Full wwPDB X-ray Structure Validation Report (i)

Mar 14, 2026 – 04:52 PM UTC

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

This is a 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:

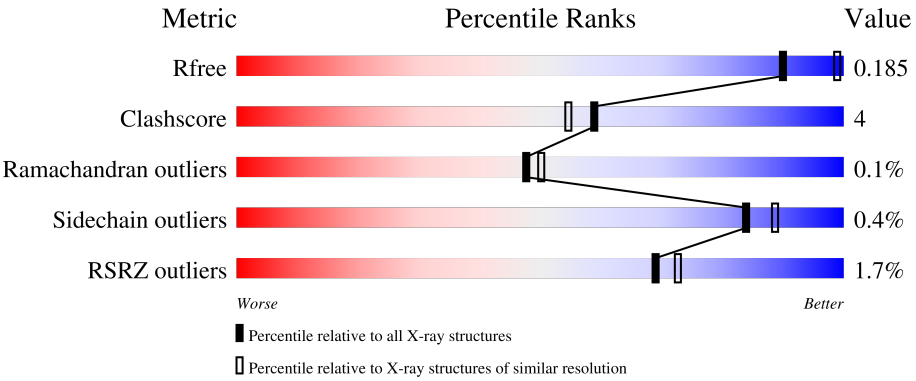
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 Å.

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



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

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

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

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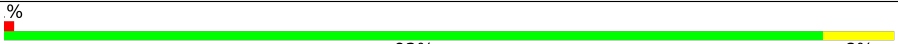
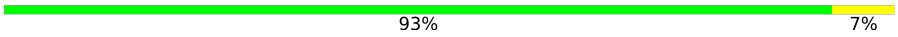
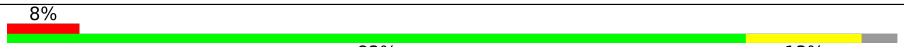
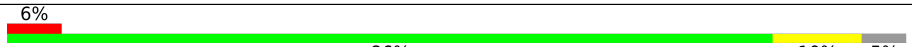
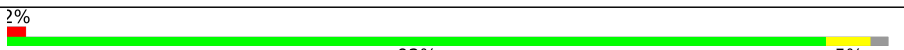
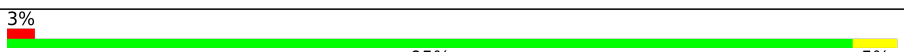
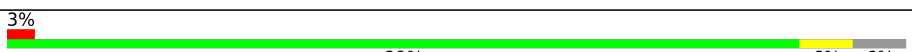
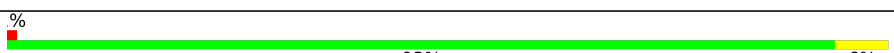
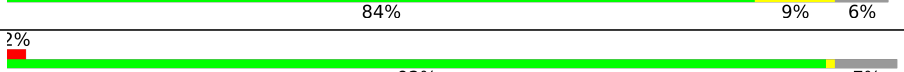
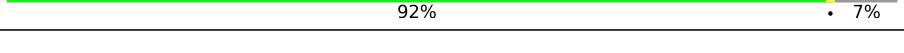
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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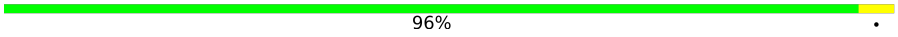
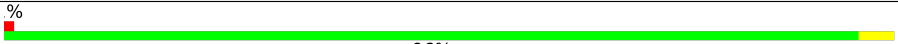
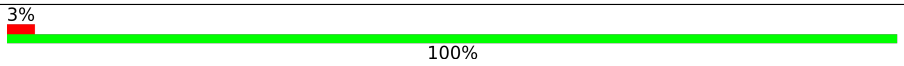
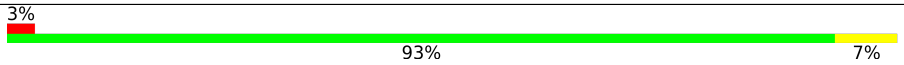
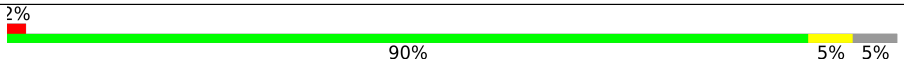
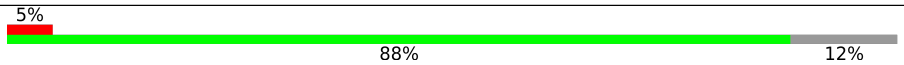
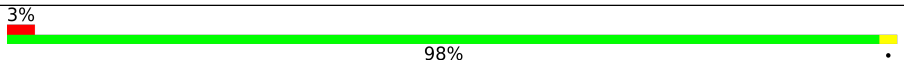
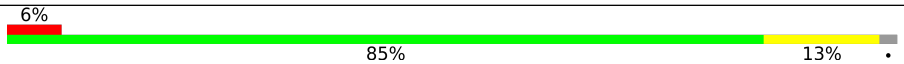
Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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
23	CLA	A	405	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	2303	X	-	-	-
23	CLA	D	2304	X	-	-	-
23	CLA	a	2609	X	-	-	-
23	CLA	a	2613	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	408	X	-	-	-
23	CLA	d	409	X	-	-	-
31	JOX	a	2617	-	X	-	-

2 Entry composition (i)

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

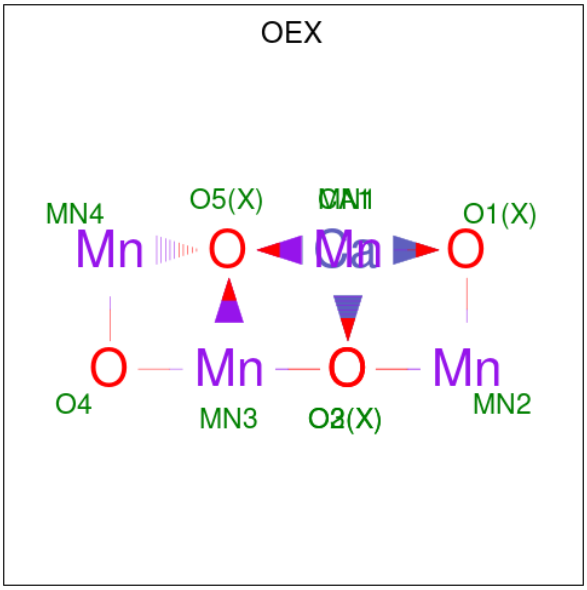
- Molecule 18 is a protein called Photosystem II reaction center protein X.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			456	312	70	72	2			

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



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

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

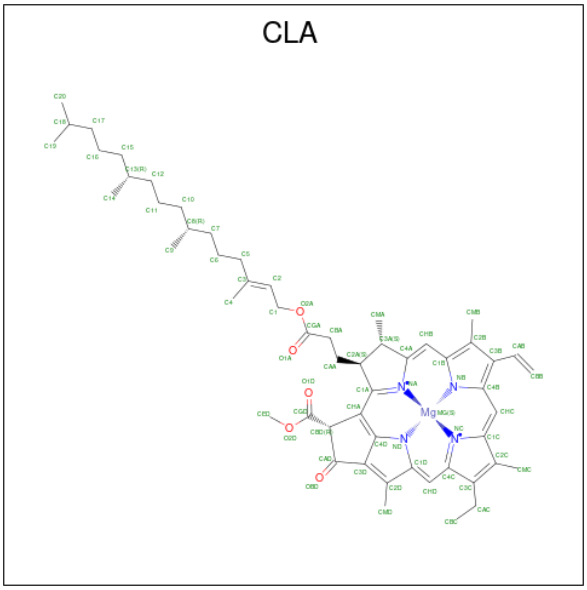
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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

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

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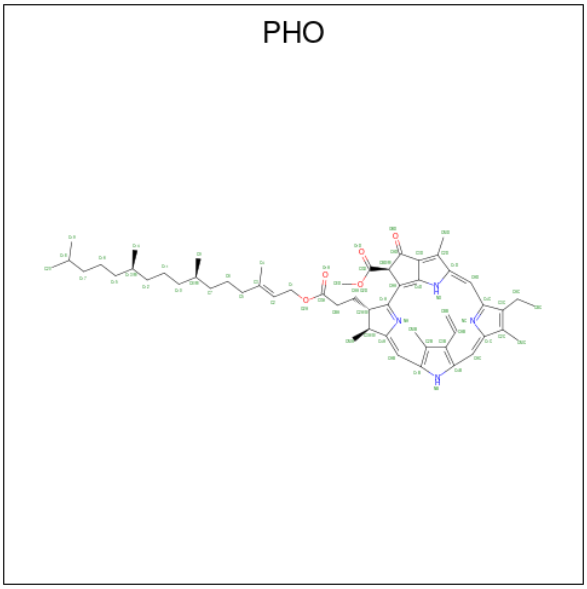
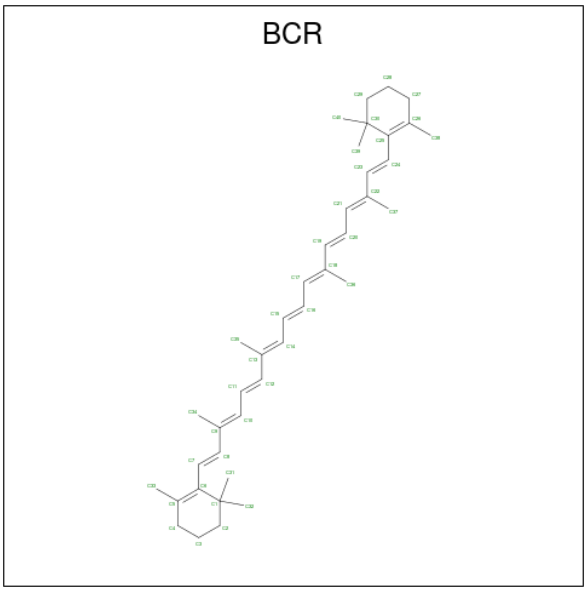
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



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

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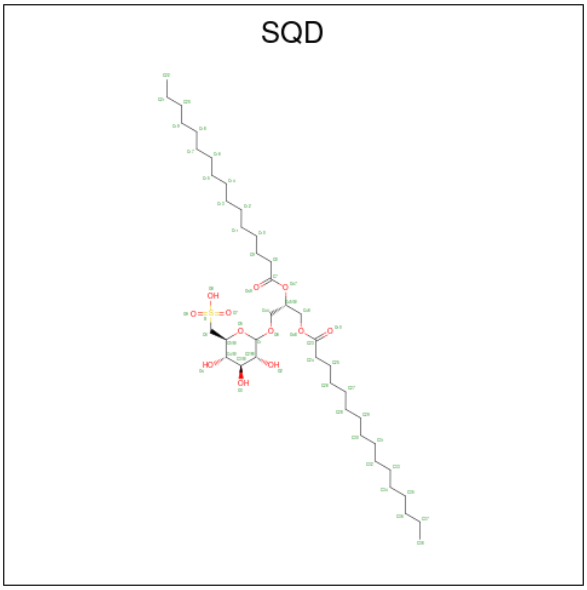
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	z	1	Total C 40 40	0	0

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



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

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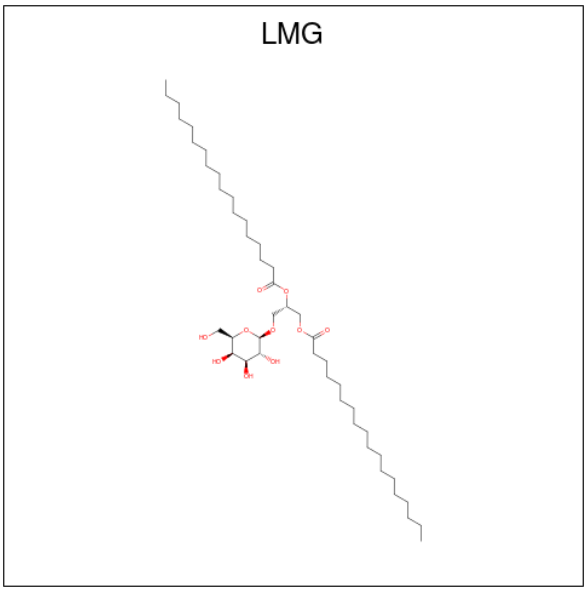
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	a	1	Total C O S 48 35 12 1	0	0
26	b	1	Total C O S 48 35 12 1	0	0
26	d	1	Total C O S 33 23 9 1	0	0
26	l	1	Total C O S 54 41 12 1	0	0

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



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

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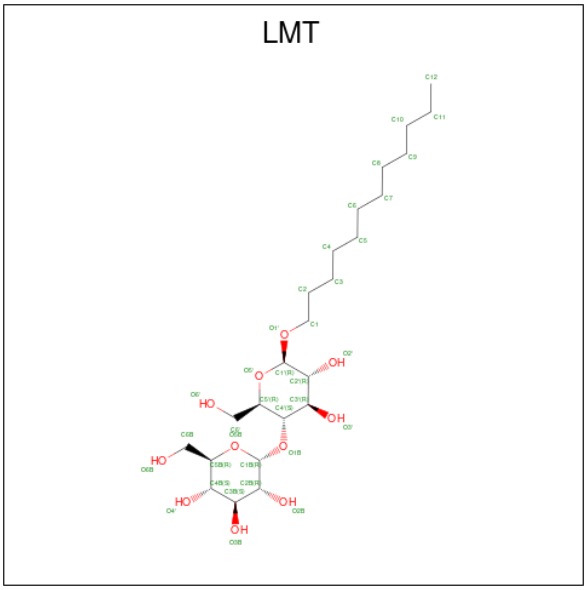
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 51 41 10	0	0
27	d	1	Total C O 51 41 10	0	0
27	m	1	Total C O 51 41 10	0	0

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



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

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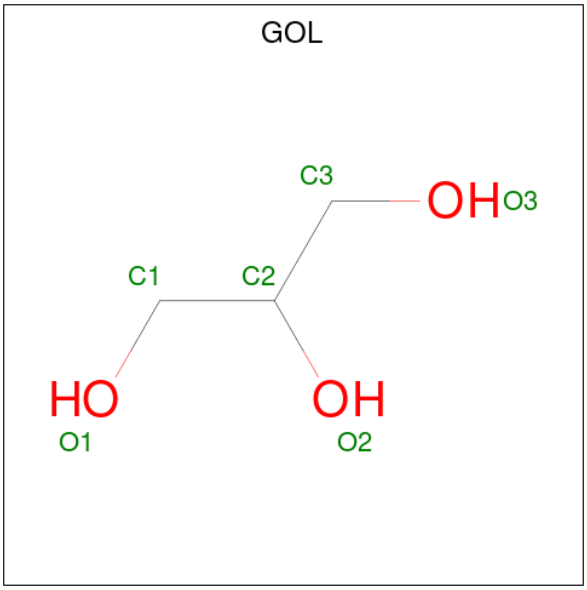
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	T	1	Total C O 24 18 6	0	0
28	Z	1	Total C O 35 24 11	0	0
28	d	1	Total C O 35 24 11	0	0
28	d	1	Total C O 25 19 6	0	0
28	f	1	Total C O 24 18 6	0	0
28	i	1	Total C O 24 18 6	0	0
28	j	1	Total C O 34 23 11	0	0
28	m	1	Total C O 35 24 11	0	0
28	m	1	Total C O 35 24 11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

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



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

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

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

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

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

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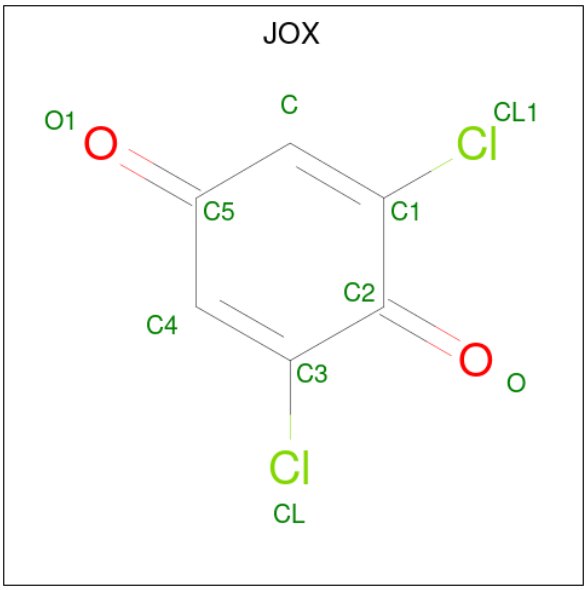
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	4	Total C O 59 54 5	0	0
30	d	2	Total C O 55 48 7	0	0
30	e	1	Total C 15 15	0	0
30	i	1	Total C O 19 15 4	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C 16 16	0	0
30	l	1	Total C O 16 14 2	0	0
30	m	1	Total C O 15 13 2	0	0
30	t	1	Total C 8 8	0	0
30	x	1	Total C O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

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



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

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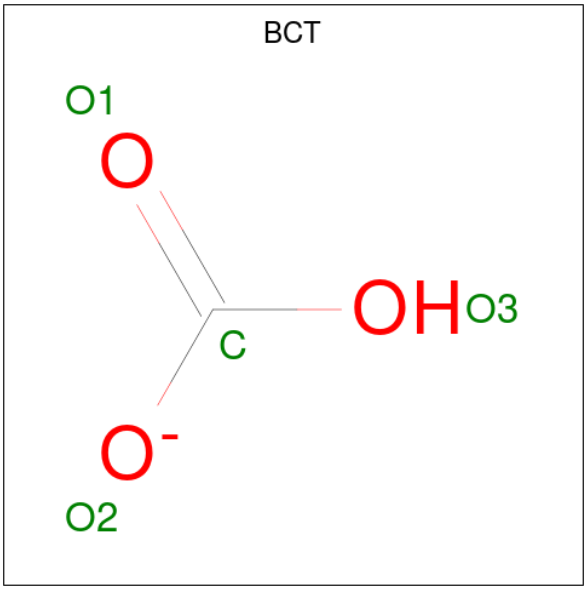
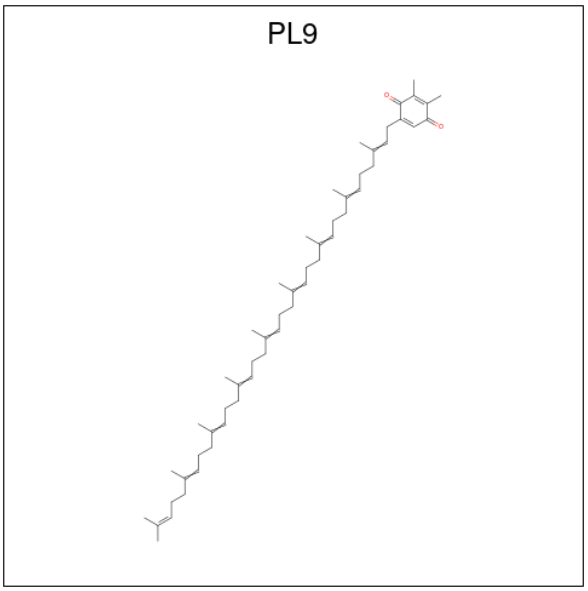
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C Cl O 10 6 2 2	0	0
31	a	1	Total C Cl O 10 6 2 2	0	0
31	a	1	Total C Cl O 10 6 2 2	0	0

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



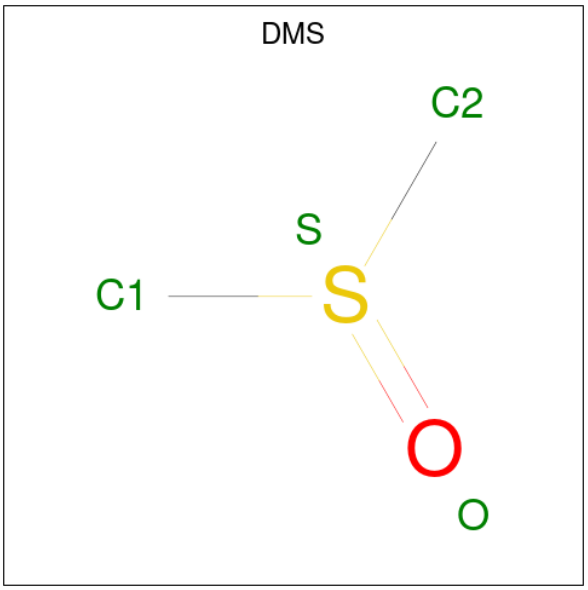
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 4 1 3	0	0
32	a	1	Total C O 4 1 3	0	0

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



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

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



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

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

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

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

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

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

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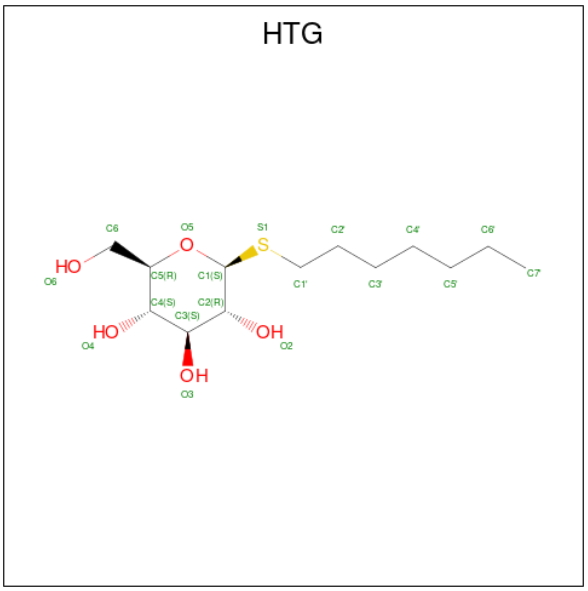
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		

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

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	1
			38	26	10	2		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	H	1	Total	C	O	S	0	0
			17	12	4	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		

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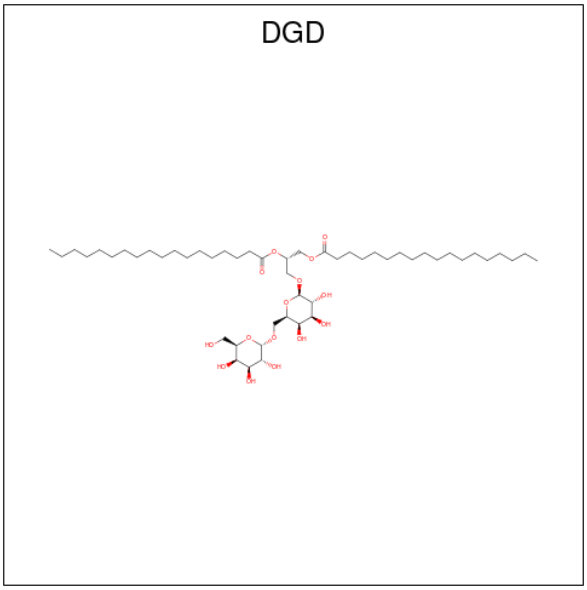
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			58	43	15		

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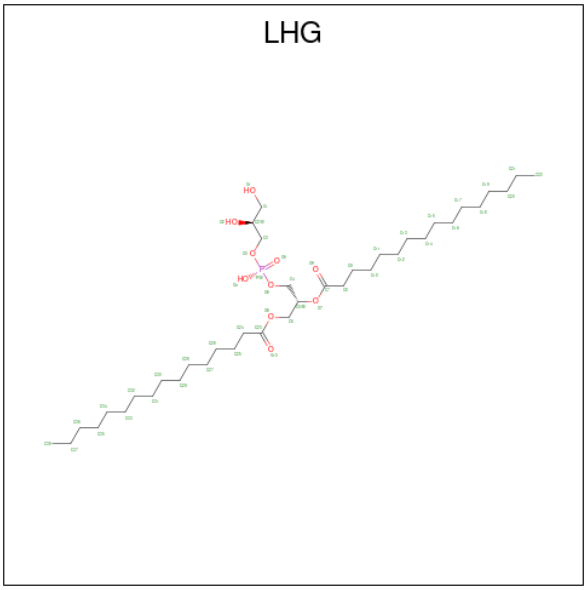
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 53 42 11	0	0
37	H	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	h	1	Total C O 62 47 15	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 39 28 10 1	0	0
38	E	1	Total C O P 40 29 10 1	0	0
38	L	1	Total C O P 49 38 10 1	0	0

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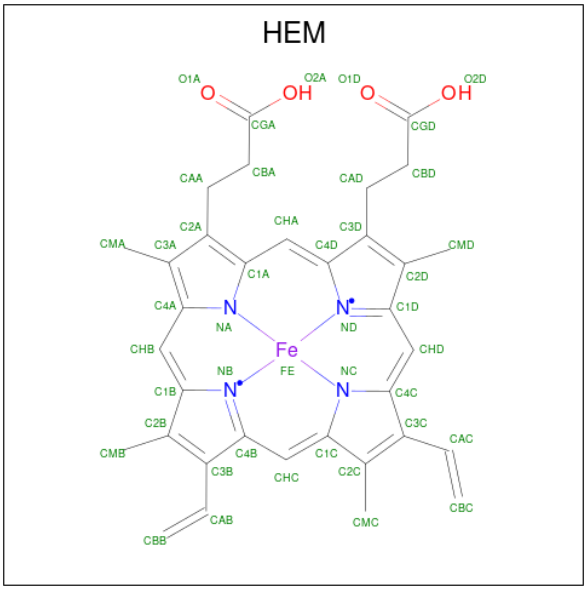
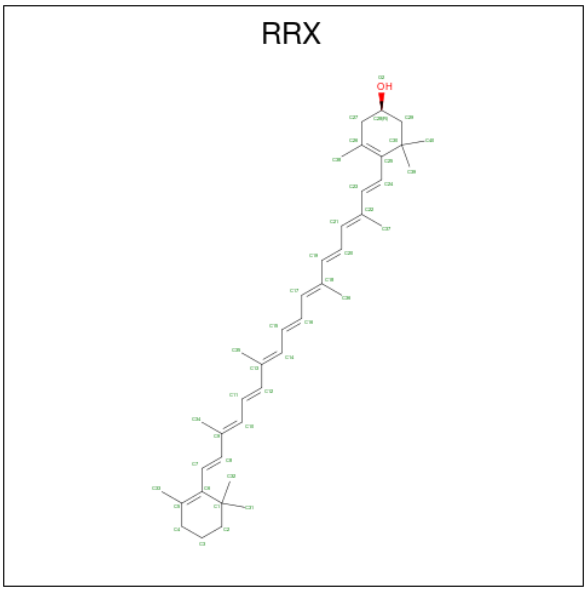
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	d	1	Total C O P 43 32 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	e	1	Total C O P 40 29 10 1	0	0
38	l	1	Total C O P 49 38 10 1	0	0

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



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

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

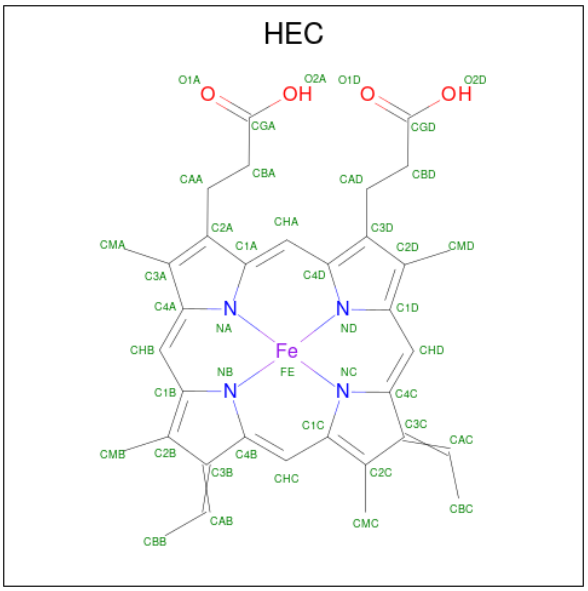


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	H	1	Total C O 41 40 1	0	0
40	h	1	Total C O 41 40 1	0	0

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

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

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



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	133	Total	O	0	0
			133	133		
43	B	302	Total	O	0	0
			302	302		
43	C	192	Total	O	0	0
			192	192		
43	D	146	Total	O	0	1
			147	147		
43	E	25	Total	O	0	0
			25	25		
43	F	9	Total	O	0	0
			9	9		
43	H	41	Total	O	0	0
			41	41		
43	I	8	Total	O	0	0
			8	8		
43	J	10	Total	O	0	0
			10	10		
43	K	10	Total	O	0	0
			10	10		

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

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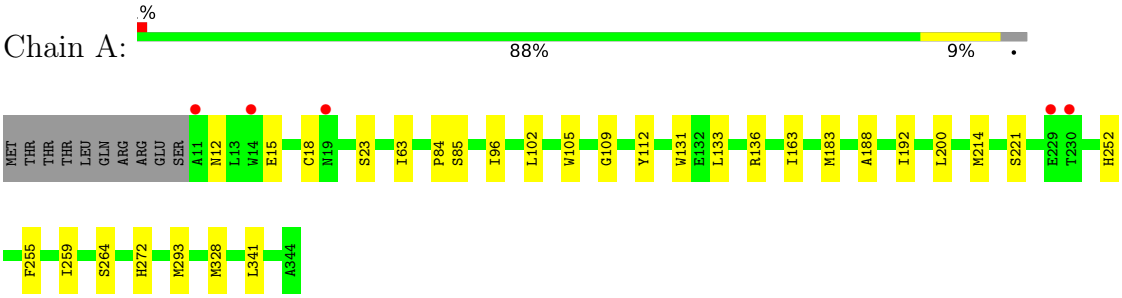
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	o	143	Total O 144 144	0	1
43	t	10	Total O 10 10	0	0
43	u	78	Total O 78 78	0	0
43	v	93	Total O 93 93	0	0
43	y	6	Total O 6 6	0	0
43	x	4	Total O 4 4	0	0
43	z	6	Total O 6 6	0	0

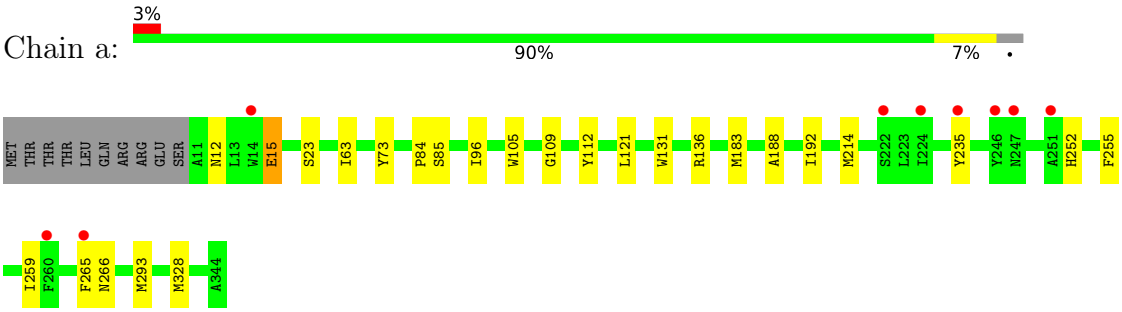
3 Residue-property plots (i)

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

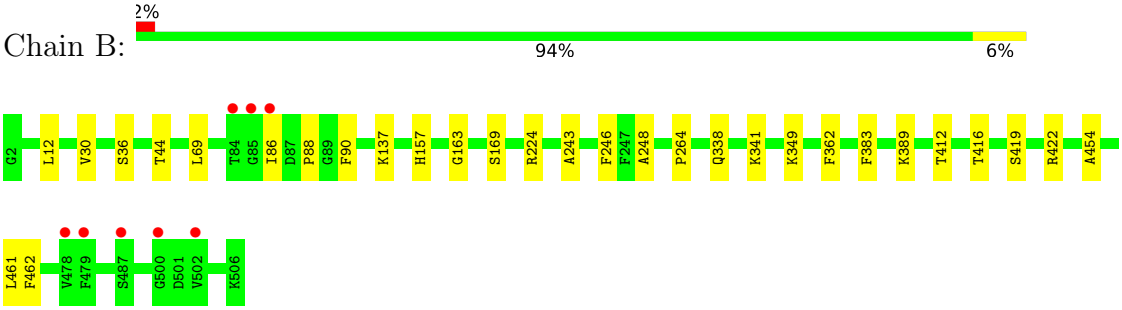
• Molecule 1: Photosystem II protein D1



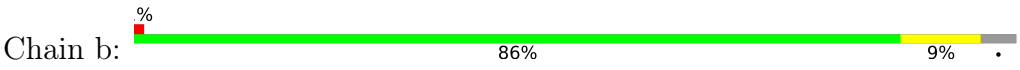
• Molecule 1: Photosystem II protein D1

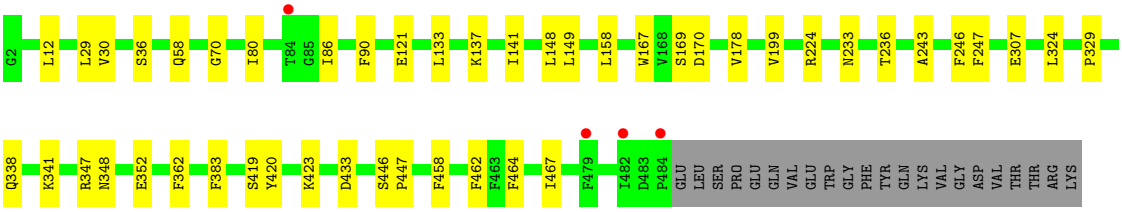


• Molecule 2: Photosystem II CP47 reaction center protein

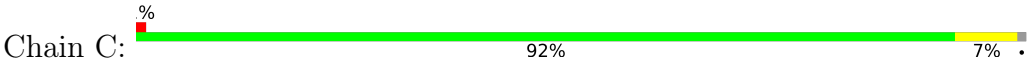


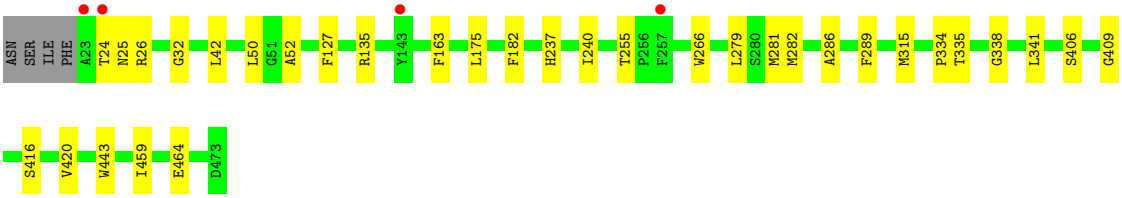
• Molecule 2: Photosystem II CP47 reaction center protein



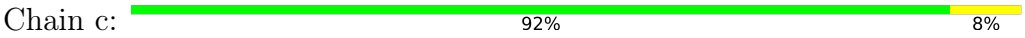


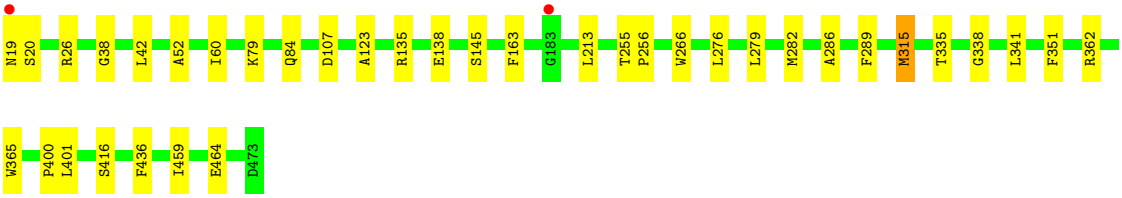
• Molecule 3: Photosystem II CP43 reaction center protein



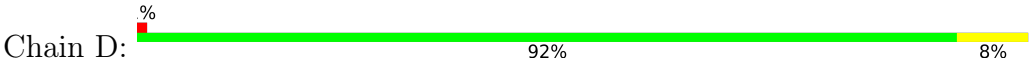


• Molecule 3: Photosystem II CP43 reaction center protein

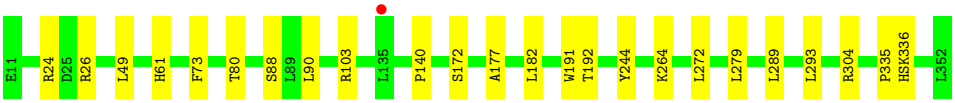




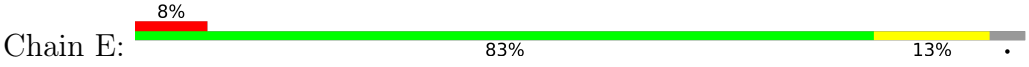
• Molecule 4: Photosystem II D2 protein

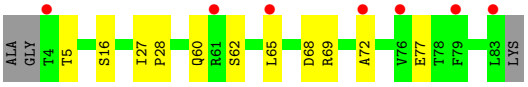


• Molecule 4: Photosystem II D2 protein

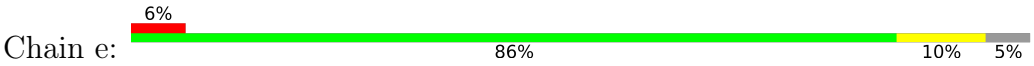


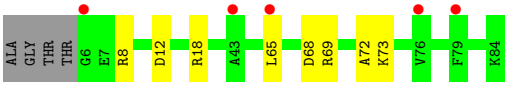
• Molecule 5: Cytochrome b559 subunit alpha



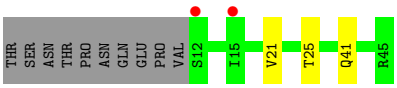


• Molecule 5: Cytochrome b559 subunit alpha

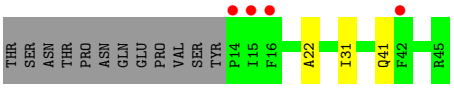




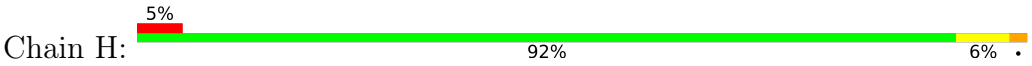
• Molecule 6: Cytochrome b559 subunit beta

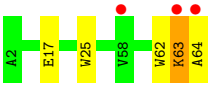


• Molecule 6: Cytochrome b559 subunit beta

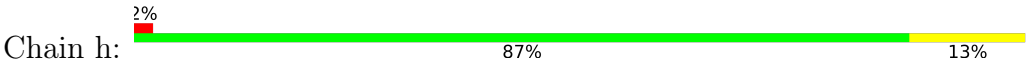


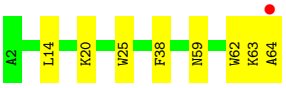
• Molecule 7: Photosystem II reaction center protein H



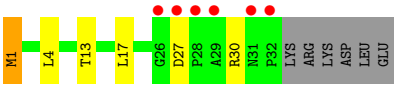


• Molecule 7: Photosystem II reaction center protein H



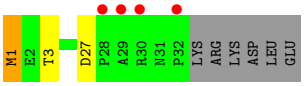


• Molecule 8: Photosystem II reaction center protein I



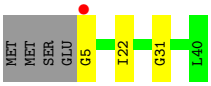
• Molecule 8: Photosystem II reaction center protein I

Chain i:



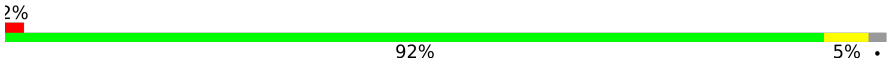
• Molecule 9: Photosystem II reaction center protein J

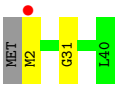
Chain J:



• Molecule 9: Photosystem II reaction center protein J

Chain j:





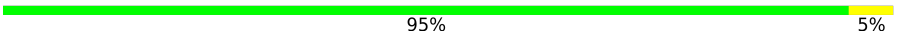
• Molecule 10: Photosystem II reaction center protein K

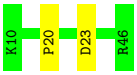
Chain K:

There are no outlier residues recorded for this chain.

• Molecule 10: Photosystem II reaction center protein K

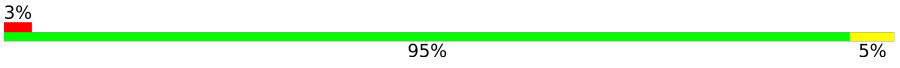
Chain k:





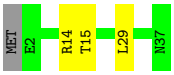
• Molecule 11: Photosystem II reaction center protein L

Chain L:



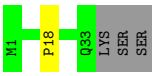
• Molecule 11: Photosystem II reaction center protein L

Chain l:



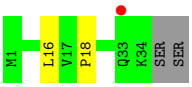
• Molecule 12: Photosystem II reaction center protein M

Chain M:



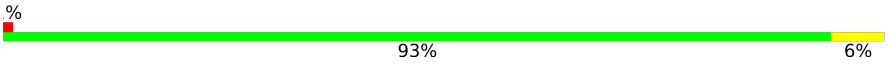
• Molecule 12: Photosystem II reaction center protein M

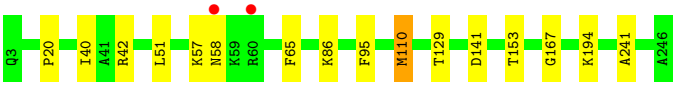
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

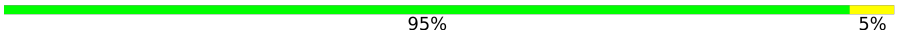
Chain O:

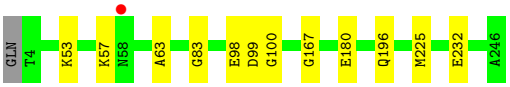




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

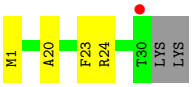
Chain o:





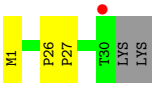
• Molecule 14: Photosystem II reaction center protein T

Chain T:



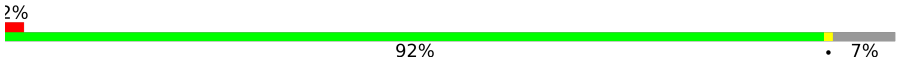
• Molecule 14: Photosystem II reaction center protein T

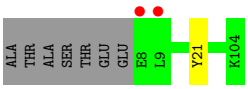
Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



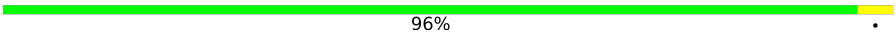


• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

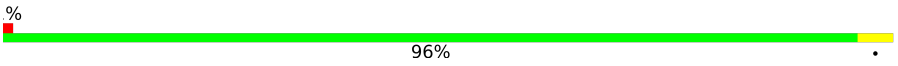
• Molecule 16: Cytochrome c-550

Chain V:



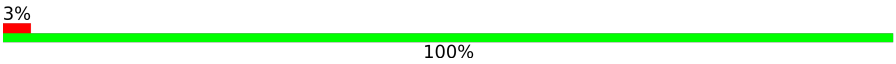
• Molecule 16: Cytochrome c-550

Chain v:



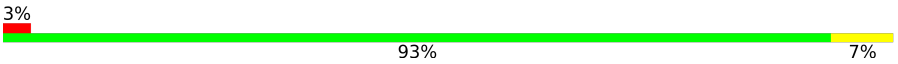
• Molecule 17: Photosystem II reaction center protein Ycf12

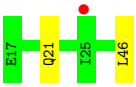
Chain Y:



• Molecule 17: Photosystem II reaction center protein Ycf12

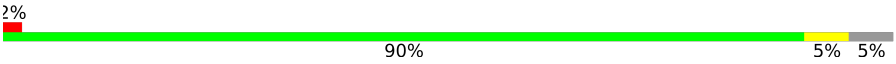
Chain y:

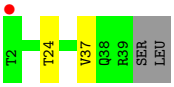




• Molecule 18: Photosystem II reaction center protein X

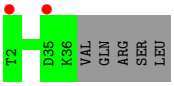
Chain X:





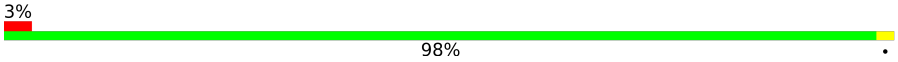
• Molecule 18: Photosystem II reaction center protein X

Chain x:



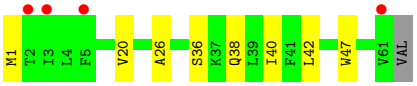
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

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

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	U	12	0	15	0	0
29	V	6	0	8	0	0
29	a	12	0	16	1	0
29	b	12	0	16	4	0
29	c	18	0	24	1	0
29	d	6	0	8	0	0
29	o	6	0	8	0	0
29	u	6	0	8	0	0
29	v	18	0	24	0	0
30	A	37	0	0	0	0
30	B	65	0	0	0	0
30	C	50	0	0	0	0
30	D	48	0	0	0	0
30	E	15	0	0	0	0
30	I	40	0	0	0	0
30	J	5	0	0	0	0
30	T	13	0	0	0	0
30	Y	12	0	0	0	0
30	a	42	0	0	0	0
30	b	64	0	0	0	0
30	c	59	0	0	0	0
30	d	55	0	0	0	0
30	e	15	0	0	0	0
30	i	19	0	0	0	0
30	j	16	0	0	0	0
30	k	16	0	0	0	0
30	l	16	0	0	0	0
30	m	15	0	0	0	0
30	t	8	0	0	0	0
30	x	18	0	0	0	0
31	A	20	0	0	0	0
31	a	20	0	0	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	A	39	0	59	4	0
33	D	55	0	80	0	0
33	d	55	0	80	1	0
33	x	39	0	59	2	0
34	A	28	0	42	1	0
34	B	52	0	78	6	0
34	C	40	0	60	1	0
34	D	20	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	4	0	6	0	0
34	O	56	0	84	1	0
34	T	8	0	12	0	0
34	U	12	0	18	1	0
34	V	40	0	60	2	0
34	X	4	0	6	0	0
34	a	20	0	30	1	0
34	b	44	0	66	1	0
34	c	72	0	108	3	0
34	d	24	0	36	1	0
34	l	4	0	6	0	0
34	o	52	0	78	3	0
34	t	4	0	6	0	0
34	u	12	0	18	0	0
34	v	40	0	60	1	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	o	1	0	0	0	0
36	B	95	0	130	4	0
36	C	57	0	78	3	0
36	H	17	0	22	2	0
36	I	19	0	26	2	0
36	V	19	0	26	0	0
36	b	95	0	130	10	0
36	c	57	0	78	0	0
36	d	38	0	52	3	0
36	i	19	0	26	1	0
36	o	19	0	26	2	0
37	C	182	0	238	6	0
37	D	53	0	71	3	0
37	H	62	0	82	0	0
37	c	186	0	246	2	0
37	h	62	0	82	0	0
38	D	137	0	196	4	0
38	E	40	0	53	0	0
38	L	49	0	74	1	0
38	d	141	0	207	6	0
38	e	40	0	53	1	0
38	l	49	0	74	2	0
39	F	43	0	30	1	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	u	78	0	0	0	0
43	v	93	0	0	0	0
43	x	4	0	0	0	0
43	y	6	0	0	0	0
43	z	6	0	0	0	0
All	All	53814	0	52371	454	0

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

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:20:PRO:HG3	29:O:302:GOL:H12	1.64	0.79
2:b:433:ASP:HB2	29:b:631:GOL:H11	1.66	0.77
28:d:401:LMT:H22	36:o:301:HTG:H1	1.66	0.76
4:d:192:THR:HG23	23:d:408:CLA:HBC2	1.71	0.73
13:O:194:LYS:NZ	43:O:401:HOH:O	2.23	0.70
23:c:506:CLA:HBB2	27:c:522:LMG:H412	1.72	0.70
1:a:252:HIS:NE2	1:a:265:PHE:O	2.26	0.69
1:A:12:ASN:HB3	1:A:15:GLU:HG3	1.73	0.69
34:B:647:DMS:H12	28:d:401:LMT:H3'	1.75	0.68
3:c:315:MET:HG2	3:c:351:PHE:CZ	2.29	0.67
39:e:103:HEM:HMC2	39:e:103:HEM:HBC2	1.77	0.67
26:D:2302:SQD:H252	26:D:2302:SQD:H92	1.77	0.66
23:C:507:CLA:HMC2	23:C:508:CLA:H102	1.79	0.65
5:e:18:ARG:HB2	9:j:2:MET:HB3	1.79	0.65
2:B:169:SER:HB3	29:B:648:GOL:H2	1.79	0.64
2:B:44:THR:HG22	28:B:634:LMT:H6D	1.78	0.64
7:H:25:TRP:CD1	36:H:101:HTG:H1	2.32	0.64
23:C:504:CLA:HBB1	27:C:527:LMG:H221	1.80	0.63
23:c:504:CLA:C4D	23:c:506:CLA:H2	2.28	0.62
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.80	0.62
2:b:420:TYR:CE2	36:b:625:HTG:H2'1	2.34	0.62
26:l:101:SQD:H462	26:l:101:SQD:H1	1.82	0.62
2:b:133:LEU:HD12	34:b:639:DMS:H22	1.80	0.62
5:e:8:ARG:HH21	5:e:12:ASP:HB3	1.65	0.62
23:a:2610:CLA:H142	27:d:414:LMG:H241	1.81	0.62
23:b:618:CLA:H18	38:d:412:LHG:H202	1.82	0.61
5:E:27:ILE:HG12	39:F:101:HEM:HMC3	1.82	0.61
28:A:414:LMT:H6'1	4:D:304:ARG:HH12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:THR:N	34:B:642:DMS:O	2.34	0.60
23:A:407:CLA:H192	33:A:422:PL9:H252	1.83	0.59
34:B:644:DMS:H11	11:L:1:MET:HB3	1.84	0.59
3:c:107:ASP:OD2	27:c:522:LMG:O2	2.20	0.59
29:a:2602:GOL:H31	36:o:301:HTG:H1'1	1.85	0.59
28:B:623:LMT:H42	26:D:2302:SQD:H241	1.85	0.59
3:c:315:MET:HG3	3:c:365:TRP:HZ3	1.66	0.59
2:B:90:PHE:H	36:B:627:HTG:H61	1.68	0.59
25:T:102:BCR:H19C	25:b:623:BCR:H363	1.85	0.59
23:C:503:CLA:H61	23:C:513:CLA:H42	1.85	0.58
28:A:414:LMT:O4'	4:D:304:ARG:NH2	2.36	0.58
25:B:633:BCR:HC8	25:B:633:BCR:H321	1.85	0.58
23:b:620:CLA:H2	23:b:621:CLA:HBB2	1.85	0.58
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.86	0.58
1:A:102:LEU:HD11	28:A:420:LMT:H42	1.85	0.58
5:E:68:ASP:O	5:E:72:ALA:HB2	2.04	0.57
19:z:47:TRP:CE2	28:z:102:LMT:H102	2.39	0.57
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	1.85	0.57
2:B:248:ALA:HA	23:B:604:CLA:H42	1.86	0.57
2:b:36:SER:OG	25:b:623:BCR:H362	2.05	0.57
37:C:519:DGD:HA32	27:D:2312:LMG:H121	1.87	0.56
4:D:61:HIS:HD2	43:D:2528:HOH:O	1.88	0.56
28:d:404:LMT:H112	36:d:407:HTG:H6'2	1.87	0.56
23:b:616:CLA:H101	23:b:618:CLA:H143	1.86	0.56
1:A:183:MET:HA	23:A:405:CLA:HMD1	1.88	0.56
4:D:192:THR:HG23	23:D:2303:CLA:HBC2	1.86	0.56
2:b:341:LYS:NZ	36:b:625:HTG:S1	2.77	0.56
26:A:412:SQD:H381	9:J:22:ILE:HD11	1.88	0.55
37:C:518:DGD:HA82	37:C:518:DGD:HAF2	1.89	0.55
3:C:50:LEU:HD11	23:C:514:CLA:HBB1	1.89	0.55
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.88	0.55
1:A:200:LEU:HG	37:C:519:DGD:HAT2	1.89	0.55
26:B:621:SQD:H242	11:l:14:ARG:HD3	1.89	0.54
3:C:182:PHE:HA	36:C:521:HTG:H61	1.88	0.54
25:T:102:BCR:H321	25:T:102:BCR:HC8	1.88	0.54
1:a:136:ARG:NH2	8:i:27:ASP:OD1	2.39	0.54
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.89	0.54
2:b:347[A]:ARG:NH2	43:b:706:HOH:O	2.40	0.54
23:C:502:CLA:HBB2	23:C:508:CLA:H92	1.90	0.54
25:B:618:BCR:H383	26:B:621:SQD:H101	1.88	0.54
28:A:414:LMT:O3'	28:A:414:LMT:O2B	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:619:BCR:H363	25:B:633:BCR:H19C	1.89	0.54
25:Y:302:BCR:H321	25:Y:302:BCR:HC8	1.89	0.54
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.07	0.53
23:c:509:CLA:H2	25:c:517:BCR:H10C	1.91	0.53
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.91	0.53
3:C:24:THR:O	3:C:26:ARG:N	2.42	0.53
3:c:60:ILE:HG22	23:c:506:CLA:HHD	1.90	0.53
24:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.91	0.52
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	1.91	0.52
5:E:60:GLN:NE2	5:E:62:SER:O	2.42	0.52
23:B:616:CLA:H2	23:B:617:CLA:HBB2	1.91	0.52
2:B:341:LYS:NZ	36:B:624[B]:HTG:S1	2.82	0.52
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.39	0.52
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.92	0.52
1:a:136:ARG:HD2	43:a:2769:HOH:O	2.09	0.52
4:d:304:ARG:HH12	28:d:401:LMT:H6'1	1.74	0.51
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.10	0.51
25:D:2305:BCR:H383	27:D:2312:LMG:H171	1.90	0.51
3:c:38:GLY:HA3	23:c:514:CLA:HMD2	1.92	0.51
3:c:256:PRO:HA	23:c:509:CLA:HED2	1.92	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
23:c:504:CLA:H202	23:c:510:CLA:HBB1	1.92	0.51
4:d:244:TYR:OH	4:d:264:LYS:HE2	2.11	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
5:E:16:SER:HB3	9:J:5:GLY:HA2	1.93	0.51
1:a:183:MET:HA	23:a:2609:CLA:HMD1	1.91	0.51
2:B:349:LYS:NZ	43:B:706:HOH:O	2.43	0.51
34:B:637:DMS:H11	43:B:891:HOH:O	2.11	0.51
23:B:606:CLA:C14	23:B:611:CLA:HED2	2.41	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.46	0.51
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.92	0.51
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.46	0.51
23:c:514:CLA:H171	19:z:20:VAL:HA	1.92	0.51
13:O:58:ASN:ND2	2:b:307[B]:GLU:OE2	2.44	0.50
16:V:18:THR:O	34:V:206:DMS:H22	2.12	0.50
23:d:402:CLA:HMB1	23:d:402:CLA:HBB1	1.93	0.50
36:d:407:HTG:H2	7:h:25:TRP:NE1	2.26	0.50
19:z:47:TRP:CE3	28:z:102:LMT:H81	2.47	0.50
23:b:620:CLA:H2	23:b:621:CLA:CBB	2.41	0.50
1:A:23:SER:HA	34:A:430:DMS:H13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:304:ARG:NH2	28:d:401:LMT:O4'	2.36	0.50
23:B:617:CLA:HBB1	23:B:617:CLA:HMB3	1.94	0.50
2:b:141:ILE:HG21	23:b:620:CLA:HBB1	1.93	0.50
2:b:464:PHE:CZ	38:d:412:LHG:H252	2.46	0.50
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.93	0.50
26:a:2615:SQD:H262	38:d:403:LHG:H121	1.93	0.49
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.95	0.49
23:b:614:CLA:NC	40:h:101:RRX:H56	2.27	0.49
23:A:407:CLA:H152	33:A:422:PL9:H222	1.95	0.49
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.49
28:A:420:LMT:H51	8:I:4:LEU:HD22	1.95	0.49
8:I:13:THR:O	8:I:17:LEU:HG	2.12	0.49
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.48	0.49
7:h:59:ASN:O	7:h:64:ALA:HB3	2.13	0.49
26:D:2308:SQD:H321	18:X:24:THR:HA	1.94	0.49
23:C:507:CLA:H51	23:C:507:CLA:H102	1.95	0.49
8:i:1:FME:HG3	28:i:103:LMT:H6D	1.95	0.49
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.48	0.48
3:c:286:ALA:HB2	23:c:505:CLA:HMD2	1.93	0.48
38:l:103:LHG:H321	12:m:18:PRO:HB3	1.96	0.48
4:D:23:LYS:NZ	26:D:2302:SQD:H462	2.28	0.48
7:h:38:PHE:HB2	40:h:101:RRX:C10	2.43	0.48
2:B:416:THR:HG23	36:B:624[B]:HTG:H6'1	1.95	0.48
23:c:508:CLA:HAA1	23:c:508:CLA:HBD	1.95	0.48
4:d:335:PRO:HB2	5:e:65[B]:LEU:HD13	1.96	0.48
23:C:504:CLA:HBB1	27:C:527:LMG:H391	1.96	0.48
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.77	0.48
4:D:126:MET:HE3	4:D:143:ALA:O	2.13	0.48
37:D:2307:DGD:HBW2	37:D:2307:DGD:O1A	2.14	0.48
3:c:279:LEU:HD22	23:c:512:CLA:HED2	1.96	0.48
23:A:405:CLA:CBD	23:A:406:CLA:HAC2	2.43	0.48
2:B:36[A]:SER:OG	25:B:619:BCR:H362	2.14	0.48
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.96	0.48
7:H:63:LYS:NZ	43:H:202:HOH:O	2.47	0.48
2:b:12:LEU:HB2	23:b:617:CLA:HMC2	1.96	0.48
23:c:505:CLA:H102	23:c:506:CLA:CHB	2.44	0.48
27:c:521:LMG:O5	28:j:2701:LMT:H2B	2.14	0.48
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.96	0.48
23:a:2613:CLA:H161	23:a:2613:CLA:H122	1.71	0.47
29:b:644:GOL:H31	7:h:62:TRP:CZ3	2.49	0.47
34:o:307:DMS:H21	43:o:425:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:410:CLA:H18	23:C:506:CLA:H142	1.95	0.47
2:B:461:LEU:HD22	38:D:2309:LHG:H301	1.96	0.47
34:B:638:DMS:H21	15:U:21:TYR:CZ	2.49	0.47
1:a:121[B]:LEU:HD11	23:c:508:CLA:H122	1.95	0.47
2:b:58:GLN:C	2:b:329:PRO:HB3	2.40	0.47
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.48	0.47
4:d:61:HIS:HD2	43:d:627:HOH:O	1.95	0.47
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.95	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.97	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.50	0.47
23:C:504:CLA:HAB	23:C:513:CLA:H41	1.97	0.47
3:c:52:ALA:HB2	23:c:514:CLA:HMA2	1.96	0.47
1:A:252:HIS:CE1	1:A:264:SER:HB3	2.49	0.47
7:H:25:TRP:CD2	36:H:101:HTG:H1'2	2.50	0.47
1:a:12[A]:ASN:OD1	1:a:15:GLU:HB2	2.13	0.47
23:b:611:CLA:H72	25:b:624:BCR:H311	1.97	0.47
2:B:86:ILE:HD12	2:B:88:PRO:HD3	1.97	0.47
13:o:232:GLU:HG2	34:o:314:DMS:H11	1.96	0.47
3:c:42:LEU:HD21	23:c:514:CLA:H2A	1.97	0.47
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.30	0.47
27:c:501:LMG:H382	37:c:518:DGD:HB52	1.98	0.46
37:c:519:DGD:HA81	37:c:519:DGD:HAE2	1.46	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.97	0.46
2:B:264:PRO:HB3	29:B:648:GOL:H11	1.96	0.46
23:a:2610:CLA:HMD3	4:d:182:LEU:HD11	1.97	0.46
23:c:509:CLA:HMC2	23:c:510:CLA:H102	1.96	0.46
2:B:341:LYS:NZ	43:B:708:HOH:O	2.43	0.46
19:z:47:TRP:CD2	28:z:102:LMT:H102	2.50	0.46
23:A:406:CLA:H203	23:A:406:CLA:H162	1.70	0.46
23:a:2609:CLA:CBD	23:d:402:CLA:HAC2	2.44	0.46
3:C:163:PHE:CD2	23:C:513:CLA:HAB	2.51	0.46
5:e:68:ASP:O	5:e:72:ALA:HB2	2.15	0.46
23:B:610:CLA:HMA2	23:B:611:CLA:C2C	2.45	0.46
23:c:504:CLA:C3D	23:c:506:CLA:H2	2.46	0.46
19:z:26:ALA:HB3	19:z:40:ILE:HD11	1.97	0.46
23:b:614:CLA:HMA3	23:b:615:CLA:C1C	2.46	0.46
37:C:518:DGD:HBF1	37:C:518:DGD:HBE2	1.59	0.46
38:L:101:LHG:H321	12:M:18:PRO:HB3	1.98	0.46
23:b:618:CLA:H141	38:d:412:LHG:H182	1.97	0.46
25:b:622:BCR:H313	27:m:2802:LMG:H111	1.97	0.46
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:101:BCR:H24C	25:K:101:BCR:H371	1.76	0.45
2:b:80:ILE:HD11	2:b:167:TRP:CZ3	2.52	0.45
2:b:149:LEU:HD21	23:b:611:CLA:HBB2	1.98	0.45
2:b:423:LYS:HG3	36:b:625:HTG:H1'1	1.98	0.45
23:B:615:CLA:H62	23:B:615:CLA:H41	1.63	0.45
29:B:632:GOL:H2	34:U:503:DMS:H12	1.98	0.45
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.45
13:O:57:LYS:HE2	2:b:338:GLN:HA	1.97	0.45
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.97	0.45
25:b:622:BCR:H24C	25:b:622:BCR:H371	1.77	0.45
13:o:180:GLU:CD	13:o:180:GLU:H	2.24	0.45
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.46	0.45
27:d:414:LMG:H292	27:d:414:LMG:H151	1.99	0.45
23:B:616:CLA:H111	23:B:616:CLA:H152	1.56	0.45
40:H:102:RRX:H47	40:H:102:RRX:H43	1.72	0.45
4:d:61:HIS:HE1	4:d:80:THR:O	1.99	0.45
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.51	0.45
28:A:414:LMT:O2'	36:b:602:HTG:H5	2.17	0.45
23:A:410:CLA:H151	23:A:410:CLA:H112	1.58	0.45
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.86	0.45
2:b:233:ASN:O	2:b:236:THR:HG22	2.17	0.45
23:b:606:CLA:HAA2	36:b:626:HTG:H62	1.97	0.45
23:B:615:CLA:H71	23:B:615:CLA:H112	1.74	0.45
25:B:633:BCR:H331	25:B:633:BCR:HC7	1.53	0.45
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.99	0.45
3:C:266:TRP:CZ3	23:C:508:CLA:HAC2	2.51	0.45
11:L:9:PRO:HA	28:m:2803:LMT:H6D	1.98	0.45
2:b:348:ASN:OD1	2:b:352[A]:GLU:HG2	2.17	0.45
25:b:623:BCR:H331	25:b:623:BCR:C8	2.47	0.45
25:c:517:BCR:H15C	25:c:517:BCR:H351	1.84	0.45
23:C:510:CLA:H141	23:C:513:CLA:HMD3	1.99	0.45
38:D:2311:LHG:H312	38:D:2311:LHG:H342	1.68	0.45
33:A:422:PL9:H452	4:D:39:PRO:HG3	1.98	0.44
23:B:607:CLA:H142	23:B:607:CLA:H111	1.73	0.44
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.16	0.44
1:a:131:TRP:CH2	23:c:508:CLA:HAA2	2.52	0.44
23:c:514:CLA:HMB1	25:k:302:BCR:H382	1.98	0.44
1:A:133:LEU:HD23	4:D:256:ILE:HG12	2.00	0.44
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.47	0.44
27:c:501:LMG:O5	29:c:530:GOL:H31	2.17	0.44
3:C:127:PHE:CZ	28:Z:101:LMT:H22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
13:O:194:LYS:HE3	34:O:307:DMS:H11	2.00	0.44
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.53	0.44
2:b:423:LYS:NZ	36:b:625:HTG:H62	2.32	0.44
3:c:362:ARG:HD3	34:c:536:DMS:O	2.18	0.44
13:o:196:GLN:NE2	34:o:314:DMS:O	2.50	0.44
14:T:23:PHE:CD1	26:l:101:SQD:H45	2.52	0.44
25:T:102:BCR:H11C	25:T:102:BCR:H341	1.87	0.44
23:b:615:CLA:H92	23:b:615:CLA:H61	1.84	0.44
6:f:22:ALA:HB2	33:x:1301:PL9:H353	1.99	0.44
23:B:604:CLA:H143	23:B:609:CLA:HAC1	1.99	0.44
3:C:443:TRP:CZ2	23:C:509:CLA:HMD1	2.52	0.44
1:a:23:SER:HA	34:a:2624:DMS:S	2.56	0.44
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.48	0.44
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.53	0.44
33:d:411:PL9:H411	11:l:29:LEU:HD23	1.99	0.44
16:v:27:LEU:HD21	34:v:209:DMS:H23	1.98	0.44
2:B:454:ALA:HB2	27:B:622:LMG:H172	1.99	0.44
40:H:102:RRX:H26	40:H:102:RRX:H22	1.85	0.44
3:c:123:ALA:HB1	28:z:102:LMT:H101	1.99	0.44
23:B:606:CLA:H152	23:B:606:CLA:H112	1.77	0.44
23:B:611:CLA:HHC	23:B:611:CLA:HBB1	2.00	0.44
23:D:2303:CLA:HAA2	23:D:2303:CLA:HBD	2.00	0.44
7:H:62:TRP:C	7:H:64:ALA:H	2.25	0.44
28:M:101:LMT:H5'	43:t:208:HOH:O	2.18	0.44
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.53	0.44
23:c:516:CLA:H61	23:c:516:CLA:H2	1.75	0.44
4:d:49:LEU:HD13	25:d:410:BCR:C15	2.48	0.44
19:z:38:GLN:O	19:z:42:LEU:HG	2.18	0.44
23:B:614:CLA:H121	23:B:614:CLA:H162	1.66	0.44
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.99	0.44
13:O:110:MET:HE2	13:O:110:MET:HB3	1.80	0.44
3:c:145:SER:H	34:c:543:DMS:H13	1.83	0.44
2:B:137:LYS:NZ	7:H:17:GLU:OE1	2.45	0.43
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.00	0.43
13:O:129:THR:HA	13:O:141:ASP:O	2.18	0.43
1:a:63:ILE:HB	3:c:335:THR:HG21	1.99	0.43
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.00	0.43
29:B:648:GOL:H32	7:H:62:TRP:CE3	2.53	0.43
6:F:21:VAL:O	6:F:25:THR:HG23	2.18	0.43
40:H:102:RRX:H32	40:H:102:RRX:H28	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:LYS:HZ1	29:B:632:GOL:H31	1.82	0.43
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.53	0.43
23:b:612:CLA:H91	23:b:612:CLA:H112	1.82	0.43
4:d:140:PRO:HD2	34:d:418:DMS:H23	1.99	0.43
36:d:407:HTG:H3'2	36:d:407:HTG:H6'1	1.82	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.43
33:A:422:PL9:H211	23:D:2303:CLA:H141	2.01	0.43
26:b:601:SQD:H191	26:b:601:SQD:H161	1.70	0.43
36:b:603:HTG:O2	36:b:604:HTG:S1	2.71	0.43
27:c:501:LMG:H192	27:c:501:LMG:H161	1.77	0.43
27:c:501:LMG:H202	27:c:501:LMG:H231	1.80	0.43
5:e:8:ARG:NH2	5:e:12:ASP:HB3	2.33	0.43
27:A:413:LMG:H372	37:C:517:DGD:HB32	2.00	0.43
2:b:90:PHE:CE2	23:b:611:CLA:H151	2.54	0.43
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.00	0.43
3:c:436:PHE:CE1	23:c:507:CLA:H202	2.53	0.43
23:c:516:CLA:H172	27:c:522:LMG:H411	2.00	0.43
23:B:611:CLA:H161	23:B:611:CLA:H203	1.80	0.43
23:C:514:CLA:H171	25:C:515:BCR:H373	1.99	0.43
2:B:419:SER:HA	2:B:422:ARG:NH1	2.34	0.43
23:C:506:CLA:HBC2	25:C:516:BCR:H341	1.99	0.43
1:a:73:TYR:HA	28:d:401:LMT:H4B	2.00	0.43
2:b:341:LYS:NZ	36:b:625:HTG:O2	2.33	0.43
7:h:20:LYS:HE3	7:h:20:LYS:HB2	1.77	0.43
40:h:101:RRX:H32	40:h:101:RRX:H28	1.78	0.43
2:B:462:PHE:CE2	23:B:614:CLA:HMB3	2.54	0.43
25:Y:302:BCR:H351	25:Y:302:BCR:H15C	1.72	0.43
2:b:137:LYS:HD2	7:h:14:LEU:O	2.17	0.43
3:c:338:GLY:HA3	3:c:341:LEU:O	2.18	0.43
4:d:26:ARG:NH2	26:d:417:SQD:O7	2.50	0.43
25:B:633:BCR:H11C	25:B:633:BCR:H341	1.84	0.43
3:C:409:GLY:HA2	29:C:526:GOL:H2	2.01	0.43
13:O:86:LYS:NZ	43:O:404:HOH:O	2.44	0.43
14:t:26:PRO:HA	14:t:27:PRO:HD3	1.97	0.43
28:A:414:LMT:H41	36:b:602:HTG:H3'2	2.00	0.43
23:C:507:CLA:H43	23:C:507:CLA:H11	1.82	0.43
23:C:507:CLA:HBA1	23:C:507:CLA:H3A	1.65	0.43
2:b:170:ASP:O	29:b:644:GOL:H12	2.19	0.43
3:c:279:LEU:HD12	3:c:282:MET:HE3	2.01	0.43
23:c:506:CLA:H112	23:c:506:CLA:H72	1.76	0.43
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:3:THR:HB	36:i:102:HTG:H1'1	2.01	0.43
8:I:1:FME:CN	36:I:101:HTG:H61	2.48	0.42
1:a:252:HIS:CD2	1:a:266:ASN:HA	2.54	0.42
3:c:26:ARG:NH2	17:y:46:LEU:OXT	2.38	0.42
3:c:138:GLU:OE2	43:c:601:HOH:O	2.21	0.42
23:c:506:CLA:HBB1	27:c:522:LMG:H231	2.01	0.42
3:C:338:GLY:HA3	3:C:341:LEU:O	2.19	0.42
23:C:504:CLA:HMC3	23:C:514:CLA:H191	2.00	0.42
25:C:516:BCR:H341	25:C:516:BCR:H11C	1.90	0.42
2:b:29:LEU:HD23	26:l:101:SQD:H211	2.00	0.42
2:b:30:VAL:HG12	23:b:610:CLA:HHD	2.01	0.42
3:c:163:PHE:CD1	23:c:515:CLA:H201	2.54	0.42
4:d:73:PHE:CZ	27:d:414:LMG:H192	2.54	0.42
23:d:402:CLA:H162	23:d:402:CLA:H203	1.71	0.42
38:e:101:LHG:H222	33:x:1301:PL9:H221	2.02	0.42
7:h:62:TRP:C	7:h:64:ALA:H	2.27	0.42
23:A:407:CLA:H142	23:A:407:CLA:H112	1.86	0.42
36:B:625:HTG:O6	36:B:625:HTG:O4	2.35	0.42
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.00	0.42
2:b:324:LEU:HA	4:d:293[A]:LEU:HG	2.00	0.42
23:b:621:CLA:H151	23:b:621:CLA:H111	1.88	0.42
24:A:408:PHO:H61	24:A:408:PHO:H2	1.90	0.42
23:A:410:CLA:H152	23:C:507:CLA:H13	2.00	0.42
25:B:620:BCR:H382	26:a:2603:SQD:H242	2.00	0.42
4:D:84:SER:O	5:E:69:ARG:HB2	2.20	0.42
2:b:462:PHE:CE2	23:b:618:CLA:HMB3	2.53	0.42
1:A:131:TRP:CH2	23:C:506:CLA:HAA2	2.54	0.42
25:B:620:BCR:H331	25:B:620:BCR:C8	2.50	0.42
14:T:20:ALA:O	14:T:24:ARG:HB3	2.20	0.42
3:c:135:ARG:O	3:c:135:ARG:HD3	2.20	0.42
3:c:315:MET:HG2	3:c:351:PHE:HZ	1.78	0.42
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.55	0.42
23:C:505:CLA:H161	23:C:511:CLA:H93	2.02	0.42
37:D:2307:DGD:HBW2	37:D:2307:DGD:HB92	1.86	0.42
3:c:19:ASN:HB3	3:c:20:SER:H	1.68	0.42
16:v:122:GLU:HG3	16:v:126:LEU:HD12	2.02	0.42
25:z:101:BCR:H15C	25:z:101:BCR:H351	1.73	0.42
23:B:605:CLA:H41	23:B:605:CLA:H62	1.88	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.42
24:a:2612:PHO:ND	24:a:2612:PHO:NC	2.67	0.42
24:a:2612:PHO:HMC2	4:d:279:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:419:SER:OG	36:b:625:HTG:H2'2	2.20	0.42
26:d:417:SQD:H462	26:d:417:SQD:O9	2.20	0.42
13:o:99:ASP:OD1	13:o:100:GLY:N	2.50	0.42
1:A:341:LEU:HD13	29:C:526:GOL:H32	2.01	0.42
34:B:647:DMS:H23	28:d:401:LMT:H5'	2.02	0.42
3:C:135:ARG:O	3:C:135:ARG:HD3	2.20	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.18	0.42
23:b:611:CLA:H162	23:b:611:CLA:H122	1.63	0.42
3:c:276:LEU:HD23	23:c:512:CLA:HED1	2.02	0.42
3:C:32:GLY:HA3	34:C:536:DMS:H13	2.01	0.42
23:C:514:CLA:HMD1	28:Z:101:LMT:H5'	2.01	0.42
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.42
1:a:85:SER:HA	1:a:109:GLY:HA3	2.02	0.42
23:b:608:CLA:CGA	23:b:608:CLA:H3A	2.50	0.42
25:y:101:BCR:H11C	25:y:101:BCR:H341	1.92	0.42
1:A:163:ILE:HD11	37:C:517:DGD:HA22	2.02	0.41
4:D:225:ASP:HB3	34:D:2320:DMS:H13	2.02	0.41
4:D:266:TRP:CG	38:D:2310:LHG:HC2	2.55	0.41
8:I:4:LEU:HD13	36:I:101:HTG:H4'1	2.02	0.41
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.01	0.41
1:A:18:CYS:SG	8:I:30:ARG:NH2	2.93	0.41
3:C:406:SER:HA	3:C:420:VAL:HG23	2.01	0.41
23:b:615:CLA:H203	23:b:615:CLA:H152	2.01	0.41
23:c:508:CLA:H93	23:c:508:CLA:H111	1.91	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.01	0.41
23:C:514:CLA:HAA1	36:C:525:HTG:H1'2	2.02	0.41
23:D:2304:CLA:H141	23:D:2304:CLA:H161	1.88	0.41
3:c:213:LEU:HD12	23:c:509:CLA:H202	2.02	0.41
3:c:266:TRP:CZ3	23:c:510:CLA:HAC2	2.55	0.41
3:c:436:PHE:CZ	23:c:507:CLA:H202	2.55	0.41
27:d:414:LMG:H191	27:d:414:LMG:H162	1.97	0.41
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.55	0.41
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.50	0.41
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.03	0.41
25:b:624:BCR:H15C	25:b:624:BCR:H351	1.93	0.41
38:d:413:LHG:HC62	11:l:15:THR:HG23	2.02	0.41
12:m:16[A]:LEU:HD23	12:m:16[A]:LEU:HA	1.90	0.41
25:z:101:BCR:H11C	25:z:101:BCR:H341	1.90	0.41
23:C:502:CLA:H42	23:C:503:CLA:HMD3	2.03	0.41
23:C:505:CLA:H91	23:C:505:CLA:H112	1.82	0.41
23:C:513:CLA:C1B	25:C:515:BCR:H401	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:2307:DGD:HA62	37:D:2307:DGD:HA92	1.76	0.41
2:b:148[B]:LEU:HD23	23:b:609:CLA:H191	2.03	0.41
4:d:293[A]:LEU:HD12	4:d:293[A]:LEU:HA	1.93	0.41
24:A:409:PHO:ND	24:A:409:PHO:NC	2.69	0.41
2:B:30:VAL:HG12	23:B:606:CLA:HHD	2.02	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.02	0.41
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.55	0.41
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.03	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.88	0.41
16:V:128:ASP:OD2	34:V:212:DMS:H12	2.21	0.41
26:a:2603:SQD:H282	26:a:2603:SQD:H312	1.79	0.41
3:c:400:PRO:C	3:c:401:LEU:HD12	2.45	0.41
2:B:69:LEU:HD12	23:B:606:CLA:HBA1	2.02	0.41
23:B:613:CLA:HAA1	23:B:613:CLA:HBD	2.03	0.41
23:C:503:CLA:H193	36:C:521:HTG:H3'1	2.03	0.41
1:a:235:TYR:HD1	1:a:235:TYR:HA	1.75	0.41
25:a:2614:BCR:H11C	25:a:2614:BCR:H341	1.89	0.41
25:a:2614:BCR:H24C	25:a:2614:BCR:H371	1.96	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
23:b:608:CLA:CAD	23:b:610:CLA:H12	2.51	0.41
34:c:535:DMS:H21	43:c:697:HOH:O	2.21	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.41
28:A:420:LMT:H2'	28:A:420:LMT:H11	1.81	0.40
23:B:602:CLA:H91	23:B:602:CLA:H112	1.85	0.40
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.98	0.40
2:b:169:SER:HB3	29:b:644:GOL:H2	2.02	0.40
2:b:458:PHE:HB3	23:b:609:CLA:HBC2	2.02	0.40
38:d:412:LHG:O9	38:l:103:LHG:HC81	2.20	0.40
39:e:103:HEM:HMC2	6:f:31:ILE:HG13	2.03	0.40
13:o:83:GLY:HA2	13:o:98:GLU:HG2	2.02	0.40
13:o:225[B]:MET:HE3	13:o:225[B]:MET:HB3	1.95	0.40
28:A:414:LMT:H51	28:A:414:LMT:H22	1.74	0.40
23:c:515:CLA:H3A	23:c:515:CLA:HBA2	1.80	0.40
4:d:272:LEU:C	4:d:272:LEU:HD23	2.46	0.40
27:A:413:LMG:H201	27:A:413:LMG:H231	2.00	0.40
2:B:338:GLN:HA	13:o:57:LYS:HE2	2.04	0.40
25:D:2305:BCR:H20C	25:D:2305:BCR:H361	1.93	0.40
38:D:2311:LHG:H141	38:D:2311:LHG:H332	2.03	0.40
23:a:2609:CLA:CAD	23:d:402:CLA:HAC2	2.51	0.40
2:b:86:ILE:H	2:b:86:ILE:HG13	1.75	0.40
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:247:PHE:CD1	23:b:607:CLA:H121	2.56	0.40
26:A:412:SQD:H302	23:C:509:CLA:H71	2.03	0.40
27:A:413:LMG:H402	3:C:281:MET:HG3	2.04	0.40
23:B:604:CLA:CGA	23:B:604:CLA:H3A	2.50	0.40
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.22	0.40
23:b:620:CLA:H92	23:b:620:CLA:H61	1.88	0.40
13:o:53:LYS:HE2	13:o:63:ALA:HB3	2.03	0.40
24:A:409:PHO:H42	24:A:409:PHO:H11	1.83	0.40
23:A:410:CLA:H18	23:C:506:CLA:C14	2.52	0.40
2:B:157:HIS:HA	2:B:163:GLY:HA3	2.02	0.40
3:C:24:THR:C	3:C:26:ARG:H	2.30	0.40
23:C:514:CLA:H3A	23:C:514:CLA:HBA1	1.58	0.40
23:d:402:CLA:C4A	23:d:402:CLA:HBA1	2.51	0.40
25:d:410:BCR:H11C	25:d:410:BCR:H341	1.95	0.40
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.53	0.40
26:l:101:SQD:H341	26:l:101:SQD:H311	1.79	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	34
1	a	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	36	34
2	B	510/505 (101%)	501 (98%)	9 (2%)	0	100	100
2	b	490/505 (97%)	484 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	441 (98%)	8 (2%)	2 (0%)	30	26
3	c	453/455 (100%)	444 (98%)	8 (2%)	1 (0%)	43	44
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	341/342 (100%)	335 (98%)	6 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	3
7	h	62/63 (98%)	59 (95%)	2 (3%)	1 (2%)	7	3
8	I	30/38 (79%)	29 (97%)	1 (3%)	0	100	100
8	i	30/38 (79%)	30 (100%)	0	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	245/244 (100%)	240 (98%)	5 (2%)	0	100	100
13	o	245/244 (100%)	240 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	36/40 (90%)	36 (100%)	0	0	100	100
18	x	34/40 (85%)	34 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5191/5346 (97%)	5103 (98%)	81 (2%)	7 (0%)	48 50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ASN
3	C	416	SER
3	c	416	SER
7	H	63	LYS
7	h	63	LYS
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	268/279 (96%)	268 (100%)	0	100 100
1	a	272/279 (98%)	271 (100%)	1 (0%)	84 89
2	B	406/403 (101%)	405 (100%)	1 (0%)	87 92
2	b	389/403 (96%)	386 (99%)	3 (1%)	73 79
3	C	354/356 (99%)	351 (99%)	3 (1%)	73 79
3	c	355/356 (100%)	352 (99%)	3 (1%)	73 79
4	D	275/276 (100%)	274 (100%)	1 (0%)	84 89
4	d	277/276 (100%)	275 (99%)	2 (1%)	76 82
5	E	69/72 (96%)	67 (97%)	2 (3%)	37 39
5	e	66/72 (92%)	66 (100%)	0	100 100
6	F	26/38 (68%)	26 (100%)	0	100 100
6	f	25/38 (66%)	25 (100%)	0	100 100
7	H	53/53 (100%)	53 (100%)	0	100 100
7	h	54/53 (102%)	54 (100%)	0	100 100

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

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	255	THR
3	C	289	PHE
3	C	315	MET
4	D	90	LEU

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Mol	Chain	Res	Type
5	E	5	THR
5	E	65	LEU
13	O	110	MET
1	a	15	GLU
2	b	121	GLU
2	b	362	PHE
2	b	467	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	24	ARG
4	d	90	LEU
15	u	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	296	ASN
2	B	14	ASN
2	B	331	ASN
2	B	374	ASN
3	C	418	ASN
4	D	186	GLN
4	D	255	GLN
4	D	301	GLN
5	E	74	GLN
19	Z	58	ASN
1	a	165	GLN
1	a	252	HIS
1	a	296	ASN
2	b	282	GLN
2	b	394	GLN
3	c	19	ASN
3	c	201	ASN
3	c	415	ASN
4	d	186	GLN
15	u	78	ASN
15	u	81	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.65	0	8,9,11	1.51	2 (25%)
4	HSK	d	336[B]	-	10,11,12	2.22	3 (30%)	5,14,16	3.84	4 (80%)
19	FME	Z	1	19	8,9,10	0.65	0	8,9,11	1.54	2 (25%)
14	FME	t	1	14	8,9,10	0.74	0	8,9,11	1.56	3 (37%)
12	FME	M	1	12	8,9,10	0.66	0	8,9,11	1.04	0
19	FME	z	1	19	8,9,10	0.61	0	8,9,11	1.42	2 (25%)
4	HSK	d	336[A]	-	10,10,12	9.05	2 (20%)	5,12,16	2.08	3 (60%)
14	FME	T	1	14	8,9,10	0.84	1 (12%)	8,9,11	1.52	1 (12%)
8	FME	I	1	8	8,9,10	0.59	0	8,9,11	1.51	3 (37%)
12	FME	m	1	12	8,9,10	0.57	0	8,9,11	1.05	0
4	HSK	D	336[B]	-	10,11,12	2.38	3 (30%)	5,14,16	3.59	4 (80%)
4	HSK	D	336[A]	-	10,10,12	8.82	2 (20%)	5,12,16	1.80	2 (40%)

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

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[A]	HSK	OM-ND1	-28.05	0.86	1.38
4	D	336[A]	HSK	OM-ND1	-27.26	0.87	1.38
4	D	336[B]	HSK	CG-ND1	-5.86	1.32	1.40
4	d	336[B]	HSK	CG-ND1	-5.25	1.33	1.40
4	D	336[A]	HSK	CG-ND1	-4.84	1.34	1.40
4	d	336[A]	HSK	CG-ND1	-4.47	1.34	1.40
4	D	336[B]	HSK	OM-ND1	2.85	1.43	1.38
4	d	336[B]	HSK	OM-ND1	2.75	1.43	1.38
4	d	336[B]	HSK	CE1-ND1	-2.36	1.33	1.37
4	D	336[B]	HSK	CE1-ND1	-2.25	1.33	1.37
14	T	1	FME	O-C	2.00	1.27	1.20

