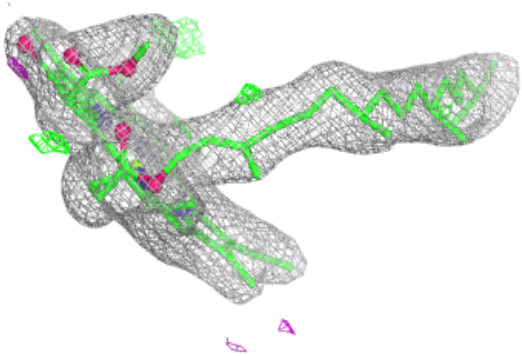


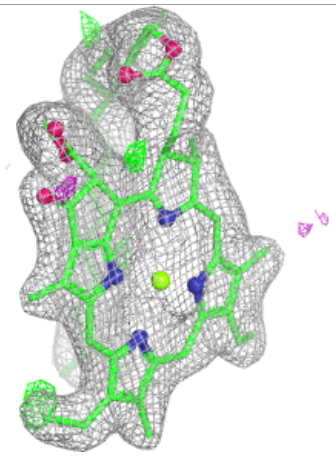


Electron density around CLA c 509:

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

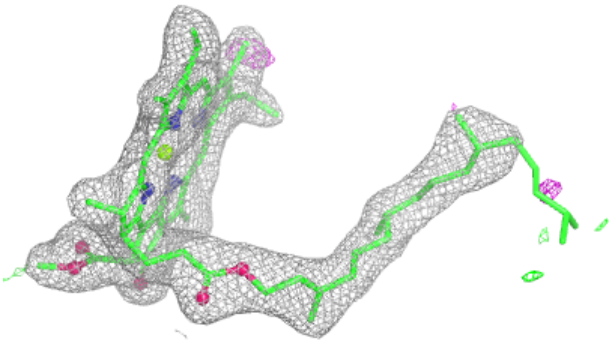


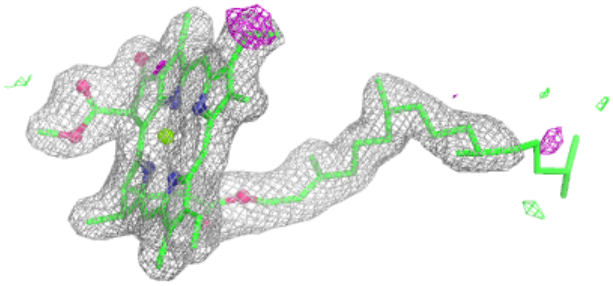


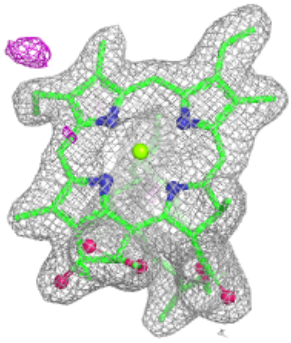


Electron density around CLA c 510:

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

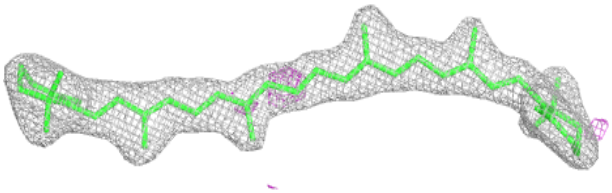


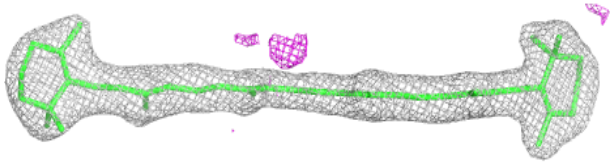


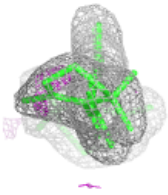


Electron density around BCR c 517:

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

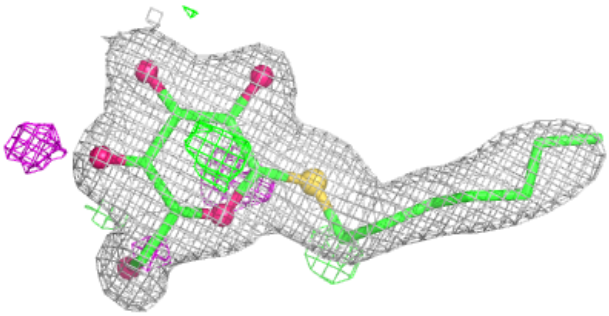


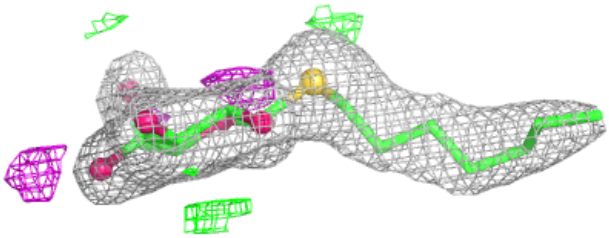


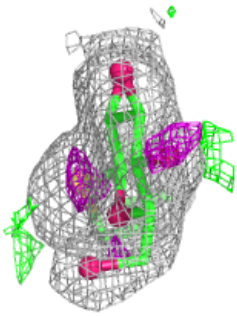


Electron density around HTG o 301:

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

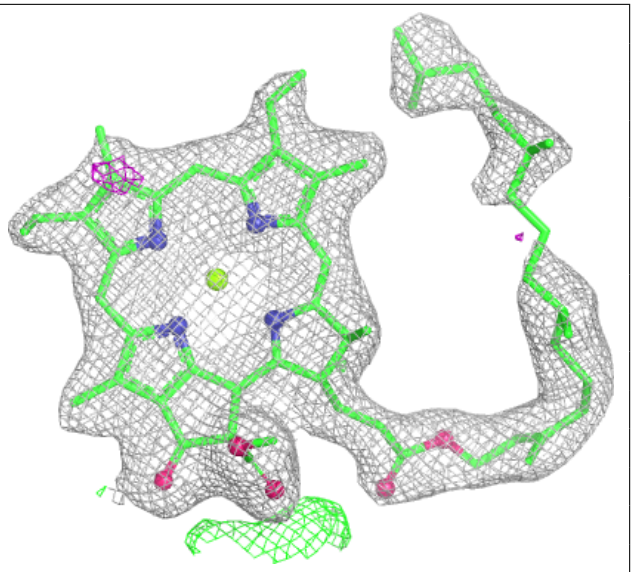


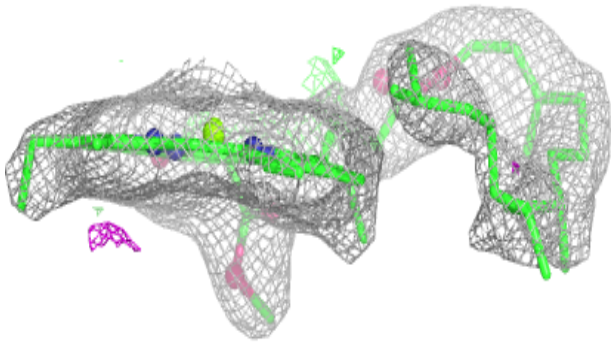


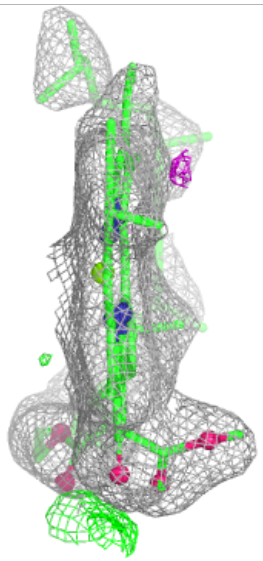


Electron density around CLA c 514:

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

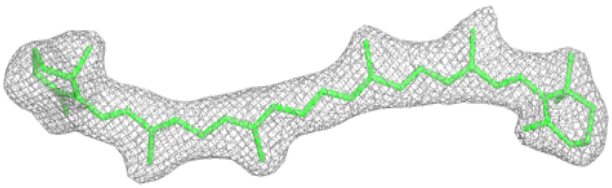


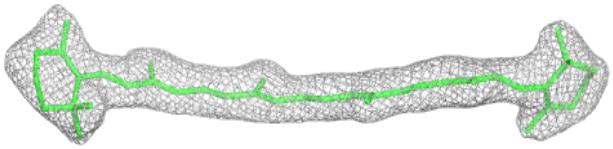


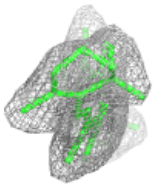


Electron density around BCR k 302:

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

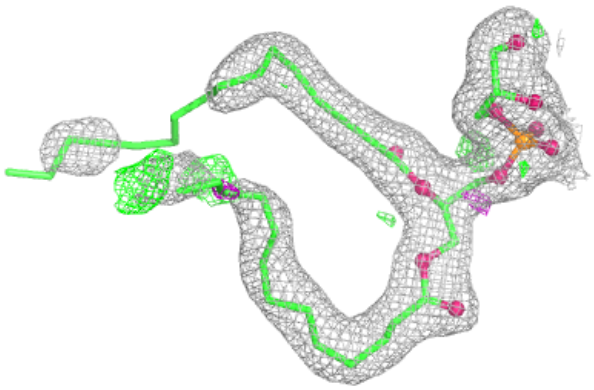


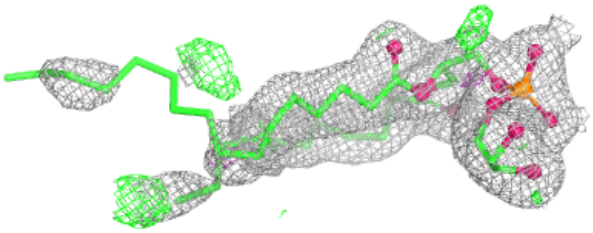


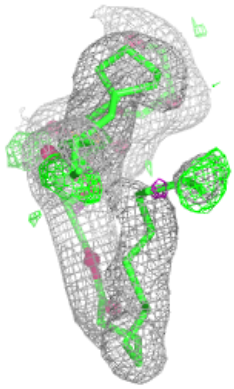


Electron density around LHG D 411:

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

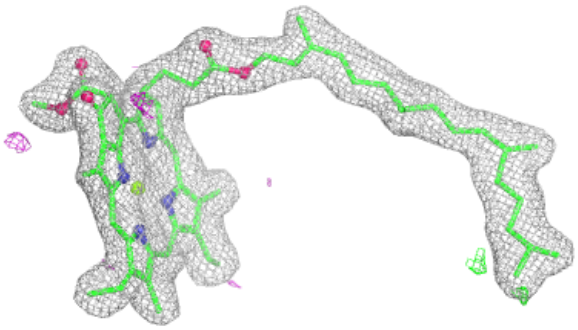


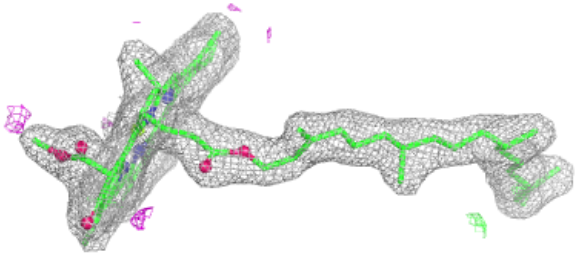


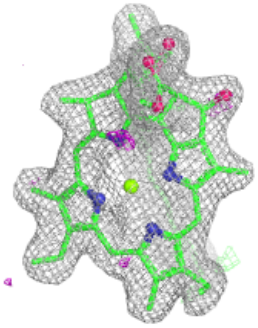


Electron density around CLA B 610:

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

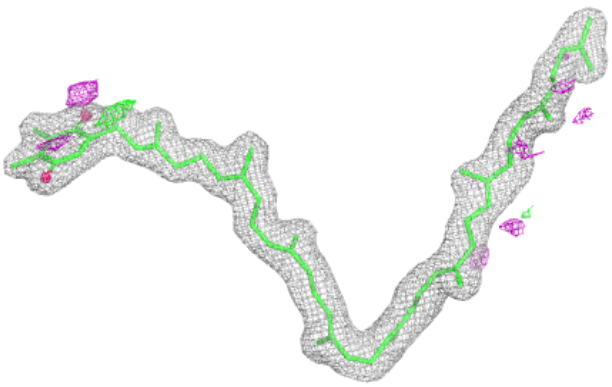


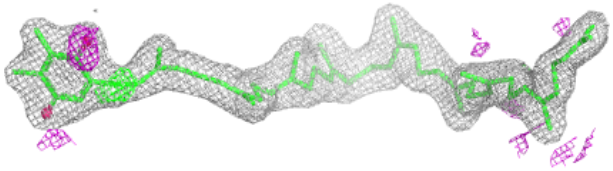


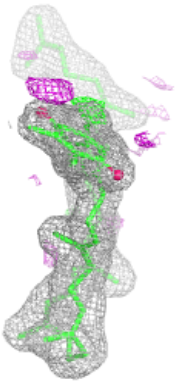


Electron density around PL9 D 406:

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

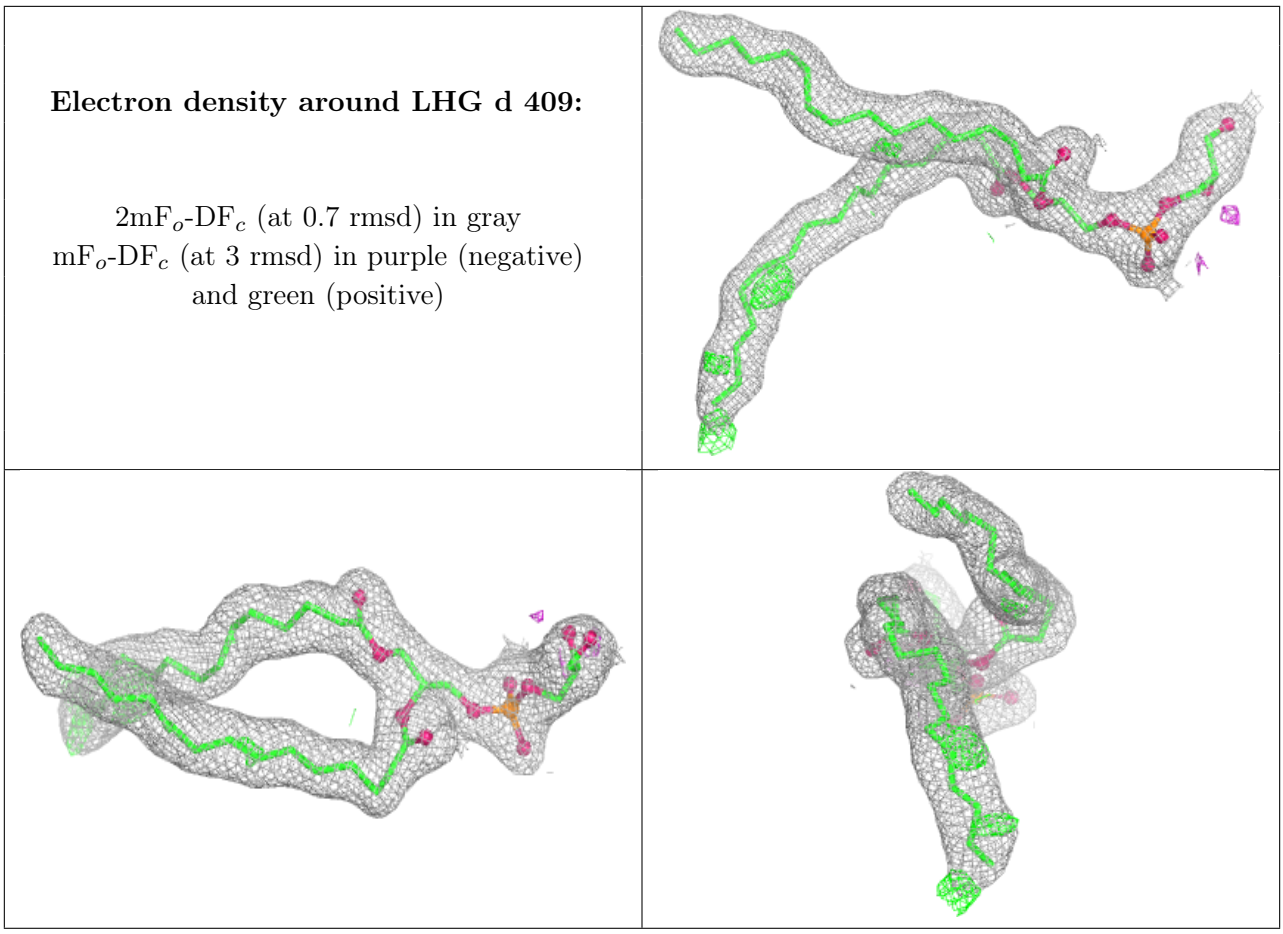






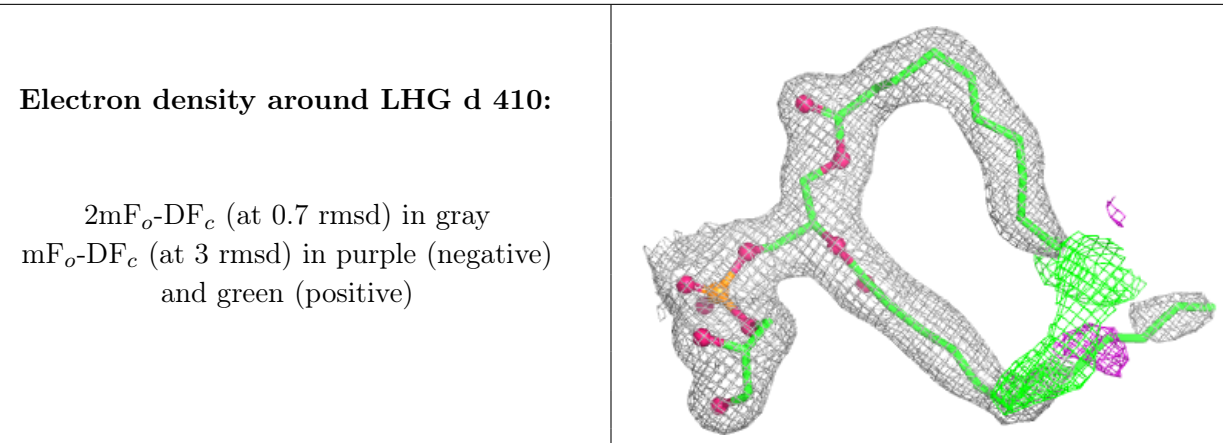
Electron density around LHG d 409:

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



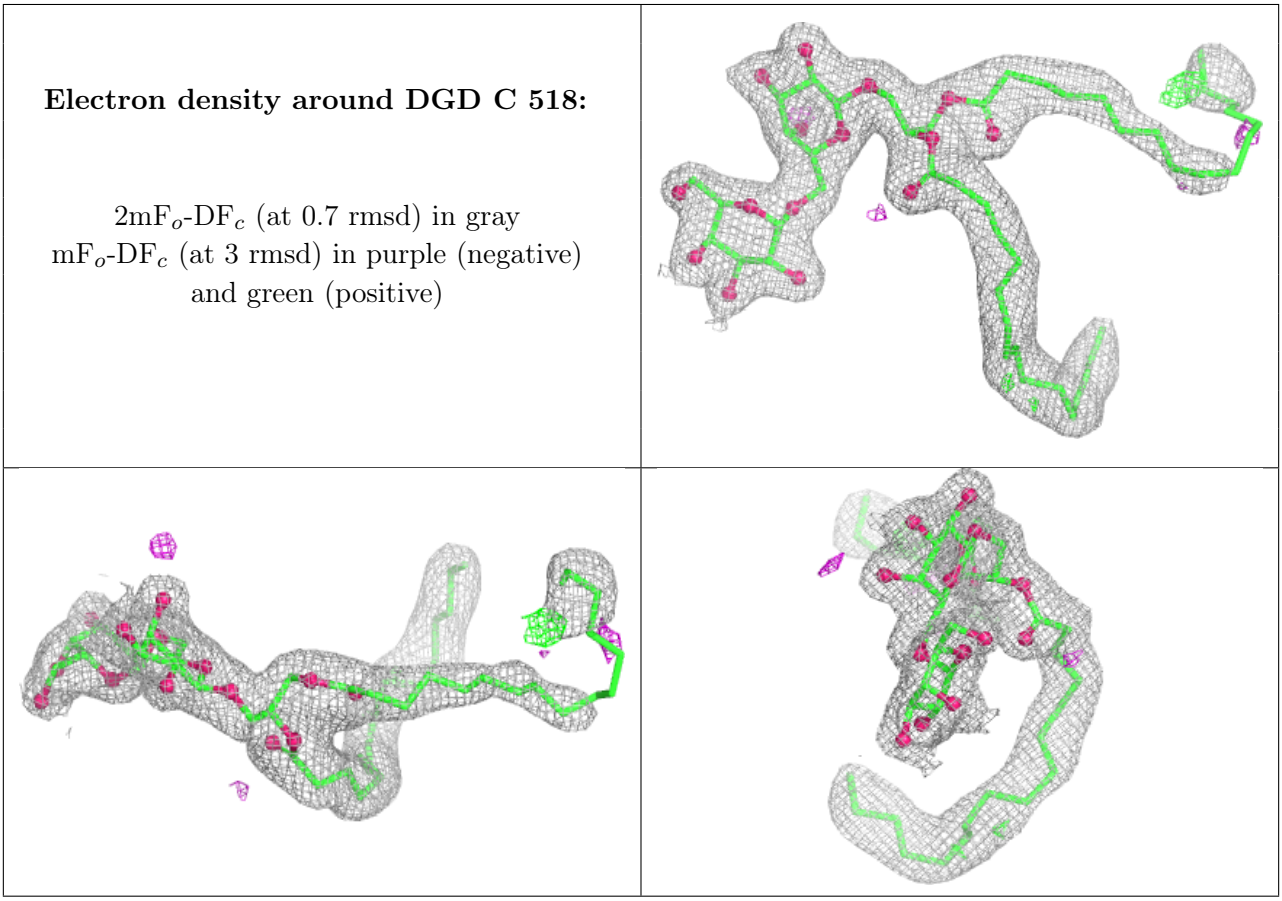
Electron density around LHG d 410:

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



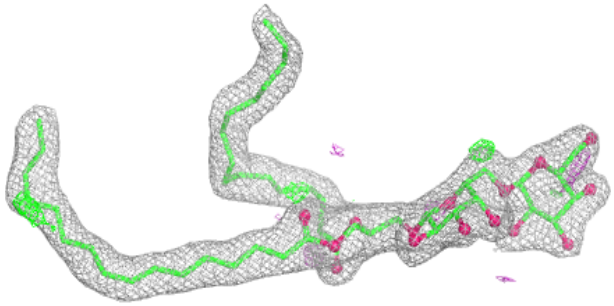
Electron density around DGD C 518:

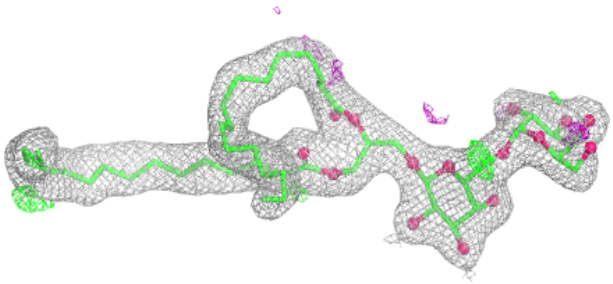
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

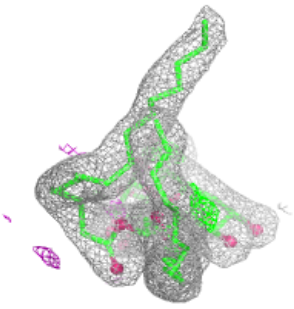


Electron density around DGD H 102:

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

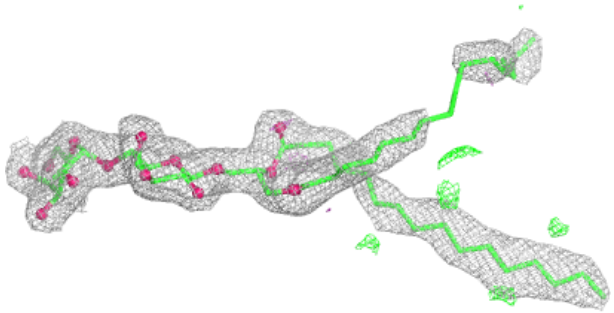


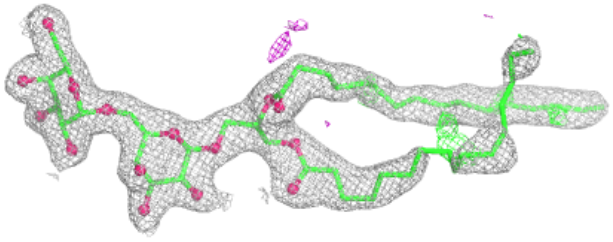


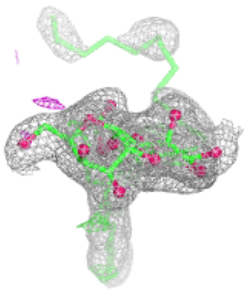


Electron density around DGD c 518:

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

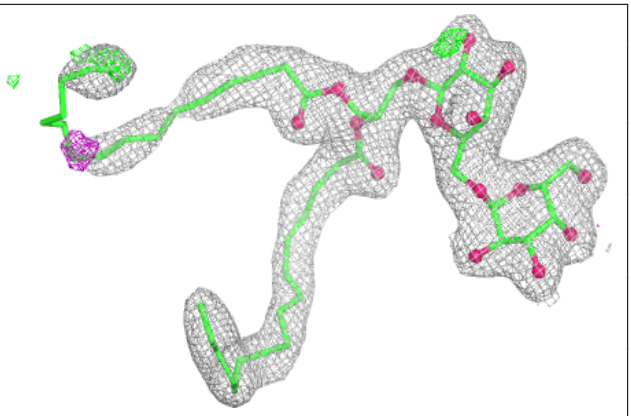


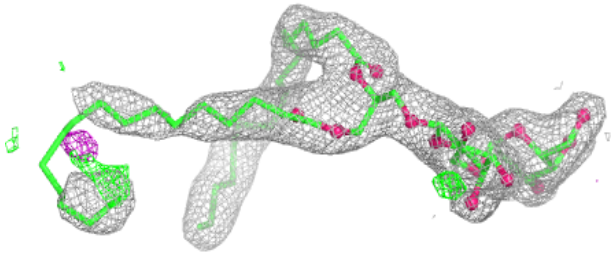


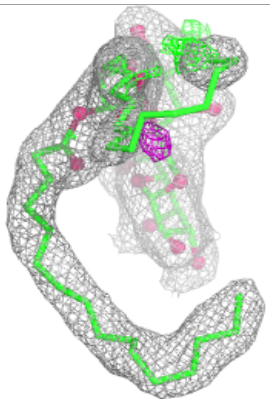


Electron density around DGD c 519:

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

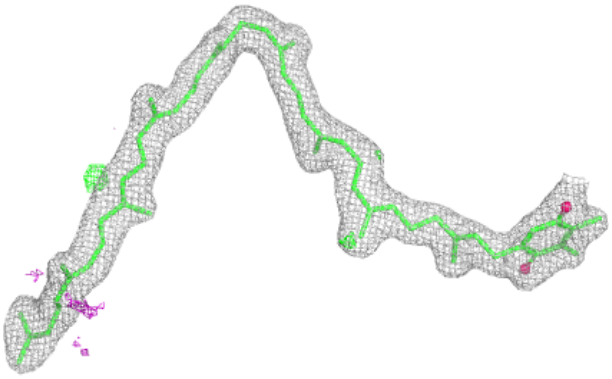


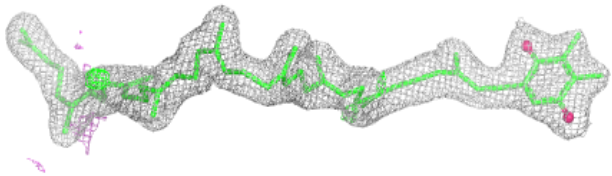


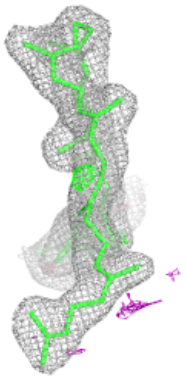


Electron density around PL9 d 407:

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

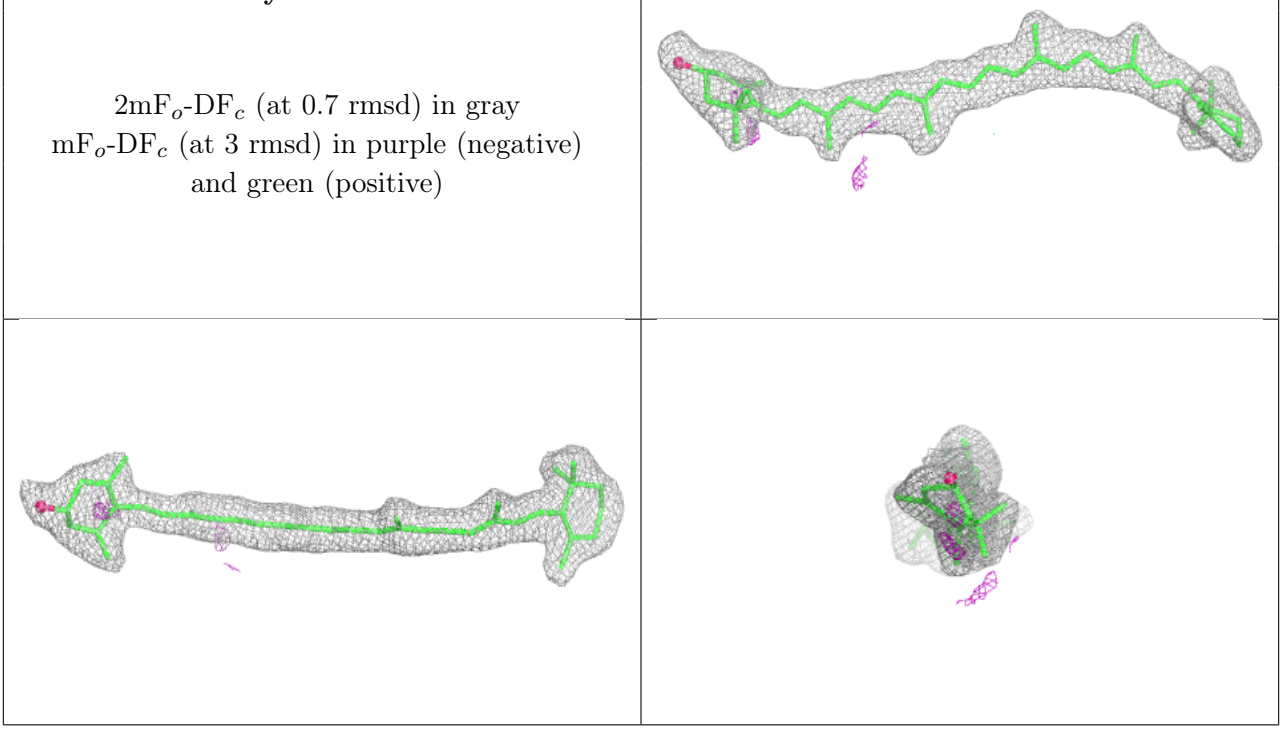






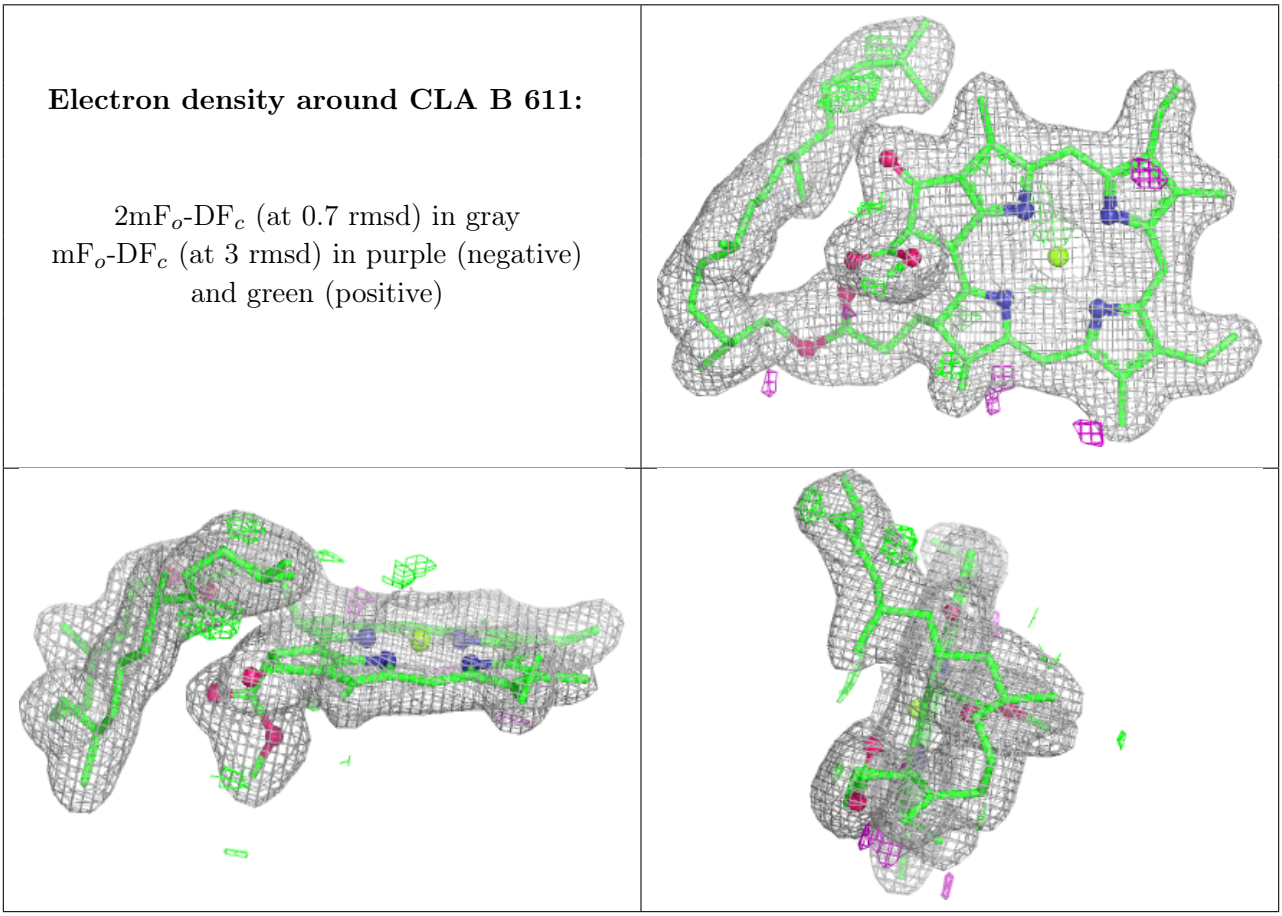
Electron density around RRX H 101:

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



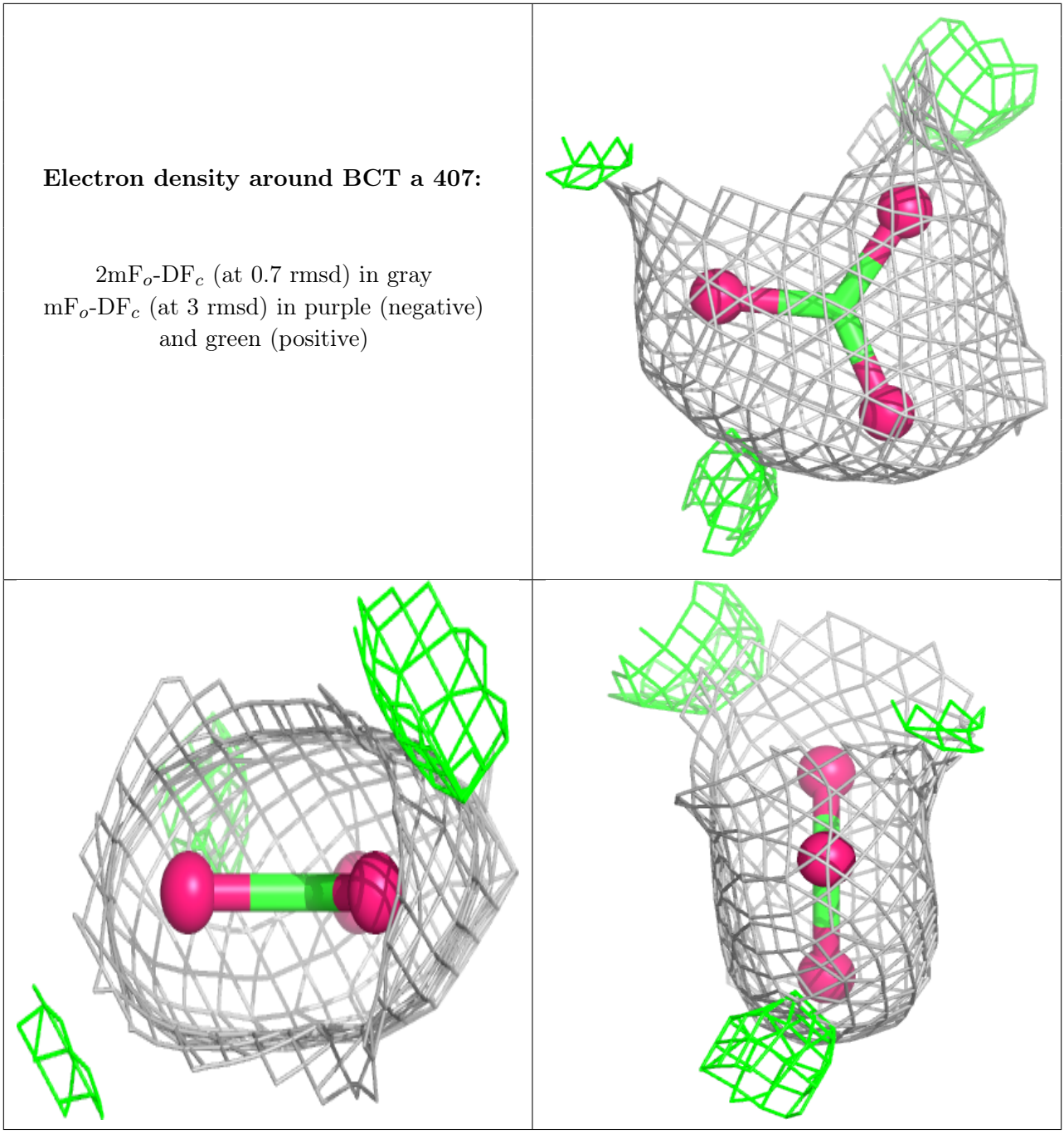
Electron density around CLA B 611:

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



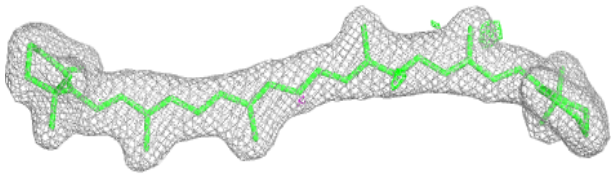
Electron density around BCT a 407:

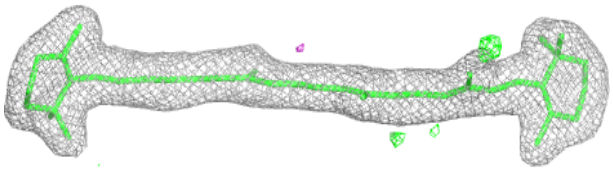
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

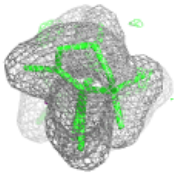


Electron density around BCR A 410:

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

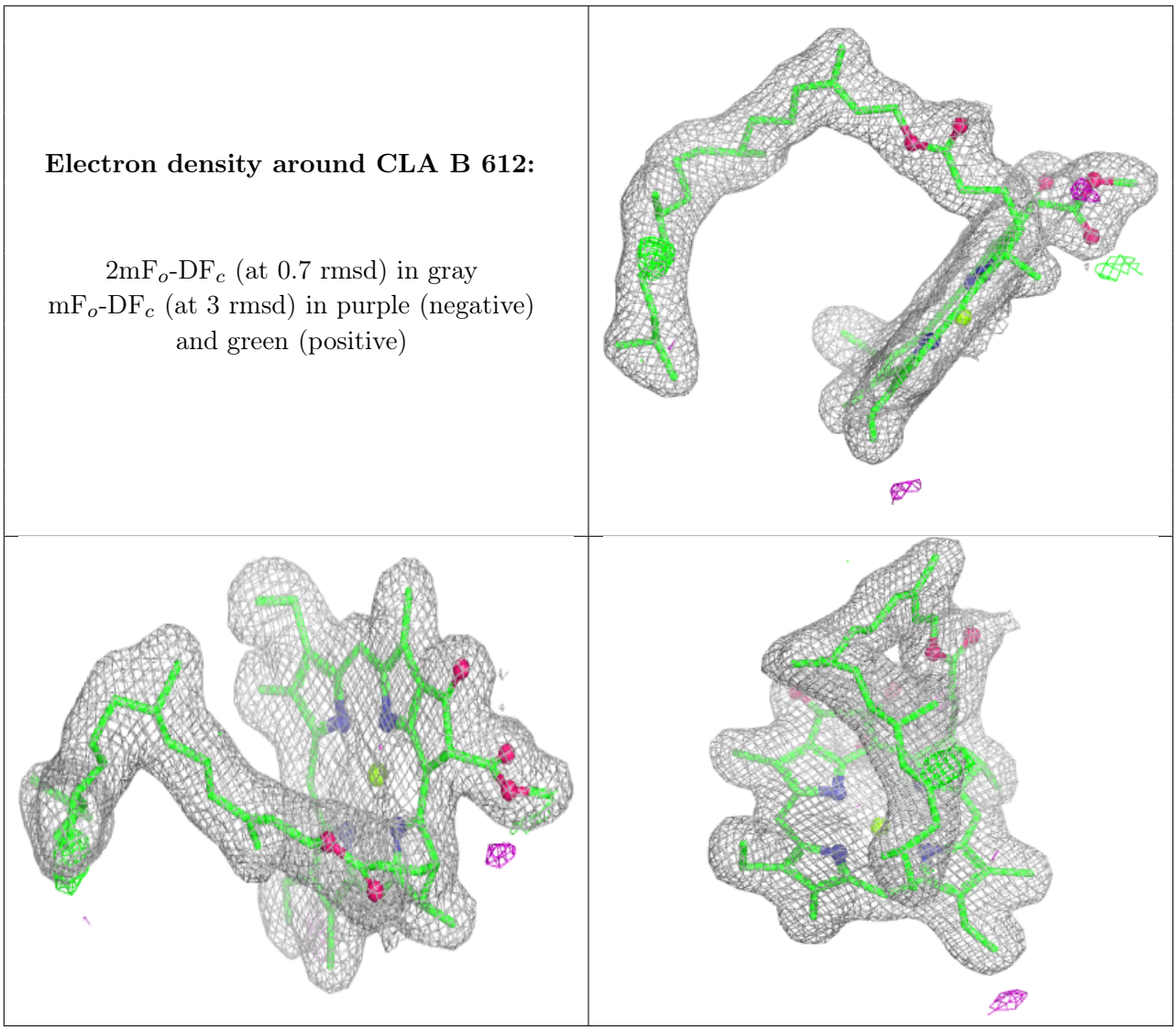






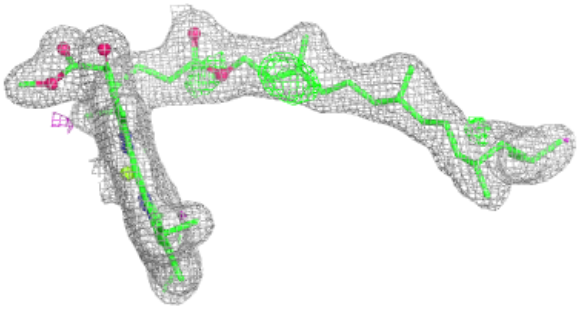
Electron density around CLA B 612:

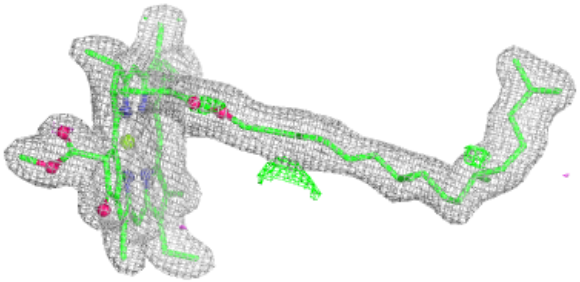
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

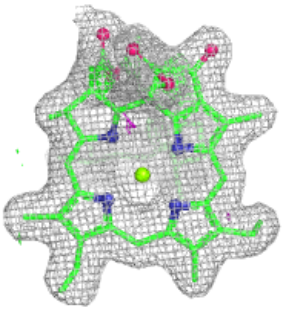


Electron density around CLA B 606:

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

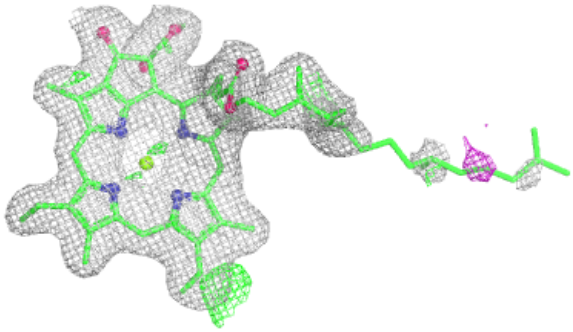


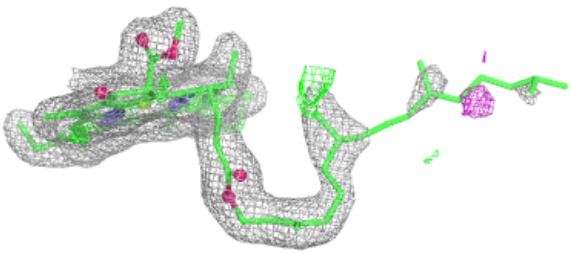


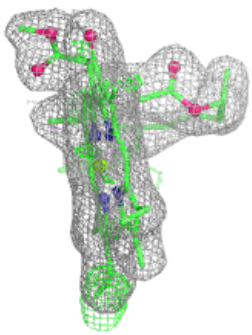


Electron density around CLA a 410:

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

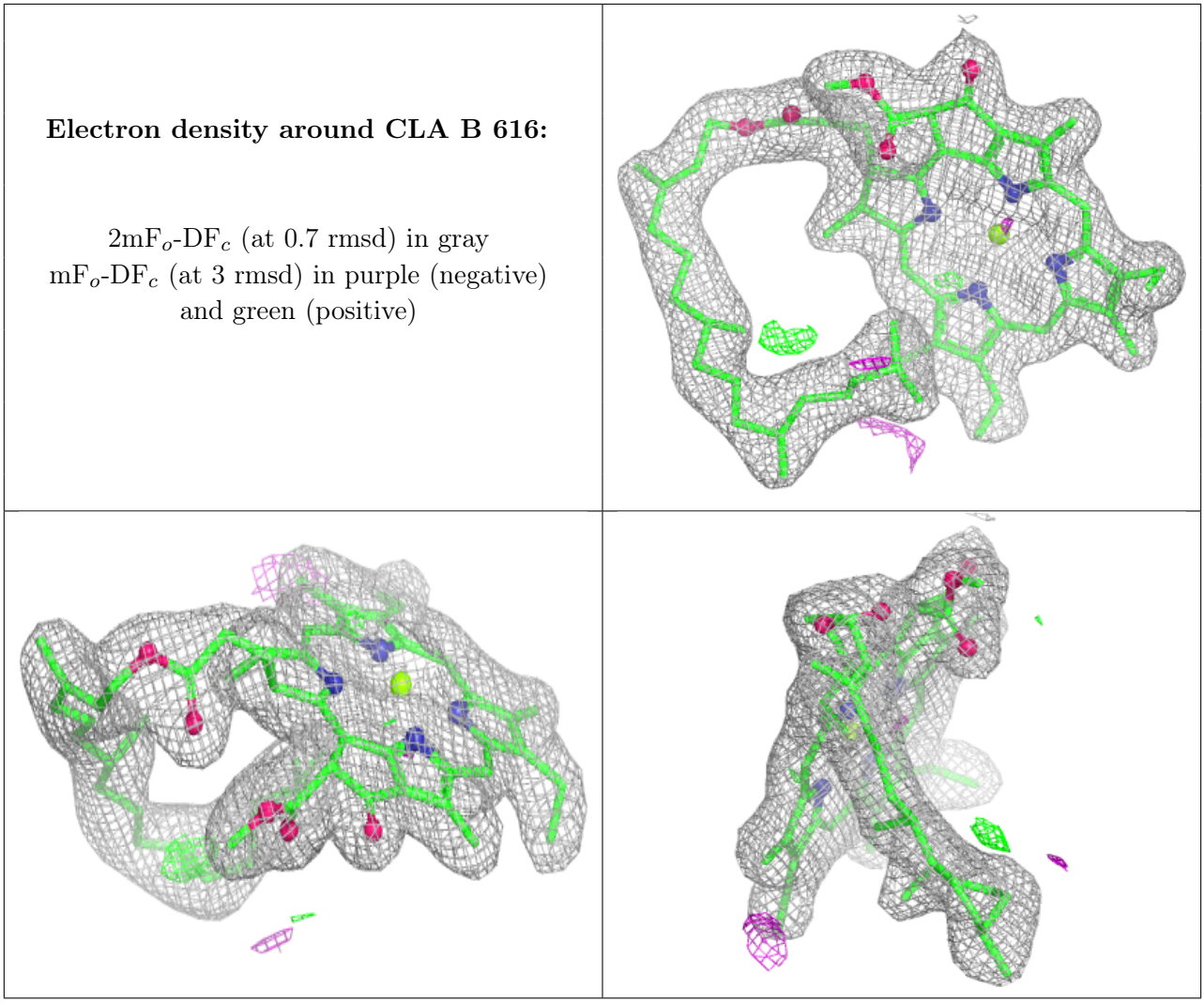






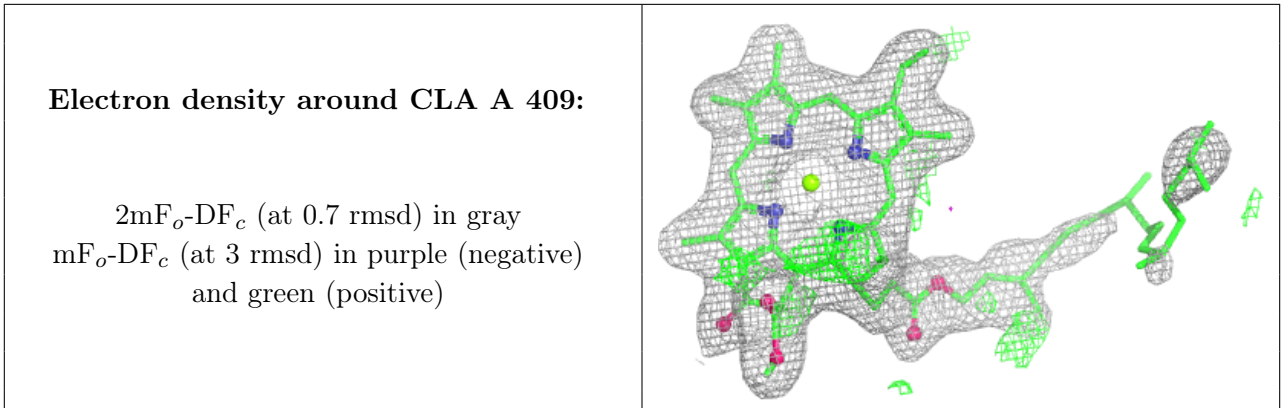
Electron density around CLA B 616:

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



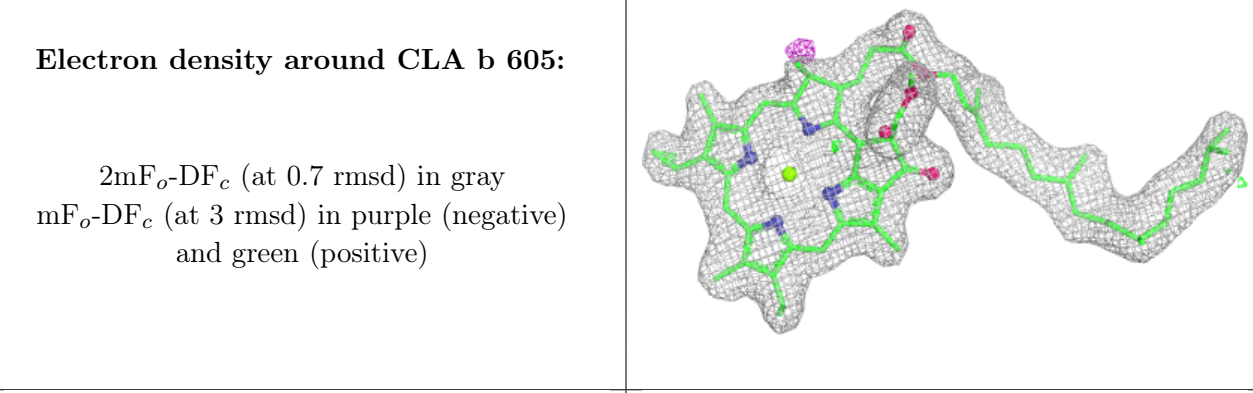
Electron density around CLA A 409:

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



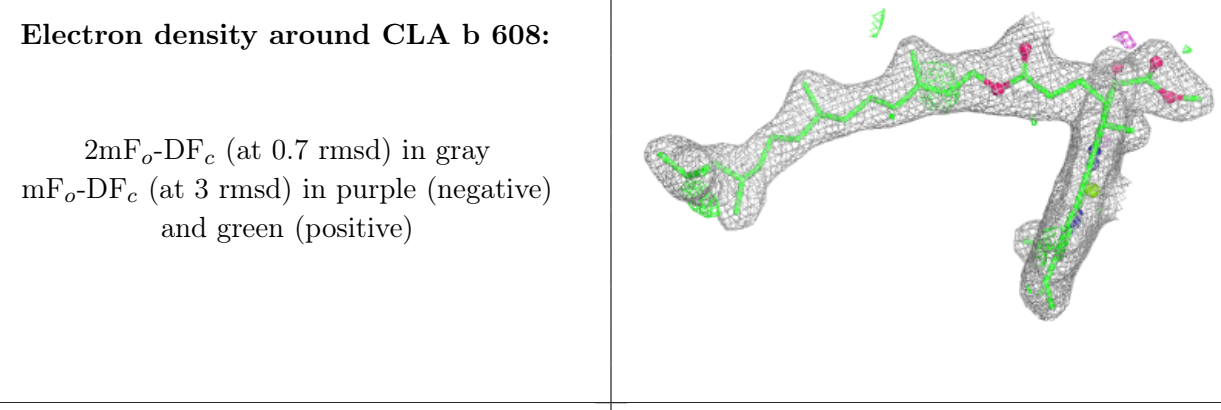
Electron density around CLA b 605:

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



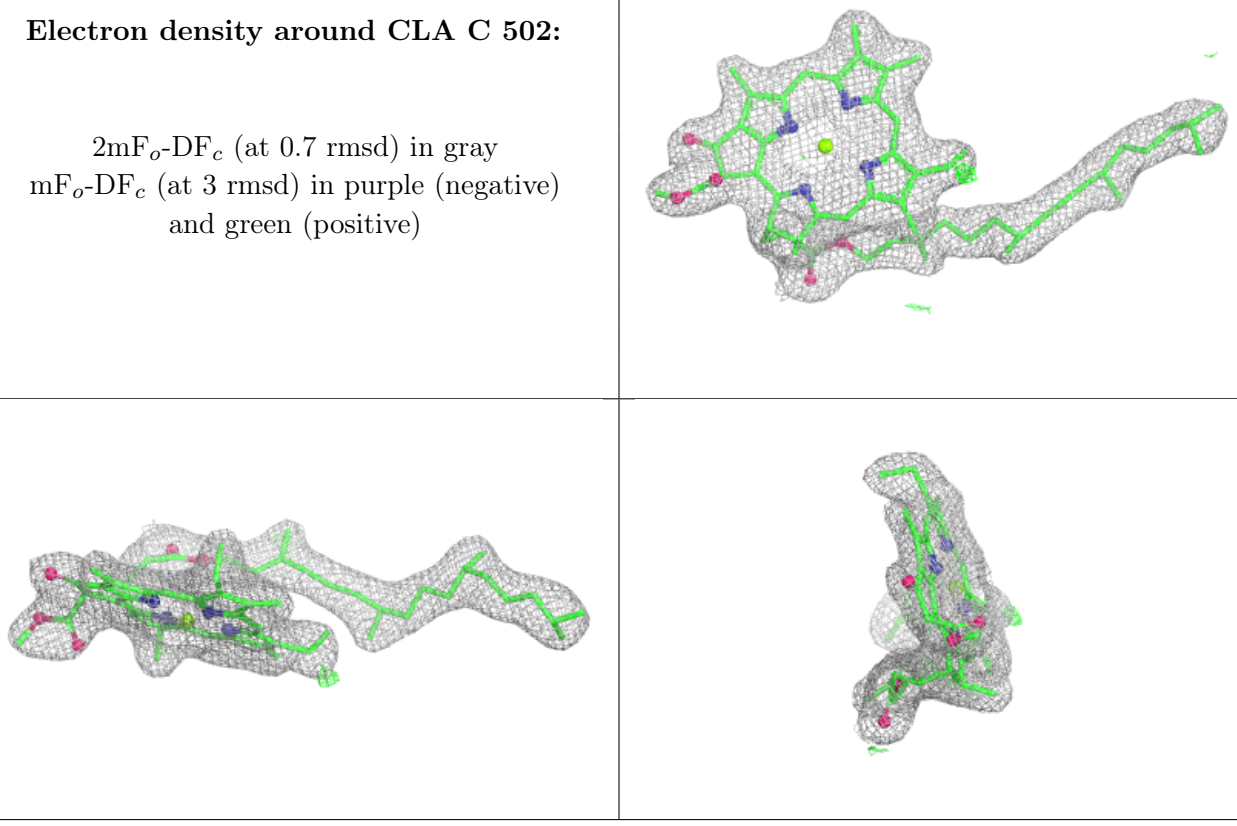
Electron density around CLA b 608:

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



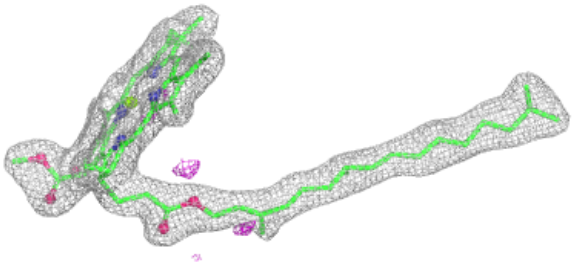
Electron density around CLA C 502:

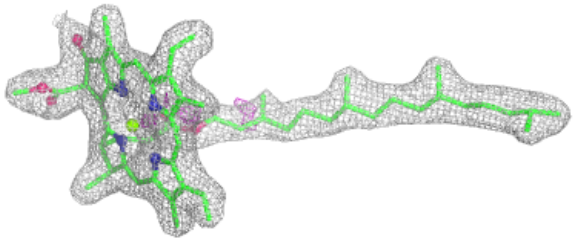
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

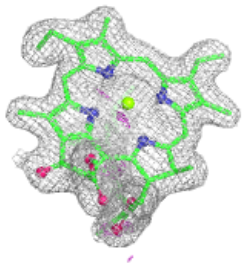


Electron density around CLA b 610:

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

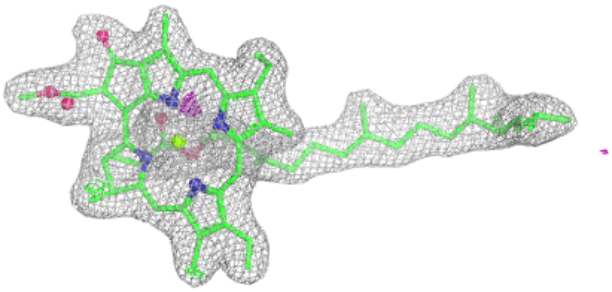


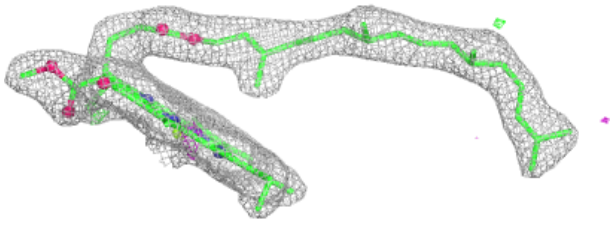


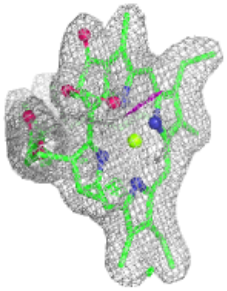


Electron density around CLA b 611:

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

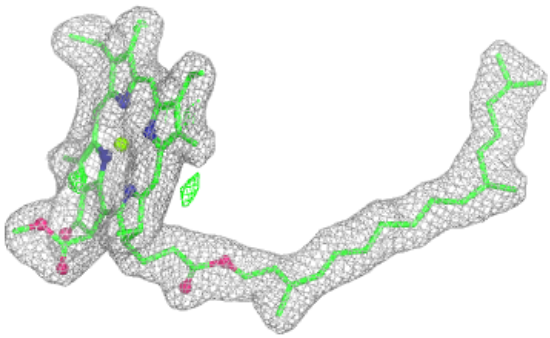


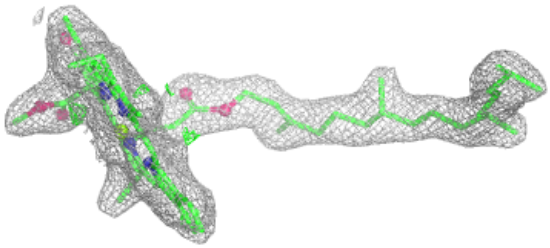


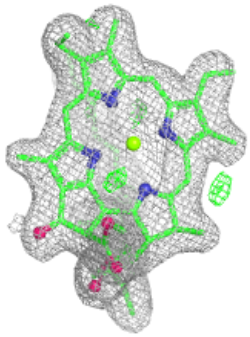


Electron density around CLA b 612:

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

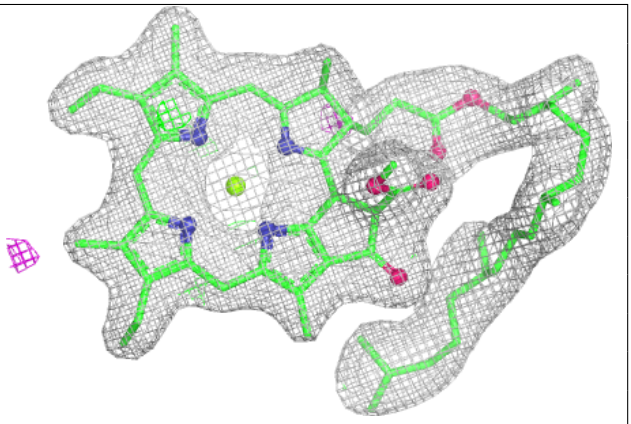


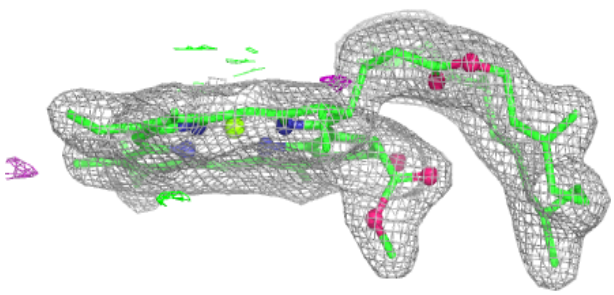


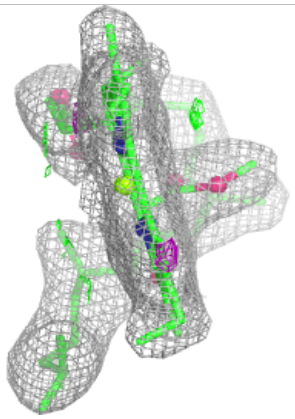


Electron density around CLA b 613:

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

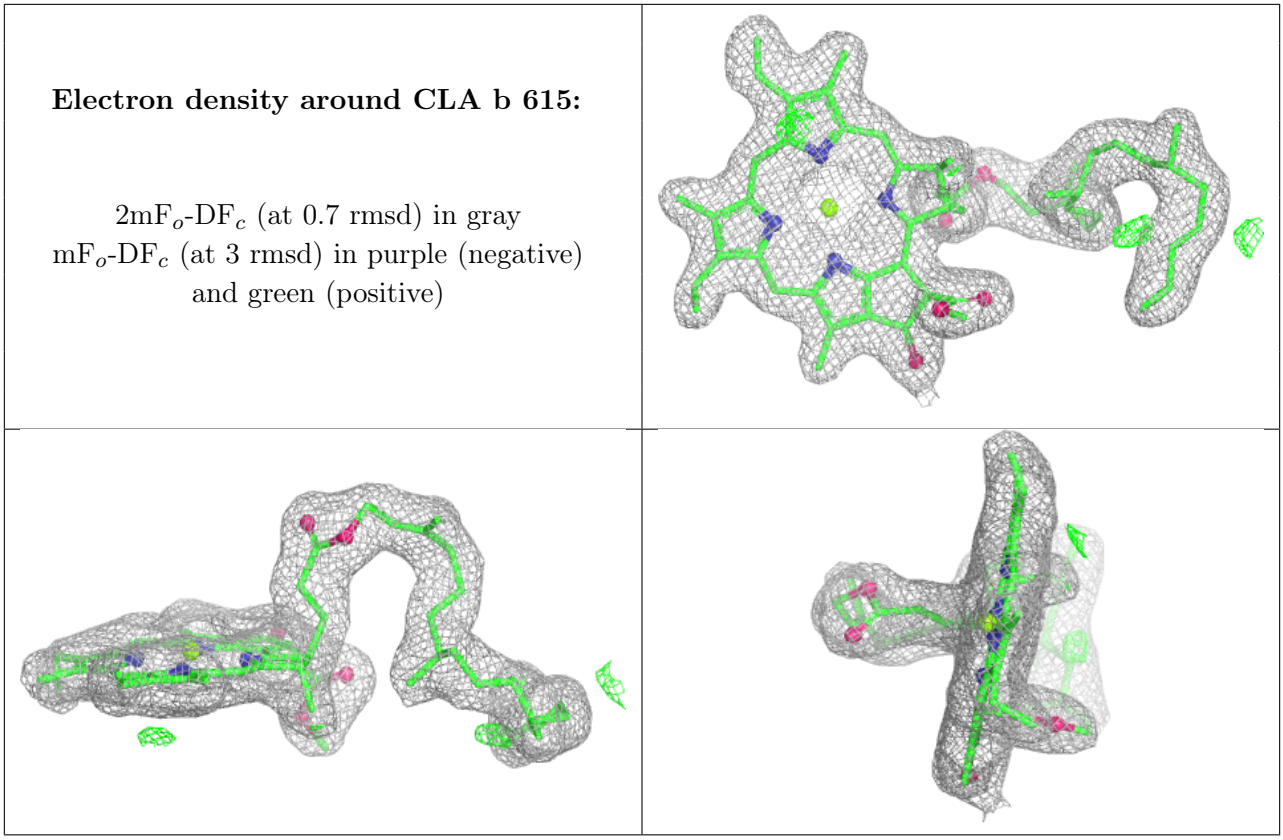






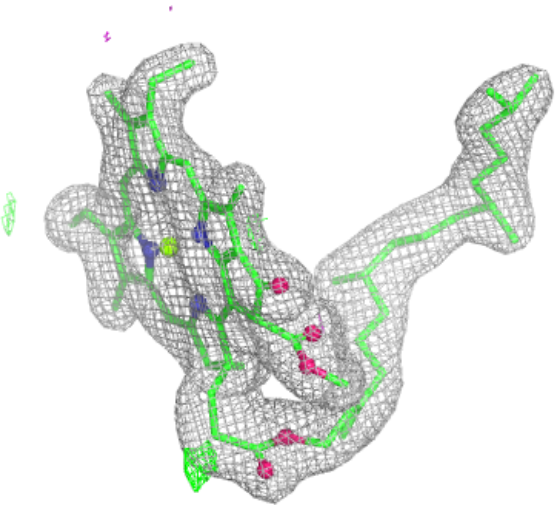
Electron density around CLA b 615:

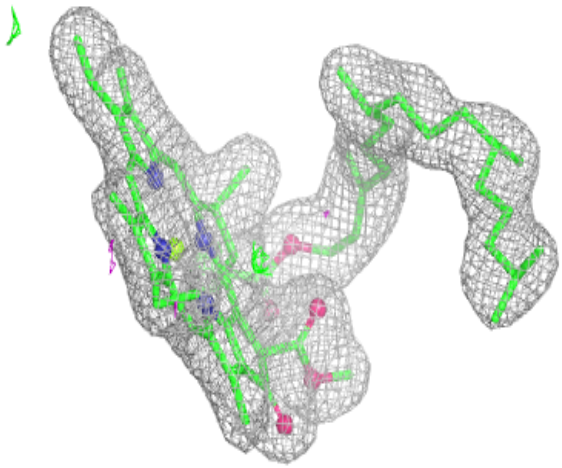
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

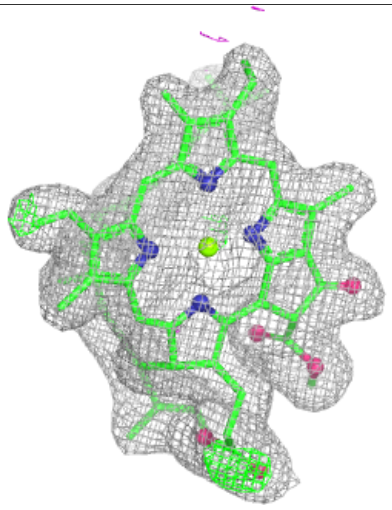


Electron density around CLA b 616:

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

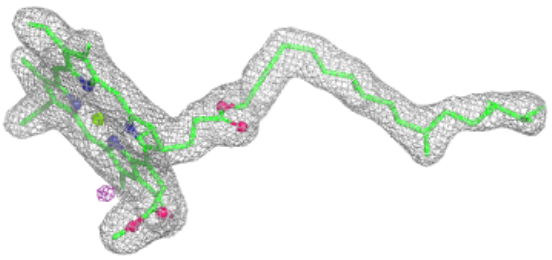


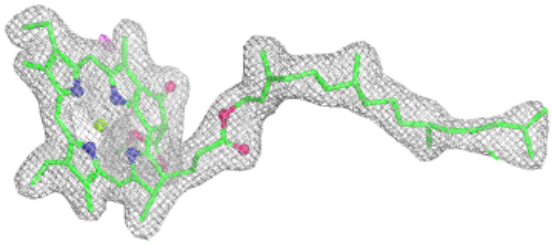


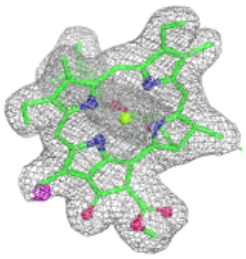


Electron density around CLA C 503:

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

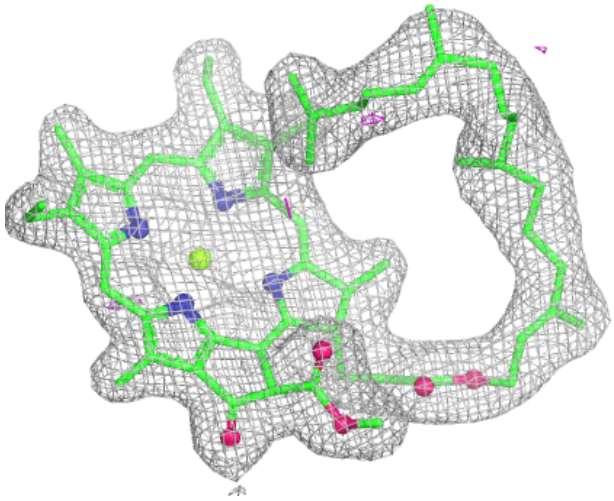


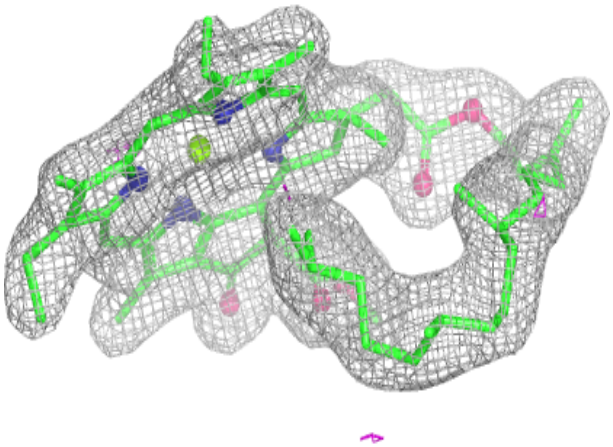


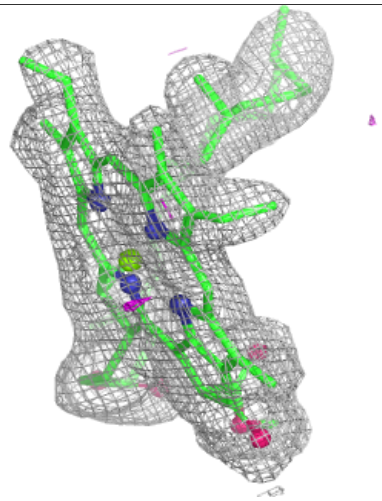


Electron density around CLA b 618:

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

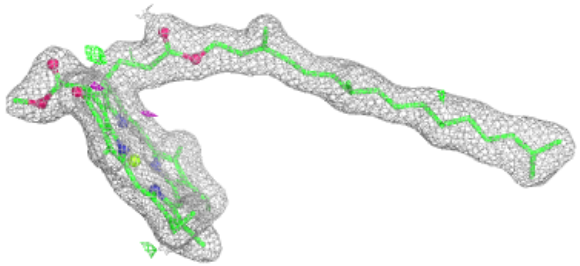


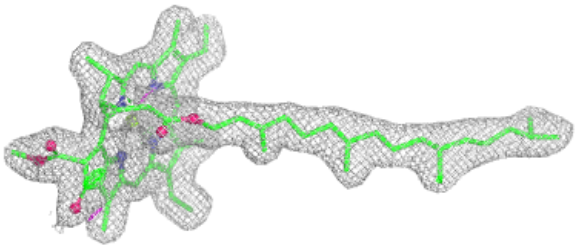


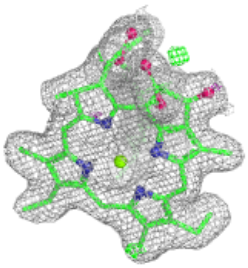


Electron density around CLA B 608:

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

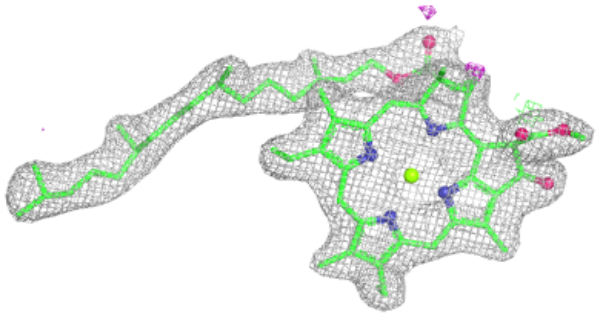


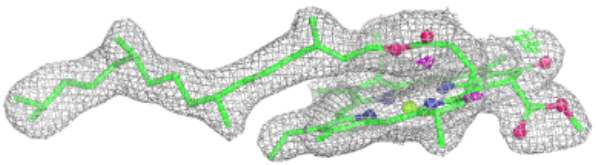


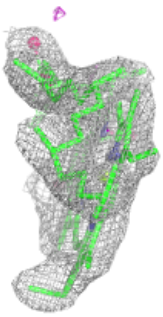


Electron density around CLA c 503:

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

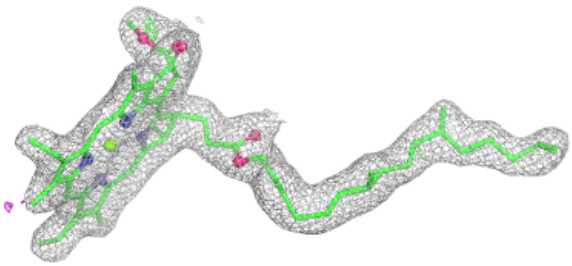


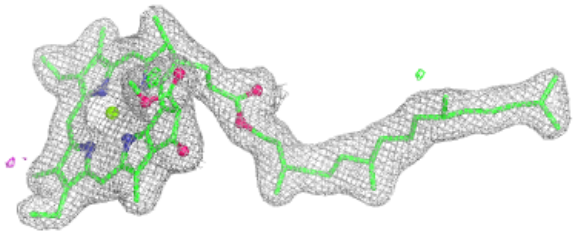


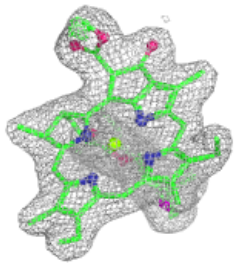


Electron density around CLA c 504:

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

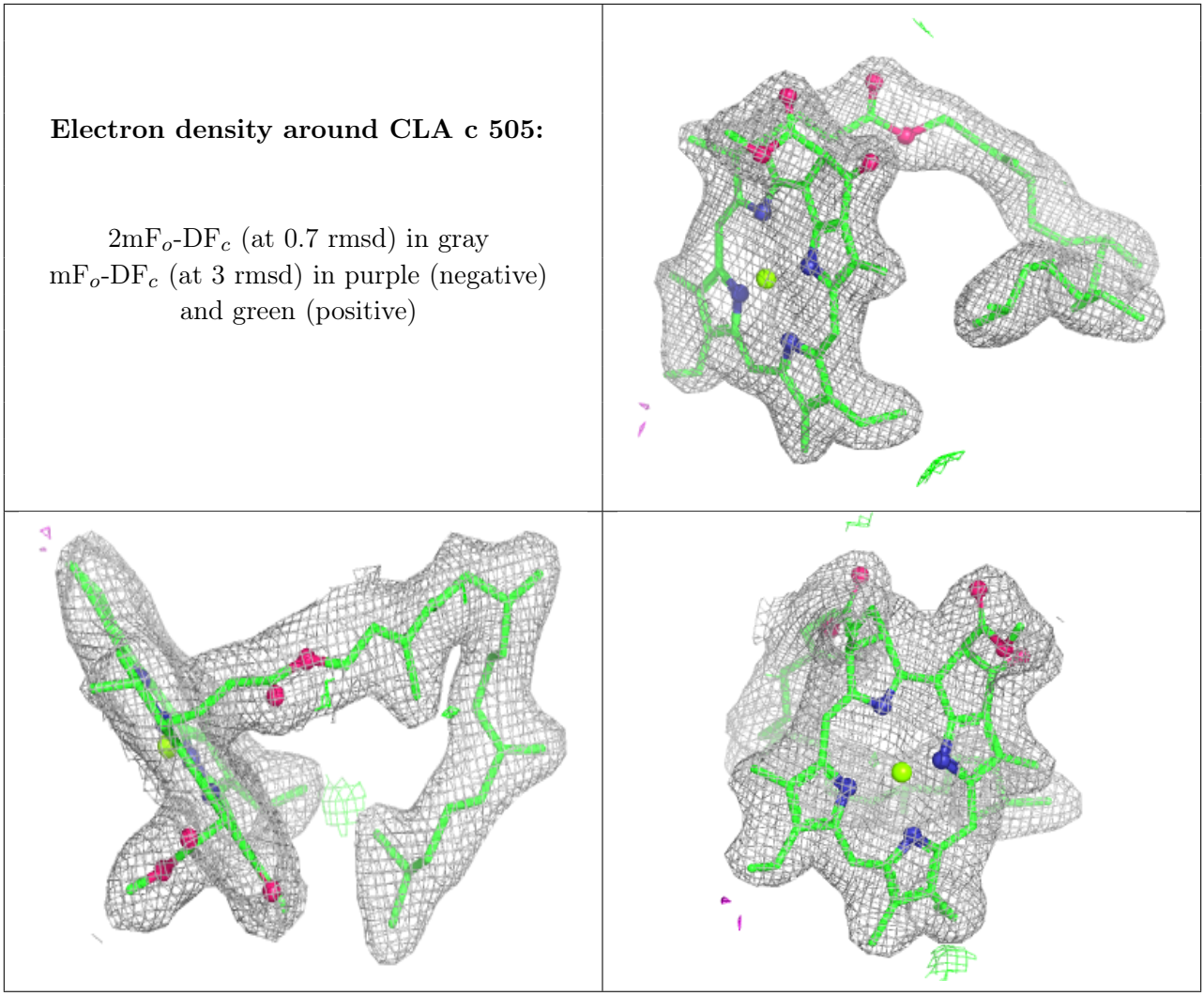






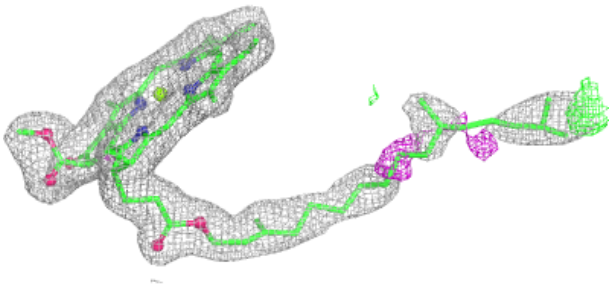
Electron density around CLA c 505:

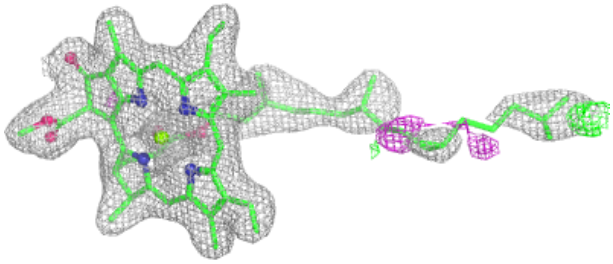
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

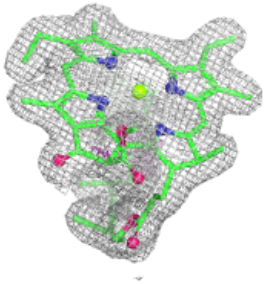


Electron density around CLA C 505:

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

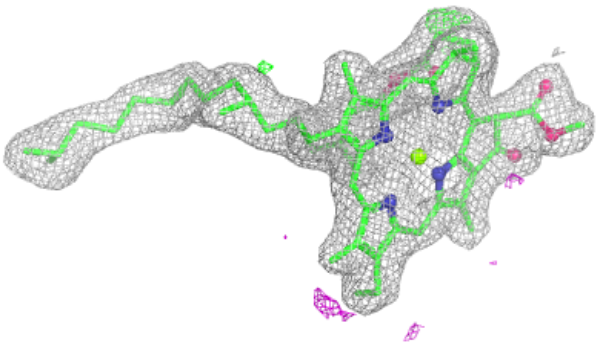


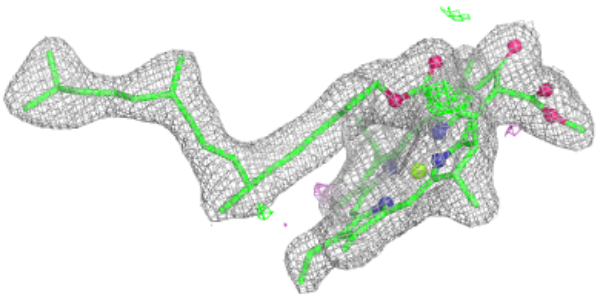


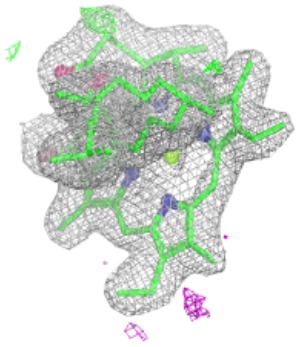


Electron density around CLA c 507:

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

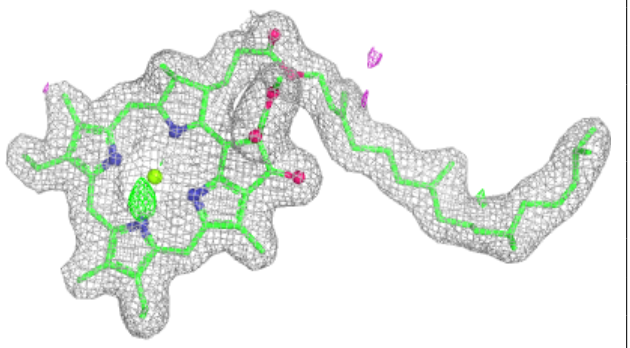


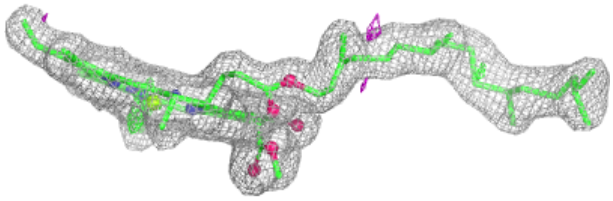


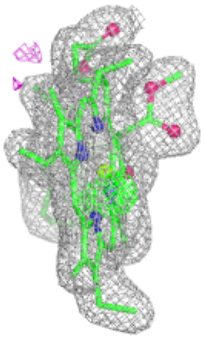


Electron density around CLA B 603:

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

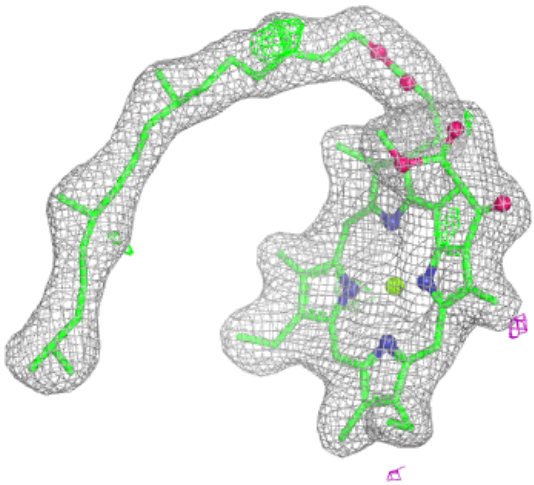


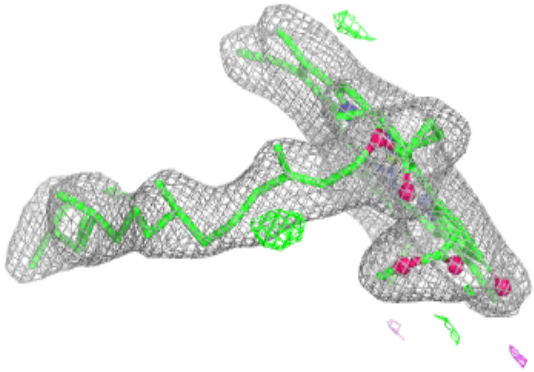


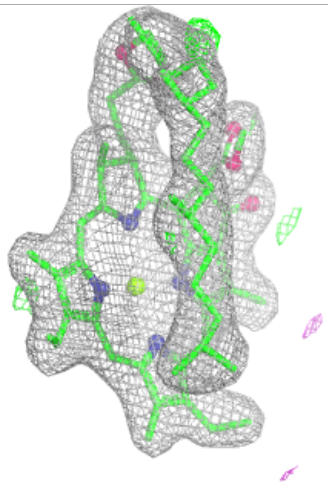


Electron density around CLA C 508:

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

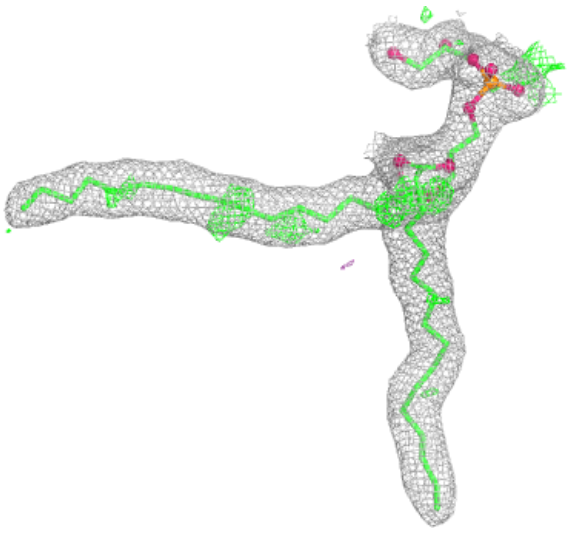


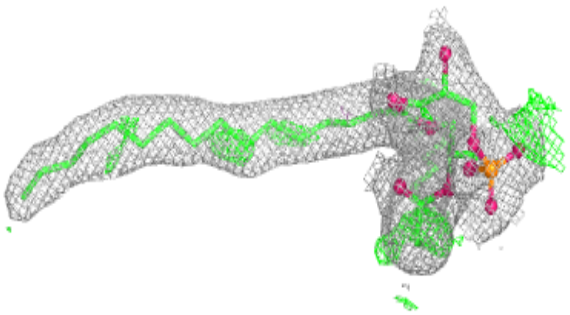


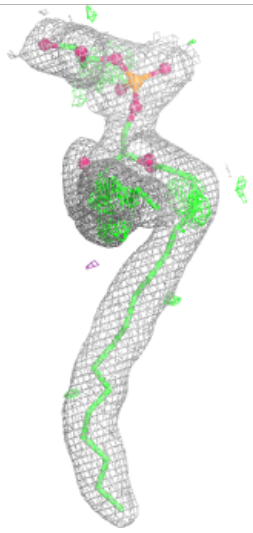


Electron density around LHG B 640:

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

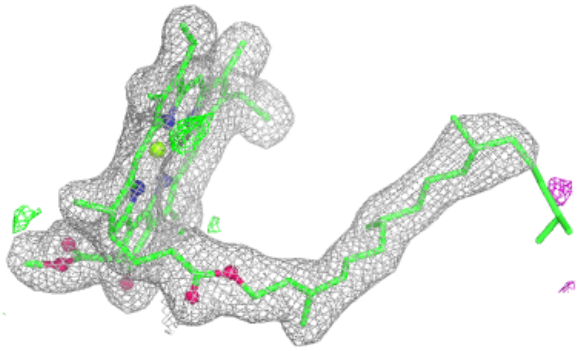


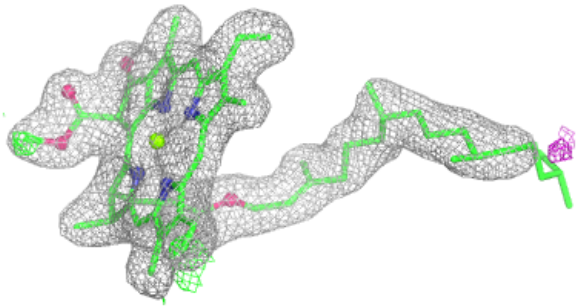


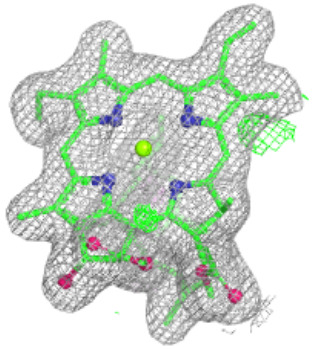


Electron density around CLA C 509:

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

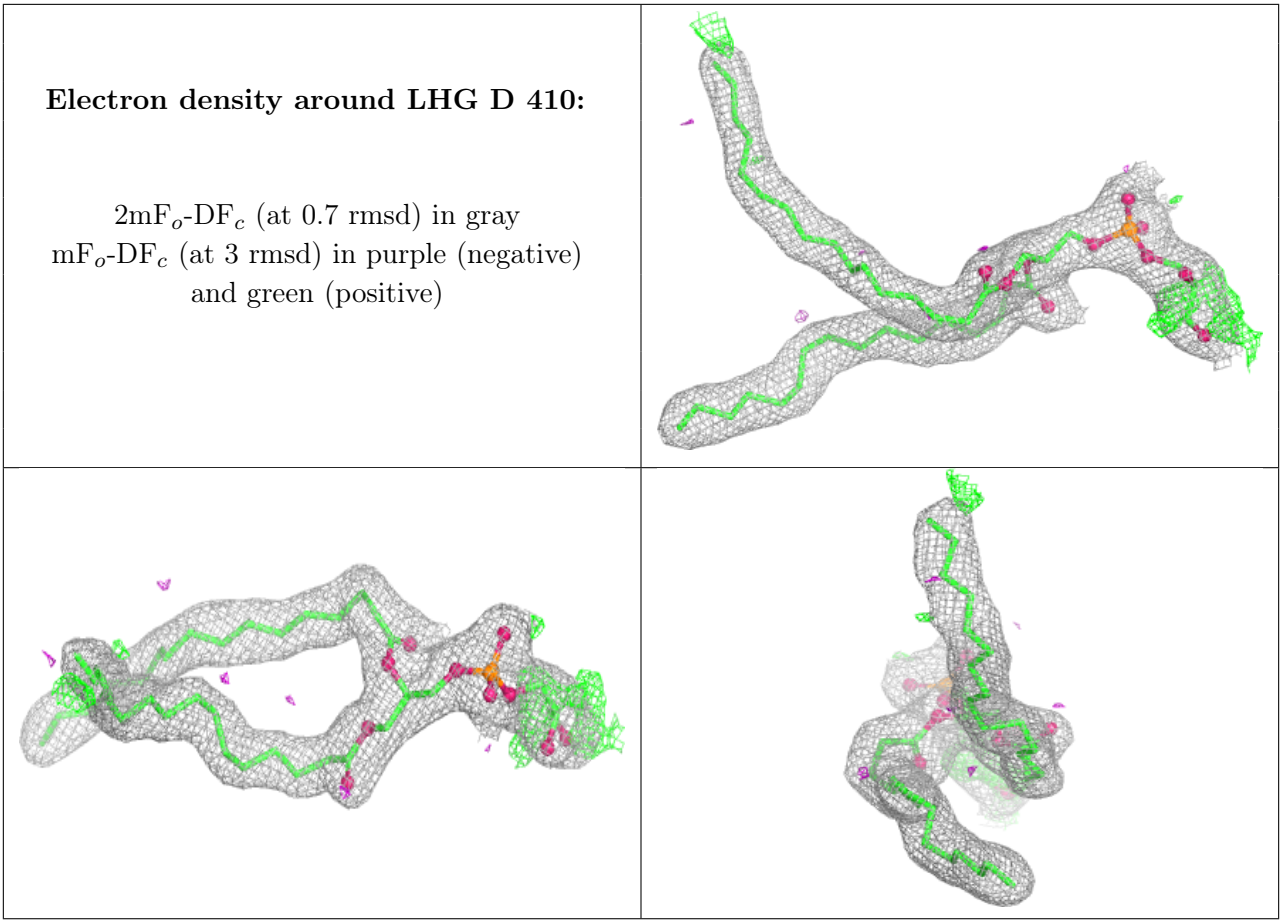






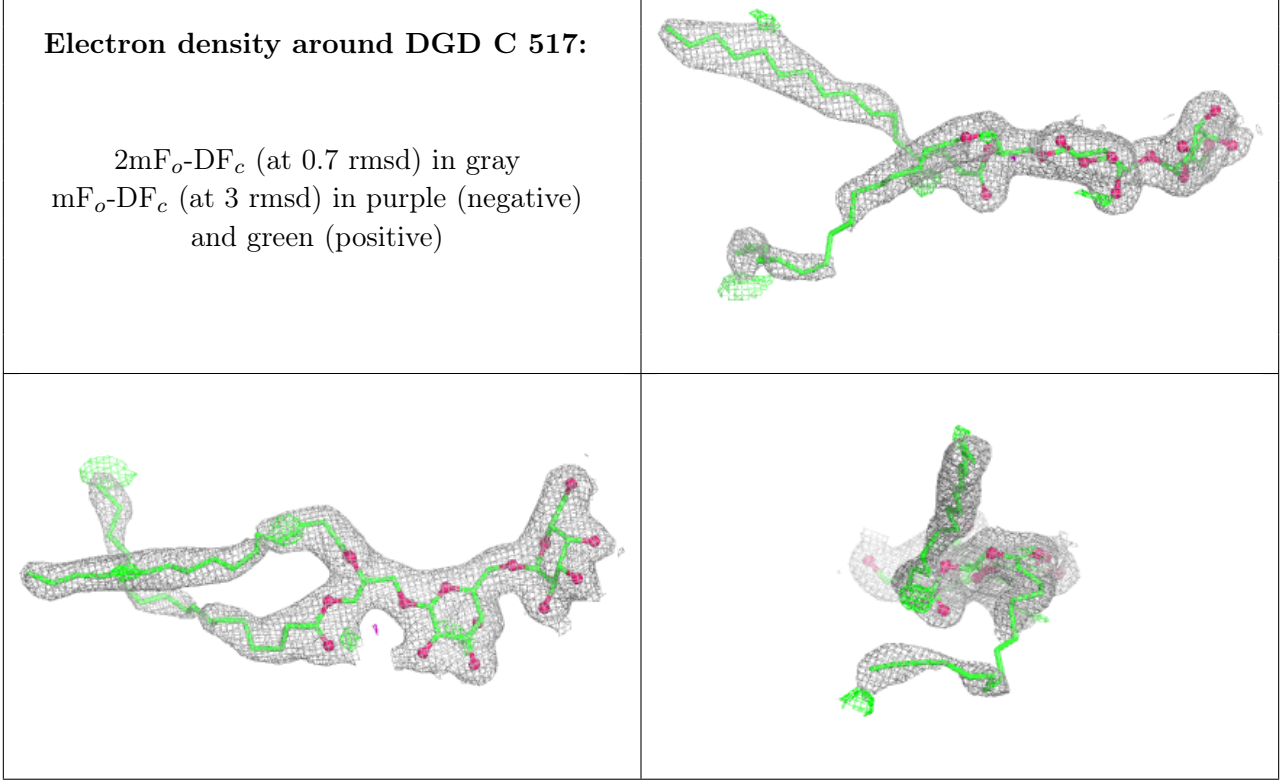
Electron density around LHG D 410:

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



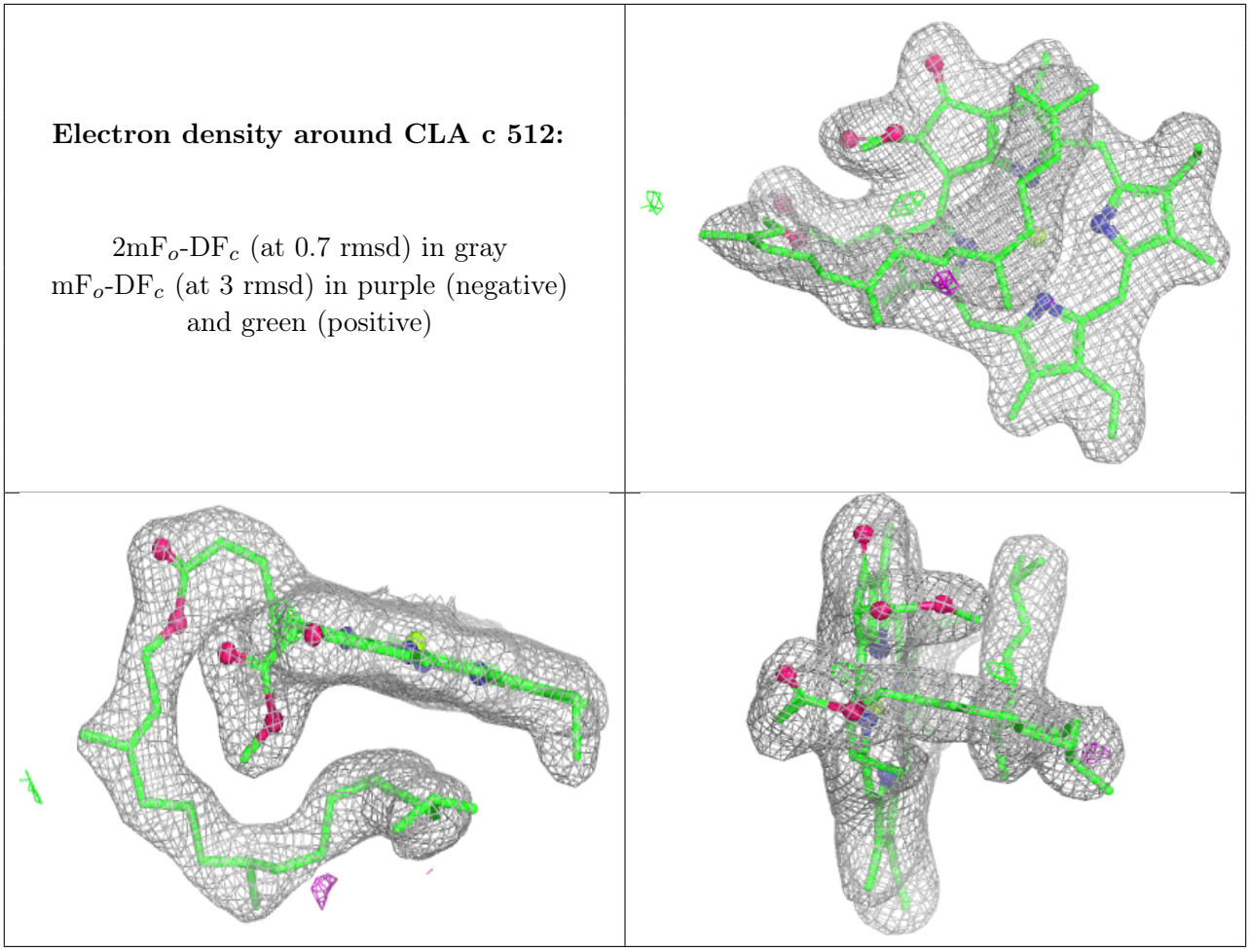
Electron density around DGD C 517:

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



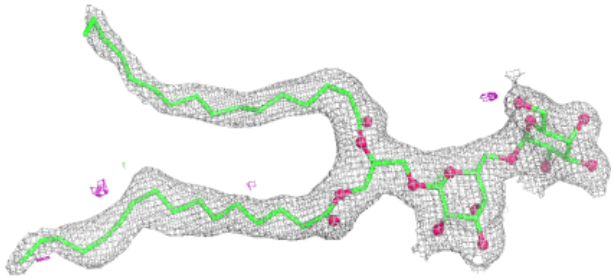
Electron density around CLA c 512:

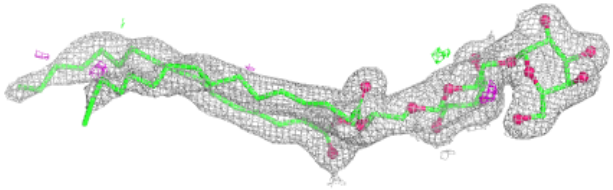
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

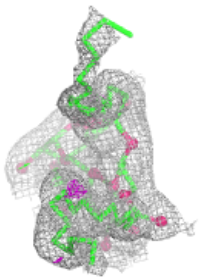


Electron density around DGD C 519:

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

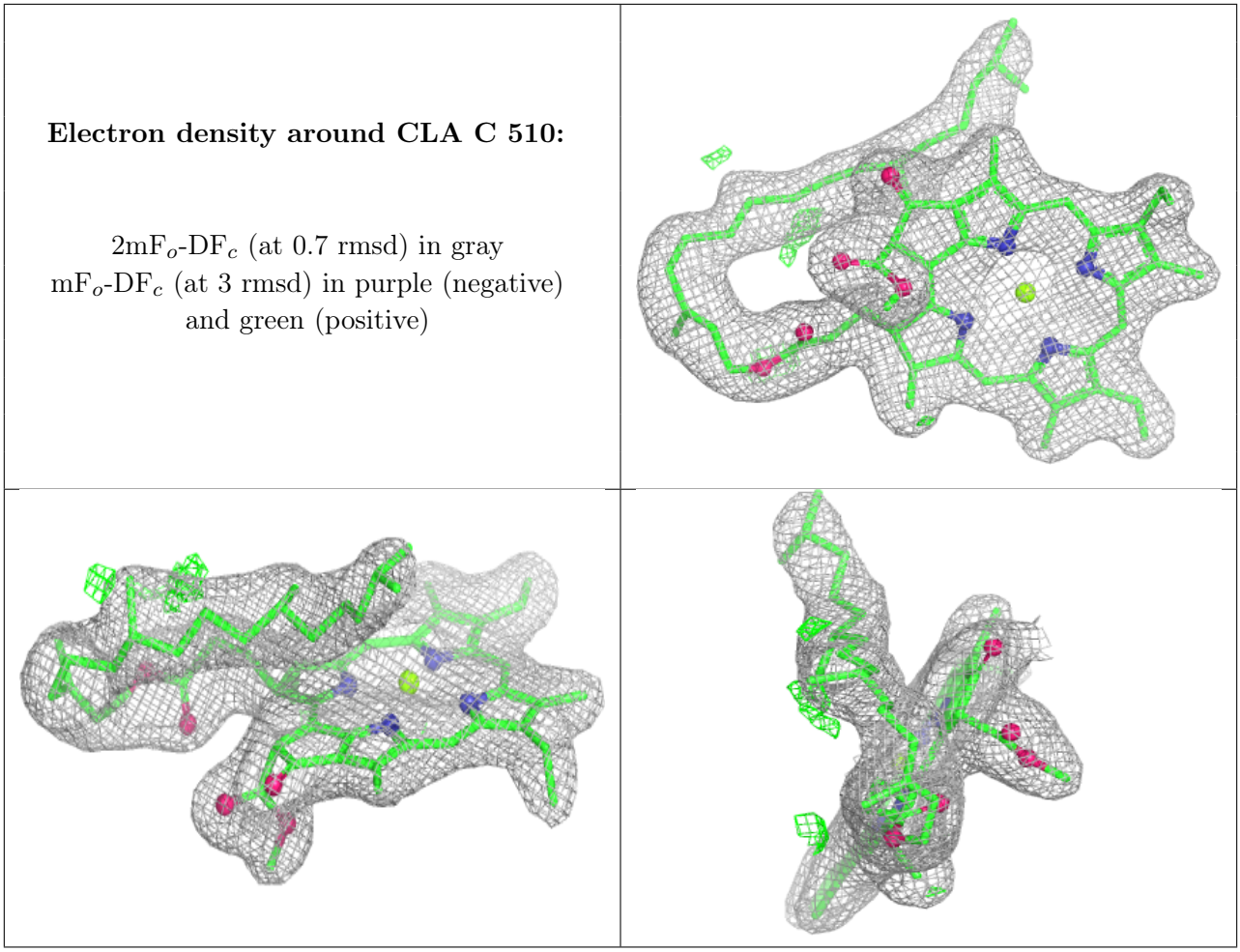






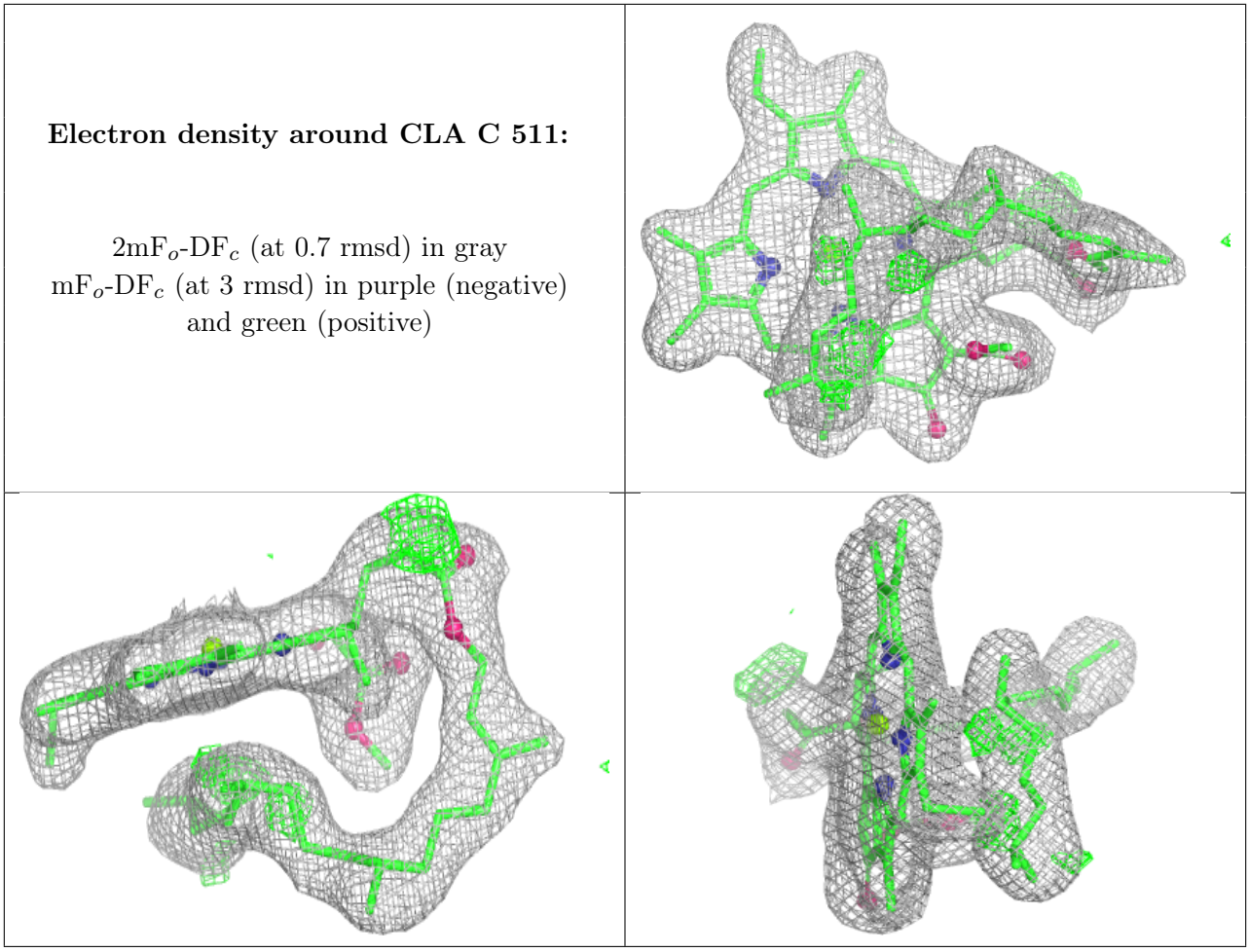
Electron density around CLA C 510:

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



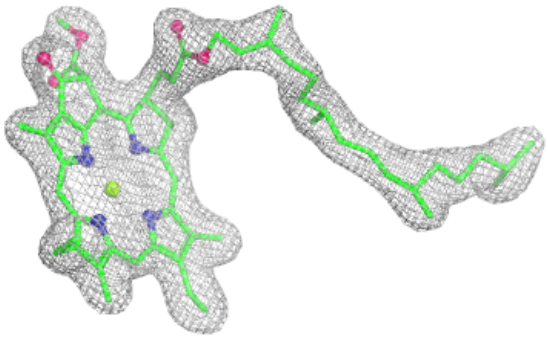
Electron density around CLA C 511:

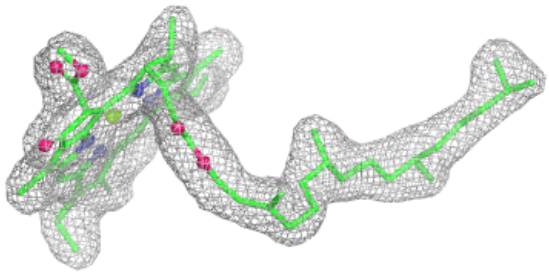
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

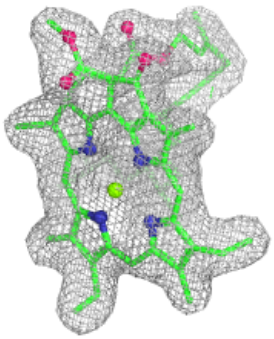


Electron density around CLA C 512:

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

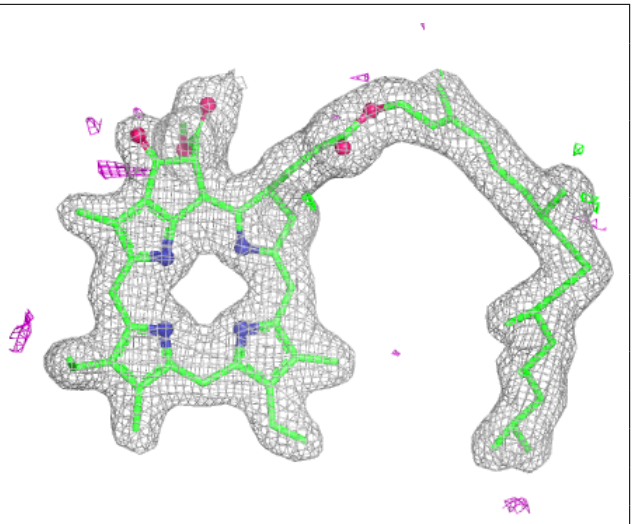


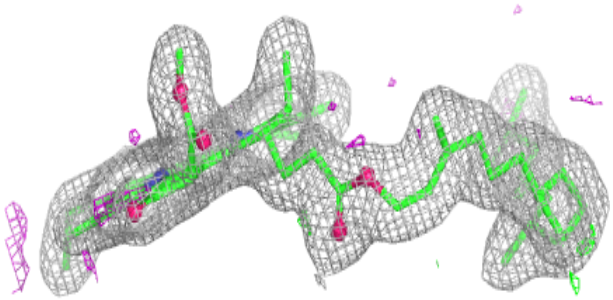




Electron density around PHO A 408:

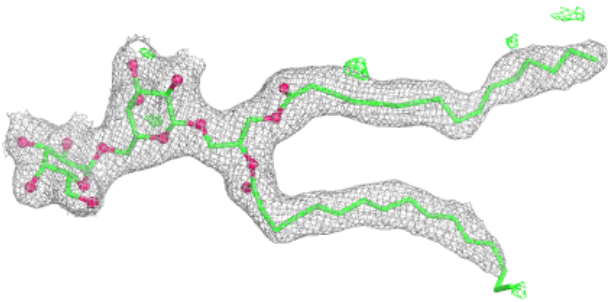
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

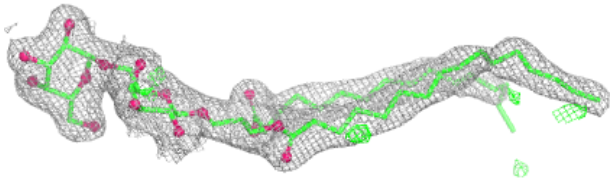


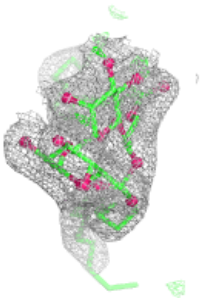


Electron density around DGD c 520:

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

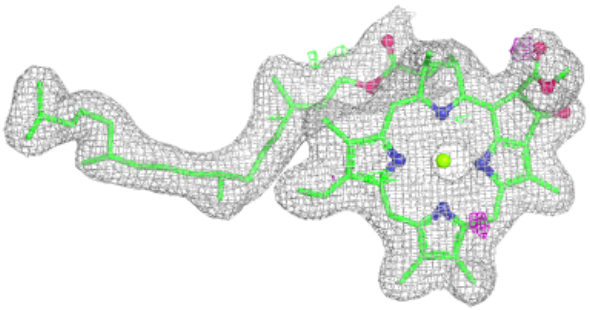


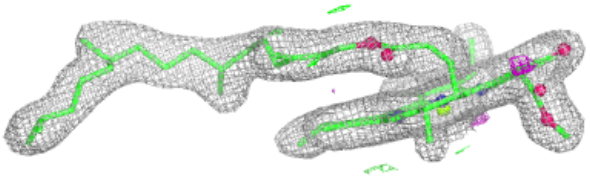


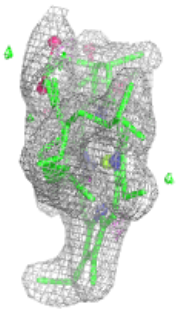


Electron density around CLA B 604:

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

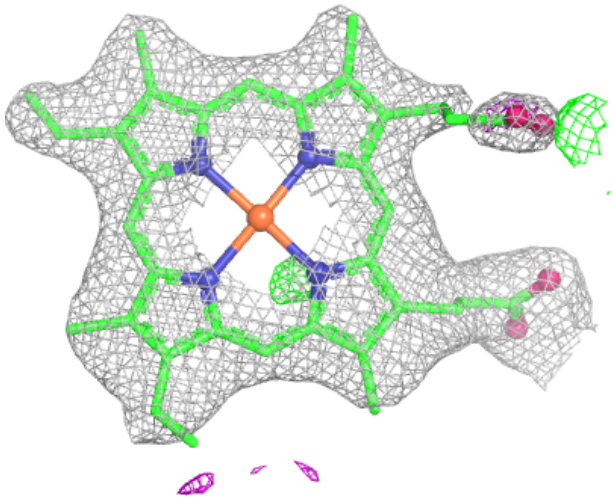


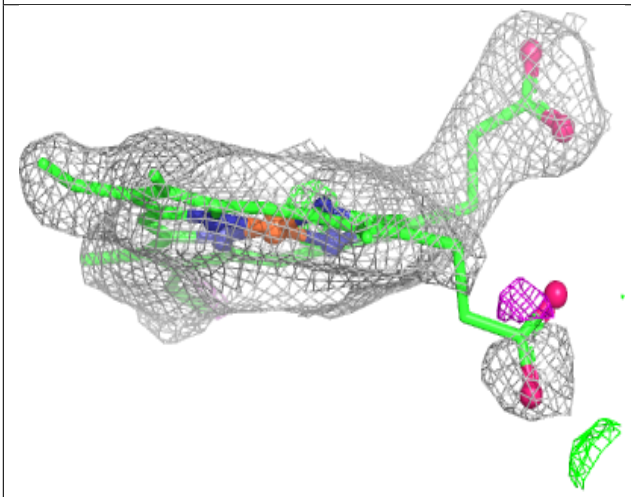


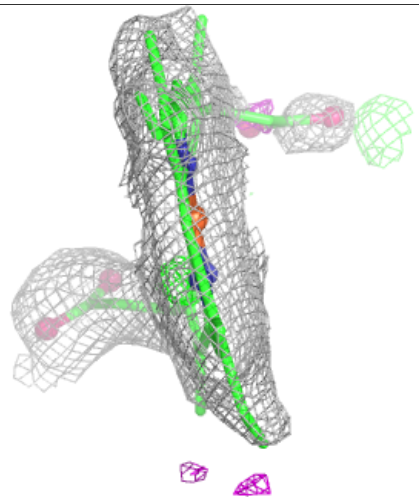


Electron density around HEM f 101:

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

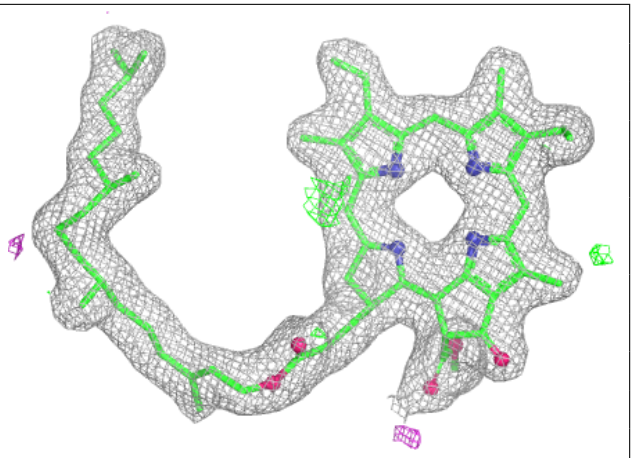


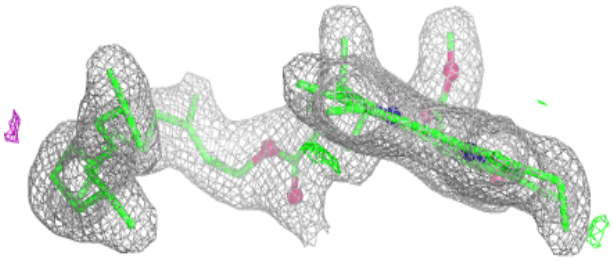


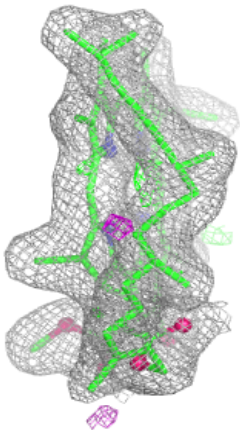


Electron density around PHO a 411:

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

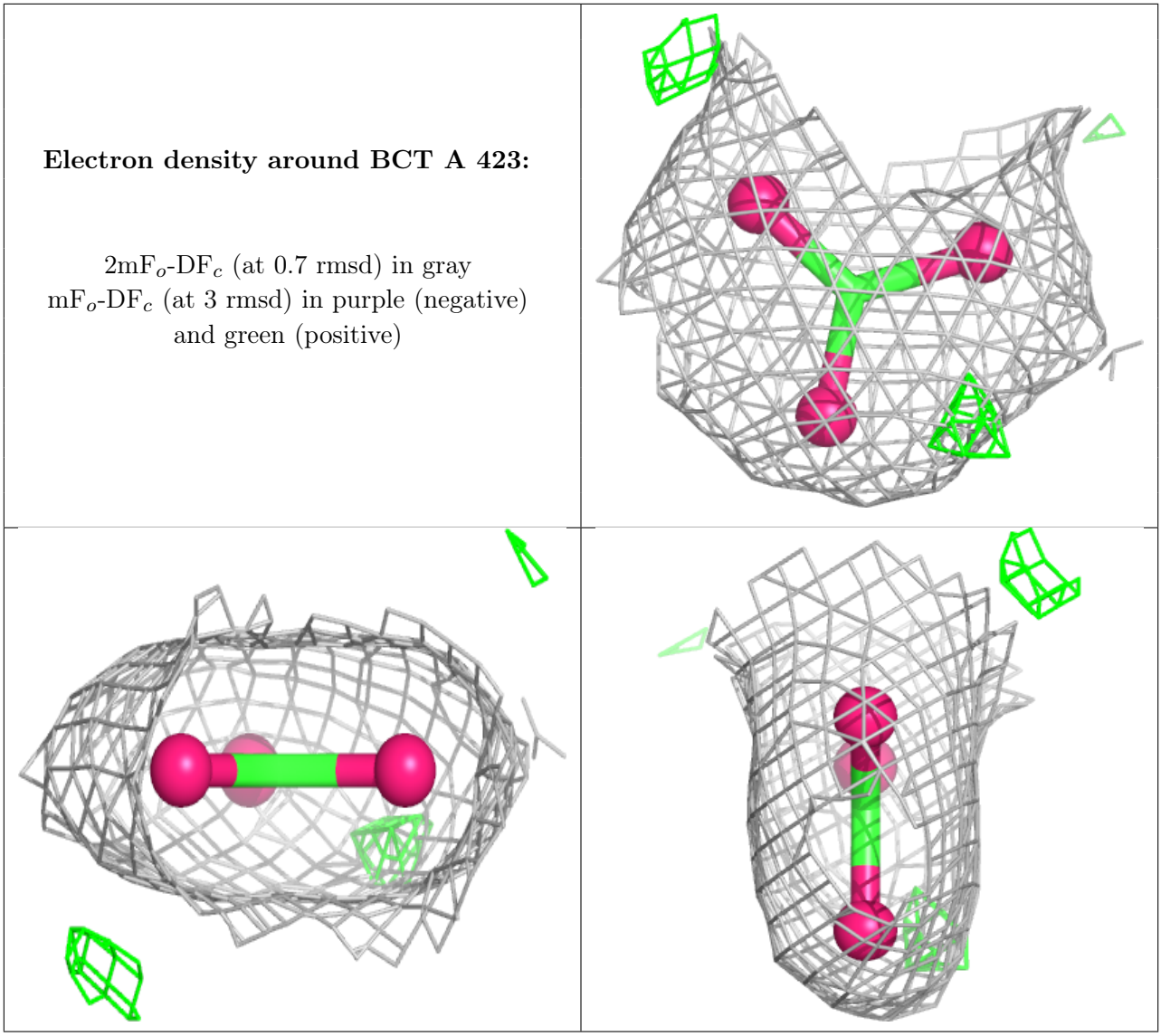






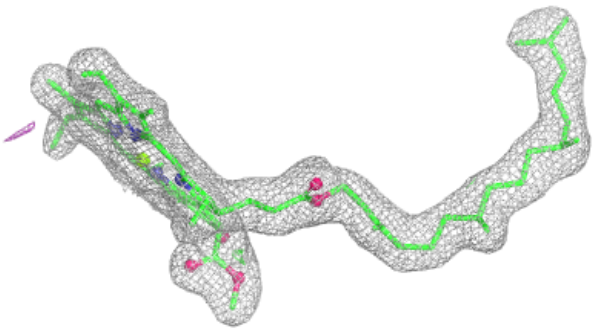
Electron density around BCT A 423:

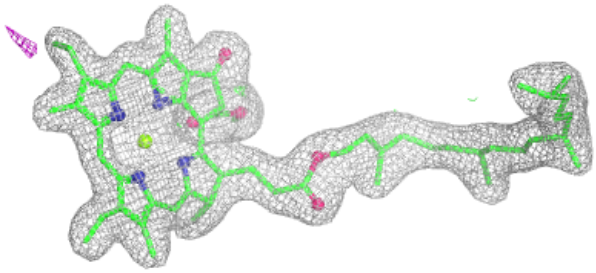
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

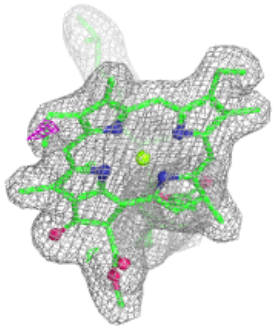


Electron density around CLA d 404:

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

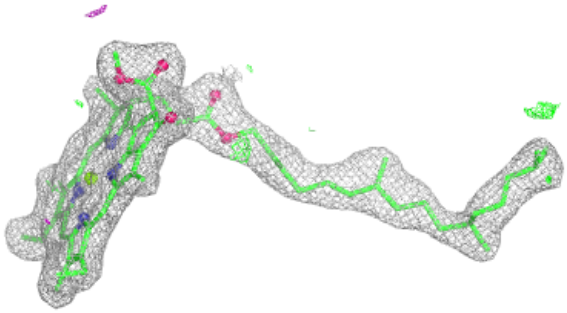


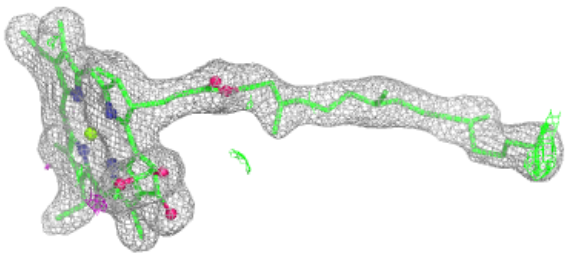


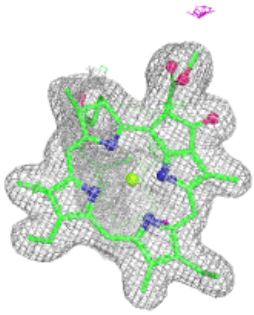


Electron density around CLA B 605:

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

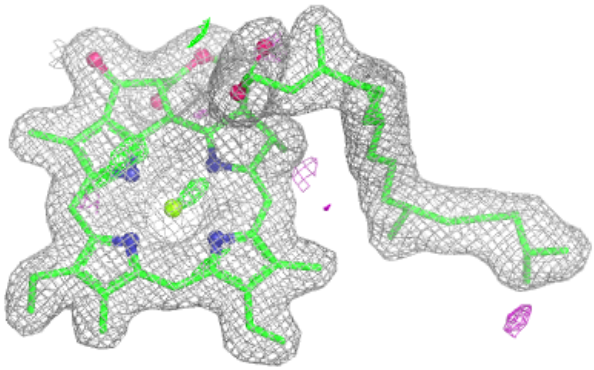


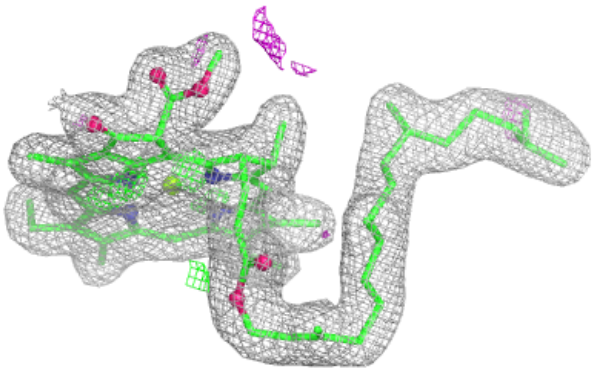


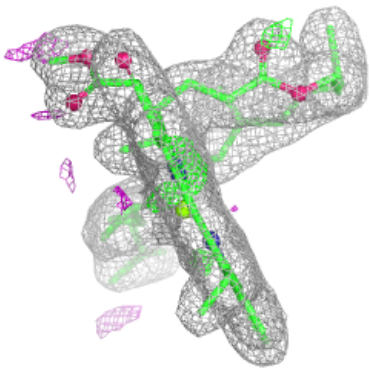


Electron density around CLA A 406:

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

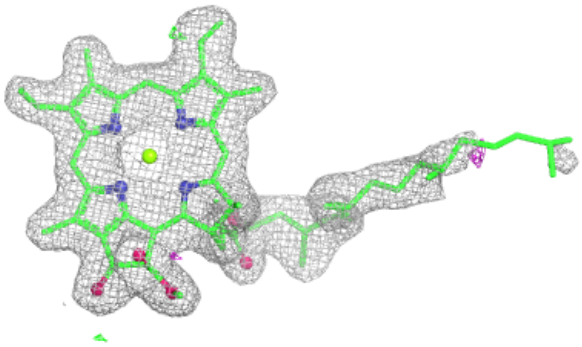


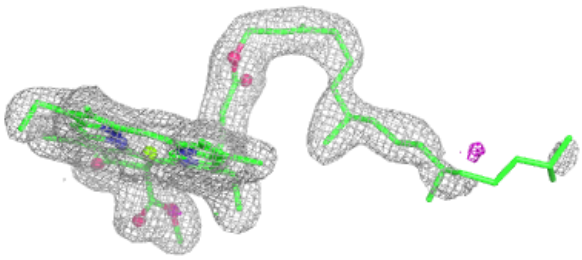


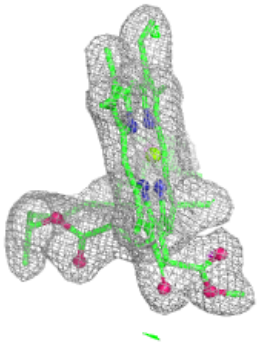


Electron density around CLA A 407:

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

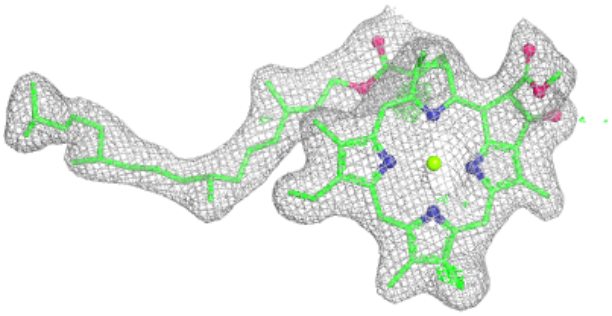


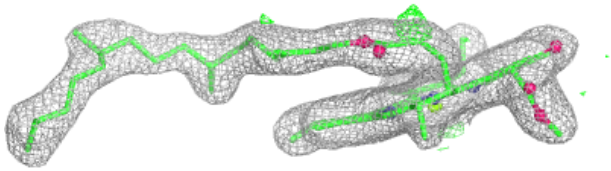


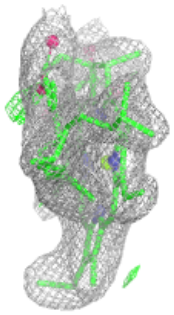


Electron density around CLA b 606:

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

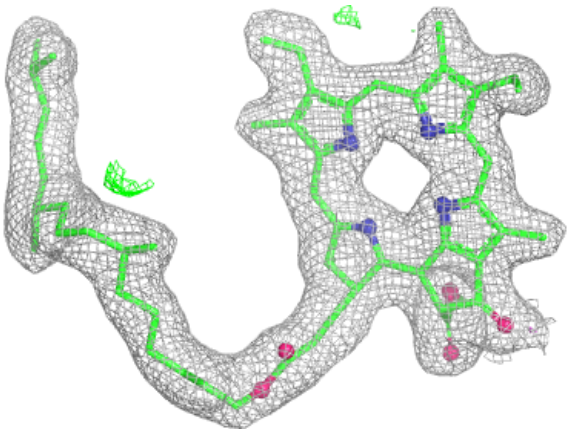


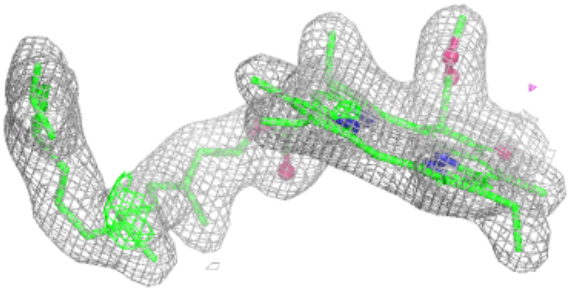


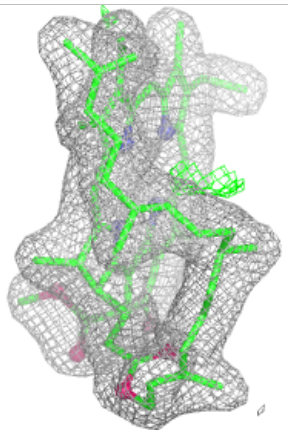


Electron density around PHO d 401:

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

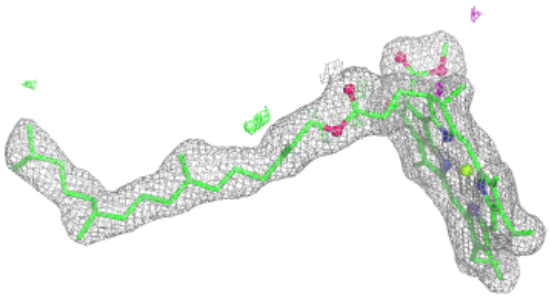


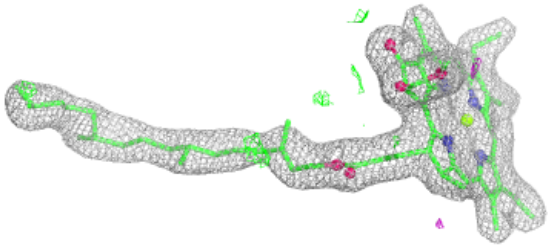


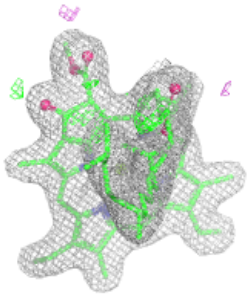


Electron density around CLA b 607:

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

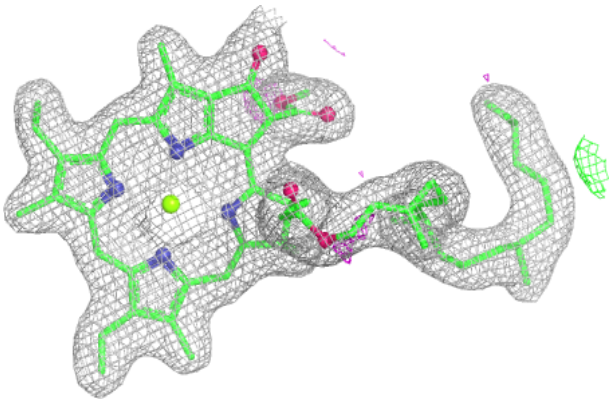


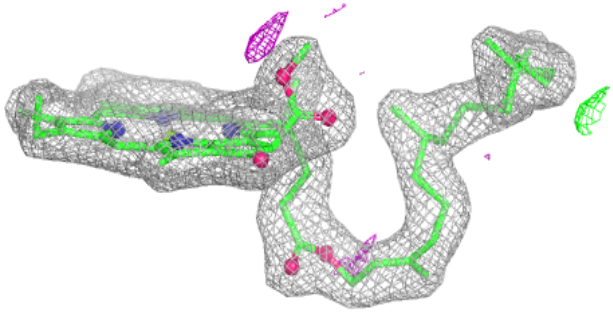


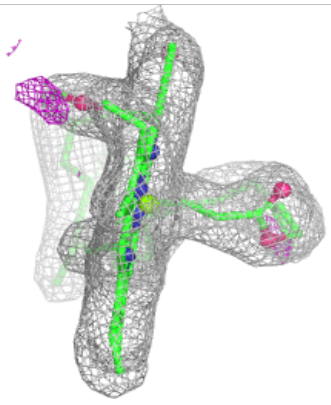


Electron density around CLA B 613:

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

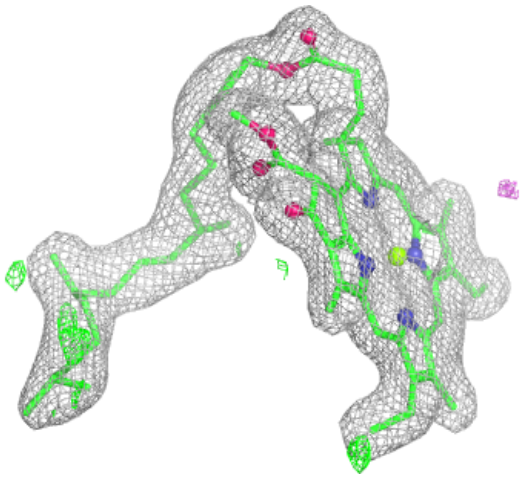


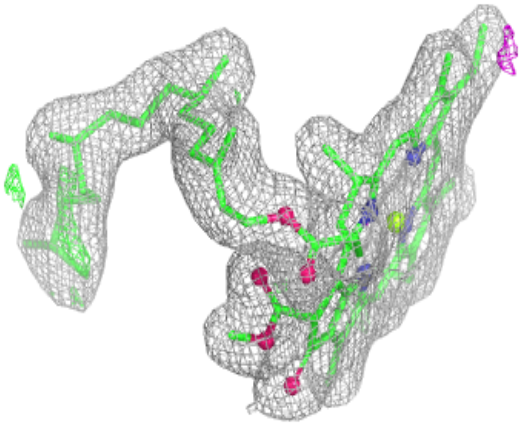


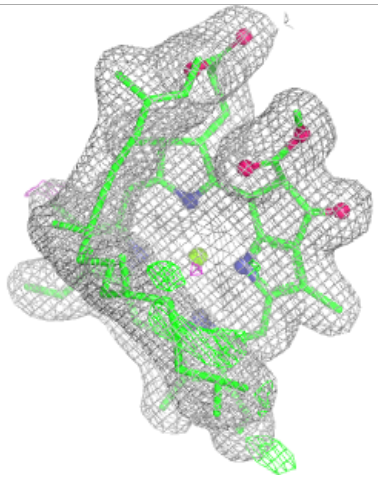


Electron density around CLA B 614:

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

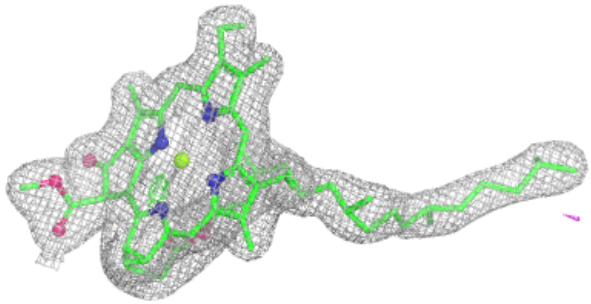


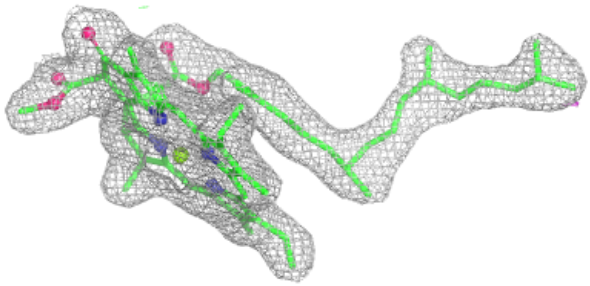


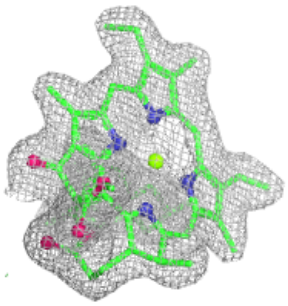


Electron density around CLA C 506:

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

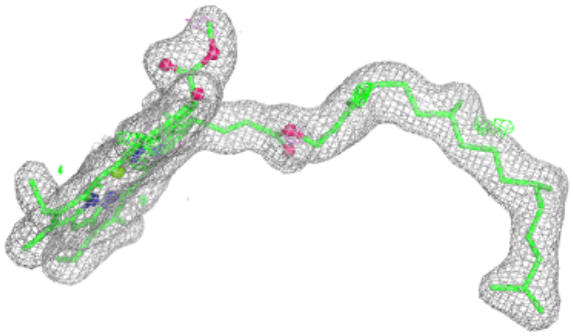


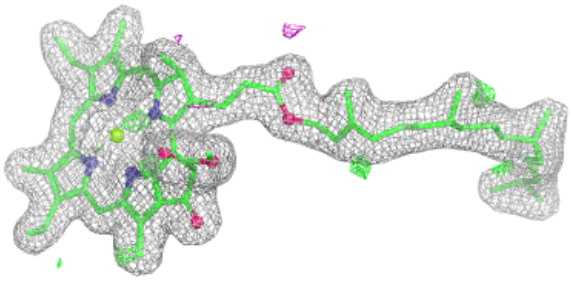


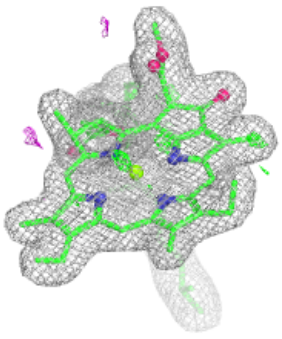


Electron density around CLA D 403:

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

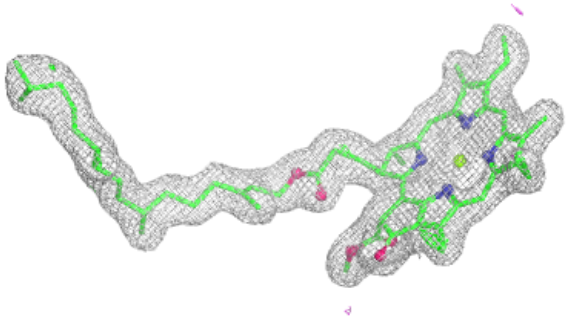


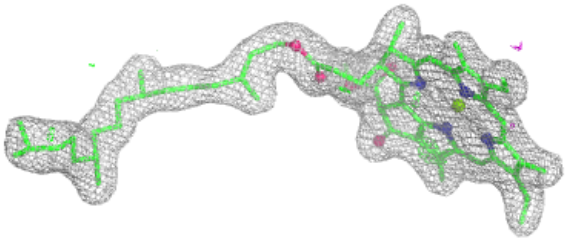


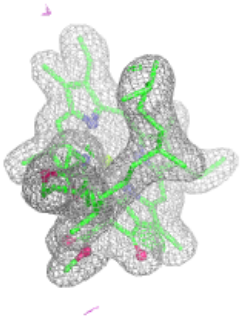


Electron density around CLA A 405:

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

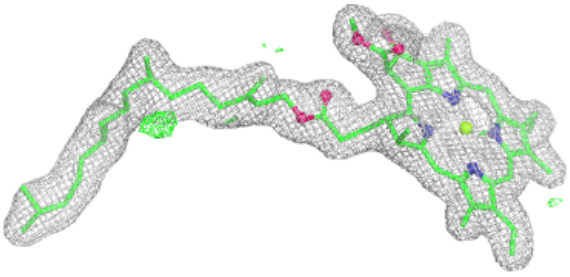


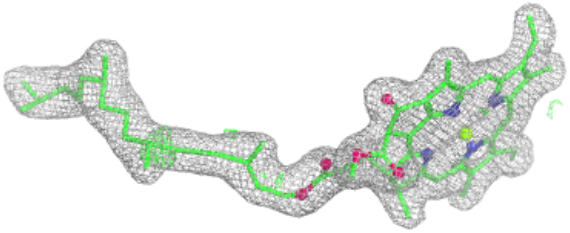


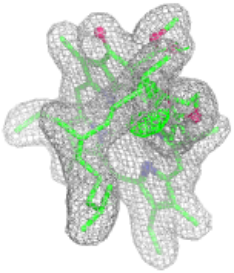


Electron density around CLA a 408:

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

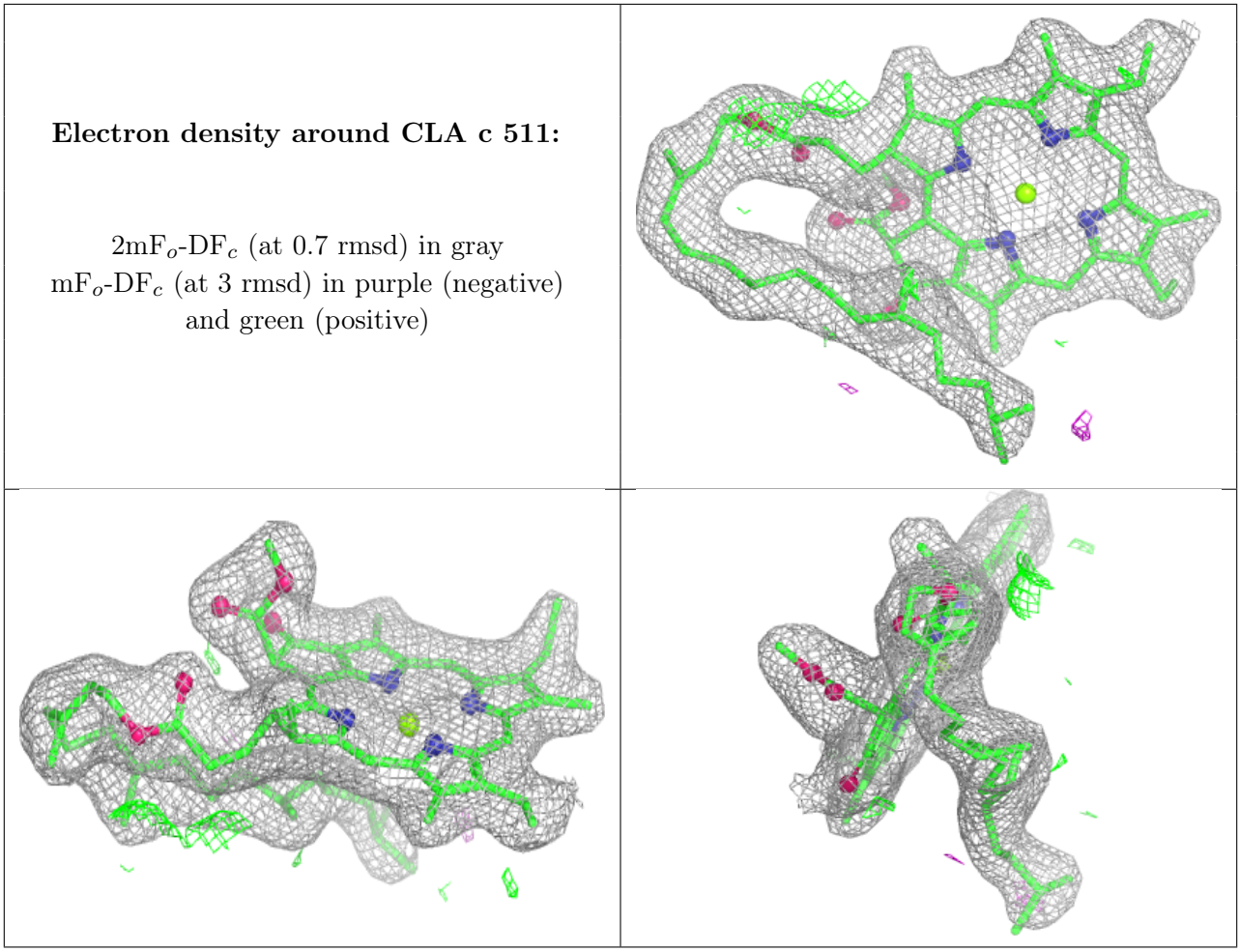






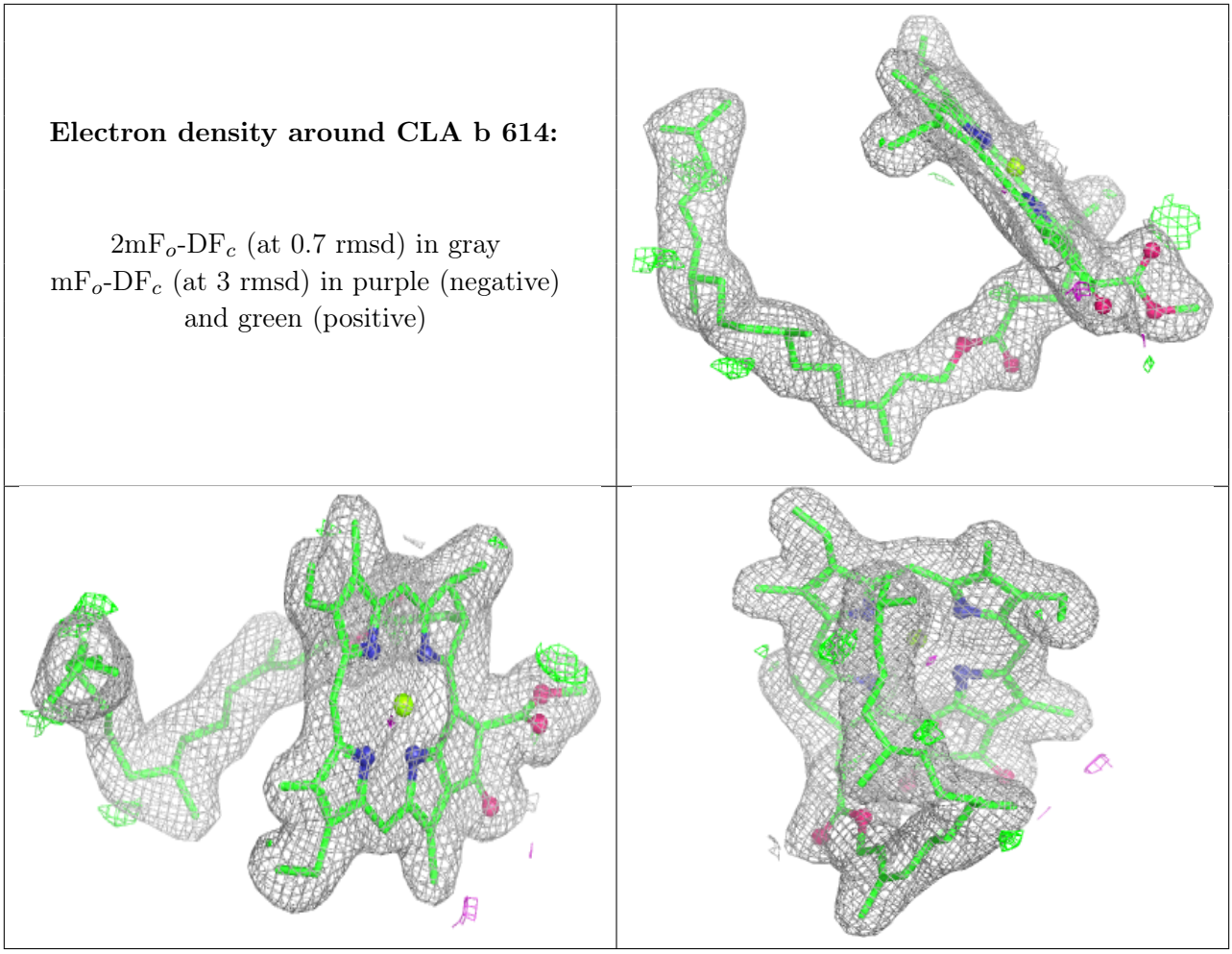
Electron density around CLA c 511:

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



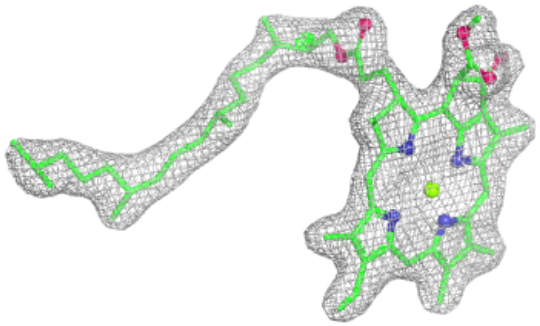
Electron density around CLA b 614:

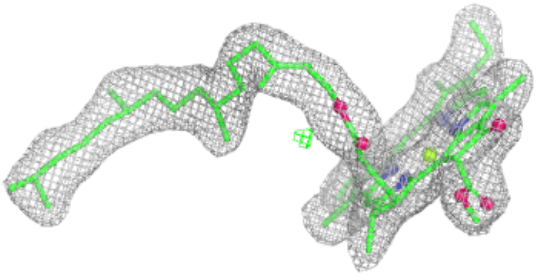
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA c 513:

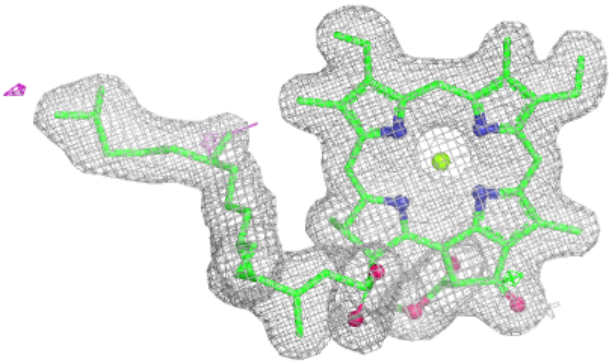
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

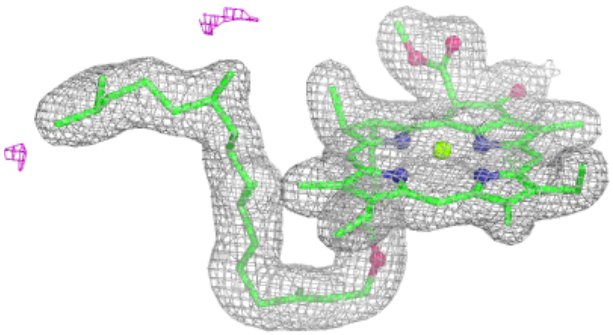


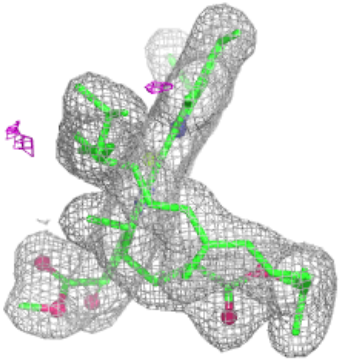


Electron density around CLA a 409:

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

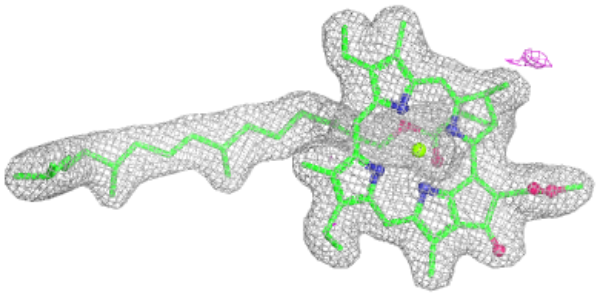


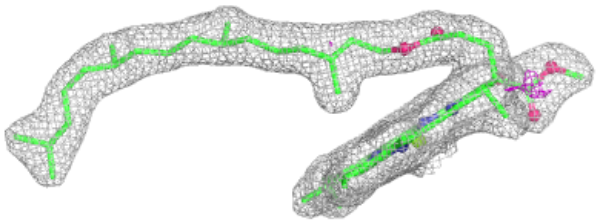




Electron density around CLA B 609:

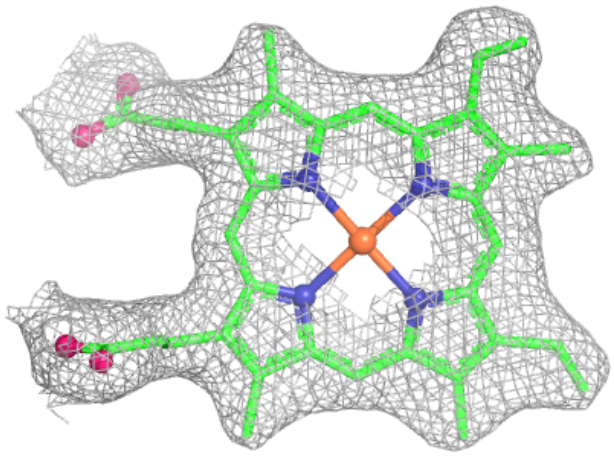
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

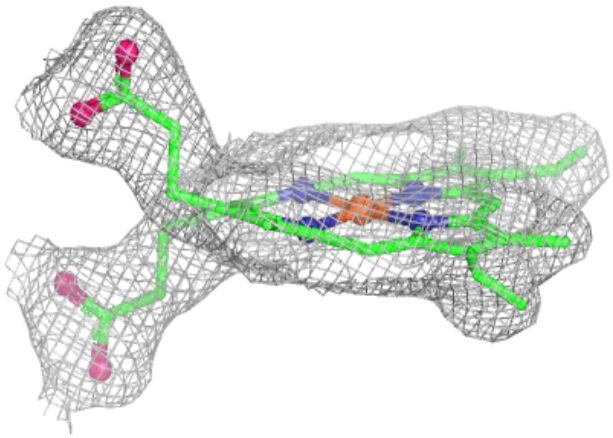


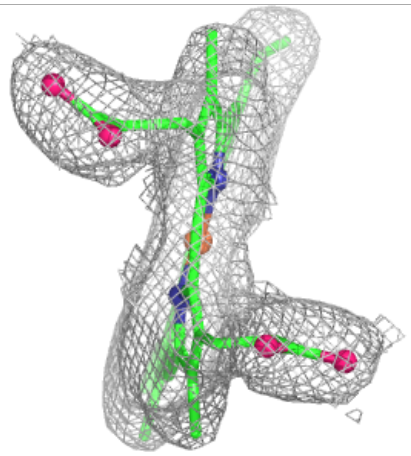


Electron density around HEM F 101:

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

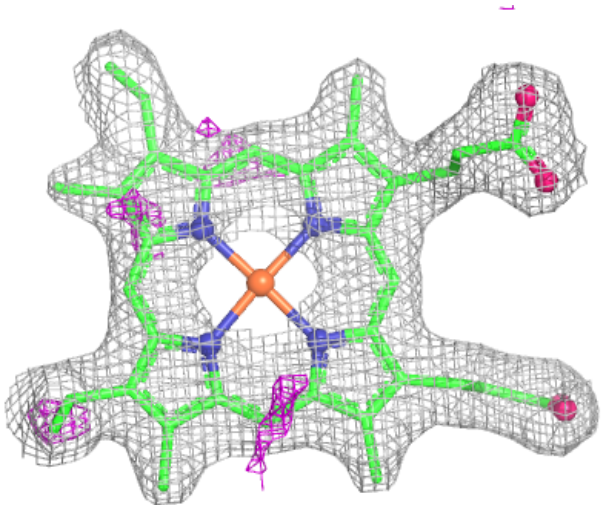


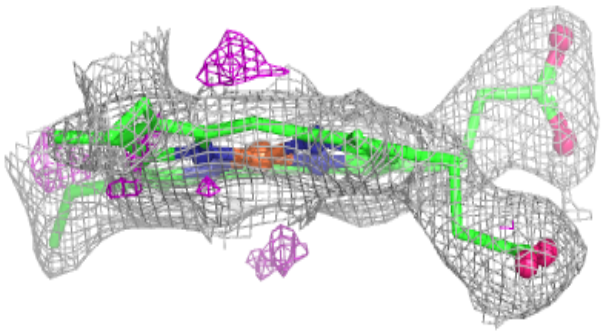


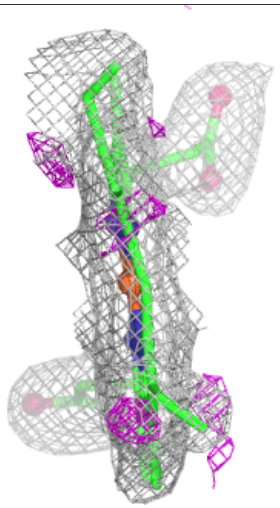


Electron density around HEC v 1603:

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

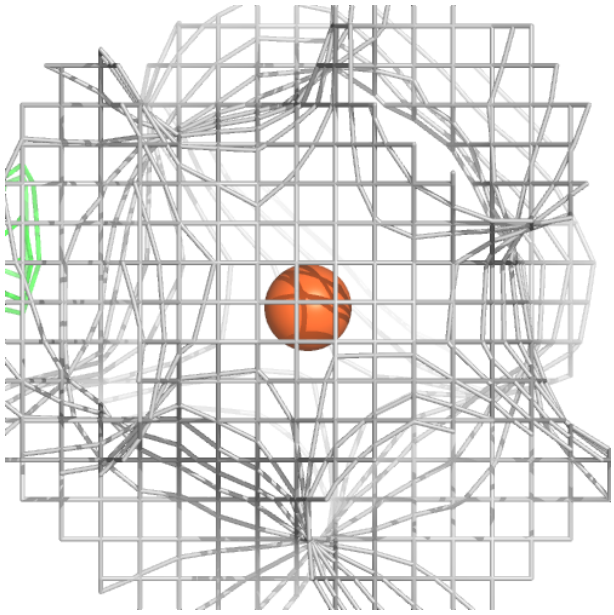


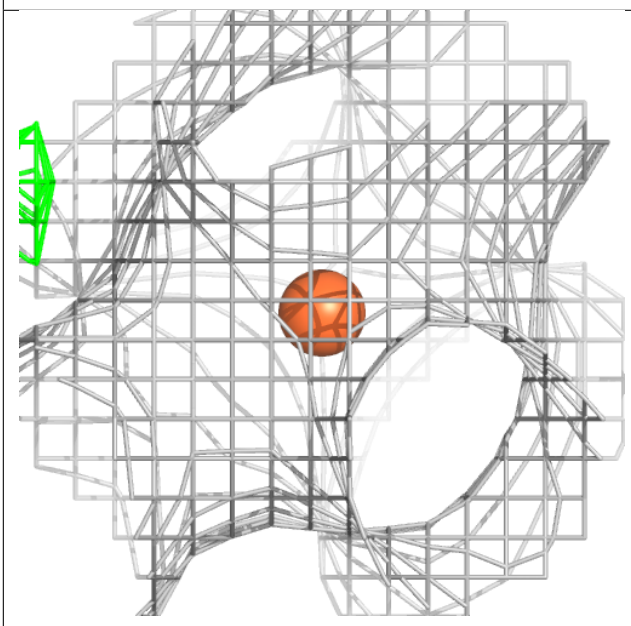


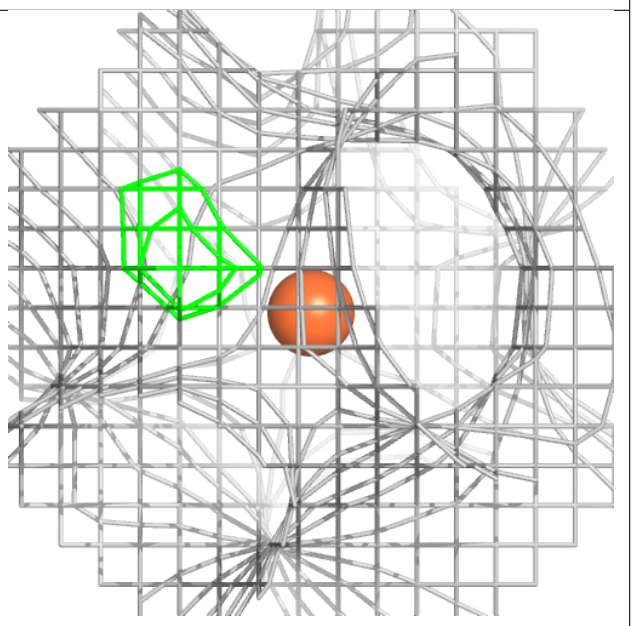


Electron density around FE2 A 402:

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

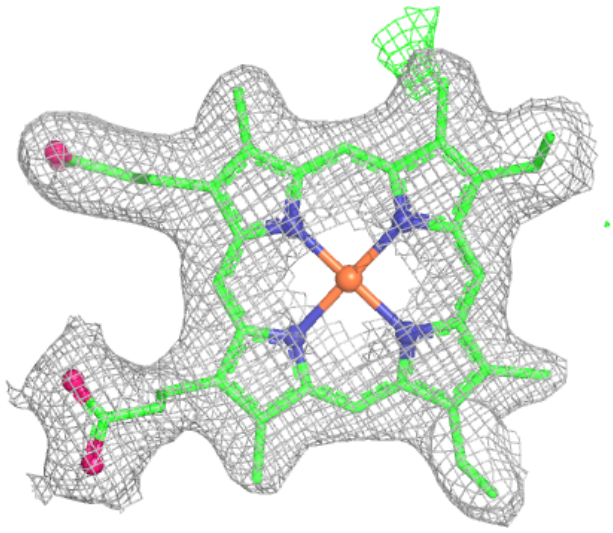


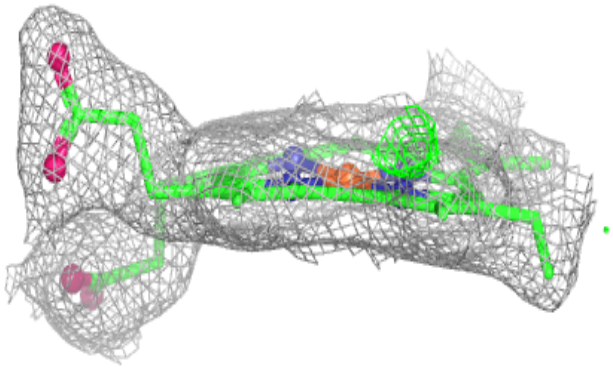


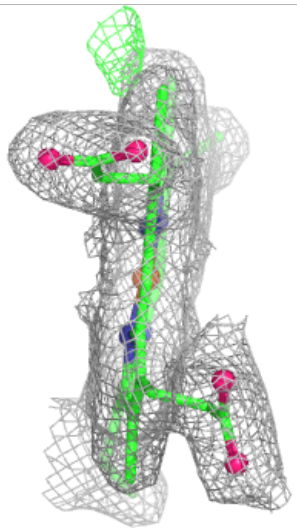


Electron density around HEC V 202:

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

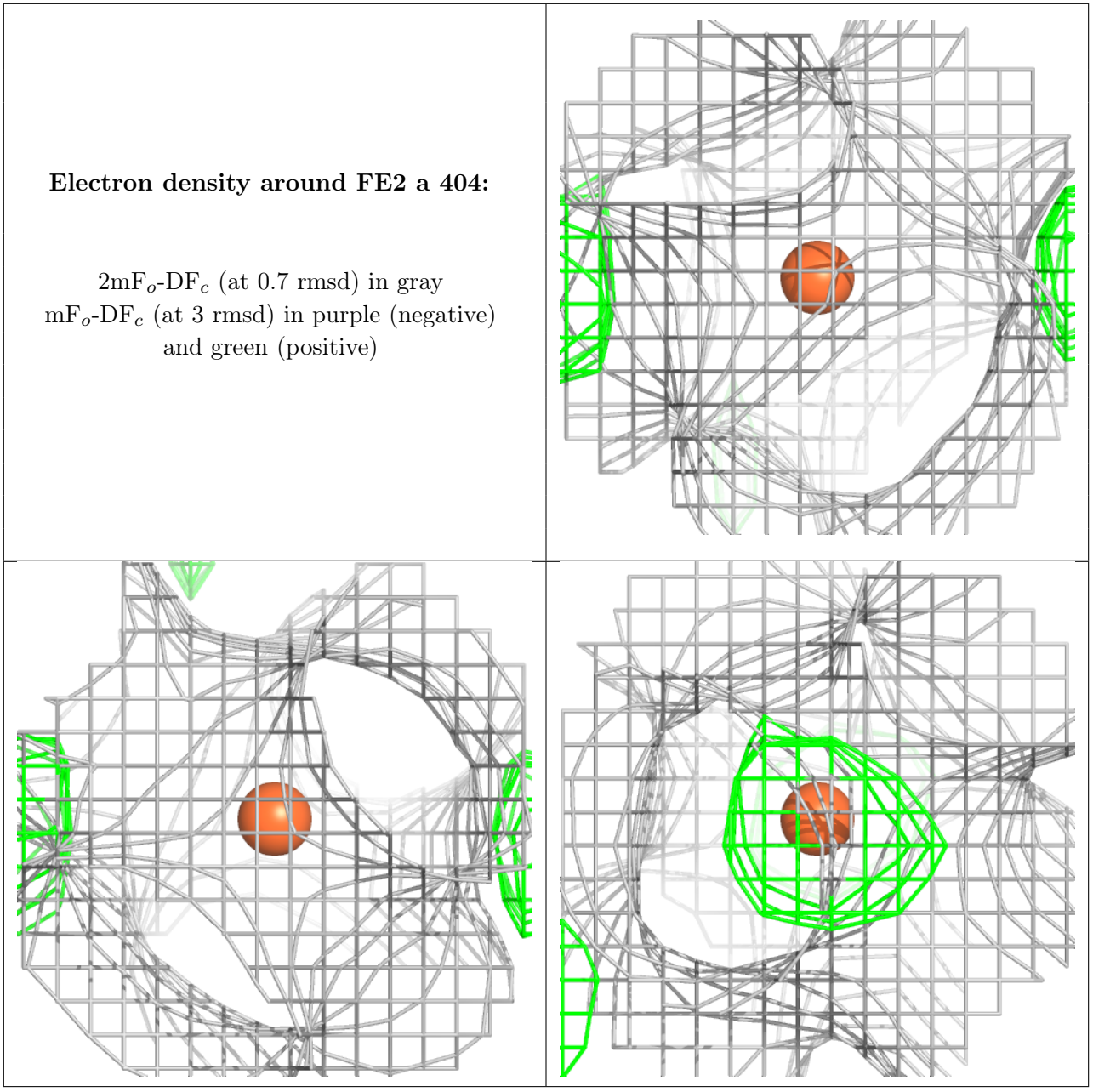






Electron density around FE2 a 404:

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



6.5 Other polymers

There are no such residues in this entry.