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	336[B]	HSK	ND1-CE1-NE2	-6.46	104.09	111.54
4	D	336[B]	HSK	ND1-CE1-NE2	-6.23	104.35	111.54
4	d	336[B]	HSK	CB-CG-ND1	3.42	128.66	122.89
4	d	336[B]	HSK	CD2-NE2-CE1	3.27	109.51	105.24
4	D	336[B]	HSK	CD2-NE2-CE1	3.11	109.31	105.24
4	d	336[B]	HSK	CE1-ND1-CG	3.00	115.05	108.87
4	d	336[A]	HSK	ND1-CE1-NE2	-2.96	108.13	111.54
4	D	336[B]	HSK	CE1-ND1-CG	2.81	114.64	108.87
4	D	336[B]	HSK	CB-CG-ND1	2.67	127.39	122.89
4	D	336[A]	HSK	ND1-CE1-NE2	-2.55	108.60	111.54
8	i	1	FME	CA-N-CN	-2.51	118.97	122.82
4	d	336[A]	HSK	CD2-NE2-CE1	2.43	108.41	105.24
19	Z	1	FME	CA-N-CN	-2.42	119.10	122.82
19	z	1	FME	O-C-CA	-2.36	118.71	124.77
4	d	336[A]	HSK	CB-CG-ND1	2.28	126.74	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O-C-CA	-2.22	119.05	124.77
19	Z	1	FME	O1-CN-N	-2.20	119.64	125.32
4	D	336[A]	HSK	CD2-NE2-CE1	2.20	108.11	105.24
14	t	1	FME	O1-CN-N	-2.17	119.71	125.32
8	I	1	FME	O-C-CA	-2.13	119.29	124.77
14	T	1	FME	O-C-CA	-2.12	119.31	124.77
14	t	1	FME	CA-N-CN	-2.12	119.56	122.82
8	i	1	FME	O1-CN-N	-2.11	119.88	125.32
19	z	1	FME	O1-CN-N	-2.10	119.90	125.32
8	I	1	FME	O1-CN-N	-2.03	120.06	125.32
8	I	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	B	602	43	69,73,73	2.63	24 (34%)	82,113,113	2.21	26 (31%)
36	HTG	c	524	-	19,19,19	0.96	2 (10%)	23,24,24	1.29	2 (8%)
27	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.06	3 (5%)
29	GOL	c	529	-	5,5,5	0.95	0	5,5,5	1.06	0
34	DMS	o	309	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
29	GOL	E	104	-	5,5,5	1.05	0	5,5,5	0.95	0
23	CLA	c	515	3	69,73,73	2.63	25 (36%)	82,113,113	2.44	30 (36%)
31	JOX	A	418	-	10,10,10	2.12	4 (40%)	14,14,14	3.41	10 (71%)
36	HTG	B	625	-	19,19,19	0.97	1 (5%)	23,24,24	1.90	4 (17%)
23	CLA	B	615	2	69,73,73	2.37	21 (30%)	82,113,113	2.51	31 (37%)
37	DGD	C	519	-	59,59,67	0.92	2 (3%)	73,73,81	1.29	7 (9%)
34	DMS	O	306	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
37	DGD	H	103	-	63,63,67	0.91	2 (3%)	77,77,81	1.09	7 (9%)
34	DMS	b	636	-	3,3,3	2.75	1 (33%)	3,3,3	0.51	0
34	DMS	c	540	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
34	DMS	c	548	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
34	DMS	a	2621	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	LHG	l	103	-	48,48,48	0.88	2 (4%)	51,54,54	1.04	4 (7%)
23	CLA	b	612	43	69,73,73	2.37	24 (34%)	82,113,113	2.36	28 (34%)
23	CLA	b	617	2	69,73,73	2.33	21 (30%)	82,113,113	2.48	26 (31%)
34	DMS	t	102	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
34	DMS	b	635	-	3,3,3	2.77	1 (33%)	3,3,3	0.63	0
28	LMT	i	103	-	24,24,36	0.52	0	29,29,47	1.08	2 (6%)
25	BCR	Y	302	-	41,41,41	0.83	0	56,56,56	1.77	10 (17%)
27	LMG	A	413	-	51,51,55	0.93	2 (3%)	59,59,63	1.24	6 (10%)
34	DMS	V	208	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
25	BCR	b	623	-	41,41,41	0.88	0	56,56,56	1.21	6 (10%)
23	CLA	C	503	3	69,73,73	2.60	24 (34%)	82,113,113	2.38	28 (34%)
25	BCR	K	101	-	41,41,41	0.70	0	56,56,56	1.34	10 (17%)
34	DMS	B	636	-	3,3,3	2.63	1 (33%)	3,3,3	0.60	0
34	DMS	U	503	-	3,3,3	2.76	1 (33%)	3,3,3	0.55	0
34	DMS	v	212	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.83	0
34	DMS	b	640	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
28	LMT	m	2803	-	36,36,36	0.42	0	47,47,47	0.83	0
36	HTG	b	604	-	19,19,19	0.98	2 (10%)	23,24,24	1.54	4 (17%)
34	DMS	o	310	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
34	DMS	b	637	-	3,3,3	2.81	1 (33%)	3,3,3	0.69	0
23	CLA	A	406	43	69,73,73	2.30	24 (34%)	82,113,113	2.63	32 (39%)
23	CLA	B	605	2	69,73,73	2.43	22 (31%)	82,113,113	2.37	28 (34%)
34	DMS	o	312	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
28	LMT	F	102	-	24,24,36	0.47	0	29,29,47	0.73	0
38	LHG	d	413	-	48,48,48	0.82	2 (4%)	51,54,54	1.00	4 (7%)
36	HTG	I	101	-	19,19,19	1.01	2 (10%)	23,24,24	1.68	4 (17%)
34	DMS	C	532	-	3,3,3	2.69	1 (33%)	3,3,3	0.74	0
29	GOL	v	204	-	5,5,5	0.92	0	5,5,5	1.03	0
23	CLA	B	610	2	69,73,73	2.63	22 (31%)	82,113,113	2.36	28 (34%)
26	SQD	a	2603	-	52,54,54	0.97	2 (3%)	62,65,65	1.11	3 (4%)
34	DMS	o	315	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
34	DMS	c	546	-	3,3,3	2.76	1 (33%)	3,3,3	0.58	0
34	DMS	B	637	-	3,3,3	2.75	1 (33%)	3,3,3	0.52	0
28	LMT	d	401	-	36,36,36	0.48	0	47,47,47	0.82	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	617	2	69,73,73	2.51	22 (31%)	82,113,113	2.42	28 (34%)
37	DGD	D	2307	-	53,53,67	0.96	2 (3%)	61,61,81	1.20	6 (9%)
34	DMS	O	310	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	PHO	A	409	-	58,69,69	2.81	15 (25%)	55,99,99	2.95	13 (23%)
34	DMS	v	214	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
34	DMS	C	535	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
34	DMS	O	311	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
34	DMS	T	104	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
38	LHG	D	2311	-	38,38,48	0.96	2 (5%)	41,44,54	1.13	4 (9%)
34	DMS	c	539	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
34	DMS	d	422	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
34	DMS	a	2624	-	3,3,3	2.81	1 (33%)	3,3,3	0.72	0
28	LMT	A	420	-	24,24,36	0.42	0	29,29,47	0.95	0
34	DMS	c	541	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
23	CLA	c	505	3	69,73,73	2.43	25 (36%)	82,113,113	2.27	24 (29%)
34	DMS	v	210	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
34	DMS	v	206	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
34	DMS	c	542	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
23	CLA	b	606	43	69,73,73	2.64	25 (36%)	82,113,113	2.21	28 (34%)
38	LHG	E	101	-	39,39,48	1.06	2 (5%)	42,45,54	1.14	3 (7%)
20	OEX	A	401	3,1,43	0,15,15	-	-	-		
26	SQD	a	2615	-	46,48,54	0.95	2 (4%)	56,59,65	1.75	12 (21%)
23	CLA	B	604	2	69,73,73	2.54	23 (33%)	82,113,113	2.47	28 (34%)
29	GOL	B	630	-	5,5,5	1.02	0	5,5,5	1.00	0
23	CLA	A	410	1	69,73,73	2.32	24 (34%)	82,113,113	2.48	29 (35%)
23	CLA	b	621	2	69,73,73	2.55	21 (30%)	82,113,113	2.55	29 (35%)
34	DMS	D	2319	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
23	CLA	B	606	2	69,73,73	2.34	23 (33%)	82,113,113	2.38	27 (32%)
34	DMS	c	538	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
34	DMS	V	206	-	3,3,3	2.77	1 (33%)	3,3,3	0.75	0
29	GOL	U	501	-	5,5,5	1.06	0	5,5,5	1.00	0
36	HTG	i	102	-	19,19,19	1.03	1 (5%)	23,24,24	1.73	3 (13%)
34	DMS	D	2317	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
34	DMS	B	645	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
34	DMS	V	211	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	511	3	69,73,73	2.61	23 (33%)	82,113,113	2.41	31 (37%)
29	GOL	C	524	-	5,5,5	0.86	0	5,5,5	1.04	0
29	GOL	v	202	-	5,5,5	1.05	0	5,5,5	0.96	0
29	GOL	v	203	-	5,5,5	0.98	0	5,5,5	1.22	1 (20%)
29	GOL	a	2618	-	5,5,5	0.90	0	5,5,5	1.12	1 (20%)
36	HTG	b	625	-	19,19,19	0.82	1 (5%)	23,24,24	1.46	4 (17%)
28	LMT	j	2701	41	34,34,36	0.57	1 (2%)	44,44,47	1.07	3 (6%)
34	DMS	c	532	-	3,3,3	2.82	1 (33%)	3,3,3	0.82	0
28	LMT	A	414	-	34,34,36	0.49	0	45,45,47	1.18	4 (8%)
23	CLA	b	613	2	69,73,73	2.50	24 (34%)	82,113,113	2.41	32 (39%)
23	CLA	d	408	4	69,73,73	2.39	23 (33%)	82,113,113	2.46	28 (34%)
39	HEM	e	103	6,5	50,50,50	1.96	10 (20%)	67,82,82	1.39	6 (8%)
28	LMT	m	2804	-	36,36,36	0.45	0	47,47,47	1.14	5 (10%)
23	CLA	B	613	2	69,73,73	2.33	23 (33%)	82,113,113	2.43	26 (31%)
29	GOL	U	502	-	5,5,5	1.32	1 (20%)	5,5,5	0.87	0
34	DMS	B	639	-	3,3,3	2.76	1 (33%)	3,3,3	0.61	0
29	GOL	c	531	-	5,5,5	0.99	0	5,5,5	0.93	0
29	GOL	O	302	-	5,5,5	0.97	0	5,5,5	1.11	0
34	DMS	B	635	-	3,3,3	2.76	1 (33%)	3,3,3	0.54	0
25	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.29	5 (8%)
25	BCR	a	2614	-	41,41,41	0.82	0	56,56,56	1.31	6 (10%)
33	PL9	x	1301	-	38,38,55	0.44	0	45,45,69	1.72	11 (24%)
29	GOL	B	648	-	5,5,5	0.93	0	5,5,5	1.01	0
34	DMS	O	312	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
36	HTG	C	521	-	19,19,19	0.90	2 (10%)	23,24,24	0.95	1 (4%)
34	DMS	b	634	-	3,3,3	2.68	1 (33%)	3,3,3	0.36	0
34	DMS	O	314	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
34	DMS	d	418	-	3,3,3	2.71	1 (33%)	3,3,3	0.64	0
23	CLA	C	507	3	69,73,73	2.56	23 (33%)	82,113,113	2.55	30 (36%)
34	DMS	C	529	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
26	SQD	D	2302	-	52,54,54	1.00	3 (5%)	62,65,65	1.39	9 (14%)
23	CLA	B	614	2	69,73,73	2.34	21 (30%)	82,113,113	2.43	28 (34%)
28	LMT	f	101	-	24,24,36	0.46	0	29,29,47	0.76	0
25	BCR	A	411	-	41,41,41	0.77	0	56,56,56	1.40	8 (14%)
25	BCR	b	624	-	41,41,41	0.71	0	56,56,56	1.60	12 (21%)
34	DMS	d	421	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	b	622	-	41,41,41	0.80	0	56,56,56	1.40	8 (14%)
34	DMS	V	202	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
34	DMS	c	549	-	3,3,3	2.78	1 (33%)	3,3,3	0.64	0
42	HEC	v	201	16	46,50,50	2.03	8 (17%)	58,82,82	1.46	8 (13%)
34	DMS	A	430	-	3,3,3	2.79	1 (33%)	3,3,3	0.62	0
34	DMS	O	309	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
34	DMS	o	307	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
29	GOL	a	2602	-	5,5,5	0.87	0	5,5,5	1.11	0
23	CLA	b	611	2	69,73,73	2.62	23 (33%)	82,113,113	2.33	27 (32%)
23	CLA	B	616	2	69,73,73	2.41	21 (30%)	82,113,113	2.50	31 (37%)
34	DMS	C	533	-	3,3,3	2.70	1 (33%)	3,3,3	0.36	0
34	DMS	A	426	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
31	JOX	A	419	-	10,10,10	2.06	4 (40%)	14,14,14	4.92	11 (78%)
36	HTG	b	602	-	19,19,19	0.96	1 (5%)	23,24,24	0.98	1 (4%)
23	CLA	B	603	2	69,73,73	2.52	24 (34%)	82,113,113	2.40	30 (36%)
29	GOL	u	501	-	5,5,5	1.32	0	5,5,5	0.89	0
25	BCR	D	2305	-	41,41,41	0.85	1 (2%)	56,56,56	1.65	9 (16%)
23	CLA	b	607	2	69,73,73	2.49	24 (34%)	82,113,113	2.37	28 (34%)
34	DMS	V	213	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
34	DMS	d	420	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
26	SQD	d	417	-	31,32,54	1.99	4 (12%)	33,36,65	1.50	4 (12%)
34	DMS	B	641	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
38	LHG	e	101	-	39,39,48	1.08	2 (5%)	42,45,54	1.09	3 (7%)
29	GOL	O	304	-	5,5,5	0.90	0	5,5,5	1.06	0
34	DMS	H	104	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
38	LHG	D	2309	-	48,48,48	0.90	2 (4%)	51,54,54	1.17	5 (9%)
34	DMS	c	535	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
29	GOL	O	305	-	5,5,5	0.92	0	5,5,5	0.98	0
31	JOX	a	2617	-	10,10,10	1.92	4 (40%)	14,14,14	5.02	14 (100%)
25	BCR	z	101	-	41,41,41	0.76	0	56,56,56	1.52	10 (17%)
34	DMS	v	207	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
23	CLA	b	618	2	69,73,73	2.41	24 (34%)	82,113,113	2.35	27 (32%)
34	DMS	C	531	-	3,3,3	2.77	1 (33%)	3,3,3	0.52	0
34	DMS	v	211	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
34	DMS	v	208	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	LHG	D	2310	-	48,48,48	0.87	2 (4%)	51,54,54	0.97	3 (5%)
27	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.08	4 (6%)
29	GOL	b	631	-	5,5,5	1.13	0	5,5,5	0.65	0
23	CLA	B	612	2	69,73,73	2.53	22 (31%)	82,113,113	2.47	31 (37%)
27	LMG	D	2312	41	47,47,55	0.91	3 (6%)	55,55,63	0.88	2 (3%)
29	GOL	b	644	-	5,5,5	0.71	0	5,5,5	1.30	1 (20%)
34	DMS	D	2320	-	3,3,3	2.72	1 (33%)	3,3,3	0.46	0
29	GOL	J	301	-	5,5,5	1.02	0	5,5,5	0.95	0
34	DMS	c	536	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
34	DMS	o	305	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
34	DMS	c	547	-	3,3,3	2.76	1 (33%)	3,3,3	0.62	0
34	DMS	o	313	-	3,3,3	2.77	1 (33%)	3,3,3	0.62	0
23	CLA	c	514	3	69,73,73	2.44	23 (33%)	82,113,113	2.31	30 (36%)
34	DMS	u	502	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
23	CLA	C	509	3	69,73,73	2.50	24 (34%)	82,113,113	2.36	27 (32%)
27	LMG	m	2802	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	2 (3%)
23	CLA	B	608	43	69,73,73	2.40	21 (30%)	82,113,113	2.37	30 (36%)
29	GOL	A	417	-	5,5,5	0.92	0	5,5,5	1.10	0
36	HTG	B	627	-	19,19,19	0.93	1 (5%)	23,24,24	1.24	2 (8%)
23	CLA	c	506	3	69,73,73	2.54	23 (33%)	82,113,113	2.30	25 (30%)
34	DMS	O	317	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
34	DMS	X	101	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
28	LMT	d	404	-	25,25,36	0.52	0	30,30,47	0.91	2 (6%)
25	BCR	B	619	-	41,41,41	0.83	0	56,56,56	1.20	5 (8%)
34	DMS	O	315	-	3,3,3	2.75	1 (33%)	3,3,3	0.54	0
34	DMS	d	419	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
23	CLA	C	506	3	69,73,73	2.67	23 (33%)	82,113,113	2.22	29 (35%)
28	LMT	M	101	-	36,36,36	0.47	0	47,47,47	1.28	7 (14%)
23	CLA	c	512	3	69,73,73	2.54	24 (34%)	82,113,113	2.40	27 (32%)
33	PL9	D	2306	-	55,55,55	0.70	2 (3%)	68,69,69	1.56	16 (23%)
34	DMS	c	545	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
20	OEX	a	2604	3,1,43	0,15,15	-	-	-		
24	PHO	A	408	-	58,69,69	2.69	14 (24%)	55,99,99	2.82	14 (25%)
37	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	6 (7%)
37	DGD	c	520	-	63,63,67	0.89	3 (4%)	77,77,81	0.87	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	509	3	69,73,73	2.61	25 (36%)	82,113,113	2.39	30 (36%)
34	DMS	O	316	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
23	CLA	C	513	3	69,73,73	2.83	24 (34%)	82,113,113	2.37	28 (34%)
34	DMS	B	640	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
37	DGD	C	517	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	5 (6%)
27	LMG	c	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.13	4 (6%)
40	RRX	h	101	-	42,42,42	0.71	0	56,58,58	1.41	9 (16%)
36	HTG	b	626	-	19,19,19	1.04	2 (10%)	23,24,24	1.31	1 (4%)
23	CLA	C	514	3	69,73,73	2.48	25 (36%)	82,113,113	2.33	25 (30%)
23	CLA	B	607	2	69,73,73	2.46	21 (30%)	82,113,113	2.31	28 (34%)
34	DMS	T	105	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
33	PL9	d	411	-	55,55,55	0.71	2 (3%)	68,69,69	1.59	15 (22%)
34	DMS	u	504	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
23	CLA	d	409	4	69,73,73	2.52	23 (33%)	82,113,113	2.38	30 (36%)
23	CLA	c	516	3	69,73,73	2.49	25 (36%)	82,113,113	2.30	27 (32%)
25	BCR	c	517	-	41,41,41	0.78	0	56,56,56	1.58	9 (16%)
23	CLA	b	614	2	69,73,73	2.59	24 (34%)	82,113,113	2.24	28 (34%)
36	HTG	o	301	-	19,19,19	0.81	1 (5%)	23,24,24	1.05	2 (8%)
34	DMS	D	2316	-	3,3,3	2.78	1 (33%)	3,3,3	0.54	0
34	DMS	b	633	-	3,3,3	2.56	1 (33%)	3,3,3	0.36	0
34	DMS	a	2623	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
29	GOL	A	415	-	5,5,5	0.85	0	5,5,5	1.17	1 (20%)
34	DMS	O	319	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
23	CLA	a	2609	1	69,73,73	2.50	24 (34%)	82,113,113	2.39	28 (34%)
36	HTG	H	101	-	17,17,19	1.13	2 (11%)	20,21,24	1.63	4 (20%)
34	DMS	b	642	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
34	DMS	V	212	-	3,3,3	2.74	1 (33%)	3,3,3	0.65	0
36	HTG	B	624[B]	-	19,19,19	0.87	1 (5%)	23,24,24	1.75	6 (26%)
25	BCR	C	516	-	41,41,41	0.77	0	56,56,56	1.55	8 (14%)
34	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
34	DMS	o	308	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
23	CLA	c	513	3	69,73,73	2.58	25 (36%)	82,113,113	2.29	29 (35%)
23	CLA	c	507	43	69,73,73	2.26	21 (30%)	82,113,113	2.52	25 (30%)
34	DMS	B	646	-	3,3,3	2.76	1 (33%)	3,3,3	0.72	0
34	DMS	B	642	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	c	521	-	49,49,55	0.92	2 (4%)	57,57,63	1.14	5 (8%)
34	DMS	O	313	-	3,3,3	2.77	1 (33%)	3,3,3	0.62	0
36	HTG	c	523	-	19,19,19	0.93	2 (10%)	23,24,24	1.35	3 (13%)
23	CLA	D	2303	4	69,73,73	2.13	22 (31%)	82,113,113	2.55	28 (34%)
33	PL9	A	422	-	38,38,55	0.42	0	45,45,69	1.89	14 (31%)
26	SQD	b	601	-	46,48,54	0.97	2 (4%)	56,59,65	1.41	9 (16%)
34	DMS	a	2620	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
23	CLA	b	619	2	69,73,73	2.43	25 (36%)	82,113,113	2.53	33 (40%)
23	CLA	C	502	3	69,73,73	2.66	25 (36%)	82,113,113	2.23	25 (30%)
34	DMS	c	533	-	3,3,3	2.67	1 (33%)	3,3,3	0.41	0
34	DMS	o	314	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
34	DMS	A	424	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
28	LMT	Z	101	-	36,36,36	0.45	0	47,47,47	0.91	2 (4%)
38	LHG	d	412	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
34	DMS	l	104	-	3,3,3	2.75	1 (33%)	3,3,3	0.53	0
23	CLA	b	615	43	69,73,73	2.50	25 (36%)	82,113,113	2.36	29 (35%)
34	DMS	c	537	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
39	HEM	F	101	6,5	50,50,50	1.89	10 (20%)	67,82,82	1.33	4 (5%)
42	HEC	V	201	16	46,50,50	2.02	7 (15%)	58,82,82	1.39	5 (8%)
23	CLA	b	609	2	69,73,73	2.76	22 (31%)	82,113,113	2.38	29 (35%)
34	DMS	o	316	-	3,3,3	2.79	1 (33%)	3,3,3	0.61	0
34	DMS	c	544	-	3,3,3	2.79	1 (33%)	3,3,3	0.57	0
23	CLA	B	609	2	69,73,73	2.47	24 (34%)	82,113,113	2.30	28 (34%)
34	DMS	C	530	-	3,3,3	2.73	1 (33%)	3,3,3	0.48	0
26	SQD	B	621	-	52,54,54	1.00	3 (5%)	62,65,65	1.42	8 (12%)
34	DMS	C	537	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
36	HTG	d	415	-	19,19,19	0.96	2 (10%)	23,24,24	1.32	1 (4%)
23	CLA	d	402	43	69,73,73	2.45	21 (30%)	82,113,113	2.49	29 (35%)
34	DMS	C	528	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
23	CLA	b	608	2	69,73,73	2.52	24 (34%)	82,113,113	2.41	30 (36%)
34	DMS	u	503	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
34	DMS	v	213	-	3,3,3	2.72	1 (33%)	3,3,3	0.47	0
34	DMS	A	427	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
34	DMS	c	543	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0
34	DMS	v	209	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HTG	c	526	-	19,19,19	0.91	2 (10%)	23,24,24	1.09	1 (4%)
23	CLA	C	512	3	69,73,73	2.56	22 (31%)	82,113,113	2.30	28 (34%)
34	DMS	b	643	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
37	DGD	c	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.04	4 (5%)
34	DMS	C	534	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
34	DMS	V	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
29	GOL	O	303	-	5,5,5	0.95	0	5,5,5	1.02	0
23	CLA	c	511	3	69,73,73	2.74	24 (34%)	82,113,113	2.33	24 (29%)
27	LMG	C	527	-	51,51,55	0.96	2 (3%)	59,59,63	1.28	6 (10%)
34	DMS	c	534	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
34	DMS	a	2622	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
36	HTG	V	204	-	19,19,19	0.88	1 (5%)	23,24,24	1.68	4 (17%)
38	LHG	d	403	-	42,42,48	0.98	2 (4%)	45,48,54	0.93	3 (6%)
31	JOX	a	2619	-	10,10,10	1.98	6 (60%)	14,14,14	2.35	5 (35%)
34	DMS	B	638	-	3,3,3	2.60	1 (33%)	3,3,3	0.35	0
25	BCR	y	101	-	41,41,41	0.78	0	56,56,56	1.57	11 (19%)
23	CLA	c	510	43	69,73,73	2.51	23 (33%)	82,113,113	2.52	31 (37%)
34	DMS	o	304	-	3,3,3	2.60	1 (33%)	3,3,3	0.33	0
24	PHO	a	2611	-	58,69,69	2.63	11 (18%)	55,99,99	2.81	17 (30%)
25	BCR	C	515	-	41,41,41	0.79	0	56,56,56	1.49	8 (14%)
25	BCR	d	410	-	41,41,41	0.83	0	56,56,56	1.68	5 (8%)
23	CLA	A	407	43	69,73,73	2.21	23 (33%)	82,113,113	2.47	33 (40%)
23	CLA	B	611	43	69,73,73	2.34	25 (36%)	82,113,113	2.51	30 (36%)
34	DMS	O	307	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
25	BCR	B	620	-	41,41,41	0.76	0	56,56,56	1.19	8 (14%)
34	DMS	V	210	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
25	BCR	B	633	-	41,41,41	0.70	0	56,56,56	1.74	13 (23%)
28	LMT	T	103	-	24,24,36	0.61	1 (4%)	29,29,47	0.94	2 (6%)
37	DGD	h	102	-	63,63,67	0.89	2 (3%)	77,77,81	1.03	5 (6%)
28	LMT	J	303	-	24,24,36	0.55	1 (4%)	29,29,47	0.95	1 (3%)
40	RRX	H	102	-	42,42,42	0.69	0	56,58,58	1.48	7 (12%)
38	LHG	L	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.08	5 (9%)
34	DMS	V	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
23	CLA	a	2613	1	69,73,73	2.25	22 (31%)	82,113,113	2.45	30 (36%)
26	SQD	l	101	-	52,54,54	1.00	3 (5%)	62,65,65	1.67	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	c	522	-	51,51,55	0.99	3 (5%)	59,59,63	1.35	7 (11%)
34	DMS	o	306	-	3,3,3	2.76	1 (33%)	3,3,3	0.65	0
29	GOL	c	530	-	5,5,5	0.97	0	5,5,5	0.87	0
23	CLA	C	504	3	69,73,73	2.49	23 (33%)	82,113,113	2.31	27 (32%)
29	GOL	V	203	-	5,5,5	0.94	0	5,5,5	0.99	0
34	DMS	b	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
23	CLA	b	610	2	69,73,73	2.33	23 (33%)	82,113,113	2.60	27 (32%)
29	GOL	D	2301	-	5,5,5	1.05	0	5,5,5	0.86	0
23	CLA	C	510	3	69,73,73	2.53	25 (36%)	82,113,113	2.41	29 (35%)
29	GOL	B	632	-	5,5,5	0.99	0	5,5,5	0.98	0
26	SQD	D	2308	-	43,45,54	1.06	2 (4%)	53,56,65	1.27	7 (13%)
34	DMS	A	425	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
23	CLA	C	505	43	69,73,73	2.36	25 (36%)	82,113,113	2.39	31 (37%)
23	CLA	C	508	43	69,73,73	2.65	23 (33%)	82,113,113	2.44	28 (34%)
34	DMS	U	504	-	3,3,3	2.76	1 (33%)	3,3,3	0.66	0
34	DMS	v	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
36	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	2.10	4 (17%)
29	GOL	o	303	-	5,5,5	1.03	0	5,5,5	1.01	0
36	HTG	b	603	-	19,19,19	0.87	1 (5%)	23,24,24	1.79	4 (17%)
34	DMS	B	647	-	3,3,3	2.74	1 (33%)	3,3,3	0.61	0
29	GOL	d	416	-	5,5,5	0.93	0	5,5,5	1.07	0
23	CLA	A	405	1	69,73,73	2.33	22 (31%)	82,113,113	2.41	30 (36%)
36	HTG	C	525	-	19,19,19	1.00	2 (10%)	23,24,24	1.55	4 (17%)
34	DMS	b	641	-	3,3,3	2.75	1 (33%)	3,3,3	0.42	0
34	DMS	U	505	-	3,3,3	2.75	1 (33%)	3,3,3	0.64	0
34	DMS	V	207	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
34	DMS	B	643	-	3,3,3	2.79	1 (33%)	3,3,3	0.56	0
23	CLA	a	2610	43	69,73,73	2.34	22 (31%)	82,113,113	2.48	31 (37%)
23	CLA	c	508	3	69,73,73	2.54	23 (33%)	82,113,113	2.41	23 (28%)
34	DMS	o	311	-	3,3,3	2.82	1 (33%)	3,3,3	0.61	0
36	HTG	d	407	-	19,19,19	1.05	2 (10%)	23,24,24	1.51	5 (21%)
25	BCR	T	102	-	41,41,41	0.70	0	56,56,56	1.87	14 (25%)
32	BCT	A	421	21	3,3,3	0.52	0	2,3,3	1.07	0
24	PHO	a	2612	-	58,69,69	2.69	12 (20%)	55,99,99	3.11	15 (27%)
36	HTG	B	626	-	19,19,19	0.92	2 (10%)	23,24,24	1.32	1 (4%)
23	CLA	b	616	2	69,73,73	2.33	23 (33%)	82,113,113	2.39	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	d	423	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
28	LMT	z	102	-	33,33,36	0.54	0	43,43,47	1.08	5 (11%)
28	LMT	B	634	-	36,36,36	0.54	1 (2%)	47,47,47	0.86	0
34	DMS	b	638	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
27	LMG	d	414	41	51,51,55	0.91	2 (3%)	59,59,63	0.86	1 (1%)
25	BCR	k	302	-	41,41,41	0.71	0	56,56,56	1.48	13 (23%)
34	DMS	B	644	-	3,3,3	2.74	1 (33%)	3,3,3	0.48	0
23	CLA	c	504	3	69,73,73	2.39	22 (31%)	82,113,113	2.51	28 (34%)
34	DMS	D	2318	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
26	SQD	A	412	-	44,46,54	0.98	2 (4%)	54,57,65	1.52	11 (20%)
37	DGD	C	518	-	63,63,67	0.88	3 (4%)	77,77,81	1.05	6 (7%)
23	CLA	D	2304	4	69,73,73	2.21	22 (31%)	82,113,113	2.44	29 (35%)
28	LMT	B	623	-	36,36,36	0.41	0	47,47,47	1.35	4 (8%)
32	BCT	a	2608	21	3,3,3	0.53	0	2,3,3	1.05	0
34	DMS	A	429	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
36	HTG	B	624[A]	-	19,19,19	0.83	1 (5%)	23,24,24	1.20	2 (8%)
34	DMS	C	536	-	3,3,3	2.73	1 (33%)	3,3,3	0.49	0
29	GOL	C	526	-	5,5,5	1.16	1 (20%)	5,5,5	1.04	0
34	DMS	O	318	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
23	CLA	b	620	2	69,73,73	2.46	23 (33%)	82,113,113	2.20	33 (40%)
34	DMS	A	428	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	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
23	CLA	B	602	43	1/1/15/20	9/39/115/115	-
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
27	LMG	B	622	-	-	16/46/66/70	0/1/1/1
23	CLA	c	511	3	1/1/15/20	3/39/115/115	-
29	GOL	c	529	-	-	0/4/4/4	-
27	LMG	C	527	-	-	14/46/66/70	0/1/1/1
29	GOL	c	531	-	-	2/4/4/4	-
23	CLA	C	513	3	1/1/15/20	9/39/115/115	-
29	GOL	E	104	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	515	3	1/1/15/20	6/39/115/115	-
29	GOL	O	302	-	-	2/4/4/4	-
36	HTG	B	625	-	-	1/10/30/30	0/1/1/1
23	CLA	B	615	2	1/1/15/20	10/39/115/115	-
31	JOX	A	418	-	-	-	0/1/1/1
37	DGD	C	519	-	-	14/47/87/95	0/2/2/2
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	BCR	a	2614	-	-	2/29/63/63	0/2/2/2
33	PL9	x	1301	-	-	12/42/42/73	-
37	DGD	C	517	-	-	18/51/91/95	0/2/2/2
27	LMG	c	501	-	-	11/46/66/70	0/1/1/1
40	RRX	h	101	-	-	1/29/65/65	0/2/2/2
29	GOL	B	648	-	-	0/4/4/4	-
23	CLA	C	514	3	-	7/39/115/115	-
23	CLA	B	607	2	1/1/15/20	3/39/115/115	-
36	HTG	b	626	-	-	6/10/30/30	0/1/1/1
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
37	DGD	H	103	-	-	12/51/91/95	0/2/2/2
36	HTG	C	521	-	-	2/10/30/30	0/1/1/1
38	LHG	d	403	-	-	6/47/47/53	-
31	JOX	a	2619	-	-	-	0/1/1/1
33	PL9	d	411	-	-	3/53/73/73	0/1/1/1
38	LHG	l	103	-	-	14/53/53/53	-
23	CLA	b	612	43	1/1/15/20	0/39/115/115	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	507	3	1/1/15/20	16/39/115/115	-
23	CLA	d	409	4	1/1/15/20	6/39/115/115	-
23	CLA	b	617	2	1/1/15/20	2/39/115/115	-
23	CLA	c	516	3	1/1/15/20	8/39/115/115	-
26	SQD	D	2302	-	-	14/49/69/69	0/1/1/1
25	BCR	c	517	-	-	2/29/63/63	0/2/2/2
23	CLA	c	510	43	1/1/15/20	10/39/115/115	-
23	CLA	B	614	2	1/1/15/20	5/39/115/115	-
24	PHO	a	2611	-	-	3/37/103/103	0/5/6/6
25	BCR	Y	302	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	i	103	-	-	8/15/35/61	0/1/1/2
28	LMT	f	101	-	-	4/15/35/61	0/1/1/2
23	CLA	b	614	2	1/1/15/20	6/39/115/115	-
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	5/29/63/63	0/2/2/2
25	BCR	b	624	-	-	2/29/63/63	0/2/2/2
36	HTG	o	301	-	-	6/10/30/30	0/1/1/1
27	LMG	A	413	-	-	20/46/66/70	0/1/1/1
25	BCR	b	622	-	-	2/29/63/63	0/2/2/2
25	BCR	d	410	-	-	7/29/63/63	0/2/2/2
25	BCR	b	623	-	-	0/29/63/63	0/2/2/2
23	CLA	A	407	43	-	5/39/115/115	-
42	HEC	v	201	16	-	6/14/54/54	-
23	CLA	C	503	3	1/1/15/20	5/39/115/115	-
29	GOL	A	415	-	-	2/4/4/4	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	43	1/1/15/20	4/39/115/115	-
29	GOL	a	2602	-	-	3/4/4/4	-
23	CLA	b	611	2	1/1/15/20	9/39/115/115	-
23	CLA	B	616	2	1/1/15/20	7/39/115/115	-
23	CLA	a	2609	1	1/1/15/20	4/39/115/115	-
36	HTG	H	101	-	-	2/8/25/30	0/1/1/1
36	HTG	B	624[B]	-	-	3/10/30/30	0/1/1/1
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
31	JOX	A	419	-	-	-	0/1/1/1
36	HTG	b	602	-	-	4/10/30/30	0/1/1/1
23	CLA	B	603	2	1/1/15/20	1/39/115/115	-
28	LMT	M	102	-	-	3/21/61/61	0/2/2/2
29	GOL	u	501	-	-	0/4/4/4	-
25	BCR	D	2305	-	-	8/29/63/63	0/2/2/2
28	LMT	m	2803	-	-	2/21/61/61	0/2/2/2
23	CLA	b	607	2	1/1/15/20	2/39/115/115	-
23	CLA	c	513	3	1/1/15/20	6/39/115/115	-
36	HTG	b	604	-	-	1/10/30/30	0/1/1/1
23	CLA	c	507	43	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	633	-	-	3/29/63/63	0/2/2/2
28	LMT	T	103	-	-	9/15/35/61	0/1/1/2
23	CLA	A	406	43	-	2/39/115/115	-
23	CLA	B	605	2	1/1/15/20	6/39/115/115	-
37	DGD	c	519	-	-	17/51/91/95	0/2/2/2
28	LMT	F	102	-	-	5/15/35/61	0/1/1/2
27	LMG	c	521	-	-	14/44/64/70	0/1/1/1
37	DGD	h	102	-	-	12/51/91/95	0/2/2/2
38	LHG	d	413	-	-	10/53/53/53	-
28	LMT	J	303	-	-	5/15/35/61	0/1/1/2
40	RRX	H	102	-	-	1/29/65/65	0/2/2/2
36	HTG	c	523	-	-	0/10/30/30	0/1/1/1
23	CLA	D	2303	4	1/1/15/20	2/39/115/115	-
36	HTG	I	101	-	-	6/10/30/30	0/1/1/1
38	LHG	L	101	-	-	15/53/53/53	-
26	SQD	d	417	-	-	12/33/33/69	-
38	LHG	e	101	-	-	13/44/44/53	-
29	GOL	v	204	-	-	0/4/4/4	-
29	GOL	O	304	-	-	2/4/4/4	-
33	PL9	A	422	-	-	12/42/42/73	-
26	SQD	b	601	-	-	16/43/63/69	0/1/1/1
23	CLA	B	610	2	1/1/15/20	4/39/115/115	-
26	SQD	a	2603	-	-	16/49/69/69	0/1/1/1
38	LHG	D	2309	-	-	13/53/53/53	-
23	CLA	b	619	2	1/1/15/20	6/39/115/115	-
23	CLA	C	502	3	1/1/15/20	3/39/115/115	-
31	JOX	a	2617	-	-	-	0/1/1/1
28	LMT	d	401	-	-	8/21/61/61	0/2/2/2
23	CLA	B	617	2	1/1/15/20	8/39/115/115	-
37	DGD	D	2307	-	-	24/47/68/95	0/1/1/2
23	CLA	a	2613	1	1/1/15/20	8/39/115/115	-
24	PHO	A	409	-	-	2/37/103/103	0/5/6/6
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
23	CLA	b	618	2	1/1/15/20	5/39/115/115	-
26	SQD	l	101	-	-	23/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	522	-	-	5/46/66/70	0/1/1/1
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
29	GOL	c	530	-	-	4/4/4/4	-
38	LHG	D	2311	-	-	8/43/43/53	-
38	LHG	d	412	-	-	13/53/53/53	-
23	CLA	C	504	3	-	5/39/115/115	-
29	GOL	V	203	-	-	0/4/4/4	-
38	LHG	D	2310	-	-	6/53/53/53	-
23	CLA	b	610	2	1/1/15/20	3/39/115/115	-
27	LMG	C	520	-	-	12/46/66/70	0/1/1/1
28	LMT	A	420	-	-	6/15/35/61	0/1/1/2
29	GOL	D	2301	-	-	2/4/4/4	-
23	CLA	B	612	2	1/1/15/20	3/39/115/115	-
27	LMG	D	2312	41	-	6/42/62/70	0/1/1/1
23	CLA	C	510	3	1/1/15/20	6/39/115/115	-
23	CLA	c	505	3	1/1/15/20	5/39/115/115	-
29	GOL	b	631	-	-	0/4/4/4	-
29	GOL	B	632	-	-	2/4/4/4	-
29	GOL	b	644	-	-	2/4/4/4	-
23	CLA	b	615	43	1/1/15/20	5/39/115/115	-
26	SQD	D	2308	-	-	16/40/60/69	0/1/1/1
23	CLA	C	505	43	1/1/15/20	7/39/115/115	-
29	GOL	J	301	-	-	4/4/4/4	-
23	CLA	C	508	43	1/1/15/20	9/39/115/115	-
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
29	GOL	o	303	-	-	0/4/4/4	-
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
23	CLA	b	606	43	1/1/15/20	10/39/115/115	-
38	LHG	E	101	-	-	13/44/44/53	-
26	SQD	a	2615	-	-	7/43/63/69	0/1/1/1
23	CLA	B	604	2	1/1/15/20	7/39/115/115	-
29	GOL	B	630	-	-	0/4/4/4	-
29	GOL	d	416	-	-	2/4/4/4	-
39	HEM	F	101	6,5	-	4/14/54/54	-
42	HEC	V	201	16	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	609	2	1/1/15/20	1/39/115/115	-
23	CLA	A	405	1	1/1/15/20	2/39/115/115	-
23	CLA	c	514	3	1/1/15/20	3/39/115/115	-
23	CLA	A	410	1	1/1/15/20	8/39/115/115	-
23	CLA	b	621	2	1/1/15/20	12/39/115/115	-
23	CLA	C	509	3	1/1/15/20	4/39/115/115	-
27	LMG	m	2802	-	-	11/46/66/70	0/1/1/1
36	HTG	C	525	-	-	0/10/30/30	0/1/1/1
23	CLA	B	608	43	1/1/15/20	3/39/115/115	-
29	GOL	A	417	-	-	3/4/4/4	-
23	CLA	B	606	2	1/1/15/20	9/39/115/115	-
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1
23	CLA	B	609	2	-	1/39/115/115	-
26	SQD	B	621	-	-	22/49/69/69	0/1/1/1
29	GOL	U	501	-	-	0/4/4/4	-
23	CLA	c	506	3	-	4/39/115/115	-
36	HTG	i	102	-	-	6/10/30/30	0/1/1/1
23	CLA	c	508	3	1/1/15/20	8/39/115/115	-
23	CLA	a	2610	43	-	13/39/115/115	-
28	LMT	d	404	-	-	5/17/37/61	0/1/1/2
36	HTG	d	407	-	-	7/10/30/30	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
24	PHO	a	2612	-	-	1/37/103/103	0/5/6/6
23	CLA	C	511	3	1/1/15/20	5/39/115/115	-
23	CLA	C	506	3	1/1/15/20	6/39/115/115	-
23	CLA	d	402	43	1/1/15/20	3/39/115/115	-
29	GOL	C	524	-	-	2/4/4/4	-
29	GOL	v	202	-	-	2/4/4/4	-
29	GOL	v	203	-	-	1/4/4/4	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
36	HTG	d	415	-	-	2/10/30/30	0/1/1/1
23	CLA	b	608	2	1/1/15/20	3/39/115/115	-
23	CLA	b	616	2	1/1/15/20	4/39/115/115	-
29	GOL	a	2618	-	-	1/4/4/4	-
28	LMT	z	102	-	-	12/16/56/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	B	634	-	-	8/21/61/61	0/2/2/2
36	HTG	b	625	-	-	2/10/30/30	0/1/1/1
27	LMG	d	414	41	-	11/46/66/70	0/1/1/1
25	BCR	k	302	-	-	0/29/63/63	0/2/2/2
28	LMT	j	2701	41	-	3/17/57/61	0/2/2/2
23	CLA	C	512	3	1/1/15/20	2/39/115/115	-
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
28	LMT	A	414	-	-	8/19/59/61	0/2/2/2
23	CLA	b	613	2	-	1/39/115/115	-
28	LMT	M	101	-	-	6/21/61/61	0/2/2/2
23	CLA	c	504	3	1/1/15/20	4/39/115/115	-
23	CLA	d	408	4	1/1/15/20	2/39/115/115	-
26	SQD	A	412	-	-	7/41/61/69	0/1/1/1
37	DGD	C	518	-	-	17/51/91/95	0/2/2/2
23	CLA	c	512	3	1/1/15/20	5/39/115/115	-
23	CLA	D	2304	4	1/1/15/20	6/39/115/115	-
33	PL9	D	2306	-	-	3/53/73/73	0/1/1/1
39	HEM	e	103	6,5	-	4/14/54/54	-
28	LMT	B	623	-	-	12/21/61/61	0/2/2/2
28	LMT	m	2804	-	-	9/21/61/61	0/2/2/2
37	DGD	c	518	-	-	15/51/91/95	0/2/2/2
36	HTG	B	624[A]	-	-	2/10/30/30	0/1/1/1
23	CLA	B	613	2	1/1/15/20	3/39/115/115	-
29	GOL	C	526	-	-	2/4/4/4	-
29	GOL	U	502	-	-	2/4/4/4	-
24	PHO	A	408	-	-	4/37/103/103	0/5/6/6
23	CLA	b	620	2	1/1/15/20	5/39/115/115	-
37	DGD	c	520	-	-	10/51/91/95	0/2/2/2
29	GOL	O	303	-	-	0/4/4/4	-
23	CLA	c	509	3	1/1/15/20	9/39/115/115	-
29	GOL	O	305	-	-	1/4/4/4	-

All (1995) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	MG-NA	10.59	2.31	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	MG-NA	10.29	2.30	2.06
23	c	506	CLA	MG-NA	10.17	2.30	2.06
23	c	511	CLA	MG-ND	-9.74	1.86	2.05
24	a	2611	PHO	C1D-C2D	9.44	1.49	1.39
23	b	609	CLA	MG-ND	-9.39	1.87	2.05
23	C	513	CLA	MG-NA	9.27	2.28	2.06
23	C	503	CLA	MG-NA	9.25	2.28	2.06
23	c	514	CLA	MG-NA	9.22	2.28	2.06
23	B	602	CLA	MG-NA	9.19	2.28	2.06
23	B	612	CLA	MG-NA	9.16	2.28	2.06
24	a	2612	PHO	C1D-C2D	9.11	1.49	1.39
23	b	621	CLA	MG-NA	8.95	2.27	2.06
23	C	506	CLA	MG-NA	8.92	2.27	2.06
24	A	408	PHO	C1D-C2D	8.89	1.49	1.39
23	b	621	CLA	MG-ND	-8.84	1.88	2.05
23	b	614	CLA	MG-NA	8.78	2.27	2.06
23	B	616	CLA	MG-NA	8.69	2.26	2.06
24	A	408	PHO	C1B-C2B	8.62	1.49	1.39
24	A	409	PHO	C1B-C2B	8.60	1.49	1.39
23	C	513	CLA	MG-ND	-8.51	1.88	2.05
23	c	504	CLA	MG-NA	8.51	2.26	2.06
23	b	611	CLA	MG-ND	-8.51	1.88	2.05
24	A	409	PHO	C1D-C2D	8.47	1.48	1.39
23	b	609	CLA	MG-NA	8.38	2.26	2.06
23	c	515	CLA	MG-ND	-8.37	1.89	2.05
24	a	2612	PHO	C1B-C2B	8.36	1.48	1.39
23	B	617	CLA	MG-NA	8.34	2.26	2.06
24	A	409	PHO	C3B-C4B	8.31	1.49	1.41
23	b	609	CLA	MG-NC	8.31	2.26	2.06
23	C	502	CLA	MG-NC	8.29	2.26	2.06
23	c	509	CLA	MG-ND	-8.25	1.89	2.05
23	B	608	CLA	MG-NA	8.23	2.25	2.06
23	C	504	CLA	MG-NA	8.19	2.25	2.06
23	b	606	CLA	MG-NC	7.96	2.25	2.06
23	C	511	CLA	MG-NA	7.96	2.25	2.06
23	C	510	CLA	MG-NA	7.96	2.25	2.06
23	a	2609	CLA	MG-ND	-7.95	1.90	2.05
23	b	620	CLA	MG-NA	7.92	2.25	2.06
23	c	511	CLA	MG-NC	7.87	2.25	2.06
23	B	610	CLA	MG-NC	7.84	2.24	2.06
23	b	608	CLA	MG-NA	7.84	2.24	2.06
24	a	2612	PHO	C3B-C4B	7.81	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	MG-ND	-7.79	1.90	2.05
24	a	2611	PHO	C1B-C2B	7.76	1.48	1.39
39	F	101	HEM	C3D-C2D	7.74	1.53	1.36
23	B	603	CLA	MG-ND	-7.73	1.90	2.05
23	c	508	CLA	MG-NA	7.69	2.24	2.06
23	B	607	CLA	MG-NA	7.68	2.24	2.06
39	e	103	HEM	C3D-C2D	7.68	1.53	1.36
23	C	507	CLA	MG-ND	-7.66	1.90	2.05
23	c	513	CLA	MG-ND	-7.66	1.90	2.05
23	c	510	CLA	MG-NA	7.64	2.24	2.06
23	B	604	CLA	MG-NA	7.63	2.24	2.06
23	C	504	CLA	MG-NC	7.54	2.24	2.06
23	c	508	CLA	MG-ND	-7.48	1.91	2.05
23	B	603	CLA	MG-NA	7.46	2.24	2.06
23	c	512	CLA	MG-NA	7.44	2.23	2.06
23	B	604	CLA	MG-NC	7.41	2.23	2.06
23	C	511	CLA	MG-ND	-7.37	1.91	2.05
23	B	617	CLA	MG-ND	-7.35	1.91	2.05
23	b	606	CLA	MG-NA	7.32	2.23	2.06
23	b	613	CLA	MG-ND	-7.31	1.91	2.05
26	d	417	SQD	C6-S	-7.31	1.67	1.77
23	c	510	CLA	MG-ND	-7.26	1.91	2.05
23	C	506	CLA	MG-ND	-7.25	1.91	2.05
23	b	611	CLA	MG-NC	7.25	2.23	2.06
23	C	514	CLA	MG-NC	7.22	2.23	2.06
23	B	609	CLA	MG-ND	-7.21	1.91	2.05
23	b	618	CLA	MG-NC	7.20	2.23	2.06
23	B	606	CLA	MG-NA	7.19	2.23	2.06
23	c	513	CLA	MG-NA	7.12	2.23	2.06
24	A	408	PHO	C4D-CHA	7.11	1.50	1.39
23	B	607	CLA	MG-NC	7.07	2.23	2.06
23	d	408	CLA	MG-NA	7.04	2.23	2.06
23	b	615	CLA	MG-NA	7.03	2.23	2.06
23	b	619	CLA	MG-ND	-7.02	1.91	2.05
23	c	515	CLA	MG-NA	7.01	2.22	2.06
23	b	611	CLA	MG-NA	6.97	2.22	2.06
23	B	605	CLA	MG-NA	6.97	2.22	2.06
23	d	402	CLA	MG-ND	-6.93	1.92	2.05
23	c	516	CLA	MG-NA	6.92	2.22	2.06
23	C	503	CLA	MG-ND	-6.91	1.92	2.05
24	A	409	PHO	C3B-C2B	6.86	1.49	1.40
23	b	612	CLA	MG-NA	6.86	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	PHO	C4D-CHA	6.83	1.49	1.39
23	c	509	CLA	MG-NA	6.76	2.22	2.06
23	B	610	CLA	MG-NA	6.76	2.22	2.06
24	a	2611	PHO	C3B-C2B	6.76	1.49	1.40
42	V	201	HEC	CAB-C3B	6.75	1.56	1.35
23	b	613	CLA	MG-NA	6.75	2.22	2.06
23	c	507	CLA	MG-NA	6.73	2.22	2.06
23	b	614	CLA	MG-NC	6.70	2.22	2.06
23	B	612	CLA	MG-ND	-6.68	1.92	2.05
23	b	607	CLA	MG-NC	6.68	2.22	2.06
23	c	509	CLA	MG-NC	6.67	2.22	2.06
23	C	513	CLA	MG-NB	6.65	2.19	2.05
23	B	609	CLA	MG-NA	6.63	2.22	2.06
23	c	512	CLA	MG-ND	-6.63	1.92	2.05
23	b	610	CLA	MG-NA	6.63	2.22	2.06
24	a	2611	PHO	C4D-CHA	6.57	1.49	1.39
23	C	507	CLA	MG-NA	6.57	2.21	2.06
24	A	408	PHO	C3B-C2B	6.55	1.49	1.40
23	C	506	CLA	MG-NC	6.53	2.21	2.06
23	A	406	CLA	MG-ND	-6.51	1.92	2.05
42	V	201	HEC	CAC-C3C	6.50	1.56	1.35
23	d	409	CLA	MG-NC	6.49	2.21	2.06
23	C	509	CLA	MG-ND	-6.48	1.92	2.05
23	B	613	CLA	MG-ND	-6.45	1.93	2.05
23	C	502	CLA	MG-NA	6.45	2.21	2.06
23	C	510	CLA	MG-ND	-6.43	1.93	2.05
23	b	616	CLA	MG-NA	6.41	2.21	2.06
23	b	615	CLA	MG-ND	-6.40	1.93	2.05
23	d	409	CLA	MG-NA	6.40	2.21	2.06
23	b	607	CLA	MG-NA	6.39	2.21	2.06
23	c	506	CLA	MG-NC	6.38	2.21	2.06
42	v	201	HEC	CAC-C3C	6.37	1.55	1.35
23	C	507	CLA	MG-NC	6.36	2.21	2.06
24	a	2612	PHO	C3B-C2B	6.32	1.48	1.40
23	C	508	CLA	MG-NB	-6.31	1.93	2.05
23	d	409	CLA	MG-ND	-6.31	1.93	2.05
23	A	405	CLA	MG-NA	6.29	2.21	2.06
23	c	505	CLA	MG-NA	6.29	2.21	2.06
23	B	605	CLA	MG-ND	-6.26	1.93	2.05
42	v	201	HEC	CAB-C3B	6.26	1.55	1.35
23	B	614	CLA	MG-NA	6.20	2.21	2.06
23	a	2610	CLA	MG-NA	6.20	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2609	CLA	MG-NC	6.17	2.20	2.06
23	c	512	CLA	MG-NC	6.16	2.20	2.06
23	B	605	CLA	MG-NC	6.16	2.20	2.06
23	c	504	CLA	MG-ND	-6.13	1.93	2.05
23	d	408	CLA	MG-NC	6.13	2.20	2.06
23	B	610	CLA	C1D-ND	6.12	1.45	1.37
23	D	2304	CLA	C3C-C2C	6.12	1.50	1.36
23	b	617	CLA	MG-ND	-6.08	1.93	2.05
23	b	608	CLA	MG-NC	6.08	2.20	2.06
23	c	510	CLA	MG-NC	6.06	2.20	2.06
24	a	2611	PHO	C3B-C4B	6.04	1.47	1.41
23	C	513	CLA	MG-NC	6.03	2.20	2.06
26	d	417	SQD	O47-C7	6.02	1.46	1.33
23	b	606	CLA	C3C-C2C	6.01	1.49	1.36
23	B	602	CLA	MG-NC	6.00	2.20	2.06
23	b	610	CLA	MG-NC	5.99	2.20	2.06
23	c	516	CLA	MG-NC	5.96	2.20	2.06
23	B	602	CLA	C3C-C2C	5.95	1.49	1.36
23	C	502	CLA	MG-ND	-5.95	1.94	2.05
24	a	2612	PHO	C4D-CHA	5.91	1.48	1.39
23	b	618	CLA	MG-NA	5.90	2.20	2.06
23	c	511	CLA	C3C-C2C	5.89	1.49	1.36
23	C	509	CLA	C3C-C2C	5.88	1.49	1.36
23	c	506	CLA	C3C-C2C	5.88	1.49	1.36
23	C	505	CLA	MG-NC	5.87	2.20	2.06
23	C	509	CLA	MG-NC	5.87	2.20	2.06
23	B	610	CLA	C3C-C2C	5.87	1.49	1.36
23	d	409	CLA	C3C-C2C	5.86	1.49	1.36
23	B	616	CLA	MG-ND	-5.85	1.94	2.05
23	d	408	CLA	MG-ND	-5.83	1.94	2.05
23	b	607	CLA	MG-ND	-5.82	1.94	2.05
23	C	514	CLA	C1D-ND	5.82	1.45	1.37
23	C	511	CLA	C3C-C2C	5.82	1.49	1.36
23	a	2610	CLA	MG-ND	-5.81	1.94	2.05
23	a	2613	CLA	C3C-C2C	5.81	1.49	1.36
23	c	516	CLA	MG-ND	-5.81	1.94	2.05
24	A	408	PHO	C3D-C2D	5.80	1.49	1.39
23	b	612	CLA	C3C-C2C	5.80	1.49	1.36
23	C	513	CLA	C3C-C2C	5.79	1.49	1.36
23	C	503	CLA	C3C-C2C	5.78	1.49	1.36
23	a	2613	CLA	MG-NC	5.78	2.20	2.06
23	b	614	CLA	C3C-C2C	5.77	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C3C-C2C	5.76	1.49	1.36
23	C	502	CLA	C1D-ND	5.75	1.45	1.37
23	B	611	CLA	C3C-C2C	5.75	1.49	1.36
23	C	507	CLA	C3C-C2C	5.75	1.49	1.36
23	C	506	CLA	C3C-C2C	5.74	1.49	1.36
23	c	515	CLA	C3C-C2C	5.73	1.49	1.36
23	b	608	CLA	C3C-C2C	5.73	1.49	1.36
23	c	509	CLA	C1D-ND	5.73	1.45	1.37
23	D	2303	CLA	C3C-C2C	5.73	1.49	1.36
23	b	611	CLA	C1D-ND	5.73	1.45	1.37
23	B	607	CLA	C3C-C2C	5.72	1.49	1.36
23	b	618	CLA	C3C-C2C	5.72	1.49	1.36
24	A	408	PHO	C3B-C4B	5.72	1.47	1.41
23	c	515	CLA	C1D-ND	5.71	1.45	1.37
23	C	510	CLA	C3C-C2C	5.71	1.49	1.36
23	A	405	CLA	C3C-C2C	5.71	1.49	1.36
23	b	615	CLA	C1D-ND	5.70	1.45	1.37
23	b	606	CLA	C1D-ND	5.70	1.45	1.37
23	c	508	CLA	MG-NC	5.69	2.19	2.06
23	B	615	CLA	MG-NA	5.68	2.19	2.06
23	b	615	CLA	C3C-C2C	5.68	1.49	1.36
23	b	620	CLA	MG-NC	5.67	2.19	2.06
23	c	511	CLA	MG-NB	5.67	2.17	2.05
23	c	509	CLA	C3C-C2C	5.67	1.49	1.36
23	B	611	CLA	MG-NC	5.66	2.19	2.06
23	b	617	CLA	MG-NC	5.66	2.19	2.06
23	C	514	CLA	MG-ND	-5.66	1.94	2.05
23	c	505	CLA	MG-NC	5.66	2.19	2.06
23	d	402	CLA	MG-NA	5.65	2.19	2.06
23	C	504	CLA	C3C-C2C	5.65	1.49	1.36
23	b	610	CLA	C3C-C2C	5.63	1.48	1.36
23	c	508	CLA	C1D-ND	5.62	1.45	1.37
23	C	512	CLA	C3C-C2C	5.61	1.48	1.36
23	C	514	CLA	C3C-C2C	5.61	1.48	1.36
23	b	607	CLA	C3C-C2C	5.59	1.48	1.36
23	b	609	CLA	C1D-ND	5.59	1.45	1.37
23	c	513	CLA	C1D-ND	5.59	1.45	1.37
23	A	405	CLA	MG-ND	-5.58	1.94	2.05
23	a	2609	CLA	C3C-C2C	5.57	1.48	1.36
23	C	507	CLA	C1D-ND	5.57	1.45	1.37
23	B	615	CLA	C3C-C2C	5.56	1.48	1.36
23	c	516	CLA	C1D-ND	5.54	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3C-C2C	5.54	1.48	1.36
23	B	603	CLA	C3C-C2C	5.53	1.48	1.36
42	v	201	HEC	C3D-C2D	5.53	1.53	1.38
23	B	605	CLA	C1D-ND	5.53	1.45	1.37
23	C	502	CLA	C3C-C2C	5.53	1.48	1.36
23	b	608	CLA	MG-ND	-5.53	1.94	2.05
23	B	604	CLA	C3C-C2C	5.53	1.48	1.36
23	b	619	CLA	C1D-ND	5.52	1.45	1.37
23	C	513	CLA	CHC-C1C	5.52	1.49	1.38
23	B	604	CLA	C1D-ND	5.52	1.45	1.37
23	b	617	CLA	C3C-C2C	5.51	1.48	1.36
23	B	602	CLA	C1D-ND	5.50	1.45	1.37
23	C	506	CLA	C1D-ND	5.50	1.45	1.37
23	b	614	CLA	C1D-ND	5.50	1.45	1.37
23	C	510	CLA	C1D-ND	5.50	1.45	1.37
23	d	402	CLA	C3C-C2C	5.49	1.48	1.36
23	B	609	CLA	C3C-C2C	5.47	1.48	1.36
23	b	609	CLA	C3C-C2C	5.47	1.48	1.36
23	b	607	CLA	C1D-ND	5.47	1.45	1.37
23	c	516	CLA	C3C-C2C	5.47	1.48	1.36
23	B	608	CLA	C3C-C2C	5.46	1.48	1.36
23	c	513	CLA	C3C-C2C	5.46	1.48	1.36
23	B	613	CLA	MG-NA	5.45	2.19	2.06
23	c	512	CLA	C1D-ND	5.45	1.45	1.37
23	B	602	CLA	CHC-C1C	5.44	1.49	1.38
23	c	515	CLA	MG-NC	5.44	2.19	2.06
23	A	407	CLA	C3C-C2C	5.44	1.48	1.36
23	c	513	CLA	MG-NC	5.43	2.19	2.06
23	B	617	CLA	C1D-ND	5.42	1.45	1.37
23	c	512	CLA	C3C-C2C	5.42	1.48	1.36
23	C	502	CLA	CHC-C1C	5.42	1.49	1.38
23	c	508	CLA	C3C-C2C	5.42	1.48	1.36
23	B	614	CLA	C1D-ND	5.42	1.45	1.37
23	B	612	CLA	C1D-ND	5.42	1.45	1.37
23	b	620	CLA	C3C-C2C	5.42	1.48	1.36
23	A	410	CLA	MG-NA	5.41	2.19	2.06
23	B	611	CLA	C1D-ND	5.41	1.45	1.37
23	b	613	CLA	C3C-C2C	5.40	1.48	1.36
23	a	2609	CLA	MG-NA	5.40	2.19	2.06
23	B	617	CLA	MG-NC	5.38	2.19	2.06
24	a	2611	PHO	C3D-C2D	5.38	1.48	1.39
23	c	514	CLA	C3C-C2C	5.38	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3C-C2C	5.38	1.48	1.36
23	b	619	CLA	C3C-C2C	5.37	1.48	1.36
23	b	620	CLA	CHC-C1C	5.37	1.49	1.38
23	C	513	CLA	C1D-ND	5.35	1.44	1.37
23	D	2304	CLA	CHC-C1C	5.35	1.49	1.38
23	a	2610	CLA	C3C-C2C	5.34	1.48	1.36
24	A	409	PHO	C3D-C2D	5.34	1.48	1.39
42	V	201	HEC	C3D-C2D	5.33	1.52	1.38
23	C	508	CLA	C3C-C2C	5.33	1.48	1.36
23	d	408	CLA	C3C-C2C	5.32	1.48	1.36
23	A	410	CLA	C3C-C2C	5.32	1.48	1.36
23	c	511	CLA	C1D-ND	5.32	1.44	1.37
23	c	507	CLA	C3C-C2C	5.31	1.48	1.36
23	d	409	CLA	C1D-ND	5.31	1.44	1.37
23	b	610	CLA	MG-ND	-5.31	1.95	2.05
23	b	613	CLA	C1D-ND	5.31	1.44	1.37
23	b	614	CLA	O2D-CGD	5.30	1.46	1.33
23	b	620	CLA	C1D-ND	5.30	1.44	1.37
23	b	606	CLA	CHC-C1C	5.28	1.49	1.38
23	C	506	CLA	CHD-C1D	5.28	1.48	1.38
23	b	621	CLA	C1D-ND	5.28	1.44	1.37
24	a	2612	PHO	C3D-C2D	5.27	1.48	1.39
23	B	612	CLA	C3C-C2C	5.27	1.48	1.36
23	C	514	CLA	CHC-C1C	5.27	1.49	1.38
23	C	505	CLA	MG-NA	5.27	2.18	2.06
23	B	607	CLA	CHC-C1C	5.26	1.49	1.38
23	B	607	CLA	C1D-ND	5.26	1.44	1.37
23	b	619	CLA	MG-NA	5.26	2.18	2.06
23	b	606	CLA	CHD-C1D	5.26	1.48	1.38
23	C	504	CLA	C1D-ND	5.25	1.44	1.37
23	c	516	CLA	CHC-C1C	5.25	1.49	1.38
23	c	504	CLA	C3C-C2C	5.25	1.48	1.36
23	B	609	CLA	C1D-ND	5.25	1.44	1.37
23	B	603	CLA	C1D-ND	5.24	1.44	1.37
23	c	510	CLA	C3C-C2C	5.24	1.48	1.36
23	C	508	CLA	MG-NC	5.23	2.18	2.06
23	B	606	CLA	MG-NC	5.23	2.18	2.06
23	B	617	CLA	C3C-C2C	5.22	1.48	1.36
23	B	614	CLA	O2D-CGD	5.21	1.46	1.33
23	B	604	CLA	CHC-C1C	5.21	1.48	1.38
23	a	2610	CLA	C1D-ND	5.20	1.44	1.37
23	b	616	CLA	C3C-C2C	5.19	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	O2D-CGD	5.19	1.46	1.33
23	a	2613	CLA	C1D-ND	5.18	1.44	1.37
23	C	508	CLA	C1D-ND	5.18	1.44	1.37
23	B	605	CLA	C3C-C2C	5.18	1.47	1.36
23	B	614	CLA	C3C-C2C	5.18	1.47	1.36
23	c	505	CLA	CHC-C1C	5.18	1.48	1.38
23	A	410	CLA	C1D-ND	5.18	1.44	1.37
23	C	506	CLA	CHC-C1C	5.17	1.48	1.38
23	b	615	CLA	CHC-C1C	5.16	1.48	1.38
23	A	406	CLA	MG-NA	5.15	2.18	2.06
23	b	608	CLA	C1D-ND	5.15	1.44	1.37
39	F	101	HEM	FE-ND	5.15	2.10	1.94
23	C	507	CLA	O2D-CGD	5.14	1.45	1.33
23	A	406	CLA	C3C-C2C	5.14	1.47	1.36
23	C	505	CLA	C1D-ND	5.12	1.44	1.37
23	c	506	CLA	CHC-C1C	5.12	1.48	1.38
23	c	505	CLA	C1D-ND	5.12	1.44	1.37
23	d	402	CLA	MG-NB	5.12	2.15	2.05
23	b	610	CLA	C1D-ND	5.11	1.44	1.37
23	c	509	CLA	O2D-CGD	5.11	1.45	1.33
23	B	602	CLA	CHD-C1D	5.11	1.48	1.38
23	b	621	CLA	O2D-CGD	5.10	1.45	1.33
23	b	606	CLA	O2D-CGD	5.10	1.45	1.33
23	B	606	CLA	C1D-ND	5.10	1.44	1.37
39	e	103	HEM	FE-ND	5.10	2.10	1.94
23	B	616	CLA	C3C-C2C	5.09	1.47	1.36
23	B	614	CLA	MG-ND	-5.09	1.95	2.05
23	D	2303	CLA	MG-NC	5.09	2.18	2.06
23	B	606	CLA	C3C-C2C	5.09	1.47	1.36
23	A	410	CLA	MG-NC	5.08	2.18	2.06
23	B	609	CLA	CHC-C1C	5.08	1.48	1.38
23	C	502	CLA	CHD-C1D	5.08	1.48	1.38
23	b	614	CLA	CHC-C1C	5.08	1.48	1.38
23	b	621	CLA	C3C-C2C	5.08	1.47	1.36
23	B	613	CLA	C3C-C2C	5.08	1.47	1.36
23	b	613	CLA	MG-NC	5.07	2.18	2.06
23	d	402	CLA	C1D-ND	5.07	1.44	1.37
23	b	616	CLA	C1D-ND	5.06	1.44	1.37
23	C	509	CLA	CHC-C1C	5.06	1.48	1.38
23	c	515	CLA	CHC-C1C	5.06	1.48	1.38
23	c	511	CLA	CHC-C1C	5.06	1.48	1.38
23	B	615	CLA	CHC-C1C	5.06	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C1D-ND	5.05	1.44	1.37
23	C	507	CLA	CHC-C1C	5.05	1.48	1.38
23	c	507	CLA	O2D-CGD	5.04	1.45	1.33
23	C	509	CLA	C1D-ND	5.03	1.44	1.37
23	b	606	CLA	MG-ND	-5.03	1.95	2.05
23	B	615	CLA	C1D-ND	5.02	1.44	1.37
23	a	2610	CLA	CHC-C1C	5.01	1.48	1.38
23	B	602	CLA	O2D-CGD	5.01	1.45	1.33
23	C	503	CLA	CHC-C1C	5.01	1.48	1.38
23	b	613	CLA	O2D-CGD	5.00	1.45	1.33
23	c	515	CLA	MG-NB	5.00	2.15	2.05
23	d	409	CLA	CHC-C1C	5.00	1.48	1.38
23	b	614	CLA	CHD-C1D	4.99	1.48	1.38
23	C	504	CLA	CHC-C1C	4.99	1.48	1.38
23	c	514	CLA	CHC-C1C	4.99	1.48	1.38
23	A	407	CLA	CHC-C1C	4.98	1.48	1.38
23	b	619	CLA	O2D-CGD	4.98	1.45	1.33
23	c	506	CLA	C1D-ND	4.98	1.44	1.37
23	b	620	CLA	O2D-CGD	4.98	1.45	1.33
23	b	619	CLA	MG-NC	4.97	2.18	2.06
23	b	607	CLA	O2D-CGD	4.97	1.45	1.33
23	B	611	CLA	CHC-C1C	4.96	1.48	1.38
23	c	507	CLA	CHC-C1C	4.96	1.48	1.38
23	b	617	CLA	C1D-ND	4.95	1.44	1.37
23	c	513	CLA	CHC-C1C	4.95	1.48	1.38
23	c	510	CLA	C1D-ND	4.95	1.44	1.37
23	A	410	CLA	CHC-C1C	4.95	1.48	1.38
23	c	505	CLA	O2D-CGD	4.94	1.45	1.33
23	c	514	CLA	C1D-ND	4.94	1.44	1.37
23	b	619	CLA	CHC-C1C	4.94	1.48	1.38
23	B	608	CLA	C1D-ND	4.94	1.44	1.37
23	C	505	CLA	CHC-C1C	4.94	1.48	1.38
23	c	513	CLA	O2D-CGD	4.94	1.45	1.33
23	c	505	CLA	MG-ND	-4.94	1.96	2.05
23	a	2613	CLA	O2D-CGD	4.94	1.45	1.33
23	C	505	CLA	O2D-CGD	4.93	1.45	1.33
23	c	507	CLA	MG-ND	-4.92	1.96	2.05
23	B	606	CLA	CHC-C1C	4.92	1.48	1.38
23	B	604	CLA	MG-ND	-4.92	1.96	2.05
23	C	511	CLA	MG-NB	4.92	2.15	2.05
23	B	610	CLA	CHC-C1C	4.91	1.48	1.38
23	b	612	CLA	MG-ND	-4.91	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	O2D-CGD	4.91	1.45	1.33
23	C	509	CLA	MG-NB	4.91	2.15	2.05
23	a	2609	CLA	C1D-ND	4.91	1.44	1.37
23	C	511	CLA	CHC-C1C	4.90	1.48	1.38
23	c	514	CLA	CHD-C1D	4.90	1.48	1.38
24	A	409	PHO	O2D-CGD	4.90	1.45	1.33
23	c	509	CLA	CHD-C1D	4.90	1.48	1.38
24	a	2611	PHO	O2D-CGD	4.89	1.45	1.33
23	C	512	CLA	CHC-C1C	4.89	1.48	1.38
39	e	103	HEM	FE-NB	4.89	2.09	1.94
23	d	409	CLA	O2D-CGD	4.88	1.45	1.33
23	a	2613	CLA	CHC-C1C	4.88	1.48	1.38
23	C	511	CLA	MG-NC	4.88	2.17	2.06
23	B	616	CLA	O2D-CGD	4.88	1.45	1.33
23	b	609	CLA	CHC-C1C	4.88	1.48	1.38
23	B	612	CLA	CHC-C1C	4.87	1.48	1.38
23	c	504	CLA	CHC-C1C	4.87	1.48	1.38
23	b	607	CLA	CHC-C1C	4.87	1.48	1.38
23	d	402	CLA	O2D-CGD	4.86	1.45	1.33
23	C	511	CLA	C1D-ND	4.86	1.44	1.37
23	C	510	CLA	O2D-CGD	4.85	1.45	1.33
23	C	514	CLA	CHD-C1D	4.85	1.47	1.38
23	c	511	CLA	CHD-C1D	4.85	1.47	1.38
23	B	616	CLA	C1D-ND	4.85	1.44	1.37
23	b	618	CLA	CHC-C1C	4.84	1.48	1.38
23	B	614	CLA	CHC-C1C	4.84	1.48	1.38
23	b	616	CLA	O2D-CGD	4.83	1.45	1.33
23	C	506	CLA	O2D-CGD	4.83	1.45	1.33
23	C	514	CLA	O2D-CGD	4.83	1.45	1.33
23	B	613	CLA	CHC-C1C	4.83	1.48	1.38
23	B	613	CLA	CHB-C1B	4.83	1.50	1.39
23	C	503	CLA	C1D-ND	4.82	1.44	1.37
23	C	512	CLA	C1D-ND	4.82	1.44	1.37
24	a	2612	PHO	O2D-CGD	4.82	1.45	1.33
23	B	603	CLA	CHD-C1D	4.82	1.47	1.38
23	B	603	CLA	CHC-C1C	4.82	1.48	1.38
23	b	608	CLA	CHC-C1C	4.82	1.48	1.38
23	b	618	CLA	O2D-CGD	4.81	1.45	1.33
23	b	607	CLA	CHD-C1D	4.81	1.47	1.38
23	A	407	CLA	O2D-CGD	4.81	1.45	1.33
23	b	615	CLA	MG-NC	4.80	2.17	2.06
23	B	617	CLA	O2D-CGD	4.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CHB-C1B	4.80	1.50	1.39
23	A	407	CLA	C1D-ND	4.80	1.44	1.37
23	c	509	CLA	CHC-C1C	4.79	1.48	1.38
23	B	607	CLA	CHD-C1D	4.79	1.47	1.38
23	A	410	CLA	CHD-C1D	4.78	1.47	1.38
23	c	516	CLA	CHD-C1D	4.78	1.47	1.38
23	b	612	CLA	MG-NC	4.78	2.17	2.06
23	C	511	CLA	CHB-C1B	4.78	1.50	1.39
23	C	508	CLA	O2D-CGD	4.77	1.45	1.33
24	A	408	PHO	O2D-CGD	4.77	1.44	1.33
23	D	2304	CLA	O2D-CGD	4.76	1.44	1.33
23	B	614	CLA	MG-NC	4.76	2.17	2.06
23	c	512	CLA	O2D-CGD	4.76	1.44	1.33
23	c	516	CLA	O2D-CGD	4.75	1.44	1.33
23	b	611	CLA	CHC-C1C	4.75	1.48	1.38
23	d	408	CLA	CHC-C1C	4.75	1.48	1.38
23	C	502	CLA	O2D-CGD	4.75	1.44	1.33
23	A	405	CLA	C1D-ND	4.75	1.44	1.37
23	C	513	CLA	O2D-CGD	4.74	1.44	1.33
23	b	616	CLA	CHD-C1D	4.74	1.47	1.38
23	b	611	CLA	O2D-CGD	4.74	1.44	1.33
23	b	613	CLA	CHC-C1C	4.74	1.48	1.38
23	b	617	CLA	O2D-CGD	4.74	1.44	1.33
23	B	606	CLA	CHD-C1D	4.73	1.47	1.38
23	C	510	CLA	CHC-C1C	4.73	1.48	1.38
34	c	532	DMS	O-S	4.73	1.81	1.50
23	C	512	CLA	CHD-C1D	4.73	1.47	1.38
23	A	410	CLA	MG-ND	-4.73	1.96	2.05
34	o	311	DMS	O-S	4.72	1.81	1.50
23	C	503	CLA	O2D-CGD	4.72	1.44	1.33
23	C	512	CLA	MG-ND	-4.72	1.96	2.05
23	A	406	CLA	C1D-ND	4.72	1.44	1.37
23	C	509	CLA	O2D-CGD	4.72	1.44	1.33
23	B	608	CLA	CHC-C1C	4.71	1.47	1.38
23	C	513	CLA	CHD-C1D	4.71	1.47	1.38
23	b	608	CLA	O2D-CGD	4.70	1.44	1.33
34	b	637	DMS	O-S	4.70	1.81	1.50
23	c	512	CLA	CHC-C1C	4.70	1.47	1.38
23	B	607	CLA	CHC-C4B	4.70	1.49	1.39
34	c	544	DMS	O-S	4.70	1.81	1.50
23	b	612	CLA	O2D-CGD	4.70	1.44	1.33
23	C	503	CLA	CHD-C1D	4.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	O2D-CGD	4.69	1.44	1.33
34	a	2624	DMS	O-S	4.69	1.81	1.50
23	c	508	CLA	CHC-C1C	4.69	1.47	1.38
23	B	616	CLA	CHC-C1C	4.69	1.47	1.38
23	C	512	CLA	O2D-CGD	4.68	1.44	1.33
23	b	617	CLA	CHC-C1C	4.68	1.47	1.38
23	B	604	CLA	CHC-C4B	4.68	1.49	1.39
34	A	430	DMS	O-S	4.67	1.81	1.50
34	B	643	DMS	O-S	4.67	1.81	1.50
23	B	608	CLA	O2D-CGD	4.67	1.44	1.33
23	c	506	CLA	CHB-C1B	4.67	1.49	1.39
23	a	2609	CLA	CHC-C1C	4.67	1.47	1.38
34	o	316	DMS	O-S	4.67	1.81	1.50
23	b	608	CLA	CHD-C1D	4.67	1.47	1.38
23	B	607	CLA	O2D-CGD	4.67	1.44	1.33
34	c	549	DMS	O-S	4.67	1.81	1.50
23	C	502	CLA	CHC-C4B	4.66	1.49	1.39
34	o	313	DMS	O-S	4.66	1.81	1.50
34	D	2316	DMS	O-S	4.66	1.81	1.50
23	B	610	CLA	CHD-C1D	4.66	1.47	1.38
23	d	402	CLA	CHC-C1C	4.66	1.47	1.38
23	b	610	CLA	O2D-CGD	4.65	1.44	1.33
34	V	206	DMS	O-S	4.65	1.80	1.50
23	b	616	CLA	CHC-C1C	4.65	1.47	1.38
23	C	505	CLA	CHD-C1D	4.65	1.47	1.38
34	C	531	DMS	O-S	4.65	1.80	1.50
23	c	513	CLA	CHD-C1D	4.65	1.47	1.38
34	B	639	DMS	O-S	4.65	1.80	1.50
23	c	510	CLA	O2D-CGD	4.64	1.44	1.33
23	B	617	CLA	CHC-C1C	4.64	1.47	1.38
34	O	313	DMS	O-S	4.64	1.80	1.50
34	U	503	DMS	O-S	4.64	1.80	1.50
34	T	105	DMS	O-S	4.64	1.80	1.50
34	B	635	DMS	O-S	4.63	1.80	1.50
34	O	314	DMS	O-S	4.63	1.80	1.50
34	b	635	DMS	O-S	4.63	1.80	1.50
23	B	606	CLA	O2D-CGD	4.63	1.44	1.33
23	C	509	CLA	MG-NA	4.63	2.17	2.06
34	O	308	DMS	O-S	4.63	1.80	1.50
34	O	312	DMS	O-S	4.63	1.80	1.50
34	c	546	DMS	O-S	4.63	1.80	1.50
34	b	643	DMS	O-S	4.63	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	MG-NA	4.63	2.17	2.06
23	b	609	CLA	O2D-CGD	4.63	1.44	1.33
34	v	206	DMS	O-S	4.63	1.80	1.50
34	l	104	DMS	O-S	4.63	1.80	1.50
34	U	504	DMS	O-S	4.63	1.80	1.50
34	A	428	DMS	O-S	4.62	1.80	1.50
34	c	547	DMS	O-S	4.62	1.80	1.50
23	A	405	CLA	O2D-CGD	4.62	1.44	1.33
34	D	2317	DMS	O-S	4.62	1.80	1.50
34	O	315	DMS	O-S	4.62	1.80	1.50
34	V	205	DMS	O-S	4.62	1.80	1.50
34	C	528	DMS	O-S	4.62	1.80	1.50
34	b	641	DMS	O-S	4.62	1.80	1.50
23	c	504	CLA	O2D-CGD	4.62	1.44	1.33
34	c	542	DMS	O-S	4.62	1.80	1.50
34	B	646	DMS	O-S	4.62	1.80	1.50
34	B	644	DMS	O-S	4.62	1.80	1.50
34	t	102	DMS	O-S	4.62	1.80	1.50
34	c	540	DMS	O-S	4.62	1.80	1.50
34	B	637	DMS	O-S	4.62	1.80	1.50
34	A	426	DMS	O-S	4.61	1.80	1.50
34	c	537	DMS	O-S	4.61	1.80	1.50
34	o	309	DMS	O-S	4.61	1.80	1.50
34	c	538	DMS	O-S	4.61	1.80	1.50
34	A	429	DMS	O-S	4.61	1.80	1.50
23	c	515	CLA	O2D-CGD	4.61	1.44	1.33
34	B	641	DMS	O-S	4.61	1.80	1.50
34	B	645	DMS	O-S	4.61	1.80	1.50
34	b	636	DMS	O-S	4.61	1.80	1.50
34	V	208	DMS	O-S	4.61	1.80	1.50
34	o	306	DMS	O-S	4.61	1.80	1.50
34	c	545	DMS	O-S	4.61	1.80	1.50
34	V	211	DMS	O-S	4.61	1.80	1.50
23	B	608	CLA	MG-NC	4.60	2.17	2.06
34	o	305	DMS	O-S	4.60	1.80	1.50
34	D	2319	DMS	O-S	4.60	1.80	1.50
34	U	505	DMS	O-S	4.60	1.80	1.50
34	d	423	DMS	O-S	4.60	1.80	1.50
34	v	210	DMS	O-S	4.60	1.80	1.50
34	a	2620	DMS	O-S	4.60	1.80	1.50
34	C	537	DMS	O-S	4.60	1.80	1.50
34	O	317	DMS	O-S	4.60	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	647	DMS	O-S	4.60	1.80	1.50
34	v	214	DMS	O-S	4.60	1.80	1.50
23	C	504	CLA	CHC-C4B	4.60	1.49	1.39
34	O	311	DMS	O-S	4.60	1.80	1.50
34	V	210	DMS	O-S	4.59	1.80	1.50
34	O	309	DMS	O-S	4.59	1.80	1.50
34	T	104	DMS	O-S	4.59	1.80	1.50
34	v	208	DMS	O-S	4.59	1.80	1.50
34	o	315	DMS	O-S	4.59	1.80	1.50
34	X	101	DMS	O-S	4.59	1.80	1.50
34	V	212	DMS	O-S	4.59	1.80	1.50
23	B	603	CLA	O2D-CGD	4.59	1.44	1.33
34	v	211	DMS	O-S	4.59	1.80	1.50
34	v	212	DMS	O-S	4.59	1.80	1.50
23	C	508	CLA	MG-ND	-4.59	1.96	2.05
34	O	319	DMS	O-S	4.59	1.80	1.50
34	H	104	DMS	O-S	4.59	1.80	1.50
34	c	541	DMS	O-S	4.59	1.80	1.50
34	b	639	DMS	O-S	4.59	1.80	1.50
23	B	604	CLA	O2D-CGD	4.59	1.44	1.33
34	c	539	DMS	O-S	4.59	1.80	1.50
23	C	511	CLA	O2D-CGD	4.59	1.44	1.33
34	c	548	DMS	O-S	4.59	1.80	1.50
34	b	642	DMS	O-S	4.59	1.80	1.50
34	o	310	DMS	O-S	4.58	1.80	1.50
23	b	613	CLA	CHD-C1D	4.58	1.47	1.38
34	C	536	DMS	O-S	4.58	1.80	1.50
34	A	427	DMS	O-S	4.58	1.80	1.50
34	b	638	DMS	O-S	4.58	1.80	1.50
34	V	207	DMS	O-S	4.58	1.80	1.50
23	d	402	CLA	CHD-C1D	4.58	1.47	1.38
34	a	2621	DMS	O-S	4.58	1.80	1.50
34	V	213	DMS	O-S	4.58	1.80	1.50
34	C	530	DMS	O-S	4.58	1.80	1.50
23	C	508	CLA	CHC-C1C	4.58	1.47	1.38
23	B	602	CLA	O2A-CGA	4.58	1.46	1.33
34	O	318	DMS	O-S	4.58	1.80	1.50
23	B	611	CLA	MG-ND	-4.58	1.96	2.05
23	d	408	CLA	O2A-CGA	4.58	1.46	1.33
23	b	614	CLA	CHB-C1B	4.58	1.49	1.39
34	O	306	DMS	O-S	4.58	1.80	1.50
27	m	2802	LMG	O8-C28	4.58	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHB-C1B	4.57	1.49	1.39
34	d	419	DMS	O-S	4.57	1.80	1.50
34	D	2320	DMS	O-S	4.57	1.80	1.50
34	v	209	DMS	O-S	4.57	1.80	1.50
34	v	213	DMS	O-S	4.57	1.80	1.50
34	o	308	DMS	O-S	4.57	1.80	1.50
34	d	421	DMS	O-S	4.57	1.80	1.50
34	u	504	DMS	O-S	4.57	1.80	1.50
34	u	502	DMS	O-S	4.57	1.80	1.50
34	a	2622	DMS	O-S	4.57	1.80	1.50
34	d	420	DMS	O-S	4.56	1.80	1.50
34	O	310	DMS	O-S	4.56	1.80	1.50
23	b	620	CLA	MG-ND	-4.56	1.96	2.05
34	C	534	DMS	O-S	4.56	1.80	1.50
34	d	422	DMS	O-S	4.56	1.80	1.50
23	c	513	CLA	CHB-C1B	4.56	1.49	1.39
34	B	640	DMS	O-S	4.56	1.80	1.50
34	b	640	DMS	O-S	4.56	1.80	1.50
23	A	407	CLA	CHD-C1D	4.56	1.47	1.38
23	A	410	CLA	O2D-CGD	4.56	1.44	1.33
39	e	103	HEM	FE-NA	4.56	2.10	1.95
34	o	314	DMS	O-S	4.56	1.80	1.50
34	v	205	DMS	O-S	4.56	1.80	1.50
34	V	202	DMS	O-S	4.56	1.80	1.50
34	d	418	DMS	O-S	4.56	1.80	1.50
34	V	209	DMS	O-S	4.56	1.80	1.50
23	c	512	CLA	CHD-C1D	4.56	1.47	1.38
34	c	543	DMS	O-S	4.55	1.80	1.50
34	A	425	DMS	O-S	4.55	1.80	1.50
34	c	536	DMS	O-S	4.55	1.80	1.50
34	C	535	DMS	O-S	4.55	1.80	1.50
23	b	612	CLA	CHD-C1D	4.55	1.47	1.38
34	a	2623	DMS	O-S	4.55	1.80	1.50
34	O	307	DMS	O-S	4.55	1.80	1.50
23	B	611	CLA	CHD-C1D	4.55	1.47	1.38
23	a	2610	CLA	O2D-CGD	4.55	1.44	1.33
34	c	535	DMS	O-S	4.55	1.80	1.50
34	u	503	DMS	O-S	4.55	1.80	1.50
34	C	533	DMS	O-S	4.54	1.80	1.50
23	B	615	CLA	CHB-C1B	4.54	1.49	1.39
34	b	634	DMS	O-S	4.54	1.80	1.50
23	B	603	CLA	MG-NC	4.54	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	534	DMS	O-S	4.54	1.80	1.50
34	v	207	DMS	O-S	4.54	1.80	1.50
23	b	612	CLA	CHC-C1C	4.54	1.47	1.38
34	o	307	DMS	O-S	4.53	1.80	1.50
23	C	510	CLA	MG-NC	4.53	2.17	2.06
23	B	615	CLA	MG-NB	4.53	2.14	2.05
23	b	610	CLA	CHC-C1C	4.53	1.47	1.38
34	o	312	DMS	O-S	4.53	1.80	1.50
23	C	508	CLA	CHD-C1D	4.53	1.47	1.38
23	C	504	CLA	CHB-C1B	4.53	1.49	1.39
23	C	512	CLA	CHB-C1B	4.53	1.49	1.39
23	B	612	CLA	O2D-CGD	4.52	1.44	1.33
23	b	611	CLA	CHD-C1D	4.52	1.47	1.38
34	B	642	DMS	O-S	4.52	1.80	1.50
23	B	609	CLA	CHD-C1D	4.52	1.47	1.38
23	C	507	CLA	CHD-C1D	4.52	1.47	1.38
23	B	612	CLA	MG-NC	4.52	2.17	2.06
34	O	316	DMS	O-S	4.51	1.80	1.50
23	b	620	CLA	CHD-C1D	4.51	1.47	1.38
34	C	529	DMS	O-S	4.51	1.80	1.50
23	B	610	CLA	CHB-C1B	4.51	1.49	1.39
23	A	406	CLA	O2D-CGD	4.51	1.44	1.33
26	l	101	SQD	O47-C7	4.50	1.47	1.34
23	d	409	CLA	CHD-C1D	4.49	1.47	1.38
27	c	522	LMG	O7-C10	4.49	1.47	1.34
23	B	605	CLA	CHD-C1D	4.49	1.47	1.38
23	c	508	CLA	CHD-C1D	4.49	1.47	1.38
23	D	2303	CLA	CHC-C1C	4.49	1.47	1.38
23	A	406	CLA	O2A-CGA	4.49	1.46	1.33
23	c	510	CLA	CHD-C1D	4.49	1.47	1.38
37	C	519	DGD	O1G-C1A	4.49	1.46	1.33
23	b	619	CLA	CHD-C1D	4.48	1.47	1.38
34	A	424	DMS	O-S	4.48	1.79	1.50
23	c	511	CLA	O2D-CGD	4.48	1.44	1.33
23	B	613	CLA	CHD-C1D	4.48	1.47	1.38
34	C	532	DMS	O-S	4.48	1.79	1.50
23	b	615	CLA	O2D-CGD	4.48	1.44	1.33
23	c	507	CLA	C1D-ND	4.48	1.43	1.37
34	c	533	DMS	O-S	4.48	1.79	1.50
27	C	527	LMG	O7-C10	4.48	1.46	1.34
26	a	2603	SQD	O47-C7	4.47	1.46	1.34
23	B	611	CLA	O2D-CGD	4.46	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	CHB-C1B	4.46	1.49	1.39
23	b	618	CLA	CHD-C1D	4.46	1.47	1.38
26	B	621	SQD	O47-C7	4.46	1.46	1.34
38	e	101	LHG	O8-C23	4.46	1.46	1.33
24	A	409	PHO	OBD-CAD	4.45	1.28	1.22
23	C	509	CLA	CHD-C1D	4.45	1.47	1.38
23	b	615	CLA	CHD-C1D	4.45	1.47	1.38
23	b	614	CLA	O2A-CGA	4.45	1.46	1.33
23	b	621	CLA	CHB-C1B	4.44	1.49	1.39
23	b	606	CLA	CHC-C4B	4.44	1.49	1.39
23	c	506	CLA	O2D-CGD	4.44	1.44	1.33
23	c	505	CLA	CHD-C1D	4.44	1.47	1.38
34	D	2318	DMS	O-S	4.44	1.79	1.50
23	B	605	CLA	O2D-CGD	4.43	1.44	1.33
37	D	2307	DGD	O1G-C1A	4.43	1.46	1.33
23	B	603	CLA	CHB-C1B	4.43	1.49	1.39
24	a	2611	PHO	OBD-CAD	4.43	1.28	1.22
23	C	509	CLA	O2A-CGA	4.43	1.46	1.33
23	c	504	CLA	C1D-ND	4.42	1.43	1.37
23	C	514	CLA	CHC-C4B	4.42	1.49	1.39
23	B	615	CLA	MG-ND	-4.42	1.97	2.05
23	C	503	CLA	CHB-C1B	4.42	1.49	1.39
23	C	513	CLA	CHB-C1B	4.42	1.49	1.39
23	b	617	CLA	CHB-C1B	4.41	1.49	1.39
23	a	2609	CLA	CHD-C1D	4.41	1.47	1.38
26	D	2302	SQD	O47-C7	4.41	1.46	1.34
34	B	636	DMS	O-S	4.41	1.79	1.50
23	C	502	CLA	CHB-C1B	4.40	1.49	1.39
23	c	516	CLA	O2A-CGA	4.40	1.46	1.33
23	B	602	CLA	CHD-C4C	4.39	1.49	1.39
27	C	520	LMG	O8-C28	4.39	1.46	1.33
23	C	510	CLA	CHD-C1D	4.39	1.47	1.38
23	B	602	CLA	CHC-C4B	4.39	1.49	1.39
23	C	510	CLA	O2A-CGA	4.38	1.46	1.33
23	a	2613	CLA	CHB-C1B	4.38	1.49	1.39
23	B	615	CLA	O2A-CGA	4.38	1.46	1.33
34	B	638	DMS	O-S	4.38	1.79	1.50
38	E	101	LHG	O8-C23	4.38	1.46	1.33
23	B	608	CLA	O2A-CGA	4.38	1.46	1.33
23	b	621	CLA	CHC-C1C	4.38	1.47	1.38
23	C	504	CLA	CHD-C1D	4.37	1.46	1.38
26	d	417	SQD	O48-C23	4.37	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	CHB-C1B	4.36	1.49	1.39
23	C	502	CLA	CHD-C4C	4.36	1.49	1.39
23	B	609	CLA	CHB-C1B	4.36	1.49	1.39
26	D	2308	SQD	O47-C7	4.36	1.46	1.34
38	e	101	LHG	O7-C7	4.35	1.46	1.34
37	D	2307	DGD	O2G-C1B	4.35	1.46	1.34
27	c	501	LMG	O8-C28	4.35	1.46	1.33
23	B	617	CLA	CHD-C1D	4.35	1.46	1.38
23	A	405	CLA	CHC-C1C	4.35	1.47	1.38
23	b	615	CLA	CHC-C4B	4.34	1.49	1.39
23	b	606	CLA	O2A-CGA	4.34	1.46	1.33
23	B	616	CLA	CHB-C1B	4.34	1.49	1.39
23	B	610	CLA	O2A-CGA	4.34	1.46	1.33
23	D	2304	CLA	CHB-C1B	4.34	1.49	1.39
34	o	304	DMS	O-S	4.34	1.78	1.50
23	c	505	CLA	CHB-C1B	4.33	1.49	1.39
23	C	503	CLA	O2A-CGA	4.33	1.46	1.33
23	d	402	CLA	OBD-CAD	4.33	1.29	1.22
37	H	103	DGD	O1G-C1A	4.33	1.46	1.33
23	b	608	CLA	CHB-C1B	4.33	1.49	1.39
23	C	509	CLA	CHB-C1B	4.33	1.49	1.39
23	b	606	CLA	CHD-C4C	4.32	1.49	1.39
23	D	2303	CLA	O2A-CGA	4.32	1.45	1.33
23	d	402	CLA	CHB-C1B	4.32	1.49	1.39
23	B	605	CLA	CHB-C1B	4.32	1.49	1.39
23	D	2303	CLA	O2D-CGD	4.32	1.43	1.33
23	c	514	CLA	O2D-CGD	4.31	1.43	1.33
23	d	408	CLA	O2D-CGD	4.31	1.43	1.33
23	C	513	CLA	CHC-C4B	4.31	1.49	1.39
23	B	609	CLA	O2D-CGD	4.31	1.43	1.33
23	C	511	CLA	CHD-C1D	4.30	1.46	1.38
23	c	510	CLA	OBD-CAD	4.30	1.29	1.22
23	b	609	CLA	CHB-C1B	4.29	1.49	1.39
34	b	633	DMS	O-S	4.29	1.78	1.50
23	b	614	CLA	CHC-C4B	4.29	1.49	1.39
23	B	608	CLA	CHC-C4B	4.29	1.49	1.39
26	D	2308	SQD	O48-C23	4.29	1.45	1.33
23	c	515	CLA	CHB-C1B	4.28	1.49	1.39
23	B	604	CLA	CHD-C1D	4.28	1.46	1.38
23	B	617	CLA	CHB-C1B	4.28	1.49	1.39
27	B	622	LMG	O8-C28	4.28	1.45	1.33
23	b	620	CLA	C3D-C2D	4.28	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	CHD-C4C	4.28	1.48	1.39
23	C	513	CLA	O2A-CGA	4.28	1.45	1.33
23	B	614	CLA	CHD-C1D	4.27	1.46	1.38
24	a	2612	PHO	OBD-CAD	4.27	1.27	1.22
23	B	608	CLA	CHB-C1B	4.27	1.49	1.39
23	b	619	CLA	O2A-CGA	4.26	1.45	1.33
23	b	616	CLA	MG-NC	4.26	2.16	2.06
23	B	615	CLA	CHD-C1D	4.26	1.46	1.38
23	d	408	CLA	CHB-C1B	4.26	1.49	1.39
23	B	605	CLA	CHC-C1C	4.26	1.47	1.38
23	C	508	CLA	CHC-C4B	4.26	1.49	1.39
23	b	621	CLA	O2A-CGA	4.26	1.45	1.33
23	B	608	CLA	CHD-C1D	4.26	1.46	1.38
23	b	618	CLA	CHB-C1B	4.26	1.49	1.39
23	C	504	CLA	O2D-CGD	4.26	1.43	1.33
23	C	510	CLA	CHB-C1B	4.25	1.48	1.39
38	E	101	LHG	O7-C7	4.25	1.46	1.34
23	A	405	CLA	OBD-CAD	4.24	1.29	1.22
23	D	2304	CLA	C1D-ND	4.24	1.43	1.37
23	C	514	CLA	CHB-C1B	4.24	1.48	1.39
23	b	611	CLA	CHB-C1B	4.24	1.48	1.39
23	C	506	CLA	O2A-CGA	4.23	1.45	1.33
23	B	615	CLA	CHC-C4B	4.23	1.48	1.39
23	a	2610	CLA	O2A-CGA	4.23	1.45	1.33
23	b	606	CLA	CHB-C1B	4.23	1.48	1.39
23	b	612	CLA	C1D-ND	4.22	1.43	1.37
23	b	609	CLA	CHC-C4B	4.22	1.48	1.39
23	D	2303	CLA	CHC-C4B	4.22	1.48	1.39
23	a	2610	CLA	CHB-C1B	4.22	1.48	1.39
23	C	503	CLA	CHC-C4B	4.22	1.48	1.39
27	c	501	LMG	O7-C10	4.22	1.46	1.34
23	c	511	CLA	O2A-CGA	4.22	1.45	1.33
23	c	506	CLA	CHD-C1D	4.21	1.46	1.38
23	a	2613	CLA	CHD-C1D	4.21	1.46	1.38
27	c	522	LMG	O8-C28	4.21	1.45	1.33
23	c	504	CLA	CHB-C1B	4.21	1.48	1.39
23	b	617	CLA	CHD-C1D	4.21	1.46	1.38
23	c	510	CLA	CHC-C1C	4.21	1.46	1.38
23	b	609	CLA	CHD-C1D	4.21	1.46	1.38
23	b	615	CLA	CHB-C1B	4.21	1.48	1.39
27	C	527	LMG	O8-C28	4.20	1.45	1.33
23	C	512	CLA	O2A-CGA	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	O2A-CGA	4.20	1.45	1.33
23	b	611	CLA	O2A-CGA	4.20	1.45	1.33
26	a	2603	SQD	O48-C23	4.20	1.45	1.33
23	B	614	CLA	CHB-C1B	4.19	1.48	1.39
23	C	508	CLA	CHB-C1B	4.19	1.48	1.39
23	b	613	CLA	O2A-CGA	4.19	1.45	1.33
23	c	505	CLA	C3D-C2D	4.19	1.50	1.39
23	B	604	CLA	O2A-CGA	4.18	1.45	1.33
23	C	505	CLA	CHD-C4C	4.18	1.48	1.39
23	c	514	CLA	O2A-CGA	4.18	1.45	1.33
23	c	514	CLA	CHD-C4C	4.18	1.48	1.39
23	B	609	CLA	O2A-CGA	4.18	1.45	1.33
23	c	515	CLA	O2A-CGA	4.18	1.45	1.33
23	b	617	CLA	O2A-CGA	4.18	1.45	1.33
23	c	514	CLA	CHB-C1B	4.18	1.48	1.39
23	b	618	CLA	MG-ND	-4.18	1.97	2.05
23	A	405	CLA	CHB-C1B	4.18	1.48	1.39
23	C	508	CLA	O2A-CGA	4.17	1.45	1.33
23	D	2304	CLA	CHD-C4C	4.17	1.48	1.39
23	D	2304	CLA	MG-NC	4.17	2.16	2.06
23	c	505	CLA	CHC-C4B	4.17	1.48	1.39
24	A	408	PHO	O2A-CGA	4.17	1.45	1.33
23	c	516	CLA	CHB-C1B	4.17	1.48	1.39
27	c	521	LMG	O8-C28	4.17	1.45	1.33
23	B	615	CLA	O2D-CGD	4.17	1.43	1.33
23	c	504	CLA	CHC-C4B	4.17	1.48	1.39
23	B	614	CLA	O2A-CGA	4.17	1.45	1.33
23	b	608	CLA	CHC-C4B	4.17	1.48	1.39
27	A	413	LMG	O8-C28	4.16	1.45	1.33
24	A	408	PHO	OBD-CAD	4.16	1.27	1.22
23	c	510	CLA	CHB-C1B	4.16	1.48	1.39
26	B	621	SQD	O48-C23	4.16	1.45	1.33
27	A	413	LMG	O7-C10	4.15	1.46	1.34
23	b	621	CLA	CHD-C1D	4.15	1.46	1.38
23	D	2303	CLA	CHB-C1B	4.15	1.48	1.39
27	B	622	LMG	O7-C10	4.15	1.46	1.34
23	c	510	CLA	O2A-CGA	4.15	1.45	1.33
23	C	503	CLA	OBD-CAD	4.15	1.29	1.22
23	C	507	CLA	CHB-C1B	4.15	1.48	1.39
23	c	507	CLA	CHC-C4B	4.15	1.48	1.39
23	A	405	CLA	CHD-C1D	4.14	1.46	1.38
23	d	409	CLA	CHB-C1B	4.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	O2A-CGA	4.14	1.45	1.33
23	d	402	CLA	C3D-C2D	4.14	1.50	1.39
23	B	612	CLA	CHD-C1D	4.13	1.46	1.38
23	c	504	CLA	CHD-C1D	4.13	1.46	1.38
23	b	607	CLA	CHB-C1B	4.12	1.48	1.39
23	a	2613	CLA	O2A-CGA	4.12	1.45	1.33
38	d	412	LHG	O8-C23	4.12	1.45	1.33
27	m	2802	LMG	O7-C10	4.12	1.45	1.34
23	b	611	CLA	CHC-C4B	4.12	1.48	1.39
23	c	509	CLA	O2A-CGA	4.11	1.45	1.33
23	a	2609	CLA	CHB-C1B	4.11	1.48	1.39
23	c	506	CLA	CHC-C4B	4.11	1.48	1.39
23	B	603	CLA	CHC-C4B	4.11	1.48	1.39
23	D	2304	CLA	C3D-C2D	4.11	1.50	1.39
23	C	509	CLA	CHC-C4B	4.11	1.48	1.39
23	a	2609	CLA	O2D-CGD	4.11	1.43	1.33
26	D	2302	SQD	O48-C23	4.11	1.45	1.33
38	L	101	LHG	O8-C23	4.11	1.45	1.33
23	b	613	CLA	CHB-C1B	4.11	1.48	1.39
23	b	620	CLA	CHB-C1B	4.11	1.48	1.39
23	c	513	CLA	OBD-CAD	4.11	1.29	1.22
23	B	602	CLA	MG-ND	-4.10	1.97	2.05
37	c	520	DGD	O1G-C1A	4.10	1.45	1.33
23	b	607	CLA	O2A-CGA	4.10	1.45	1.33
23	B	614	CLA	CHC-C4B	4.10	1.48	1.39
23	B	611	CLA	MG-NA	4.10	2.16	2.06
23	b	612	CLA	CHB-C1B	4.09	1.48	1.39
23	c	512	CLA	O2A-CGA	4.09	1.45	1.33
23	a	2610	CLA	CHD-C1D	4.09	1.46	1.38
27	d	414	LMG	O8-C28	4.09	1.45	1.33
23	C	505	CLA	CHB-C1B	4.09	1.48	1.39
23	c	507	CLA	CHD-C1D	4.09	1.46	1.38
23	c	508	CLA	CHB-C1B	4.09	1.48	1.39
23	c	511	CLA	CHC-C4B	4.09	1.48	1.39
23	C	514	CLA	CHD-C4C	4.08	1.48	1.39
23	b	614	CLA	CHD-C4C	4.08	1.48	1.39
23	A	406	CLA	CHC-C1C	4.08	1.46	1.38
23	C	502	CLA	OBD-CAD	4.08	1.29	1.22
23	B	613	CLA	OBD-CAD	4.08	1.29	1.22
23	B	606	CLA	CHC-C4B	4.07	1.48	1.39
23	C	514	CLA	O2A-CGA	4.07	1.45	1.33
23	D	2303	CLA	MG-NA	4.07	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	MG-NC	4.07	2.15	2.06
23	c	514	CLA	OBD-CAD	4.07	1.29	1.22
23	C	504	CLA	O2A-CGA	4.07	1.45	1.33
23	c	515	CLA	CHD-C1D	4.07	1.46	1.38
38	D	2309	LHG	O8-C23	4.07	1.45	1.33
23	C	512	CLA	CHD-C4C	4.06	1.48	1.39
37	h	102	DGD	O2G-C1B	4.06	1.45	1.34
23	a	2613	CLA	C3D-C2D	4.06	1.50	1.39
23	B	605	CLA	OBD-CAD	4.06	1.29	1.22
26	b	601	SQD	O48-C23	4.06	1.45	1.33
23	c	513	CLA	CHC-C4B	4.06	1.48	1.39
23	b	608	CLA	O2A-CGA	4.06	1.45	1.33
23	c	516	CLA	CHC-C4B	4.06	1.48	1.39
23	c	509	CLA	CHB-C1B	4.05	1.48	1.39
23	d	409	CLA	O2A-CGA	4.05	1.45	1.33
23	A	407	CLA	O2A-CGA	4.05	1.45	1.33
23	B	609	CLA	MG-NB	4.05	2.13	2.05
23	D	2304	CLA	CHC-C4B	4.05	1.48	1.39
23	C	506	CLA	CHC-C4B	4.04	1.48	1.39
23	B	612	CLA	CHB-C1B	4.04	1.48	1.39
23	B	611	CLA	CHC-C4B	4.04	1.48	1.39
26	b	601	SQD	O47-C7	4.04	1.45	1.34
23	b	606	CLA	C3D-C2D	4.03	1.50	1.39
23	C	507	CLA	CHC-C4B	4.03	1.48	1.39
42	v	201	HEC	CBC-CAC	-4.03	1.34	1.49
23	a	2609	CLA	CHC-C4B	4.03	1.48	1.39
38	d	403	LHG	O7-C7	4.02	1.45	1.34
23	B	613	CLA	C1D-ND	4.02	1.43	1.37
23	D	2304	CLA	O2A-CGA	4.02	1.45	1.33
23	c	504	CLA	O2A-CGA	4.02	1.45	1.33
23	b	620	CLA	O2A-CGA	4.02	1.45	1.33
37	C	519	DGD	O2G-C1B	4.01	1.45	1.34
26	l	101	SQD	O48-C23	4.01	1.45	1.33
23	c	515	CLA	C3D-C2D	4.01	1.49	1.39
23	b	613	CLA	CHC-C4B	4.01	1.48	1.39
38	l	103	LHG	O8-C23	4.01	1.45	1.33
37	c	519	DGD	O2G-C1B	4.00	1.45	1.34
23	B	609	CLA	CHC-C4B	4.00	1.48	1.39
26	A	412	SQD	O47-C7	4.00	1.45	1.34
23	c	515	CLA	CHD-C4C	4.00	1.48	1.39
23	C	512	CLA	C3D-C2D	4.00	1.49	1.39
23	c	508	CLA	CHC-C4B	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	408	CLA	C1D-ND	3.98	1.43	1.37
23	b	619	CLA	CHC-C4B	3.98	1.48	1.39
23	c	507	CLA	CHB-C1B	3.98	1.48	1.39
26	A	412	SQD	O48-C23	3.98	1.45	1.33
23	A	407	CLA	C3D-C2D	3.98	1.49	1.39
37	h	102	DGD	O1G-C1A	3.98	1.44	1.33
23	d	409	CLA	CHC-C4B	3.98	1.48	1.39
26	a	2615	SQD	O48-C23	3.97	1.44	1.33
23	C	513	CLA	CHD-C4C	3.97	1.48	1.39
23	c	505	CLA	O2A-CGA	3.97	1.44	1.33
23	D	2304	CLA	CHD-C1D	3.97	1.46	1.38
23	a	2610	CLA	CHD-C4C	3.97	1.48	1.39
23	a	2613	CLA	CHD-C4C	3.97	1.48	1.39
23	B	616	CLA	CHD-C1D	3.97	1.46	1.38
23	c	509	CLA	CHD-C4C	3.97	1.48	1.39
23	C	509	CLA	CHD-C4C	3.97	1.48	1.39
23	d	409	CLA	OBD-CAD	3.97	1.29	1.22
23	d	408	CLA	CHD-C1D	3.97	1.46	1.38
23	B	617	CLA	O2A-CGA	3.96	1.44	1.33
23	A	407	CLA	OBD-CAD	3.96	1.29	1.22
37	H	103	DGD	O2G-C1B	3.96	1.45	1.34
23	C	506	CLA	OBD-CAD	3.96	1.29	1.22
23	B	606	CLA	O2A-CGA	3.96	1.44	1.33
23	A	405	CLA	C3D-C2D	3.96	1.49	1.39
23	C	503	CLA	C3D-C2D	3.95	1.49	1.39
23	C	507	CLA	CHD-C4C	3.95	1.48	1.39
23	B	605	CLA	CHC-C4B	3.94	1.48	1.39
23	c	508	CLA	O2A-CGA	3.94	1.44	1.33
27	D	2312	LMG	O8-C28	3.94	1.44	1.33
23	c	505	CLA	CHD-C4C	3.94	1.48	1.39
23	a	2609	CLA	OBD-CAD	3.94	1.29	1.22
23	d	402	CLA	CHD-C4C	3.94	1.48	1.39
23	A	406	CLA	CHB-C1B	3.94	1.48	1.39
23	B	609	CLA	C3D-C2D	3.94	1.49	1.39
23	C	510	CLA	OBD-CAD	3.94	1.29	1.22
42	V	201	HEC	CBC-CAC	-3.94	1.34	1.49
23	B	605	CLA	CHD-C4C	3.94	1.48	1.39
37	c	519	DGD	O1G-C1A	3.94	1.44	1.33
23	b	617	CLA	CHC-C4B	3.93	1.48	1.39
23	C	511	CLA	C3D-C2D	3.93	1.49	1.39
23	b	613	CLA	CHD-C4C	3.93	1.48	1.39
23	B	603	CLA	O2A-CGA	3.93	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	518	DGD	O1G-C1A	3.93	1.44	1.33
23	B	604	CLA	CHB-C1B	3.93	1.48	1.39
23	b	615	CLA	O2A-CGA	3.93	1.44	1.33
23	B	603	CLA	CHD-C4C	3.93	1.48	1.39
23	B	606	CLA	CHB-C1B	3.92	1.48	1.39
23	B	616	CLA	CHC-C4B	3.92	1.48	1.39
23	A	407	CLA	CHD-C4C	3.92	1.48	1.39
23	B	617	CLA	CHC-C4B	3.92	1.48	1.39
23	B	611	CLA	CHB-C1B	3.91	1.48	1.39
38	D	2310	LHG	O7-C7	3.91	1.45	1.34
23	c	512	CLA	CHC-C4B	3.91	1.48	1.39
23	B	613	CLA	O2A-CGA	3.91	1.44	1.33
23	b	607	CLA	C3D-C2D	3.91	1.49	1.39
23	C	506	CLA	CHD-C4C	3.91	1.48	1.39
23	A	410	CLA	C3D-C2D	3.90	1.49	1.39
23	b	610	CLA	CHB-C1B	3.90	1.48	1.39
23	c	506	CLA	O2A-CGA	3.90	1.44	1.33
23	b	607	CLA	CHD-C4C	3.90	1.48	1.39
23	A	405	CLA	CHC-C4B	3.90	1.48	1.39
23	C	508	CLA	OBD-CAD	3.90	1.29	1.22
23	b	616	CLA	CHD-C4C	3.90	1.48	1.39
23	A	406	CLA	MG-NC	3.90	2.15	2.06
23	D	2304	CLA	MG-NA	3.90	2.15	2.06
37	c	520	DGD	O2G-C1B	3.89	1.45	1.34
23	b	618	CLA	CHC-C4B	3.89	1.48	1.39
23	B	602	CLA	C3D-C2D	3.89	1.49	1.39
23	C	509	CLA	C3D-C2D	3.89	1.49	1.39
23	b	612	CLA	O2A-CGA	3.89	1.44	1.33
23	d	409	CLA	CHD-C4C	3.89	1.48	1.39
27	C	520	LMG	O7-C10	3.88	1.45	1.34
23	a	2609	CLA	CHD-C4C	3.88	1.48	1.39
23	a	2610	CLA	C3D-C2D	3.88	1.49	1.39
23	c	516	CLA	C3D-C2D	3.88	1.49	1.39
23	C	505	CLA	C3D-C2D	3.88	1.49	1.39
23	B	610	CLA	CHC-C4B	3.88	1.48	1.39
23	B	612	CLA	C3D-C2D	3.88	1.49	1.39
23	A	410	CLA	O2A-CGA	3.88	1.44	1.33
23	b	614	CLA	MG-ND	-3.88	1.98	2.05
23	A	410	CLA	CHC-C4B	3.87	1.48	1.39
23	B	607	CLA	O2A-CGA	3.87	1.44	1.33
23	C	511	CLA	CHC-C4B	3.87	1.48	1.39
23	C	503	CLA	CHD-C4C	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C3D-C2D	3.87	1.49	1.39
23	c	511	CLA	C3D-C2D	3.87	1.49	1.39
23	b	614	CLA	OBD-CAD	3.87	1.29	1.22
38	d	403	LHG	O8-C23	3.87	1.44	1.33
23	b	608	CLA	OBD-CAD	3.87	1.29	1.22
23	b	620	CLA	CHD-C4C	3.87	1.48	1.39
23	c	513	CLA	O2A-CGA	3.87	1.44	1.33
23	c	512	CLA	CHD-C4C	3.87	1.48	1.39
23	c	510	CLA	CHC-C4B	3.87	1.48	1.39
23	b	614	CLA	C3D-C2D	3.86	1.49	1.39
23	C	505	CLA	CHC-C4B	3.86	1.48	1.39
23	A	407	CLA	MG-NC	3.86	2.15	2.06
23	b	607	CLA	CHC-C4B	3.86	1.48	1.39
23	b	610	CLA	CHC-C4B	3.86	1.48	1.39
23	B	608	CLA	CHD-C4C	3.86	1.48	1.39
23	A	410	CLA	OBD-CAD	3.86	1.29	1.22
23	C	510	CLA	CHD-C4C	3.86	1.48	1.39
23	b	609	CLA	O2A-CGA	3.86	1.44	1.33
37	C	518	DGD	O2G-C1B	3.86	1.45	1.34
23	c	512	CLA	OBD-CAD	3.86	1.29	1.22
27	d	414	LMG	O7-C10	3.86	1.45	1.34
23	B	610	CLA	OBD-CAD	3.86	1.29	1.22
23	B	607	CLA	CHB-C1B	3.85	1.48	1.39
23	C	511	CLA	CHD-C4C	3.85	1.48	1.39
23	B	607	CLA	CHD-C4C	3.85	1.48	1.39
23	A	410	CLA	CHD-C4C	3.85	1.48	1.39
23	b	609	CLA	C4D-CHA	3.85	1.51	1.38
37	C	518	DGD	O1G-C1A	3.84	1.44	1.33
23	B	612	CLA	CHC-C4B	3.84	1.48	1.39
23	c	514	CLA	CHC-C4B	3.84	1.48	1.39
23	B	616	CLA	O2A-CGA	3.84	1.44	1.33
23	B	616	CLA	OBD-CAD	3.84	1.29	1.22
23	d	409	CLA	C3D-C2D	3.84	1.49	1.39
26	a	2615	SQD	O47-C7	3.84	1.45	1.34
23	B	617	CLA	C3D-C2D	3.84	1.49	1.39
23	b	618	CLA	O2A-CGA	3.83	1.44	1.33
23	b	612	CLA	CHC-C4B	3.83	1.48	1.39
23	C	511	CLA	OBD-CAD	3.83	1.29	1.22
27	c	521	LMG	O7-C10	3.83	1.45	1.34
23	b	617	CLA	MG-NA	3.83	2.15	2.06
23	C	505	CLA	MG-ND	-3.83	1.98	2.05
23	c	505	CLA	OBD-CAD	3.82	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHD-C4C	3.82	1.47	1.39
24	a	2612	PHO	O2A-CGA	3.82	1.44	1.33
23	c	513	CLA	C3D-C2D	3.82	1.49	1.39
23	C	503	CLA	MG-NC	3.82	2.15	2.06
23	C	505	CLA	O2A-CGA	3.81	1.44	1.33
23	c	509	CLA	C3D-C2D	3.81	1.49	1.39
23	B	608	CLA	C3D-C2D	3.81	1.49	1.39
23	c	507	CLA	CHD-C4C	3.81	1.47	1.39
23	b	610	CLA	O2A-CGA	3.81	1.44	1.33
23	C	514	CLA	MG-NB	3.81	2.13	2.05
23	B	606	CLA	MG-ND	-3.81	1.98	2.05
42	v	201	HEC	CBB-CAB	-3.80	1.35	1.49
23	c	509	CLA	CHC-C4B	3.80	1.47	1.39
23	B	610	CLA	C3D-C2D	3.80	1.49	1.39
23	c	506	CLA	CHD-C4C	3.80	1.47	1.39
23	C	502	CLA	C3D-C2D	3.80	1.49	1.39
23	c	513	CLA	CHD-C4C	3.79	1.47	1.39
23	b	606	CLA	OBD-CAD	3.79	1.29	1.22
38	D	2311	LHG	O8-C23	3.78	1.44	1.33
23	b	619	CLA	CHB-C1B	3.78	1.47	1.39
23	c	514	CLA	C3D-C2D	3.78	1.49	1.39
23	c	511	CLA	CHB-C1B	3.78	1.47	1.39
23	A	410	CLA	CHB-C1B	3.78	1.47	1.39
23	b	619	CLA	CHD-C4C	3.78	1.47	1.39
23	D	2303	CLA	CHD-C4C	3.78	1.47	1.39
23	C	509	CLA	OBD-CAD	3.78	1.29	1.22
23	b	620	CLA	CHC-C4B	3.78	1.47	1.39
23	C	510	CLA	CHC-C4B	3.77	1.47	1.39
23	b	616	CLA	MG-ND	-3.77	1.98	2.05
23	C	513	CLA	C3D-C2D	3.77	1.49	1.39
23	B	612	CLA	CHD-C4C	3.77	1.47	1.39
23	b	616	CLA	O2A-CGA	3.77	1.44	1.33
24	A	409	PHO	CHA-CBD	-3.77	1.47	1.51
23	D	2303	CLA	CHD-C1D	3.77	1.45	1.38
23	b	611	CLA	C3D-C2D	3.76	1.49	1.39
23	c	515	CLA	CHC-C4B	3.76	1.47	1.39
24	A	409	PHO	O2A-CGA	3.76	1.44	1.33
23	b	615	CLA	CHD-C4C	3.75	1.47	1.39
23	b	616	CLA	C3D-C2D	3.75	1.49	1.39
23	B	616	CLA	C3D-C2D	3.75	1.49	1.39
38	d	413	LHG	O7-C7	3.75	1.44	1.34
23	B	615	CLA	OBD-CAD	3.74	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	OBD-CAD	3.74	1.28	1.22
23	C	512	CLA	OBD-CAD	3.74	1.28	1.22
23	A	406	CLA	CHD-C1D	3.74	1.45	1.38
23	B	614	CLA	CHD-C4C	3.74	1.47	1.39
23	b	616	CLA	MG-NB	3.73	2.13	2.05
23	B	609	CLA	MG-NC	3.73	2.15	2.06
23	d	408	CLA	C3D-C2D	3.73	1.49	1.39
36	d	407	HTG	C1'-S1	-3.73	1.76	1.81
38	d	412	LHG	O7-C7	3.73	1.44	1.34
23	B	603	CLA	C3D-C2D	3.73	1.49	1.39
23	c	516	CLA	CHD-C4C	3.73	1.47	1.39
23	D	2303	CLA	C1D-ND	3.72	1.42	1.37
23	A	405	CLA	CHD-C4C	3.72	1.47	1.39
23	B	608	CLA	MG-ND	-3.72	1.98	2.05
23	A	407	CLA	CHB-C1B	3.72	1.47	1.39
23	b	612	CLA	C3D-C2D	3.72	1.49	1.39
37	C	517	DGD	O2G-C1B	3.72	1.44	1.34
23	C	512	CLA	CHC-C4B	3.72	1.47	1.39
23	B	604	CLA	CHD-C4C	3.72	1.47	1.39
23	c	507	CLA	O2A-CGA	3.71	1.44	1.33
23	c	504	CLA	OBD-CAD	3.71	1.28	1.22
23	b	611	CLA	CHD-C4C	3.71	1.47	1.39
36	i	102	HTG	C1'-S1	-3.71	1.76	1.81
23	A	407	CLA	C1B-NB	-3.70	1.33	1.37
23	c	515	CLA	OBD-CAD	3.70	1.28	1.22
23	B	615	CLA	C4B-NB	-3.70	1.33	1.37
23	A	406	CLA	CHC-C4B	3.70	1.47	1.39
23	c	508	CLA	CHD-C4C	3.70	1.47	1.39
36	H	101	HTG	C1'-S1	-3.70	1.76	1.81
23	A	406	CLA	OBD-CAD	3.70	1.28	1.22
23	A	407	CLA	CHC-C4B	3.70	1.47	1.39
23	B	614	CLA	OBD-CAD	3.69	1.28	1.22
23	B	611	CLA	C3D-C2D	3.69	1.49	1.39
23	B	602	CLA	OBD-CAD	3.69	1.28	1.22
23	B	611	CLA	CHD-C4C	3.68	1.47	1.39
23	B	612	CLA	O2A-CGA	3.68	1.44	1.33
23	A	406	CLA	C3D-C2D	3.67	1.49	1.39
23	b	610	CLA	CHD-C1D	3.67	1.45	1.38
38	L	101	LHG	O7-C7	3.67	1.44	1.34
23	C	502	CLA	MG-NB	3.67	2.13	2.05
23	c	511	CLA	CHD-C4C	3.67	1.47	1.39
23	B	603	CLA	OBD-CAD	3.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	418	JOX	C1-CL1	3.67	1.80	1.73
23	b	609	CLA	CHD-C4C	3.66	1.47	1.39
23	C	508	CLA	CHD-C4C	3.66	1.47	1.39
23	b	617	CLA	C3D-C2D	3.66	1.49	1.39
24	a	2611	PHO	O2A-CGA	3.66	1.44	1.33
23	d	402	CLA	C1B-NB	-3.66	1.33	1.37
23	B	615	CLA	C3D-C2D	3.65	1.49	1.39
23	b	609	CLA	C3D-C2D	3.65	1.48	1.39
23	C	513	CLA	OBD-CAD	3.65	1.28	1.22
23	C	504	CLA	C3D-C2D	3.65	1.48	1.39
23	B	617	CLA	CHD-C4C	3.65	1.47	1.39
23	B	608	CLA	OBD-CAD	3.65	1.28	1.22
23	B	606	CLA	C3D-C2D	3.65	1.48	1.39
23	C	514	CLA	OBD-CAD	3.65	1.28	1.22
23	b	609	CLA	OBD-CAD	3.65	1.28	1.22
36	b	626	HTG	C1'-S1	-3.65	1.76	1.81
23	b	612	CLA	CHD-C4C	3.64	1.47	1.39
23	b	615	CLA	OBD-CAD	3.64	1.28	1.22
23	d	402	CLA	O2A-CGA	3.64	1.44	1.33
23	B	609	CLA	CHD-C4C	3.63	1.47	1.39
23	d	402	CLA	CHC-C4B	3.62	1.47	1.39
23	a	2610	CLA	CHC-C4B	3.62	1.47	1.39
37	C	517	DGD	O1G-C1A	3.62	1.43	1.33
23	b	610	CLA	C3D-C2D	3.61	1.48	1.39
23	B	607	CLA	MG-ND	-3.61	1.98	2.05
31	A	418	JOX	C3-CL	3.61	1.79	1.73
23	C	511	CLA	O2A-CGA	3.61	1.43	1.33
23	c	507	CLA	C3D-C2D	3.61	1.48	1.39
23	b	613	CLA	OBD-CAD	3.60	1.28	1.22
23	c	511	CLA	C1B-NB	-3.60	1.33	1.37
23	a	2610	CLA	OBD-CAD	3.60	1.28	1.22
23	b	621	CLA	CHC-C4B	3.60	1.47	1.39
23	b	620	CLA	OBD-CAD	3.59	1.28	1.22
23	B	607	CLA	C3D-C2D	3.59	1.48	1.39
23	B	606	CLA	CHD-C4C	3.59	1.47	1.39
23	D	2304	CLA	OBD-CAD	3.59	1.28	1.22
37	c	518	DGD	O2G-C1B	3.58	1.44	1.34
23	B	611	CLA	O2A-CGA	3.58	1.43	1.33
23	B	613	CLA	CHC-C4B	3.58	1.47	1.39
23	c	510	CLA	CHD-C4C	3.58	1.47	1.39
23	C	514	CLA	C3D-C2D	3.57	1.48	1.39
23	c	514	CLA	MG-ND	-3.57	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	OBD-CAD	3.57	1.28	1.22
23	b	615	CLA	C3D-C2D	3.56	1.48	1.39
23	B	612	CLA	MG-NB	3.56	2.12	2.05
23	c	504	CLA	CHD-C4C	3.56	1.47	1.39
36	C	525	HTG	C1'-S1	-3.56	1.76	1.81
31	A	419	JOX	C1-CL1	3.56	1.79	1.73
23	c	512	CLA	C3D-C2D	3.55	1.48	1.39
38	D	2310	LHG	O8-C23	3.55	1.43	1.33
23	B	604	CLA	C3D-C2D	3.55	1.48	1.39
23	D	2303	CLA	C3D-C2D	3.55	1.48	1.39
23	c	508	CLA	C3D-C2D	3.55	1.48	1.39
36	I	101	HTG	C1'-S1	-3.55	1.76	1.81
23	b	616	CLA	CHC-C4B	3.55	1.47	1.39
23	a	2609	CLA	O2A-CGA	3.54	1.43	1.33
23	b	608	CLA	C3D-C2D	3.54	1.48	1.39
38	D	2311	LHG	O7-C7	3.53	1.44	1.34
23	C	504	CLA	CHD-C4C	3.53	1.47	1.39
23	c	510	CLA	C3D-C2D	3.53	1.48	1.39
23	b	608	CLA	CHD-C4C	3.53	1.47	1.39
23	B	616	CLA	CHD-C4C	3.53	1.47	1.39
23	A	405	CLA	MG-NC	3.52	2.14	2.06
42	V	201	HEC	CBB-CAB	-3.52	1.36	1.49
23	b	612	CLA	OBD-CAD	3.52	1.28	1.22
23	B	613	CLA	C1B-NB	-3.51	1.33	1.37
23	B	612	CLA	OBD-CAD	3.51	1.28	1.22
23	c	504	CLA	C3D-C2D	3.51	1.48	1.39
23	B	607	CLA	OBD-CAD	3.51	1.28	1.22
23	B	606	CLA	OBD-CAD	3.51	1.28	1.22
23	A	405	CLA	C1B-NB	-3.51	1.33	1.37
23	b	619	CLA	OBD-CAD	3.51	1.28	1.22
23	A	405	CLA	O2A-CGA	3.50	1.43	1.33
23	b	613	CLA	C3D-C2D	3.50	1.48	1.39
23	B	605	CLA	C3D-C2D	3.50	1.48	1.39
27	D	2312	LMG	O7-C10	3.49	1.44	1.34
23	B	609	CLA	C1B-NB	-3.49	1.33	1.37
23	A	407	CLA	MG-NA	3.49	2.14	2.06
23	b	618	CLA	OBD-CAD	3.48	1.28	1.22
23	b	608	CLA	MG-NB	-3.47	1.98	2.05
23	d	408	CLA	CHD-C4C	3.47	1.47	1.39
23	a	2613	CLA	OBD-CAD	3.47	1.28	1.22
23	b	611	CLA	OBD-CAD	3.47	1.28	1.22
23	B	613	CLA	CHD-C4C	3.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	C1B-NB	-3.46	1.33	1.37
23	B	614	CLA	C3D-C2D	3.46	1.48	1.39
23	b	618	CLA	C3D-C2D	3.46	1.48	1.39
23	c	506	CLA	C3D-C2D	3.45	1.48	1.39
23	a	2609	CLA	C3D-C2D	3.45	1.48	1.39
23	c	508	CLA	OBD-CAD	3.45	1.28	1.22
23	b	617	CLA	CHD-C4C	3.44	1.47	1.39
36	b	602	HTG	C1'-S1	-3.44	1.76	1.81
23	C	508	CLA	C3D-C2D	3.43	1.48	1.39
23	C	507	CLA	C3D-C2D	3.43	1.48	1.39
38	D	2309	LHG	O7-C7	3.43	1.44	1.34
23	d	408	CLA	OBD-CAD	3.42	1.28	1.22
23	b	621	CLA	C3D-C2D	3.42	1.48	1.39
23	C	508	CLA	C4D-CHA	3.41	1.50	1.38
23	B	605	CLA	O2A-CGA	3.41	1.43	1.33
23	b	607	CLA	OBD-CAD	3.41	1.28	1.22
23	B	611	CLA	OBD-CAD	3.40	1.28	1.22
23	c	507	CLA	OBD-CAD	3.40	1.28	1.22
23	A	406	CLA	CHD-C4C	3.40	1.46	1.39
36	d	415	HTG	C1'-S1	-3.40	1.76	1.81
23	b	610	CLA	CHD-C4C	3.39	1.46	1.39
23	d	408	CLA	CHC-C4B	3.39	1.47	1.39
23	B	613	CLA	C3D-C2D	3.39	1.48	1.39
23	B	615	CLA	C1B-NB	-3.38	1.33	1.37
23	B	610	CLA	CHD-C4C	3.37	1.46	1.39
23	B	612	CLA	C4D-CHA	3.37	1.49	1.38
23	B	616	CLA	C4B-NB	-3.37	1.33	1.37
23	B	617	CLA	C4D-CHA	3.37	1.49	1.38
23	C	511	CLA	C1B-NB	-3.36	1.33	1.37
36	B	625	HTG	C1'-S1	-3.36	1.76	1.81
39	F	101	HEM	FE-NA	3.36	2.06	1.95
23	D	2304	CLA	C1B-NB	-3.36	1.33	1.37
23	c	506	CLA	C4D-CHA	3.36	1.49	1.38
36	c	524	HTG	C1'-S1	-3.36	1.76	1.81
38	l	103	LHG	O7-C7	3.35	1.43	1.34
23	d	409	CLA	C1B-NB	-3.35	1.33	1.37
23	b	619	CLA	C3D-C2D	3.35	1.48	1.39
23	a	2613	CLA	CHC-C4B	3.35	1.46	1.39
36	b	604	HTG	C1'-S1	-3.34	1.76	1.81
23	C	505	CLA	C1B-NB	-3.34	1.33	1.37
23	c	512	CLA	C1B-C2B	3.33	1.50	1.43
23	C	506	CLA	C3D-C2D	3.33	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	OBD-CAD	3.32	1.28	1.22
23	C	507	CLA	OBD-CAD	3.32	1.28	1.22
23	a	2610	CLA	MG-NC	3.32	2.14	2.06
23	b	621	CLA	MG-NC	3.32	2.14	2.06
23	a	2609	CLA	C1B-NB	-3.31	1.33	1.37
23	B	608	CLA	C4D-CHA	3.31	1.49	1.38
23	c	509	CLA	OBD-CAD	3.31	1.28	1.22
23	B	609	CLA	OBD-CAD	3.30	1.28	1.22
23	b	616	CLA	OBD-CAD	3.30	1.28	1.22
23	b	615	CLA	C4D-CHA	3.29	1.49	1.38
23	c	516	CLA	OBD-CAD	3.29	1.28	1.22
23	B	616	CLA	C1B-C2B	3.28	1.50	1.43
23	a	2613	CLA	C1B-NB	-3.28	1.33	1.37
23	C	510	CLA	C4B-NB	-3.28	1.33	1.37
23	b	620	CLA	C4D-CHA	3.27	1.49	1.38
23	C	514	CLA	MG-NA	3.26	2.14	2.06
23	C	512	CLA	C4B-NB	-3.25	1.33	1.37
23	C	512	CLA	C4D-CHA	3.25	1.49	1.38
23	B	608	CLA	C1B-C2B	3.24	1.50	1.43
23	b	612	CLA	C1B-NB	-3.22	1.33	1.37
23	c	513	CLA	MG-NB	3.22	2.12	2.05
23	B	612	CLA	C1B-NB	-3.21	1.33	1.37
23	B	602	CLA	C4D-CHA	3.21	1.49	1.38
23	c	510	CLA	C4D-CHA	3.21	1.49	1.38
23	B	611	CLA	C4B-NB	-3.21	1.33	1.37
23	b	621	CLA	C1B-C2B	3.21	1.50	1.43
23	b	621	CLA	CHD-C4C	3.21	1.46	1.39
36	b	625	HTG	C1'-S1	-3.21	1.76	1.81
39	F	101	HEM	FE-NB	3.21	2.04	1.94
36	V	204	HTG	C1'-S1	-3.20	1.76	1.81
23	B	604	CLA	C4D-CHA	3.20	1.49	1.38
23	d	402	CLA	C1B-C2B	3.20	1.50	1.43
36	B	627	HTG	C1'-S1	-3.20	1.76	1.81
23	a	2613	CLA	MG-ND	-3.19	1.99	2.05
23	C	504	CLA	OBD-CAD	3.19	1.28	1.22
23	B	615	CLA	MG-NC	3.19	2.13	2.06
23	a	2609	CLA	MG-NB	3.19	2.12	2.05
36	B	624[B]	HTG	C1'-S1	-3.18	1.76	1.81
23	C	505	CLA	OBD-CAD	3.18	1.28	1.22
23	b	615	CLA	C1B-NB	-3.18	1.33	1.37
23	b	613	CLA	C4B-NB	-3.18	1.33	1.37
23	b	612	CLA	C1B-C2B	3.18	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C4B-NB	-3.17	1.33	1.37
23	C	510	CLA	C4D-CHA	3.17	1.49	1.38
36	c	526	HTG	C1'-S1	-3.16	1.77	1.81
23	C	503	CLA	C4D-CHA	3.16	1.49	1.38
23	C	502	CLA	C4D-CHA	3.15	1.49	1.38
38	d	413	LHG	O8-C23	3.15	1.42	1.33
23	B	615	CLA	C4D-CHA	3.14	1.49	1.38
23	A	410	CLA	C4D-CHA	3.14	1.49	1.38
23	c	515	CLA	C4D-CHA	3.14	1.49	1.38
23	C	507	CLA	C1B-NB	-3.14	1.33	1.37
23	B	615	CLA	C1B-C2B	3.14	1.50	1.43
23	C	504	CLA	C1B-C2B	3.13	1.50	1.43
23	B	605	CLA	C4D-CHA	3.13	1.49	1.38
23	b	606	CLA	C4D-CHA	3.13	1.49	1.38
36	c	523	HTG	C1'-S1	-3.13	1.77	1.81
23	c	512	CLA	C4D-CHA	3.12	1.49	1.38
23	B	607	CLA	C4D-CHA	3.12	1.49	1.38
23	b	611	CLA	C4D-CHA	3.12	1.49	1.38
23	C	513	CLA	C4D-CHA	3.12	1.49	1.38
23	A	406	CLA	C1B-NB	-3.12	1.33	1.37
23	b	621	CLA	OBD-CAD	3.12	1.27	1.22
23	D	2303	CLA	OBD-CAD	3.11	1.27	1.22
23	A	406	CLA	C4B-NB	-3.11	1.33	1.37
23	C	506	CLA	C4D-CHA	3.11	1.49	1.38
23	b	612	CLA	C4D-CHA	3.10	1.49	1.38
23	B	604	CLA	OBD-CAD	3.10	1.27	1.22
39	e	103	HEM	CAB-C3B	3.10	1.55	1.47
23	b	621	CLA	C4D-CHA	3.09	1.49	1.38
36	B	626	HTG	C1'-S1	-3.09	1.77	1.81
23	C	512	CLA	C1B-C2B	3.09	1.50	1.43
23	c	508	CLA	C4D-CHA	3.08	1.48	1.38
23	C	511	CLA	C4D-CHA	3.07	1.48	1.38
23	c	507	CLA	C4D-CHA	3.07	1.48	1.38
23	C	505	CLA	C4D-CHA	3.07	1.48	1.38
23	b	610	CLA	C4B-NB	-3.07	1.33	1.37
23	c	514	CLA	MG-NC	3.07	2.13	2.06
23	c	504	CLA	MG-NC	3.06	2.13	2.06
39	F	101	HEM	CAC-C3C	3.05	1.55	1.47
39	e	103	HEM	CAC-C3C	3.05	1.55	1.47
23	C	504	CLA	C4D-CHA	3.05	1.48	1.38
23	B	603	CLA	C1B-C2B	3.05	1.50	1.43
23	B	614	CLA	C1B-NB	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	C1B-C2B	3.05	1.50	1.43
23	B	616	CLA	C4D-CHA	3.04	1.48	1.38
36	C	521	HTG	C1'-S1	-3.04	1.77	1.81
23	C	510	CLA	C1B-C2B	3.04	1.50	1.43
23	c	515	CLA	C1B-C2B	3.04	1.50	1.43
23	b	619	CLA	C1B-NB	-3.04	1.33	1.37
23	d	408	CLA	C1B-C2B	3.03	1.50	1.43
23	b	607	CLA	C4D-CHA	3.03	1.48	1.38
23	C	511	CLA	C1C-C2C	3.03	1.50	1.44
23	b	610	CLA	C4D-CHA	3.03	1.48	1.38
23	B	604	CLA	C1B-C2B	3.03	1.50	1.43
23	c	513	CLA	C4D-CHA	3.02	1.48	1.38
23	b	618	CLA	C4D-CHA	3.02	1.48	1.38
23	A	407	CLA	MG-NB	-3.02	1.99	2.05
23	a	2610	CLA	C1B-NB	-3.02	1.33	1.37
23	a	2613	CLA	C1B-C2B	3.02	1.50	1.43
23	c	514	CLA	C4D-CHA	3.02	1.48	1.38
31	a	2619	JOX	C3-CL	3.01	1.78	1.73
23	b	615	CLA	MG-NB	3.01	2.11	2.05
23	B	606	CLA	C1B-C2B	3.01	1.50	1.43
39	F	101	HEM	FE-NC	3.00	2.05	1.95
23	c	510	CLA	C1B-C2B	3.00	1.50	1.43
23	c	508	CLA	C1B-C2B	3.00	1.50	1.43
23	d	408	CLA	C1C-NC	-3.00	1.33	1.37
23	B	611	CLA	C4D-CHA	2.99	1.48	1.38
23	B	604	CLA	C1C-C2C	2.99	1.50	1.44
23	c	508	CLA	C4B-NB	-2.99	1.33	1.37
23	C	507	CLA	C4D-CHA	2.98	1.48	1.38
23	B	616	CLA	C1B-NB	-2.98	1.33	1.37
23	b	619	CLA	C1B-C2B	2.98	1.50	1.43
23	C	511	CLA	C1B-C2B	2.98	1.50	1.43
23	B	614	CLA	C4D-CHA	2.98	1.48	1.38
23	c	516	CLA	C4D-CHA	2.97	1.48	1.38
23	B	605	CLA	C1B-C2B	2.97	1.50	1.43
36	b	603	HTG	C1'-S1	-2.96	1.77	1.81
39	F	101	HEM	CAB-C3B	2.95	1.55	1.47
23	b	616	CLA	C4D-CHA	2.95	1.48	1.38
23	a	2613	CLA	C4D-CHA	2.95	1.48	1.38
36	B	624[A]	HTG	C1'-S1	-2.95	1.77	1.81
23	b	610	CLA	OBD-CAD	2.95	1.27	1.22
23	b	614	CLA	C4D-CHA	2.95	1.48	1.38
23	B	611	CLA	C1B-NB	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C4D-CHA	2.94	1.48	1.38
36	C	522	HTG	C1'-S1	-2.94	1.77	1.81
23	b	613	CLA	C4D-CHA	2.94	1.48	1.38
23	B	603	CLA	C4D-CHA	2.94	1.48	1.38
23	B	613	CLA	C1B-C2B	2.93	1.50	1.43
23	c	506	CLA	C1B-C2B	2.93	1.50	1.43
23	a	2613	CLA	C4B-NB	-2.93	1.34	1.37
23	a	2609	CLA	C1B-C2B	2.93	1.50	1.43
23	A	407	CLA	MG-ND	-2.93	2.00	2.05
23	B	609	CLA	C4B-NB	-2.93	1.34	1.37
23	b	621	CLA	C4B-NB	-2.92	1.34	1.37
23	c	516	CLA	C1B-C2B	2.92	1.50	1.43
23	d	402	CLA	MG-NC	2.92	2.13	2.06
23	b	617	CLA	C4D-CHA	2.91	1.48	1.38
23	C	512	CLA	MG-NB	2.91	2.11	2.05
23	D	2304	CLA	C4D-CHA	2.91	1.48	1.38
23	b	610	CLA	C1B-C2B	2.91	1.49	1.43
23	d	408	CLA	C4D-CHA	2.91	1.48	1.38
31	a	2619	JOX	C1-CL1	2.90	1.78	1.73
23	b	608	CLA	C1B-C2B	2.90	1.49	1.43
23	d	409	CLA	C1B-C2B	2.90	1.49	1.43
23	b	607	CLA	C1B-C2B	2.89	1.49	1.43
23	A	405	CLA	C4D-CHA	2.89	1.48	1.38
23	C	506	CLA	C1B-C2B	2.89	1.49	1.43
23	c	513	CLA	C1B-NB	-2.88	1.34	1.37
23	C	505	CLA	C4B-NB	-2.88	1.34	1.37
23	B	609	CLA	C4D-CHA	2.88	1.48	1.38
23	c	504	CLA	C4D-CHA	2.88	1.48	1.38
23	C	506	CLA	C4C-C3C	2.88	1.49	1.45
23	A	407	CLA	C4D-CHA	2.88	1.48	1.38
23	D	2304	CLA	C1B-C2B	2.88	1.49	1.43
23	B	611	CLA	MG-NB	2.87	2.11	2.05
23	b	621	CLA	C1C-NC	-2.87	1.33	1.37
23	b	616	CLA	C4B-NB	-2.87	1.34	1.37
23	b	618	CLA	C1B-C2B	2.87	1.49	1.43
23	B	614	CLA	C1B-C2B	2.86	1.49	1.43
23	b	611	CLA	MG-NB	2.86	2.11	2.05
23	c	513	CLA	C4B-NB	-2.85	1.34	1.37
24	a	2612	PHO	C3A-C2A	-2.85	1.52	1.54
23	b	608	CLA	C4D-CHA	2.85	1.48	1.38
23	d	402	CLA	C4B-NB	-2.85	1.34	1.37
23	B	606	CLA	C4D-CHA	2.85	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	2303	CLA	C4D-CHA	2.85	1.48	1.38
23	c	507	CLA	C1B-C2B	2.85	1.49	1.43
23	c	513	CLA	C1B-C2B	2.85	1.49	1.43
23	b	619	CLA	C4D-CHA	2.85	1.48	1.38
23	B	617	CLA	OBD-CAD	2.84	1.27	1.22
23	c	509	CLA	C1B-NB	-2.84	1.34	1.37
23	C	509	CLA	C1B-C2B	2.84	1.49	1.43
23	b	616	CLA	C1B-C2B	2.84	1.49	1.43
23	b	609	CLA	C1B-C2B	2.83	1.49	1.43
23	C	509	CLA	C4D-CHA	2.83	1.48	1.38
23	C	504	CLA	C1C-C2C	2.83	1.50	1.44
23	D	2303	CLA	C1B-C2B	2.83	1.49	1.43
23	A	405	CLA	C1B-C2B	2.83	1.49	1.43
23	c	515	CLA	C1B-NB	-2.83	1.34	1.37
23	b	620	CLA	C1B-C2B	2.83	1.49	1.43
23	A	406	CLA	C1B-C2B	2.83	1.49	1.43
23	a	2610	CLA	C1B-C2B	2.82	1.49	1.43
23	c	505	CLA	C4D-CHA	2.82	1.48	1.38
23	b	619	CLA	MG-NB	2.82	2.11	2.05
23	B	610	CLA	C4D-CHA	2.81	1.48	1.38
23	c	509	CLA	C4D-CHA	2.81	1.48	1.38
33	D	2306	PL9	C6-C5	2.81	1.49	1.35
23	C	502	CLA	C1B-NB	-2.81	1.34	1.37
23	d	408	CLA	C1B-NB	-2.81	1.34	1.37
23	d	409	CLA	C4D-CHA	2.81	1.48	1.38
23	d	409	CLA	C4B-NB	-2.81	1.34	1.37
23	C	513	CLA	C1B-C2B	2.81	1.49	1.43
23	b	614	CLA	C1B-C2B	2.80	1.49	1.43
23	C	503	CLA	C1B-NB	-2.80	1.34	1.37
23	C	508	CLA	C1B-C2B	2.80	1.49	1.43
23	c	508	CLA	C1C-NC	-2.79	1.33	1.37
23	c	507	CLA	C1B-NB	-2.78	1.34	1.37
23	c	512	CLA	C1C-C2C	2.78	1.50	1.44
23	B	617	CLA	C4B-NB	-2.78	1.34	1.37
23	b	615	CLA	C1B-C2B	2.78	1.49	1.43
23	B	616	CLA	MG-NC	2.77	2.12	2.06
23	b	612	CLA	MG-NB	2.77	2.11	2.05
23	d	402	CLA	C4D-CHA	2.77	1.47	1.38
23	a	2609	CLA	C4D-CHA	2.77	1.47	1.38
23	a	2610	CLA	C4D-CHA	2.77	1.47	1.38
23	b	616	CLA	C1B-NB	-2.77	1.34	1.37
23	b	613	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1B-NB	-2.77	1.34	1.37
23	c	505	CLA	C1B-C2B	2.77	1.49	1.43
23	c	504	CLA	C4B-NB	-2.76	1.34	1.37
23	b	617	CLA	C1B-C2B	2.76	1.49	1.43
31	a	2617	JOX	C3-CL	2.76	1.78	1.73
23	C	503	CLA	MG-NB	2.75	2.11	2.05
23	b	607	CLA	C1C-NC	-2.75	1.33	1.37
23	B	610	CLA	C1B-C2B	2.74	1.49	1.43
36	o	301	HTG	C1'-S1	-2.73	1.77	1.81
23	B	617	CLA	C1C-NC	-2.73	1.33	1.37
23	a	2613	CLA	MG-NA	2.73	2.12	2.06
23	b	613	CLA	C1B-NB	-2.73	1.34	1.37
23	b	612	CLA	C4B-NB	-2.73	1.34	1.37
23	c	511	CLA	C4D-CHA	2.73	1.47	1.38
23	C	513	CLA	C1C-C2C	2.73	1.50	1.44
31	A	419	JOX	C3-CL	2.73	1.78	1.73
23	C	514	CLA	C1B-C2B	2.73	1.49	1.43
23	B	605	CLA	C1B-NB	-2.72	1.34	1.37
23	C	503	CLA	C4B-NB	-2.72	1.34	1.37
23	A	410	CLA	C1B-C2B	2.72	1.49	1.43
23	C	509	CLA	C1B-NB	-2.72	1.34	1.37
23	d	409	CLA	C4C-C3C	2.71	1.49	1.45
23	b	618	CLA	C1B-NB	-2.71	1.34	1.37
23	D	2303	CLA	C1B-NB	-2.71	1.34	1.37
23	b	607	CLA	C4C-C3C	2.70	1.49	1.45
23	C	510	CLA	C1B-NB	-2.70	1.34	1.37
23	b	607	CLA	C4B-NB	-2.69	1.34	1.37
23	b	610	CLA	C1C-NC	-2.69	1.33	1.37
24	a	2612	PHO	C4B-NB	-2.68	1.33	1.38
23	c	504	CLA	C1B-C2B	2.68	1.49	1.43
23	C	510	CLA	C1C-C2C	2.68	1.50	1.44
23	C	514	CLA	C4D-CHA	2.68	1.47	1.38
23	B	602	CLA	C1B-C2B	2.67	1.49	1.43
23	b	609	CLA	C1B-NB	-2.67	1.34	1.37
23	C	503	CLA	C1B-C2B	2.67	1.49	1.43
23	c	506	CLA	MG-ND	-2.67	2.00	2.05
23	C	502	CLA	C1B-C2B	2.66	1.49	1.43
23	c	516	CLA	C1B-NB	-2.66	1.34	1.37
26	d	417	SQD	O47-C45	-2.66	1.43	1.46
23	b	617	CLA	C4B-NB	-2.66	1.34	1.37
23	c	505	CLA	C1C-C2C	2.66	1.49	1.44
23	A	410	CLA	C1B-NB	-2.65	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C1B-NB	-2.65	1.34	1.37
23	b	614	CLA	C1B-NB	-2.65	1.34	1.37
24	a	2611	PHO	C4B-NB	-2.65	1.33	1.38
23	b	617	CLA	C1C-C2C	2.64	1.49	1.44
23	B	608	CLA	C4B-NB	-2.64	1.34	1.37
23	B	609	CLA	C1B-C2B	2.64	1.49	1.43
23	C	512	CLA	C4C-C3C	2.64	1.49	1.45
23	b	611	CLA	C1B-C2B	2.64	1.49	1.43
23	C	507	CLA	C1C-NC	-2.64	1.33	1.37
23	b	606	CLA	C4C-C3C	2.64	1.49	1.45
23	c	512	CLA	C4C-C3C	2.63	1.49	1.45
23	B	603	CLA	C1B-NB	-2.63	1.34	1.37
23	B	603	CLA	C4C-C3C	2.63	1.49	1.45
23	C	510	CLA	C4C-C3C	2.63	1.49	1.45
23	b	606	CLA	C1B-C2B	2.62	1.49	1.43
23	B	613	CLA	C4B-NB	-2.62	1.34	1.37
24	A	409	PHO	C4B-NB	-2.62	1.33	1.38
23	b	606	CLA	C1B-NB	-2.62	1.34	1.37
23	B	613	CLA	C4D-CHA	2.62	1.47	1.38
23	B	611	CLA	C3B-C4B	2.62	1.50	1.42
23	B	612	CLA	C4B-NB	-2.61	1.34	1.37
23	c	509	CLA	C1C-NC	-2.61	1.33	1.37
23	C	507	CLA	C4B-NB	-2.61	1.34	1.37
23	B	611	CLA	C1B-C2B	2.60	1.49	1.43
23	C	514	CLA	C1C-C2C	2.60	1.49	1.44
31	A	419	JOX	C-C1	2.60	1.40	1.35
23	b	615	CLA	C4B-NB	-2.59	1.34	1.37
23	C	508	CLA	C1C-NC	-2.59	1.33	1.37
33	d	411	PL9	C6-C5	2.59	1.48	1.35
23	C	514	CLA	C1B-NB	-2.59	1.34	1.37
23	c	510	CLA	C1C-NC	-2.59	1.33	1.37
23	c	511	CLA	C1B-C2B	2.58	1.49	1.43
23	A	410	CLA	C4C-C3C	2.58	1.49	1.45
23	c	516	CLA	C4B-NB	-2.58	1.34	1.37
23	d	408	CLA	C4B-NB	-2.58	1.34	1.37
23	c	506	CLA	C1C-C2C	2.57	1.49	1.44
23	c	504	CLA	C1C-NC	-2.57	1.33	1.37
23	C	511	CLA	C4B-NB	-2.57	1.34	1.37
23	c	512	CLA	C1C-NC	-2.57	1.33	1.37
23	d	408	CLA	C4C-C3C	2.57	1.49	1.45
23	c	514	CLA	C4B-NB	-2.56	1.34	1.37
29	U	502	GOL	O2-C2	-2.56	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1C-C2C	2.56	1.49	1.44
23	b	619	CLA	C4B-NB	-2.56	1.34	1.37
23	b	619	CLA	C4C-C3C	2.56	1.49	1.45
23	c	511	CLA	C1C-C2C	2.56	1.49	1.44
23	B	607	CLA	C1B-C2B	2.56	1.49	1.43
23	B	617	CLA	C1B-C2B	2.56	1.49	1.43
23	c	507	CLA	C4B-NB	-2.56	1.34	1.37
31	a	2617	JOX	C4-C3	2.56	1.40	1.35
23	c	507	CLA	MG-NC	2.55	2.12	2.06
23	b	607	CLA	C1B-NB	-2.54	1.34	1.37
23	C	506	CLA	C1B-NB	-2.54	1.34	1.37
31	a	2619	JOX	C4-C3	2.53	1.40	1.35
23	c	505	CLA	C1B-NB	-2.53	1.34	1.37
23	C	503	CLA	C1C-C2C	2.53	1.49	1.44
31	a	2617	JOX	C1-CL1	2.53	1.77	1.73
23	C	505	CLA	C1B-C2B	2.53	1.49	1.43
23	c	508	CLA	C1C-C2C	2.53	1.49	1.44
23	C	506	CLA	C4B-NB	-2.53	1.34	1.37
23	a	2609	CLA	C4B-NB	-2.53	1.34	1.37
23	A	405	CLA	C1C-C2C	2.52	1.49	1.44
23	b	609	CLA	C1C-C2C	2.52	1.49	1.44
23	C	513	CLA	C4B-NB	-2.52	1.34	1.37
31	a	2617	JOX	C-C1	2.52	1.40	1.35
23	c	516	CLA	C1C-C2C	2.51	1.49	1.44
23	C	514	CLA	C3D-C4D	-2.51	1.38	1.44
23	b	616	CLA	C3B-C2B	2.51	1.49	1.41
23	B	614	CLA	C1C-C2C	2.50	1.49	1.44
23	b	614	CLA	C1C-C2C	2.50	1.49	1.44
24	a	2612	PHO	CHA-CBD	-2.50	1.48	1.51
23	C	504	CLA	C1C-NC	-2.49	1.34	1.37
23	c	514	CLA	C3B-C4B	2.49	1.50	1.42
24	A	409	PHO	C1D-ND	-2.49	1.34	1.38
23	b	618	CLA	C1C-NC	-2.49	1.34	1.37
23	A	406	CLA	C1C-NC	-2.48	1.34	1.37
23	B	602	CLA	C3B-C4B	2.48	1.50	1.42
23	d	409	CLA	C1C-C2C	2.48	1.49	1.44
23	b	609	CLA	C4B-NB	-2.48	1.34	1.37
23	b	618	CLA	C3B-C2B	2.48	1.49	1.41
23	b	608	CLA	C1C-C2C	2.48	1.49	1.44
23	B	612	CLA	C1B-C2B	2.48	1.49	1.43
23	b	614	CLA	C1D-C2D	2.48	1.50	1.45
24	A	409	PHO	C3D-C4D	-2.47	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C1C-NC	-2.47	1.34	1.37
23	B	608	CLA	C1B-NB	-2.47	1.34	1.37
23	b	615	CLA	C3B-C4B	2.47	1.49	1.42
24	A	408	PHO	C1B-NB	-2.47	1.34	1.38
23	C	506	CLA	C1C-NC	-2.47	1.34	1.37
23	c	508	CLA	C1B-NB	-2.47	1.34	1.37
23	B	615	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	609	CLA	C4C-C3C	2.46	1.49	1.45
31	A	418	JOX	C-C1	2.46	1.39	1.35
23	C	502	CLA	C1C-C2C	2.46	1.49	1.44
23	c	511	CLA	C3B-C2B	2.46	1.49	1.41
23	B	602	CLA	C1C-C2C	2.46	1.49	1.44
23	A	410	CLA	C4B-NB	-2.46	1.34	1.37
23	c	509	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	509	CLA	C4C-C3C	2.46	1.49	1.45
23	b	620	CLA	C3B-C4B	2.46	1.49	1.42
23	A	407	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	617	CLA	C1C-NC	-2.46	1.34	1.37
23	C	505	CLA	C1C-C2C	2.46	1.49	1.44
23	A	406	CLA	C3B-C2B	2.46	1.49	1.41
23	c	504	CLA	C1C-C2C	2.45	1.49	1.44
23	A	406	CLA	MG-NB	2.45	2.10	2.05
23	B	611	CLA	C4C-C3C	2.45	1.49	1.45
23	b	621	CLA	C1B-NB	-2.45	1.34	1.37
23	b	607	CLA	C1C-C2C	2.45	1.49	1.44
23	C	513	CLA	C3B-C4B	2.45	1.49	1.42
23	B	613	CLA	C1C-NC	-2.45	1.34	1.37
23	b	613	CLA	C1C-NC	-2.45	1.34	1.37
23	b	606	CLA	C1C-C2C	2.45	1.49	1.44
23	c	515	CLA	C1C-C2C	2.44	1.49	1.44
23	b	606	CLA	C3B-C4B	2.44	1.49	1.42
23	A	407	CLA	C1B-C2B	2.44	1.48	1.43
23	c	511	CLA	C4B-NB	-2.44	1.34	1.37
23	B	602	CLA	C3B-C2B	2.44	1.49	1.41
23	d	408	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	502	CLA	C1C-NC	-2.44	1.34	1.37
23	c	512	CLA	C4B-NB	-2.44	1.34	1.37
23	b	613	CLA	MG-NB	2.44	2.10	2.05
23	C	511	CLA	C4C-C3C	2.43	1.49	1.45
36	b	626	HTG	C1-S1	-2.43	1.76	1.80
23	C	510	CLA	C3B-C2B	2.43	1.49	1.41
23	B	606	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C4C-C3C	2.43	1.49	1.45
23	c	512	CLA	C1B-NB	-2.43	1.34	1.37
23	D	2303	CLA	C1C-C2C	2.42	1.49	1.44
23	B	617	CLA	C3B-C2B	2.42	1.49	1.41
31	A	419	JOX	C4-C3	2.42	1.39	1.35
23	C	505	CLA	MG-NB	2.42	2.10	2.05
28	j	2701	LMT	O1'-C1'	2.42	1.44	1.40
23	a	2610	CLA	C4B-NB	-2.42	1.34	1.37
23	c	510	CLA	C1B-NB	-2.42	1.34	1.37
23	A	405	CLA	C4C-C3C	2.42	1.49	1.45
23	C	502	CLA	C3B-C4B	2.42	1.49	1.42
23	c	509	CLA	C4B-NB	-2.42	1.34	1.37
23	A	405	CLA	C4B-NB	-2.41	1.34	1.37
23	D	2304	CLA	C4B-NB	-2.41	1.34	1.37
23	B	613	CLA	C3B-C2B	2.41	1.49	1.41
23	B	610	CLA	C4C-C3C	2.41	1.49	1.45
23	c	509	CLA	C1B-C2B	2.41	1.48	1.43
23	B	613	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	616	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	618	CLA	C4C-C3C	2.41	1.49	1.45
23	B	605	CLA	C4C-C3C	2.41	1.49	1.45
23	B	607	CLA	C1C-C2C	2.40	1.49	1.44
23	c	508	CLA	C4C-C3C	2.40	1.49	1.45
23	a	2609	CLA	C1C-C2C	2.40	1.49	1.44
23	b	621	CLA	C3B-C2B	2.40	1.49	1.41
23	a	2610	CLA	C3B-C4B	2.40	1.49	1.42
23	B	617	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	609	CLA	C1C-C2C	2.39	1.49	1.44
23	b	608	CLA	C1C-NC	-2.39	1.34	1.37
23	a	2609	CLA	C3B-C2B	2.39	1.49	1.41
23	c	514	CLA	C1C-C2C	2.39	1.49	1.44
23	b	617	CLA	C3B-C2B	2.39	1.49	1.41
23	b	610	CLA	C3B-C2B	2.39	1.49	1.41
23	b	620	CLA	C1B-NB	-2.39	1.34	1.37
23	C	505	CLA	C3D-C4D	-2.38	1.38	1.44
26	D	2302	SQD	O6-C1	2.38	1.44	1.40
23	b	614	CLA	C4C-C3C	2.38	1.49	1.45
23	C	506	CLA	C1C-C2C	2.38	1.49	1.44
23	A	407	CLA	C3B-C4B	2.38	1.49	1.42
23	b	610	CLA	C1B-NB	-2.38	1.34	1.37
23	c	512	CLA	C3B-C2B	2.37	1.49	1.41
23	C	503	CLA	C3B-C2B	2.37	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C1B-NB	-2.37	1.34	1.37
23	B	604	CLA	C1C-NC	-2.37	1.34	1.37
23	c	510	CLA	C3B-C2B	2.37	1.49	1.41
23	b	619	CLA	C1C-C2C	2.37	1.49	1.44
23	B	611	CLA	C1C-NC	-2.37	1.34	1.37
23	C	512	CLA	C3B-C2B	2.37	1.49	1.41
23	C	502	CLA	C3D-C4D	-2.37	1.38	1.44
23	C	511	CLA	C1C-NC	-2.37	1.34	1.37
23	B	617	CLA	C1B-NB	-2.36	1.34	1.37
23	C	504	CLA	C3B-C2B	2.36	1.49	1.41
23	B	614	CLA	C1C-NC	-2.36	1.34	1.37
23	B	602	CLA	C4B-NB	-2.36	1.34	1.37
23	A	406	CLA	C1C-C2C	2.36	1.49	1.44
23	b	611	CLA	C1B-NB	-2.36	1.34	1.37
23	B	612	CLA	C3B-C2B	2.36	1.49	1.41
23	B	613	CLA	C1C-C2C	2.36	1.49	1.44
23	B	607	CLA	C3B-C2B	2.36	1.49	1.41
23	B	605	CLA	C3B-C2B	2.36	1.49	1.41
23	C	510	CLA	C1C-NC	-2.36	1.34	1.37
23	C	509	CLA	C4B-NB	-2.35	1.34	1.37
23	c	514	CLA	C1B-NB	-2.35	1.34	1.37
28	B	634	LMT	O1'-C1'	2.35	1.44	1.40
23	C	507	CLA	C3D-C4D	-2.35	1.38	1.44
23	A	410	CLA	C1C-C2C	2.35	1.49	1.44
23	B	606	CLA	C4B-NB	-2.35	1.34	1.37
23	C	504	CLA	MG-ND	-2.35	2.01	2.05
23	C	502	CLA	C4B-NB	-2.35	1.34	1.37
42	v	201	HEC	CMC-C2C	2.35	1.55	1.50
42	v	201	HEC	CMD-C2D	2.35	1.55	1.50
23	C	509	CLA	C3B-C2B	2.34	1.49	1.41
23	B	604	CLA	C1B-NB	-2.34	1.34	1.37
23	C	514	CLA	C4B-NB	-2.34	1.34	1.37
26	B	621	SQD	O6-C1	2.34	1.44	1.40
23	b	607	CLA	C3B-C4B	2.34	1.49	1.42
23	c	511	CLA	C3D-C4D	-2.33	1.38	1.44
23	a	2609	CLA	C1C-NC	-2.33	1.34	1.37
23	c	506	CLA	C4B-NB	-2.33	1.34	1.37
23	B	604	CLA	C3B-C4B	2.33	1.49	1.42
23	B	606	CLA	C1B-NB	-2.33	1.34	1.37
23	b	611	CLA	C3B-C2B	2.33	1.49	1.41
23	b	607	CLA	C3B-C2B	2.33	1.49	1.41
23	c	516	CLA	MG-NB	2.33	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C1C-C2C	2.33	1.49	1.44
23	C	509	CLA	C3B-C4B	2.33	1.49	1.42
23	C	503	CLA	C4C-C3C	2.33	1.49	1.45
39	F	101	HEM	CMB-C2B	2.33	1.55	1.50
23	c	513	CLA	C3B-C2B	2.33	1.49	1.41
23	C	514	CLA	C3B-C4B	2.32	1.49	1.42
23	B	606	CLA	C3B-C4B	2.32	1.49	1.42
23	c	515	CLA	C4B-NB	-2.32	1.34	1.37
23	c	514	CLA	C3B-C2B	2.32	1.49	1.41
23	C	508	CLA	C3B-C2B	2.32	1.49	1.41
23	B	604	CLA	C4C-C3C	2.32	1.49	1.45
23	b	608	CLA	C3B-C4B	2.32	1.49	1.42
28	T	103	LMT	O1'-C1'	2.31	1.44	1.40
23	b	609	CLA	C1C-NC	-2.31	1.34	1.37
23	B	614	CLA	C3B-C2B	2.31	1.49	1.41
23	a	2610	CLA	C1C-NC	-2.31	1.34	1.37
23	a	2613	CLA	C1C-NC	-2.31	1.34	1.37
24	A	408	PHO	C4B-NB	-2.31	1.34	1.38
42	V	201	HEC	CMC-C2C	2.31	1.55	1.50
23	A	410	CLA	C1C-NC	-2.31	1.34	1.37
23	b	609	CLA	C3B-C2B	2.31	1.49	1.41
23	c	507	CLA	C4C-C3C	2.31	1.49	1.45
23	c	509	CLA	C4C-C3C	2.30	1.48	1.45
23	B	603	CLA	C4B-NB	-2.30	1.34	1.37
23	c	516	CLA	C4C-C3C	2.30	1.48	1.45
23	D	2304	CLA	C3B-C2B	2.30	1.48	1.41
23	B	610	CLA	C1C-NC	-2.30	1.34	1.37
23	C	505	CLA	C4C-C3C	2.30	1.48	1.45
23	b	606	CLA	C3B-C2B	2.30	1.48	1.41
23	C	505	CLA	C1C-NC	-2.29	1.34	1.37
23	b	615	CLA	C1C-C2C	2.29	1.49	1.44
23	b	612	CLA	C1C-C2C	2.29	1.49	1.44
23	c	515	CLA	C3B-C2B	2.29	1.48	1.41
23	c	505	CLA	C3B-C2B	2.29	1.48	1.41
23	D	2303	CLA	C3B-C2B	2.29	1.48	1.41
23	b	618	CLA	C1C-C2C	2.29	1.49	1.44
23	c	509	CLA	C3B-C4B	2.29	1.49	1.42
23	C	508	CLA	C1C-C2C	2.29	1.49	1.44
23	C	506	CLA	C3B-C2B	2.28	1.48	1.41
23	a	2609	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	611	CLA	C1C-C2C	2.28	1.49	1.44
23	A	407	CLA	C4B-NB	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	621	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	603	CLA	C3B-C2B	2.27	1.48	1.41
23	c	516	CLA	C3B-C2B	2.27	1.48	1.41
23	c	509	CLA	C3B-C2B	2.27	1.48	1.41
23	B	605	CLA	C1C-C2C	2.27	1.49	1.44
23	b	612	CLA	C3B-C4B	2.27	1.49	1.42
23	c	507	CLA	C1C-C2C	2.27	1.49	1.44
23	B	602	CLA	C1D-C2D	2.27	1.49	1.45
23	c	514	CLA	C4C-C3C	2.27	1.48	1.45
36	H	101	HTG	C1-S1	-2.27	1.76	1.80
23	d	408	CLA	C3B-C2B	2.26	1.48	1.41
23	C	512	CLA	C1C-C2C	2.26	1.49	1.44
23	A	405	CLA	C3B-C2B	2.26	1.48	1.41
23	B	608	CLA	C4C-C3C	2.26	1.48	1.45
23	d	409	CLA	C3B-C2B	2.26	1.48	1.41
23	b	620	CLA	C3B-C2B	2.26	1.48	1.41
23	A	410	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	606	CLA	C1C-NC	-2.26	1.34	1.37
23	c	507	CLA	C3B-C2B	2.25	1.48	1.41
23	c	505	CLA	C4B-NB	-2.25	1.34	1.37
23	B	606	CLA	C3B-C2B	2.25	1.48	1.41
23	b	614	CLA	C1C-NC	-2.25	1.34	1.37
23	D	2303	CLA	C4C-C3C	2.25	1.48	1.45
23	c	510	CLA	C4C-C3C	2.25	1.48	1.45
23	b	611	CLA	C4B-NB	-2.25	1.34	1.37
23	B	610	CLA	C1B-NB	-2.25	1.34	1.37
23	C	512	CLA	C3B-C4B	2.24	1.49	1.42
23	b	608	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	608	CLA	C1B-NB	-2.24	1.34	1.37
23	B	603	CLA	C3B-C4B	2.24	1.49	1.42
23	C	513	CLA	C3D-C4D	-2.24	1.39	1.44
23	a	2613	CLA	C3B-C4B	2.24	1.49	1.42
36	d	407	HTG	C1-S1	-2.24	1.77	1.80
36	b	604	HTG	C1-S1	-2.23	1.77	1.80
23	b	606	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	611	CLA	C1C-C2C	2.23	1.49	1.44
23	c	509	CLA	C1C-C2C	2.23	1.49	1.44
23	c	510	CLA	C1C-C2C	2.23	1.49	1.44
23	c	506	CLA	C4C-C3C	2.23	1.48	1.45
23	C	505	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C3B-C4B	2.23	1.49	1.42
23	B	609	CLA	C3B-C2B	2.23	1.48	1.41
23	b	618	CLA	C4B-NB	-2.23	1.34	1.37
36	c	524	HTG	C1-S1	-2.23	1.77	1.80
36	B	626	HTG	C1-S1	-2.23	1.77	1.80
23	b	619	CLA	C3D-C4D	-2.22	1.39	1.44
23	a	2609	CLA	C3B-C4B	2.22	1.49	1.42
31	a	2619	JOX	C-C1	2.22	1.39	1.35
23	C	513	CLA	C3B-C2B	2.22	1.48	1.41
37	c	520	DGD	O2G-C2G	-2.22	1.41	1.46
23	B	607	CLA	C4C-C3C	2.22	1.48	1.45
23	B	604	CLA	C4B-NB	-2.22	1.34	1.37
23	D	2304	CLA	C3B-C4B	2.22	1.49	1.42
23	a	2610	CLA	MG-NB	2.22	2.10	2.05
24	A	409	PHO	C3A-C2A	-2.22	1.52	1.54
23	B	615	CLA	C4C-C3C	2.21	1.48	1.45
23	B	614	CLA	C4B-NB	-2.21	1.35	1.37
23	b	620	CLA	MG-NB	2.21	2.10	2.05
23	C	509	CLA	C1C-C2C	2.21	1.49	1.44
23	b	613	CLA	C4C-C3C	2.21	1.48	1.45
23	b	612	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	602	CLA	C1C-NC	-2.21	1.34	1.37
23	c	511	CLA	C3B-C4B	2.21	1.49	1.42
24	A	409	PHO	C1B-NB	-2.21	1.34	1.38
23	C	511	CLA	C3B-C2B	2.21	1.48	1.41
42	V	201	HEC	CMD-C2D	2.21	1.55	1.50
23	B	612	CLA	C3D-C4D	-2.21	1.39	1.44
23	C	508	CLA	C4B-NB	-2.21	1.35	1.37
23	b	610	CLA	C3B-C4B	2.20	1.49	1.42
23	b	615	CLA	C3B-C2B	2.20	1.48	1.41
23	B	603	CLA	MG-NB	2.20	2.10	2.05
23	b	606	CLA	C1C-NC	-2.20	1.34	1.37
23	c	505	CLA	MG-NB	2.20	2.10	2.05
23	C	504	CLA	C1B-NB	-2.20	1.35	1.37
23	C	514	CLA	C4C-C3C	2.19	1.48	1.45
23	a	2613	CLA	C3B-C2B	2.19	1.48	1.41
23	B	608	CLA	C3B-C2B	2.19	1.48	1.41
25	D	2305	BCR	C30-C25	-2.19	1.51	1.53
23	C	504	CLA	C3B-C4B	2.19	1.49	1.42
23	c	504	CLA	C3B-C2B	2.19	1.48	1.41
23	B	603	CLA	C1C-C2C	2.18	1.49	1.44
23	C	506	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	514	CLA	C3B-C2B	2.18	1.48	1.41
23	B	610	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	505	CLA	C3B-C4B	2.18	1.49	1.42
23	A	410	CLA	C3B-C2B	2.17	1.48	1.41
23	b	613	CLA	C3B-C2B	2.17	1.48	1.41
23	B	610	CLA	C1C-C2C	2.17	1.48	1.44
23	b	619	CLA	C3B-C2B	2.17	1.48	1.41
23	D	2303	CLA	C3D-C4D	-2.17	1.39	1.44
31	A	418	JOX	C4-C5	-2.16	1.40	1.45
23	C	510	CLA	C3D-C4D	-2.16	1.39	1.44
23	C	505	CLA	C3B-C2B	2.16	1.48	1.41
23	B	605	CLA	C4B-NB	-2.16	1.35	1.37
23	c	508	CLA	C3B-C2B	2.16	1.48	1.41
23	c	504	CLA	C1B-NB	-2.16	1.35	1.37
23	c	511	CLA	C1C-NC	-2.16	1.34	1.37
23	C	507	CLA	C1B-C2B	2.15	1.48	1.43
23	a	2610	CLA	C1C-C2C	2.15	1.48	1.44
23	A	410	CLA	C3B-C4B	2.15	1.49	1.42
39	e	103	HEM	CMC-C2C	2.15	1.55	1.50
31	a	2619	JOX	C4-C5	-2.14	1.40	1.45
23	b	612	CLA	C3B-C2B	2.14	1.48	1.41
23	B	607	CLA	C3D-C4D	-2.14	1.39	1.44
23	a	2613	CLA	C3D-C4D	-2.14	1.39	1.44
23	C	503	CLA	C1C-NC	-2.14	1.34	1.37
23	B	603	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	606	CLA	C3D-C4D	-2.14	1.39	1.44
23	b	620	CLA	C4C-C3C	2.14	1.48	1.45
23	c	508	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	608	CLA	C3B-C4B	2.14	1.49	1.42
23	B	616	CLA	C1C-NC	-2.13	1.34	1.37
23	c	505	CLA	C3D-C4D	-2.13	1.39	1.44
23	c	505	CLA	C4C-C3C	2.13	1.48	1.45
23	c	515	CLA	C3B-C4B	2.13	1.49	1.42
23	b	614	CLA	C4B-NB	-2.13	1.35	1.37
23	b	618	CLA	C3D-C4D	-2.13	1.39	1.44
36	C	521	HTG	C1-S1	-2.13	1.77	1.80
23	c	516	CLA	C3B-C4B	2.12	1.48	1.42
23	d	409	CLA	C3B-C4B	2.12	1.48	1.42
23	D	2304	CLA	MG-NB	2.12	2.10	2.05
36	c	523	HTG	C1-S1	-2.12	1.77	1.80
23	b	612	CLA	C1C-NC	-2.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C1C-C2C	2.12	1.48	1.44
27	D	2312	LMG	O7-C8	-2.12	1.41	1.46
26	l	101	SQD	O6-C1	2.12	1.43	1.40
23	d	409	CLA	C3D-C4D	-2.12	1.39	1.44
23	A	407	CLA	C1C-NC	-2.12	1.34	1.37
23	A	406	CLA	C3B-C4B	2.11	1.48	1.42
23	B	609	CLA	C3B-C4B	2.11	1.48	1.42
23	b	619	CLA	C3B-C4B	2.11	1.48	1.42
23	C	503	CLA	C3B-C4B	2.11	1.48	1.42
23	c	513	CLA	C3B-C4B	2.11	1.48	1.42
23	b	619	CLA	C1C-NC	-2.11	1.34	1.37
29	C	526	GOL	O2-C2	-2.10	1.37	1.43
23	D	2303	CLA	C3B-C4B	2.10	1.48	1.42
23	b	616	CLA	C4C-C3C	2.10	1.48	1.45
23	c	513	CLA	C3D-C4D	-2.10	1.39	1.44
23	b	608	CLA	C4C-C3C	2.10	1.48	1.45
23	C	504	CLA	C4B-NB	-2.10	1.35	1.37
23	c	516	CLA	C1C-NC	-2.10	1.34	1.37
23	c	506	CLA	C1B-NB	-2.09	1.35	1.37
23	C	510	CLA	C3B-C4B	2.09	1.48	1.42
23	b	620	CLA	C1C-C2C	2.09	1.48	1.44
23	c	513	CLA	C1C-C2C	2.09	1.48	1.44
39	e	103	HEM	CMA-C3A	2.09	1.55	1.50
23	D	2303	CLA	C4B-NB	-2.09	1.35	1.37
23	C	508	CLA	C3D-C4D	-2.09	1.39	1.44
23	B	612	CLA	C3B-C4B	2.09	1.48	1.42
23	D	2304	CLA	C3D-C4D	-2.09	1.39	1.44
39	F	101	HEM	CMA-C3A	2.09	1.55	1.50
23	B	616	CLA	C3B-C2B	2.08	1.48	1.41
31	a	2619	JOX	C-C5	-2.08	1.40	1.45
23	c	515	CLA	C3D-C4D	-2.08	1.39	1.44
23	d	408	CLA	C1C-C2C	2.07	1.48	1.44
36	C	525	HTG	C1-S1	-2.07	1.77	1.80
23	b	614	CLA	C3B-C4B	2.07	1.48	1.42
23	b	606	CLA	C1D-C2D	2.07	1.49	1.45
23	c	506	CLA	C3B-C2B	2.07	1.48	1.41
23	c	514	CLA	C1C-NC	-2.06	1.34	1.37
23	A	407	CLA	C1C-C2C	2.06	1.48	1.44
23	c	516	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	515	CLA	C4C-C3C	2.06	1.48	1.45
23	b	615	CLA	C1C-NC	-2.06	1.34	1.37
36	d	415	HTG	C1-S1	-2.06	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	2304	CLA	C1D-C2D	2.06	1.49	1.45
23	B	611	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	504	CLA	C4C-C3C	2.06	1.48	1.45
23	d	402	CLA	C1C-NC	-2.06	1.34	1.37
23	b	611	CLA	C3B-C4B	2.06	1.48	1.42
23	C	514	CLA	C1C-NC	-2.06	1.34	1.37
23	c	512	CLA	C3B-C4B	2.06	1.48	1.42
39	e	103	HEM	CMB-C2B	2.06	1.55	1.50
37	C	517	DGD	O2G-C2G	-2.06	1.41	1.46
23	b	611	CLA	C1C-NC	-2.05	1.34	1.37
23	d	402	CLA	C3B-C2B	2.05	1.48	1.41
24	A	408	PHO	CBD-CGD	-2.05	1.49	1.52
38	L	101	LHG	O7-C5	-2.05	1.41	1.46
23	b	615	CLA	C4C-C3C	2.05	1.48	1.45
42	v	201	HEC	C3C-C2C	-2.05	1.34	1.41
23	B	610	CLA	C3B-C4B	2.05	1.48	1.42
33	D	2306	PL9	C2-C3	2.05	1.39	1.34
23	B	616	CLA	C3D-C4D	-2.04	1.39	1.44
23	C	504	CLA	CBD-CAD	-2.04	1.47	1.56
28	J	303	LMT	O1'-C1'	2.04	1.43	1.40
23	c	512	CLA	C3D-C4D	-2.04	1.39	1.44
23	C	510	CLA	MG-NB	2.04	2.09	2.05
23	C	513	CLA	C1C-NC	-2.04	1.34	1.37
23	B	609	CLA	C3D-C4D	-2.04	1.39	1.44
23	b	607	CLA	C3D-C4D	-2.04	1.39	1.44
23	b	610	CLA	C3D-C4D	-2.03	1.39	1.44
36	c	526	HTG	C1-S1	-2.03	1.77	1.80
39	e	103	HEM	FE-NC	2.03	2.01	1.95
23	A	405	CLA	C1C-NC	-2.03	1.34	1.37
23	c	506	CLA	C3D-C4D	-2.03	1.39	1.44
36	I	101	HTG	C1-S1	-2.03	1.77	1.80
23	C	502	CLA	C3B-C2B	2.02	1.48	1.41
23	A	406	CLA	C4C-C3C	2.02	1.48	1.45
24	A	408	PHO	C1D-ND	-2.02	1.35	1.38
39	F	101	HEM	CMD-C2D	2.02	1.54	1.50
23	C	507	CLA	C3B-C2B	2.02	1.48	1.41
23	B	617	CLA	C4C-C3C	2.02	1.48	1.45
23	B	602	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	614	CLA	C3B-C2B	2.02	1.48	1.41
24	A	408	PHO	C3D-C4D	-2.02	1.38	1.41
23	c	515	CLA	C1C-NC	-2.02	1.34	1.37
23	c	513	CLA	C1C-NC	-2.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C1D-C2D	2.02	1.49	1.45
23	B	609	CLA	C1C-NC	-2.01	1.34	1.37
23	c	509	CLA	C1D-C2D	2.01	1.49	1.45
23	C	508	CLA	C4C-C3C	2.01	1.48	1.45
27	c	522	LMG	O1-C1	2.01	1.43	1.40
23	C	509	CLA	C3D-C4D	-2.01	1.39	1.44
37	C	518	DGD	O3G-C1D	2.01	1.43	1.40
33	d	411	PL9	C2-C3	2.01	1.39	1.34
23	c	513	CLA	C4C-C3C	2.01	1.48	1.45
23	b	608	CLA	C3B-C2B	2.01	1.47	1.41
23	b	620	CLA	C3D-C4D	-2.01	1.39	1.44
24	a	2611	PHO	CHA-CBD	-2.01	1.49	1.51
23	b	606	CLA	C4B-NB	-2.00	1.35	1.37
23	b	616	CLA	C1C-C2C	2.00	1.48	1.44
23	b	618	CLA	C3B-C4B	2.00	1.48	1.42
23	c	505	CLA	C1C-NC	-2.00	1.34	1.37
23	B	613	CLA	CBD-CAD	-2.00	1.47	1.56
23	B	605	CLA	CBD-CAD	-2.00	1.47	1.56
23	c	510	CLA	C3D-C4D	-2.00	1.39	1.44
23	C	502	CLA	C1D-C2D	2.00	1.49	1.45

All (2680) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	408	PHO	C2D-C1D-ND	11.31	117.61	109.43
24	A	409	PHO	C2D-C1D-ND	10.96	117.35	109.43
23	c	504	CLA	C1D-ND-C4D	-10.91	98.66	106.31
24	a	2612	PHO	C2D-C1D-ND	10.65	117.13	109.43
24	a	2611	PHO	C2D-C1D-ND	10.26	116.84	109.43
31	A	419	JOX	C2-C3-CL	-10.25	107.56	115.82
23	b	617	CLA	C1D-ND-C4D	-10.24	99.13	106.31
23	B	613	CLA	C1D-ND-C4D	-10.23	99.14	106.31
23	a	2610	CLA	C1D-ND-C4D	-10.18	99.17	106.31
23	a	2609	CLA	C1D-ND-C4D	-10.04	99.27	106.31
23	A	406	CLA	C1D-ND-C4D	-10.02	99.28	106.31
23	c	507	CLA	C1D-ND-C4D	-9.97	99.32	106.31
23	b	610	CLA	C1D-ND-C4D	-9.97	99.32	106.31
23	D	2303	CLA	C1D-ND-C4D	-9.84	99.41	106.31
23	B	610	CLA	C1D-ND-C4D	-9.81	99.43	106.31
23	B	614	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	b	621	CLA	C1D-ND-C4D	-9.77	99.46	106.31
23	c	511	CLA	C1D-ND-C4D	-9.66	99.54	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	408	CLA	C1D-ND-C4D	-9.53	99.62	106.31
23	C	514	CLA	C1D-ND-C4D	-9.41	99.71	106.31
23	b	619	CLA	C1D-ND-C4D	-9.39	99.72	106.31
23	b	608	CLA	C1D-ND-C4D	-9.39	99.72	106.31
23	C	507	CLA	C1D-ND-C4D	-9.39	99.72	106.31
23	b	613	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	B	609	CLA	C1D-ND-C4D	-9.37	99.74	106.31
23	B	616	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	C	509	CLA	C1D-ND-C4D	-9.34	99.76	106.31
23	B	615	CLA	C1D-ND-C4D	-9.32	99.78	106.31
23	c	512	CLA	C1D-ND-C4D	-9.29	99.79	106.31
23	A	407	CLA	C1D-ND-C4D	-9.27	99.81	106.31
31	a	2617	JOX	C2-C1-CL1	-9.25	108.36	115.82
23	C	511	CLA	C1D-ND-C4D	-9.23	99.83	106.31
23	c	505	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	B	612	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	b	618	CLA	C1D-ND-C4D	-9.13	99.91	106.31
23	A	410	CLA	C1D-ND-C4D	-9.10	99.93	106.31
23	d	409	CLA	C1D-ND-C4D	-9.08	99.94	106.31
23	B	606	CLA	C1D-ND-C4D	-9.08	99.94	106.31
24	a	2611	PHO	O2D-CGD-CBD	9.07	120.91	110.95
23	D	2304	CLA	C1D-ND-C4D	-9.05	99.97	106.31
23	B	605	CLA	C1D-ND-C4D	-9.04	99.97	106.31
23	a	2613	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	A	405	CLA	C1D-ND-C4D	-9.00	100.00	106.31
23	c	508	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	C	503	CLA	C1D-ND-C4D	-8.94	100.04	106.31
23	c	515	CLA	C1D-ND-C4D	-8.88	100.08	106.31
23	d	402	CLA	C1D-ND-C4D	-8.86	100.10	106.31
23	B	604	CLA	C1D-ND-C4D	-8.86	100.10	106.31
23	b	615	CLA	C1D-ND-C4D	-8.83	100.12	106.31
23	c	516	CLA	C1D-ND-C4D	-8.82	100.12	106.31
23	c	509	CLA	C1D-ND-C4D	-8.78	100.15	106.31
23	b	611	CLA	C1D-ND-C4D	-8.77	100.16	106.31
23	c	510	CLA	C1D-ND-C4D	-8.74	100.18	106.31
23	b	616	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	c	514	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	C	504	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	B	611	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	b	614	CLA	C1D-ND-C4D	-8.66	100.23	106.31
23	B	603	CLA	C1D-ND-C4D	-8.65	100.24	106.31
23	B	608	CLA	C1D-ND-C4D	-8.63	100.26	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	617	CLA	C1D-ND-C4D	-8.60	100.28	106.31
23	c	513	CLA	C1D-ND-C4D	-8.58	100.29	106.31
23	C	508	CLA	C1D-ND-C4D	-8.53	100.33	106.31
24	A	408	PHO	C3B-C4B-NB	8.52	113.02	107.46
23	C	513	CLA	C1D-ND-C4D	-8.52	100.33	106.31
24	a	2612	PHO	C3B-C4B-NB	8.50	113.01	107.46
23	C	505	CLA	C1D-ND-C4D	-8.46	100.38	106.31
23	c	506	CLA	C1D-ND-C4D	-8.43	100.39	106.31
23	C	510	CLA	C1D-ND-C4D	-8.40	100.42	106.31
23	b	607	CLA	C1D-ND-C4D	-8.40	100.42	106.31
23	b	612	CLA	C1D-ND-C4D	-8.36	100.45	106.31
23	B	607	CLA	C1D-ND-C4D	-8.27	100.51	106.31
23	C	502	CLA	C1D-ND-C4D	-8.18	100.57	106.31
24	a	2612	PHO	C2B-C1B-NB	8.09	115.28	109.43
23	C	512	CLA	C1D-ND-C4D	-8.07	100.65	106.31
23	b	609	CLA	C1D-ND-C4D	-8.03	100.68	106.31
31	a	2617	JOX	C2-C3-CL	-7.97	109.39	115.82
23	C	507	CLA	C1-C2-C3	-7.91	113.24	126.20
23	C	506	CLA	C1D-ND-C4D	-7.87	100.79	106.31
24	A	409	PHO	O2D-CGD-CBD	7.83	119.55	110.95
23	b	620	CLA	C1D-ND-C4D	-7.81	100.83	106.31
23	b	606	CLA	C1D-ND-C4D	-7.61	100.97	106.31
24	a	2612	PHO	O2D-CGD-CBD	7.59	119.29	110.95
23	B	602	CLA	C1D-ND-C4D	-7.56	101.01	106.31
36	C	522	HTG	C1'-S1-C1	7.34	116.30	100.45
24	A	409	PHO	C1-C2-C3	-7.26	114.30	126.20
23	b	619	CLA	CMD-C2D-C1D	7.25	137.50	124.73
23	C	507	CLA	CMD-C2D-C1D	7.20	137.41	124.73
24	a	2611	PHO	C3B-C4B-NB	7.14	112.11	107.46
23	B	604	CLA	O2D-CGD-CBD	7.09	123.63	111.23
26	l	101	SQD	O6-C1-C2	7.03	118.95	108.27
31	A	419	JOX	C3-C4-C5	-7.03	117.45	120.54
23	c	510	CLA	O2D-CGD-CBD	7.00	123.46	111.23
23	c	504	CLA	C2D-C1D-ND	6.95	117.01	110.13
23	A	406	CLA	C2D-C1D-ND	6.92	116.97	110.13
23	C	514	CLA	CMD-C2D-C1D	6.88	136.84	124.73
23	B	605	CLA	CMD-C2D-C1D	6.88	136.84	124.73
23	b	615	CLA	CMD-C2D-C1D	6.83	136.76	124.73
23	C	502	CLA	CMD-C2D-C1D	6.82	136.74	124.73
23	b	610	CLA	C2D-C1D-ND	6.79	116.85	110.13
24	A	408	PHO	O2D-CGD-CBD	6.76	118.37	110.95
23	b	614	CLA	CMD-C2D-C1D	6.71	136.54	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	C2D-C1D-ND	6.64	116.70	110.13
23	B	602	CLA	CMD-C2D-C1D	6.63	136.41	124.73
23	b	621	CLA	C2D-C1D-ND	6.62	116.68	110.13
23	D	2303	CLA	C2D-C1D-ND	6.61	116.67	110.13
23	B	616	CLA	C2D-C1D-ND	6.59	116.65	110.13
23	b	618	CLA	CMD-C2D-C1D	6.58	136.31	124.73
24	A	409	PHO	C3B-C4B-NB	6.57	111.75	107.46
31	A	419	JOX	C1-C2-C3	6.57	120.02	114.12
23	c	508	CLA	CMD-C2D-C1D	6.56	136.28	124.73
36	b	603	HTG	C1'-S1-C1	6.56	114.61	100.45
24	A	409	PHO	C2B-C1B-NB	6.56	114.17	109.43
31	a	2617	JOX	C1-C-C5	-6.54	117.66	120.54
23	b	613	CLA	CMD-C2D-C1D	6.54	136.25	124.73
23	C	506	CLA	CMD-C2D-C1D	6.53	136.23	124.73
23	c	508	CLA	O2D-CGD-CBD	6.53	122.64	111.23
23	C	508	CLA	O2D-CGD-CBD	6.51	122.61	111.23
23	c	509	CLA	CMD-C2D-C1D	6.51	136.19	124.73
31	A	419	JOX	C-C1-C2	-6.49	118.17	123.21
23	c	507	CLA	C2D-C1D-ND	6.48	116.53	110.13
23	a	2610	CLA	C2D-C1D-ND	6.45	116.51	110.13
23	b	606	CLA	O2D-CGD-CBD	6.44	122.48	111.23
23	C	505	CLA	CMD-C2D-C1D	6.43	136.05	124.73
23	B	612	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	B	604	CLA	CMD-C2D-C1D	6.42	136.04	124.73
23	B	610	CLA	CMD-C2D-C1D	6.39	135.99	124.73
23	b	617	CLA	C2D-C1D-ND	6.38	116.44	110.13
23	C	510	CLA	O2D-CGD-CBD	6.38	122.38	111.23
23	b	606	CLA	CMD-C2D-C1D	6.31	135.84	124.73
23	C	513	CLA	O2D-CGD-CBD	6.30	122.24	111.23
23	d	409	CLA	CMD-C2D-C1D	6.29	135.81	124.73
23	C	502	CLA	O2D-CGD-CBD	6.29	122.23	111.23
23	B	615	CLA	CMD-C2D-C1D	6.29	135.80	124.73
23	c	515	CLA	O2D-CGD-CBD	6.28	122.21	111.23
23	c	516	CLA	CMD-C2D-C1D	6.28	135.79	124.73
23	C	508	CLA	CMD-C2D-C1D	6.27	135.77	124.73
23	b	608	CLA	CMD-C2D-C1D	6.26	135.75	124.73
23	B	613	CLA	C2D-C1D-ND	6.25	116.31	110.13
23	d	408	CLA	CMD-C2D-C1D	6.24	135.72	124.73
23	C	504	CLA	CMD-C2D-C1D	6.23	135.70	124.73
23	B	614	CLA	CMD-C2D-C1D	6.22	135.68	124.73
23	c	506	CLA	CMD-C2D-C1D	6.22	135.68	124.73
23	b	621	CLA	CMD-C2D-C1D	6.21	135.66	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	2303	CLA	CMD-C2D-C1D	6.20	135.64	124.73
31	A	418	JOX	C1-C2-C3	6.19	119.68	114.12
23	c	510	CLA	CMD-C2D-C1D	6.17	135.59	124.73
26	a	2615	SQD	O6-C1-C2	6.17	117.64	108.27
23	C	510	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	B	617	CLA	O2D-CGD-CBD	6.16	122.00	111.23
23	B	603	CLA	CMD-C2D-C1D	6.16	135.57	124.73
24	a	2611	PHO	C2B-C1B-NB	6.15	113.88	109.43
23	B	612	CLA	CMD-C2D-C1D	6.14	135.55	124.73
23	c	507	CLA	CMD-C2D-C1D	6.13	135.53	124.73
23	d	408	CLA	C2D-C1D-ND	6.13	116.19	110.13
23	B	611	CLA	CMD-C2D-C1D	6.12	135.51	124.73
24	a	2612	PHO	C4D-ND-C1D	-6.10	101.57	108.87
23	C	503	CLA	O2D-CGD-CBD	6.09	121.87	111.23
23	b	616	CLA	CMD-C2D-C1D	6.08	135.43	124.73
31	a	2617	JOX	C1-C2-C3	6.07	119.58	114.12
23	C	511	CLA	O2D-CGD-CBD	6.07	121.85	111.23
23	b	607	CLA	O2D-CGD-CBD	6.07	121.84	111.23
23	b	609	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	A	410	CLA	CMD-C2D-C1D	6.06	135.40	124.73
23	B	607	CLA	CMD-C2D-C1D	6.06	135.39	124.73
23	B	608	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	c	513	CLA	CMD-C2D-C1D	6.03	135.34	124.73
23	C	513	CLA	CMD-C2D-C1D	6.02	135.33	124.73
23	b	611	CLA	CMD-C2D-C1D	6.01	135.31	124.73
31	A	418	JOX	C4-C3-C2	-6.00	118.55	123.21
23	b	609	CLA	C1-C2-C3	-6.00	116.37	126.20
36	i	102	HTG	C1'-S1-C1	6.00	113.40	100.45
23	C	509	CLA	O2D-CGD-CBD	5.99	121.70	111.23
24	A	408	PHO	C4D-ND-C1D	-5.98	101.70	108.87
23	B	609	CLA	C2D-C1D-ND	5.98	116.04	110.13
23	a	2610	CLA	CMD-C2D-C1D	5.98	135.25	124.73
23	c	515	CLA	C2D-C1D-ND	5.96	116.02	110.13
24	A	408	PHO	C2B-C1B-NB	5.95	113.73	109.43
23	A	407	CLA	CMD-C2D-C1D	5.95	135.21	124.73
23	b	607	CLA	CMD-C2D-C1D	5.94	135.20	124.73
23	B	606	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	B	602	CLA	O2D-CGD-CBD	5.93	121.59	111.23
23	D	2304	CLA	O2D-CGD-CBD	5.92	121.58	111.23
23	C	512	CLA	CMD-C2D-C1D	5.92	135.16	124.73
23	B	617	CLA	CMD-C2D-C1D	5.92	135.15	124.73
23	c	512	CLA	CMD-C2D-C1D	5.91	135.14	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	C2D-C1D-ND	5.91	115.97	110.13
31	A	418	JOX	C-C1-C2	-5.91	118.62	123.21
23	b	612	CLA	C2D-C1D-ND	5.90	115.96	110.13
23	b	621	CLA	O2D-CGD-CBD	5.89	121.53	111.23
23	C	508	CLA	C2D-C1D-ND	5.89	115.96	110.13
23	b	610	CLA	CMD-C2D-C1D	5.89	135.09	124.73
23	C	504	CLA	C2D-C1D-ND	5.88	115.95	110.13
23	b	619	CLA	O2D-CGD-CBD	5.88	121.51	111.23
23	C	503	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	a	2612	PHO	C1-C2-C3	-5.86	116.59	126.20
23	A	410	CLA	C2D-C1D-ND	5.84	115.91	110.13
23	c	507	CLA	O2D-CGD-CBD	5.82	121.40	111.23
23	c	506	CLA	C2D-C1D-ND	5.81	115.88	110.13
23	D	2304	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	d	402	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	b	612	CLA	CMD-C2D-C1D	5.79	134.93	124.73
24	A	409	PHO	C4D-ND-C1D	-5.79	101.93	108.87
23	c	511	CLA	C2D-C1D-ND	5.79	115.86	110.13
23	C	509	CLA	C2D-C1D-ND	5.77	115.84	110.13
24	a	2612	PHO	C3D-C4D-ND	5.77	115.10	107.71
23	B	615	CLA	O2D-CGD-CBD	5.76	121.31	111.23
23	a	2609	CLA	C2D-C1D-ND	5.76	115.83	110.13
23	A	405	CLA	CMD-C2D-C1D	5.76	134.87	124.73
23	b	615	CLA	C2D-C1D-ND	5.76	115.82	110.13
23	a	2613	CLA	C2D-C1D-ND	5.75	115.82	110.13
23	b	610	CLA	O2D-CGD-CBD	5.75	121.28	111.23
23	C	506	CLA	O2D-CGD-CBD	5.71	121.21	111.23
25	d	410	BCR	C24-C23-C22	-5.71	117.80	126.23
23	c	505	CLA	C2D-C1D-ND	5.70	115.77	110.13
26	D	2302	SQD	O47-C7-C8	5.69	123.80	111.48
23	B	616	CLA	CMD-C2D-C1D	5.69	134.74	124.73
23	B	610	CLA	C2D-C1D-ND	5.68	115.75	110.13
23	B	615	CLA	C2D-C1D-ND	5.67	115.74	110.13
23	a	2609	CLA	CMD-C2D-C1D	5.66	134.70	124.73
23	A	405	CLA	C2D-C1D-ND	5.64	115.70	110.13
23	b	616	CLA	C2D-C1D-ND	5.63	115.70	110.13
24	a	2611	PHO	C4D-ND-C1D	-5.63	102.13	108.87
23	C	511	CLA	C2D-C1D-ND	5.62	115.69	110.13
23	d	409	CLA	C2D-C1D-ND	5.60	115.67	110.13
23	b	611	CLA	C2D-C1D-ND	5.60	115.66	110.13
36	B	625	HTG	C1'-S1-C1	5.59	112.52	100.45
23	b	618	CLA	C2D-C1D-ND	5.58	115.65	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	CMD-C2D-C1D	5.58	134.55	124.73
23	B	617	CLA	C2D-C1D-ND	5.57	115.64	110.13
23	b	619	CLA	C2D-C1D-ND	5.54	115.61	110.13
23	C	505	CLA	O2D-CGD-CBD	5.54	120.92	111.23
23	b	613	CLA	C2D-C1D-ND	5.53	115.60	110.13
24	A	409	PHO	C3D-C4D-ND	5.52	114.78	107.71
23	D	2304	CLA	CMD-C2D-C1D	5.52	134.45	124.73
23	c	514	CLA	CMD-C2D-C1D	5.51	134.44	124.73
23	B	607	CLA	O2D-CGD-CBD	5.51	120.86	111.23
23	D	2303	CLA	O2D-CGD-CBD	5.50	120.85	111.23
23	C	512	CLA	C2D-C1D-ND	5.50	115.57	110.13
23	c	510	CLA	C2D-C1D-ND	5.49	115.56	110.13
23	A	407	CLA	C2D-C1D-ND	5.49	115.56	110.13
24	a	2611	PHO	C3D-C4D-ND	5.47	114.72	107.71
23	B	607	CLA	C2D-C1D-ND	5.45	115.52	110.13
23	c	514	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	c	516	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	B	605	CLA	C2D-C1D-ND	5.42	115.49	110.13
23	C	513	CLA	C2D-C1D-ND	5.42	115.49	110.13
23	b	608	CLA	C2D-C1D-ND	5.41	115.48	110.13
23	C	507	CLA	C2D-C1D-ND	5.41	115.48	110.13
23	b	609	CLA	C2D-C1D-ND	5.39	115.46	110.13
23	B	606	CLA	CMD-C2D-C1D	5.38	134.20	124.73
23	B	613	CLA	CMD-C2D-C1D	5.38	134.20	124.73
23	B	603	CLA	C2D-C1D-ND	5.38	115.45	110.13
25	B	633	BCR	C33-C5-C6	-5.36	118.63	124.48
36	d	415	HTG	C1'-S1-C1	5.36	112.02	100.45
23	B	611	CLA	C2D-C1D-ND	5.36	115.43	110.13
39	F	101	HEM	C4D-ND-C1D	5.35	111.55	105.21
24	A	408	PHO	C3D-C4D-ND	5.35	114.57	107.71
23	B	604	CLA	C2D-C1D-ND	5.34	115.41	110.13
23	C	503	CLA	CMD-C2D-C1D	5.34	134.12	124.73
23	A	406	CLA	CMD-C2D-C1D	5.33	134.12	124.73
23	C	505	CLA	C2D-C1D-ND	5.33	115.41	110.13
39	e	103	HEM	C4D-ND-C1D	5.33	111.52	105.21
23	C	510	CLA	C2D-C1D-ND	5.33	115.40	110.13
23	c	511	CLA	O2D-CGD-CBD	5.31	120.51	111.23
23	c	510	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
23	b	609	CLA	O2D-CGD-CBD	5.28	120.47	111.23
23	b	607	CLA	C2D-C1D-ND	5.25	115.32	110.13
23	b	608	CLA	O2D-CGD-CBD	5.25	120.41	111.23
23	B	608	CLA	O2D-CGD-CBD	5.25	120.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	611	CLA	O2D-CGD-CBD	5.25	120.40	111.23
23	B	611	CLA	C1-C2-C3	-5.23	117.63	126.20
23	B	608	CLA	CMD-C2D-C1D	5.23	133.94	124.73
23	c	508	CLA	C2D-C1D-ND	5.22	115.30	110.13
23	B	612	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
23	A	406	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
23	B	612	CLA	O2D-CGD-CBD	5.16	120.26	111.23
23	b	620	CLA	C2D-C1D-ND	5.16	115.23	110.13
26	l	101	SQD	O47-C7-C8	5.12	122.55	111.48
23	b	614	CLA	C2D-C1D-ND	5.12	115.19	110.13
23	A	406	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
36	I	101	HTG	C1'-S1-C1	5.11	111.47	100.45
23	B	611	CLA	O2D-CGD-CBD	5.10	120.14	111.23
26	d	417	SQD	O47-C7-O49	-5.08	119.19	125.70
37	C	519	DGD	O2G-C1B-C2B	5.07	122.45	111.48
23	C	511	CLA	CMD-C2D-C1D	5.06	133.63	124.73
23	b	621	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
25	Y	302	BCR	C15-C14-C13	-5.04	120.21	127.28
36	B	626	HTG	C1'-S1-C1	5.04	111.32	100.45
23	b	617	CLA	O2D-CGD-CBD	5.03	120.03	111.23
23	b	610	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
23	a	2613	CLA	CMD-C2D-C1D	5.03	133.58	124.73
23	b	610	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
26	B	621	SQD	O47-C7-C8	5.01	122.33	111.48
23	A	406	CLA	CBC-CAC-C3C	-5.00	98.85	112.42
23	c	512	CLA	O2D-CGD-CBD	4.95	119.88	111.23
23	B	613	CLA	O2D-CGD-CBD	4.94	119.87	111.23
27	C	527	LMG	O7-C10-C11	4.94	122.16	111.48
23	B	614	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	B	603	CLA	O2D-CGD-CBD	4.92	119.83	111.23
23	C	514	CLA	C2D-C1D-ND	4.92	114.99	110.13
23	d	402	CLA	CMD-C2D-C1D	4.91	133.37	124.73
23	c	515	CLA	CMD-C2D-C1D	4.90	133.36	124.73
23	c	508	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	D	2303	CLA	O2D-CGD-O1D	-4.89	114.33	123.85
23	A	406	CLA	O2D-CGD-CBD	4.88	119.75	111.23
23	b	620	CLA	CMD-C2D-C1D	4.87	133.30	124.73
27	A	413	LMG	O7-C10-C11	4.86	122.00	111.48
23	B	616	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
23	c	509	CLA	O2D-CGD-CBD	4.85	119.71	111.23
23	D	2303	CLA	CHD-C4C-C3C	-4.84	117.72	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	102	BCR	C33-C5-C6	-4.83	119.21	124.48
31	A	419	JOX	C4-C3-CL	4.83	131.29	119.92
23	c	504	CLA	O2D-CGD-CBD	4.83	119.67	111.23
23	c	513	CLA	C2D-C1D-ND	4.82	114.90	110.13
23	a	2613	CLA	O2D-CGD-CBD	4.82	119.66	111.23
23	c	506	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
36	C	525	HTG	C1'-S1-C1	4.82	110.85	100.45
31	a	2617	JOX	C3-C4-C5	-4.81	118.42	120.54
23	D	2304	CLA	CHD-C4C-C3C	-4.80	117.77	124.77
42	V	201	HEC	CBB-CAB-C3B	-4.80	117.84	127.43
23	C	508	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
23	D	2303	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
23	a	2610	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	c	509	CLA	C2D-C1D-ND	4.79	114.86	110.13
23	C	509	CLA	CMD-C2D-C1D	4.79	133.16	124.73
23	B	616	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	B	606	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
23	b	612	CLA	O2D-CGD-CBD	4.75	119.54	111.23
23	d	409	CLA	O2D-CGD-CBD	4.75	119.53	111.23
23	b	612	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	b	617	CLA	CHD-C4C-C3C	-4.75	117.85	124.77
23	c	505	CLA	CMD-C2D-C1D	4.75	133.09	124.73
23	b	610	CLA	CHD-C4C-C3C	-4.75	117.85	124.77
36	V	204	HTG	C1'-S1-C1	4.74	110.70	100.45
23	b	619	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	b	617	CLA	CMD-C2D-C1D	4.73	133.06	124.73
23	B	615	CLA	CHD-C4C-C3C	-4.71	117.91	124.77
31	a	2619	JOX	C-C1-C2	-4.71	119.56	123.21
25	C	516	BCR	C7-C8-C9	-4.69	119.29	126.23
23	c	505	CLA	O2D-CGD-CBD	4.69	119.43	111.23
25	D	2305	BCR	C24-C23-C22	-4.69	119.30	126.23
23	b	613	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	C	514	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	B	616	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	d	402	CLA	O2D-CGD-CBD	4.68	119.40	111.23
23	C	504	CLA	CHD-C4C-C3C	-4.67	117.96	124.77
23	c	516	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
36	c	524	HTG	C1'-S1-C1	4.67	110.53	100.45
36	B	625	HTG	O5-C1-C2	4.67	116.75	110.32
23	B	604	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
23	A	410	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
23	d	409	CLA	C3B-C2B-C1B	-4.65	101.69	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	522	HTG	C1-O5-C5	4.65	120.90	112.56
31	a	2617	JOX	C-C1-CL1	4.64	130.84	119.92
37	D	2307	DGD	O2G-C1B-C2B	4.64	121.52	111.48
23	a	2613	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
23	A	407	CLA	CHD-C4C-C3C	-4.62	118.03	124.77
23	b	616	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	a	2609	CLA	C3D-C4D-ND	4.62	117.49	109.99
25	D	2305	BCR	C7-C8-C9	-4.61	119.42	126.23
25	D	2305	BCR	C38-C26-C25	-4.61	119.46	124.48
23	C	510	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
23	B	614	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
23	B	608	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	C	513	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	B	615	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	c	504	CLA	C3D-C4D-ND	4.58	117.43	109.99
23	a	2610	CLA	C3D-C4D-ND	4.58	117.42	109.99
23	B	606	CLA	C3B-C2B-C1B	-4.58	101.78	107.17
23	A	407	CLA	C3D-C4D-ND	4.57	117.42	109.99
31	a	2617	JOX	C4-C3-CL	4.57	130.66	119.92
27	c	501	LMG	O7-C10-C11	4.56	121.35	111.48
36	b	604	HTG	C1'-S1-C1	4.56	110.30	100.45
23	C	504	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	A	410	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	b	615	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
23	B	611	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	B	609	CLA	CMD-C2D-C1D	4.53	132.71	124.73
23	c	515	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	B	617	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	B	615	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	c	504	CLA	C3D-C2D-C1D	-4.53	99.66	105.83
23	c	506	CLA	O2D-CGD-CBD	4.52	119.14	111.23
23	B	606	CLA	CHD-C4C-C3C	-4.52	118.19	124.77
23	b	621	CLA	CHD-C4C-C3C	-4.52	118.19	124.77
25	Y	302	BCR	C38-C26-C25	-4.51	119.56	124.48
23	b	617	CLA	C3D-C4D-ND	4.51	117.32	109.99
23	B	607	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
26	A	412	SQD	O47-C7-C8	4.51	121.23	111.48
23	b	607	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
23	b	619	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	C	503	CLA	O2D-CGD-O1D	-4.50	115.09	123.85
27	c	522	LMG	O7-C10-C11	4.50	121.21	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	b	621	CLA	C1D-CHD-C4C	-4.50	116.47	126.02
23	B	611	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
36	d	407	HTG	C1'-S1-C1	4.49	110.15	100.45
36	b	626	HTG	C1'-S1-C1	4.49	110.14	100.45
23	b	611	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	C	514	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	c	512	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
25	z	101	BCR	C15-C14-C13	-4.47	121.01	127.28
25	c	517	BCR	C33-C5-C6	-4.46	119.61	124.48
23	d	402	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
23	A	406	CLA	C2C-C1C-NC	4.46	114.67	109.98
23	c	511	CLA	CMD-C2D-C1D	4.46	132.58	124.73
25	d	410	BCR	C7-C8-C9	-4.46	119.64	126.23
23	B	613	CLA	C3D-C4D-ND	4.46	117.23	109.99
23	c	505	CLA	C3D-C4D-ND	4.46	117.23	109.99
36	c	523	HTG	C1'-S1-C1	4.45	110.07	100.45
23	C	506	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
23	B	615	CLA	O2D-CGD-O1D	-4.45	115.18	123.85
23	C	502	CLA	C2D-C1D-ND	4.45	114.53	110.13
23	D	2304	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	d	408	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	B	602	CLA	C2D-C1D-ND	4.45	114.53	110.13
23	a	2613	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	d	408	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
23	d	408	CLA	C1-C2-C3	-4.44	118.92	126.20
23	C	507	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	c	516	CLA	O2D-CGD-CBD	4.44	118.99	111.23
23	d	408	CLA	C2C-C1C-NC	4.44	114.64	109.98
23	C	505	CLA	C1C-C2C-C3C	-4.44	102.31	106.98
23	C	505	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	b	618	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
25	d	410	BCR	C33-C5-C6	-4.43	119.65	124.48
23	b	619	CLA	C1-C2-C3	-4.43	118.94	126.20
23	B	605	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
23	c	511	CLA	C3D-C4D-ND	4.42	117.17	109.99
25	T	102	BCR	C7-C8-C9	-4.42	119.70	126.23
23	d	409	CLA	C3D-C2D-C1D	-4.42	99.81	105.83
23	B	610	CLA	O2D-CGD-CBD	4.41	118.95	111.23
23	B	617	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
42	v	201	HEC	CBB-CAB-C3B	-4.41	118.63	127.43
23	C	509	CLA	C3D-C2D-C1D	-4.40	99.82	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	2303	CLA	C3D-C4D-ND	4.40	117.14	109.99
37	C	519	DGD	O1G-C1A-C2A	4.40	125.26	111.83
23	C	513	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	A	407	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	b	610	CLA	C1C-C2C-C3C	-4.39	102.37	106.98
23	B	604	CLA	O2D-CGD-O1D	-4.38	115.31	123.85
23	A	406	CLA	C3B-C2B-C1B	-4.38	102.00	107.17
26	a	2603	SQD	O47-C7-C8	4.38	120.96	111.48
25	B	618	BCR	C33-C5-C6	-4.38	119.70	124.48
26	a	2615	SQD	O47-C7-C8	4.38	120.95	111.48
23	C	509	CLA	C3D-C4D-ND	4.38	117.10	109.99
23	c	507	CLA	C3B-C2B-C1B	-4.37	102.01	107.17
23	c	511	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
23	c	504	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
23	b	621	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
23	A	407	CLA	O2D-CGD-CBD	4.36	118.86	111.23
23	c	513	CLA	O2D-CGD-CBD	4.36	118.86	111.23
28	M	101	LMT	O5'-C5'-C4'	4.36	118.74	109.72
23	b	616	CLA	CHD-C4C-C3C	-4.36	118.41	124.77
23	d	402	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
31	A	419	JOX	C2-C1-CL1	-4.36	112.31	115.82
23	A	406	CLA	CHD-C4C-C3C	-4.36	118.42	124.77
23	c	504	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
23	A	405	CLA	C3D-C4D-ND	4.36	117.07	109.99
23	C	503	CLA	C1-C2-C3	-4.35	119.06	126.20
23	B	616	CLA	O2D-CGD-CBD	4.35	118.84	111.23
25	T	102	BCR	C15-C16-C17	-4.35	114.62	123.52
25	Y	302	BCR	C33-C5-C6	-4.35	119.74	124.48
23	A	410	CLA	O2D-CGD-CBD	4.34	118.82	111.23
23	b	613	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
25	d	410	BCR	C38-C26-C25	-4.34	119.75	124.48
23	A	410	CLA	C2B-C1B-NB	4.33	114.82	110.33
23	c	516	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	b	607	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
33	A	422	PL9	C27-C28-C29	-4.33	117.71	127.62
23	c	505	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
23	c	510	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
23	b	620	CLA	O2D-CGD-CBD	4.33	118.80	111.23
23	c	504	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
25	b	624	BCR	C38-C26-C25	-4.32	119.77	124.48
23	c	507	CLA	C3D-C4D-ND	4.32	117.01	109.99
23	B	605	CLA	O2D-CGD-CBD	4.32	118.79	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	CHD-C4C-C3C	-4.32	118.48	124.77
23	d	402	CLA	CHD-C4C-C3C	-4.31	118.48	124.77
23	D	2304	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	d	402	CLA	CBC-CAC-C3C	-4.31	100.73	112.42
23	c	507	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
23	B	608	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	d	402	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	B	603	CLA	C3D-C2D-C1D	-4.31	99.96	105.83
23	b	606	CLA	C2D-C1D-ND	4.30	114.39	110.13
23	c	507	CLA	CHD-C4C-C3C	-4.30	118.50	124.77
23	b	610	CLA	O2D-CGD-O1D	-4.30	115.48	123.85
23	C	503	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
23	b	606	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
23	C	504	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
23	c	509	CLA	C3D-C4D-ND	4.30	116.97	109.99
23	D	2304	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
23	C	512	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
25	y	101	BCR	C33-C5-C6	-4.29	119.80	124.48
23	d	408	CLA	O2D-CGD-CBD	4.29	118.73	111.23
23	B	610	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	d	409	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
23	d	408	CLA	C3D-C4D-ND	4.29	116.96	109.99
36	c	526	HTG	C1'-S1-C1	4.29	109.71	100.45
23	C	511	CLA	C3D-C4D-ND	4.29	116.95	109.99
23	c	511	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	A	407	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
23	B	611	CLA	CAC-C3C-C4C	4.28	130.36	124.79
23	A	406	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	C	510	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
23	b	612	CLA	CHD-C4C-C3C	-4.27	118.55	124.77
23	B	613	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
25	c	517	BCR	C7-C8-C9	-4.26	119.93	126.23
23	C	514	CLA	O2D-CGD-CBD	4.26	118.67	111.23
23	c	515	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	B	610	CLA	C3D-C4D-ND	4.26	116.90	109.99
23	B	609	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	C	504	CLA	O2D-CGD-CBD	4.25	118.66	111.23
23	b	609	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	B	612	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
23	b	614	CLA	C3D-C4D-ND	4.24	116.89	109.99
23	b	617	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
23	a	2613	CLA	C3D-C4D-ND	4.24	116.88	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	CAC-C3C-C4C	4.24	130.30	124.79
23	b	616	CLA	O2D-CGD-CBD	4.24	118.63	111.23
23	C	503	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
23	b	609	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	c	510	CLA	C2C-C1C-NC	4.22	114.42	109.98
26	A	412	SQD	O6-C1-C2	4.22	114.69	108.27
28	B	623	LMT	C1B-O5B-C5B	4.22	121.97	113.72
23	a	2610	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
23	b	617	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
23	B	615	CLA	C3D-C4D-ND	4.22	116.84	109.99
23	B	604	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
31	a	2617	JOX	C4-C3-C2	-4.21	119.94	123.21
23	c	515	CLA	C1-O2A-CGA	4.21	126.84	116.65
25	T	102	BCR	C12-C13-C14	-4.20	112.40	119.01
23	b	612	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
23	B	609	CLA	C3D-C4D-ND	4.20	116.82	109.99
23	b	614	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
26	b	601	SQD	O47-C7-C8	4.20	120.57	111.48
23	C	508	CLA	C1-C2-C3	-4.20	119.32	126.20
23	B	602	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
26	D	2308	SQD	O47-C7-C8	4.19	120.55	111.48
27	c	522	LMG	O6-C5-C4	4.18	117.24	109.70
23	B	609	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
40	H	102	RRX	C7-C8-C9	-4.17	120.06	126.23
23	b	612	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
23	c	505	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	B	607	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
23	b	613	CLA	C3D-C4D-ND	4.17	116.76	109.99
23	d	402	CLA	C3D-C4D-ND	4.17	116.76	109.99
23	c	513	CLA	C3B-C2B-C1B	-4.16	102.26	107.17
23	C	512	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
23	b	613	CLA	O2D-CGD-CBD	4.16	118.50	111.23
23	b	611	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
23	c	509	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	b	618	CLA	C3B-C2B-C1B	-4.15	102.27	107.17
36	I	101	HTG	C1-O5-C5	4.15	120.01	112.56
36	B	627	HTG	C1'-S1-C1	4.15	109.42	100.45
23	B	613	CLA	CHD-C4C-C3C	-4.15	118.72	124.77
23	A	407	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
23	c	512	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
23	D	2304	CLA	C1-C2-C3	-4.15	119.41	126.20
23	a	2613	CLA	CHD-C4C-C3C	-4.15	118.73	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
36	H	101	HTG	C1'-S1-C1	4.14	109.39	100.45
23	B	613	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
23	B	603	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
23	B	603	CLA	CAA-C2A-C3A	-4.13	101.84	113.00
23	B	608	CLA	CAA-C2A-C3A	-4.13	101.84	113.00
26	a	2615	SQD	C1-O5-C5	-4.13	105.66	113.72
23	a	2609	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
23	a	2613	CLA	C1-C2-C3	-4.12	119.44	126.20
23	B	605	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
23	a	2609	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	C	507	CLA	C3D-C4D-ND	4.12	116.68	109.99
23	b	615	CLA	CHD-C4C-C3C	-4.11	118.77	124.77
38	E	101	LHG	O7-C7-C8	4.11	120.38	111.48
23	c	506	CLA	CMB-C2B-C1B	4.11	131.68	125.42
23	c	510	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
23	b	610	CLA	C2B-C1B-NB	4.11	114.58	110.33
23	b	616	CLA	C3B-C2B-C1B	-4.10	102.33	107.17
37	c	518	DGD	O2G-C1B-C2B	4.10	120.36	111.48
23	c	514	CLA	C3B-C2B-C1B	-4.10	102.33	107.17
23	D	2303	CLA	C1C-C2C-C3C	-4.10	102.67	106.98
37	C	518	DGD	O2G-C1B-C2B	4.10	120.36	111.48
23	a	2613	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
23	C	512	CLA	C1-O2A-CGA	4.10	126.57	116.65
23	C	514	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
23	b	608	CLA	C3D-C4D-ND	4.09	116.64	109.99
23	B	605	CLA	C2C-C1C-NC	4.09	114.28	109.98
23	D	2303	CLA	C2C-C1C-NC	4.09	114.27	109.98
23	c	513	CLA	C3D-C4D-ND	4.08	116.63	109.99
23	c	504	CLA	O2D-CGD-O1D	-4.08	115.90	123.85
31	A	419	JOX	C-C1-CL1	4.08	129.52	119.92
23	b	620	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
23	c	506	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
23	B	616	CLA	C1D-CHD-C4C	-4.08	117.36	126.02
23	C	508	CLA	CHD-C4C-C3C	-4.07	118.83	124.77
25	k	302	BCR	C24-C23-C22	-4.07	120.21	126.23
23	A	405	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
33	x	1301	PL9	C27-C28-C29	-4.07	118.31	127.62
23	A	407	CLA	C1C-C2C-C3C	-4.06	102.70	106.98
23	b	614	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
23	A	407	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
24	a	2612	PHO	C4-C3-C5	4.06	122.28	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	409	CLA	C3D-C4D-ND	4.06	116.59	109.99
23	B	609	CLA	O2D-CGD-CBD	4.06	118.33	111.23
23	B	606	CLA	C3D-C4D-ND	4.06	116.58	109.99
23	d	408	CLA	C3B-C2B-C1B	-4.06	102.39	107.17
42	v	201	HEC	CBC-CAC-C3C	-4.05	119.33	127.43
40	h	101	RRX	C16-C17-C18	-4.05	121.60	127.28
23	b	619	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
33	A	422	PL9	C32-C33-C34	-4.04	118.38	127.62
23	b	616	CLA	CBC-CAC-C3C	-4.04	101.48	112.42
23	d	402	CLA	C2C-C1C-NC	4.03	114.22	109.98
23	D	2304	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
23	B	605	CLA	C1-C2-C3	-4.03	119.60	126.20
23	B	611	CLA	C3D-C4D-ND	4.03	116.53	109.99
23	c	508	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
27	m	2802	LMG	O7-C10-C11	4.02	120.18	111.48
23	A	410	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
23	A	410	CLA	C3D-C4D-ND	4.01	116.51	109.99
23	c	514	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
23	b	608	CLA	C1C-C2C-C3C	-4.01	102.77	106.98
23	b	620	CLA	C3B-C2B-C1B	-4.01	102.45	107.17
23	B	606	CLA	O2A-CGA-O1A	-4.00	113.61	123.63
23	C	507	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
23	c	514	CLA	C3D-C4D-ND	4.00	116.49	109.99
23	A	410	CLA	C1-C2-C3	-4.00	119.65	126.20
23	c	516	CLA	C3D-C4D-ND	4.00	116.48	109.99
23	B	605	CLA	C3B-C2B-C1B	-3.99	102.46	107.17
23	b	619	CLA	C3D-C4D-ND	3.99	116.47	109.99
23	b	618	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	B	602	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
37	c	519	DGD	O2G-C1B-C2B	3.98	120.08	111.48
23	a	2613	CLA	CBC-CAC-C3C	-3.97	101.64	112.42
23	B	603	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
27	c	522	LMG	C1-O6-C5	3.96	121.46	113.72
26	b	601	SQD	O8-S-C6	3.96	113.62	105.97
23	a	2609	CLA	CAA-C2A-C3A	-3.96	102.30	113.00
23	b	607	CLA	O2D-CGD-O1D	-3.96	116.14	123.85
23	c	514	CLA	CHD-C4C-C3C	-3.96	119.00	124.77
23	b	618	CLA	C3D-C4D-ND	3.96	116.42	109.99
23	A	410	CLA	C2C-C1C-NC	3.96	114.14	109.98
23	D	2304	CLA	CHD-C1D-ND	-3.96	119.24	124.80
23	c	515	CLA	C1D-CHD-C4C	-3.95	117.61	126.02
23	B	614	CLA	C3B-C2B-C1B	-3.95	102.51	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	B	614	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	C	502	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
23	C	503	CLA	C3D-C4D-ND	3.95	116.40	109.99
23	b	609	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	C	510	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
25	C	515	BCR	C38-C26-C25	-3.94	120.18	124.48
23	b	616	CLA	C3D-C4D-ND	3.93	116.38	109.99
23	D	2303	CLA	C3B-C2B-C1B	-3.93	102.54	107.17
23	b	610	CLA	C3D-C4D-ND	3.93	116.37	109.99
23	C	509	CLA	C3B-C2B-C1B	-3.93	102.54	107.17
23	d	402	CLA	CAA-C2A-C3A	-3.93	102.39	113.00
23	C	502	CLA	C3D-C4D-ND	3.92	116.37	109.99
23	b	621	CLA	C3B-C4B-NB	3.92	114.03	110.53
24	A	408	PHO	C1A-C2A-C3A	-3.92	99.11	102.84
23	b	616	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
23	C	510	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
23	C	505	CLA	C3D-C4D-ND	3.91	116.35	109.99
23	C	511	CLA	CBC-CAC-C3C	-3.91	101.82	112.42
23	C	508	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	c	507	CLA	C2C-C1C-NC	3.91	114.08	109.98
26	D	2302	SQD	C1-O5-C5	3.90	121.34	113.72
36	B	624[B]	HTG	C1'-S1-C1	3.90	108.87	100.45
23	a	2613	CLA	C2C-C1C-NC	3.90	114.07	109.98
23	B	611	CLA	CMB-C2B-C1B	3.90	131.35	125.42
23	B	611	CLA	CHD-C4C-C3C	-3.89	119.10	124.77
23	a	2610	CLA	CHD-C4C-C3C	-3.89	119.10	124.77
23	B	617	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
38	D	2309	LHG	O8-C23-C24	3.89	123.68	111.83
23	B	608	CLA	C1C-C2C-C3C	-3.88	102.89	106.98
23	A	405	CLA	C3B-C2B-C1B	-3.88	102.59	107.17
23	d	409	CLA	C2B-C1B-NB	3.88	114.35	110.33
25	C	516	BCR	C33-C5-C6	-3.88	120.25	124.48
39	F	101	HEM	CBD-CAD-C3D	-3.88	101.80	112.53
23	C	507	CLA	O2D-CGD-CBD	3.88	118.02	111.23
36	B	624[B]	HTG	C1-O5-C5	3.88	119.52	112.56
23	C	502	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	b	608	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	b	606	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	d	402	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
23	B	607	CLA	CHD-C4C-C3C	-3.87	119.13	124.77
23	c	508	CLA	C3D-C4D-ND	3.87	116.27	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	621	CLA	C3C-C4C-NC	3.86	115.38	110.43
23	c	513	CLA	CBC-CAC-C3C	-3.86	101.95	112.42
23	C	504	CLA	C1-C2-C3	-3.85	119.88	126.20
23	b	607	CLA	C3D-C4D-ND	3.85	116.25	109.99
23	B	610	CLA	C1-C2-C3	-3.85	119.89	126.20
23	c	508	CLA	C2C-C1C-NC	3.85	114.02	109.98
23	a	2610	CLA	CHD-C1D-ND	-3.85	119.39	124.80
23	B	603	CLA	C2C-C1C-NC	3.85	114.02	109.98
37	H	103	DGD	O2G-C1B-C2B	3.85	119.80	111.48
23	A	405	CLA	CHD-C4C-C3C	-3.85	119.17	124.77
27	C	520	LMG	O7-C10-C11	3.85	119.80	111.48
23	C	511	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
38	e	101	LHG	O7-C7-C8	3.84	119.80	111.48
23	C	505	CLA	C3B-C2B-C1B	-3.84	102.64	107.17
23	c	505	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	B	604	CLA	C3D-C4D-ND	3.84	116.23	109.99
23	b	611	CLA	CHD-C4C-C3C	-3.84	119.18	124.77
23	C	512	CLA	CHD-C4C-C3C	-3.83	119.18	124.77
31	a	2619	JOX	C4-C3-C2	-3.83	120.24	123.21
25	b	624	BCR	C24-C23-C22	-3.83	120.58	126.23
23	c	512	CLA	C3D-C4D-ND	3.82	116.20	109.99
23	B	603	CLA	C3D-C4D-ND	3.82	116.20	109.99
23	B	605	CLA	C3D-C4D-ND	3.82	116.20	109.99
23	C	506	CLA	C2D-C1D-ND	3.82	113.91	110.13
23	C	503	CLA	CHD-C4C-C3C	-3.81	119.21	124.77
39	e	103	HEM	CBD-CAD-C3D	-3.81	101.99	112.53
23	b	606	CLA	C3D-C4D-ND	3.81	116.18	109.99
23	a	2609	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
25	a	2614	BCR	C33-C5-C6	-3.81	120.33	124.48
23	c	512	CLA	C1-C2-C3	-3.81	119.95	126.20
23	A	405	CLA	C2C-C1C-NC	3.81	113.98	109.98
33	d	411	PL9	C42-C43-C44	-3.81	118.91	127.62
23	c	515	CLA	C3D-C4D-ND	3.80	116.16	109.99
25	b	622	BCR	C24-C23-C22	-3.79	120.63	126.23
23	c	509	CLA	C3B-C2B-C1B	-3.79	102.71	107.17
23	c	514	CLA	O2D-CGD-CBD	3.78	117.84	111.23
23	C	513	CLA	CHD-C4C-C3C	-3.78	119.26	124.77
23	c	515	CLA	CHD-C4C-C3C	-3.78	119.26	124.77
23	C	511	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
31	A	419	JOX	O-C2-C3	-3.78	118.80	122.70
23	b	615	CLA	C2B-C1B-NB	3.78	114.24	110.33
23	A	405	CLA	CAA-C2A-C3A	-3.78	102.79	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	O2D-CGD-O1D	-3.78	116.50	123.85
23	a	2610	CLA	C2B-C1B-NB	3.77	114.24	110.33
23	d	402	CLA	C3B-C4B-NB	3.77	113.90	110.53
23	B	614	CLA	C3D-C4D-ND	3.77	116.12	109.99
23	c	511	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
23	a	2609	CLA	C1D-CHD-C4C	-3.77	118.02	126.02
23	B	611	CLA	C2B-C1B-NB	3.76	114.23	110.33
23	c	507	CLA	CBC-CAC-C3C	-3.76	102.22	112.42
23	b	608	CLA	CHD-C4C-C3C	-3.76	119.29	124.77
23	c	511	CLA	C2B-C1B-NB	3.76	114.23	110.33
23	B	615	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
28	B	623	LMT	O5B-C5B-C4B	3.76	116.47	109.70
23	C	506	CLA	C3D-C4D-ND	3.76	116.09	109.99
23	c	513	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
23	C	514	CLA	CHD-C4C-C3C	-3.75	119.30	124.77
23	C	510	CLA	C1-C2-C3	-3.75	120.05	126.20
23	b	619	CLA	C2B-C1B-NB	3.74	114.21	110.33
23	c	514	CLA	C1-O2A-CGA	3.74	125.70	116.65
23	C	507	CLA	CHD-C4C-C3C	-3.74	119.33	124.77
23	d	409	CLA	C2C-C1C-NC	3.73	113.90	109.98
23	B	609	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
23	b	621	CLA	C4C-C3C-C2C	-3.73	101.46	106.89
23	C	511	CLA	C1-C2-C3	-3.73	120.09	126.20
23	b	608	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
23	a	2613	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
23	C	507	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
25	b	622	BCR	C33-C5-C6	-3.73	120.42	124.48
23	c	513	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
23	b	613	CLA	C1-C2-C3	-3.72	120.09	126.20
23	B	608	CLA	CBC-CAC-C3C	-3.72	102.32	112.42
23	B	608	CLA	C2C-C1C-NC	3.72	113.89	109.98
23	a	2610	CLA	O2D-CGD-CBD	3.72	117.74	111.23
23	C	513	CLA	C3D-C4D-ND	3.72	116.03	109.99
23	b	612	CLA	C3D-C4D-ND	3.72	116.03	109.99
40	H	102	RRX	C24-C23-C22	-3.71	120.74	126.23
23	B	608	CLA	C3D-C4D-ND	3.71	116.02	109.99
36	H	101	HTG	C5-O5-C1	3.71	117.33	111.19
23	b	617	CLA	CMC-C2C-C1C	3.71	130.83	125.03
23	B	610	CLA	CMB-C2B-C1B	3.71	131.07	125.42
38	D	2309	LHG	O7-C7-C8	3.71	119.50	111.48
23	C	510	CLA	C2C-C1C-NC	3.70	113.87	109.98
23	B	602	CLA	C3D-C4D-ND	3.70	116.00	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	618	CLA	C2C-C1C-NC	3.70	113.86	109.98
23	C	505	CLA	C2C-C1C-NC	3.69	113.86	109.98
23	c	510	CLA	C3D-C4D-ND	3.69	115.98	109.99
23	C	502	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
25	B	633	BCR	C15-C14-C13	3.69	132.45	127.28
23	b	607	CLA	C2B-C1B-NB	3.69	114.15	110.33
23	B	616	CLA	C2C-C1C-NC	3.68	113.85	109.98
23	c	508	CLA	C2B-C1B-NB	3.68	114.14	110.33
23	A	410	CLA	CHD-C4C-C3C	-3.68	119.41	124.77
23	b	610	CLA	C2C-C1C-NC	3.68	113.85	109.98
42	v	201	HEC	C4D-ND-C1D	3.67	111.81	105.82
23	b	608	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	B	612	CLA	C3D-C4D-ND	3.67	115.95	109.99
23	b	609	CLA	CAC-C3C-C4C	3.67	129.56	124.79
23	B	604	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
23	c	514	CLA	CBC-CAC-C3C	-3.66	102.49	112.42
23	b	617	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	b	621	CLA	C2C-C1C-NC	3.66	113.82	109.98
38	L	101	LHG	O8-C23-C24	3.66	122.98	111.83
23	A	410	CLA	CMA-C3A-C4A	-3.65	101.95	111.77
23	b	620	CLA	C3D-C4D-ND	3.65	115.93	109.99
23	C	504	CLA	C3D-C4D-ND	3.65	115.92	109.99
33	d	411	PL9	C7-C8-C9	-3.65	120.54	126.83
23	B	604	CLA	C2B-C1B-NB	3.65	114.11	110.33
23	c	508	CLA	CHD-C4C-C3C	-3.65	119.46	124.77
23	C	502	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
23	A	406	CLA	C2B-C1B-NB	3.64	114.10	110.33
23	b	618	CLA	C1-C2-C3	-3.64	120.23	126.20
23	A	405	CLA	O2D-CGD-CBD	3.64	117.59	111.23
25	T	102	BCR	C35-C13-C12	3.64	123.65	118.09
23	b	613	CLA	C2B-C1B-NB	3.64	114.10	110.33
23	b	611	CLA	C3D-C4D-ND	3.64	115.90	109.99
26	l	101	SQD	C1-C2-C3	-3.64	102.36	110.01
23	B	616	CLA	C3D-C4D-ND	3.64	115.90	109.99
23	C	512	CLA	C3D-C4D-ND	3.64	115.90	109.99
23	c	509	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
23	C	514	CLA	C2B-C1B-NB	3.63	114.09	110.33
40	H	102	RRX	C10-C11-C12	-3.63	112.68	123.20
23	c	515	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
26	a	2615	SQD	C1-C2-C3	-3.63	102.38	110.01
31	a	2619	JOX	C1-C2-C3	3.63	117.38	114.12
25	B	633	BCR	C15-C16-C17	-3.62	116.11	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
28	B	623	LMT	C1-O1'-C1'	-3.62	107.50	113.68
23	c	510	CLA	O2D-CGD-O1D	-3.61	116.81	123.85
23	B	616	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	c	508	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	b	613	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
27	c	521	LMG	O7-C10-C11	3.61	119.28	111.48
23	B	610	CLA	C1D-CHD-C4C	-3.60	118.36	126.02
23	C	508	CLA	C2C-C1C-NC	3.60	113.76	109.98
23	b	606	CLA	C2B-C1B-NB	3.60	114.06	110.33
23	A	405	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
23	b	615	CLA	C3D-C4D-ND	3.59	115.83	109.99
23	C	510	CLA	C3D-C4D-ND	3.59	115.82	109.99
23	c	516	CLA	C1-C2-C3	-3.59	120.32	126.20
23	C	511	CLA	C3B-C2B-C1B	-3.58	102.94	107.17
23	b	614	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
27	B	622	LMG	O7-C10-C11	3.58	119.23	111.48
23	b	618	CLA	O2D-CGD-CBD	3.58	117.48	111.23
23	C	512	CLA	C2C-C1C-NC	3.58	113.74	109.98
23	B	615	CLA	C1C-C2C-C3C	-3.58	103.22	106.98
23	c	515	CLA	CBC-CAC-C3C	-3.57	102.73	112.42
23	c	510	CLA	C2B-C1B-NB	3.57	114.03	110.33
23	C	511	CLA	C4-C3-C5	3.57	121.42	115.23
23	c	504	CLA	CBC-CAC-C3C	-3.57	102.74	112.42
28	z	102	LMT	O1B-C1B-C2B	3.57	116.87	108.09
23	B	610	CLA	C3B-C2B-C1B	-3.57	102.96	107.17
23	b	619	CLA	C2C-C1C-NC	3.57	113.73	109.98
23	C	509	CLA	C1-C2-C3	-3.57	120.35	126.20
23	B	614	CLA	C4-C3-C5	3.57	121.42	115.23
23	c	506	CLA	CHD-C4C-C3C	-3.57	119.57	124.77
23	B	605	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
27	C	520	LMG	O8-C28-C29	3.56	122.70	111.83
23	B	611	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
23	b	611	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
23	c	507	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
37	D	2307	DGD	O1G-C1A-C2A	3.56	122.68	111.83
26	l	101	SQD	C3-C4-C5	3.55	116.68	110.23
23	c	516	CLA	C2B-C1B-NB	3.55	114.01	110.33
23	b	610	CLA	C1D-CHD-C4C	-3.55	118.47	126.02
23	B	611	CLA	C4C-C3C-C2C	-3.55	101.73	106.89
25	D	2305	BCR	C33-C5-C6	-3.55	120.61	124.48
23	B	604	CLA	C4-C3-C5	3.55	121.39	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	621	CLA	C3D-C4D-ND	3.54	115.75	109.99
23	B	606	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
23	c	511	CLA	CHD-C4C-C3C	-3.54	119.61	124.77
23	C	514	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
23	B	617	CLA	CBC-CAC-C3C	-3.53	102.84	112.42
23	C	509	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	b	611	CLA	C1D-CHD-C4C	-3.53	118.52	126.02
23	B	617	CLA	C3D-C4D-ND	3.53	115.72	109.99
23	C	512	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
25	C	515	BCR	C33-C5-C6	-3.53	120.63	124.48
23	B	603	CLA	C1D-CHD-C4C	-3.53	118.52	126.02
23	b	606	CLA	C1C-C2C-C3C	-3.52	103.27	106.98
23	c	512	CLA	C1D-CHD-C4C	-3.52	118.53	126.02
23	B	616	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
23	a	2613	CLA	C3B-C4B-NB	3.52	113.67	110.53
23	b	616	CLA	C2C-C1C-NC	3.52	113.68	109.98
38	d	412	LHG	O8-C23-C24	3.51	122.54	111.83
23	C	509	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
23	b	617	CLA	C1D-CHD-C4C	-3.51	118.57	126.02
33	D	2306	PL9	C40-C39-C41	3.51	121.31	115.23
23	B	614	CLA	C2C-C1C-NC	3.50	113.66	109.98
27	C	527	LMG	O8-C28-C29	3.50	122.52	111.83
23	b	614	CLA	CBC-CAC-C3C	-3.50	102.92	112.42
23	C	506	CLA	C1D-CHD-C4C	-3.50	118.57	126.02
23	C	511	CLA	CHD-C4C-C3C	-3.50	119.67	124.77
23	A	406	CLA	C3B-C4B-NB	3.50	113.66	110.53
26	B	621	SQD	C1-O5-C5	3.50	120.56	113.72
23	B	602	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	a	2610	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	A	410	CLA	CBC-CAC-C3C	-3.50	102.93	112.42
23	c	508	CLA	C3C-C4C-NC	3.50	114.91	110.43
23	b	617	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	A	407	CLA	C2C-C1C-NC	3.49	113.65	109.98
25	B	618	BCR	C7-C8-C9	-3.49	121.07	126.23
23	c	506	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
23	b	608	CLA	C2C-C1C-NC	3.49	113.64	109.98
23	b	612	CLA	C2C-C1C-NC	3.48	113.64	109.98
23	b	619	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
23	B	603	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
23	B	617	CLA	C4-C3-C5	3.48	121.27	115.23
37	C	517	DGD	O2G-C1B-C2B	3.48	119.01	111.48
23	a	2613	CLA	CMA-C3A-C2A	-3.48	100.53	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	2609	CLA	C2C-C1C-NC	3.48	113.64	109.98
23	B	613	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
23	c	510	CLA	C4A-NA-C1A	3.48	108.27	106.68
36	V	204	HTG	O5-C1-C2	-3.48	105.52	110.32
23	B	613	CLA	C3C-C4C-NC	3.48	114.88	110.43
23	B	606	CLA	O2D-CGD-CBD	3.48	117.31	111.23
24	a	2612	PHO	C4D-CHA-CBD	3.48	110.12	108.45
38	D	2309	LHG	O8-C23-O10	-3.47	114.94	123.63
23	C	512	CLA	C4A-NA-C1A	3.47	108.26	106.68
23	B	607	CLA	C3D-C4D-ND	3.47	115.63	109.99
23	b	620	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	a	2613	CLA	C2B-C1B-NB	3.47	113.93	110.33
23	b	609	CLA	C2C-C1C-NC	3.47	113.63	109.98
23	B	617	CLA	CHD-C4C-C3C	-3.47	119.72	124.77
23	B	612	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
33	A	422	PL9	C32-C31-C29	-3.47	101.69	113.19
25	c	517	BCR	C38-C26-C25	-3.47	120.70	124.48
23	B	612	CLA	C2B-C1B-NB	3.46	113.92	110.33
23	C	504	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	C	502	CLA	CMB-C2B-C1B	3.46	130.69	125.42
23	b	615	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
23	c	512	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	c	516	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
23	C	508	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
23	c	510	CLA	C1-C2-C3	-3.45	120.54	126.20
23	c	514	CLA	C2C-C1C-NC	3.45	113.61	109.98
25	A	411	BCR	C33-C5-C6	-3.45	120.72	124.48
23	b	619	CLA	CAC-C3C-C4C	3.45	129.27	124.79
23	c	506	CLA	C3D-C4D-ND	3.45	115.59	109.99
25	C	515	BCR	C11-C10-C9	-3.44	122.45	127.28
23	A	406	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
23	C	509	CLA	CHD-C4C-C3C	-3.44	119.76	124.77
23	c	509	CLA	C2B-C1B-NB	3.44	113.89	110.33
37	h	102	DGD	O2G-C1B-C2B	3.44	118.92	111.48
23	c	513	CLA	C1D-CHD-C4C	-3.44	118.72	126.02
26	a	2615	SQD	O9-S-C6	3.44	111.89	106.76
23	b	609	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
23	b	608	CLA	O2A-CGA-O1A	-3.43	115.04	123.63
23	c	512	CLA	C2C-C1C-NC	3.43	113.58	109.98
25	z	101	BCR	C16-C17-C18	-3.43	122.47	127.28
26	B	621	SQD	C3-C4-C5	3.43	116.45	110.23
23	c	511	CLA	C1D-CHD-C4C	-3.43	118.74	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	C3B-C4B-NB	3.42	113.59	110.53
23	C	512	CLA	C3B-C4B-NB	3.42	113.59	110.53
23	c	504	CLA	CHD-C1D-ND	-3.42	119.98	124.80
23	D	2304	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
23	B	615	CLA	C2C-C1C-NC	3.42	113.58	109.98
23	c	512	CLA	CHD-C4C-C3C	-3.42	119.78	124.77
23	B	611	CLA	C1D-CHD-C4C	-3.42	118.75	126.02
23	C	510	CLA	CHD-C4C-C3C	-3.42	119.79	124.77
24	a	2612	PHO	O2D-CGD-O1D	-3.42	117.19	123.85
23	C	511	CLA	C4B-C3B-C2B	-3.41	103.06	107.30
23	B	617	CLA	C2C-C1C-NC	3.41	113.57	109.98
23	c	509	CLA	C2C-C1C-NC	3.41	113.57	109.98
23	C	505	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
23	b	608	CLA	C4-C3-C5	3.41	121.15	115.23
23	B	617	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
23	c	512	CLA	CAC-C3C-C4C	3.41	129.23	124.79
23	b	619	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
23	B	613	CLA	C2C-C1C-NC	3.41	113.56	109.98
23	B	604	CLA	CHD-C4C-C3C	-3.40	119.81	124.77
23	c	512	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
33	A	422	PL9	C17-C18-C19	-3.40	119.84	127.62
33	d	411	PL9	C37-C38-C39	-3.40	119.84	127.62
23	B	612	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
23	C	503	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
26	b	601	SQD	O5-C5-C4	3.39	115.81	109.70
23	B	617	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
23	b	606	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
25	K	101	BCR	C24-C23-C22	-3.39	121.22	126.23
36	i	102	HTG	C3-C4-C5	3.39	116.38	110.23
23	c	509	CLA	C16-C15-C13	-3.39	104.70	115.97
27	C	527	LMG	O6-C5-C4	3.39	115.80	109.70
23	B	606	CLA	C2B-C1B-NB	3.38	113.83	110.33
23	C	507	CLA	C1D-CHD-C4C	-3.38	118.83	126.02
23	c	508	CLA	C1D-CHD-C4C	-3.38	118.83	126.02
23	C	506	CLA	CAC-C3C-C4C	3.38	129.19	124.79
23	c	509	CLA	CBC-CAC-C3C	-3.38	103.26	112.42
23	D	2303	CLA	O2A-CGA-CBA	3.38	122.14	111.83
23	C	510	CLA	C2B-C1B-NB	3.38	113.83	110.33
23	b	614	CLA	CHD-C4C-C3C	-3.38	119.85	124.77
23	D	2304	CLA	C2B-C1B-NB	3.38	113.83	110.33
36	B	624[B]	HTG	O5-C1-C2	3.38	114.97	110.32
23	C	513	CLA	C1D-CHD-C4C	-3.38	118.84	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C3B-C4B-NB	3.38	113.54	110.53
23	C	504	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
23	c	508	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
23	B	616	CLA	C3B-C4B-NB	3.37	113.54	110.53
23	A	407	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
23	c	514	CLA	C2B-C1B-NB	3.37	113.82	110.33
23	b	616	CLA	C1D-CHD-C4C	-3.37	118.86	126.02
23	D	2303	CLA	CHD-C1D-ND	-3.37	120.06	124.80
23	B	608	CLA	CAC-C3C-C4C	3.36	129.17	124.79
23	C	504	CLA	C4A-NA-C1A	3.36	108.21	106.68
23	D	2303	CLA	C1-C2-C3	-3.36	120.69	126.20
23	C	507	CLA	C2B-C1B-NB	3.36	113.81	110.33
23	b	615	CLA	O2D-CGD-CBD	3.36	117.11	111.23
23	D	2303	CLA	C3C-C4C-NC	3.36	114.74	110.43
23	C	512	CLA	C1D-CHD-C4C	-3.36	118.88	126.02
23	B	606	CLA	O2A-CGA-CBA	3.36	122.08	111.83
23	B	616	CLA	C2B-C1B-NB	3.36	113.81	110.33
23	c	507	CLA	CHD-C1D-ND	-3.36	120.08	124.80
23	C	509	CLA	C2C-C1C-NC	3.36	113.51	109.98
23	B	613	CLA	CMC-C2C-C1C	3.35	130.27	125.03
23	b	607	CLA	CAC-C3C-C4C	3.35	129.15	124.79
23	b	615	CLA	C1-C2-C3	-3.35	120.71	126.20
23	c	504	CLA	C2C-C1C-NC	3.35	113.50	109.98
25	B	633	BCR	C11-C10-C9	-3.35	122.58	127.28
23	b	607	CLA	C4C-C3C-C2C	-3.35	102.02	106.89
23	A	407	CLA	CBC-CAC-C3C	-3.35	103.35	112.42
33	A	422	PL9	C12-C13-C14	-3.34	119.97	127.62
23	B	605	CLA	CHD-C4C-C3C	-3.34	119.90	124.77
23	B	606	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
40	H	102	RRX	C38-C26-C25	-3.34	120.84	124.48
23	B	606	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
23	c	505	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
23	b	619	CLA	CHD-C4C-C3C	-3.34	119.91	124.77
23	c	507	CLA	C2B-C1B-NB	3.34	113.79	110.33
23	C	507	CLA	CBC-CAC-C3C	-3.33	103.39	112.42
26	d	417	SQD	O8-S-C6	3.33	112.52	106.00
23	C	508	CLA	C1D-CHD-C4C	-3.33	118.94	126.02
23	b	616	CLA	C1-C2-C3	-3.33	120.74	126.20
23	B	612	CLA	CHD-C4C-C3C	-3.33	119.92	124.77
23	d	408	CLA	C3B-C4B-NB	3.33	113.50	110.53
23	C	513	CLA	C1-C2-C3	-3.33	120.75	126.20
23	d	402	CLA	C1-C2-C3	-3.33	120.75	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	618	CLA	CHD-C4C-C3C	-3.32	119.93	124.77
23	c	510	CLA	CMB-C2B-C1B	3.32	130.48	125.42
36	b	625	HTG	C6-C5-C4	-3.32	104.86	113.02
23	b	608	CLA	O2A-CGA-CBA	3.32	121.96	111.83
23	C	507	CLA	C2C-C1C-NC	3.32	113.47	109.98
23	c	511	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
23	C	505	CLA	CHD-C4C-C3C	-3.32	119.93	124.77
23	c	509	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
23	a	2609	CLA	CHD-C4C-C3C	-3.32	119.93	124.77
27	c	521	LMG	O8-C28-C29	3.32	121.96	111.83
23	A	410	CLA	CMA-C3A-C2A	-3.32	101.15	113.98
23	C	514	CLA	C1D-CHD-C4C	-3.32	118.97	126.02
23	B	604	CLA	CMB-C2B-C1B	3.32	130.47	125.42
23	C	506	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
23	B	602	CLA	O2A-CGA-CBA	3.31	121.94	111.83
28	M	101	LMT	C1'-O5'-C5'	3.31	120.19	113.72
36	V	204	HTG	C1-C2-C3	-3.31	104.07	110.55
23	A	406	CLA	CAA-C2A-C3A	-3.31	104.05	113.00
33	x	1301	PL9	C12-C13-C14	-3.31	120.04	127.62
23	B	606	CLA	C3C-C4C-NC	3.31	114.67	110.43
23	a	2609	CLA	C2B-C1B-NB	3.31	113.76	110.33
23	b	610	CLA	C4-C3-C5	3.31	120.97	115.23
23	b	620	CLA	CHD-C4C-C3C	-3.31	119.95	124.77
23	C	505	CLA	CBC-CAC-C3C	-3.31	103.46	112.42
23	B	607	CLA	C2B-C1B-NB	3.31	113.75	110.33
23	B	609	CLA	C3C-C4C-NC	3.30	114.66	110.43
23	d	409	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
23	c	515	CLA	CBA-CAA-C2A	-3.30	103.97	113.79
23	A	407	CLA	CMB-C2B-C1B	3.30	130.44	125.42
23	A	405	CLA	C3C-C4C-NC	3.30	114.66	110.43
25	y	101	BCR	C38-C26-C25	-3.30	120.89	124.48
23	A	410	CLA	C1D-CHD-C4C	-3.30	119.01	126.02
23	C	508	CLA	C2B-C1B-NB	3.29	113.74	110.33
37	c	519	DGD	O1G-C1A-C2A	3.29	121.88	111.83
23	b	609	CLA	CMB-C2B-C1B	3.29	130.43	125.42
23	C	506	CLA	C2C-C1C-NC	3.29	113.44	109.98
23	b	613	CLA	O2A-CGA-CBA	3.29	121.88	111.83
23	c	509	CLA	C1D-CHD-C4C	-3.29	119.03	126.02
23	b	608	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
23	a	2613	CLA	C4B-C3B-C2B	-3.29	103.22	107.30
23	b	608	CLA	CAA-C2A-C3A	-3.28	104.12	113.00
23	B	610	CLA	C4C-C3C-C2C	-3.28	102.11	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	C2B-C1B-NB	3.28	113.73	110.33
23	c	506	CLA	C2C-C1C-NC	3.28	113.43	109.98
23	c	513	CLA	C2C-C1C-NC	3.28	113.43	109.98
23	b	617	CLA	C1-C2-C3	-3.28	120.82	126.20
23	b	620	CLA	C2B-C1B-NB	3.28	113.73	110.33
23	c	516	CLA	CHD-C4C-C3C	-3.28	119.99	124.77
25	c	517	BCR	C15-C14-C13	-3.28	122.68	127.28
38	d	412	LHG	O8-C23-O10	-3.28	115.43	123.63
23	c	511	CLA	C3C-C4C-NC	3.27	114.62	110.43
23	B	607	CLA	C1D-CHD-C4C	-3.27	119.06	126.02
23	c	516	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
23	b	618	CLA	C2B-C1B-NB	3.26	113.71	110.33
23	b	617	CLA	C2C-C1C-NC	3.26	113.41	109.98
25	B	633	BCR	C7-C8-C9	-3.26	121.41	126.23
23	C	510	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
23	c	513	CLA	C2B-C1B-NB	3.26	113.71	110.33
23	b	617	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
23	c	505	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
23	b	617	CLA	C2B-C1B-NB	3.25	113.70	110.33
23	b	614	CLA	CMB-C2B-C1B	3.25	130.37	125.42
23	B	610	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
23	B	616	CLA	CBC-CAC-C3C	-3.25	103.60	112.42
23	A	410	CLA	C4-C3-C5	3.25	120.87	115.23
36	C	525	HTG	C1-O5-C5	3.25	118.39	112.56
23	b	609	CLA	C3D-C4D-ND	3.25	115.27	109.99
23	A	405	CLA	CAA-C2A-C1A	-3.25	101.33	111.97
25	B	633	BCR	C12-C13-C14	-3.24	113.91	119.01
23	b	610	CLA	C3C-C4C-NC	3.24	114.59	110.43
31	A	418	JOX	O1-C5-C4	-3.24	116.81	121.43
23	c	514	CLA	C1D-CHD-C4C	-3.24	119.13	126.02
23	c	513	CLA	CHD-C4C-C3C	-3.24	120.05	124.77
24	A	409	PHO	C4-C3-C5	3.24	120.85	115.23
25	A	411	BCR	C38-C26-C25	-3.24	120.95	124.48
23	B	606	CLA	CAC-C3C-C4C	3.23	129.00	124.79
42	V	201	HEC	CBC-CAC-C3C	-3.23	120.97	127.43
23	b	615	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
25	b	622	BCR	C7-C8-C9	-3.23	121.45	126.23
42	V	201	HEC	CBD-CAD-C3D	-3.23	103.60	112.53
23	B	609	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
23	C	503	CLA	C1D-CHD-C4C	-3.23	119.16	126.02
23	B	603	CLA	C2B-C1B-NB	3.23	113.67	110.33
23	d	402	CLA	C2B-C1B-NB	3.23	113.67	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	C1D-CHD-C4C	-3.23	119.16	126.02
25	C	515	BCR	C7-C8-C9	-3.22	121.46	126.23
38	e	101	LHG	O8-C23-C24	3.22	121.66	111.83
23	b	607	CLA	C2C-C1C-NC	3.22	113.37	109.98
23	b	612	CLA	C1D-CHD-C4C	-3.22	119.17	126.02
23	B	602	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
25	b	624	BCR	C15-C14-C13	-3.22	122.76	127.28
23	B	612	CLA	C2C-C1C-NC	3.22	113.36	109.98
23	A	406	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	B	613	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	b	613	CLA	C2C-C1C-NC	3.22	113.36	109.98
23	a	2609	CLA	CAA-C2A-C1A	-3.21	101.44	111.97
27	A	413	LMG	C8-O7-C10	-3.21	110.10	117.80
40	H	102	RRX	C16-C17-C18	-3.21	122.77	127.28
23	c	514	CLA	C4-C3-C5	3.21	120.80	115.23
27	c	521	LMG	C8-O7-C10	-3.21	110.11	117.80
23	c	506	CLA	C1D-CHD-C4C	-3.21	119.20	126.02
23	C	514	CLA	C1-C2-C3	-3.21	120.94	126.20
23	A	405	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
23	c	509	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
23	c	515	CLA	C2B-C1B-NB	3.21	113.65	110.33
23	c	515	CLA	CMB-C2B-C1B	3.20	130.30	125.42
23	a	2613	CLA	C4-C3-C5	3.20	120.79	115.23
23	A	410	CLA	C3B-C4B-NB	3.20	113.39	110.53
23	B	604	CLA	O2A-CGA-CBA	3.20	121.60	111.83
36	o	301	HTG	C1'-S1-C1	3.20	107.36	100.45
23	A	407	CLA	C4-C3-C5	3.20	120.78	115.23
23	B	613	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
37	H	103	DGD	O1G-C1A-C2A	3.19	121.58	111.83
23	c	506	CLA	C1-C2-C3	-3.19	120.96	126.20
23	B	607	CLA	CAC-C3C-C4C	3.19	128.94	124.79
23	c	508	CLA	CMB-C2B-C1B	3.19	130.28	125.42
23	b	607	CLA	C1-C2-C3	-3.19	120.97	126.20
23	c	510	CLA	CHD-C4C-C3C	-3.19	120.12	124.77
23	C	512	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
23	b	613	CLA	CHD-C4C-C3C	-3.18	120.13	124.77
33	x	1301	PL9	C32-C33-C34	-3.18	120.34	127.62
23	c	509	CLA	CAA-C2A-C3A	-3.18	104.40	113.00
23	A	405	CLA	C3B-C4B-NB	3.18	113.37	110.53
23	c	509	CLA	O2A-CGA-O1A	-3.18	115.67	123.63
24	a	2612	PHO	C1A-C2A-C3A	-3.18	99.81	102.84
42	V	201	HEC	C4D-ND-C1D	3.18	111.00	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
23	C	507	CLA	O2A-CGA-CBA	3.17	121.51	111.83
23	B	608	CLA	C1-O2A-CGA	3.17	124.33	116.65
33	D	2306	PL9	C7-C8-C9	-3.17	121.37	126.83
23	B	615	CLA	C2B-C1B-NB	3.17	113.61	110.33
23	B	610	CLA	C2C-C1C-NC	3.17	113.31	109.98
23	c	515	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
23	C	510	CLA	C3B-C4B-NB	3.17	113.36	110.53
23	B	613	CLA	C2B-C1B-NB	3.17	113.61	110.33
23	c	508	CLA	CHA-C1A-NA	-3.17	119.22	126.39
24	a	2612	PHO	CMB-C2B-C3B	3.17	131.01	124.68
23	B	603	CLA	CBC-CAC-C3C	-3.17	103.84	112.42
23	d	409	CLA	C4-C3-C5	3.17	120.72	115.23
23	B	614	CLA	C3B-C4B-NB	3.16	113.35	110.53
23	b	614	CLA	CHD-C1D-ND	-3.16	120.35	124.80
23	c	504	CLA	C2B-C1B-NB	3.16	113.60	110.33
23	c	511	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
23	B	604	CLA	C1D-CHD-C4C	-3.16	119.31	126.02
23	A	405	CLA	CMA-C3A-C4A	-3.16	103.28	111.77
23	C	504	CLA	CMC-C2C-C1C	3.16	129.97	125.03
23	A	405	CLA	C1-C2-C3	-3.16	121.02	126.20
23	C	506	CLA	CHA-C1A-NA	-3.16	119.24	126.39
23	A	405	CLA	C1D-CHD-C4C	-3.16	119.31	126.02
23	C	504	CLA	CBC-CAC-C3C	-3.16	103.87	112.42
26	d	417	SQD	O48-C23-C24	3.15	121.45	111.83
23	d	408	CLA	C3C-C4C-NC	3.15	114.47	110.43
23	b	612	CLA	CMC-C2C-C1C	3.15	129.96	125.03
23	c	510	CLA	CBC-CAC-C3C	-3.15	103.88	112.42
23	b	621	CLA	C2B-C1B-NB	3.15	113.59	110.33
23	C	502	CLA	C1D-CHD-C4C	-3.15	119.32	126.02
25	B	618	BCR	C24-C23-C22	-3.15	121.58	126.23
23	B	613	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
23	b	620	CLA	CAC-C3C-C4C	3.14	128.88	124.79
24	A	409	PHO	C1A-C2A-C3A	-3.14	99.85	102.84
23	b	621	CLA	C1-C2-C3	-3.14	121.05	126.20
23	b	612	CLA	C2B-C1B-NB	3.14	113.58	110.33
23	a	2610	CLA	O2A-CGA-O1A	-3.14	115.77	123.63
23	b	607	CLA	C1D-CHD-C4C	-3.14	119.35	126.02
23	B	604	CLA	O2A-CGA-O1A	-3.14	115.78	123.63
23	C	509	CLA	C2B-C1B-NB	3.14	113.58	110.33
23	A	405	CLA	CHD-C1D-ND	-3.13	120.39	124.80
23	B	613	CLA	C1D-CHD-C4C	-3.13	119.36	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	C2B-C1B-NB	3.13	113.57	110.33
23	b	607	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
23	C	506	CLA	C2B-C1B-NB	3.13	113.57	110.33
23	C	503	CLA	C2B-C1B-NB	3.13	113.57	110.33
23	B	614	CLA	C1D-CHD-C4C	-3.13	119.38	126.02
23	B	617	CLA	C2B-C1B-NB	3.13	113.57	110.33
24	a	2611	PHO	C1A-C2A-C3A	-3.12	99.87	102.84
23	C	511	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
23	B	603	CLA	CHD-C4C-C3C	-3.12	120.22	124.77
23	B	605	CLA	C3B-C4B-NB	3.12	113.32	110.53
23	B	614	CLA	C3C-C4C-NC	3.12	114.43	110.43
36	b	604	HTG	O5-C5-C4	3.12	115.32	109.70
23	d	402	CLA	O2A-CGA-O1A	-3.12	115.82	123.63
23	c	506	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
23	c	506	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
23	B	605	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
23	c	512	CLA	C3B-C4B-NB	3.12	113.31	110.53
25	C	516	BCR	C38-C26-C25	-3.12	121.08	124.48
23	B	612	CLA	C1D-CHD-C4C	-3.12	119.40	126.02
37	h	102	DGD	O1G-C1A-O1A	-3.11	115.84	123.63
23	C	512	CLA	C2B-C1B-NB	3.11	113.56	110.33
23	b	611	CLA	C3C-C4C-NC	3.11	114.42	110.43
23	b	613	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
23	d	408	CLA	CHD-C4C-C3C	-3.11	120.23	124.77
23	C	505	CLA	C2B-C1B-NB	3.11	113.55	110.33
31	a	2617	JOX	C-C1-C2	-3.11	120.80	123.21
23	B	608	CLA	CHD-C4C-C3C	-3.11	120.24	124.77
23	c	514	CLA	CHD-C1D-ND	-3.11	120.42	124.80
23	C	509	CLA	CAC-C3C-C4C	3.11	128.84	124.79
37	c	520	DGD	O1G-C1A-C2A	3.11	121.32	111.83
33	d	411	PL9	O1-C4-C3	-3.11	117.45	120.73
23	c	512	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	b	610	CLA	CMC-C2C-C1C	3.11	129.89	125.03
23	A	405	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	c	510	CLA	C1D-CHD-C4C	-3.11	119.42	126.02
23	C	512	CLA	CHD-C1D-ND	-3.11	120.43	124.80
36	d	407	HTG	C1-O5-C5	3.10	118.13	112.56
23	B	605	CLA	C2B-C1B-NB	3.10	113.54	110.33
23	B	614	CLA	C2B-C1B-NB	3.10	113.54	110.33
23	a	2609	CLA	C3C-C4C-NC	3.10	114.41	110.43
23	C	514	CLA	CMB-C2B-C1B	3.10	130.14	125.42
23	C	508	CLA	CMB-C2B-C1B	3.10	130.14	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	625	HTG	C1'-S1-C1	3.10	107.14	100.45
33	d	411	PL9	C40-C39-C41	3.10	120.61	115.23
23	b	608	CLA	C2B-C1B-NB	3.10	113.54	110.33
23	C	506	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
23	b	611	CLA	C2B-C1B-NB	3.10	113.54	110.33
23	b	621	CLA	CBC-CAC-C3C	-3.09	104.03	112.42
23	B	615	CLA	O2A-CGA-O1A	-3.09	115.89	123.63
23	C	508	CLA	C3D-C4D-ND	3.09	115.02	109.99
23	b	612	CLA	CBC-CAC-C3C	-3.09	104.03	112.42
23	C	511	CLA	C1-O2A-CGA	3.09	124.13	116.65
23	b	612	CLA	C3C-C4C-NC	3.09	114.39	110.43
25	b	623	BCR	C38-C26-C25	-3.09	121.11	124.48
23	B	611	CLA	C1-O2A-CGA	3.09	124.13	116.65
23	a	2609	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
23	b	617	CLA	O2A-CGA-CBA	3.09	121.25	111.83
23	a	2610	CLA	O2A-CGA-CBA	3.09	121.25	111.83
23	C	505	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
23	B	607	CLA	C1-O2A-CGA	3.09	124.12	116.65
23	C	513	CLA	CMB-C2B-C1B	3.09	130.12	125.42
23	B	615	CLA	CHD-C1D-ND	-3.08	120.46	124.80
37	H	103	DGD	C2G-O2G-C1B	-3.08	110.43	117.80
33	x	1301	PL9	C20-C19-C21	3.08	120.57	115.23
23	d	408	CLA	CMB-C2B-C1B	3.07	130.10	125.42
23	b	616	CLA	CMC-C2C-C1C	3.07	129.84	125.03
23	b	616	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
23	d	408	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
23	C	513	CLA	CBA-CAA-C2A	-3.07	104.66	113.79
28	i	103	LMT	C1'-O5'-C5'	3.07	119.71	113.72
23	B	606	CLA	C1-C2-C3	-3.07	121.17	126.20
23	C	507	CLA	C4-C3-C5	3.07	120.55	115.23
23	c	513	CLA	C3B-C4B-NB	3.07	113.27	110.53
23	B	608	CLA	C2B-C1B-NB	3.07	113.50	110.33
23	b	607	CLA	CAA-CBA-CGA	-3.07	104.50	113.21
23	B	612	CLA	CMC-C2C-C1C	3.06	129.82	125.03
23	B	602	CLA	C2B-C1B-NB	3.06	113.50	110.33
23	B	614	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	C	513	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	d	408	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
23	D	2303	CLA	C1D-CHD-C4C	-3.06	119.51	126.02
23	b	609	CLA	CHA-C1A-NA	-3.06	119.46	126.39
23	c	504	CLA	C1D-CHD-C4C	-3.06	119.52	126.02
23	c	512	CLA	CMC-C2C-C1C	3.06	129.81	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	417	SQD	O9-S-C6	3.06	111.35	106.73
23	c	509	CLA	O2A-CGA-CBA	3.06	121.16	111.83
23	B	606	CLA	CMC-C2C-C1C	3.06	129.81	125.03
23	b	615	CLA	C3C-C4C-NC	3.06	114.35	110.43
23	b	615	CLA	O2A-CGA-CBA	3.05	121.14	111.83
23	B	610	CLA	CHD-C4C-C3C	-3.05	120.32	124.77
23	C	509	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	d	402	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
33	x	1301	PL9	C37-C38-C39	-3.05	120.64	127.62
23	A	407	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
23	c	505	CLA	O2A-CGA-CBA	3.05	121.13	111.83
23	A	405	CLA	O2A-CGA-CBA	3.04	121.11	111.83
23	B	607	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
33	d	411	PL9	C15-C14-C16	3.04	120.51	115.23
23	C	503	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	A	405	CLA	C2B-C1B-NB	3.04	113.48	110.33
23	B	611	CLA	C2C-C1C-NC	3.04	113.17	109.98
23	b	613	CLA	C1D-CHD-C4C	-3.04	119.56	126.02
28	m	2804	LMT	C1B-C2B-C3B	3.04	116.40	110.01
23	B	615	CLA	CBC-CAC-C3C	-3.03	104.19	112.42
23	B	617	CLA	C3B-C4B-NB	3.03	113.24	110.53
25	k	302	BCR	C38-C26-C25	-3.03	121.17	124.48
23	C	509	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
23	B	609	CLA	C2B-C1B-NB	3.03	113.47	110.33
23	b	614	CLA	C2C-C1C-NC	3.03	113.17	109.98
23	B	616	CLA	C3C-C4C-NC	3.03	114.31	110.43
23	B	615	CLA	O2A-CGA-CBA	3.03	121.08	111.83
23	c	505	CLA	O2A-CGA-O1A	-3.03	116.05	123.63
23	C	513	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	B	614	CLA	O2A-CGA-CBA	3.03	121.06	111.83
23	B	611	CLA	C3C-C4C-NC	3.03	114.31	110.43
23	B	609	CLA	C1C-C2C-C3C	-3.03	103.80	106.98
23	a	2609	CLA	O2A-CGA-CBA	3.02	121.05	111.83
23	b	617	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
23	C	511	CLA	C2C-C1C-NC	3.02	113.16	109.98
28	j	2701	LMT	O1B-C4'-C3'	3.02	114.91	107.23
23	A	407	CLA	C1-C2-C3	-3.02	121.25	126.20
23	B	615	CLA	C3B-C4B-NB	3.02	113.22	110.53
23	b	610	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
23	B	616	CLA	C4-C3-C5	3.02	120.46	115.23
23	B	617	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
25	K	101	BCR	C7-C8-C9	-3.01	121.78	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	O2D-CGD-CBD	3.01	116.50	111.23
23	b	620	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
23	b	615	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
37	c	518	DGD	O2G-C1B-O1B	-3.01	116.66	123.70
23	c	505	CLA	C2C-C1C-NC	3.01	113.14	109.98
23	c	507	CLA	C4-C3-C5	3.01	120.45	115.23
23	C	509	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	B	602	CLA	C1D-CHD-C4C	-3.01	119.63	126.02
23	b	618	CLA	C3B-C4B-NB	3.01	113.22	110.53
23	b	608	CLA	C3C-C4C-NC	3.01	114.28	110.43
26	D	2308	SQD	O6-C1-C2	3.01	112.84	108.27
23	C	506	CLA	C3D-C2D-C1D	-3.01	101.73	105.83
31	A	418	JOX	C2-C3-CL	3.00	118.24	115.82
23	c	512	CLA	C3C-C4C-NC	3.00	114.28	110.43
23	b	619	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
23	c	515	CLA	C2C-C1C-NC	3.00	113.14	109.98
23	c	513	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
23	D	2303	CLA	C2B-C1B-NB	3.00	113.44	110.33
23	c	507	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	B	605	CLA	C4A-NA-C1A	3.00	108.05	106.68
23	b	611	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
25	T	102	BCR	C11-C10-C9	-3.00	123.07	127.28
38	D	2311	LHG	O8-C23-C24	3.00	120.98	111.83
23	c	510	CLA	C4-C3-C5	3.00	120.43	115.23
23	A	410	CLA	CAA-C2A-C3A	-3.00	104.90	113.00
25	y	101	BCR	C16-C17-C18	-3.00	123.08	127.28
23	B	611	CLA	CAA-C2A-C3A	-2.99	104.91	113.00
23	C	508	CLA	C3C-C4C-NC	2.99	114.27	110.43
23	c	509	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
23	c	510	CLA	C3C-C4C-NC	2.99	114.26	110.43
23	d	408	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
23	b	609	CLA	C4A-NA-C1A	2.99	108.04	106.68
26	A	412	SQD	O48-C23-C24	2.99	120.95	111.83
37	h	102	DGD	O1G-C1A-C2A	2.99	120.94	111.83
23	b	619	CLA	CBC-CAC-C3C	-2.99	104.32	112.42
23	B	616	CLA	CMC-C2C-C1C	2.99	129.70	125.03
38	d	413	LHG	O8-C23-O10	-2.99	116.16	123.63
23	B	607	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
23	a	2610	CLA	C4-C3-C5	2.98	120.41	115.23
23	b	606	CLA	C1-C2-C3	-2.98	121.31	126.20
23	d	408	CLA	O2A-CGA-CBA	2.98	120.94	111.83
23	a	2610	CLA	C2C-C1C-NC	2.98	113.11	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	508	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
23	B	612	CLA	CHA-C1A-NA	-2.98	119.64	126.39
38	L	101	LHG	O8-C23-O10	-2.98	116.17	123.63
23	b	611	CLA	C2C-C1C-NC	2.98	113.11	109.98
23	B	611	CLA	CMA-C3A-C4A	-2.98	103.78	111.77
23	c	514	CLA	C4B-C3B-C2B	-2.97	103.60	107.30
31	a	2617	JOX	C-C5-C4	2.97	123.59	117.06
23	c	506	CLA	C3C-C4C-NC	2.97	114.24	110.43
23	b	620	CLA	CED-O2D-CGD	2.97	122.66	115.92
23	b	618	CLA	C1D-CHD-C4C	-2.97	119.70	126.02
40	h	101	RRX	C10-C11-C12	-2.97	114.59	123.20
23	b	613	CLA	C3B-C4B-NB	2.97	113.18	110.53
23	B	609	CLA	O2A-CGA-CBA	2.97	120.89	111.83
38	l	103	LHG	O8-C23-C24	2.97	120.89	111.83
23	C	503	CLA	C2C-C1C-NC	2.96	113.10	109.98
23	d	402	CLA	C3C-C4C-NC	2.96	114.23	110.43
23	C	503	CLA	CBC-CAC-C3C	-2.96	104.38	112.42
23	c	509	CLA	CHD-C4C-C3C	-2.96	120.45	124.77
25	T	102	BCR	C7-C6-C5	-2.96	114.73	121.56
23	b	621	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
23	B	605	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
23	c	511	CLA	C1-C2-C3	-2.96	121.35	126.20
23	B	608	CLA	C3B-C4B-NB	2.96	113.17	110.53
23	b	618	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	b	610	CLA	C3B-C4B-NB	2.96	113.17	110.53
23	c	512	CLA	C4A-NA-C1A	2.96	108.03	106.68
26	D	2308	SQD	O7-S-C6	2.96	111.17	106.76
23	C	507	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
23	d	409	CLA	C1-C2-C3	-2.95	121.36	126.20
23	B	607	CLA	C3C-C4C-NC	2.95	114.21	110.43
23	B	602	CLA	CBC-CAC-C3C	-2.95	104.42	112.42
23	a	2609	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
23	B	602	CLA	CHD-C4C-C3C	-2.95	120.47	124.77
23	b	619	CLA	C3C-C4C-NC	2.95	114.21	110.43
23	d	402	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
26	a	2615	SQD	C45-O47-C7	-2.95	110.74	117.80
23	c	514	CLA	C3B-C4B-NB	2.95	113.16	110.53
23	b	614	CLA	O2D-CGD-CBD	2.95	116.38	111.23
23	b	616	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
23	d	408	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
36	H	101	HTG	O5-C1-C2	2.94	112.85	109.47
23	b	618	CLA	CMB-C2B-C1B	2.94	129.90	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	408	CLA	C2B-C1B-NB	2.94	113.38	110.33
23	B	606	CLA	CMB-C2B-C1B	2.94	129.90	125.42
23	B	604	CLA	CBC-CAC-C3C	-2.94	104.45	112.42
23	B	617	CLA	O2A-CGA-CBA	2.94	120.79	111.83
23	C	509	CLA	C1D-CHD-C4C	-2.94	119.78	126.02
26	A	412	SQD	C1-C2-C3	-2.94	103.83	110.01
25	C	516	BCR	C2-C1-C6	2.93	114.70	110.44
40	H	102	RRX	C20-C21-C22	-2.93	123.17	127.28
23	B	604	CLA	C3C-C4C-NC	2.93	114.19	110.43
23	b	618	CLA	O2A-CGA-CBA	2.93	120.77	111.83
23	C	506	CLA	CMB-C2B-C1B	2.93	129.88	125.42
23	a	2609	CLA	CMC-C2C-C1C	2.93	129.61	125.03
26	D	2308	SQD	O48-C23-C24	2.93	120.77	111.83
23	C	504	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
33	D	2306	PL9	C25-C24-C26	2.93	120.31	115.23
23	B	605	CLA	CMC-C2C-C1C	2.93	129.61	125.03
23	D	2304	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
23	b	618	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
23	C	510	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
23	B	612	CLA	C1-O2A-CGA	2.92	123.73	116.65
23	c	511	CLA	C4-C3-C5	2.92	120.30	115.23
23	A	407	CLA	CHD-C1D-ND	-2.92	120.69	124.80
23	c	511	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
33	D	2306	PL9	C37-C38-C39	-2.92	120.94	127.62
23	A	406	CLA	CHD-C1D-ND	-2.92	120.69	124.80
23	b	616	CLA	CHD-C1D-ND	-2.92	120.70	124.80
23	C	505	CLA	CHD-C1D-ND	-2.92	120.70	124.80
23	c	506	CLA	CAC-C3C-C4C	2.91	128.58	124.79
23	B	616	CLA	CAC-C3C-C4C	2.91	128.58	124.79
23	a	2613	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
23	A	410	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
23	b	610	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
23	d	409	CLA	CHD-C4C-C3C	-2.91	120.53	124.77
23	c	507	CLA	C3B-C4B-NB	2.91	113.13	110.53
23	c	504	CLA	C1-O2A-CGA	2.91	123.69	116.65
23	B	610	CLA	C3C-C4C-NC	2.91	114.16	110.43
23	C	510	CLA	C3C-C4C-NC	2.91	114.15	110.43
26	a	2615	SQD	O8-S-C6	2.90	111.58	105.97
23	c	509	CLA	C4-C3-C5	2.90	120.27	115.23
23	c	505	CLA	CMB-C2B-C1B	2.90	129.84	125.42
33	D	2306	PL9	C42-C43-C44	-2.90	120.98	127.62
23	c	516	CLA	C4C-C3C-C2C	-2.90	102.67	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	2610	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	B	607	CLA	C2C-C1C-NC	2.90	113.03	109.98
23	C	504	CLA	CMB-C2B-C1B	2.90	129.83	125.42
23	B	604	CLA	C2C-C1C-NC	2.90	113.02	109.98
23	a	2609	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
23	b	621	CLA	O2A-CGA-CBA	2.90	120.66	111.83
23	B	604	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
23	b	606	CLA	C1D-CHD-C4C	-2.89	119.87	126.02
23	b	608	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
27	B	622	LMG	O8-C28-C29	2.89	120.65	111.83
23	b	609	CLA	C3C-C4C-NC	2.89	114.13	110.43
28	j	2701	LMT	C3'-C4'-C5'	-2.89	104.52	110.93
37	C	517	DGD	O3G-C3G-C2G	-2.89	103.79	110.82
23	B	602	CLA	C4A-NA-C1A	2.89	108.00	106.68
23	b	607	CLA	C1-O2A-CGA	2.89	123.65	116.65
23	b	619	CLA	CMB-C2B-C1B	2.89	129.82	125.42
26	a	2603	SQD	O7-S-C6	2.89	111.07	106.76
23	C	502	CLA	CBC-CAC-C3C	-2.89	104.58	112.42
23	C	508	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
23	C	504	CLA	C3C-C4C-NC	2.89	114.13	110.43
23	b	611	CLA	CMC-C2C-C1C	2.89	129.55	125.03
23	d	409	CLA	C3B-C4B-NB	2.89	113.11	110.53
36	B	625	HTG	C1-C2-C3	2.89	116.19	110.55
23	b	620	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
23	c	516	CLA	O2A-CGA-CBA	2.88	120.63	111.83
23	c	511	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
23	B	604	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
23	c	516	CLA	CAC-C3C-C4C	2.88	128.54	124.79
23	b	614	CLA	C2B-C1B-NB	2.88	113.31	110.33
23	b	612	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
31	A	419	JOX	O1-C5-C	-2.88	117.33	121.43
23	C	509	CLA	C3C-C4C-NC	2.88	114.12	110.43
23	b	621	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
28	J	303	LMT	C1'-O5'-C5'	2.88	119.34	113.72
23	b	613	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
23	B	612	CLA	C1-C2-C3	-2.88	121.48	126.20
23	c	515	CLA	CMA-C3A-C4A	-2.88	104.04	111.77
23	C	507	CLA	C3C-C4C-NC	2.87	114.11	110.43
23	b	609	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
23	C	513	CLA	C3C-C4C-NC	2.87	114.11	110.43
23	C	505	CLA	CAA-C2A-C3A	-2.87	105.23	113.00
38	D	2310	LHG	O8-C23-O10	-2.87	116.44	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	m	2802	LMG	O8-C28-C29	2.87	120.59	111.83
23	A	407	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
25	B	619	BCR	C38-C26-C25	-2.87	121.35	124.48
23	b	612	CLA	CHD-C1D-ND	-2.87	120.76	124.80
31	A	418	JOX	C-C5-C4	2.87	123.36	117.06
23	D	2303	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
23	a	2610	CLA	C3C-C4C-NC	2.87	114.10	110.43
38	l	103	LHG	O7-C7-C8	2.87	117.68	111.48
23	b	611	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	a	2611	PHO	O2D-CGD-O1D	-2.86	118.28	123.85
23	b	621	CLA	CHA-C1A-NA	-2.86	119.92	126.39
40	h	101	RRX	C38-C26-C25	-2.86	121.37	124.48
23	b	615	CLA	C2C-C1C-NC	2.86	112.98	109.98
23	b	621	CLA	CAC-C3C-C4C	2.86	128.51	124.79
23	c	510	CLA	C3B-C4B-NB	2.86	113.08	110.53
25	y	101	BCR	C15-C14-C13	-2.85	123.28	127.28
23	B	615	CLA	C4A-NA-C1A	2.85	107.98	106.68
23	b	609	CLA	C6-C5-C3	-2.85	106.53	113.47
23	a	2610	CLA	CED-O2D-CGD	2.85	122.38	115.92
23	B	616	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
23	C	510	CLA	O2A-CGA-CBA	2.85	120.52	111.83
23	c	516	CLA	C2C-C1C-NC	2.85	112.97	109.98
23	C	507	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
23	C	511	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
23	B	610	CLA	C2B-C1B-NB	2.85	113.28	110.33
23	B	613	CLA	C4-C3-C5	2.84	120.16	115.23
23	C	514	CLA	C4-C3-C5	2.84	120.16	115.23
23	C	506	CLA	O2A-CGA-CBA	2.84	120.50	111.83
23	b	615	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	b	609	CLA	CHD-C4C-C3C	-2.84	120.63	124.77
23	C	514	CLA	CBC-CAC-C3C	-2.84	104.72	112.42
23	A	410	CLA	C3C-C4C-NC	2.84	114.07	110.43
37	c	518	DGD	C2G-O2G-C1B	-2.84	111.00	117.80
23	C	512	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
23	b	609	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	c	507	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
23	d	402	CLA	CMA-C3A-C2A	-2.83	103.02	113.98
23	C	503	CLA	C3C-C4C-NC	2.83	114.06	110.43
25	k	302	BCR	C31-C1-C6	-2.83	105.80	110.24
23	b	615	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
23	D	2303	CLA	CBC-CAC-C3C	-2.83	104.74	112.42
23	A	406	CLA	C3C-C4C-NC	2.83	114.06	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CMB-C2B-C1B	2.83	129.73	125.42
23	b	620	CLA	C1-C2-C3	-2.83	121.56	126.20
25	c	517	BCR	C21-C20-C19	-2.83	115.00	123.20
23	B	602	CLA	CHD-C1D-ND	-2.83	120.82	124.80
36	C	521	HTG	C1'-S1-C1	2.83	106.56	100.45
23	C	506	CLA	C1-C2-C3	-2.83	121.56	126.20
23	C	512	CLA	CBC-CAC-C3C	-2.83	104.76	112.42
23	b	606	CLA	C2C-C1C-NC	2.82	112.95	109.98
23	C	513	CLA	CHA-C1A-NA	-2.82	120.00	126.39
23	a	2609	CLA	C3B-C4B-NB	2.82	113.05	110.53
23	b	609	CLA	C2B-C1B-NB	2.82	113.25	110.33
28	A	414	LMT	C1B-O5B-C5B	2.82	119.23	113.72
38	d	403	LHG	O8-C23-C24	2.82	120.44	111.83
26	b	601	SQD	C3-C4-C5	2.82	115.34	110.23
36	i	102	HTG	O5-C5-C4	2.82	114.78	109.70
23	b	618	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
23	b	607	CLA	C3C-C4C-NC	2.81	114.04	110.43
23	b	615	CLA	CMA-C3A-C4A	-2.81	104.21	111.77
23	c	512	CLA	C2B-C1B-NB	2.81	113.24	110.33
23	b	617	CLA	C3B-C4B-NB	2.81	113.04	110.53
23	c	506	CLA	CHA-C1A-NA	-2.81	120.02	126.39
23	C	511	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	B	608	CLA	CMB-C2B-C1B	2.81	129.70	125.42
23	B	610	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	C	508	CLA	CHA-C1A-NA	-2.81	120.03	126.39
23	C	510	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
26	a	2615	SQD	O48-C23-C24	2.81	120.40	111.83
23	b	619	CLA	O2A-CGA-CBA	2.81	120.40	111.83
23	A	406	CLA	CMA-C3A-C2A	-2.81	103.13	113.98
37	C	518	DGD	O1G-C1A-O1A	-2.81	116.61	123.63
23	C	508	CLA	CBC-CAC-C3C	-2.81	104.81	112.42
36	B	624[B]	HTG	C6-C5-C4	-2.81	106.13	113.02
25	B	633	BCR	C1-C6-C7	2.81	123.26	115.65
23	c	512	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
25	T	102	BCR	C1-C6-C7	2.80	123.25	115.65
23	b	610	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
23	C	505	CLA	CMB-C2B-C1B	2.80	129.69	125.42
26	l	101	SQD	O7-S-C6	2.80	110.94	106.76
23	D	2304	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	c	507	CLA	CMB-C2B-C1B	2.80	129.68	125.42
26	b	601	SQD	O48-C23-C24	2.80	120.37	111.83
23	b	614	CLA	C1-O2A-CGA	2.80	123.43	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	102	BCR	C15-C14-C13	2.80	131.20	127.28
23	a	2609	CLA	C7-C6-C5	-2.80	105.80	113.26
25	B	633	BCR	C35-C13-C12	2.80	122.36	118.09
23	C	511	CLA	C3C-C4C-NC	2.80	114.01	110.43
23	c	508	CLA	O2A-CGA-CBA	2.80	120.36	111.83
23	b	617	CLA	C4-C3-C5	2.80	120.08	115.23
23	b	612	CLA	C3B-C4B-NB	2.80	113.03	110.53
40	h	101	RRX	C24-C23-C22	-2.80	122.10	126.23
23	b	613	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
23	b	607	CLA	CHD-C4C-C3C	-2.79	120.70	124.77
28	A	414	LMT	C3'-C4'-C5'	-2.79	104.74	110.93
23	b	616	CLA	C2B-C1B-NB	2.79	113.22	110.33
23	B	612	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
27	A	413	LMG	C7-O1-C1	-2.79	107.81	113.80
23	D	2303	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
25	b	624	BCR	C3-C4-C5	-2.79	109.09	114.06
23	b	615	CLA	CHA-C1A-NA	-2.78	120.09	126.39
33	A	422	PL9	C40-C39-C41	2.78	120.06	115.23
23	b	614	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
23	b	616	CLA	C3B-C4B-NB	2.78	113.01	110.53
24	a	2611	PHO	C4-C3-C5	2.78	120.05	115.23
23	B	616	CLA	CHA-C1A-NA	-2.78	120.10	126.39
23	b	614	CLA	CED-O2D-CGD	2.78	122.21	115.92
23	B	609	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	B	633	BCR	C7-C6-C5	-2.78	115.16	121.56
25	b	624	BCR	C8-C7-C6	-2.77	119.59	127.00
23	B	615	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
23	B	603	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
23	a	2610	CLA	C1-C2-C3	-2.77	121.66	126.20
33	D	2306	PL9	C17-C18-C19	-2.77	121.29	127.62
37	C	518	DGD	O2G-C1B-O1B	-2.77	117.23	123.70
23	A	410	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
23	b	613	CLA	CAC-C3C-C4C	2.77	128.39	124.79
23	C	512	CLA	C4-C3-C5	2.77	120.03	115.23
23	B	613	CLA	CAC-C3C-C4C	2.77	128.39	124.79
25	Y	302	BCR	C10-C11-C12	-2.77	115.19	123.20
23	d	408	CLA	CHD-C1D-ND	-2.77	120.91	124.80
23	B	610	CLA	CBC-CAC-C3C	-2.77	104.92	112.42
23	c	513	CLA	C1-O2A-CGA	2.77	123.34	116.65
23	c	515	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
23	C	513	CLA	CBC-CAC-C3C	-2.76	104.93	112.42
25	C	516	BCR	C15-C14-C13	-2.76	123.40	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	O2A-CGA-CBA	2.76	120.26	111.83
33	A	422	PL9	C27-C26-C24	-2.76	104.03	113.19
38	d	403	LHG	O7-C7-C8	2.76	117.46	111.48
23	c	508	CLA	C3B-C4B-NB	2.76	112.99	110.53
23	D	2303	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	a	2613	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	D	2304	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
38	L	101	LHG	O7-C7-C8	2.76	117.45	111.48
23	B	617	CLA	C3C-C4C-NC	2.76	113.96	110.43
33	D	2306	PL9	C10-C9-C11	2.76	120.01	115.23
23	B	603	CLA	C3B-C4B-NB	2.76	112.99	110.53
38	d	413	LHG	O7-C7-C8	2.76	117.44	111.48
36	B	625	HTG	C1-O5-C5	2.75	117.50	112.56
23	c	504	CLA	C3C-C4C-NC	2.75	113.95	110.43
23	A	410	CLA	CHD-C1D-ND	-2.75	120.93	124.80
23	b	616	CLA	CAC-C3C-C4C	2.75	128.37	124.79
23	c	506	CLA	C4A-NA-C1A	2.75	107.93	106.68
23	c	510	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
23	C	513	CLA	C4A-NA-C1A	2.75	107.93	106.68
23	b	608	CLA	C6-C7-C8	-2.75	106.83	115.97
37	D	2307	DGD	O6D-C5D-C4D	2.75	114.65	109.70
23	B	603	CLA	O2A-CGA-CBA	2.74	120.20	111.83
24	a	2612	PHO	C4A-C3A-C2A	-2.74	100.23	102.84
23	b	606	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
23	B	605	CLA	C3C-C4C-NC	2.74	113.94	110.43
23	B	614	CLA	CED-O2D-CGD	2.74	122.13	115.92
25	k	302	BCR	C16-C17-C18	-2.74	123.44	127.28
23	C	504	CLA	C1-O2A-CGA	2.74	123.28	116.65
23	B	604	CLA	CMC-C2C-C1C	2.74	129.31	125.03
23	C	509	CLA	O2A-CGA-CBA	2.74	120.18	111.83
37	H	103	DGD	C3G-O3G-C1D	-2.74	107.93	113.80
23	b	611	CLA	O2A-CGA-CBA	2.73	120.17	111.83
23	d	409	CLA	C4B-C3B-C2B	-2.73	103.90	107.30
23	c	505	CLA	C3C-C4C-NC	2.73	113.93	110.43
23	a	2610	CLA	CBC-CAC-C3C	-2.73	105.02	112.42
23	c	514	CLA	CMB-C2B-C1B	2.73	129.58	125.42
23	A	406	CLA	CMC-C2C-C1C	2.73	129.30	125.03
23	C	512	CLA	CAC-C3C-C4C	2.73	128.34	124.79
38	D	2311	LHG	O7-C7-C8	2.73	117.39	111.48
23	c	505	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
23	B	612	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
38	D	2311	LHG	O8-C23-O10	-2.73	116.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C3C-C4C-NC	2.73	113.92	110.43
23	C	505	CLA	C1-O2A-CGA	2.73	123.25	116.65
23	d	409	CLA	C1D-CHD-C4C	-2.73	120.22	126.02
23	c	506	CLA	C4-C3-C5	2.73	119.96	115.23
37	h	102	DGD	C2G-O2G-C1B	-2.73	111.27	117.80
23	a	2609	CLA	CAC-C3C-C4C	2.73	128.34	124.79
25	Y	302	BCR	C37-C22-C23	2.72	122.25	118.09
24	A	408	PHO	CMA-C3A-C4A	-2.72	108.75	114.61
23	c	505	CLA	CMC-C2C-C1C	2.72	129.28	125.03
23	B	603	CLA	C3C-C4C-NC	2.72	113.91	110.43
39	e	103	HEM	CBA-CAA-C2A	-2.71	105.03	112.53
23	A	407	CLA	CHD-C4C-NC	2.71	128.44	124.23
36	C	522	HTG	O5-C1-C2	2.71	114.06	110.32
23	c	514	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	c	516	CLA	C3C-C4C-NC	2.71	113.90	110.43
23	B	609	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
23	a	2610	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
23	B	607	CLA	C4-C3-C5	2.71	119.93	115.23
23	C	514	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	C	502	CLA	C2C-C1C-NC	2.71	112.83	109.98
23	c	509	CLA	C3B-C4B-NB	2.71	112.95	110.53
23	b	608	CLA	C4B-C3B-C2B	-2.71	103.94	107.30
23	d	402	CLA	O2A-CGA-CBA	2.71	120.08	111.83
23	b	616	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
23	B	612	CLA	CHD-C1D-ND	-2.70	121.00	124.80
23	B	614	CLA	CHD-C1D-ND	-2.70	121.00	124.80
23	B	611	CLA	C4-C3-C5	2.70	119.92	115.23
23	C	504	CLA	C2B-C1B-NB	2.70	113.13	110.33
23	B	614	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
23	B	612	CLA	C3C-C4C-NC	2.70	113.89	110.43
23	b	620	CLA	CMB-C2B-C1B	2.70	129.53	125.42
23	b	611	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
23	A	405	CLA	CAA-CBA-CGA	-2.70	105.54	113.21
23	B	603	CLA	CMA-C3A-C2A	-2.70	103.55	113.98
25	A	411	BCR	C15-C16-C17	-2.70	118.00	123.52
28	j	2701	LMT	C1'-O5'-C5'	2.70	118.99	113.72
23	b	607	CLA	C3B-C4B-NB	2.70	112.94	110.53
23	b	611	CLA	C4-C3-C5	2.70	119.91	115.23
23	c	513	CLA	O2A-CGA-CBA	2.69	120.05	111.83
37	c	519	DGD	C5A-C4A-C3A	-2.69	100.75	114.37
33	d	411	PL9	C27-C28-C29	-2.69	121.46	127.62
23	C	502	CLA	CHD-C4C-C3C	-2.69	120.85	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	z	101	BCR	C38-C26-C25	-2.69	121.55	124.48
23	B	609	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
23	b	607	CLA	C4-C3-C5	2.69	119.90	115.23
24	A	409	PHO	O2D-CGD-O1D	-2.69	118.62	123.85
23	D	2304	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
23	C	506	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
37	c	519	DGD	C3A-C2A-C1A	-2.69	103.85	113.69
23	B	617	CLA	C1-C2-C3	-2.69	121.80	126.20
23	D	2304	CLA	C1D-CHD-C4C	-2.69	120.31	126.02
23	a	2609	CLA	CMA-C3A-C2A	-2.69	103.60	113.98
23	b	620	CLA	C6-C5-C3	-2.68	106.93	113.47
23	c	509	CLA	C3C-C4C-NC	2.68	113.87	110.43
23	b	618	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
23	B	612	CLA	C4A-NA-C1A	2.68	107.90	106.68
23	C	503	CLA	CHA-C1A-NA	-2.68	120.32	126.39
25	k	302	BCR	C11-C10-C9	-2.68	123.52	127.28
23	c	508	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
23	C	514	CLA	C2C-C1C-NC	2.68	112.80	109.98
37	C	517	DGD	O1G-C1A-O1A	-2.68	116.93	123.63
25	y	101	BCR	C24-C23-C22	-2.68	122.27	126.23
23	c	515	CLA	CHA-C1A-NA	-2.68	120.33	126.39
23	C	505	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
23	c	504	CLA	CMB-C2B-C1B	2.68	129.49	125.42
23	C	512	CLA	CHA-C1A-NA	-2.68	120.33	126.39
25	T	102	BCR	C3-C4-C5	-2.67	109.29	114.06
23	c	512	CLA	CMB-C2B-C1B	2.67	129.49	125.42
38	d	412	LHG	O7-C7-C8	2.67	117.26	111.48
31	A	418	JOX	O-C2-C1	-2.67	119.95	122.70
23	B	613	CLA	O2A-CGA-CBA	2.67	119.98	111.83
23	B	609	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
23	c	515	CLA	C4-C3-C5	2.67	119.86	115.23
23	B	611	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
23	B	602	CLA	C2C-C1C-NC	2.67	112.78	109.98
23	b	606	CLA	C4-C3-C5	2.66	119.85	115.23
23	B	615	CLA	CHD-C4C-NC	2.66	128.36	124.23
23	B	605	CLA	O2A-CGA-CBA	2.66	119.95	111.83
23	b	620	CLA	C2C-C1C-NC	2.66	112.78	109.98
23	C	510	CLA	C4A-NA-C1A	2.66	107.89	106.68
23	C	511	CLA	CMC-C2C-C1C	2.66	129.19	125.03
25	y	101	BCR	C34-C9-C8	2.66	122.15	118.09
38	D	2309	LHG	O7-C7-O9	-2.66	117.49	123.70
23	b	616	CLA	CMA-C3A-C4A	-2.66	104.63	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	515	CLA	C3C-C4C-NC	2.66	113.84	110.43
23	C	512	CLA	O2A-CGA-CBA	2.66	119.94	111.83
24	A	409	PHO	CMB-C2B-C3B	2.66	129.99	124.68
26	A	412	SQD	O48-C23-O10	-2.66	116.98	123.63
23	b	607	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
23	A	407	CLA	C4A-NA-C1A	-2.65	105.47	106.68
23	c	507	CLA	C3C-C4C-NC	2.65	113.83	110.43
23	B	606	CLA	C2C-C1C-NC	2.65	112.77	109.98
31	A	419	JOX	C-C5-C4	2.65	122.89	117.06
24	A	408	PHO	CMB-C2B-C3B	2.65	129.98	124.68
23	D	2304	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
23	b	611	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
23	B	610	CLA	CED-O2D-CGD	2.65	121.92	115.92
31	A	419	JOX	C4-C3-C2	-2.65	121.16	123.21
23	B	603	CLA	CAC-C3C-C4C	2.65	128.23	124.79
23	a	2613	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
23	b	612	CLA	C4C-C3C-C2C	-2.65	103.04	106.89
28	d	401	LMT	C1B-O1B-C4'	-2.65	111.70	117.98
23	C	511	CLA	C2B-C1B-NB	2.65	113.07	110.33
23	A	410	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
23	C	507	CLA	CAA-C2A-C3A	-2.65	105.85	113.00
23	B	606	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
23	c	515	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
37	C	517	DGD	O2G-C1B-O1B	-2.64	117.53	123.70
23	B	609	CLA	CMA-C3A-C2A	-2.64	103.77	113.98
23	b	618	CLA	C3C-C4C-NC	2.64	113.81	110.43
23	C	514	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
23	c	507	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
38	l	103	LHG	O8-C23-O10	-2.64	117.03	123.63
23	B	603	CLA	C4-C3-C5	2.64	119.81	115.23
23	A	405	CLA	CAC-C3C-C4C	2.64	128.22	124.79
23	c	513	CLA	C4C-C3C-C2C	-2.64	103.06	106.89
25	y	101	BCR	C21-C20-C19	-2.64	115.56	123.20
23	c	510	CLA	CHC-C4B-NB	2.64	128.00	124.05
23	b	613	CLA	CMA-C3A-C2A	-2.63	103.80	113.98
25	Y	302	BCR	C16-C17-C18	-2.63	123.58	127.28
27	c	522	LMG	O8-C28-C29	2.63	119.86	111.83
23	B	616	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
24	a	2611	PHO	C1-C2-C3	-2.63	121.89	126.20
25	C	516	BCR	C21-C20-C19	-2.63	115.58	123.20
23	B	610	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
23	B	602	CLA	C4C-C3C-C2C	-2.63	103.06	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	CAC-C3C-C4C	2.63	128.21	124.79
25	B	633	BCR	C3-C4-C5	-2.63	109.37	114.06
36	B	624[A]	HTG	C1-C2-C3	2.63	115.69	110.55
39	F	101	HEM	C2A-C1A-NA	-2.63	107.24	110.15
23	b	619	CLA	O2A-CGA-O1A	-2.62	117.06	123.63
23	c	509	CLA	CHA-C1A-NA	-2.62	120.45	126.39
23	B	611	CLA	CAA-CBA-CGA	-2.62	105.76	113.21
23	B	608	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
23	D	2303	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
23	A	407	CLA	C3B-C4B-NB	2.62	112.87	110.53
42	v	201	HEC	CMD-C2D-C1D	2.62	129.40	125.42
23	A	406	CLA	O2A-CGA-CBA	2.62	119.81	111.83
23	C	514	CLA	CHD-C1D-ND	-2.61	121.12	124.80
26	a	2615	SQD	O47-C7-O49	-2.61	117.59	123.70
33	A	422	PL9	C22-C23-C24	-2.61	121.64	127.62
23	D	2304	CLA	C2C-C1C-NC	2.61	112.73	109.98
23	c	511	CLA	C2C-C1C-NC	2.61	112.73	109.98
23	C	508	CLA	CHC-C4B-NB	2.61	127.97	124.05
23	b	609	CLA	O2A-CGA-CBA	2.61	119.80	111.83
23	B	617	CLA	CHA-C1A-NA	-2.61	120.48	126.39
23	c	505	CLA	CHD-C1D-ND	-2.61	121.13	124.80
25	T	102	BCR	C21-C20-C19	-2.61	115.64	123.20
23	B	609	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
23	B	603	CLA	CHA-C1A-NA	-2.61	120.49	126.39
26	l	101	SQD	C44-O6-C1	-2.61	108.21	113.80
23	b	616	CLA	C4A-NA-C1A	2.61	107.87	106.68
26	l	101	SQD	O48-C23-C24	2.61	119.78	111.83
23	b	621	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
23	c	511	CLA	CHA-C1A-NA	-2.61	120.49	126.39
23	C	502	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
23	b	620	CLA	CHA-C1A-NA	-2.60	120.50	126.39
23	d	409	CLA	CHD-C1D-ND	-2.60	121.14	124.80
24	a	2611	PHO	CMA-C3A-C4A	-2.60	109.00	114.61
23	B	617	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
25	C	515	BCR	C20-C21-C22	-2.60	123.63	127.28
37	C	519	DGD	O6E-C1E-O5D	-2.60	103.90	110.04
38	E	101	LHG	C5-O7-C7	-2.60	111.57	117.80
23	c	507	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
23	B	615	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
23	C	509	CLA	C3B-C4B-NB	2.60	112.85	110.53
37	H	103	DGD	O1G-C1A-O1A	-2.60	117.13	123.63
38	D	2310	LHG	O8-C23-C24	2.60	119.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
33	A	422	PL9	C37-C38-C39	-2.60	121.68	127.62
23	b	620	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
25	k	302	BCR	C33-C5-C6	-2.59	121.65	124.48
25	z	101	BCR	C33-C5-C6	-2.59	121.65	124.48
23	C	512	CLA	C3C-C4C-NC	2.59	113.75	110.43
23	b	614	CLA	C1D-CHD-C4C	-2.59	120.51	126.02
23	b	612	CLA	C1-C2-C3	-2.59	121.95	126.20
23	b	609	CLA	C3B-C4B-NB	2.59	112.84	110.53
23	c	504	CLA	CMC-C2C-C1C	2.59	129.08	125.03
23	B	616	CLA	CED-O2D-CGD	2.59	121.79	115.92
23	c	513	CLA	C3C-C4C-NC	2.59	113.75	110.43
27	C	527	LMG	C3-C4-C5	2.59	114.92	110.23
23	d	408	CLA	CMA-C3A-C2A	-2.58	103.99	113.98
23	B	612	CLA	CBC-CAC-C3C	-2.58	105.41	112.42
24	a	2611	PHO	O1D-CGD-CBD	-2.58	120.80	124.72
28	m	2804	LMT	O5'-C5'-C4'	2.58	115.06	109.72
23	c	515	CLA	C3B-C4B-NB	2.58	112.83	110.53
23	b	610	CLA	CHA-C1A-NA	-2.58	120.54	126.39
23	b	614	CLA	CHA-C1A-NA	-2.58	120.55	126.39
23	b	616	CLA	C7-C6-C5	-2.58	106.39	113.26
23	B	614	CLA	CMC-C2C-C1C	2.58	129.07	125.03
23	B	604	CLA	C1-O2A-CGA	2.58	122.89	116.65
23	B	614	CLA	CMA-C3A-C4A	-2.58	104.85	111.77
23	A	406	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
23	B	603	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
23	C	502	CLA	C2B-C1B-NB	2.57	113.00	110.33
33	x	1301	PL9	C15-C14-C16	2.57	119.70	115.23
23	c	506	CLA	CHD-C1D-ND	-2.57	121.18	124.80
23	C	506	CLA	CMA-C3A-C4A	-2.57	104.86	111.77
23	B	603	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	a	2610	CLA	C3B-C4B-NB	2.57	112.82	110.53
23	c	516	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
26	B	621	SQD	O5-C1-C2	2.57	115.64	110.37
23	C	503	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
23	c	514	CLA	O2A-CGA-CBA	2.57	119.66	111.83
23	C	504	CLA	C2C-C1C-NC	2.56	112.68	109.98
23	A	405	CLA	CMC-C2C-C1C	2.56	129.04	125.03
23	A	405	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
23	b	612	CLA	CAA-C2A-C3A	-2.56	106.07	113.00
23	a	2610	CLA	CAA-C2A-C3A	-2.56	106.07	113.00
25	B	619	BCR	C31-C1-C6	-2.56	106.22	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	v	201	HEC	C2A-C1A-NA	-2.56	107.85	110.32
40	h	101	RRX	C15-C14-C13	-2.56	123.69	127.28
23	d	409	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
23	b	608	CLA	C3B-C4B-NB	2.56	112.81	110.53
23	C	512	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
23	b	610	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
23	a	2610	CLA	C1D-CHD-C4C	-2.55	120.59	126.02
38	D	2310	LHG	O7-C7-C8	2.55	117.01	111.48
23	b	613	CLA	C3C-C4C-NC	2.55	113.70	110.43
23	B	617	CLA	CAC-C3C-C4C	2.55	128.11	124.79
23	b	613	CLA	CHD-C1D-ND	-2.55	121.21	124.80
23	D	2303	CLA	CMB-C2B-C1B	2.55	129.30	125.42
23	b	615	CLA	CAC-C3C-C4C	2.55	128.10	124.79
23	B	608	CLA	C3C-C4C-NC	2.55	113.69	110.43
28	z	102	LMT	O5B-C5B-C4B	2.55	114.29	109.70
23	A	405	CLA	CMA-C3A-C2A	-2.54	104.14	113.98
23	C	506	CLA	CHD-C4C-C3C	-2.54	121.07	124.77
23	d	402	CLA	CHD-C1D-ND	-2.54	121.22	124.80
23	B	608	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
33	d	411	PL9	C2-C1-C6	2.54	122.02	119.00
23	C	508	CLA	O2A-CGA-CBA	2.54	119.58	111.83
23	C	504	CLA	O2A-CGA-CBA	2.54	119.58	111.83
23	b	607	CLA	O2A-CGA-CBA	2.54	119.58	111.83
33	x	1301	PL9	C35-C34-C36	2.54	119.64	115.23
23	c	506	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
23	C	507	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
23	b	606	CLA	CHD-C4C-C3C	-2.54	121.08	124.77
23	A	406	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
23	c	514	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
23	C	507	CLA	CMC-C2C-C1C	2.53	128.99	125.03
23	b	611	CLA	CHA-C1A-NA	-2.53	120.66	126.39
23	b	620	CLA	C3C-C4C-NC	2.53	113.67	110.43
25	b	624	BCR	C21-C20-C19	-2.53	115.88	123.20
23	b	606	CLA	O2A-CGA-CBA	2.53	119.54	111.83
23	C	505	CLA	CMC-C2C-C1C	2.53	128.98	125.03
37	c	520	DGD	O1G-C1A-O1A	-2.53	117.31	123.63
37	C	519	DGD	O2G-C1B-O1B	-2.53	117.80	123.70
23	c	510	CLA	CHA-C1A-NA	-2.53	120.67	126.39
23	c	512	CLA	O2A-CGA-CBA	2.53	119.53	111.83
23	B	613	CLA	CHD-C1D-ND	-2.52	121.25	124.80
23	b	621	CLA	OBD-CAD-C3D	-2.52	122.52	128.42
25	B	633	BCR	C21-C20-C19	-2.52	115.89	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	CHD-C1D-ND	-2.52	121.25	124.80
26	b	601	SQD	O48-C23-O10	-2.52	117.32	123.63
25	b	623	BCR	C8-C7-C6	-2.52	120.26	127.00
37	c	519	DGD	O2G-C1B-O1B	-2.52	117.81	123.70
23	d	408	CLA	CBC-CAC-C3C	-2.52	105.60	112.42
25	B	620	BCR	C2-C3-C4	-2.52	105.75	111.28
23	D	2304	CLA	C3C-C4C-NC	2.52	113.65	110.43
23	B	615	CLA	C4C-C3C-C2C	-2.51	103.23	106.89
23	B	608	CLA	C4C-C3C-C2C	-2.51	103.23	106.89
23	C	503	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
23	B	611	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	K	101	BCR	C38-C26-C25	-2.51	121.74	124.48
25	b	624	BCR	C11-C10-C9	-2.51	123.76	127.28
23	d	409	CLA	C3C-C4C-NC	2.51	113.65	110.43
37	c	519	DGD	O1G-C1A-O1A	-2.51	117.36	123.63
23	B	616	CLA	C1-C2-C3	-2.51	122.09	126.20
25	b	624	BCR	C2-C1-C6	2.51	114.08	110.44
23	c	505	CLA	CED-O2D-CGD	2.51	121.60	115.92
25	K	101	BCR	C10-C11-C12	-2.50	115.94	123.20
23	B	615	CLA	C3C-C4C-NC	2.50	113.64	110.43
23	B	610	CLA	C3B-C4B-NB	2.50	112.76	110.53
23	c	510	CLA	CMC-C2C-C1C	2.50	128.94	125.03
23	d	402	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
37	D	2307	DGD	O1G-C1A-O1A	-2.50	117.38	123.63
23	b	619	CLA	CHD-C1D-ND	-2.50	121.29	124.80
23	B	611	CLA	O2A-CGA-CBA	2.50	119.45	111.83
31	a	2617	JOX	O-C2-C1	-2.49	120.13	122.70
23	C	510	CLA	CAC-C3C-C4C	2.49	128.03	124.79
24	A	408	PHO	O1D-CGD-CBD	-2.49	120.94	124.72
23	B	606	CLA	C4-C3-C5	2.49	119.56	115.23
23	B	614	CLA	C1-C2-C3	-2.49	122.11	126.20
23	a	2610	CLA	C11-C10-C8	-2.49	107.68	115.97
23	B	614	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
23	B	616	CLA	CBA-CAA-C2A	-2.49	106.38	113.79
23	c	506	CLA	O2A-CGA-CBA	2.49	119.43	111.83
26	A	412	SQD	O9-S-C6	2.49	110.47	106.76
23	d	409	CLA	CMC-C2C-C1C	2.49	128.93	125.03
24	A	408	PHO	C4-C3-C5	2.49	119.55	115.23
36	b	625	HTG	C1-C2-C3	2.49	115.42	110.55
23	c	516	CLA	CMC-C2C-C1C	2.49	128.92	125.03
23	C	507	CLA	CHA-C1A-NA	-2.49	120.76	126.39
23	C	507	CLA	CHD-C1D-ND	-2.49	121.30	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
23	b	612	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
23	A	405	CLA	C4-C3-C5	2.49	119.54	115.23
23	A	407	CLA	O2A-CGA-CBA	2.49	119.41	111.83
36	I	101	HTG	O5-C5-C4	2.49	114.18	109.70
23	b	608	CLA	CMC-C2C-C1C	2.48	128.91	125.03
23	C	502	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
36	c	524	HTG	C1-O5-C5	2.48	117.01	112.56
23	C	511	CLA	CMB-C2B-C1B	2.48	129.20	125.42
26	A	412	SQD	C44-O6-C1	-2.48	108.48	113.80
23	c	516	CLA	CHD-C1D-ND	-2.48	121.31	124.80
27	C	520	LMG	O8-C28-O10	-2.48	117.43	123.63
23	C	506	CLA	C4-C3-C5	2.48	119.53	115.23
38	d	403	LHG	O8-C23-O10	-2.48	117.43	123.63
23	b	613	CLA	CMC-C2C-C1C	2.48	128.91	125.03
23	C	503	CLA	CMB-C2B-C1B	2.48	129.19	125.42
23	C	511	CLA	C4A-NA-C1A	2.47	107.81	106.68
23	B	603	CLA	CMA-C3A-C4A	-2.47	105.12	111.77
23	c	514	CLA	CMC-C2C-C1C	2.47	128.90	125.03
26	A	412	SQD	C1-O5-C5	-2.47	108.89	113.72
23	b	609	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
36	b	604	HTG	C3-C4-C5	2.47	114.71	110.23
23	a	2609	CLA	O2D-CGD-CBD	2.47	115.55	111.23
23	D	2303	CLA	C3B-C4B-NB	2.47	112.73	110.53
23	a	2613	CLA	C3C-C4C-NC	2.47	113.59	110.43
23	c	504	CLA	C3B-C4B-NB	2.47	112.73	110.53
25	Y	302	BCR	C1-C6-C7	2.47	122.34	115.65
36	b	604	HTG	C1-O5-C5	2.47	116.99	112.56
23	d	409	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
25	z	101	BCR	C20-C21-C22	-2.47	123.82	127.28
38	E	101	LHG	O8-C23-C24	2.47	119.35	111.83
23	c	516	CLA	CBC-CAC-C3C	-2.47	105.74	112.42
23	c	508	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
23	b	615	CLA	CHD-C1D-ND	-2.46	121.33	124.80
33	D	2306	PL9	C22-C23-C24	-2.46	121.98	127.62
26	a	2603	SQD	O48-C23-C24	2.46	119.35	111.83
33	D	2306	PL9	C51-C49-C50	2.46	120.25	114.59
23	C	506	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
23	b	615	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
25	b	624	BCR	C10-C11-C12	-2.46	116.07	123.20
26	D	2302	SQD	O47-C7-O49	-2.46	117.96	123.70
33	x	1301	PL9	C46-C44-C45	2.46	120.25	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	CHA-C1A-NA	-2.46	120.83	126.39
23	b	619	CLA	C3B-C4B-NB	2.46	112.72	110.53
42	v	201	HEC	CBD-CAD-C3D	-2.46	105.74	112.53
25	z	101	BCR	C2-C1-C6	2.46	114.01	110.44
23	b	607	CLA	CMA-C3A-C4A	-2.46	105.17	111.77
23	b	618	CLA	CHD-C1D-ND	-2.45	121.35	124.80
23	b	621	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
36	b	603	HTG	C6-C5-C4	-2.45	107.00	113.02
25	A	411	BCR	C3-C4-C5	-2.45	109.68	114.06
38	D	2309	LHG	C5-O7-C7	-2.45	111.93	117.80
23	b	617	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
25	k	302	BCR	C8-C7-C6	-2.45	120.46	127.00
23	b	614	CLA	C3C-C4C-NC	2.45	113.57	110.43
23	b	611	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
23	c	512	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
23	d	408	CLA	C1D-CHD-C4C	-2.45	120.82	126.02
23	C	505	CLA	C3B-C4B-NB	2.44	112.71	110.53
23	d	402	CLA	CMA-C3A-C4A	-2.44	105.20	111.77
23	b	609	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
33	d	411	PL9	C53-C6-C1	2.44	120.28	115.28
23	C	505	CLA	OBD-CAD-C3D	-2.44	122.71	128.42
23	b	607	CLA	CHA-C1A-NA	-2.44	120.86	126.39
23	a	2613	CLA	CMB-C2B-C1B	2.44	129.14	125.42
33	D	2306	PL9	C53-C6-C1	2.44	120.28	115.28
23	a	2610	CLA	CMB-C2B-C1B	2.44	129.13	125.42
23	b	610	CLA	CHD-C1D-ND	-2.44	121.37	124.80
23	A	406	CLA	C1-O2A-CGA	2.44	122.55	116.65
25	K	101	BCR	C15-C14-C13	-2.44	123.86	127.28
23	B	609	CLA	CAA-C2A-C3A	-2.44	106.42	113.00
25	a	2614	BCR	C11-C10-C9	-2.43	123.86	127.28
23	C	506	CLA	C3B-C4B-NB	2.43	112.70	110.53
26	A	412	SQD	O47-C7-O49	-2.43	118.02	123.70
23	b	616	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
23	c	510	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
23	b	620	CLA	CBC-CAC-C3C	-2.43	105.84	112.42
31	a	2617	JOX	O1-C5-C4	-2.43	117.97	121.43
23	b	614	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
23	C	508	CLA	CHB-C1B-C2B	-2.43	120.39	127.43
23	b	620	CLA	C6-C7-C8	-2.43	107.90	115.97
23	b	610	CLA	C1-C2-C3	-2.42	122.22	126.20
26	b	601	SQD	C45-O47-C7	-2.42	111.99	117.80
25	Y	302	BCR	C35-C13-C14	-2.42	118.89	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	620	CLA	C4-C3-C5	2.42	119.43	115.23
23	C	511	CLA	CAA-CBA-CGA	-2.42	106.33	113.21
23	d	408	CLA	CHA-C1A-NA	-2.42	120.91	126.39
23	d	409	CLA	C6-C7-C8	-2.42	107.91	115.97
23	b	620	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
23	d	409	CLA	CHA-C1A-NA	-2.42	120.91	126.39
23	B	616	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
23	c	513	CLA	C1-C2-C3	-2.42	122.23	126.20
26	A	412	SQD	O8-S-C6	2.42	110.64	105.97
27	C	527	LMG	O8-C28-O10	-2.42	117.58	123.63
23	A	407	CLA	C3C-C4C-NC	2.42	113.53	110.43
23	C	511	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
23	b	610	CLA	C4B-C3B-C2B	-2.42	104.30	107.30
23	C	507	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
23	B	609	CLA	CMB-C2B-C1B	2.41	129.10	125.42
36	C	525	HTG	O5-C1-C2	2.41	113.64	110.32
23	B	609	CLA	C1-C2-C3	-2.41	122.24	126.20
25	b	622	BCR	C21-C20-C19	-2.41	116.21	123.20
23	A	406	CLA	CED-O2D-CGD	2.41	121.39	115.92
27	A	413	LMG	O7-C10-O9	-2.41	118.06	123.70
23	B	602	CLA	C4-C3-C5	2.41	119.41	115.23
33	D	2306	PL9	C40-C39-C38	-2.41	117.44	123.63
23	b	606	CLA	CHA-C1A-NA	-2.41	120.94	126.39
23	C	513	CLA	C4-C3-C5	2.41	119.41	115.23
25	k	302	BCR	C3-C4-C5	-2.41	109.76	114.06
23	B	603	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
23	d	402	CLA	C4C-C3C-C2C	-2.40	103.39	106.89
23	b	616	CLA	CHD-C4C-NC	2.40	127.96	124.23
23	B	608	CLA	CMC-C2C-C1C	2.40	128.79	125.03
23	B	605	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
23	A	406	CLA	CMA-C3A-C4A	-2.40	105.32	111.77
23	c	514	CLA	C4A-NA-C1A	2.40	107.77	106.68
23	c	509	CLA	CGD-CBD-CAD	-2.40	103.08	110.85
23	C	507	CLA	CED-O2D-CGD	2.40	121.36	115.92
25	k	302	BCR	C7-C8-C9	-2.40	122.69	126.23
23	B	616	CLA	CHC-C1C-C2C	-2.40	120.13	126.95
33	d	411	PL9	C22-C23-C24	-2.40	122.14	127.62
23	C	506	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
27	D	2312	LMG	O8-C28-O10	-2.40	117.63	123.63
33	d	411	PL9	C25-C24-C26	2.40	119.39	115.23
23	B	612	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
25	z	101	BCR	C11-C10-C9	-2.40	123.92	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
33	A	422	PL9	C20-C19-C21	2.39	119.39	115.23
33	d	411	PL9	C10-C9-C11	2.39	119.39	115.23
29	b	644	GOL	C3-C2-C1	-2.39	103.01	111.80
23	B	615	CLA	CAC-C3C-C4C	2.39	127.90	124.79
36	B	624[A]	HTG	O5-C5-C6	2.39	112.37	106.44
23	c	514	CLA	C4C-C3C-C2C	-2.39	103.41	106.89
28	M	101	LMT	C1-O1'-C1'	-2.39	109.60	113.68
25	K	101	BCR	C33-C5-C6	-2.39	121.88	124.48
25	a	2614	BCR	C38-C26-C25	-2.39	121.88	124.48
23	b	612	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
23	b	606	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
23	A	410	CLA	C7-C6-C5	-2.39	106.90	113.26
23	b	609	CLA	CHC-C4B-NB	2.39	127.63	124.05
28	T	103	LMT	O1'-C1'-C2'	2.39	111.90	108.27
23	D	2304	CLA	O2A-CGA-CBA	2.38	119.10	111.83
23	C	508	CLA	C4-C3-C5	2.38	119.36	115.23
28	d	404	LMT	C1'-O5'-C5'	2.38	118.37	113.72
26	B	621	SQD	O47-C7-O49	-2.38	118.14	123.70
25	b	624	BCR	C16-C17-C18	-2.38	123.94	127.28
23	b	618	CLA	CMA-C3A-C4A	-2.38	105.38	111.77
23	b	613	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
33	D	2306	PL9	C15-C14-C16	2.38	119.36	115.23
23	B	605	CLA	CHA-C1A-NA	-2.38	121.01	126.39
26	a	2615	SQD	O48-C23-O10	-2.38	117.68	123.63
28	d	404	LMT	O5'-C5'-C4'	2.38	114.64	109.72
23	B	613	CLA	C1-C2-C3	-2.38	122.31	126.20
25	z	101	BCR	C8-C7-C6	-2.38	120.65	127.00
37	C	518	DGD	O1G-C1A-C2A	2.37	119.08	111.83
25	b	622	BCR	C38-C26-C25	-2.37	121.89	124.48
24	A	409	PHO	C4-C3-C2	-2.37	117.53	123.63
23	b	606	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
23	c	504	CLA	C4-C3-C5	2.37	119.35	115.23
23	B	607	CLA	CHA-C1A-NA	-2.37	121.02	126.39
26	l	101	SQD	O47-C7-O49	-2.37	118.16	123.70
23	d	408	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
23	b	621	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
25	y	101	BCR	C1-C6-C7	2.37	122.08	115.65
23	b	619	CLA	CMC-C2C-C1C	2.37	128.74	125.03
23	B	603	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
25	y	101	BCR	C10-C11-C12	-2.37	116.33	123.20
23	B	612	CLA	O2A-CGA-CBA	2.37	119.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	414	LMG	O7-C10-C11	2.37	116.60	111.48
23	B	607	CLA	O2A-CGA-CBA	2.37	119.05	111.83
23	B	607	CLA	CMC-C2C-C1C	2.37	128.73	125.03
23	b	618	CLA	CHA-C1A-NA	-2.37	121.03	126.39
23	C	510	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
24	a	2612	PHO	C4-C3-C2	-2.36	117.56	123.63
23	C	509	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
23	c	513	CLA	CHA-C1A-NA	-2.36	121.05	126.39
23	C	513	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	a	2611	PHO	CBA-CAA-C2A	-2.36	106.83	113.78
23	c	512	CLA	CHA-C1A-NA	-2.36	121.05	126.39
31	a	2619	JOX	C2-C1-CL1	2.36	117.72	115.82
23	B	606	CLA	CHD-C1D-ND	-2.36	121.49	124.80
23	C	503	CLA	CHD-C1D-ND	-2.36	121.49	124.80
23	C	514	CLA	C3C-C4C-NC	2.36	113.45	110.43
26	D	2302	SQD	O9-S-C6	2.36	110.27	106.76
28	Z	101	LMT	C1B-O5B-C5B	2.36	118.32	113.72
24	a	2611	PHO	CMB-C2B-C3B	2.35	129.39	124.68
23	b	615	CLA	CMC-C2C-C1C	2.35	128.71	125.03
23	c	515	CLA	C4A-NA-C1A	2.35	107.75	106.68
23	b	613	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
23	B	611	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
23	B	607	CLA	CHC-C4B-NB	2.35	127.58	124.05
23	C	505	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
23	b	608	CLA	CHB-C1B-C2B	-2.35	120.60	127.43
37	c	520	DGD	O3G-C1D-C2D	-2.35	104.71	108.27
23	B	609	CLA	C4-C3-C5	2.35	119.30	115.23
23	B	607	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
23	C	508	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
23	B	615	CLA	OBD-CAD-C3D	-2.35	122.93	128.42
23	A	407	CLA	CMC-C2C-C1C	2.35	128.70	125.03
26	D	2302	SQD	O48-C23-C24	2.35	118.99	111.83
23	b	621	CLA	C4-C3-C5	2.35	119.30	115.23
23	b	614	CLA	O2A-CGA-CBA	2.34	118.98	111.83
25	B	620	BCR	C3-C4-C5	-2.34	109.88	114.06
23	D	2304	CLA	C4-C3-C5	2.34	119.30	115.23
23	C	502	CLA	C1-C2-C3	-2.34	122.36	126.20
23	c	508	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
25	B	620	BCR	C7-C8-C9	-2.34	122.77	126.23
23	C	502	CLA	O2A-CGA-CBA	2.34	118.97	111.83
25	b	624	BCR	C33-C5-C6	-2.34	121.93	124.48
23	C	502	CLA	O2A-CGA-O1A	-2.34	117.78	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	C3C-C4C-NC	2.34	113.43	110.43
23	c	507	CLA	C4C-C3C-C2C	-2.34	103.49	106.89
23	C	502	CLA	C3C-C4C-NC	2.34	113.43	110.43
39	F	101	HEM	CBA-CAA-C2A	-2.34	106.07	112.53
23	c	513	CLA	CMC-C2C-C1C	2.34	128.69	125.03
23	c	509	CLA	CAC-C3C-C4C	2.34	127.83	124.79
28	M	101	LMT	O1B-C1B-C2B	2.34	113.83	108.09
23	c	515	CLA	CHB-C4A-NA	2.34	127.77	124.40
31	a	2617	JOX	O-C2-C3	-2.33	120.29	122.70
23	c	504	CLA	C4B-C3B-C2B	-2.33	104.40	107.30
23	B	602	CLA	CHA-C1A-NA	-2.33	121.11	126.39
23	B	603	CLA	CHD-C1D-ND	-2.33	121.52	124.80
25	b	624	BCR	C32-C1-C6	-2.33	106.59	110.24
37	c	520	DGD	O3G-C3G-C2G	-2.33	105.16	110.82
23	b	619	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
23	b	621	CLA	CHD-C1D-C2D	-2.33	120.64	125.49
23	c	511	CLA	C3B-C4B-NB	2.33	112.61	110.53
23	C	506	CLA	C4B-C3B-C2B	-2.32	104.41	107.30
23	b	617	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
37	D	2307	DGD	C1D-O6D-C5D	2.32	118.26	113.72
23	B	602	CLA	C4B-C3B-C2B	-2.32	104.41	107.30
25	c	517	BCR	C16-C17-C18	-2.32	124.02	127.28
28	B	623	LMT	O1B-C4'-C5'	-2.32	103.39	109.48
33	x	1301	PL9	C40-C39-C41	2.32	119.26	115.23
25	B	619	BCR	C20-C21-C22	-2.32	124.02	127.28
23	b	619	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
23	C	511	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	C	511	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	a	2611	PHO	CBC-CAC-C3C	-2.32	109.55	112.87
23	b	616	CLA	C4C-C3C-C2C	-2.32	103.52	106.89
23	c	510	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	B	611	CLA	CMC-C2C-C1C	2.32	128.65	125.03
23	B	604	CLA	CMA-C3A-C2A	-2.32	105.03	113.98
23	C	507	CLA	CHB-C1B-C2B	-2.32	120.71	127.43
27	C	520	LMG	O7-C10-O9	-2.31	118.29	123.70
23	b	607	CLA	CHD-C1D-ND	-2.31	121.55	124.80
23	B	611	CLA	CHA-C1A-NA	-2.31	121.16	126.39
23	d	402	CLA	CHB-C4A-NA	2.31	127.73	124.40
23	C	503	CLA	C4A-NA-C1A	2.31	107.73	106.68
26	B	621	SQD	O48-C23-C24	2.31	118.88	111.83
23	c	513	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
33	D	2306	PL9	C30-C29-C31	2.31	119.24	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
25	D	2305	BCR	C15-C14-C13	-2.31	124.04	127.28
25	b	622	BCR	C15-C14-C13	-2.31	124.04	127.28
23	a	2613	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
38	d	413	LHG	O8-C23-C24	2.31	118.87	111.83
23	B	605	CLA	C4C-C3C-C2C	-2.31	103.53	106.89
23	B	616	CLA	CHD-C1D-ND	-2.30	121.56	124.80
23	B	609	CLA	CBC-CAC-C3C	-2.30	106.17	112.42
23	a	2613	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
36	b	625	HTG	O6-C6-C5	-2.30	103.49	111.33
23	B	612	CLA	C3B-C4B-NB	2.30	112.58	110.53
25	B	618	BCR	C21-C20-C19	-2.30	116.53	123.20
23	c	514	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
23	C	502	CLA	CHD-C1D-ND	-2.30	121.56	124.80
25	c	517	BCR	C31-C1-C6	-2.30	106.64	110.24
23	b	608	CLA	C5-C3-C2	-2.30	116.01	121.17
23	d	409	CLA	CBC-CAC-C3C	-2.30	106.19	112.42
23	c	506	CLA	C2B-C1B-NB	2.30	112.71	110.33
23	B	607	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
23	a	2613	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
23	c	516	CLA	C3B-C4B-NB	2.30	112.58	110.53
27	B	622	LMG	C9-C8-C7	-2.30	106.43	111.78
23	C	510	CLA	CHA-C1A-NA	-2.30	121.19	126.39
23	b	621	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
23	A	407	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
26	B	621	SQD	O7-S-C6	2.29	110.18	106.76
23	B	612	CLA	C7-C6-C5	-2.29	107.16	113.26
28	M	101	LMT	C1'-C2'-C3'	-2.29	105.19	110.01
23	A	407	CLA	CMA-C3A-C2A	-2.29	105.13	113.98
23	B	613	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
23	B	607	CLA	CHD-C1D-ND	-2.29	121.58	124.80
23	B	615	CLA	CMC-C2C-C1C	2.29	128.61	125.03
23	b	614	CLA	C4-C3-C5	2.29	119.20	115.23
23	c	515	CLA	C1-C2-C3	-2.29	122.45	126.20
33	x	1301	PL9	C42-C43-C44	-2.29	120.02	127.64
23	b	608	CLA	CMB-C2B-C1B	2.29	128.90	125.42
25	K	101	BCR	C3-C4-C5	-2.29	109.98	114.06
39	e	103	HEM	C1B-NB-C4B	2.29	107.91	105.21
27	c	522	LMG	C8-O7-C10	-2.28	112.33	117.80
23	B	617	CLA	CMA-C3A-C4A	-2.28	105.64	111.77
23	B	617	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	c	516	CLA	CAA-C2A-C3A	-2.28	106.84	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	2308	SQD	C44-O6-C1	-2.28	108.91	113.80
23	C	505	CLA	C3C-C4C-NC	2.28	113.35	110.43
25	c	517	BCR	C3-C4-C5	-2.28	109.99	114.06
33	D	2306	PL9	C12-C13-C14	-2.28	122.41	127.62
23	B	608	CLA	O2A-CGA-CBA	2.28	118.78	111.83
29	v	203	GOL	C3-C2-C1	-2.28	103.45	111.80
25	k	302	BCR	C21-C20-C19	-2.28	116.61	123.20
23	b	613	CLA	CHA-C1A-NA	-2.28	121.24	126.39
23	A	407	CLA	CHB-C1B-C2B	-2.27	120.82	127.43
23	c	506	CLA	CMC-C2C-C1C	2.27	128.59	125.03
23	C	508	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
23	c	516	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
23	c	515	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
23	C	511	CLA	C4-C3-C2	-2.27	117.80	123.63
23	B	605	CLA	CMB-C2B-C1B	2.27	128.88	125.42
23	C	513	CLA	CMA-C3A-C4A	-2.27	105.67	111.77
23	B	612	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
23	b	619	CLA	OBD-CAD-C3D	-2.27	123.11	128.42
23	b	618	CLA	C4-C3-C5	2.27	119.16	115.23
23	b	613	CLA	C11-C12-C13	-2.27	108.43	115.97
25	C	515	BCR	C8-C7-C6	-2.27	120.94	127.00
33	d	411	PL9	C40-C39-C38	-2.27	117.81	123.63
23	A	406	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
23	b	613	CLA	C11-C10-C8	-2.27	108.44	115.97
23	A	406	CLA	C4-C3-C5	2.26	119.16	115.23
23	B	610	CLA	CHA-C1A-NA	-2.26	121.27	126.39
23	C	510	CLA	CMC-C2C-C1C	2.26	128.57	125.03
23	b	614	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
23	c	513	CLA	CAC-C3C-C4C	2.26	127.73	124.79
37	h	102	DGD	C3G-O3G-C1D	-2.26	108.95	113.80
23	c	509	CLA	CHB-C1B-C2B	-2.26	120.88	127.43
25	B	620	BCR	C15-C16-C17	-2.26	118.90	123.52
31	A	418	JOX	O-C2-C3	-2.26	120.38	122.70
33	A	422	PL9	C42-C43-C44	-2.25	120.12	127.64
23	C	511	CLA	CHA-C1A-NA	-2.25	121.29	126.39
23	b	615	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
23	b	607	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
23	C	513	CLA	CMC-C2C-C1C	2.25	128.56	125.03
23	b	609	CLA	CHD-C1D-C2D	-2.25	120.80	125.49
25	Y	302	BCR	C35-C13-C12	2.25	121.52	118.09
23	b	609	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	D	2305	BCR	C10-C11-C12	-2.25	116.68	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	2613	CLA	CMC-C2C-C1C	2.25	128.55	125.03
23	C	504	CLA	CHD-C4C-NC	2.25	127.72	124.23
23	B	608	CLA	CHD-C1D-ND	-2.25	121.64	124.80
23	c	516	CLA	CHA-C1A-NA	-2.25	121.30	126.39
25	A	411	BCR	C7-C8-C9	-2.25	122.91	126.23
23	B	605	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
23	B	602	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
23	b	614	CLA	C4B-C3B-C2B	-2.25	104.51	107.30
23	C	505	CLA	C4C-C3C-C2C	-2.24	103.62	106.89
23	b	608	CLA	CHD-C1D-ND	-2.24	121.64	124.80
23	b	610	CLA	O2A-CGA-CBA	2.24	118.68	111.83
23	d	402	CLA	CMB-C2B-C1B	2.24	128.83	125.42
23	C	514	CLA	O2A-CGA-CBA	2.24	118.67	111.83
23	b	617	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
23	c	505	CLA	CHA-C1A-NA	-2.24	121.32	126.39
23	C	505	CLA	C7-C6-C5	-2.24	107.29	113.26
23	c	515	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
23	B	616	CLA	CHD-C4C-NC	2.24	127.70	124.23
24	A	408	PHO	C1-O2A-CGA	2.24	122.06	116.65
28	m	2804	LMT	C1-O1'-C1'	-2.24	109.86	113.68
23	B	614	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
23	b	617	CLA	CHB-C4A-NA	2.23	127.62	124.40
23	b	606	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
23	B	612	CLA	OBD-CAD-C3D	-2.23	123.19	128.42
23	c	513	CLA	C4-C3-C5	2.23	119.11	115.23
23	B	614	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
33	x	1301	PL9	C25-C24-C23	-2.23	117.89	123.63
23	B	608	CLA	CHA-C1A-NA	-2.23	121.34	126.39
26	B	621	SQD	O9-S-C6	2.23	110.09	106.76
23	B	604	CLA	CHD-C1D-ND	-2.23	121.66	124.80
25	A	411	BCR	C31-C1-C6	-2.23	106.75	110.24
25	d	410	BCR	C21-C20-C19	-2.23	116.75	123.20
23	c	514	CLA	CHA-C1A-NA	-2.23	121.35	126.39
23	B	617	CLA	CHC-C1C-C2C	-2.22	120.62	126.95
23	c	509	CLA	C1-C2-C3	-2.22	122.55	126.20
23	b	619	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
23	b	615	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
36	d	407	HTG	O5-C5-C4	2.22	113.71	109.70
23	c	505	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
25	k	302	BCR	C20-C21-C22	-2.22	124.16	127.28
33	A	422	PL9	C25-C24-C26	2.22	119.08	115.23
23	C	504	CLA	CHA-C1A-NA	-2.22	121.36	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	2305	BCR	C16-C17-C18	-2.22	124.16	127.28
25	b	622	BCR	C3-C4-C5	-2.22	110.10	114.06
23	b	620	CLA	C1-O2A-CGA	2.22	122.02	116.65
23	B	605	CLA	CHD-C1D-ND	-2.22	121.68	124.80
23	B	608	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
25	C	516	BCR	C11-C10-C9	-2.22	124.17	127.28
33	A	422	PL9	C15-C14-C16	2.22	119.08	115.23
23	D	2304	CLA	CMC-C2C-C1C	2.22	128.50	125.03
28	m	2804	LMT	C1B-O5B-C5B	2.22	118.05	113.72
25	Y	302	BCR	C34-C9-C8	2.22	121.47	118.09
23	a	2613	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
23	C	502	CLA	C4-C3-C5	2.22	119.07	115.23
23	a	2613	CLA	CHD-C4C-NC	2.22	127.67	124.23
23	A	405	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
26	a	2615	SQD	C44-O6-C1	-2.21	109.05	113.80
23	A	407	CLA	CAA-CBA-CGA	2.21	119.49	113.21
23	b	616	CLA	C3C-C4C-NC	2.21	113.27	110.43
23	b	606	CLA	CAC-C3C-C4C	2.21	127.67	124.79
23	D	2304	CLA	C3B-C4B-NB	2.21	112.50	110.53
33	A	422	PL9	C46-C44-C45	2.21	119.68	114.59
25	A	411	BCR	C8-C7-C6	-2.21	121.09	127.00
39	e	103	HEM	CHC-C1C-NC	2.21	126.86	124.45
23	B	610	CLA	C7-C6-C5	-2.21	107.37	113.26
23	b	614	CLA	C4D-CHA-C1A	2.21	123.88	121.24
23	b	606	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
23	A	410	CLA	CMC-C2C-C1C	2.21	128.49	125.03
40	h	101	RRX	C7-C8-C9	-2.21	122.97	126.23
36	H	101	HTG	C5-C4-C3	2.21	112.86	109.64
25	B	620	BCR	C10-C11-C12	-2.21	116.80	123.20
25	z	101	BCR	C37-C22-C23	2.21	121.46	118.09
23	A	407	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
23	B	612	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
23	C	506	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
26	D	2302	SQD	O5-C1-C2	2.20	114.90	110.37
23	A	407	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
37	H	103	DGD	O2G-C1B-O1B	-2.20	118.56	123.70
23	B	602	CLA	CAC-C3C-C4C	2.20	127.65	124.79
23	D	2303	CLA	CAC-C3C-C2C	2.20	131.60	127.56
23	B	609	CLA	CHA-C1A-NA	-2.20	121.41	126.39
31	A	418	JOX	C1-C-C5	-2.20	119.57	120.54
23	C	510	CLA	CMB-C2B-C1B	2.20	128.77	125.42
23	B	615	CLA	CMB-C2B-C1B	2.20	128.77	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	522	HTG	O5-C5-C4	2.20	113.66	109.70
24	a	2612	PHO	CMA-C3A-C4A	-2.20	109.88	114.61
23	c	509	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
23	B	606	CLA	C12-C11-C10	-2.20	103.43	113.28
23	C	503	CLA	C1-O2A-CGA	2.20	121.97	116.65
23	b	606	CLA	CHD-C1D-ND	-2.20	121.71	124.80
28	T	103	LMT	C1-O1'-C1'	-2.20	109.93	113.68
23	c	513	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
25	y	101	BCR	C32-C1-C6	-2.19	106.80	110.24
23	C	512	CLA	C1-C2-C3	-2.19	122.60	126.20
23	A	406	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
23	b	612	CLA	CAA-CBA-CGA	2.19	119.44	113.21
37	C	518	DGD	O6E-C5E-C6E	2.19	111.87	106.44
23	B	605	CLA	CAC-C3C-C4C	2.19	127.64	124.79
23	a	2609	CLA	C1-C2-C3	-2.19	122.61	126.20
36	b	603	HTG	O5-C5-C4	2.19	113.64	109.70
23	b	612	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
23	C	504	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
28	A	414	LMT	O1B-C1B-O5B	-2.19	104.94	110.69
37	c	520	DGD	O2G-C1B-C2B	2.19	116.21	111.48
23	B	602	CLA	CMC-C2C-C1C	2.18	128.44	125.03
33	D	2306	PL9	C35-C34-C36	2.18	119.02	115.23
23	d	409	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	b	620	CLA	C11-C10-C8	-2.18	108.72	115.97
23	c	504	CLA	C1-C2-C3	-2.18	122.63	126.20
23	B	611	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
23	B	608	CLA	C4A-NA-C1A	2.18	107.67	106.68
23	A	406	CLA	CAA-CBA-CGA	2.18	119.39	113.21
23	c	510	CLA	O2A-CGA-CBA	2.18	118.48	111.83
27	A	413	LMG	O8-C28-C29	2.18	118.47	111.83
23	B	609	CLA	CMC-C2C-C1C	2.18	128.44	125.03
23	c	511	CLA	C6-C7-C8	-2.18	108.73	115.97
25	B	633	BCR	C33-C5-C4	2.18	118.23	113.60
33	d	411	PL9	C35-C34-C36	2.18	119.00	115.23
26	D	2302	SQD	O7-S-C6	2.18	110.00	106.76
33	D	2306	PL9	C47-C48-C49	-2.18	120.39	127.64
38	L	101	LHG	O4-P-O5	2.18	122.56	112.44
24	A	408	PHO	C4D-CHA-CBD	2.17	109.50	108.45
23	b	612	CLA	CMB-C2B-C1B	2.17	128.73	125.42
26	b	601	SQD	C46-C45-C44	-2.17	106.72	111.78
23	C	507	CLA	C3B-C4B-NB	2.17	112.47	110.53
23	C	509	CLA	CMB-C2B-C1B	2.17	128.72	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
36	d	407	HTG	C4-C3-C2	-2.17	107.02	110.83
23	b	620	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
25	T	102	BCR	C36-C18-C19	2.17	121.40	118.09
25	y	101	BCR	C23-C24-C25	-2.17	121.21	127.00
23	b	618	CLA	CBC-CAC-C3C	-2.16	106.55	112.42
23	C	505	CLA	C1-C2-C3	-2.16	122.65	126.20
25	K	101	BCR	C20-C21-C22	-2.16	124.24	127.28
23	B	607	CLA	CBC-CAC-C3C	-2.16	106.56	112.42
23	b	612	CLA	C4A-NA-C1A	2.16	107.67	106.68
25	b	623	BCR	C40-C30-C25	-2.16	106.85	110.24
23	c	508	CLA	C4B-C3B-C2B	-2.16	104.61	107.30
40	H	102	RRX	C21-C20-C19	-2.16	116.94	123.20
23	b	611	CLA	CAC-C3C-C4C	2.16	127.60	124.79
23	b	616	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	C	503	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
23	C	510	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
25	a	2614	BCR	C8-C7-C6	-2.16	121.23	127.00
23	a	2609	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
27	c	501	LMG	C30-C29-C28	-2.16	105.79	113.69
23	c	507	CLA	O2A-CGA-CBA	2.16	118.42	111.83
25	T	102	BCR	C16-C17-C18	-2.16	124.25	127.28
28	Z	101	LMT	C1-O1'-C1'	-2.15	110.00	113.68
23	d	408	CLA	CAC-C3C-C4C	2.15	127.59	124.79
23	c	507	CLA	CHD-C4C-NC	2.15	127.57	124.23
24	a	2611	PHO	C1-O2A-CGA	2.15	121.86	116.65
23	B	613	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	B	602	CLA	C1-C2-C3	-2.15	122.67	126.20
23	A	410	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
23	b	617	CLA	OBD-CAD-C3D	-2.15	123.40	128.42
28	M	101	LMT	C1B-O1B-C4'	-2.15	112.89	117.98
23	A	406	CLA	C1-C2-C3	-2.15	122.68	126.20
38	L	101	LHG	O7-C7-O9	-2.15	118.69	123.70
23	B	604	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
23	C	507	CLA	C4-C3-C2	-2.15	118.12	123.63
23	C	508	CLA	CMC-C2C-C1C	2.14	128.38	125.03
23	c	504	CLA	CHD-C4C-NC	2.14	127.55	124.23
23	C	505	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
23	B	603	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
28	m	2804	LMT	O5B-C1B-C2B	2.14	114.77	110.37
29	A	415	GOL	C3-C2-C1	-2.14	103.94	111.80
23	a	2609	CLA	CHD-C1D-ND	-2.14	121.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	C6-C7-C8	-2.14	108.85	115.97
23	D	2303	CLA	CMC-C2C-C1C	2.14	128.38	125.03
23	b	608	CLA	CHA-C1A-NA	-2.14	121.55	126.39
23	c	514	CLA	C1-C2-C3	-2.14	122.70	126.20
23	D	2303	CLA	CHD-C4C-NC	2.13	127.54	124.23
25	k	302	BCR	C15-C14-C13	-2.13	124.29	127.28
23	B	609	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
23	C	509	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
23	b	620	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
23	b	619	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
23	b	610	CLA	CHD-C4C-NC	2.13	127.53	124.23
40	h	101	RRX	C20-C21-C22	-2.13	124.29	127.28
25	K	101	BCR	C2-C3-C4	-2.13	106.59	111.28
27	c	501	LMG	O8-C28-C29	2.13	118.33	111.83
26	D	2308	SQD	O48-C23-O10	-2.13	118.30	123.63
25	B	619	BCR	C29-C28-C27	-2.13	106.60	111.28
23	B	610	CLA	O2A-CGA-CBA	2.13	118.32	111.83
23	b	620	CLA	CMC-C2C-C1C	2.13	128.36	125.03
36	I	101	HTG	O5-C1-C2	2.13	113.25	110.32
23	c	514	CLA	CHD-C4C-NC	2.13	127.53	124.23
23	C	507	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
31	A	418	JOX	C-C1-CL1	2.12	124.91	119.92
23	C	513	CLA	C1-O2A-CGA	2.12	121.79	116.65
23	b	614	CLA	CAC-C3C-C4C	2.12	127.55	124.79
26	b	601	SQD	O47-C7-O49	-2.12	118.74	123.70
23	B	602	CLA	CMB-C2B-C1B	2.12	128.65	125.42
23	C	506	CLA	C4A-NA-C1A	2.12	107.65	106.68
23	A	407	CLA	CHA-C1A-NA	-2.12	121.59	126.39
23	b	618	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
23	A	406	CLA	CHD-C4C-NC	2.12	127.52	124.23
23	B	616	CLA	C4A-NA-C1A	2.12	107.65	106.68
23	b	616	CLA	CHA-C1A-NA	-2.12	121.59	126.39
42	V	201	HEC	C2A-C1A-NA	-2.12	108.28	110.32
25	a	2614	BCR	C29-C30-C25	2.12	113.52	110.44
23	B	614	CLA	CHA-C1A-NA	-2.12	121.60	126.39
23	C	508	CLA	C3B-C4B-NB	2.11	112.42	110.53
25	B	618	BCR	C15-C14-C13	-2.11	124.31	127.28
23	C	510	CLA	CHD-C1D-ND	-2.11	121.83	124.80
23	C	509	CLA	C11-C12-C13	-2.11	108.94	115.97
26	A	412	SQD	C45-O47-C7	-2.11	112.74	117.80
23	B	606	CLA	C4B-C3B-C2B	-2.11	104.67	107.30
37	C	519	DGD	O1G-C1A-O1A	-2.11	118.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	BCR	C16-C17-C18	-2.11	124.31	127.28
42	v	201	HEC	C3D-C4D-ND	-2.11	107.81	110.15
23	b	611	CLA	C3B-C4B-NB	2.11	112.42	110.53
26	a	2615	SQD	O5-C1-C2	-2.11	106.03	110.37
23	B	611	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
27	c	521	LMG	O7-C10-O9	-2.11	118.77	123.70
33	d	411	PL9	C47-C48-C49	-2.11	120.61	127.64
23	B	614	CLA	CHD-C4C-NC	2.11	127.50	124.23
23	b	619	CLA	CHA-C1A-NA	-2.11	121.62	126.39
23	b	613	CLA	OBD-CAD-C3D	-2.11	123.49	128.42
23	C	512	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
23	C	513	CLA	C2C-C1C-NC	2.11	112.19	109.98
23	a	2610	CLA	CMC-C2C-C1C	2.11	128.32	125.03
23	B	614	CLA	CMB-C2B-C1B	2.10	128.62	125.42
23	B	617	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
23	C	504	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
28	A	414	LMT	C3B-C4B-C5B	2.10	114.04	110.23
23	c	512	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
38	e	101	LHG	O8-C23-O10	-2.10	118.37	123.63
31	a	2617	JOX	O1-C5-C	-2.10	118.44	121.43
23	C	503	CLA	C3B-C4B-NB	2.10	112.41	110.53
23	D	2304	CLA	CHB-C4A-NA	2.10	127.43	124.40
36	B	627	HTG	C1-O5-C5	2.10	116.32	112.56
23	d	409	CLA	O2A-CGA-CBA	2.09	118.22	111.83
24	A	409	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
39	e	103	HEM	C3B-C4B-NB	-2.09	107.97	109.47
23	b	620	CLA	CHD-C1D-ND	-2.09	121.86	124.80
23	c	511	CLA	CHD-C1D-C2D	-2.09	121.14	125.49
25	D	2305	BCR	C15-C16-C17	-2.09	119.24	123.52
23	B	604	CLA	CHA-C1A-NA	-2.09	121.66	126.39
23	A	410	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
23	b	607	CLA	CMA-C3A-C2A	-2.09	105.90	113.98
23	c	509	CLA	CHD-C1D-ND	-2.09	121.86	124.80
23	B	605	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
27	c	521	LMG	O8-C28-O10	-2.09	118.41	123.63
25	C	515	BCR	C23-C24-C25	-2.09	121.43	127.00
23	a	2610	CLA	CHA-C1A-NA	-2.08	121.67	126.39
23	C	514	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
23	c	510	CLA	C6-C7-C8	-2.08	109.04	115.97
23	b	613	CLA	CMB-C2B-C1B	2.08	128.59	125.42
23	c	510	CLA	OBD-CAD-C3D	-2.08	123.55	128.42
28	z	102	LMT	C1B-O5B-C5B	2.08	117.78	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	623	BCR	C29-C30-C25	2.08	113.46	110.44
25	z	101	BCR	C3-C4-C5	-2.08	110.35	114.06
25	B	620	BCR	C38-C26-C25	-2.08	122.22	124.48
23	B	610	CLA	CAC-C3C-C4C	2.08	127.49	124.79
23	b	614	CLA	CMC-C2C-C1C	2.08	128.28	125.03
23	B	608	CLA	C4-C3-C5	2.08	118.83	115.23
23	B	615	CLA	C4-C3-C5	2.08	118.83	115.23
27	D	2312	LMG	C9-C8-C7	-2.08	106.94	111.78
23	d	409	CLA	CMA-C3A-C2A	-2.08	105.95	113.98
23	d	409	CLA	CMB-C2B-C1B	2.08	128.58	125.42
23	b	619	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
26	D	2302	SQD	C9-C8-C7	-2.08	106.09	113.69
23	d	409	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
23	D	2304	CLA	CMB-C2B-C1B	2.08	128.58	125.42
40	h	101	RRX	C11-C10-C9	-2.07	124.37	127.28
23	c	516	CLA	C4-C3-C5	2.07	118.83	115.23
23	C	511	CLA	C11-C10-C8	-2.07	109.07	115.97
23	a	2610	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
23	b	611	CLA	C11-C10-C8	-2.07	109.08	115.97
23	C	514	CLA	CED-O2D-CGD	2.07	120.61	115.92
36	B	624[B]	HTG	C1-C2-C3	2.07	114.60	110.55
36	V	204	HTG	O5-C5-C4	2.07	113.43	109.70
23	b	606	CLA	C3C-C4C-NC	2.07	113.08	110.43
23	D	2303	CLA	CHC-C1C-C2C	-2.07	121.07	126.95
37	H	103	DGD	C3E-C4E-C5E	-2.07	106.48	110.23
36	B	624[B]	HTG	O5-C5-C4	2.07	113.42	109.70
23	B	617	CLA	CHC-C4B-NB	2.07	127.15	124.05
36	b	603	HTG	C1-O5-C5	2.06	116.27	112.56
23	D	2304	CLA	C11-C10-C8	-2.06	109.11	115.97
23	b	606	CLA	CMB-C2B-C1B	2.06	128.56	125.42
23	b	620	CLA	C3B-C4B-NB	2.06	112.37	110.53
37	C	517	DGD	C2G-O2G-C1B	-2.06	112.86	117.80
29	a	2618	GOL	C3-C2-C1	-2.06	104.24	111.80
23	C	513	CLA	C6-C5-C3	2.06	118.49	113.47
36	c	523	HTG	C6-C5-C4	-2.06	107.96	113.02
27	c	501	LMG	C8-O7-C10	-2.06	112.87	117.80
31	a	2619	JOX	C-C5-C4	2.06	121.58	117.06
26	D	2308	SQD	O9-S-C6	2.06	109.83	106.76
23	c	504	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
36	o	301	HTG	O5-C5-C6	2.06	111.54	106.44
23	b	613	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
37	D	2307	DGD	O2G-C1B-O1B	-2.06	118.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	z	102	LMT	C1'-O5'-C5'	2.06	117.73	113.72
27	C	527	LMG	O7-C10-O9	-2.06	118.90	123.70
23	C	504	CLA	C4-C3-C5	2.05	118.80	115.23
23	C	513	CLA	CHD-C1D-ND	-2.05	121.91	124.80
25	b	623	BCR	C29-C28-C27	-2.05	106.76	111.28
23	b	611	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
23	b	620	CLA	O2A-CGA-CBA	2.05	118.09	111.83
23	c	504	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
23	b	611	CLA	C1-C2-C3	-2.05	122.83	126.20
26	D	2302	SQD	O8-S-C6	2.05	109.93	105.97
23	C	512	CLA	CMC-C2C-C1C	2.05	128.24	125.03
23	C	503	CLA	O2A-C1-C2	2.05	115.99	108.11
28	i	103	LMT	C3'-C4'-C5'	2.05	113.95	110.23
23	b	606	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
25	A	411	BCR	C2-C3-C4	-2.05	106.77	111.28
23	C	504	CLA	CHD-C1D-ND	-2.05	121.92	124.80
42	v	201	HEC	C1D-C2D-C3D	-2.05	104.47	106.82
23	b	621	CLA	CMB-C2B-C1B	2.05	128.53	125.42
36	C	525	HTG	C4-C3-C2	-2.05	107.24	110.83
23	A	410	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
23	b	612	CLA	C4-C3-C5	2.04	118.78	115.23
23	B	606	CLA	CHA-C1A-NA	-2.04	121.76	126.39
23	b	617	CLA	CHD-C1D-ND	-2.04	121.93	124.80
36	d	407	HTG	C6-C5-C4	-2.04	108.00	113.02
23	c	504	CLA	O2A-CGA-CBA	2.04	118.06	111.83
23	B	610	CLA	C1-O2A-CGA	2.04	121.59	116.65
23	a	2609	CLA	C4-C3-C5	2.04	118.77	115.23
23	a	2610	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
23	c	511	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
23	b	616	CLA	CHB-C4A-NA	2.04	127.34	124.40
38	D	2311	LHG	O7-C7-O9	-2.04	118.94	123.70
24	A	408	PHO	CBA-CAA-C2A	-2.04	107.77	113.78
27	A	413	LMG	O6-C5-C4	2.04	113.37	109.70
25	b	623	BCR	C28-C27-C26	-2.04	110.42	114.06
23	c	505	CLA	CHD-C4C-NC	2.04	127.39	124.23
23	c	515	CLA	CHD-C1D-C2D	-2.04	121.25	125.49
23	c	516	CLA	CMB-C2B-C1B	2.04	128.52	125.42
37	C	519	DGD	C2G-O2G-C1B	-2.04	112.92	117.80
23	b	619	CLA	C4-C3-C2	-2.04	118.40	123.63
36	b	602	HTG	O5-C1-C2	2.03	113.12	110.32
23	c	513	CLA	CHD-C1D-ND	-2.03	121.94	124.80
23	c	510	CLA	CHC-C1C-C2C	-2.03	121.17	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	2613	CLA	CHD-C1D-ND	-2.03	121.94	124.80
23	C	505	CLA	CAA-CBA-CGA	2.03	118.98	113.21
23	b	608	CLA	CAA-C2A-C1A	-2.03	105.32	111.97
25	c	517	BCR	C37-C22-C23	2.03	121.19	118.09
23	C	510	CLA	OBD-CAD-C3D	-2.03	123.67	128.42
40	h	101	RRX	C34-C9-C8	2.03	121.19	118.09
23	C	514	CLA	CHC-C1C-C2C	-2.03	121.18	126.95
37	C	519	DGD	O4D-C4D-C3D	-2.03	105.59	110.38
23	C	514	CLA	CMC-C2C-C1C	2.03	128.20	125.03
23	b	619	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	B	610	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
23	b	615	CLA	C4-C3-C5	2.03	118.75	115.23
23	B	604	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
25	B	619	BCR	C11-C10-C9	-2.03	124.44	127.28
23	B	608	CLA	CAA-CBA-CGA	2.03	118.96	113.21
23	c	513	CLA	C11-C10-C8	-2.03	109.23	115.97
23	B	613	CLA	C2A-C1A-CHA	-2.02	120.35	123.87
23	C	509	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	d	408	CLA	C4-C3-C5	2.02	118.74	115.23
25	a	2614	BCR	C15-C14-C13	-2.02	124.44	127.28
23	d	402	CLA	CAA-CBA-CGA	2.02	118.95	113.21
28	M	101	LMT	C1B-O5B-C5B	2.02	117.67	113.72
25	B	620	BCR	C24-C23-C22	-2.02	123.25	126.23
38	l	103	LHG	O7-C7-O9	-2.02	118.98	123.70
23	B	615	CLA	CHC-C1C-NC	2.02	127.35	124.31
25	k	302	BCR	C10-C11-C12	-2.02	117.35	123.20
25	B	633	BCR	C23-C24-C25	-2.02	121.61	127.00
36	c	523	HTG	C1-O5-C5	2.02	116.18	112.56
23	b	608	CLA	CMA-C3A-C2A	-2.02	106.18	113.98
25	b	622	BCR	C16-C17-C18	-2.02	124.45	127.28
23	B	610	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
28	z	102	LMT	C3'-C4'-C5'	-2.02	106.46	110.93
23	C	506	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
23	B	615	CLA	CMA-C3A-C2A	-2.01	106.19	113.98
25	D	2305	BCR	C30-C25-C24	2.01	121.11	115.65
38	d	413	LHG	C5-O7-C7	-2.01	112.98	117.80
23	C	508	CLA	C4A-NA-C1A	2.01	107.60	106.68
37	C	518	DGD	O3G-C3G-C2G	2.01	115.71	110.82
27	c	522	LMG	C4-C3-C2	-2.01	107.30	110.83
23	b	606	CLA	C4-C3-C2	-2.01	118.46	123.63
23	b	615	CLA	C11-C12-C13	-2.01	109.28	115.97
23	D	2304	CLA	C1-O2A-CGA	2.01	121.51	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	102	BCR	C33-C5-C4	2.01	117.88	113.60
23	a	2610	CLA	CAA-CBA-CGA	2.01	118.91	113.21
23	b	609	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
25	C	516	BCR	C31-C1-C6	-2.01	107.10	110.24
23	b	616	CLA	C1-O2A-CGA	2.01	121.50	116.65
27	c	522	LMG	O7-C10-O9	-2.00	119.02	123.70
37	c	518	DGD	C6D-O5D-C1E	2.00	118.09	113.80
23	c	512	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
24	a	2611	PHO	C4A-C3A-C2A	-2.00	100.93	102.84
25	K	101	BCR	C21-C20-C19	-2.00	117.39	123.20
23	C	505	CLA	C4A-NA-C1A	2.00	107.59	106.68
23	C	510	CLA	CBC-CAC-C3C	-2.00	106.99	112.42
25	B	620	BCR	C2-C1-C6	2.00	113.35	110.44
23	B	606	CLA	C10-C8-C7	-2.00	101.92	112.07
23	B	607	CLA	OBD-CAD-C3D	-2.00	123.74	128.42
23	b	615	CLA	CMB-C2B-C1B	2.00	128.47	125.42

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	405	CLA	ND
23	A	410	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	B	617	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	2303	CLA	ND
23	D	2304	CLA	ND
23	a	2609	CLA	ND
23	a	2613	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	b	620	CLA	ND
23	b	621	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	c	515	CLA	ND
23	c	516	CLA	ND
23	d	402	CLA	ND
23	d	408	CLA	ND
23	d	409	CLA	ND

All (1213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB
23	B	611	CLA	C14-C13-C15-C16
23	B	615	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	C	514	CLA	C4B-C3B-CAB-CBB
23	D	2304	CLA	C4-C3-C5-C6
23	b	610	CLA	C4-C3-C5-C6
23	b	614	CLA	C2B-C3B-CAB-CBB
23	b	614	CLA	C4B-C3B-CAB-CBB
23	b	619	CLA	CAD-CBD-CGD-O1D
23	b	619	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	C4B-C3B-CAB-CBB
23	c	506	CLA	C4B-C3B-CAB-CBB
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	515	CLA	C4B-C3B-CAB-CBB
25	B	633	BCR	C11-C12-C13-C14
25	B	633	BCR	C13-C14-C15-C16
25	D	2305	BCR	C7-C8-C9-C10
25	D	2305	BCR	C21-C22-C23-C24
25	D	2305	BCR	C37-C22-C23-C24
25	T	102	BCR	C11-C12-C13-C14
25	Y	302	BCR	C21-C22-C23-C24
25	d	410	BCR	C7-C8-C9-C10
25	d	410	BCR	C21-C22-C23-C24
25	d	410	BCR	C37-C22-C23-C24
25	y	101	BCR	C21-C22-C23-C24
26	B	621	SQD	O5-C1-O6-C44
26	B	621	SQD	O49-C7-O47-C45
26	B	621	SQD	C8-C7-O47-C45
26	B	621	SQD	C5-C6-S-O7
26	B	621	SQD	C5-C6-S-O8
26	B	621	SQD	C5-C6-S-O9
26	D	2302	SQD	O49-C7-O47-C45
26	D	2308	SQD	C8-C7-O47-C45
26	D	2308	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
26	D	2308	SQD	C5-C6-S-O9
26	a	2603	SQD	O6-C44-C45-O47
26	a	2603	SQD	C5-C6-S-O7
26	a	2603	SQD	C5-C6-S-O8
26	a	2603	SQD	C5-C6-S-O9
26	b	601	SQD	C5-C6-S-O7
26	b	601	SQD	C5-C6-S-O8
26	b	601	SQD	C5-C6-S-O9
26	d	417	SQD	O49-C7-O47-C45
26	l	101	SQD	O5-C1-O6-C44
26	l	101	SQD	O49-C7-O47-C45
26	l	101	SQD	C8-C7-O47-C45
26	l	101	SQD	C5-C6-S-O7
26	l	101	SQD	C5-C6-S-O9
27	C	527	LMG	O9-C10-O7-C8
27	C	527	LMG	C11-C10-O7-C8
27	c	501	LMG	O9-C10-O7-C8
28	A	414	LMT	C2'-C1'-O1'-C1
28	A	414	LMT	O5'-C1'-O1'-C1
28	A	414	LMT	C2-C1-O1'-C1'
28	A	420	LMT	O5'-C1'-O1'-C1
28	B	623	LMT	C2-C1-O1'-C1'
28	F	102	LMT	C2'-C1'-O1'-C1
28	F	102	LMT	O5'-C1'-O1'-C1
28	f	101	LMT	C2'-C1'-O1'-C1
28	f	101	LMT	O5'-C1'-O1'-C1
28	z	102	LMT	C2'-C1'-O1'-C1
28	z	102	LMT	O5'-C1'-O1'-C1
29	B	632	GOL	O1-C1-C2-C3
29	C	524	GOL	O1-C1-C2-O2
29	C	524	GOL	O1-C1-C2-C3
29	J	301	GOL	O1-C1-C2-C3
29	J	301	GOL	C1-C2-C3-O3
29	J	301	GOL	O2-C2-C3-O3
29	O	302	GOL	C1-C2-C3-O3
29	O	304	GOL	O1-C1-C2-C3
29	U	502	GOL	C1-C2-C3-O3
29	b	644	GOL	O1-C1-C2-C3
33	A	422	PL9	C12-C11-C9-C8
33	A	422	PL9	C12-C11-C9-C10
33	x	1301	PL9	C18-C19-C21-C22
33	x	1301	PL9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
36	I	101	HTG	C2-C1-S1-C1'
36	I	101	HTG	O5-C1-S1-C1'
36	V	204	HTG	O5-C1-S1-C1'
36	b	626	HTG	O5-C1-S1-C1'
36	d	407	HTG	C2-C1-S1-C1'
36	d	407	HTG	O5-C1-S1-C1'
36	d	415	HTG	O5-C1-S1-C1'
36	i	102	HTG	O5-C1-S1-C1'
37	D	2307	DGD	C2B-C1B-O2G-C2G
37	D	2307	DGD	C2D-C1D-O3G-C3G
37	D	2307	DGD	O6D-C1D-O3G-C3G
38	D	2310	LHG	C4-O6-P-O4
38	E	101	LHG	C4-O6-P-O3
38	E	101	LHG	C4-O6-P-O5
38	L	101	LHG	C4-O6-P-O3
38	L	101	LHG	C4-O6-P-O4
38	d	412	LHG	O2-C2-C3-O3
38	d	413	LHG	O1-C1-C2-C3
38	e	101	LHG	O10-C23-O8-C6
38	e	101	LHG	C24-C23-O8-C6
38	l	103	LHG	C4-O6-P-O3
38	l	103	LHG	C4-O6-P-O4
42	V	201	HEC	C2B-C3B-CAB-CBB
42	V	201	HEC	C4B-C3B-CAB-CBB
42	V	201	HEC	C2C-C3C-CAC-CBC
42	V	201	HEC	C4C-C3C-CAC-CBC
42	v	201	HEC	C2B-C3B-CAB-CBB
42	v	201	HEC	C4B-C3B-CAB-CBB
42	v	201	HEC	C2C-C3C-CAC-CBC
42	v	201	HEC	C4C-C3C-CAC-CBC
23	C	507	CLA	C15-C16-C17-C18
23	b	611	CLA	C10-C11-C12-C13
26	D	2308	SQD	O10-C23-O48-C46
26	D	2308	SQD	O49-C7-O47-C45
37	D	2307	DGD	O1B-C1B-O2G-C2G
26	D	2302	SQD	C8-C7-O47-C45
27	c	501	LMG	C11-C10-O7-C8
23	B	615	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	b	608	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	D	2304	CLA	C2-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
23	D	2304	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
23	b	621	CLA	C3-C5-C6-C7
26	D	2308	SQD	C24-C23-O48-C46
25	T	102	BCR	C13-C14-C15-C16
23	B	605	CLA	C3-C5-C6-C7
23	c	516	CLA	C3-C5-C6-C7
23	d	409	CLA	C3-C5-C6-C7
38	E	101	LHG	C24-C23-O8-C6
36	b	626	HTG	O5-C5-C6-O6
28	z	102	LMT	O5B-C5B-C6B-O6B
28	T	103	LMT	O5'-C5'-C6'-O6'
36	I	101	HTG	S1-C1'-C2'-C3'
23	B	606	CLA	C4-C3-C5-C6
23	B	606	CLA	C2-C3-C5-C6
23	B	615	CLA	C2-C3-C5-C6
23	b	608	CLA	C2-C3-C5-C6
23	b	619	CLA	C2-C3-C5-C6
38	E	101	LHG	O10-C23-O8-C6
33	A	422	PL9	C9-C11-C12-C13
33	A	422	PL9	C14-C16-C17-C18
33	x	1301	PL9	C9-C11-C12-C13
33	x	1301	PL9	C14-C16-C17-C18
28	T	103	LMT	O5'-C1'-O1'-C1
28	d	401	LMT	O5'-C1'-O1'-C1
28	d	404	LMT	O5'-C1'-O1'-C1
28	i	103	LMT	O5'-C1'-O1'-C1
28	A	414	LMT	C2-C3-C4-C5
36	i	102	HTG	O5-C5-C6-O6
28	Z	101	LMT	O5B-C5B-C6B-O6B
28	B	634	LMT	O5'-C5'-C6'-O6'
36	B	626	HTG	C4-C5-C6-O6
28	z	102	LMT	C4B-C5B-C6B-O6B
28	B	634	LMT	C4'-C5'-C6'-O6'
37	C	517	DGD	CCB-CDB-CEB-CFB
23	b	619	CLA	C4-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
23	A	410	CLA	C14-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C9
23	B	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C11-C12-C13-C14
23	C	507	CLA	C14-C13-C15-C16
23	a	2610	CLA	C11-C12-C13-C14
23	c	507	CLA	C11-C12-C13-C14
26	B	621	SQD	C2-C1-O6-C44
28	J	303	LMT	C2'-C1'-O1'-C1
28	T	103	LMT	C2'-C1'-O1'-C1
28	d	401	LMT	C2'-C1'-O1'-C1
28	d	404	LMT	C2'-C1'-O1'-C1
28	i	103	LMT	C2'-C1'-O1'-C1
37	C	518	DGD	C8A-C9A-CAA-CBA
25	B	633	BCR	C11-C12-C13-C35
25	D	2305	BCR	C7-C8-C9-C34
25	T	102	BCR	C11-C12-C13-C35
25	Y	302	BCR	C37-C22-C23-C24
25	b	624	BCR	C37-C22-C23-C24
25	d	410	BCR	C7-C8-C9-C34
25	y	101	BCR	C37-C22-C23-C24
36	B	624[A]	HTG	S1-C1'-C2'-C3'
36	b	602	HTG	S1-C1'-C2'-C3'
28	Z	101	LMT	O5B-C1B-O1B-C4'
27	C	520	LMG	C10-C11-C12-C13
28	i	103	LMT	O5'-C5'-C6'-O6'
36	d	407	HTG	O5-C5-C6-O6
28	Z	101	LMT	C4B-C5B-C6B-O6B
36	i	102	HTG	C4-C5-C6-O6
37	c	518	DGD	C8A-C9A-CAA-CBA
23	a	2609	CLA	C15-C16-C17-C18
23	B	616	CLA	C13-C15-C16-C17
28	J	303	LMT	O5'-C5'-C6'-O6'
29	J	301	GOL	O1-C1-C2-O2
29	v	202	GOL	O2-C2-C3-O3
36	B	626	HTG	O5-C5-C6-O6
37	h	102	DGD	C9A-CAA-CBA-CCA
36	V	204	HTG	C4-C5-C6-O6
23	A	410	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	B	617	CLA	C12-C13-C15-C16
23	b	611	CLA	C12-C13-C15-C16
23	b	618	CLA	C11-C12-C13-C15
27	B	622	LMG	C15-C16-C17-C18
37	H	103	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
23	d	409	CLA	C4-C3-C5-C6
37	c	519	DGD	C1B-C2B-C3B-C4B
28	d	401	LMT	O1'-C1-C2-C3
33	A	422	PL9	C19-C21-C22-C23
33	x	1301	PL9	C24-C26-C27-C28
28	B	623	LMT	O1'-C1-C2-C3
23	C	514	CLA	C10-C11-C12-C13
23	a	2613	CLA	C5-C6-C7-C8
23	b	606	CLA	C10-C11-C12-C13
23	c	515	CLA	C10-C11-C12-C13
28	z	102	LMT	O5'-C5'-C6'-O6'
28	T	103	LMT	C4'-C5'-C6'-O6'
26	D	2302	SQD	C23-C24-C25-C26
27	m	2802	LMG	C10-C11-C12-C13
37	C	517	DGD	C1B-C2B-C3B-C4B
37	C	518	DGD	C1B-C2B-C3B-C4B
28	Z	101	LMT	C2B-C1B-O1B-C4'
28	J	303	LMT	O5'-C1'-O1'-C1
36	b	626	HTG	C4-C5-C6-O6
23	B	614	CLA	C10-C11-C12-C13
23	D	2304	CLA	C8-C10-C11-C12
23	b	616	CLA	C13-C15-C16-C17
23	c	516	CLA	C10-C11-C12-C13
27	m	2802	LMG	C30-C31-C32-C33
38	d	403	LHG	C34-C35-C36-C37
23	d	409	CLA	C8-C10-C11-C12
23	C	508	CLA	C15-C16-C17-C18
23	d	409	CLA	C2-C3-C5-C6
36	o	301	HTG	C4-C5-C6-O6
26	B	621	SQD	C7-C8-C9-C10
23	B	615	CLA	C3-C5-C6-C7
27	B	622	LMG	C10-C11-C12-C13
38	d	412	LHG	C1-C2-C3-O3
23	B	604	CLA	C5-C6-C7-C8
37	D	2307	DGD	O6D-C5D-C6D-O5D
23	b	621	CLA	C5-C6-C7-C8
23	b	621	CLA	C13-C15-C16-C17
28	B	623	LMT	O5B-C1B-O1B-C4'
23	B	617	CLA	C5-C6-C7-C8
23	B	617	CLA	C10-C11-C12-C13
23	C	510	CLA	C13-C15-C16-C17
26	D	2302	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
27	c	521	LMG	C11-C10-O7-C8
28	F	102	LMT	C1-C2-C3-C4
27	c	521	LMG	O9-C10-O7-C8
28	j	2701	LMT	C2'-C1'-O1'-C1
23	C	511	CLA	C8-C10-C11-C12
33	x	1301	PL9	C34-C36-C37-C38
23	C	504	CLA	CBD-CGD-O2D-CED
23	b	620	CLA	C10-C11-C12-C13
23	c	512	CLA	C8-C10-C11-C12
29	A	415	GOL	O1-C1-C2-C3
29	A	417	GOL	C1-C2-C3-O3
29	C	526	GOL	O1-C1-C2-C3
29	D	2301	GOL	O1-C1-C2-C3
29	a	2602	GOL	O1-C1-C2-C3
29	c	530	GOL	C1-C2-C3-O3
29	c	531	GOL	C1-C2-C3-O3
29	d	416	GOL	C1-C2-C3-O3
29	v	202	GOL	C1-C2-C3-O3
38	D	2310	LHG	O1-C1-C2-C3
38	D	2311	LHG	O1-C1-C2-C3
38	d	412	LHG	O1-C1-C2-C3
23	C	502	CLA	C16-C17-C18-C19
23	c	509	CLA	C15-C16-C17-C18
23	B	602	CLA	CBA-CGA-O2A-C1
28	A	420	LMT	C1-C2-C3-C4
23	c	516	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C16-C17-C18-C20
28	i	103	LMT	C1-C2-C3-C4
27	d	414	LMG	O6-C5-C6-O5
28	A	414	LMT	C1-C2-C3-C4
38	l	103	LHG	C33-C34-C35-C36
27	C	527	LMG	O6-C5-C6-O5
23	B	606	CLA	C10-C11-C12-C13
23	c	513	CLA	C8-C10-C11-C12
26	l	101	SQD	C31-C32-C33-C34
38	L	101	LHG	C33-C34-C35-C36
28	Z	101	LMT	C2-C1-O1'-C1'
29	A	417	GOL	O2-C2-C3-O3
29	O	302	GOL	O2-C2-C3-O3
29	U	502	GOL	O2-C2-C3-O3
29	b	644	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	c	530	GOL	O2-C2-C3-O3
38	d	413	LHG	O1-C1-C2-O2
37	D	2307	DGD	C3B-C4B-C5B-C6B
23	C	503	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C4B-C3B-CAB-CBB
37	c	519	DGD	C1A-C2A-C3A-C4A
23	B	607	CLA	C2A-CAA-CBA-CGA
23	c	511	CLA	C11-C10-C8-C7
27	C	520	LMG	C16-C17-C18-C19
28	M	101	LMT	O5B-C5B-C6B-O6B
28	d	401	LMT	C5-C6-C7-C8
23	C	513	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C3A-C2A-CAA-CBA
26	D	2302	SQD	O10-C23-O48-C46
36	B	627	HTG	C4-C5-C6-O6
26	D	2302	SQD	C17-C18-C19-C20
27	A	413	LMG	C30-C31-C32-C33
36	H	101	HTG	C3'-C4'-C5'-C6'
37	C	518	DGD	C4B-C5B-C6B-C7B
26	l	101	SQD	C29-C30-C31-C32
37	C	518	DGD	C5A-C6A-C7A-C8A
23	B	602	CLA	O1A-CGA-O2A-C1
28	z	102	LMT	C7-C8-C9-C10
37	C	517	DGD	C4A-C5A-C6A-C7A
38	D	2309	LHG	C32-C33-C34-C35
26	a	2603	SQD	C34-C35-C36-C37
27	c	501	LMG	C11-C12-C13-C14
28	B	634	LMT	C9-C10-C11-C12
37	C	518	DGD	CBB-CCB-CDB-CEB
37	D	2307	DGD	C1B-C2B-C3B-C4B
36	I	101	HTG	O5-C5-C6-O6
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	C	514	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
23	c	506	CLA	C2B-C3B-CAB-CBB
23	c	515	CLA	C2B-C3B-CAB-CBB
25	Y	302	BCR	C1-C6-C7-C8
25	Y	302	BCR	C5-C6-C7-C8
25	c	517	BCR	C1-C6-C7-C8
25	c	517	BCR	C5-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	y	101	BCR	C5-C6-C7-C8
23	b	618	CLA	C8-C10-C11-C12
26	a	2603	SQD	C31-C32-C33-C34
27	A	413	LMG	C38-C39-C40-C41
37	C	517	DGD	C5B-C6B-C7B-C8B
37	c	518	DGD	CBB-CCB-CDB-CEB
26	a	2615	SQD	C23-C24-C25-C26
27	d	414	LMG	C19-C20-C21-C22
27	B	622	LMG	C37-C38-C39-C40
27	C	527	LMG	C34-C35-C36-C37
37	c	518	DGD	C4B-C5B-C6B-C7B
26	B	621	SQD	C27-C28-C29-C30
27	C	527	LMG	C33-C34-C35-C36
37	c	519	DGD	CCA-CDA-CEA-CFA
28	T	103	LMT	C9-C10-C11-C12
23	c	509	CLA	C11-C10-C8-C9
26	b	601	SQD	C24-C25-C26-C27
28	i	103	LMT	C6-C7-C8-C9
27	C	520	LMG	C31-C32-C33-C34
26	a	2603	SQD	O5-C1-O6-C44
28	B	634	LMT	O5'-C1'-O1'-C1
28	j	2701	LMT	O5'-C1'-O1'-C1
37	D	2307	DGD	C4D-C5D-C6D-O5D
27	c	521	LMG	C36-C37-C38-C39
36	V	204	HTG	O5-C5-C6-O6
26	a	2603	SQD	C2-C1-O6-C44
28	B	634	LMT	C2'-C1'-O1'-C1
37	c	519	DGD	C4B-C5B-C6B-C7B
28	f	101	LMT	C1-C2-C3-C4
23	c	508	CLA	C16-C17-C18-C20
27	A	413	LMG	C11-C10-O7-C8
27	m	2802	LMG	C11-C10-O7-C8
27	c	522	LMG	O6-C5-C6-O5
28	B	623	LMT	C7-C8-C9-C10
25	C	515	BCR	C37-C22-C23-C24
38	E	101	LHG	C7-C8-C9-C10
26	l	101	SQD	C15-C16-C17-C18
23	A	410	CLA	C3-C5-C6-C7
36	o	301	HTG	O5-C5-C6-O6
28	A	414	LMT	O1'-C1-C2-C3
23	A	407	CLA	C16-C17-C18-C20
23	b	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C16-C17-C18-C19
23	c	516	CLA	C16-C17-C18-C19
23	b	621	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
27	D	2312	LMG	C35-C36-C37-C38
27	A	413	LMG	C35-C36-C37-C38
27	c	521	LMG	C10-C11-C12-C13
27	B	622	LMG	C36-C37-C38-C39
38	E	101	LHG	O6-C4-C5-O7
27	c	501	LMG	C36-C37-C38-C39
37	C	518	DGD	C3B-C4B-C5B-C6B
23	a	2613	CLA	C10-C11-C12-C13
26	l	101	SQD	C11-C10-C9-C8
28	T	103	LMT	C6-C7-C8-C9
26	D	2308	SQD	C23-C24-C25-C26
36	B	625	HTG	O5-C5-C6-O6
28	i	103	LMT	C2-C3-C4-C5
26	a	2603	SQD	C24-C25-C26-C27
28	j	2701	LMT	O5B-C5B-C6B-O6B
38	D	2309	LHG	C24-C25-C26-C27
23	C	502	CLA	C16-C17-C18-C20
23	C	507	CLA	C16-C17-C18-C19
38	l	103	LHG	C13-C14-C15-C16
28	m	2804	LMT	C3'-C4'-O1B-C1B
23	b	614	CLA	C2-C3-C5-C6
37	c	518	DGD	C3B-C4B-C5B-C6B
38	L	101	LHG	C13-C14-C15-C16
23	b	611	CLA	C2A-CAA-CBA-CGA
38	D	2311	LHG	C27-C28-C29-C30
26	B	621	SQD	C28-C29-C30-C31
27	B	622	LMG	C30-C31-C32-C33
28	B	634	LMT	C11-C10-C9-C8
28	z	102	LMT	C6-C7-C8-C9
37	C	517	DGD	O6E-C5E-C6E-O5E
37	c	518	DGD	CDB-CEB-CFB-CGB
29	a	2602	GOL	O1-C1-C2-O2
38	D	2310	LHG	O1-C1-C2-O2
27	D	2312	LMG	C36-C37-C38-C39
38	d	403	LHG	C32-C33-C34-C35
23	C	513	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	C1A-C2A-CAA-CBA
23	b	616	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
26	D	2302	SQD	C24-C25-C26-C27
28	B	623	LMT	C4B-C5B-C6B-O6B
28	F	102	LMT	O5'-C5'-C6'-O6'
27	A	413	LMG	O9-C10-O7-C8
28	Z	101	LMT	C2-C3-C4-C5
36	V	204	HTG	C2'-C3'-C4'-C5'
37	D	2307	DGD	CCB-CDB-CEB-CFB
23	B	611	CLA	C12-C13-C15-C16
23	B	616	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
26	A	412	SQD	C30-C31-C32-C33
38	D	2309	LHG	C23-C24-C25-C26
38	L	101	LHG	C30-C31-C32-C33
23	B	617	CLA	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
24	a	2611	PHO	C2-C3-C5-C6
27	m	2802	LMG	C13-C14-C15-C16
28	m	2804	LMT	C5'-C4'-O1B-C1B
23	A	410	CLA	C11-C12-C13-C14
23	B	614	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C10-C8-C9
23	c	508	CLA	C11-C12-C13-C14
38	D	2311	LHG	C25-C26-C27-C28
26	l	101	SQD	C28-C29-C30-C31
38	d	412	LHG	C29-C30-C31-C32
23	c	510	CLA	C5-C6-C7-C8
28	A	420	LMT	C2'-C1'-O1'-C1
26	d	417	SQD	C44-C45-C46-O48
26	l	101	SQD	C44-C45-C46-O48
27	A	413	LMG	C7-C8-C9-O8
27	c	521	LMG	C7-C8-C9-O8
28	M	101	LMT	C11-C10-C9-C8
37	c	518	DGD	O6E-C5E-C6E-O5E
23	C	509	CLA	C5-C6-C7-C8
23	c	512	CLA	C13-C15-C16-C17
27	A	413	LMG	C37-C38-C39-C40
23	c	516	CLA	CBA-CGA-O2A-C1
28	m	2804	LMT	O5B-C5B-C6B-O6B
23	A	407	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C16-C17-C18-C19
27	A	413	LMG	C21-C22-C23-C24
36	c	526	HTG	C2'-C3'-C4'-C5'
37	c	518	DGD	C9A-CAA-CBA-CCA
38	d	412	LHG	C25-C26-C27-C28
37	C	517	DGD	O6D-C5D-C6D-O5D
23	A	410	CLA	C8-C10-C11-C12
26	b	601	SQD	C23-C24-C25-C26
23	C	511	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
28	B	623	LMT	C1-C2-C3-C4
23	B	617	CLA	C2-C3-C5-C6
23	b	621	CLA	C2-C3-C5-C6
23	B	615	CLA	C5-C6-C7-C8
38	L	101	LHG	C11-C10-C9-C8
23	c	516	CLA	C16-C17-C18-C20
37	h	102	DGD	C7A-C8A-C9A-CAA
27	D	2312	LMG	O6-C5-C6-O5
25	b	624	BCR	C21-C22-C23-C24
23	C	507	CLA	C5-C6-C7-C8
38	D	2309	LHG	C25-C26-C27-C28
38	l	103	LHG	C30-C31-C32-C33
23	B	611	CLA	C2A-CAA-CBA-CGA
37	c	520	DGD	CBA-CCA-CDA-CEA
26	l	101	SQD	C32-C33-C34-C35
37	c	520	DGD	C7B-C8B-C9B-CAB
26	l	101	SQD	C23-C24-C25-C26
37	H	103	DGD	C7A-C8A-C9A-CAA
26	B	621	SQD	C24-C23-O48-C46
26	B	621	SQD	C46-C45-O47-C7
26	l	101	SQD	C46-C45-O47-C7
27	A	413	LMG	C36-C37-C38-C39
23	a	2610	CLA	C8-C10-C11-C12
27	B	622	LMG	C29-C30-C31-C32
38	d	412	LHG	C26-C27-C28-C29
38	l	103	LHG	C11-C10-C9-C8
37	C	519	DGD	C5B-C6B-C7B-C8B
38	e	101	LHG	C1-C2-C3-O3
37	c	520	DGD	C9B-CAB-CBB-CCB
23	a	2613	CLA	CBA-CGA-O2A-C1
38	E	101	LHG	C26-C27-C28-C29
27	C	520	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
26	D	2302	SQD	C34-C35-C36-C37
33	d	411	PL9	C13-C14-C16-C17
26	l	101	SQD	C12-C13-C14-C15
38	L	101	LHG	C12-C13-C14-C15
26	b	601	SQD	C11-C12-C13-C14
38	d	403	LHG	C28-C29-C30-C31
26	d	417	SQD	C27-C28-C29-C30
26	b	601	SQD	C25-C26-C27-C28
26	A	412	SQD	C11-C12-C13-C14
38	D	2309	LHG	C11-C10-C9-C8
27	c	501	LMG	C40-C41-C42-C43
36	b	625	HTG	C4'-C5'-C6'-C7'
26	l	101	SQD	C27-C28-C29-C30
23	C	512	CLA	CBA-CGA-O2A-C1
37	c	520	DGD	C2A-C1A-O1G-C1G
36	b	626	HTG	C1'-C2'-C3'-C4'
26	B	621	SQD	C29-C30-C31-C32
27	B	622	LMG	C32-C33-C34-C35
38	E	101	LHG	C13-C14-C15-C16
38	l	103	LHG	C7-C8-C9-C10
33	A	422	PL9	C15-C14-C16-C17
28	B	623	LMT	C3'-C4'-O1B-C1B
27	m	2802	LMG	O9-C10-O7-C8
28	M	101	LMT	C2-C1-O1'-C1'
29	B	632	GOL	O1-C1-C2-O2
38	d	412	LHG	O1-C1-C2-O2
23	B	615	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C6-C7-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	b	616	CLA	C14-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C9
37	C	517	DGD	CAA-CBA-CCA-CDA
23	C	513	CLA	C4B-C3B-CAB-CBB
23	b	620	CLA	C4B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
37	D	2307	DGD	CDB-CEB-CFB-CGB
26	D	2302	SQD	C2-C1-O6-C44
27	B	622	LMG	C17-C18-C19-C20
27	C	520	LMG	C39-C40-C41-C42
37	h	102	DGD	CDA-CEA-CFA-CGA
38	E	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
38	e	101	LHG	O6-C4-C5-C6
26	a	2615	SQD	C30-C31-C32-C33
36	d	407	HTG	C3'-C4'-C5'-C6'
37	H	103	DGD	CDA-CEA-CFA-CGA
23	B	615	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C10-C8-C7
23	b	616	CLA	C12-C13-C15-C16
23	b	621	CLA	C11-C10-C8-C7
23	c	508	CLA	C11-C12-C13-C15
23	c	508	CLA	C12-C13-C15-C16
23	B	607	CLA	C10-C11-C12-C13
23	c	516	CLA	O1A-CGA-O2A-C1
28	d	401	LMT	C9-C10-C11-C12
38	D	2309	LHG	C29-C30-C31-C32
38	l	103	LHG	C12-C13-C14-C15
23	B	610	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
24	a	2611	PHO	C4-C3-C5-C6
23	C	513	CLA	C10-C11-C12-C13
23	C	506	CLA	C2-C3-C5-C6
26	D	2302	SQD	C7-C8-C9-C10
37	C	517	DGD	C2B-C3B-C4B-C5B
23	C	512	CLA	O1A-CGA-O2A-C1
37	C	517	DGD	C4D-C5D-C6D-O5D
38	e	101	LHG	C15-C16-C17-C18
36	d	407	HTG	C4'-C5'-C6'-C7'
37	C	518	DGD	C9A-CAA-CBA-CCA
37	c	519	DGD	C8A-C9A-CAA-CBA
36	d	415	HTG	S1-C1'-C2'-C3'
37	c	519	DGD	C5B-C6B-C7B-C8B
37	c	519	DGD	C6A-C7A-C8A-C9A
28	M	101	LMT	C1-C2-C3-C4
28	B	623	LMT	C5'-C4'-O1B-C1B
26	B	621	SQD	C44-C45-C46-O48
26	a	2603	SQD	O6-C44-C45-C46
28	F	102	LMT	O1'-C1-C2-C3
38	D	2309	LHG	C9-C10-C11-C12
23	d	402	CLA	C2C-C3C-CAC-CBC
27	m	2802	LMG	C31-C32-C33-C34
37	C	519	DGD	C6A-C7A-C8A-C9A
33	d	411	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	C33-C34-C35-C36
33	A	422	PL9	C13-C14-C16-C17
33	D	2306	PL9	C13-C14-C16-C17
23	B	617	CLA	C3-C5-C6-C7
37	D	2307	DGD	C4A-C5A-C6A-C7A
37	c	519	DGD	CBB-CCB-CDB-CEB
23	c	516	CLA	O1D-CGD-O2D-CED
37	C	518	DGD	C6A-C7A-C8A-C9A
23	a	2613	CLA	O1A-CGA-O2A-C1
23	b	620	CLA	C2B-C3B-CAB-CBB
25	B	618	BCR	C1-C6-C7-C8
25	C	516	BCR	C1-C6-C7-C8
25	D	2305	BCR	C23-C24-C25-C30
25	b	622	BCR	C1-C6-C7-C8
25	d	410	BCR	C23-C24-C25-C30
38	e	101	LHG	O2-C2-C3-O3
28	Z	101	LMT	O1'-C1-C2-C3
38	D	2309	LHG	C17-C18-C19-C20
27	C	520	LMG	C37-C38-C39-C40
23	B	614	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
26	d	417	SQD	O47-C45-C46-O48
38	L	101	LHG	C7-C8-C9-C10
33	D	2306	PL9	C15-C14-C16-C17
23	B	612	CLA	C2-C3-C5-C6
23	b	621	CLA	CBA-CGA-O2A-C1
28	d	404	LMT	C6-C7-C8-C9
26	B	621	SQD	O10-C23-O48-C46
23	b	621	CLA	C11-C10-C8-C9
23	c	508	CLA	C14-C13-C15-C16
23	c	510	CLA	C14-C13-C15-C16
36	B	626	HTG	C2'-C3'-C4'-C5'
37	h	102	DGD	C6B-C7B-C8B-C9B
36	d	407	HTG	C4-C5-C6-O6
27	d	414	LMG	C36-C37-C38-C39
36	B	627	HTG	O5-C5-C6-O6
37	H	103	DGD	C7B-C8B-C9B-CAB
28	f	101	LMT	O1'-C1-C2-C3
38	e	101	LHG	C10-C11-C12-C13
33	D	2306	PL9	C39-C41-C42-C43
33	d	411	PL9	C39-C41-C42-C43
36	B	624[B]	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
29	A	415	GOL	O1-C1-C2-O2
29	C	526	GOL	O1-C1-C2-O2
29	O	305	GOL	O2-C2-C3-O3
29	a	2602	GOL	O2-C2-C3-O3
29	a	2618	GOL	O1-C1-C2-O2
29	v	203	GOL	O2-C2-C3-O3
26	d	417	SQD	C26-C27-C28-C29
37	H	103	DGD	C6B-C7B-C8B-C9B
40	H	102	RRX	C9-C10-C11-C12
40	h	101	RRX	C9-C10-C11-C12
37	c	518	DGD	C6B-C7B-C8B-C9B
27	m	2802	LMG	C33-C34-C35-C36
26	B	621	SQD	C11-C10-C9-C8
23	c	513	CLA	CBA-CGA-O2A-C1
37	c	518	DGD	C6A-C7A-C8A-C9A
23	B	615	CLA	C8-C10-C11-C12
23	b	613	CLA	C13-C15-C16-C17
26	A	412	SQD	C34-C35-C36-C37
23	A	407	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C10-C8-C7
36	c	526	HTG	S1-C1'-C2'-C3'
26	a	2615	SQD	C32-C33-C34-C35
27	m	2802	LMG	C20-C21-C22-C23
38	L	101	LHG	C10-C11-C12-C13
37	C	518	DGD	CDB-CEB-CFB-CGB
25	C	515	BCR	C21-C22-C23-C24
26	d	417	SQD	C30-C31-C32-C33
26	D	2308	SQD	C5-C6-S-O8
26	l	101	SQD	C5-C6-S-O8
27	c	522	LMG	C8-C7-O1-C1
37	C	518	DGD	C2G-C3G-O3G-C1D
37	C	518	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
28	m	2804	LMT	C6-C7-C8-C9
23	b	607	CLA	C2A-CAA-CBA-CGA
38	D	2310	LHG	C34-C35-C36-C37
23	a	2613	CLA	C4-C3-C5-C6
37	h	102	DGD	O2G-C1B-C2B-C3B
29	c	530	GOL	O1-C1-C2-C3
38	D	2309	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	d	403	LHG	O1-C1-C2-C3
27	c	522	LMG	C37-C38-C39-C40
26	D	2308	SQD	C46-C45-O47-C7
37	C	517	DGD	C2A-C3A-C4A-C5A
23	c	513	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	O1A-C1A-O1G-C1G
37	D	2307	DGD	C6A-C7A-C8A-C9A
38	e	101	LHG	O6-C4-C5-O7
26	D	2302	SQD	O6-C44-C45-C46
27	c	501	LMG	C7-C8-C9-O8
36	C	521	HTG	S1-C1'-C2'-C3'
23	a	2613	CLA	C2-C3-C5-C6
26	d	417	SQD	C34-C35-C36-C37
37	D	2307	DGD	C7A-C8A-C9A-CAA
37	h	102	DGD	C7B-C8B-C9B-CAB
36	V	204	HTG	C2-C1-S1-C1'
36	i	102	HTG	C2-C1-S1-C1'
26	B	621	SQD	O47-C45-C46-O48
26	D	2302	SQD	O6-C44-C45-O47
26	D	2308	SQD	O47-C45-C46-O48
27	C	527	LMG	O7-C8-C9-O8
37	D	2307	DGD	O1G-C1G-C2G-O2G
23	C	507	CLA	C11-C12-C13-C14
38	d	412	LHG	C15-C16-C17-C18
23	b	621	CLA	O1A-CGA-O2A-C1
26	B	621	SQD	C31-C32-C33-C34
26	b	601	SQD	C28-C29-C30-C31
28	d	401	LMT	C11-C10-C9-C8
23	B	603	CLA	C13-C15-C16-C17
28	d	404	LMT	O1'-C1-C2-C3
26	l	101	SQD	C34-C35-C36-C37
38	l	103	LHG	C11-C12-C13-C14
26	D	2308	SQD	C33-C34-C35-C36
37	C	517	DGD	C6B-C7B-C8B-C9B
38	D	2309	LHG	C33-C34-C35-C36
37	c	518	DGD	C5B-C6B-C7B-C8B
23	C	506	CLA	C4-C3-C5-C6
26	a	2615	SQD	C26-C27-C28-C29
37	h	102	DGD	C8A-C9A-CAA-CBA
36	b	604	HTG	O5-C5-C6-O6
38	d	412	LHG	C13-C14-C15-C16
36	B	624[B]	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C1A-C2A-CAA-CBA
23	B	606	CLA	C4B-C3B-CAB-CBB
23	a	2610	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
27	A	413	LMG	C29-C28-O8-C9
27	A	413	LMG	C12-C13-C14-C15
23	A	406	CLA	C2C-C3C-CAC-CBC
38	l	103	LHG	C10-C11-C12-C13
27	C	520	LMG	C11-C12-C13-C14
23	A	410	CLA	C11-C10-C8-C7
23	B	604	CLA	C11-C10-C8-C7
23	C	514	CLA	C12-C13-C15-C16
23	a	2610	CLA	C11-C10-C8-C7
23	a	2610	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C7
23	c	515	CLA	C12-C13-C15-C16
37	h	102	DGD	C5B-C6B-C7B-C8B
38	L	101	LHG	C11-C12-C13-C14
37	H	103	DGD	O2G-C1B-C2B-C3B
27	D	2312	LMG	C12-C13-C14-C15
27	C	527	LMG	C31-C32-C33-C34
38	D	2309	LHG	C26-C27-C28-C29
38	d	403	LHG	C2-C3-O3-P
27	d	414	LMG	C30-C31-C32-C33
38	d	412	LHG	C30-C31-C32-C33
37	H	103	DGD	C5B-C6B-C7B-C8B
23	C	505	CLA	C15-C16-C17-C18
38	e	101	LHG	C13-C14-C15-C16
23	A	407	CLA	C11-C10-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
26	a	2603	SQD	C35-C36-C37-C38
27	A	413	LMG	O10-C28-O8-C9
26	a	2603	SQD	C32-C33-C34-C35
37	H	103	DGD	C8A-C9A-CAA-CBA
27	A	413	LMG	C22-C23-C24-C25
37	c	518	DGD	O6D-C5D-C6D-O5D
26	a	2603	SQD	O5-C5-C6-S
37	C	519	DGD	C8A-C9A-CAA-CBA
23	b	617	CLA	C8-C10-C11-C12
26	A	412	SQD	O6-C44-C45-O47
27	A	413	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
27	c	521	LMG	O7-C8-C9-O8
37	H	103	DGD	O1G-C1G-C2G-O2G
26	b	601	SQD	C2-C1-O6-C44
26	D	2308	SQD	C44-C45-C46-O48
37	D	2307	DGD	O1G-C1G-C2G-C3G
37	H	103	DGD	O1G-C1G-C2G-C3G
37	h	102	DGD	O1G-C1G-C2G-C3G
26	D	2302	SQD	C9-C10-C11-C12
26	d	417	SQD	C32-C33-C34-C35
26	l	101	SQD	C17-C18-C19-C20
38	e	101	LHG	C19-C20-C21-C22
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	b	606	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
28	z	102	LMT	C4-C5-C6-C7
38	D	2311	LHG	O10-C23-O8-C6
27	d	414	LMG	C29-C30-C31-C32
26	b	601	SQD	O5-C1-O6-C44
37	c	519	DGD	C6B-C7B-C8B-C9B
38	D	2310	LHG	C32-C33-C34-C35
27	c	521	LMG	C19-C20-C21-C22
23	a	2609	CLA	C2C-C3C-CAC-CBC
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
38	E	101	LHG	C4-O6-P-O4
38	L	101	LHG	C4-O6-P-O5
38	d	413	LHG	C3-O3-P-O5
38	l	103	LHG	C4-O6-P-O5
23	B	606	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
38	e	101	LHG	C9-C10-C11-C12
23	c	506	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	D	2311	LHG	C2-C3-O3-P
37	c	518	DGD	C4D-C5D-C6D-O5D
27	d	414	LMG	C12-C13-C14-C15
28	z	102	LMT	C2B-C1B-O1B-C4'
27	c	521	LMG	C31-C32-C33-C34
29	D	2301	GOL	O1-C1-C2-O2
29	c	531	GOL	O2-C2-C3-O3
29	d	416	GOL	O2-C2-C3-O3
27	C	520	LMG	C33-C34-C35-C36
36	B	624[B]	HTG	S1-C1'-C2'-C3'
37	D	2307	DGD	C9A-CAA-CBA-CCA
23	b	606	CLA	CAA-CBA-CGA-O2A
26	a	2603	SQD	C33-C34-C35-C36
23	b	615	CLA	C8-C10-C11-C12
36	I	101	HTG	C1'-C2'-C3'-C4'
26	B	621	SQD	C12-C13-C14-C15
36	b	602	HTG	C2'-C3'-C4'-C5'
28	J	303	LMT	C7-C8-C9-C10
23	A	410	CLA	C11-C10-C8-C9
23	B	617	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	b	618	CLA	C11-C12-C13-C14
23	B	605	CLA	C6-C7-C8-C10
23	c	506	CLA	C10-C11-C12-C13
26	B	621	SQD	C23-C24-C25-C26
37	H	103	DGD	C9B-CAB-CBB-CCB
23	c	510	CLA	C2A-CAA-CBA-CGA
28	T	103	LMT	C11-C10-C9-C8
26	B	621	SQD	C26-C27-C28-C29
23	C	507	CLA	O1A-CGA-O2A-C1
28	m	2803	LMT	O5'-C5'-C6'-O6'
37	c	519	DGD	C2E-C1E-O5D-C6D
37	C	518	DGD	C5B-C6B-C7B-C8B
23	a	2610	CLA	C16-C17-C18-C20
27	c	522	LMG	C10-C11-C12-C13
38	L	101	LHG	C14-C15-C16-C17
26	l	101	SQD	O47-C45-C46-O48
27	c	501	LMG	O7-C8-C9-O8
37	h	102	DGD	O1G-C1G-C2G-O2G
37	c	519	DGD	C2A-C3A-C4A-C5A
23	a	2610	CLA	C16-C17-C18-C19
27	C	520	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	l	101	SQD	C13-C14-C15-C16
23	b	615	CLA	C2A-CAA-CBA-CGA
28	M	101	LMT	C7-C8-C9-C10
37	c	520	DGD	C2A-C3A-C4A-C5A
23	B	611	CLA	C2-C1-O2A-CGA
27	C	527	LMG	C7-C8-C9-O8
36	o	301	HTG	C2'-C3'-C4'-C5'
27	B	622	LMG	C28-C29-C30-C31
23	B	609	CLA	C13-C15-C16-C17
36	b	625	HTG	C2'-C1'-S1-C1
28	A	420	LMT	C5-C6-C7-C8
26	a	2603	SQD	C45-C44-O6-C1
37	c	518	DGD	C5D-C6D-O5D-C1E
23	b	615	CLA	C16-C17-C18-C19
37	C	517	DGD	C7A-C8A-C9A-CAA
33	x	1301	PL9	C40-C39-C41-C42
27	B	622	LMG	O6-C5-C6-O5
37	C	519	DGD	C2A-C3A-C4A-C5A
37	C	519	DGD	C6B-C7B-C8B-C9B
36	H	101	HTG	C2'-C3'-C4'-C5'
38	e	101	LHG	C11-C10-C9-C8
28	m	2804	LMT	C5-C6-C7-C8
23	a	2609	CLA	C16-C17-C18-C20
23	b	611	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C9
23	d	409	CLA	C6-C7-C8-C9
27	B	622	LMG	C16-C17-C18-C19
27	m	2802	LMG	C19-C20-C21-C22
23	b	611	CLA	C4B-C3B-CAB-CBB
38	D	2311	LHG	C24-C23-O8-C6
24	a	2612	PHO	C2C-C3C-CAC-CBC
38	E	101	LHG	C19-C20-C21-C22
33	x	1301	PL9	C38-C39-C41-C42
37	C	517	DGD	CBA-CCA-CDA-CEA
23	c	507	CLA	C16-C17-C18-C20
28	M	102	LMT	O5'-C5'-C6'-O6'
23	c	514	CLA	C11-C12-C13-C15
23	d	409	CLA	C6-C7-C8-C10
23	b	615	CLA	C16-C17-C18-C20
27	C	527	LMG	C39-C40-C41-C42
37	C	517	DGD	CAB-CBB-CCB-CDB
23	b	614	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
38	E	101	LHG	C14-C15-C16-C17
23	b	619	CLA	C10-C11-C12-C13
37	C	517	DGD	O6E-C1E-O5D-C6D
27	C	520	LMG	O9-C10-O7-C8
38	D	2311	LHG	C31-C32-C33-C34
37	h	102	DGD	C9B-CAB-CBB-CCB
28	m	2804	LMT	O5'-C5'-C6'-O6'
37	C	519	DGD	C4B-C5B-C6B-C7B
27	C	527	LMG	C28-C29-C30-C31
38	d	413	LHG	O2-C2-C3-O3
36	B	624[A]	HTG	C2'-C3'-C4'-C5'
23	b	621	CLA	C15-C16-C17-C18
26	A	412	SQD	O6-C44-C45-C46
37	C	519	DGD	O1G-C1G-C2G-C3G
27	c	521	LMG	C30-C31-C32-C33
38	d	413	LHG	C11-C10-C9-C8
23	b	611	CLA	C11-C10-C8-C9
23	b	621	CLA	C6-C7-C8-C9
23	B	608	CLA	C16-C17-C18-C19
27	A	413	LMG	C20-C21-C22-C23
38	l	103	LHG	C14-C15-C16-C17
23	c	509	CLA	C5-C6-C7-C8
26	b	601	SQD	C16-C17-C18-C19
28	B	623	LMT	C6-C7-C8-C9
23	C	513	CLA	O1A-CGA-O2A-C1
27	C	527	LMG	C11-C12-C13-C14
37	c	519	DGD	C9B-CAB-CBB-CCB
38	d	412	LHG	C11-C10-C9-C8
33	A	422	PL9	C35-C34-C36-C37
33	x	1301	PL9	C25-C24-C26-C27
29	O	304	GOL	O1-C1-C2-O2
28	m	2804	LMT	C2B-C1B-O1B-C4'
36	i	102	HTG	C1'-C2'-C3'-C4'
38	d	413	LHG	C34-C35-C36-C37
23	B	606	CLA	O1A-CGA-O2A-C1
23	a	2609	CLA	C4C-C3C-CAC-CBC
26	A	412	SQD	C11-C10-C9-C8
23	C	503	CLA	C16-C17-C18-C20
38	d	413	LHG	C32-C33-C34-C35
23	B	604	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	a	2610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C2B-C3B-CAB-CBB
25	B	618	BCR	C5-C6-C7-C8
25	C	515	BCR	C1-C6-C7-C8
25	C	515	BCR	C23-C24-C25-C30
25	C	516	BCR	C5-C6-C7-C8
25	D	2305	BCR	C1-C6-C7-C8
25	D	2305	BCR	C23-C24-C25-C26
25	b	622	BCR	C5-C6-C7-C8
25	d	410	BCR	C1-C6-C7-C8
25	d	410	BCR	C23-C24-C25-C26
38	e	101	LHG	C26-C27-C28-C29
37	C	519	DGD	C8B-C9B-CAB-CBB
28	z	102	LMT	O5B-C1B-O1B-C4'
25	a	2614	BCR	C19-C20-C21-C22
23	A	410	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	b	620	CLA	C12-C13-C15-C16
23	c	504	CLA	C2A-CAA-CBA-CGA
26	D	2308	SQD	C25-C26-C27-C28
23	C	504	CLA	C10-C11-C12-C13
37	D	2307	DGD	C2B-C3B-C4B-C5B
27	A	413	LMG	C11-C12-C13-C14
28	A	420	LMT	C3-C4-C5-C6
26	D	2308	SQD	C28-C29-C30-C31
26	D	2308	SQD	C34-C35-C36-C37
23	c	507	CLA	C2-C3-C5-C6
23	c	509	CLA	C2-C1-O2A-CGA
23	b	609	CLA	C13-C15-C16-C17
27	c	501	LMG	C21-C22-C23-C24
28	B	623	LMT	C3-C4-C5-C6
27	C	527	LMG	C30-C31-C32-C33
23	a	2610	CLA	C6-C7-C8-C9
26	D	2308	SQD	C31-C32-C33-C34
26	a	2603	SQD	C13-C14-C15-C16
28	A	414	LMT	C2B-C1B-O1B-C4'
24	A	408	PHO	C2C-C3C-CAC-CBC
27	C	520	LMG	O10-C28-O8-C9
27	c	501	LMG	O8-C28-C29-C30
27	c	521	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	H	103	DGD	CDB-CEB-CFB-CGB
23	C	506	CLA	C16-C17-C18-C19
39	F	101	HEM	CAD-CBD-CGD-O1D
23	B	615	CLA	C15-C16-C17-C18
28	i	103	LMT	C2-C1-O1'-C1'
33	A	422	PL9	C40-C39-C41-C42
33	x	1301	PL9	C15-C14-C16-C17
27	d	414	LMG	C35-C36-C37-C38
37	C	518	DGD	CBA-CCA-CDA-CEA
23	B	608	CLA	C16-C17-C18-C20
23	B	612	CLA	C15-C16-C17-C18
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	607	CLA	C4B-C3B-CAB-CBB
23	B	608	CLA	C4B-C3B-CAB-CBB
23	b	608	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	CAA-CBA-CGA-O2A
36	i	102	HTG	C2'-C3'-C4'-C5'
24	A	409	PHO	CHA-CBD-CGD-O1D
24	A	409	PHO	CHA-CBD-CGD-O2D
36	I	101	HTG	C4'-C5'-C6'-C7'
37	D	2307	DGD	O2G-C1B-C2B-C3B
28	A	414	LMT	O5B-C1B-O1B-C4'
23	C	507	CLA	CBA-CGA-O2A-C1
39	F	101	HEM	CAA-CBA-CGA-O2A
39	e	103	HEM	CAA-CBA-CGA-O2A
23	C	509	CLA	C10-C11-C12-C13
37	D	2307	DGD	C5D-C6D-O5D-C1E
28	T	103	LMT	C4-C5-C6-C7
27	A	413	LMG	O1-C7-C8-O7
23	B	605	CLA	C13-C15-C16-C17
37	C	519	DGD	C1A-C2A-C3A-C4A
33	x	1301	PL9	C13-C14-C16-C17
28	m	2804	LMT	O5'-C1'-O1'-C1
37	C	518	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
23	c	509	CLA	C11-C12-C13-C15
42	V	201	HEC	CAD-CBD-CGD-O2D
27	d	414	LMG	C37-C38-C39-C40
23	c	511	CLA	C15-C16-C17-C18
37	h	102	DGD	CDB-CEB-CFB-CGB
28	d	401	LMT	C1-C2-C3-C4
26	l	101	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
42	v	201	HEC	CAD-CBD-CGD-O2D
23	c	515	CLA	C14-C13-C15-C16
37	D	2307	DGD	C6B-C7B-C8B-C9B
24	a	2611	PHO	C8-C10-C11-C12
28	B	634	LMT	C4-C5-C6-C7
26	d	417	SQD	C44-C45-O47-C7
26	d	417	SQD	C46-C45-O47-C7
28	B	634	LMT	C6-C7-C8-C9
23	C	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C2-C1-O2A-CGA
26	D	2302	SQD	C16-C17-C18-C19
23	c	508	CLA	C3A-C2A-CAA-CBA
42	v	201	HEC	CAD-CBD-CGD-O1D
23	c	509	CLA	C13-C15-C16-C17
27	m	2802	LMG	C18-C19-C20-C21
28	J	303	LMT	C4'-C5'-C6'-O6'
23	d	402	CLA	C4C-C3C-CAC-CBC
27	C	520	LMG	C29-C28-O8-C9
37	C	518	DGD	C2E-C1E-O5D-C6D
27	D	2312	LMG	C30-C31-C32-C33
37	D	2307	DGD	C5A-C6A-C7A-C8A
38	D	2311	LHG	C30-C31-C32-C33
23	C	510	CLA	C15-C16-C17-C18
27	C	527	LMG	C35-C36-C37-C38
23	A	407	CLA	C13-C15-C16-C17
23	A	405	CLA	C2C-C3C-CAC-CBC
28	M	101	LMT	C5-C6-C7-C8
23	c	513	CLA	C2-C3-C5-C6
26	a	2615	SQD	C28-C29-C30-C31
23	D	2304	CLA	C16-C17-C18-C19
26	d	417	SQD	O5-C5-C6-S
39	e	103	HEM	CAA-CBA-CGA-O1A
28	B	623	LMT	C2B-C1B-O1B-C4'
23	B	613	CLA	C3-C5-C6-C7
38	d	413	LHG	C1-C2-C3-O3
23	B	614	CLA	C15-C16-C17-C18
28	M	102	LMT	C4B-C5B-C6B-O6B
42	V	201	HEC	CAD-CBD-CGD-O1D
29	A	417	GOL	O1-C1-C2-O2
29	c	530	GOL	O1-C1-C2-O2
27	D	2312	LMG	C17-C18-C19-C20
38	D	2309	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
36	o	301	HTG	S1-C1'-C2'-C3'
26	b	601	SQD	O49-C7-O47-C45
37	C	519	DGD	O1G-C1A-C2A-C3A
24	A	408	PHO	C2-C3-C5-C6
26	b	601	SQD	C14-C15-C16-C17
27	d	414	LMG	C13-C14-C15-C16
36	b	626	HTG	C3'-C4'-C5'-C6'
38	d	413	LHG	C31-C32-C33-C34
26	a	2615	SQD	O6-C44-C45-O47
23	B	604	CLA	C6-C7-C8-C9
23	B	604	CLA	C11-C10-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	a	2610	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16
26	b	601	SQD	C15-C16-C17-C18
28	i	103	LMT	O1'-C1-C2-C3
24	A	408	PHO	C4-C3-C5-C6
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C12-C13-C15-C16
23	a	2610	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C12-C13-C15
23	D	2303	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C2B-C3B-CAB-CBB
25	C	515	BCR	C5-C6-C7-C8
25	D	2305	BCR	C5-C6-C7-C8
25	a	2614	BCR	C1-C6-C7-C8
23	b	618	CLA	C2-C1-O2A-CGA
23	b	619	CLA	C2-C1-O2A-CGA
37	C	517	DGD	C2E-C1E-O5D-C6D
23	c	505	CLA	C16-C17-C18-C20
37	C	517	DGD	O2G-C1B-C2B-C3B
37	c	518	DGD	O6E-C1E-O5D-C6D
23	B	613	CLA	C8-C10-C11-C12
39	e	103	HEM	CAD-CBD-CGD-O1D
28	T	103	LMT	C1-C2-C3-C4
23	B	602	CLA	C4-C3-C5-C6
23	B	602	CLA	C2-C3-C5-C6
39	F	101	HEM	CAD-CBD-CGD-O2D
36	C	521	HTG	C2'-C1'-S1-C1
36	b	602	HTG	C2'-C1'-S1-C1
36	b	626	HTG	C2'-C1'-S1-C1
36	d	407	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
36	o	301	HTG	C2'-C1'-S1-C1
23	C	502	CLA	C2A-CAA-CBA-CGA
26	b	601	SQD	C8-C7-O47-C45
37	D	2307	DGD	C8B-C9B-CAB-CBB
38	L	101	LHG	C16-C17-C18-C19
36	B	627	HTG	C4'-C5'-C6'-C7'
37	C	518	DGD	O2G-C1B-C2B-C3B
26	B	621	SQD	C30-C31-C32-C33
28	m	2804	LMT	C2-C3-C4-C5
23	c	513	CLA	C4-C3-C5-C6
33	x	1301	PL9	C23-C24-C26-C27
28	B	623	LMT	C5-C6-C7-C8
37	c	520	DGD	CAB-CBB-CCB-CDB
28	A	420	LMT	C11-C10-C9-C8
23	C	508	CLA	C5-C6-C7-C8
23	A	405	CLA	C4C-C3C-CAC-CBC
23	a	2610	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C9
23	b	620	CLA	C14-C13-C15-C16
27	A	413	LMG	O1-C7-C8-C9
27	c	521	LMG	O1-C7-C8-C9
23	B	610	CLA	C1A-C2A-CAA-CBA
23	D	2303	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB
23	d	408	CLA	C4B-C3B-CAB-CBB
26	d	417	SQD	C24-C25-C26-C27
23	B	612	CLA	C4-C3-C5-C6
23	d	402	CLA	C15-C16-C17-C18
28	M	102	LMT	O5'-C1'-O1'-C1
28	m	2803	LMT	O5'-C1'-O1'-C1
23	C	511	CLA	CAA-CBA-CGA-O2A
23	c	513	CLA	CAA-CBA-CGA-O2A
27	c	521	LMG	O7-C10-C11-C12
28	z	102	LMT	C4'-C5'-C6'-O6'
27	c	522	LMG	O7-C8-C9-O8
38	E	101	LHG	O7-C5-C6-O8
23	a	2613	CLA	C16-C17-C18-C19
37	C	519	DGD	O6E-C5E-C6E-O5E
38	d	412	LHG	O8-C23-C24-C25
39	e	103	HEM	CAD-CBD-CGD-O2D
39	F	101	HEM	CAA-CBA-CGA-O1A
26	l	101	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	B	616	CLA	C5-C6-C7-C8
23	d	408	CLA	C2-C1-O2A-CGA
27	B	622	LMG	O8-C28-C29-C30
37	c	518	DGD	O2G-C1B-C2B-C3B
23	B	604	CLA	C6-C7-C8-C10
23	B	616	CLA	C11-C10-C8-C7
23	a	2610	CLA	C11-C12-C13-C15
37	c	520	DGD	O6D-C5D-C6D-O5D
27	c	501	LMG	C30-C31-C32-C33
38	D	2310	LHG	C16-C17-C18-C19
28	d	401	LMT	O5B-C5B-C6B-O6B
23	b	606	CLA	CBA-CGA-O2A-C1
38	L	101	LHG	C17-C18-C19-C20
23	A	406	CLA	C15-C16-C17-C18
23	B	605	CLA	C4-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
33	A	422	PL9	C33-C34-C36-C37
38	D	2309	LHG	C28-C29-C30-C31
27	B	622	LMG	O10-C28-O8-C9
37	D	2307	DGD	C9B-CAB-CBB-CCB
37	C	519	DGD	C9B-CAB-CBB-CCB
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	513	CLA	CAA-CBA-CGA-O2A
27	c	521	LMG	C12-C13-C14-C15
23	D	2304	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	C	508	CLA	C14-C13-C15-C16
23	c	512	CLA	C14-C13-C15-C16
38	d	403	LHG	C29-C30-C31-C32
37	c	520	DGD	O1G-C1A-C2A-C3A
37	C	519	DGD	O1A-C1A-C2A-C3A
37	C	519	DGD	CBA-CCA-CDA-CEA
37	c	519	DGD	C8B-C9B-CAB-CBB
27	A	413	LMG	C29-C30-C31-C32
23	b	618	CLA	CAA-CBA-CGA-O2A
23	B	617	CLA	C13-C15-C16-C17
23	C	504	CLA	C15-C16-C17-C18
23	c	515	CLA	C15-C16-C17-C18
37	C	517	DGD	O1B-C1B-C2B-C3B
23	B	606	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CAA-CBA-CGA-O1A
38	d	412	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
36	o	301	HTG	C1'-C2'-C3'-C4'
27	B	622	LMG	C8-C7-O1-C1
27	m	2802	LMG	C8-C7-O1-C1
27	d	414	LMG	C20-C21-C22-C23
26	a	2615	SQD	C31-C32-C33-C34
27	B	622	LMG	O10-C28-C29-C30
37	C	518	DGD	O1B-C1B-C2B-C3B
23	b	617	CLA	CAA-CBA-CGA-O2A
27	A	413	LMG	O8-C28-C29-C30
27	c	501	LMG	C14-C15-C16-C17
36	b	602	HTG	C4-C5-C6-O6
27	c	521	LMG	O9-C10-C11-C12
28	d	404	LMT	C3'-C4'-O1B-C1B
23	C	506	CLA	CAA-CBA-CGA-O2A
33	A	422	PL9	C38-C39-C41-C42
23	c	512	CLA	C3-C5-C6-C7
28	z	102	LMT	C11-C10-C9-C8
23	b	606	CLA	O1A-CGA-O2A-C1
27	C	527	LMG	C40-C41-C42-C43
23	B	606	CLA	CAD-CBD-CGD-O2D
23	b	621	CLA	CAD-CBD-CGD-O2D
24	A	408	PHO	CAD-CBD-CGD-O2D
26	b	601	SQD	C26-C27-C28-C29
27	B	622	LMG	C33-C34-C35-C36
23	C	511	CLA	CAA-CBA-CGA-O1A
37	c	519	DGD	O2G-C1B-C2B-C3B
33	A	422	PL9	C16-C17-C18-C19
23	a	2613	CLA	C12-C13-C15-C16
27	d	414	LMG	O7-C10-C11-C12
38	L	101	LHG	O7-C7-C8-C9
23	C	507	CLA	C10-C11-C12-C13
37	D	2307	DGD	C8A-C9A-CAA-CBA
38	l	103	LHG	O7-C7-C8-C9
38	l	103	LHG	C17-C18-C19-C20
37	c	520	DGD	O1A-C1A-C2A-C3A
38	d	413	LHG	C14-C15-C16-C17

There are no ring outliers.

180 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	622	LMG	1	0
23	c	515	CLA	2	0
36	B	625	HTG	1	0
23	B	615	CLA	2	0
37	C	519	DGD	2	0
38	l	103	LHG	2	0
23	b	612	CLA	1	0
23	b	617	CLA	1	0
28	i	103	LMT	1	0
25	Y	302	BCR	2	0
27	A	413	LMG	3	0
25	b	623	BCR	3	0
23	C	503	CLA	4	0
25	K	101	BCR	1	0
34	U	503	DMS	1	0
28	m	2803	LMT	1	0
36	b	604	HTG	1	0
23	A	406	CLA	2	0
23	B	605	CLA	1	0
38	d	413	LHG	1	0
36	I	101	HTG	2	0
23	B	610	CLA	1	0
26	a	2603	SQD	2	0
34	B	637	DMS	1	0
28	d	401	LMT	6	0
23	B	617	CLA	2	0
37	D	2307	DGD	3	0
24	A	409	PHO	3	0
38	D	2311	LHG	2	0
34	a	2624	DMS	1	0
28	A	420	LMT	3	0
23	c	505	CLA	2	0
23	b	606	CLA	1	0
26	a	2615	SQD	1	0
23	B	604	CLA	3	0
23	A	410	CLA	4	0
23	b	621	CLA	3	0
23	B	606	CLA	4	0
34	V	206	DMS	1	0
36	i	102	HTG	1	0
23	C	511	CLA	3	0
36	b	625	HTG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	j	2701	LMT	1	0
28	A	414	LMT	6	0
23	d	408	CLA	1	0
39	e	103	HEM	2	0
23	B	613	CLA	2	0
29	O	302	GOL	1	0
25	B	618	BCR	1	0
25	a	2614	BCR	2	0
33	x	1301	PL9	2	0
29	B	648	GOL	3	0
36	C	521	HTG	2	0
34	d	418	DMS	1	0
23	C	507	CLA	5	0
26	D	2302	SQD	3	0
23	B	614	CLA	3	0
25	b	624	BCR	2	0
25	b	622	BCR	2	0
34	A	430	DMS	1	0
34	o	307	DMS	1	0
29	a	2602	GOL	1	0
23	b	611	CLA	4	0
23	B	616	CLA	2	0
36	b	602	HTG	2	0
25	D	2305	BCR	2	0
23	b	607	CLA	1	0
26	d	417	SQD	2	0
38	e	101	LHG	1	0
38	D	2309	LHG	1	0
34	c	535	DMS	1	0
25	z	101	BCR	2	0
23	b	618	CLA	4	0
38	D	2310	LHG	1	0
29	b	631	GOL	1	0
27	D	2312	LMG	2	0
29	b	644	GOL	3	0
34	D	2320	DMS	1	0
34	c	536	DMS	1	0
23	c	514	CLA	5	0
23	C	509	CLA	3	0
27	m	2802	LMG	1	0
36	B	627	HTG	1	0
23	c	506	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	404	LMT	1	0
25	B	619	BCR	3	0
23	C	506	CLA	4	0
28	M	101	LMT	1	0
23	c	512	CLA	2	0
24	A	408	PHO	1	0
37	c	519	DGD	1	0
23	c	509	CLA	4	0
23	C	513	CLA	5	0
37	C	517	DGD	2	0
27	c	501	LMG	4	0
40	h	101	RRX	3	0
36	b	626	HTG	1	0
23	C	514	CLA	6	0
23	B	607	CLA	1	0
33	d	411	PL9	1	0
23	c	516	CLA	2	0
25	c	517	BCR	2	0
23	b	614	CLA	2	0
36	o	301	HTG	2	0
23	a	2609	CLA	3	0
36	H	101	HTG	2	0
34	V	212	DMS	1	0
36	B	624[B]	HTG	2	0
25	C	516	BCR	3	0
23	c	507	CLA	2	0
34	B	642	DMS	1	0
27	c	521	LMG	1	0
23	D	2303	CLA	3	0
33	A	422	PL9	4	0
26	b	601	SQD	1	0
23	C	502	CLA	5	0
34	o	314	DMS	2	0
28	Z	101	LMT	2	0
38	d	412	LHG	4	0
23	b	615	CLA	4	0
39	F	101	HEM	1	0
23	b	609	CLA	2	0
23	B	609	CLA	1	0
26	B	621	SQD	2	0
23	d	402	CLA	5	0
23	b	608	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	c	543	DMS	1	0
34	v	209	DMS	1	0
23	C	512	CLA	2	0
37	c	518	DGD	1	0
27	C	527	LMG	2	0
38	d	403	LHG	1	0
34	B	638	DMS	1	0
25	y	101	BCR	2	0
23	c	510	CLA	3	0
25	C	515	BCR	2	0
25	d	410	BCR	2	0
23	A	407	CLA	3	0
23	B	611	CLA	4	0
34	O	307	DMS	1	0
25	B	620	BCR	2	0
25	B	633	BCR	4	0
40	H	102	RRX	3	0
38	L	101	LHG	1	0
23	a	2613	CLA	1	0
26	l	101	SQD	4	0
27	c	522	LMG	4	0
29	c	530	GOL	1	0
23	C	504	CLA	6	0
34	b	639	DMS	1	0
23	b	610	CLA	2	0
23	C	510	CLA	3	0
29	B	632	GOL	2	0
26	D	2308	SQD	1	0
23	C	505	CLA	2	0
23	C	508	CLA	4	0
36	b	603	HTG	1	0
34	B	647	DMS	2	0
23	A	405	CLA	2	0
36	C	525	HTG	1	0
23	a	2610	CLA	2	0
23	c	508	CLA	4	0
36	d	407	HTG	3	0
25	T	102	BCR	3	0
24	a	2612	PHO	2	0
23	b	616	CLA	1	0
28	z	102	LMT	4	0
28	B	634	LMT	1	0

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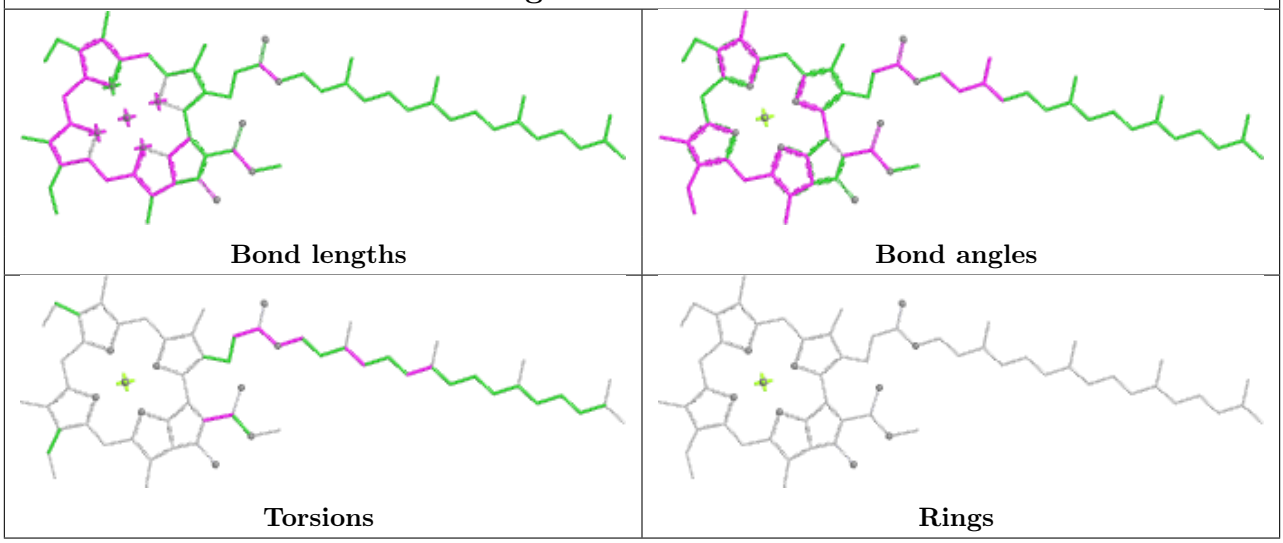
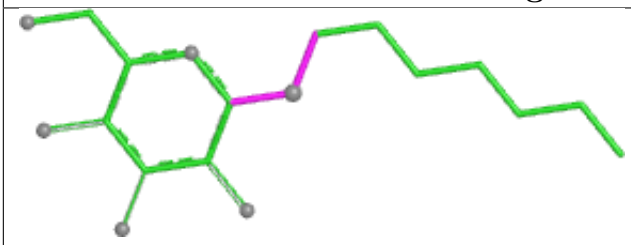
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	d	414	LMG	4	0
25	k	302	BCR	1	0
34	B	644	DMS	1	0
23	c	504	CLA	3	0
26	A	412	SQD	2	0
37	C	518	DGD	2	0
23	D	2304	CLA	1	0
28	B	623	LMT	1	0
34	C	536	DMS	1	0
29	C	526	GOL	2	0
23	b	620	CLA	4	0

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.

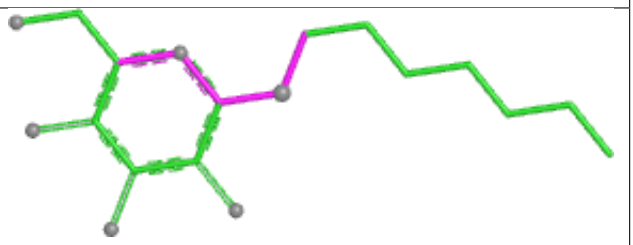
Ligand CLA B 602



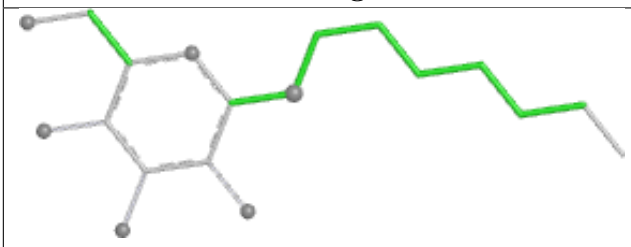
Ligand HTG c 524



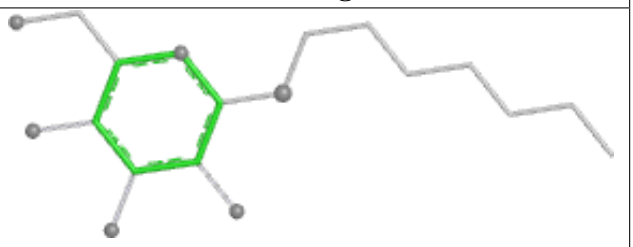
Bond lengths



Bond angles

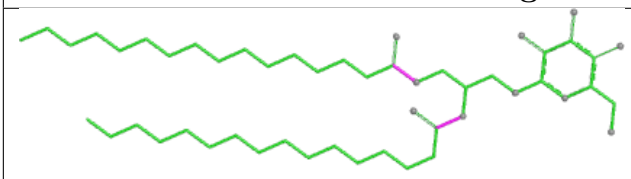


Torsions

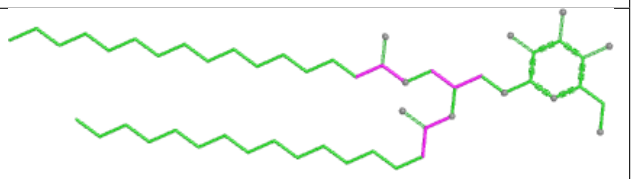


Rings

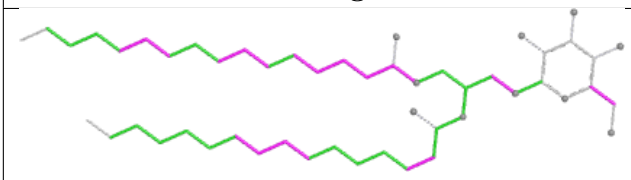
Ligand LMG B 622



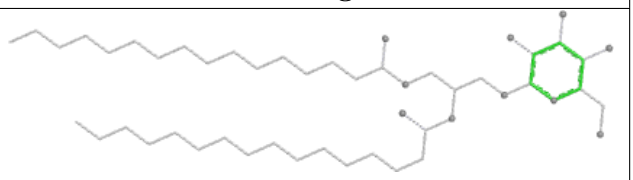
Bond lengths



Bond angles

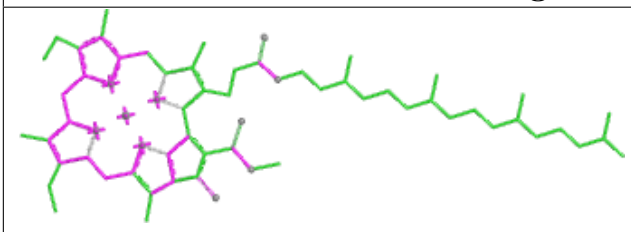


Torsions

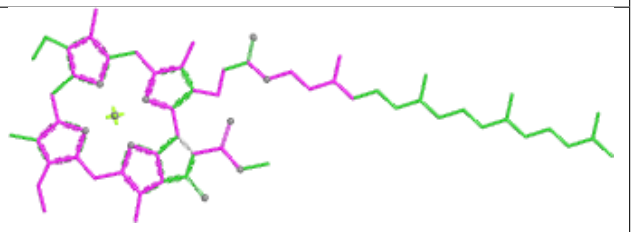


Rings

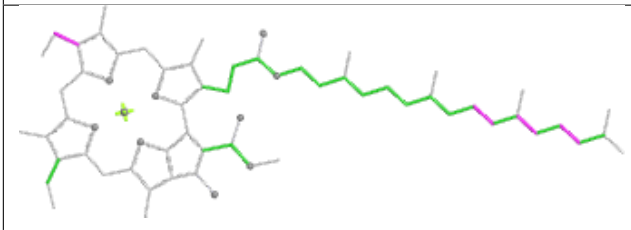
Ligand CLA c 515



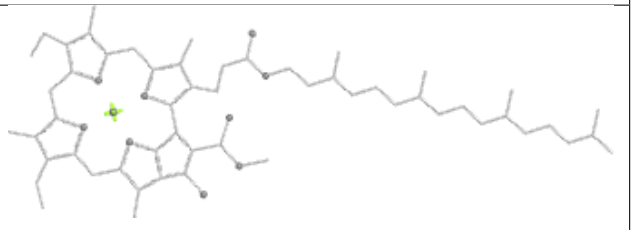
Bond lengths



Bond angles

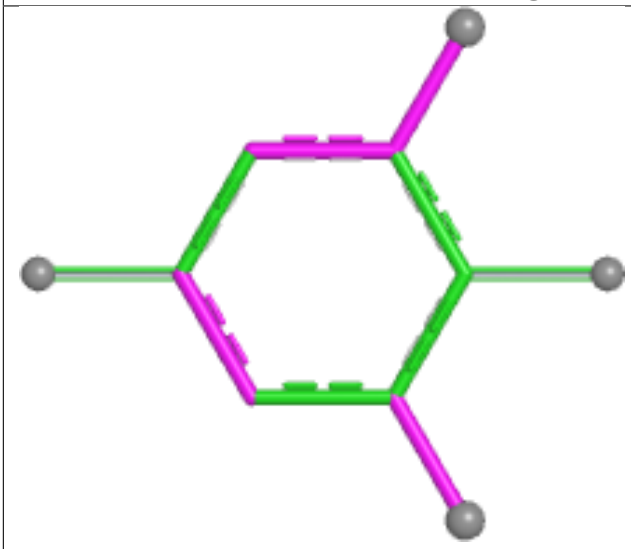


Torsions



Rings

Ligand JOX A 418



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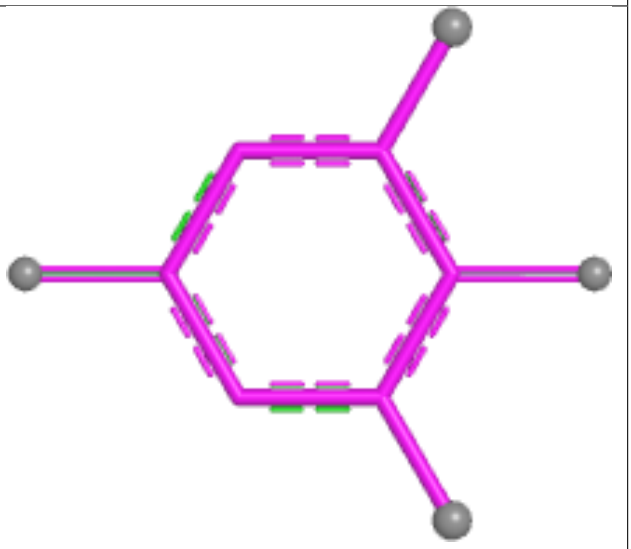
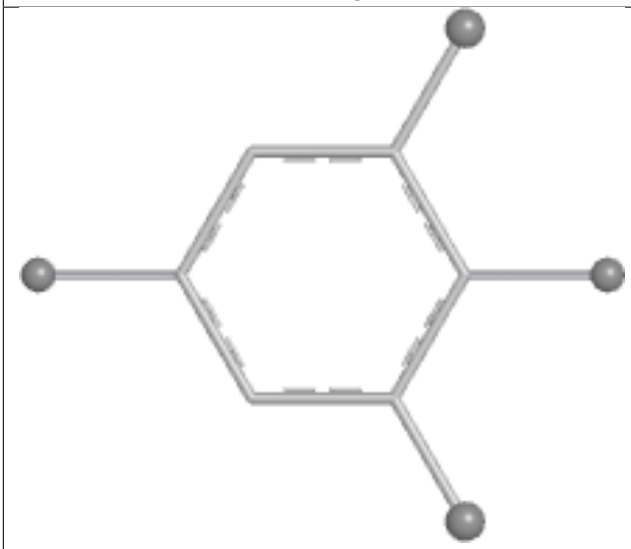


Bond angles



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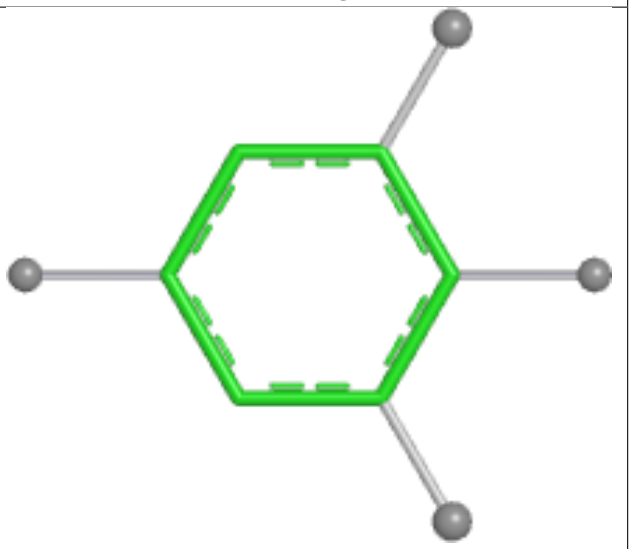
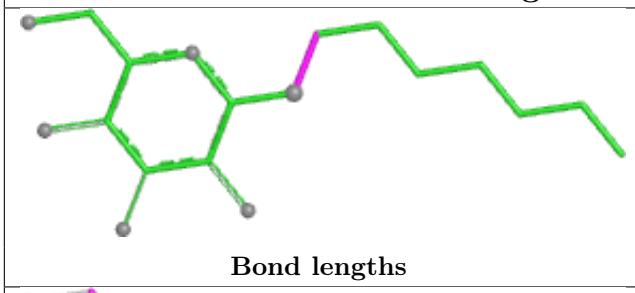


Rings

Ligand HTG B 625



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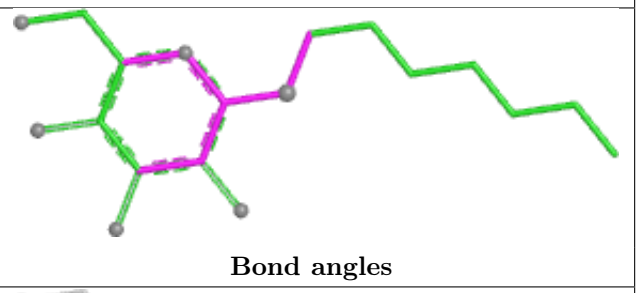
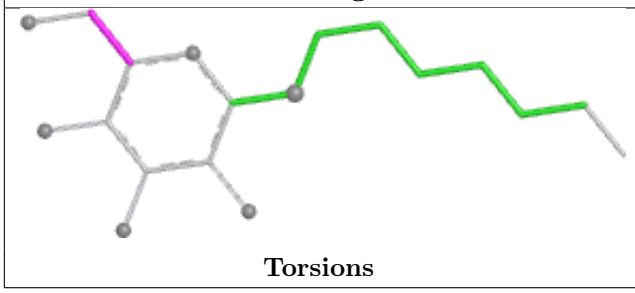


Bond angles



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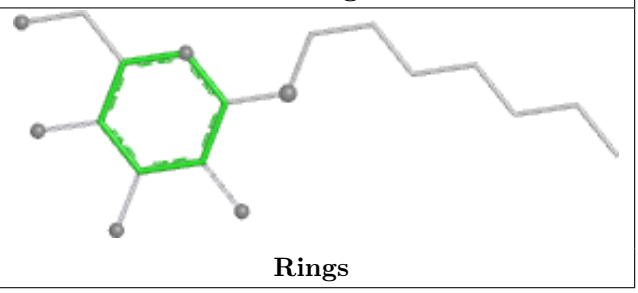
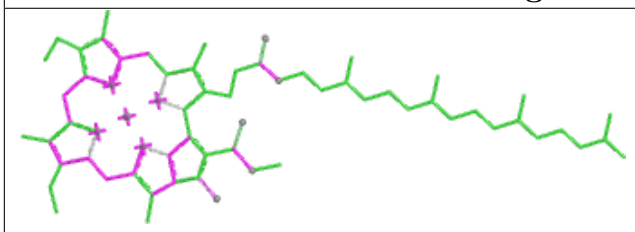


Rings

Ligand CLA B 615



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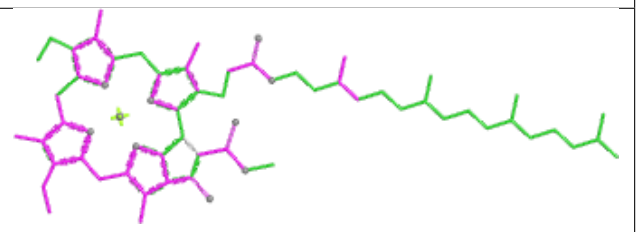
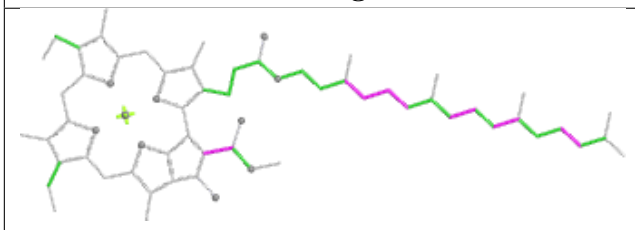


Bond angles



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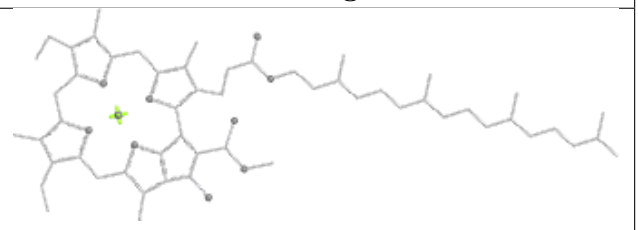
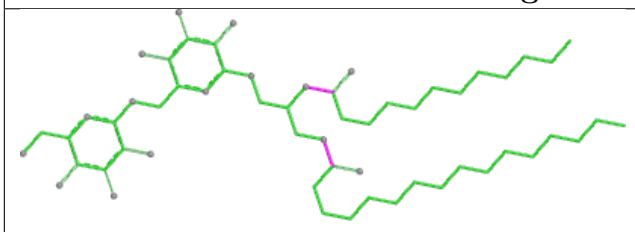


Rings

Ligand DGD C 519



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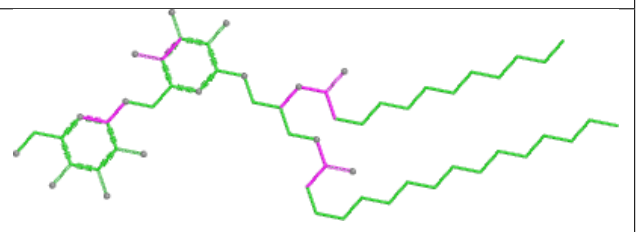
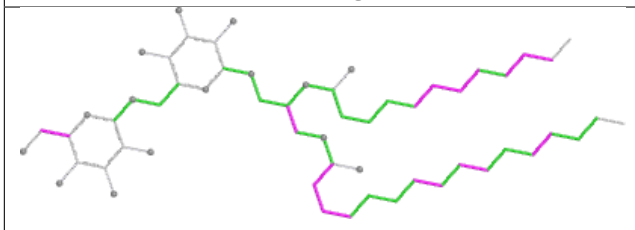
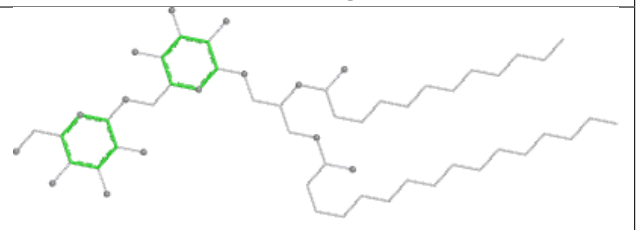


Bond angles

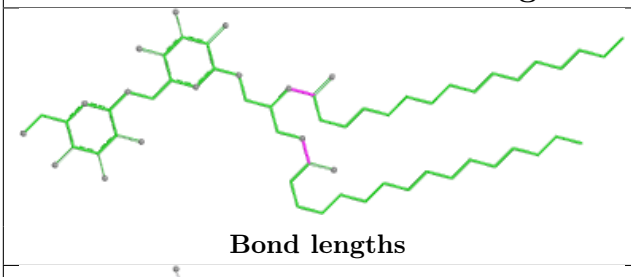


Torsions



Rings

Ligand DGD H 103



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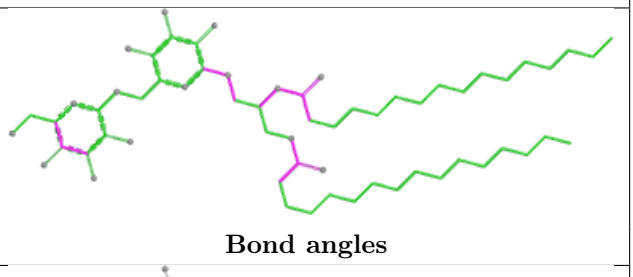
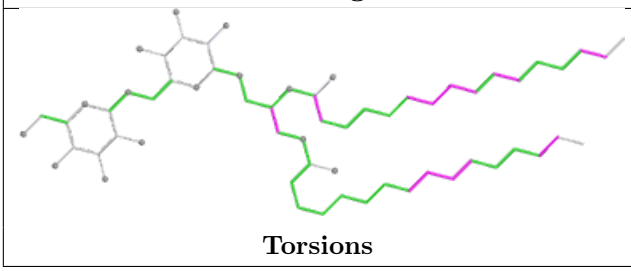


Bond angles



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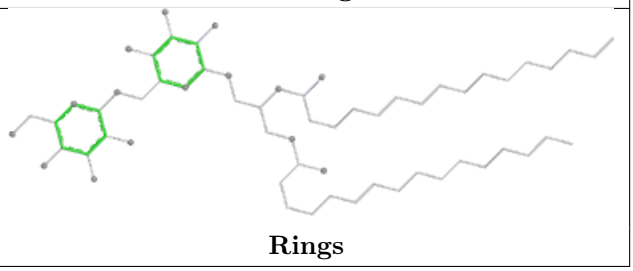
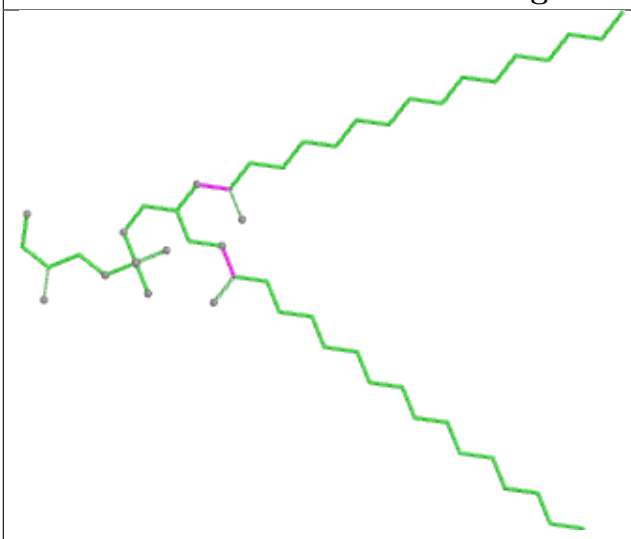


Rings

Ligand LHG l 103



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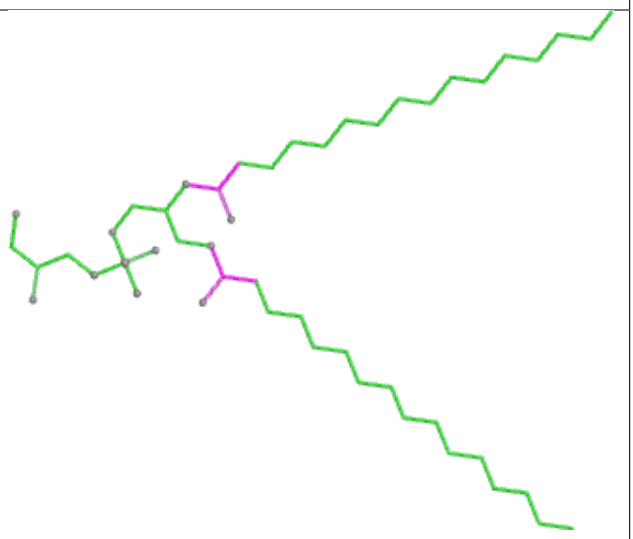
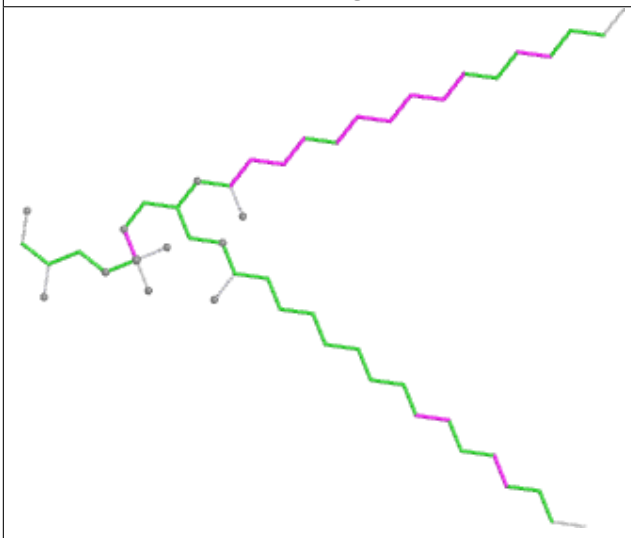


Bond angles



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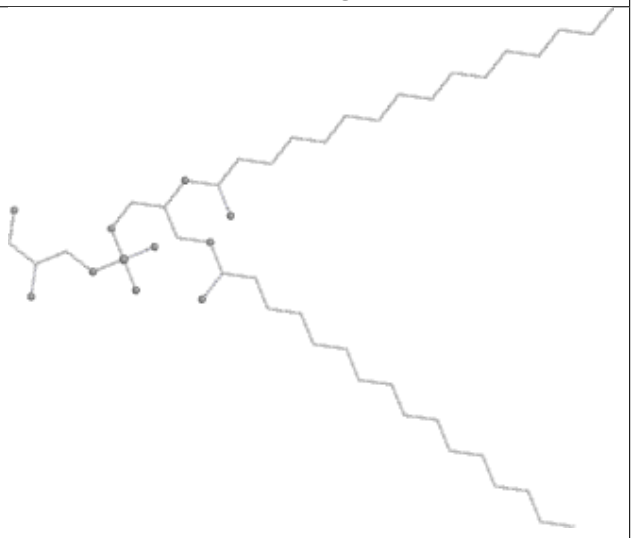
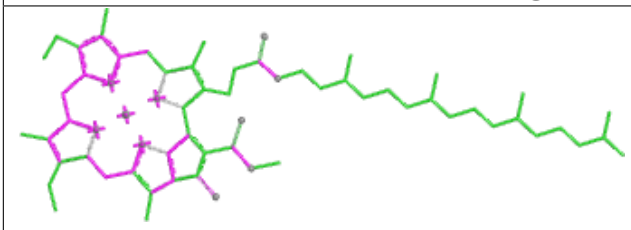


Rings

Ligand CLA b 612



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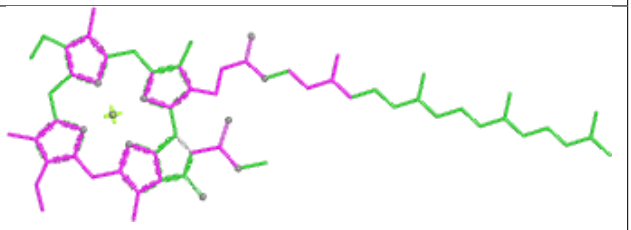
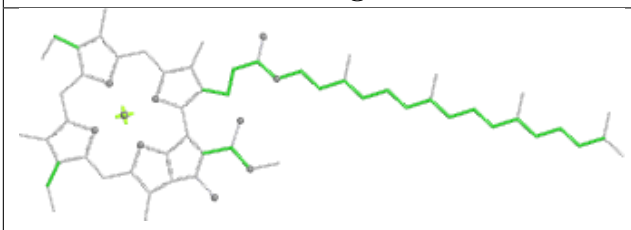


Bond angles



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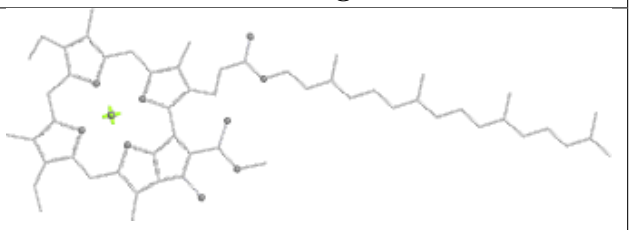
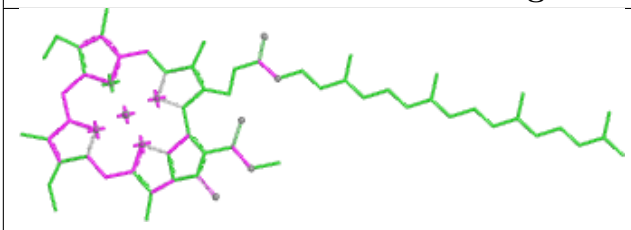


Rings

Ligand CLA b 617



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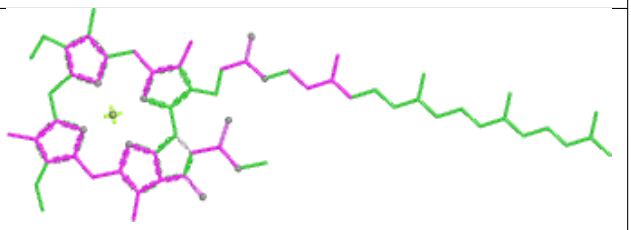
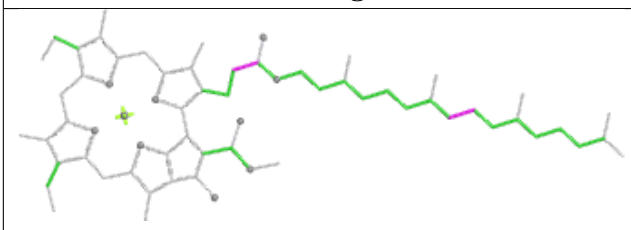
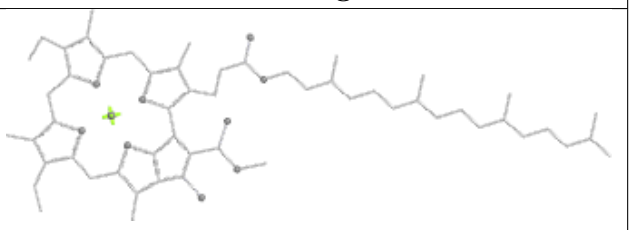


Bond angles

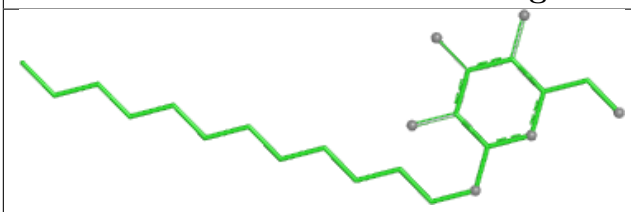


Torsions



Rings

Ligand LMT i 103



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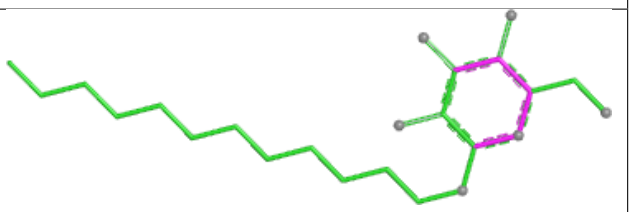
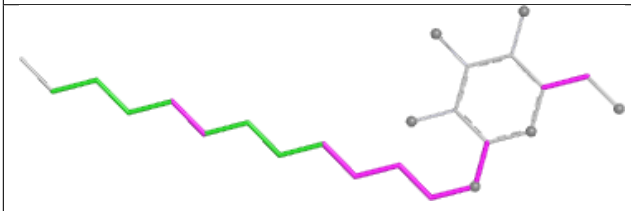


Bond angles



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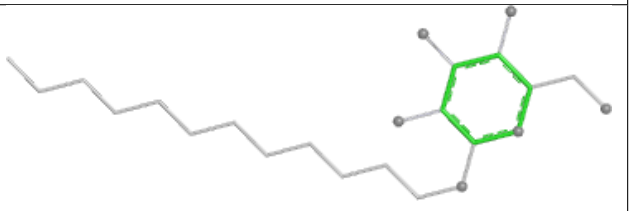
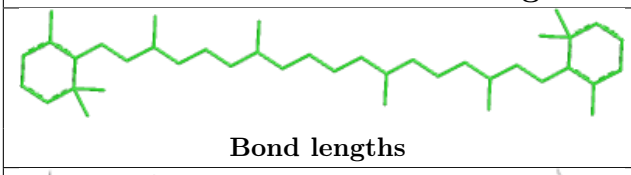


Rings

Ligand BCR Y 302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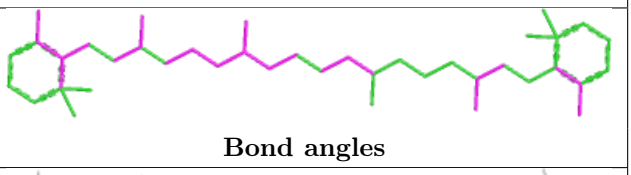
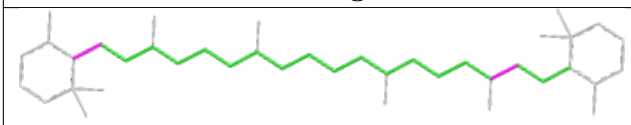
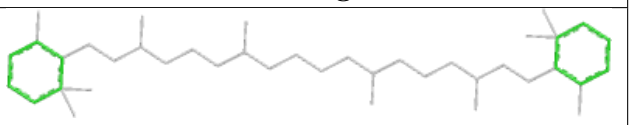
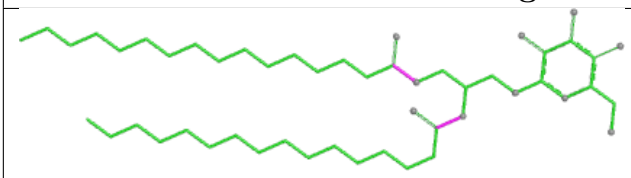

Bond angles


Torsions


Rings

Ligand LMG A 413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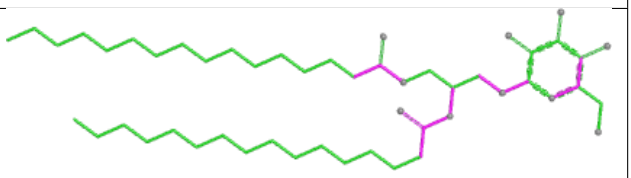
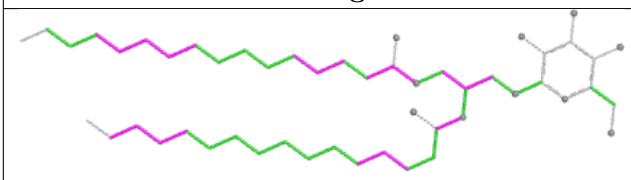

Bond angles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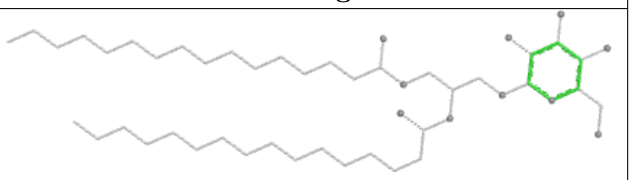
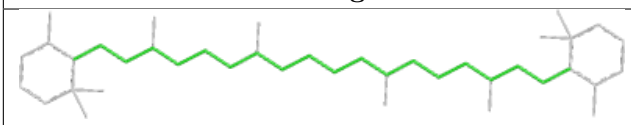
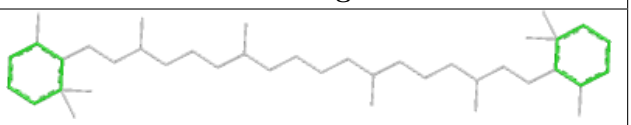

Rings

Ligand BCR b 623

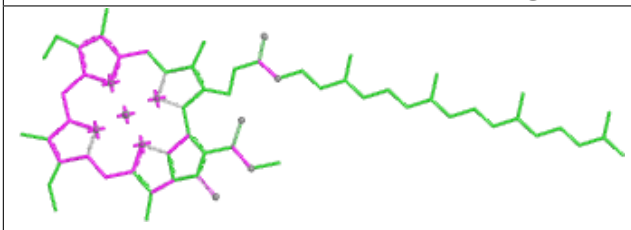
Bond lengths

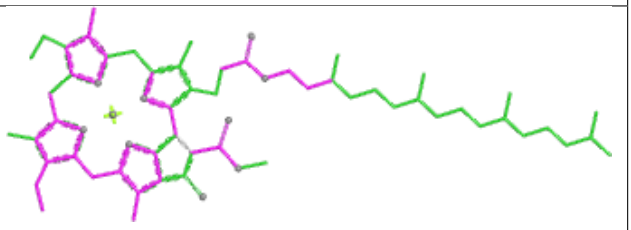
Bond angles

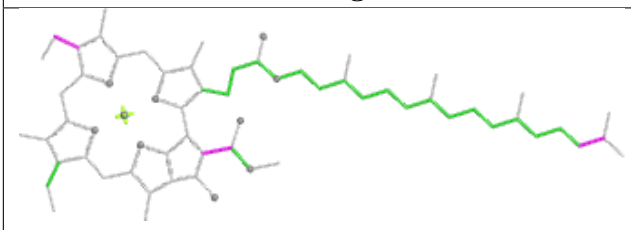

Torsions


Rings

Ligand CLA C 503


Bond lengths


Bond angles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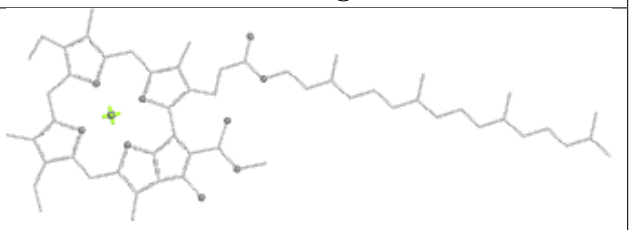
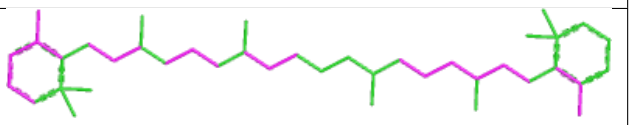
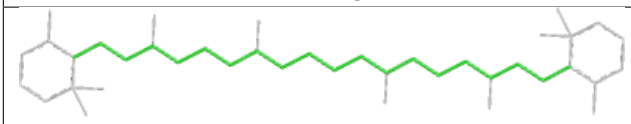
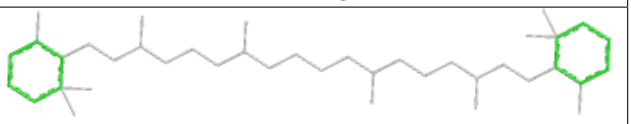

Rings

Ligand BCR K 101

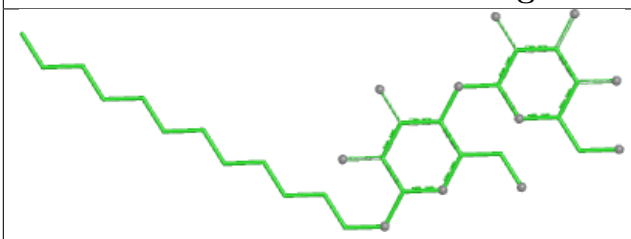
Bond lengths

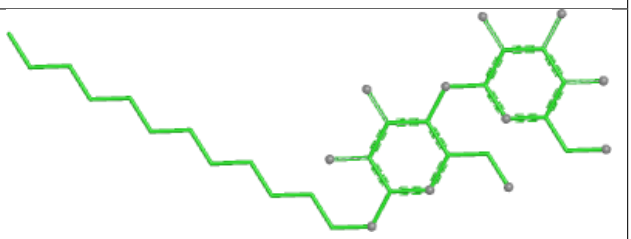

Bond angles

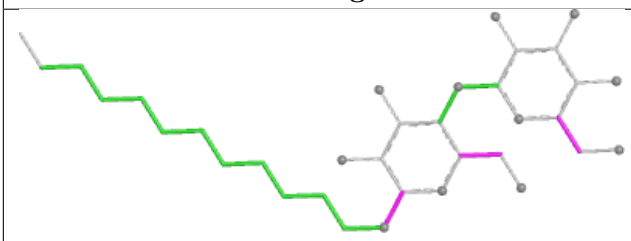

Torsions

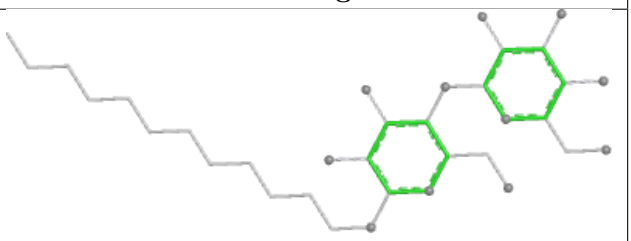

Rings

Ligand LMT M 102

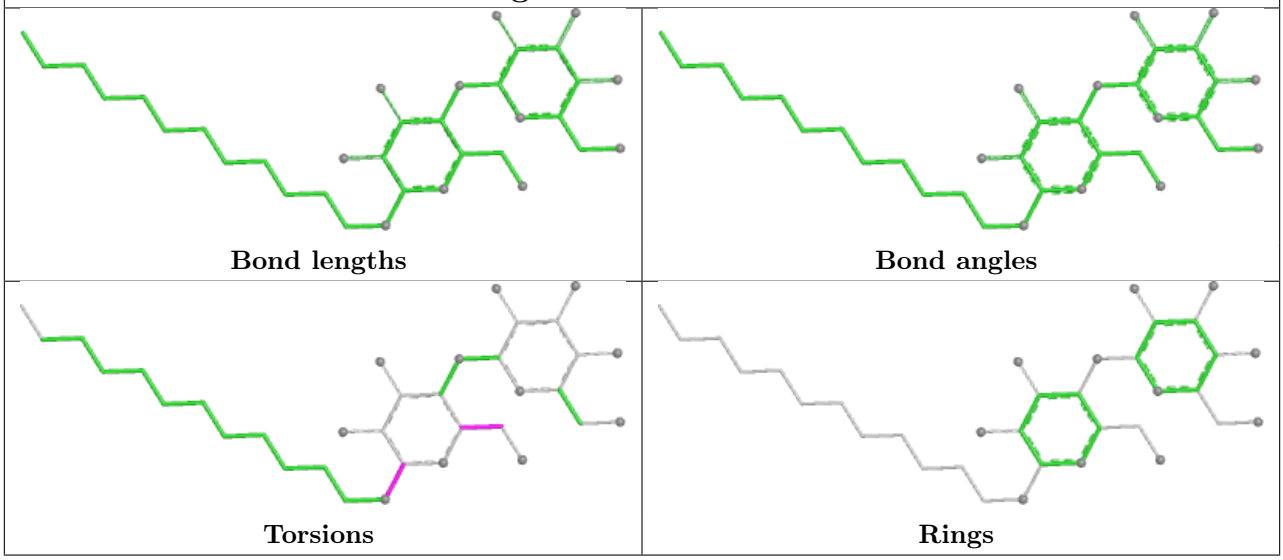

Bond lengths


Bond angles

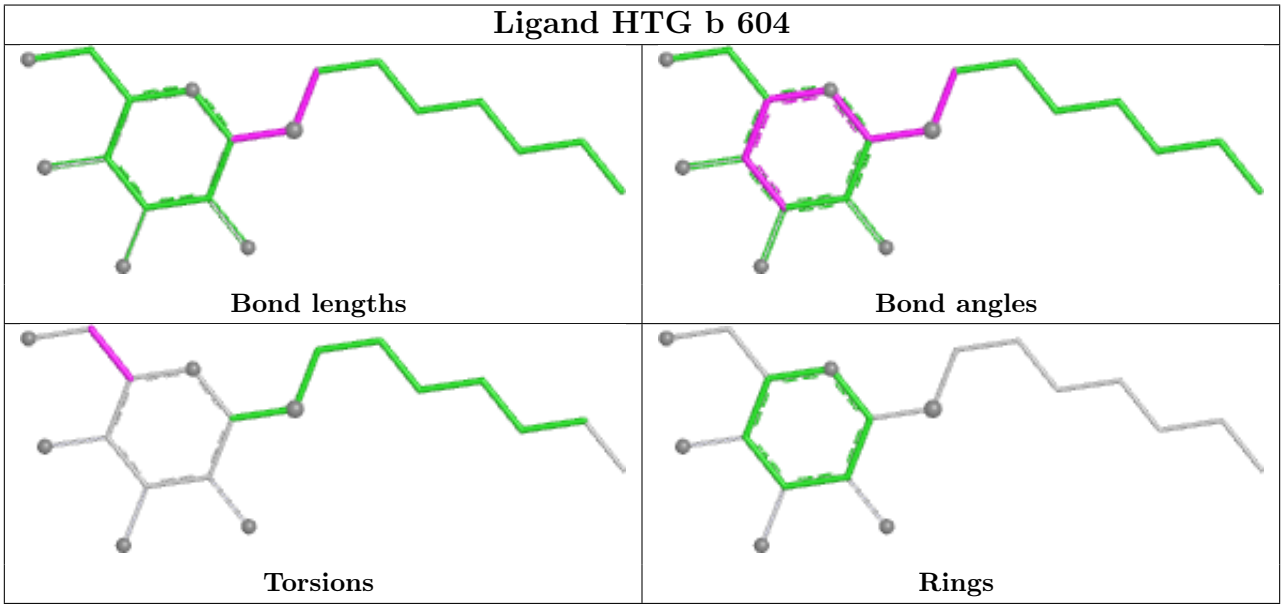

Torsions


Rings

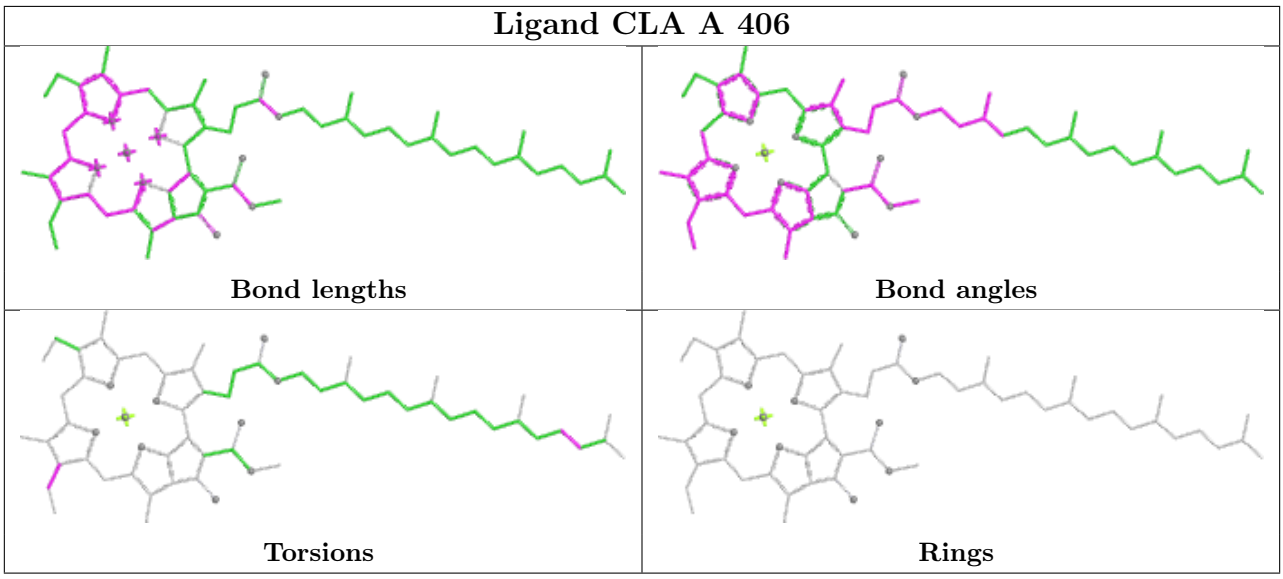
Ligand LMT m 2803



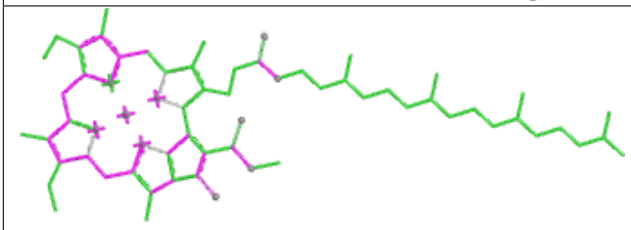
Ligand HTG b 604



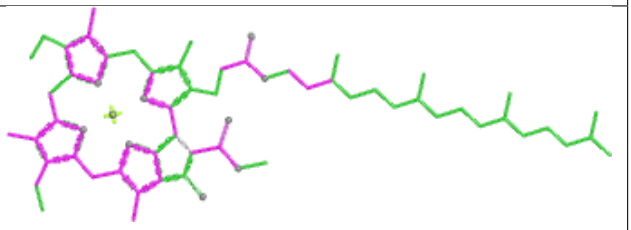
Ligand CLA A 406



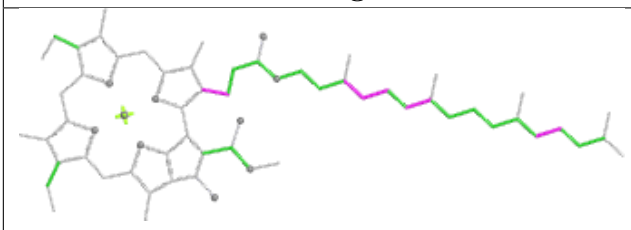
Ligand CLA B 605



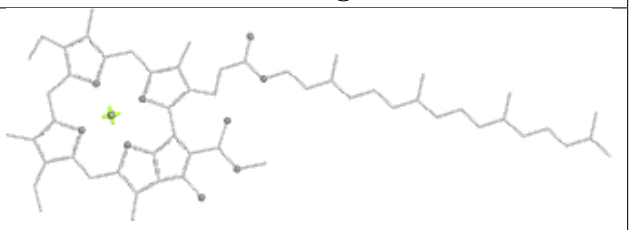
Bond lengths



Bond angles



Torsions

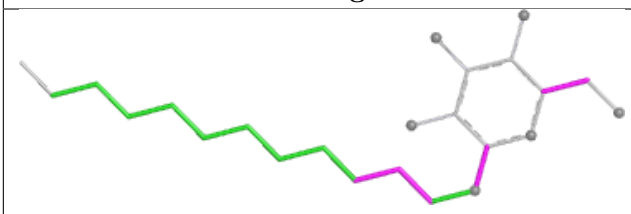


Rings

Ligand LMT F 102

Bond lengths

Bond angles



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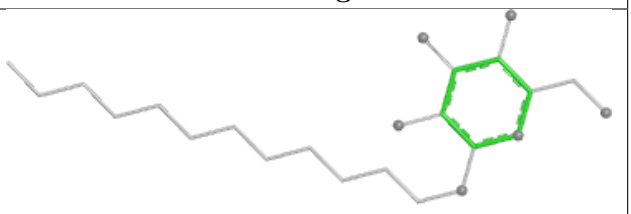
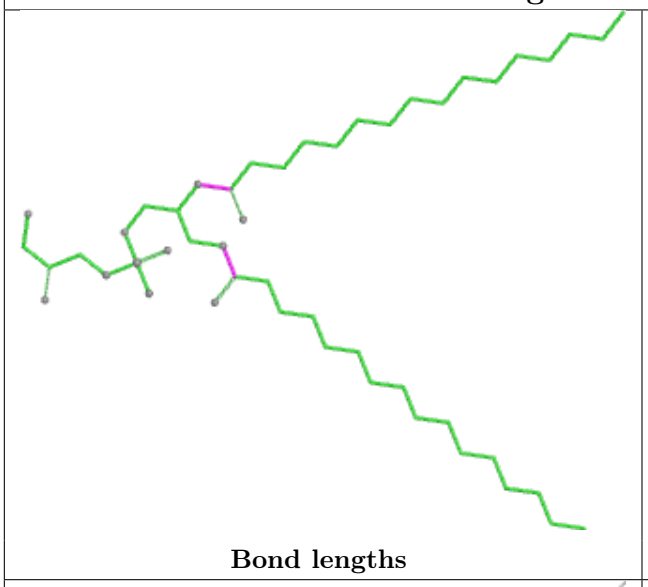
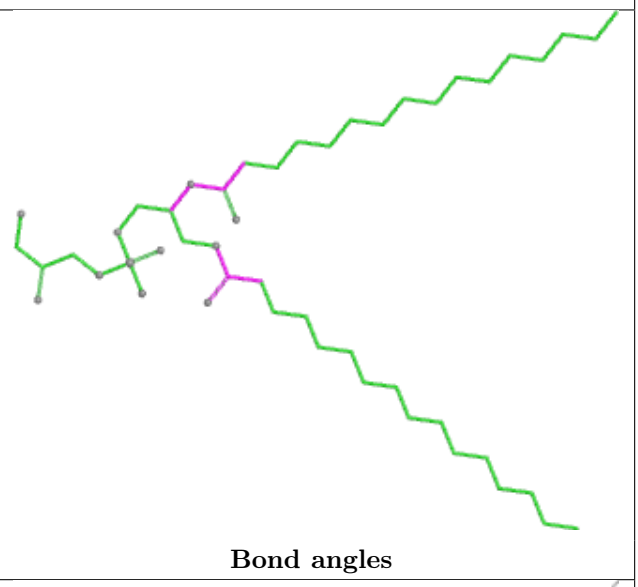


Rings

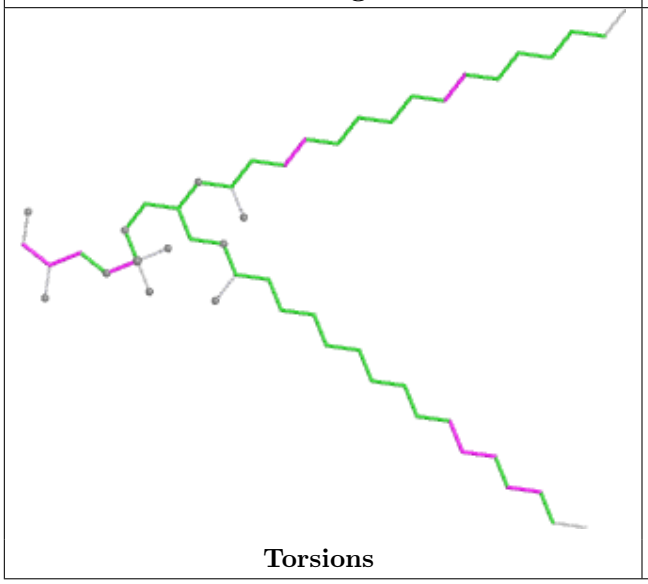
Ligand LHG d 413



Bond lengths



Bond angles



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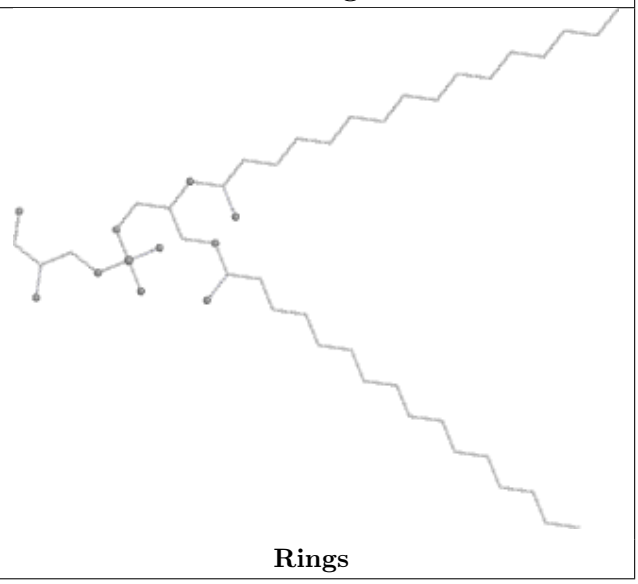
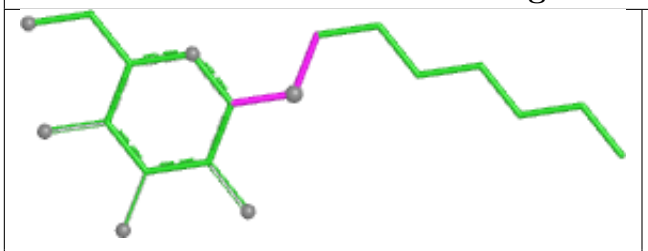


Rings

Ligand HTG I 101



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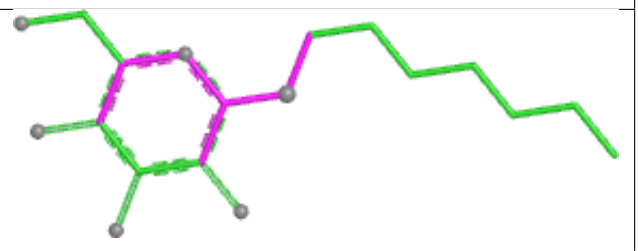
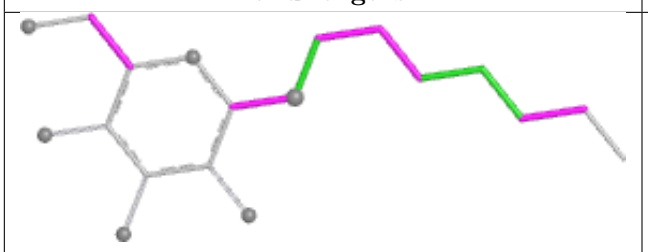


Bond angles



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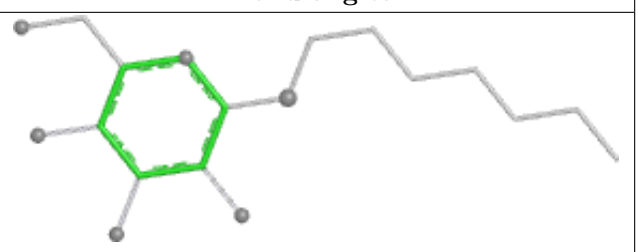
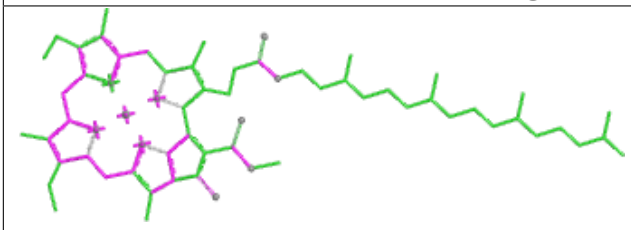


Rings

Ligand CLA B 610



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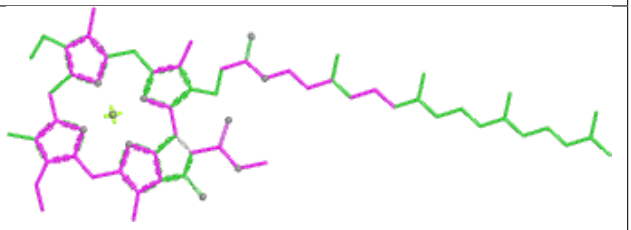
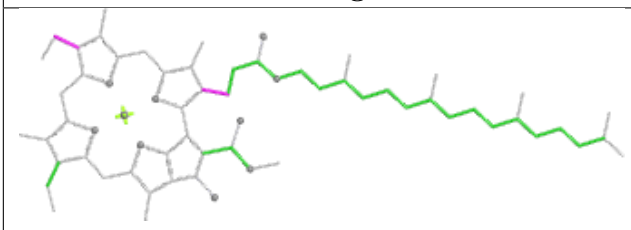


Bond angles



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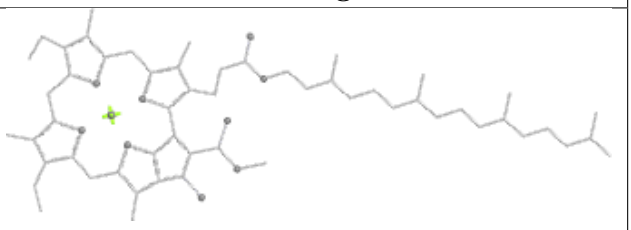
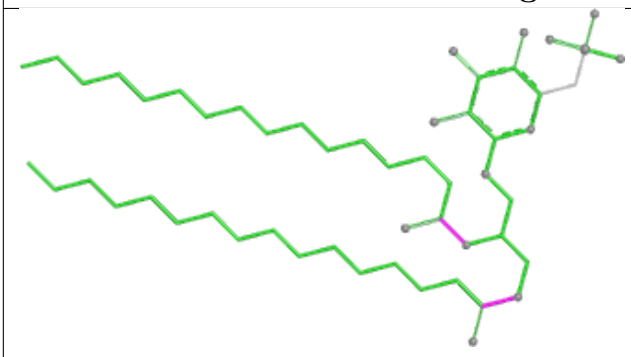


Rings

Ligand SQD a 2603



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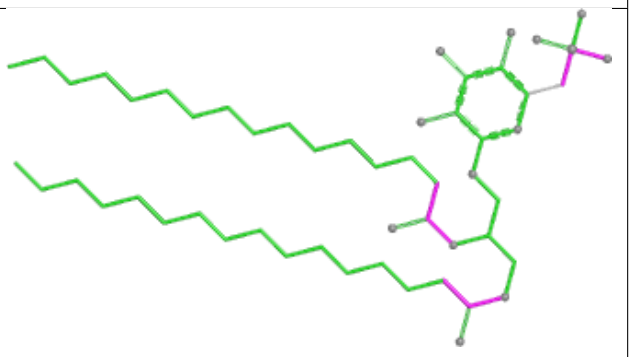
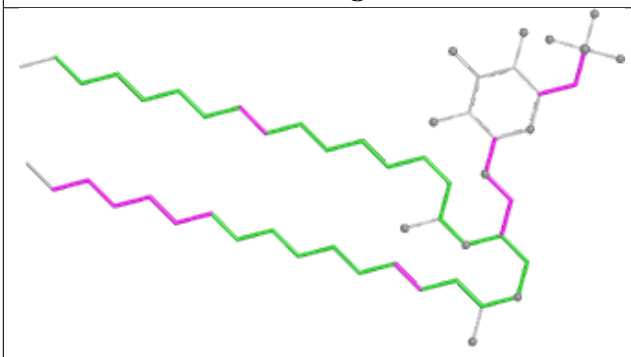


Bond angles



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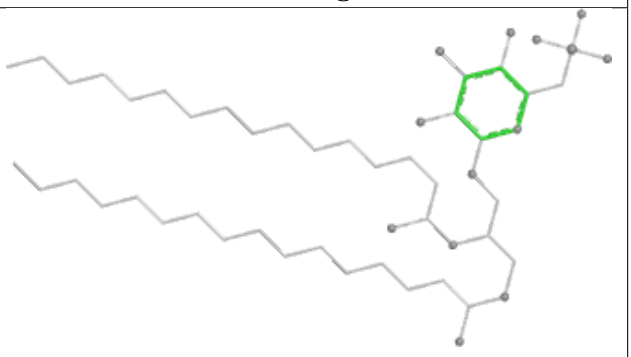
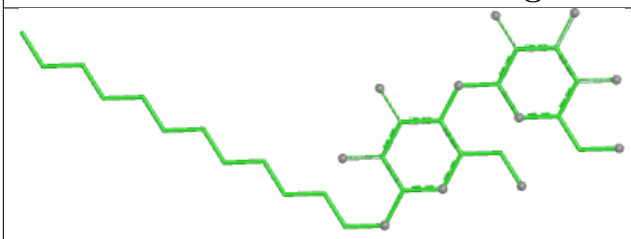


Rings

Ligand LMT d 401



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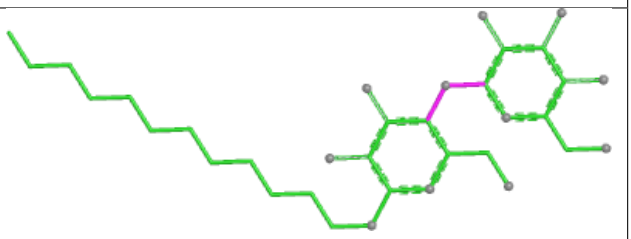
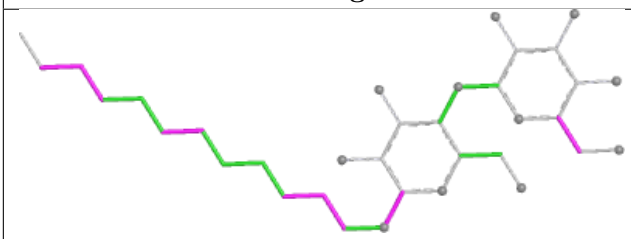


Bond angles



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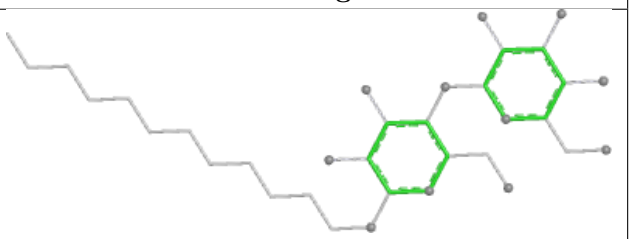
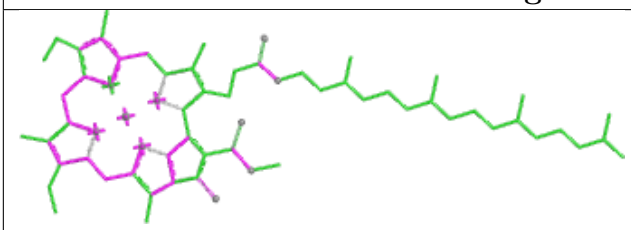


Rings

Ligand CLA B 617



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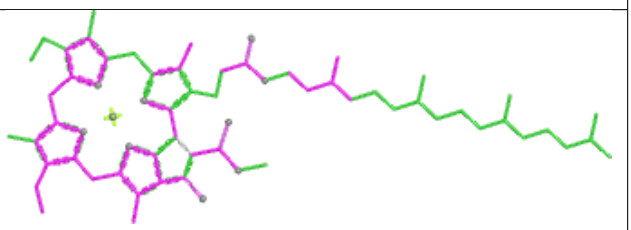
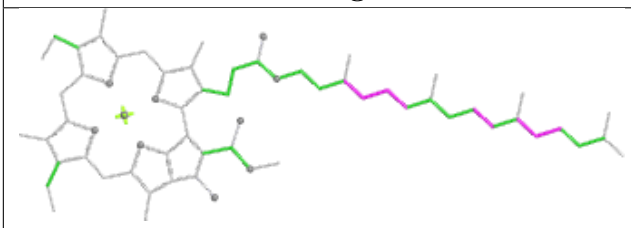


Bond angles



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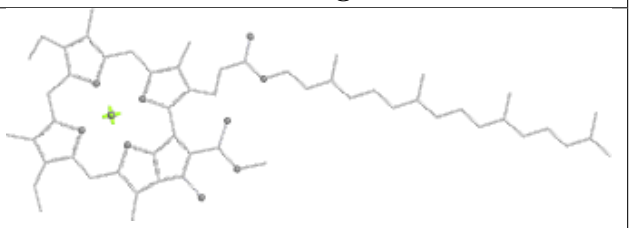
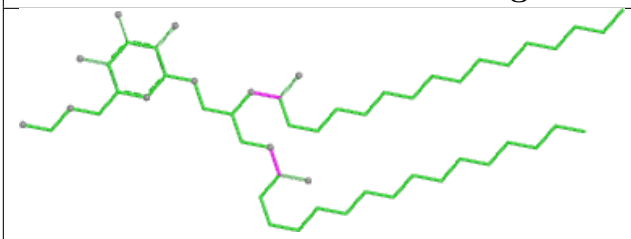


Rings

Ligand DGD D 2307



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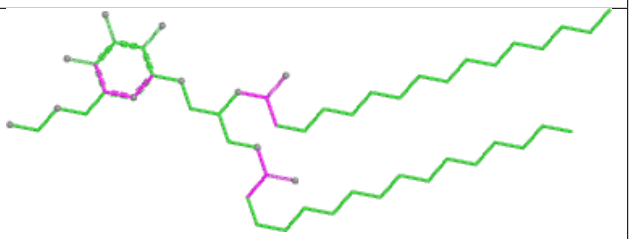

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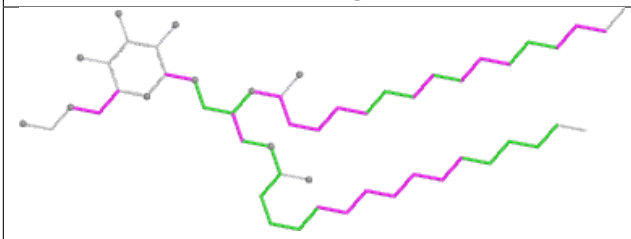

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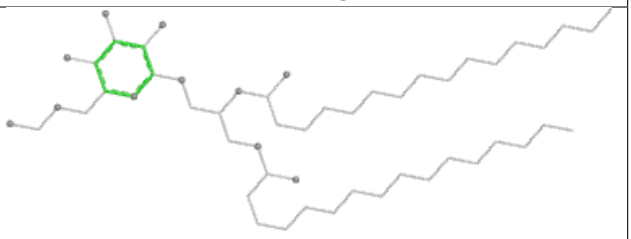
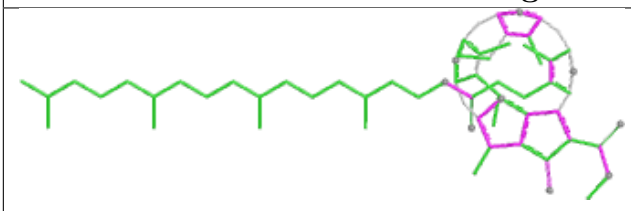


Rings

Ligand PHO A 409



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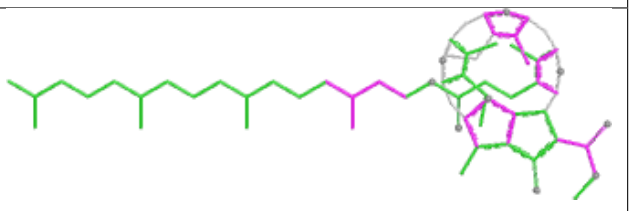
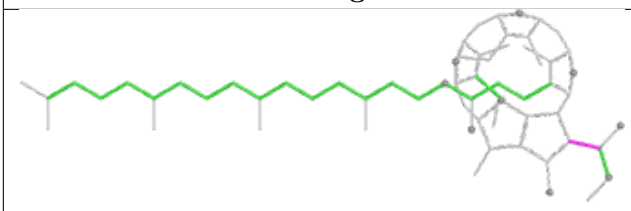


Bond angles



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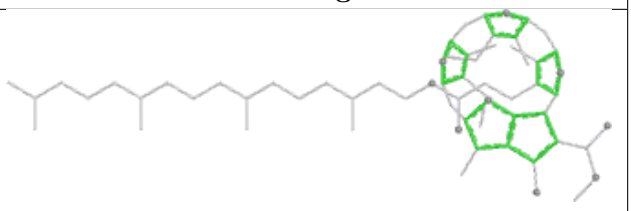
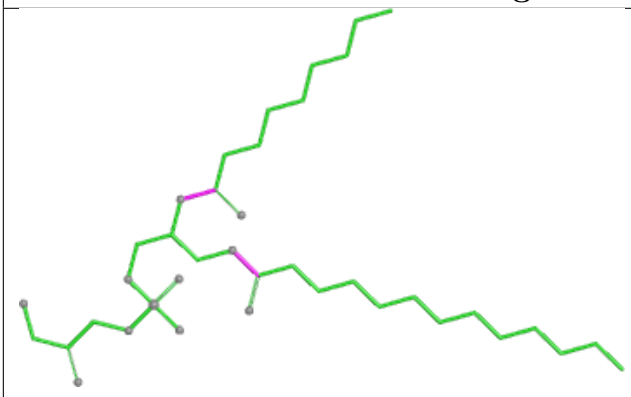


Rings

Ligand LHG D 2311



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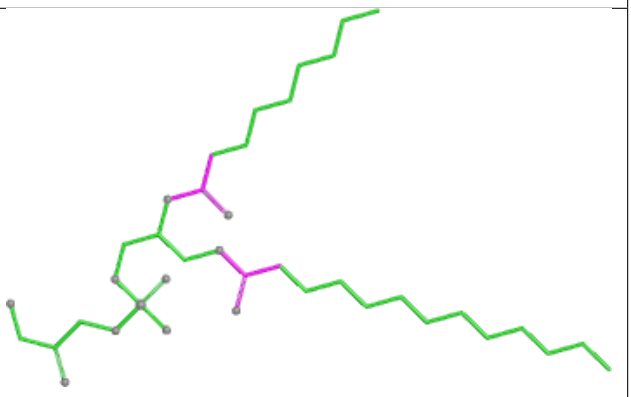
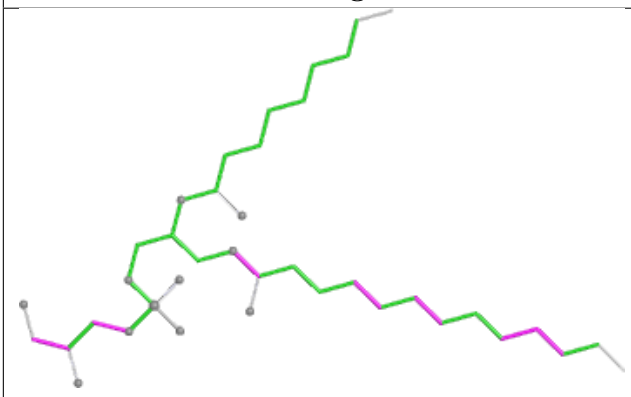


Bond angles



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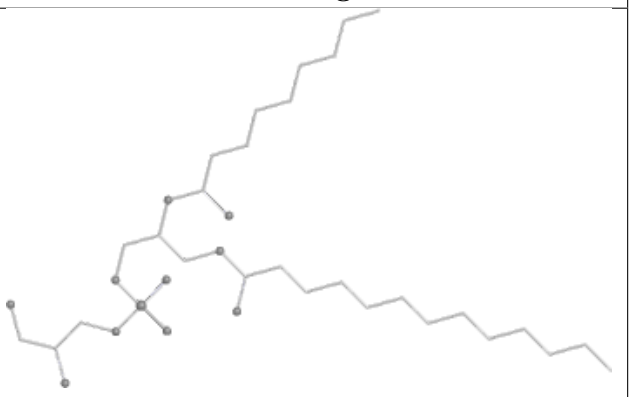
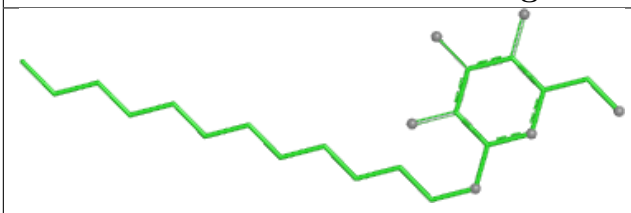


Rings

Ligand LMT A 420



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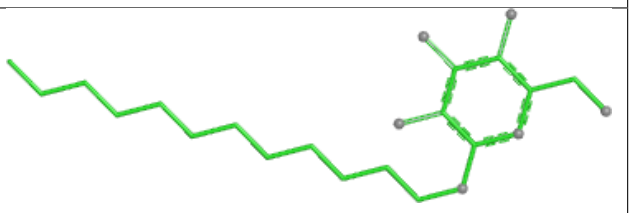
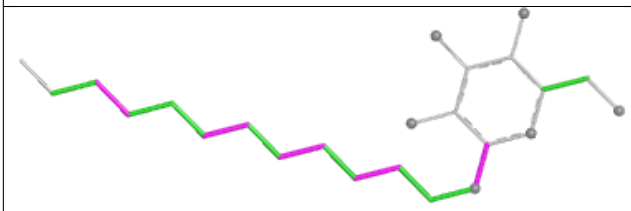
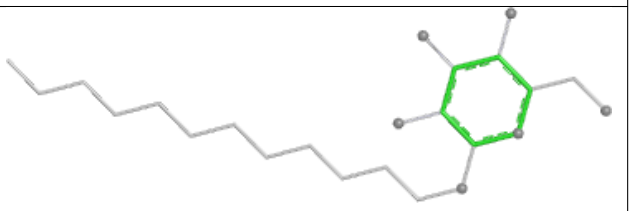


Bond angles

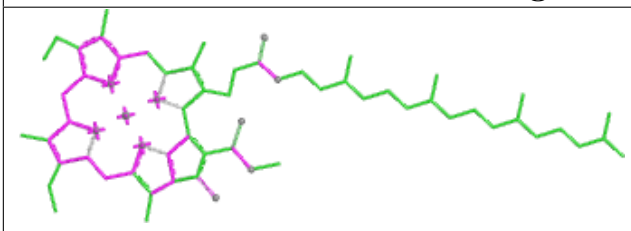


Torsions

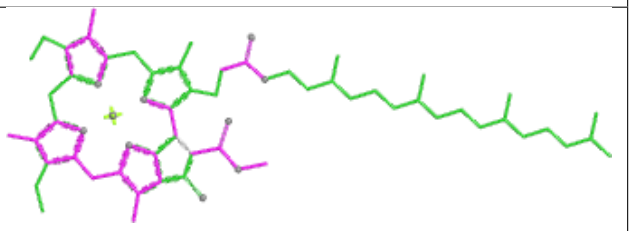


Rings

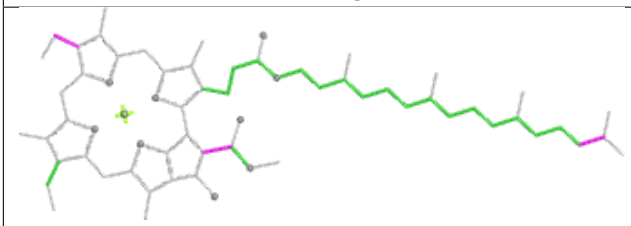
Ligand CLA c 505



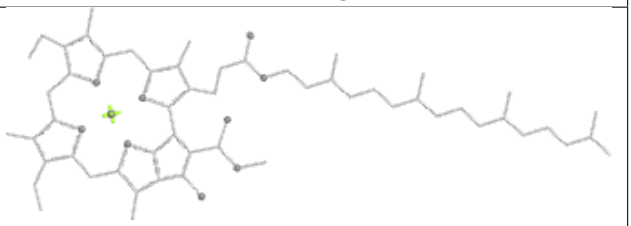
Bond lengths



Bond angles

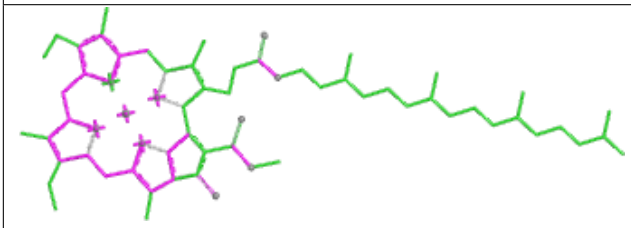


Torsions



Rings

Ligand CLA b 606



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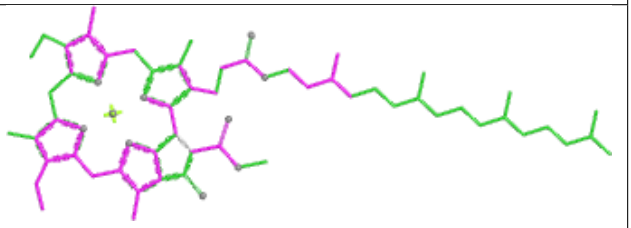
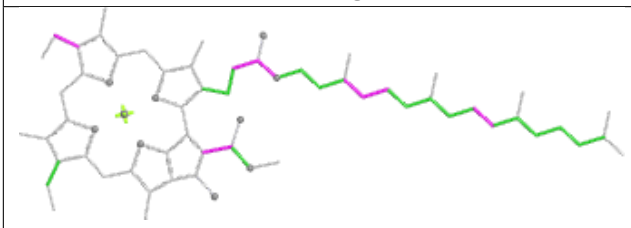
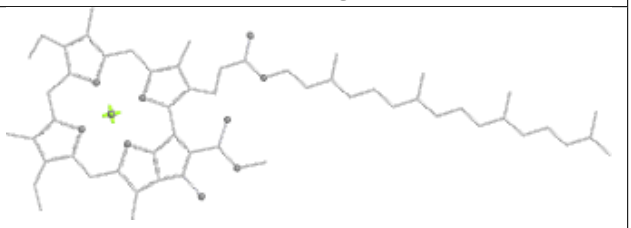


Bond angles

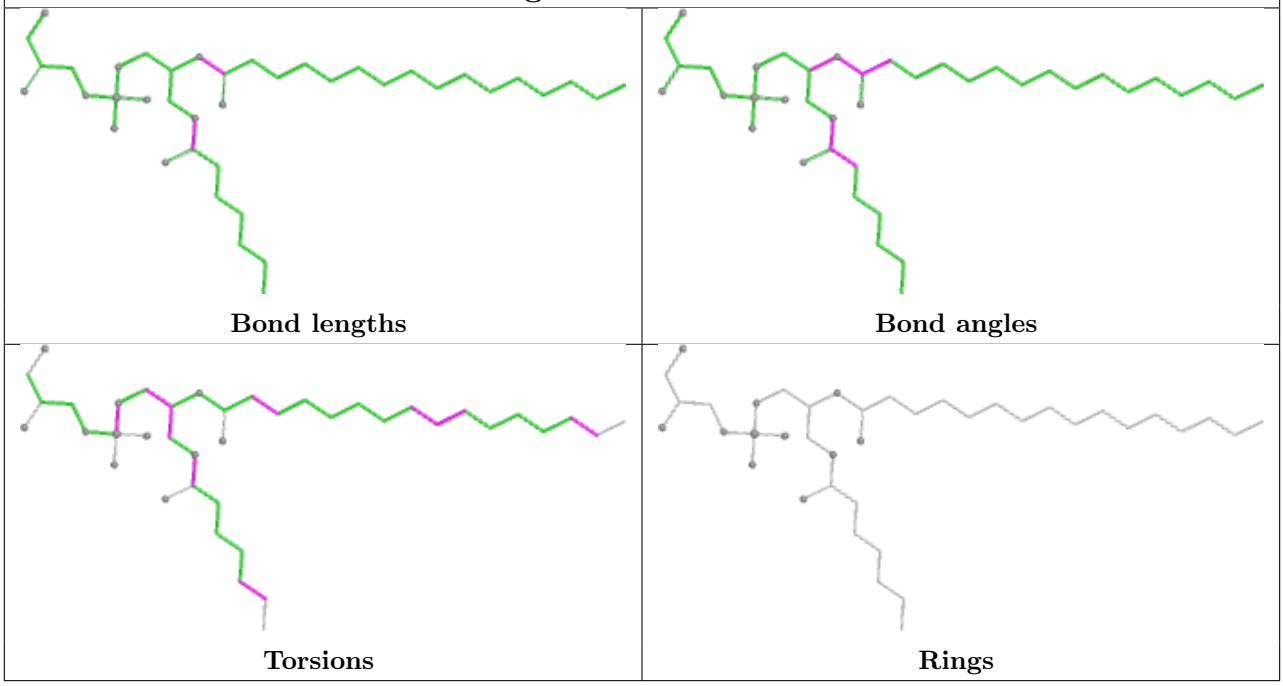


Torsions

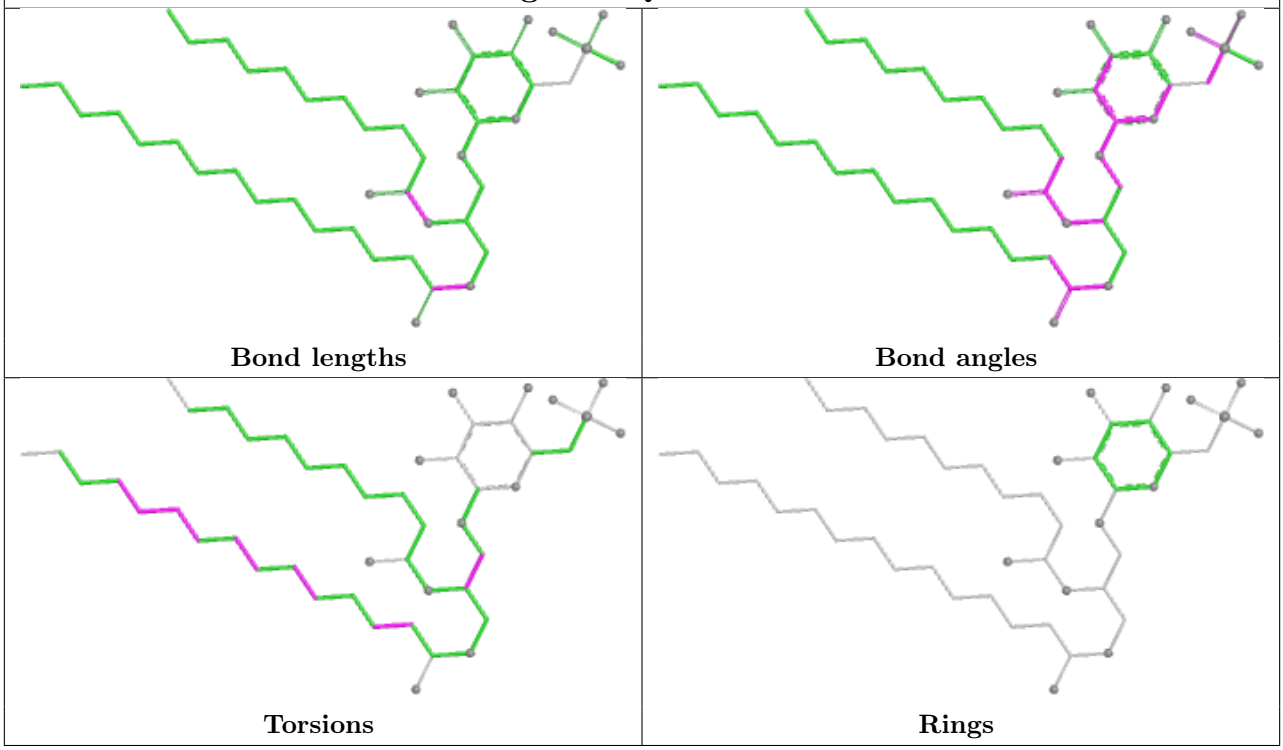


Rings

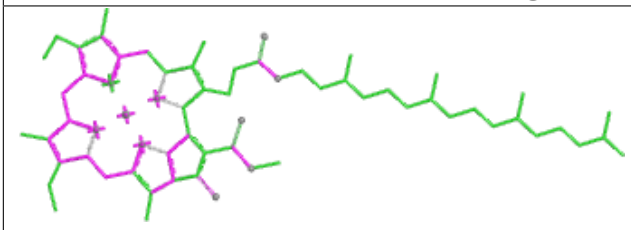
Ligand LHG E 101



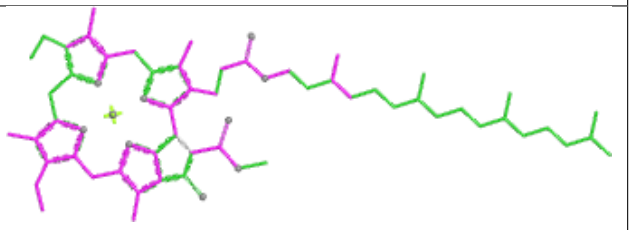
Ligand SQD a 2615



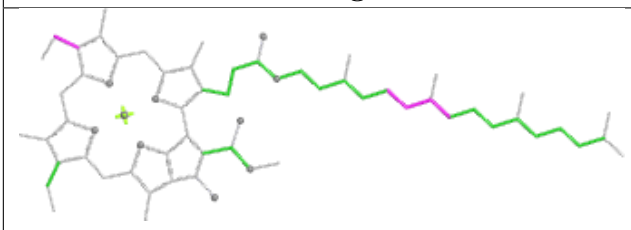
Ligand CLA B 604



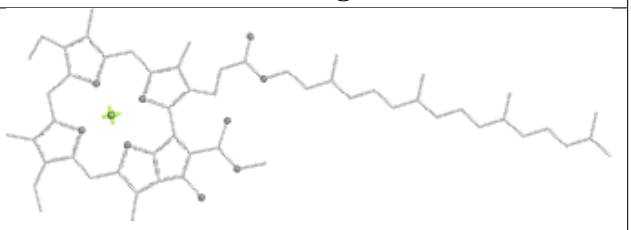
Bond lengths



Bond angles

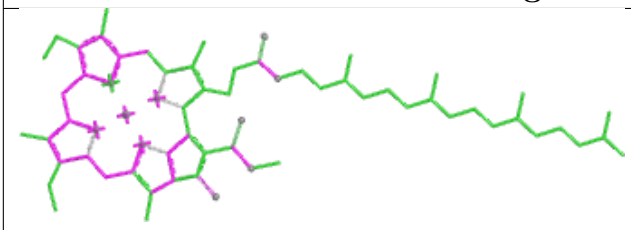


Torsions



Rings

Ligand CLA A 410



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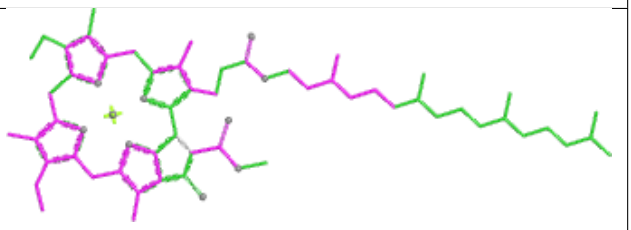
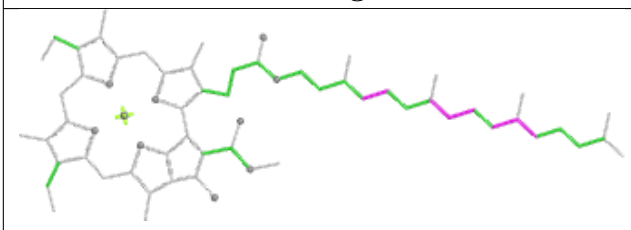
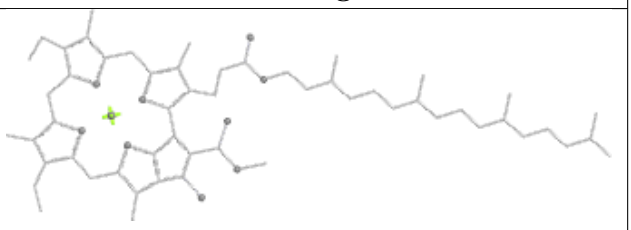


Bond angles

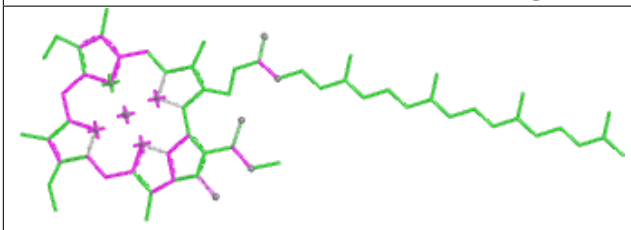


Torsions

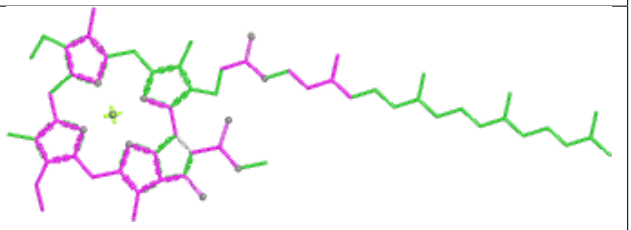


Rings

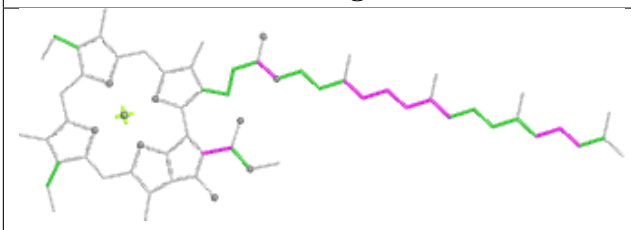
Ligand CLA b 621



Bond lengths



Bond angles



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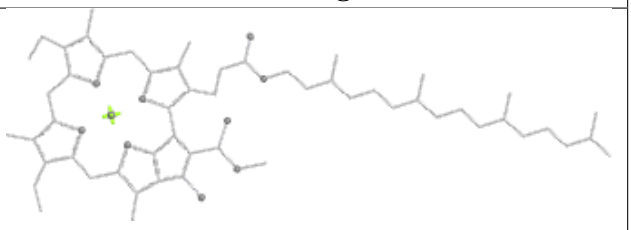
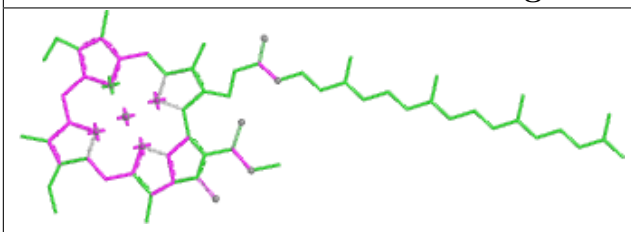


Rings

Ligand CLA B 606



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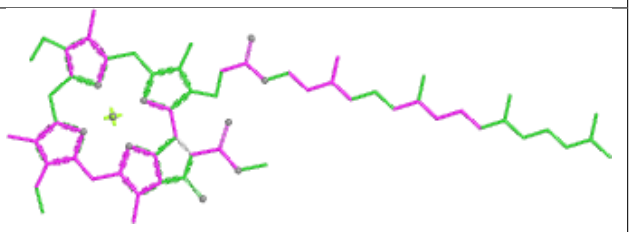
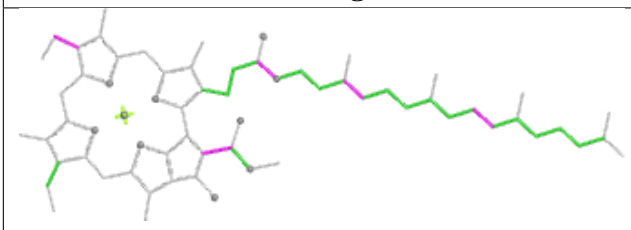
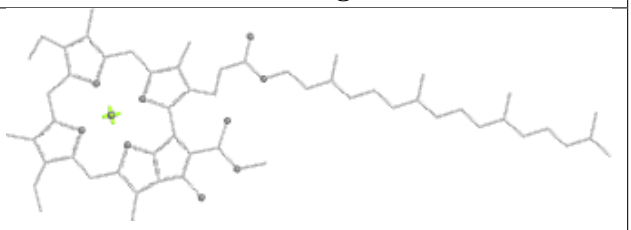


Bond angles

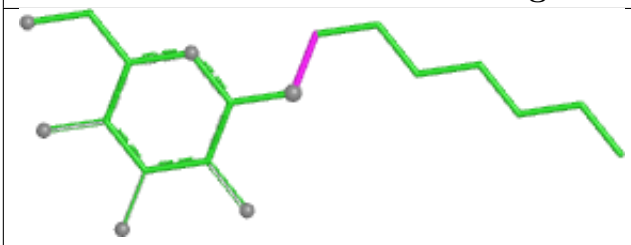


Torsions



Rings

Ligand HTG i 102



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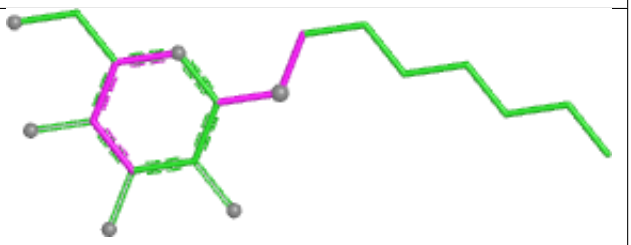
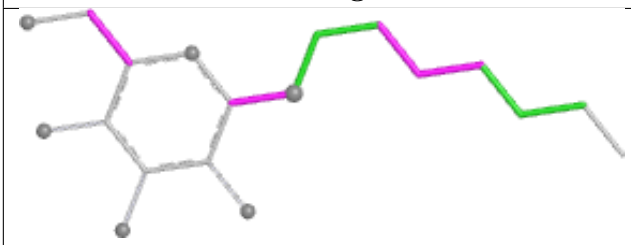


Bond angles



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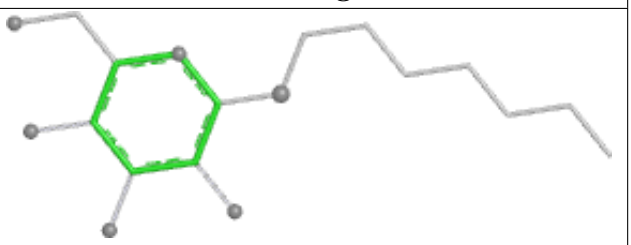
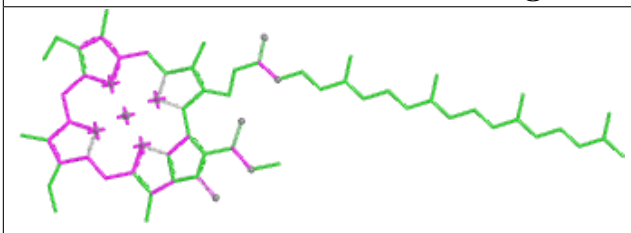


Rings

Ligand CLA C 511



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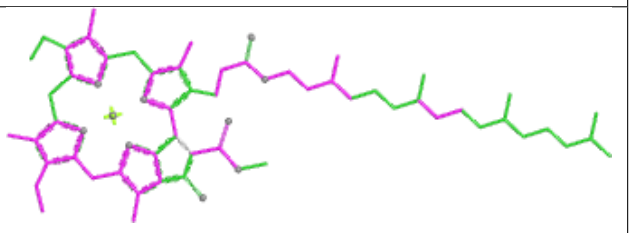
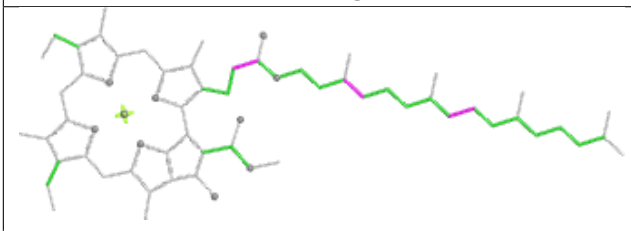
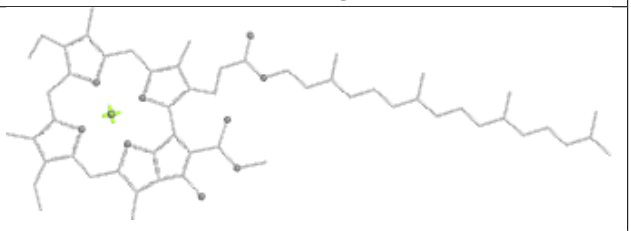


Bond angles

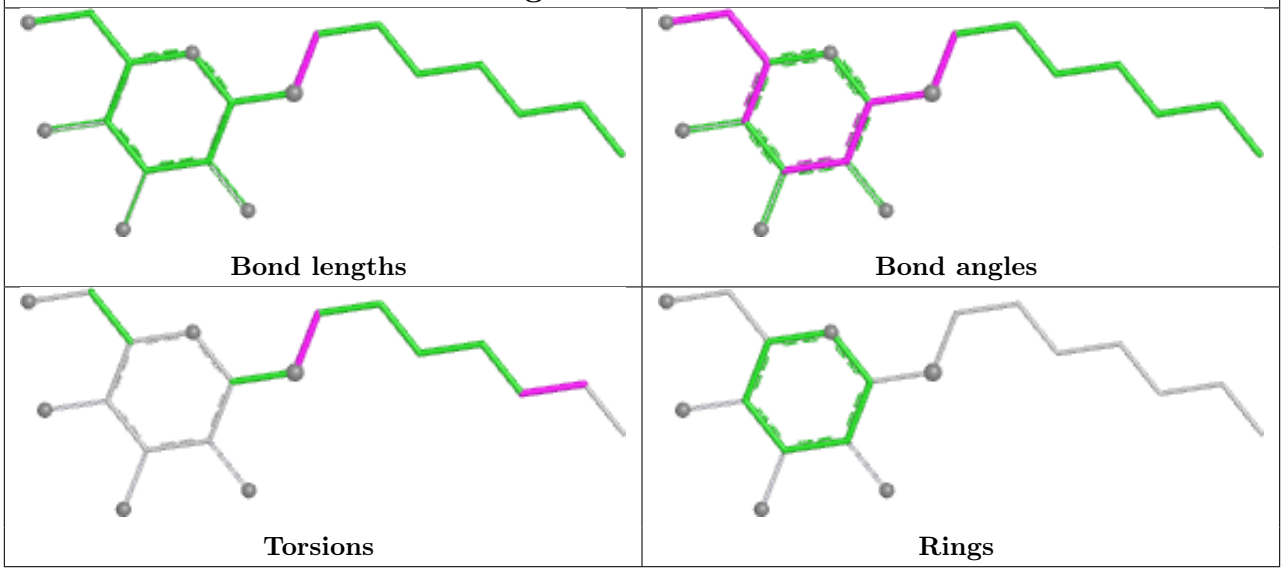


Torsions

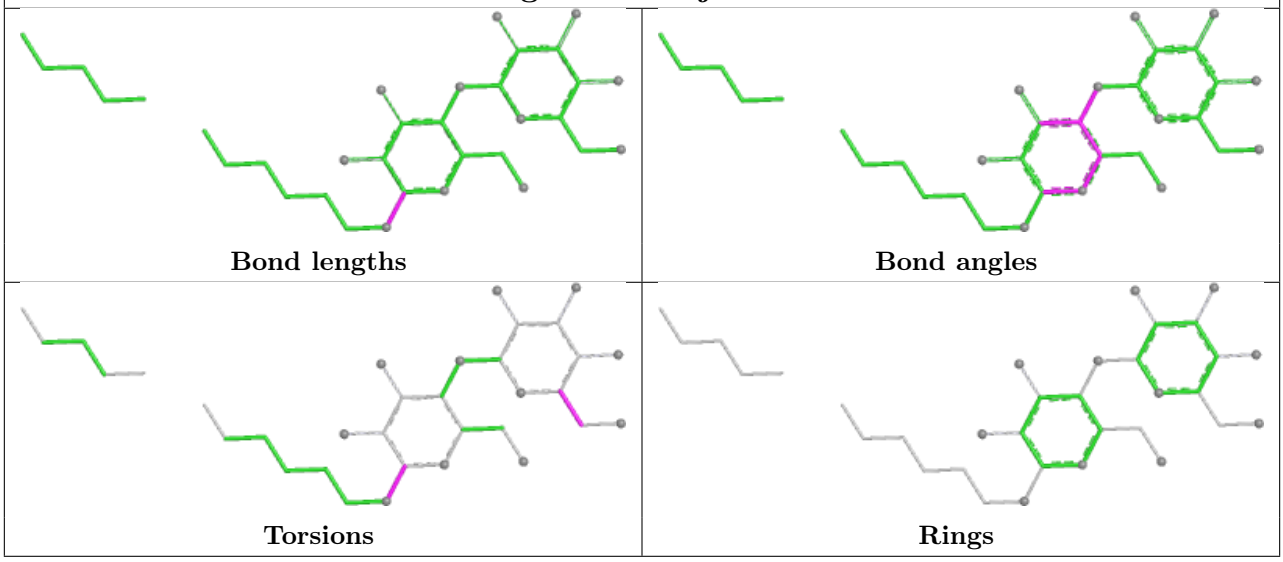


Rings

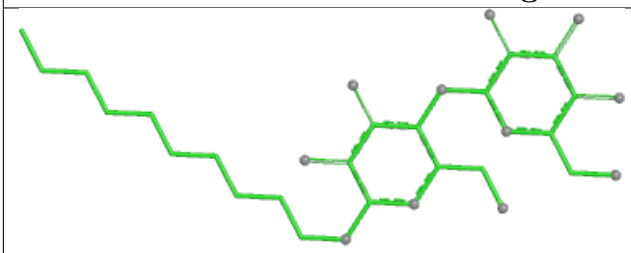
Ligand HTG b 625



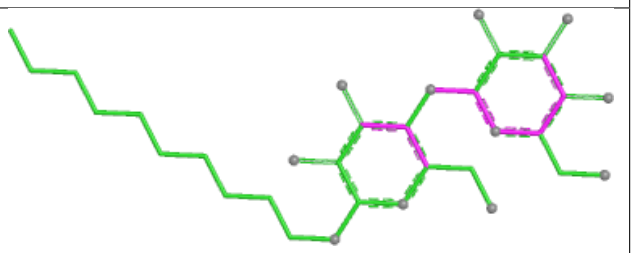
Ligand LMT j 2701



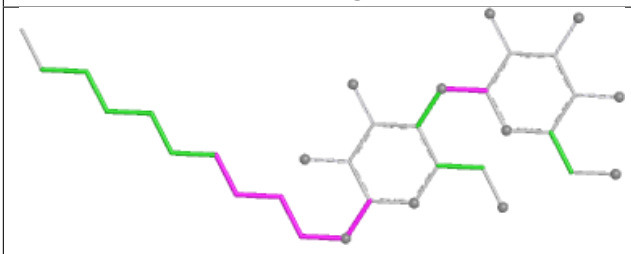
Ligand LMT A 414



Bond lengths



Bond angles



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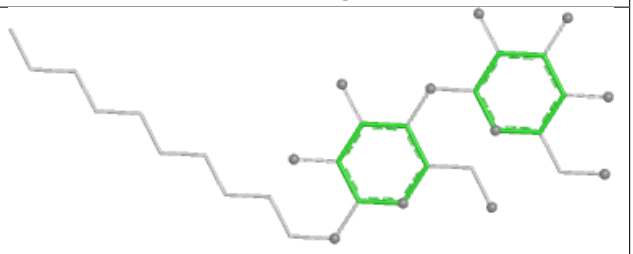
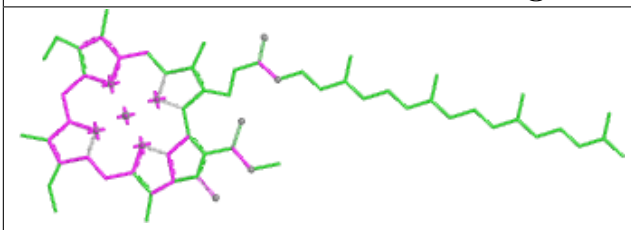


Rings

Ligand CLA b 613



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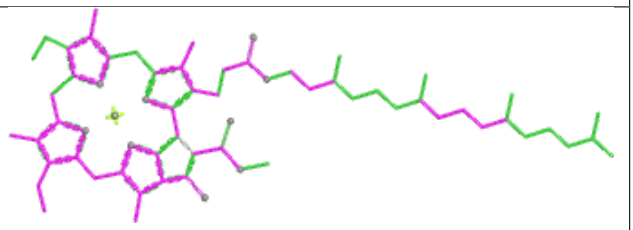
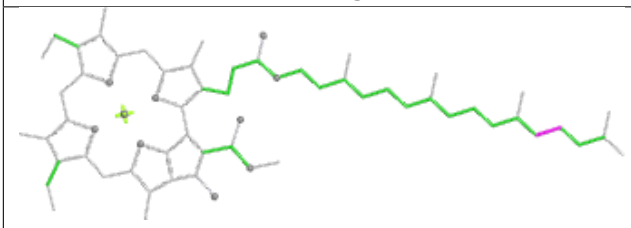
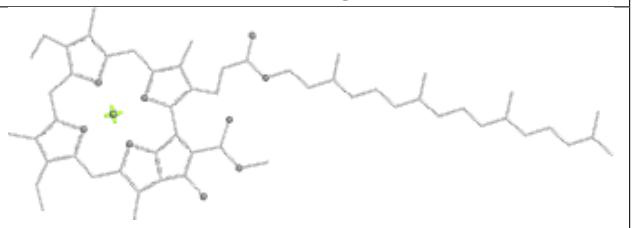


Bond angles

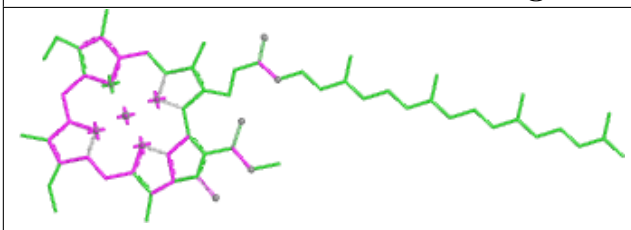


Torsions



Rings

Ligand CLA d 408



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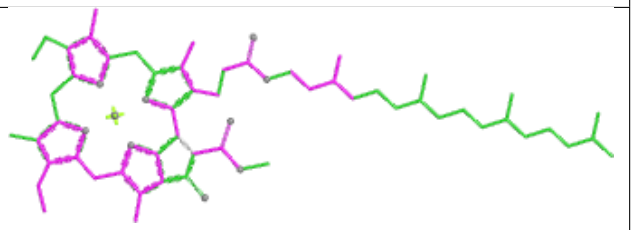
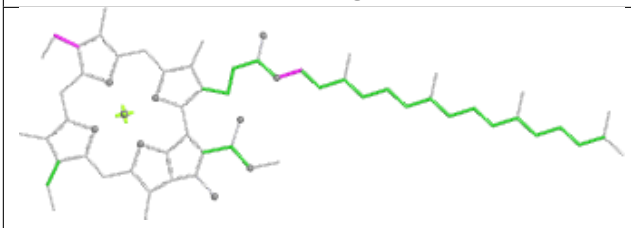


Bond angles



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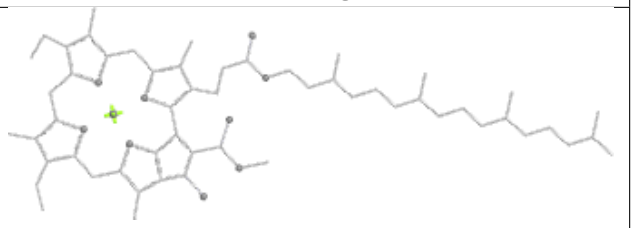
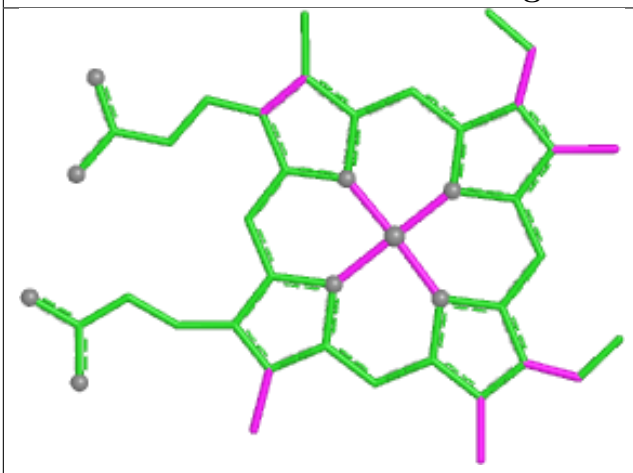
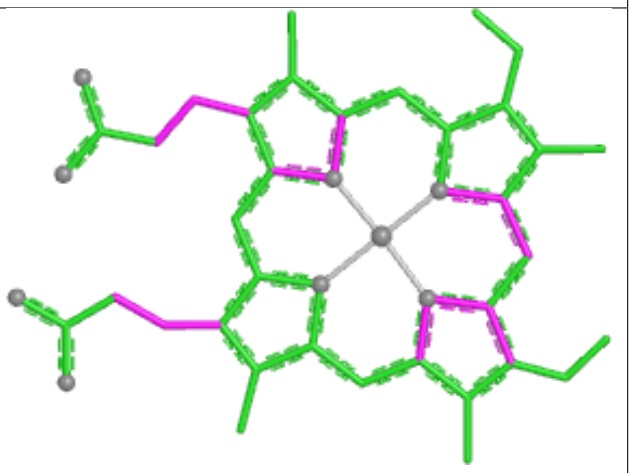


Rings

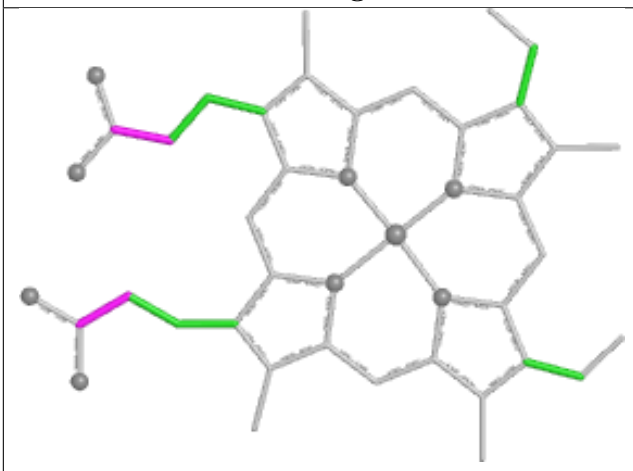
Ligand HEM e 103



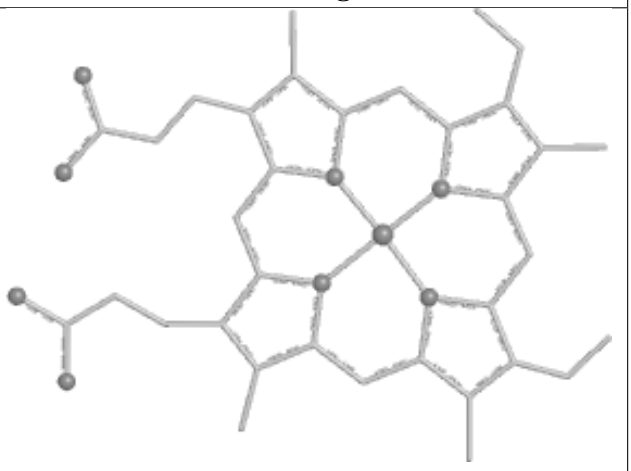
Bond lengths



Bond angles

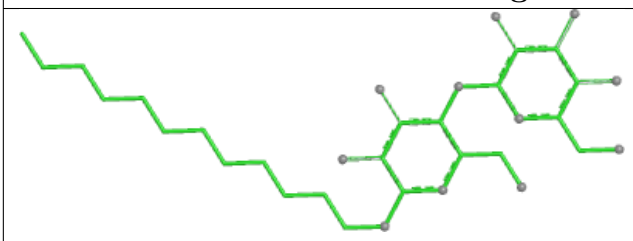


Torsions

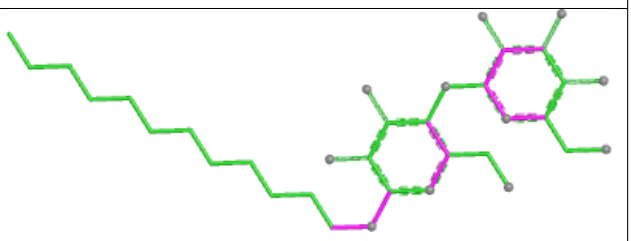


Rings

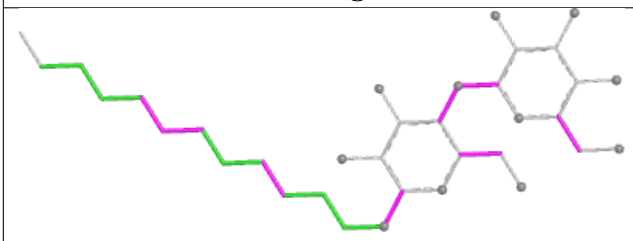
Ligand LMT m 2804



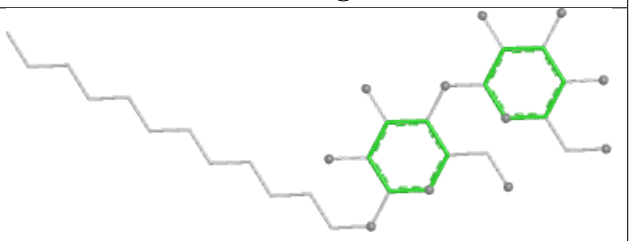
Bond lengths



Bond angles

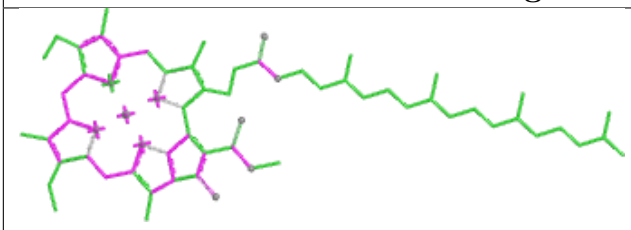


Torsions

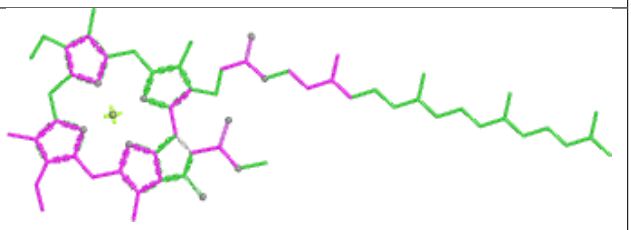


Rings

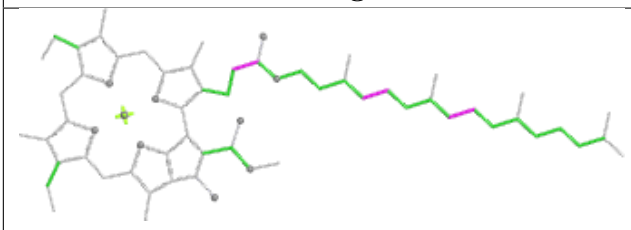
Ligand CLA B 613



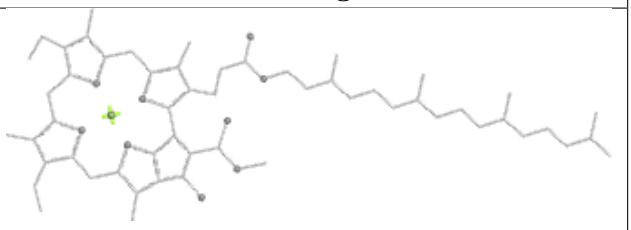
Bond lengths



Bond angles

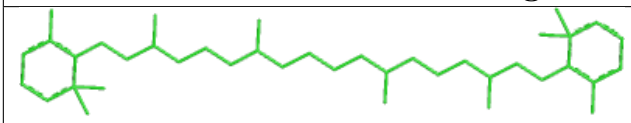


Torsions

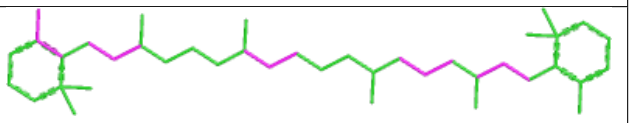


Rings

Ligand BCR B 618

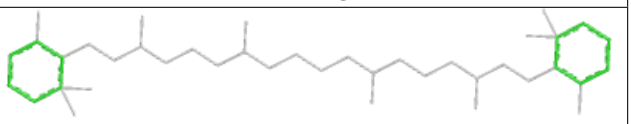


Bond lengths



Bond angles

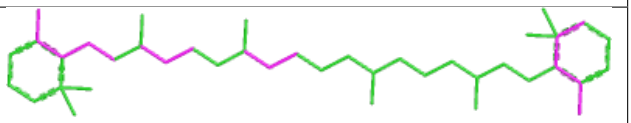
Torsions



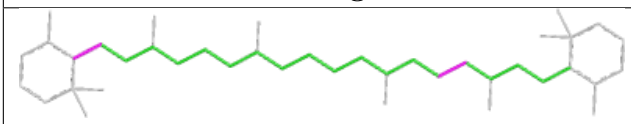
Rings

Ligand BCR a 2614

Bond lengths



Bond angles



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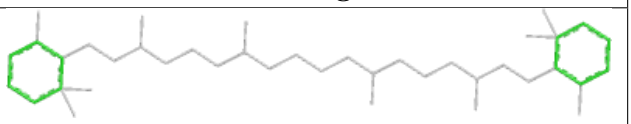
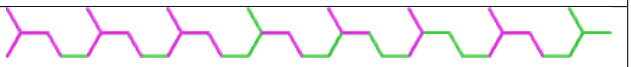


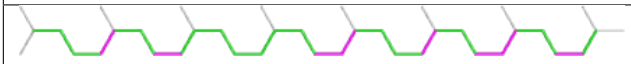
Rings

Ligand PL9 x 1301

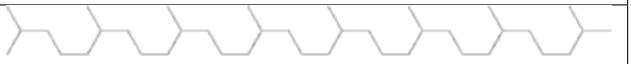
Bond lengths



Bond angles

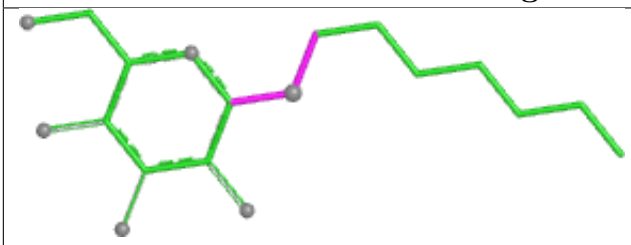


Torsions

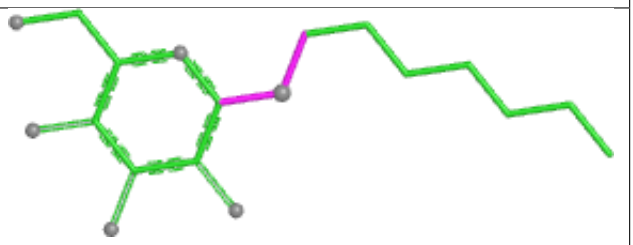


Rings

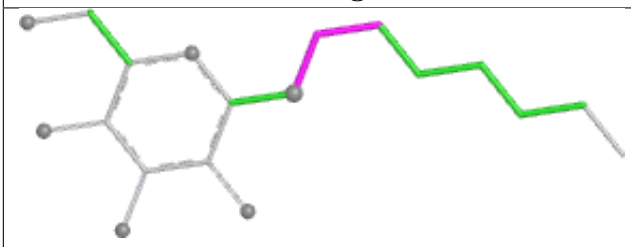
Ligand HTG C 521



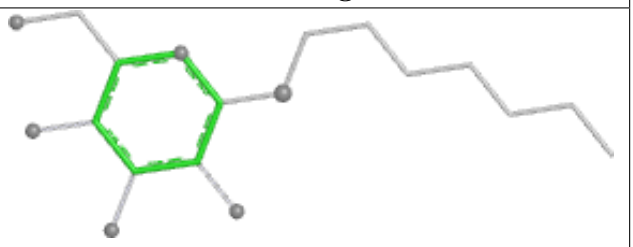
Bond lengths



Bond angles

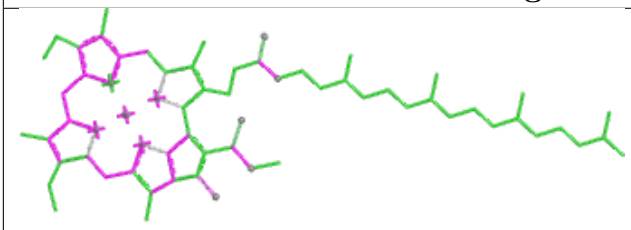


Torsions

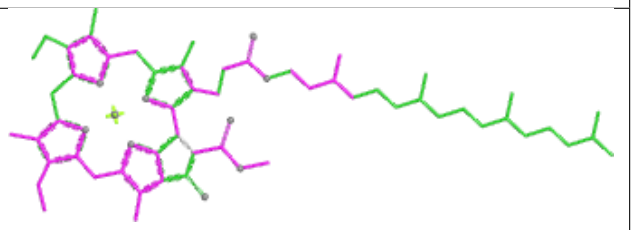


Rings

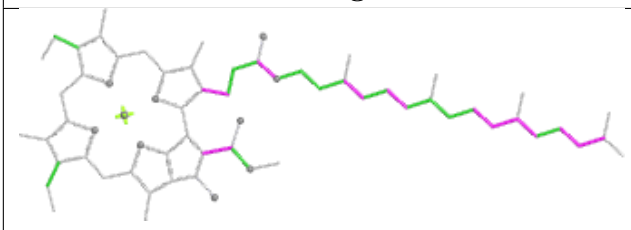
Ligand CLA C 507



Bond lengths



Bond angles



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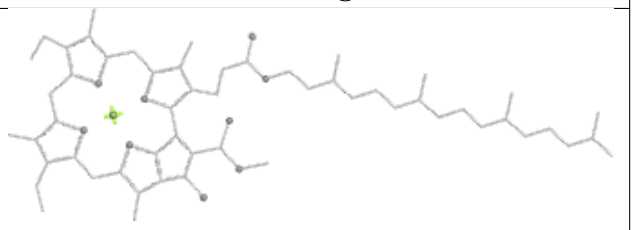
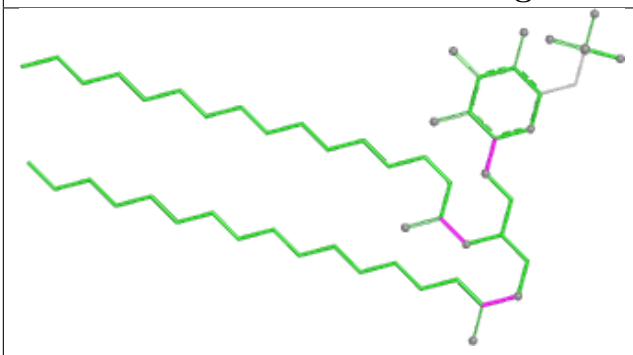
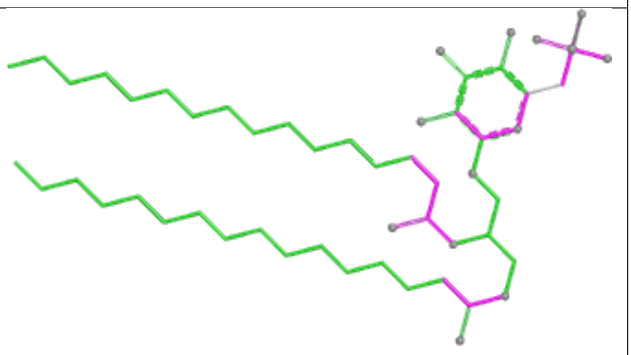


Rings

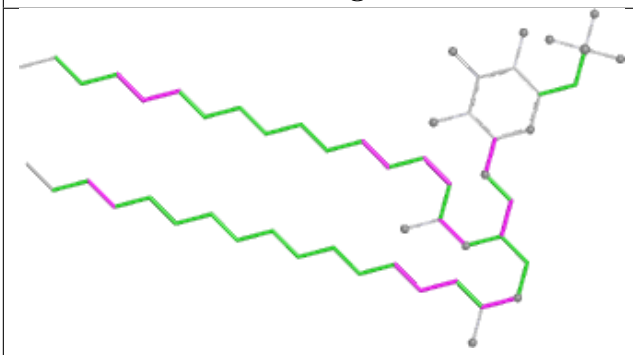
Ligand SQD D 2302



Bond lengths



Bond angles



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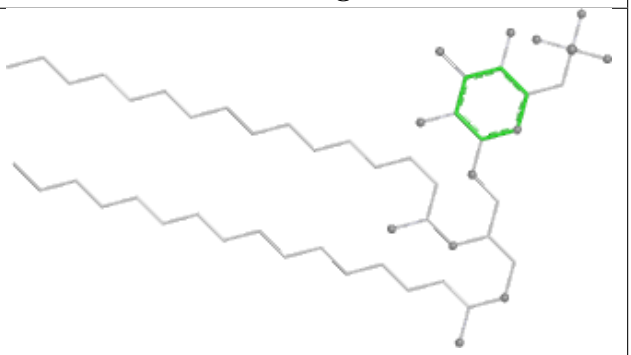
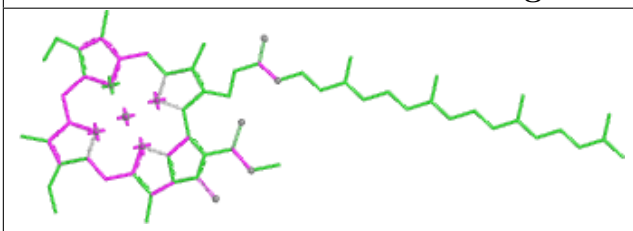
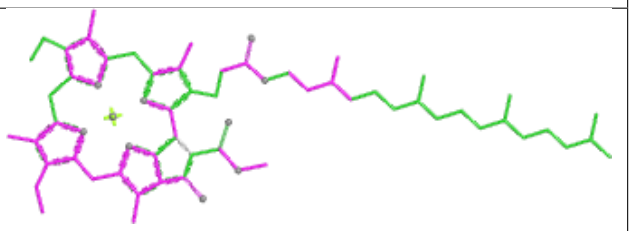


Rings

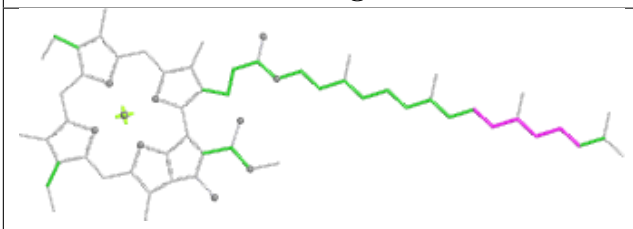
Ligand CLA B 614



Bond lengths



Bond angles



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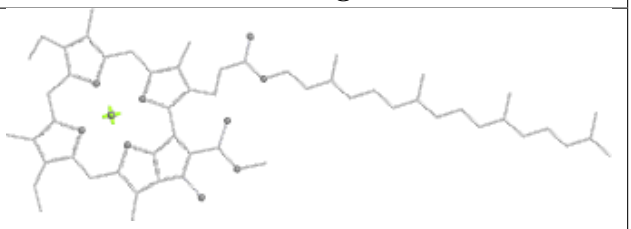
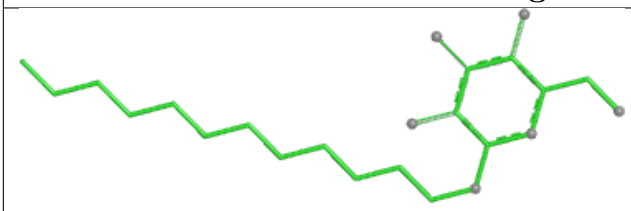
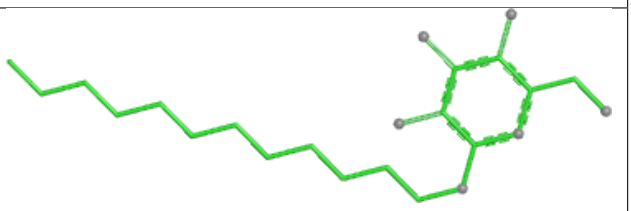
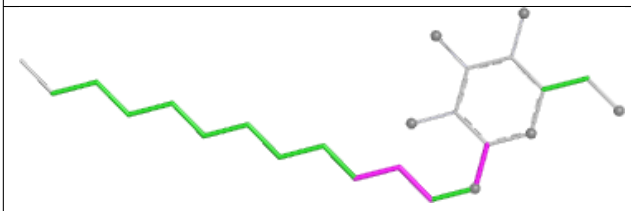


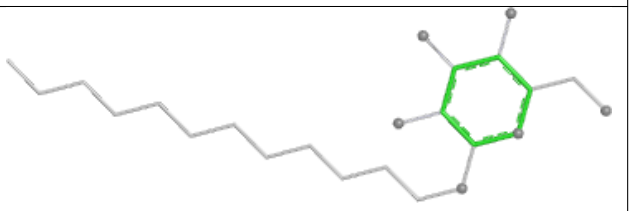
Rings

Ligand LMT f 101


Bond lengths

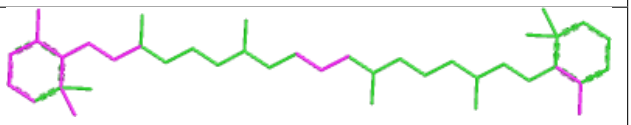

Bond angles

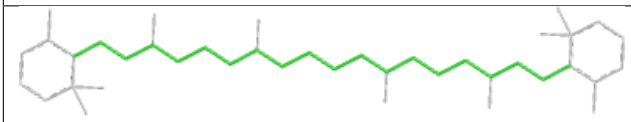

Torsions


Rings

Ligand BCR A 411

Bond lengths


Bond angles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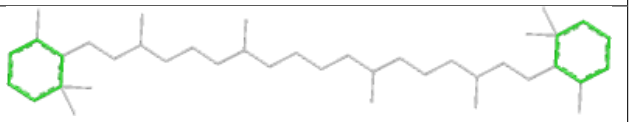
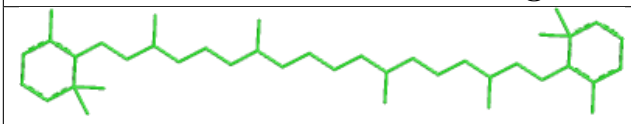

Rings

Ligand BCR b 624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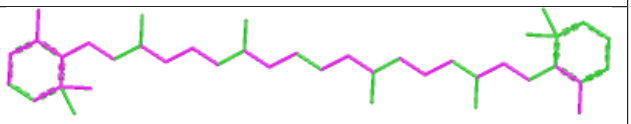
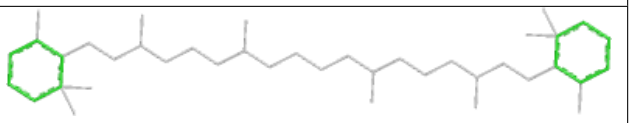
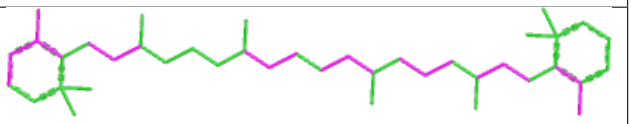

Bond angles

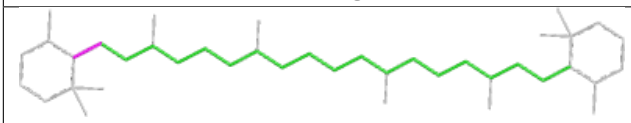
Torsions


Rings

Ligand BCR b 622

Bond lengths


Bond angles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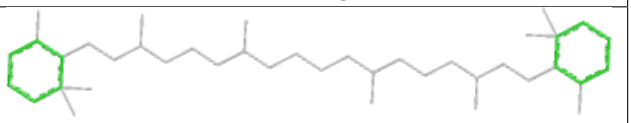
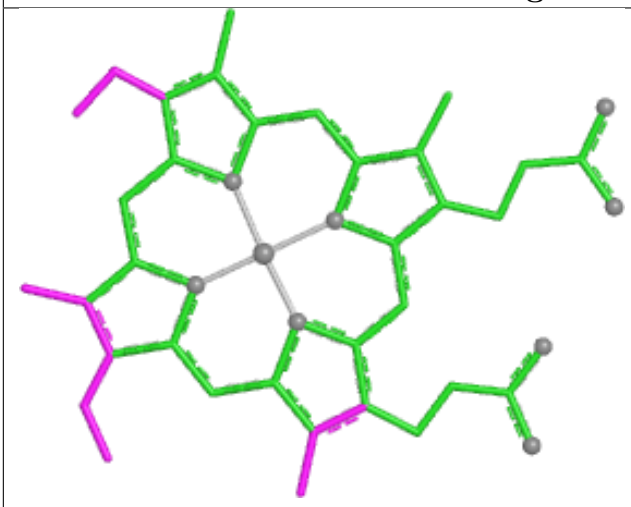
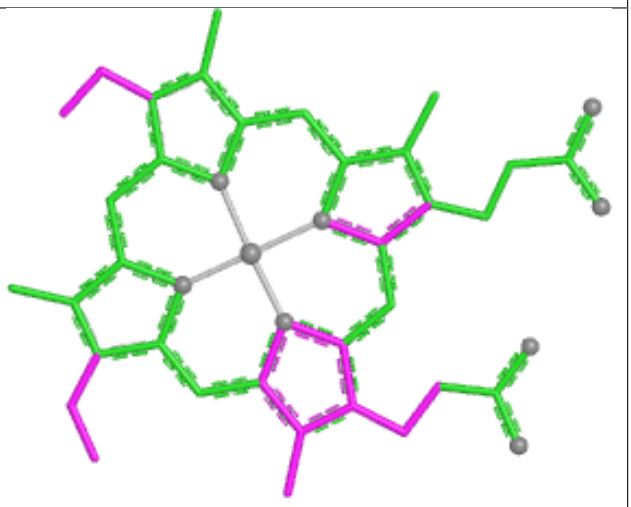

Rings

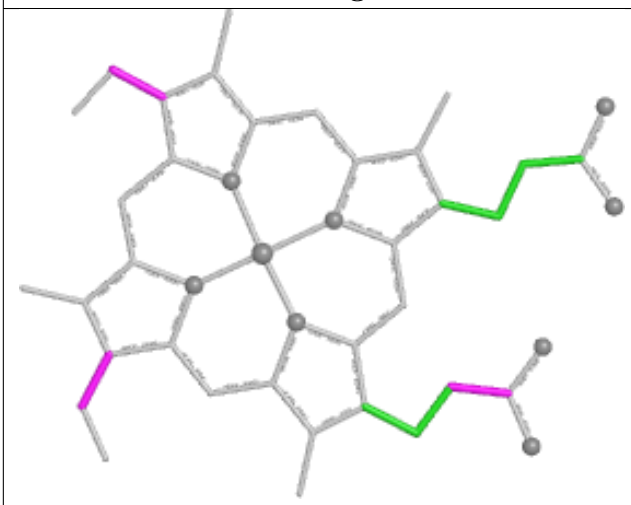
Ligand HEC v 201



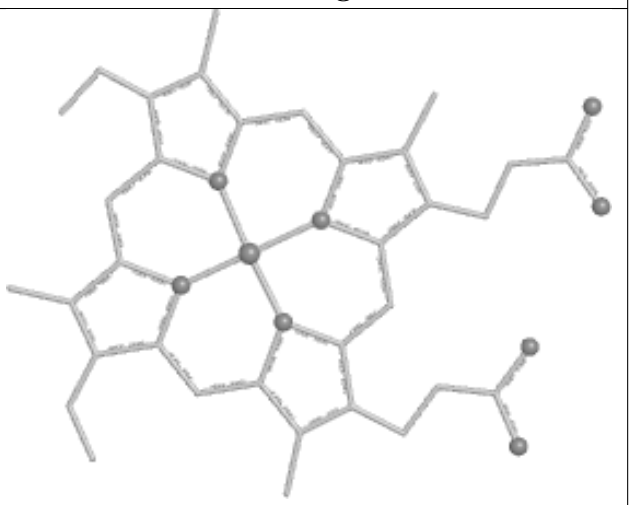
Bond lengths



Bond angles

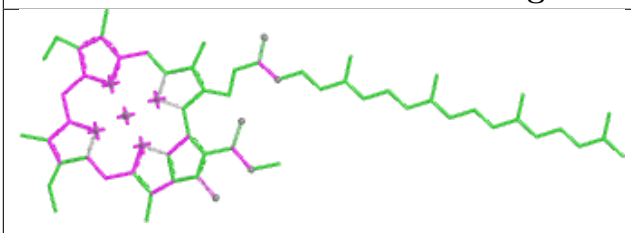


Torsions

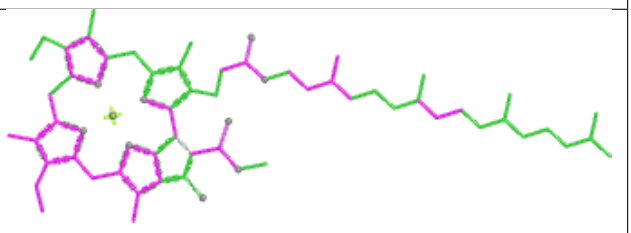


Rings

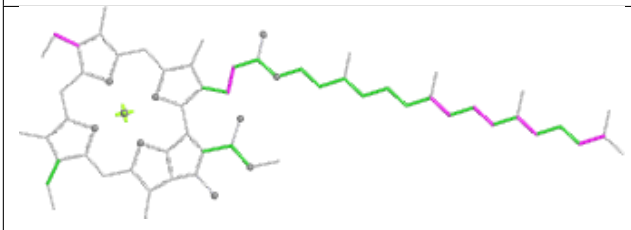
Ligand CLA b 611



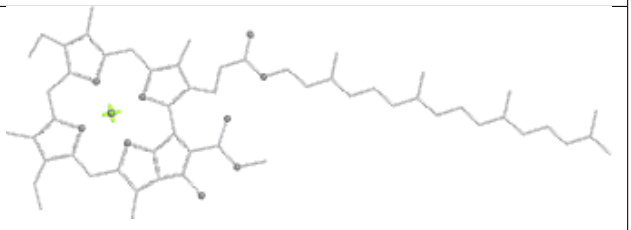
Bond lengths



Bond angles

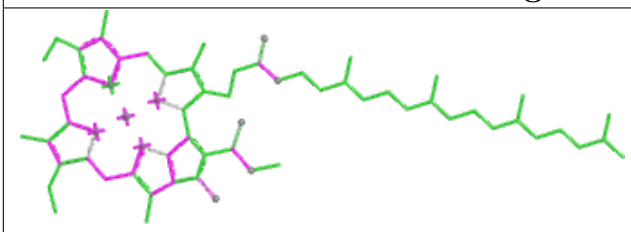


Torsions

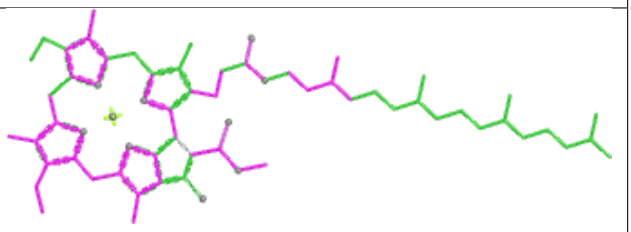


Rings

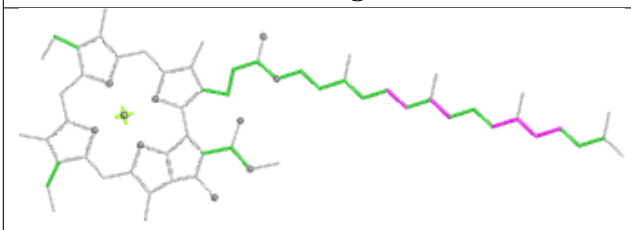
Ligand CLA B 616



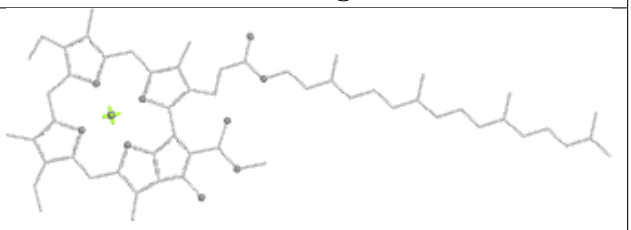
Bond lengths



Bond angles

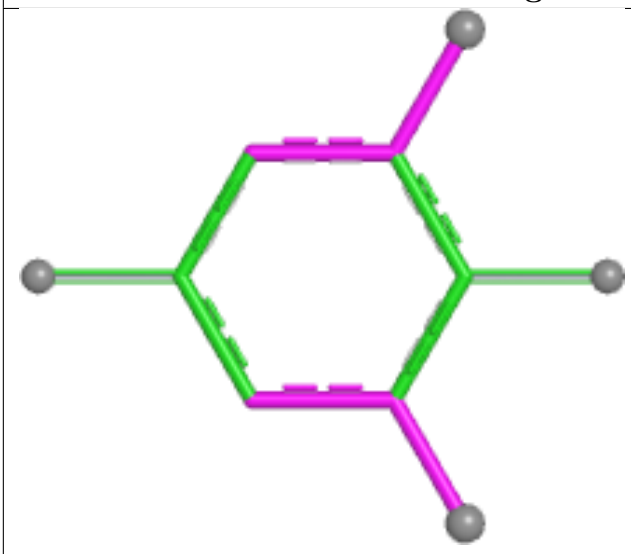


Torsions

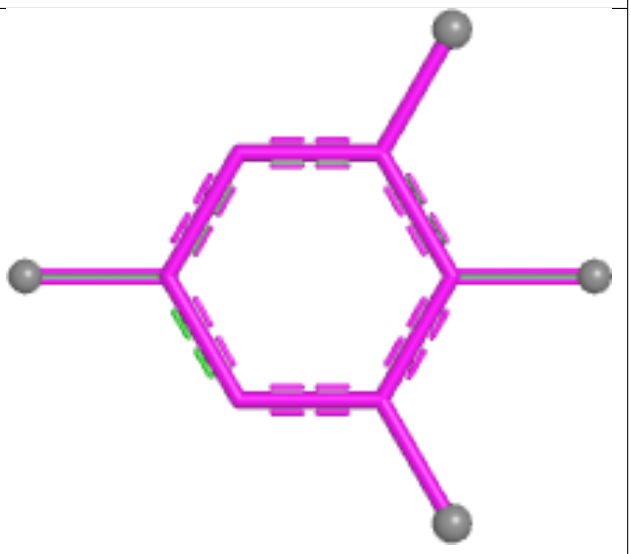


Rings

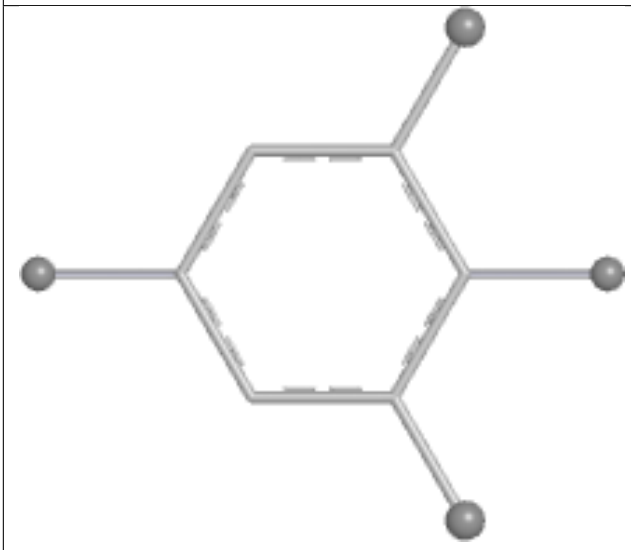
Ligand JOX A 419



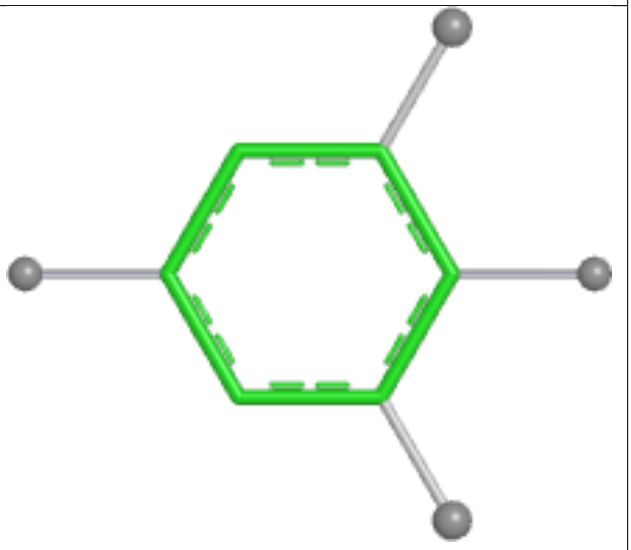
Bond lengths



Bond angles

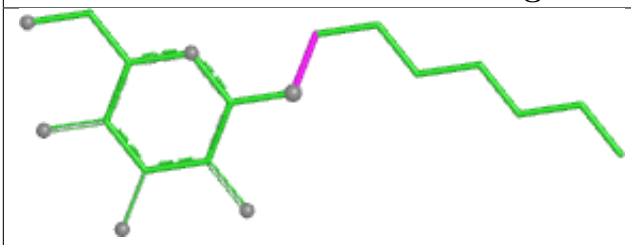


Torsions

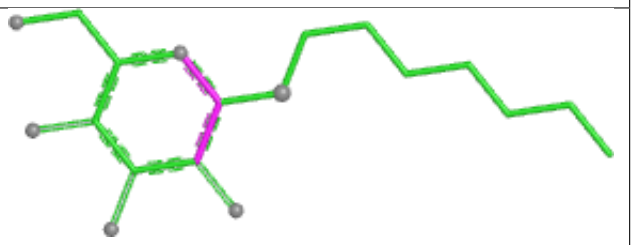


Rings

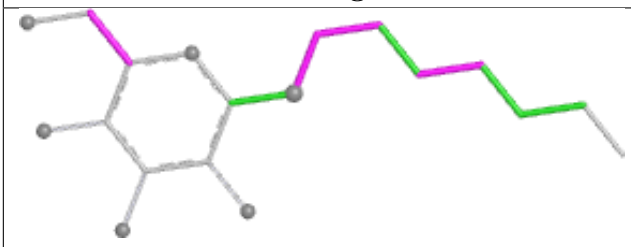
Ligand HTG b 602



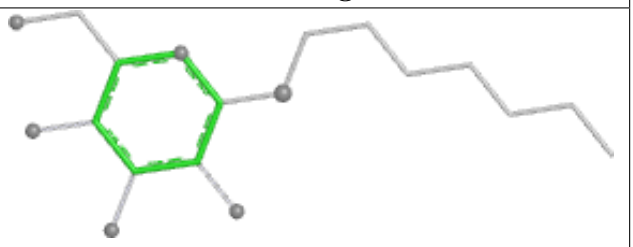
Bond lengths



Bond angles

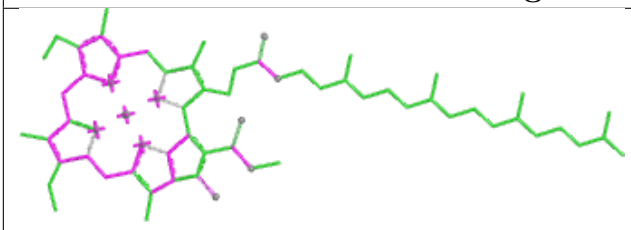


Torsions

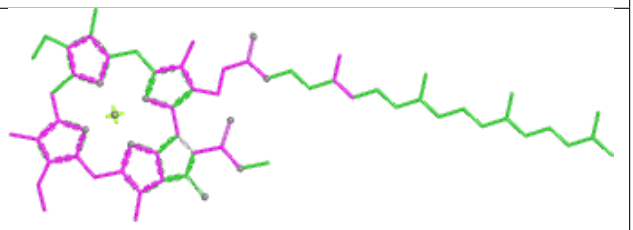


Rings

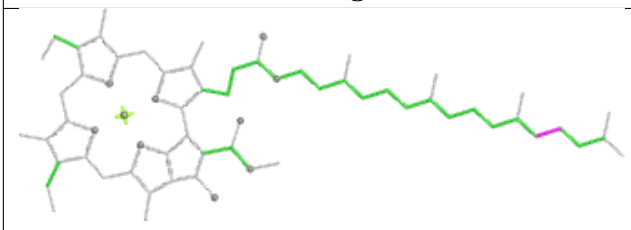
Ligand CLA B 603



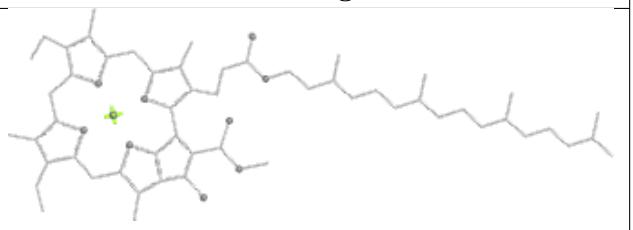
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR D 2305

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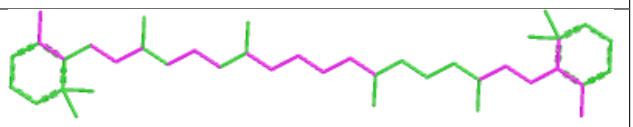

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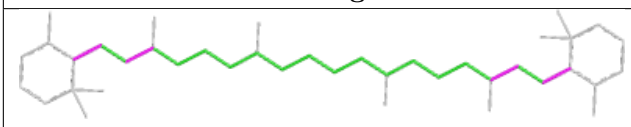
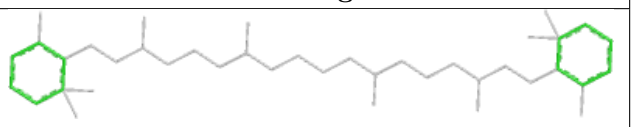
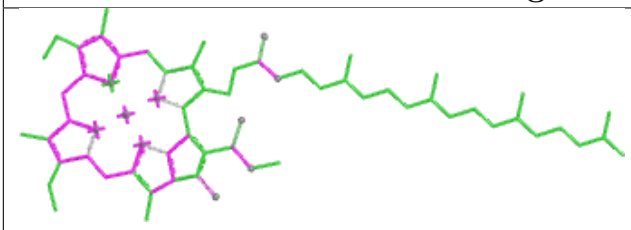


Torsions



Rings

Ligand CLA b 607



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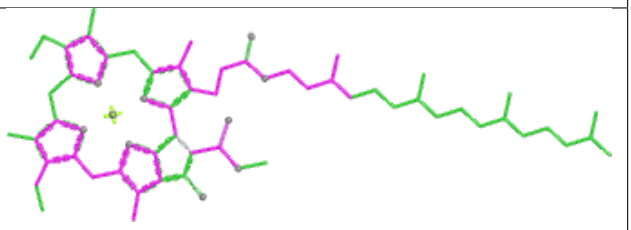
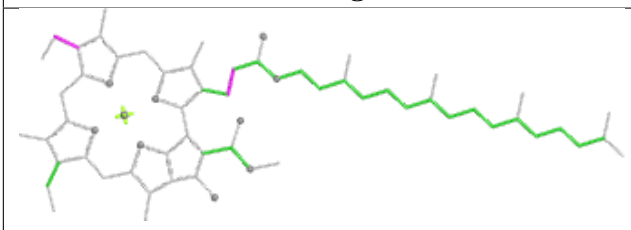


Bond angles



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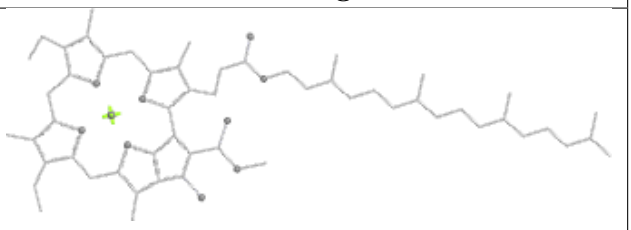
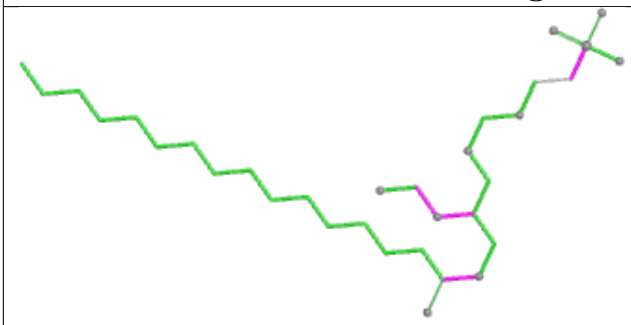


Rings

Ligand SQD d 417



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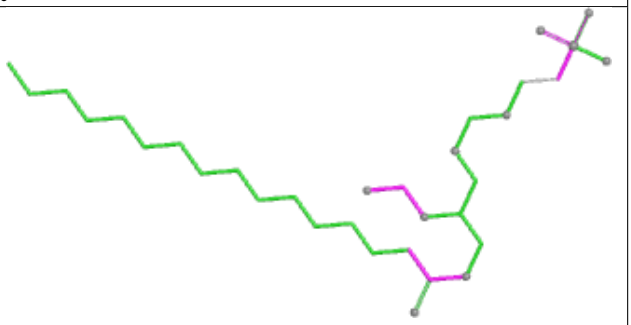
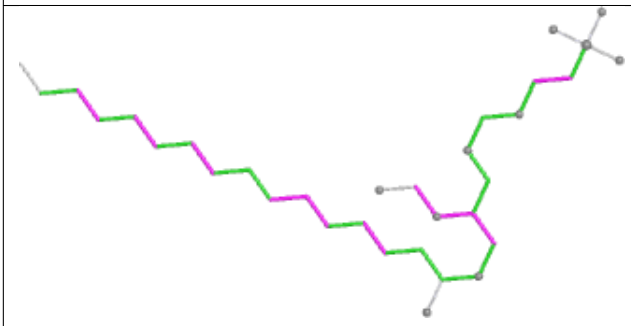


Bond angles



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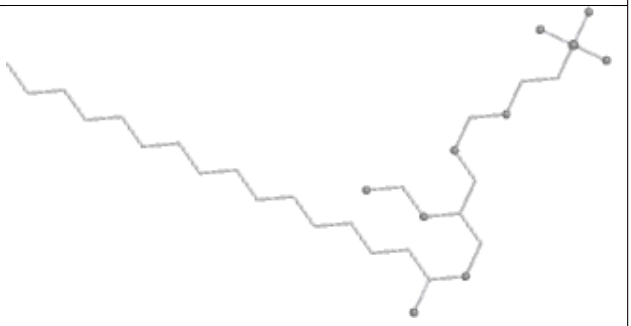
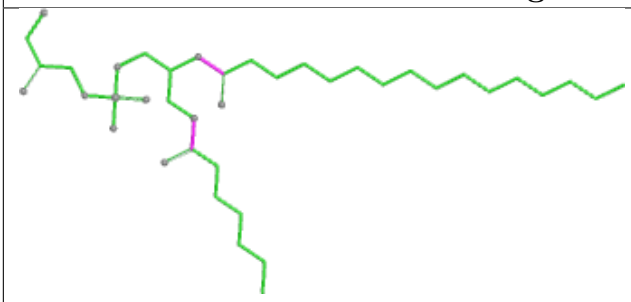


Rings

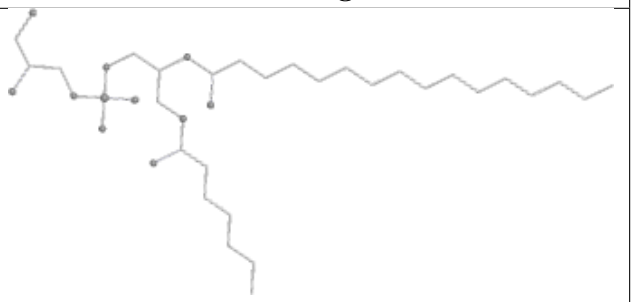
Ligand LHG e 101



Bond lengths

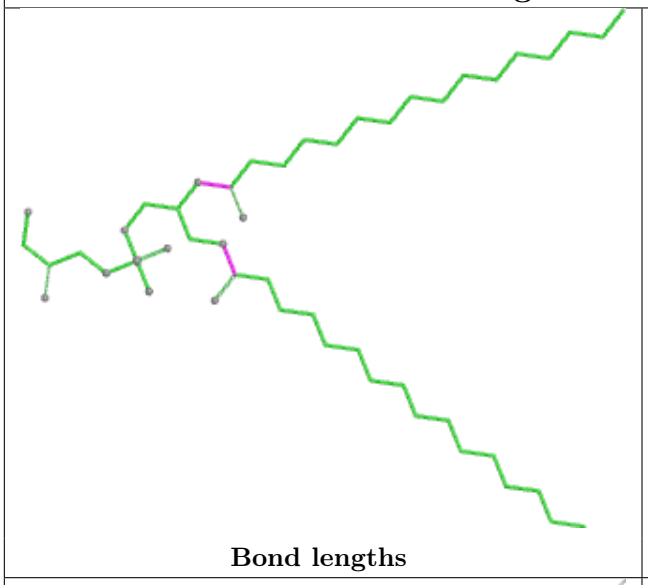
Bond angles

Torsions



Rings

Ligand LHG D 2309



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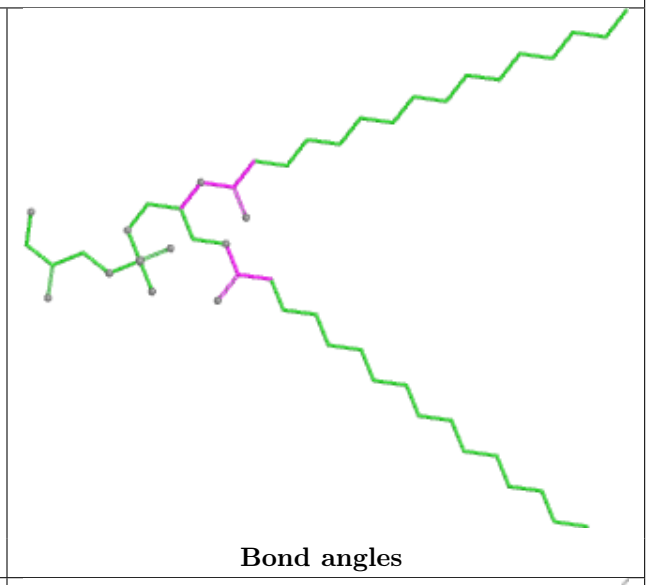
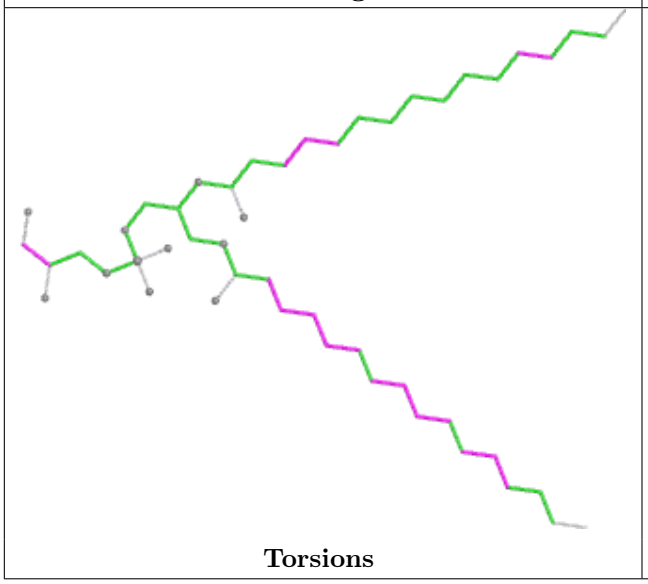


Bond angles



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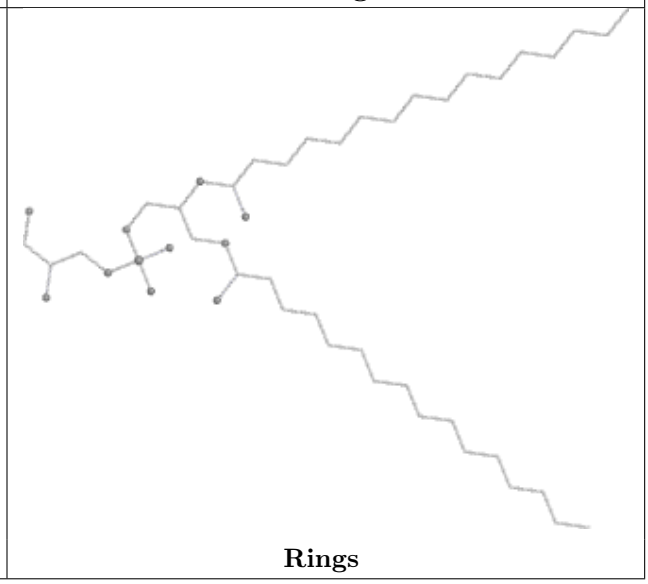
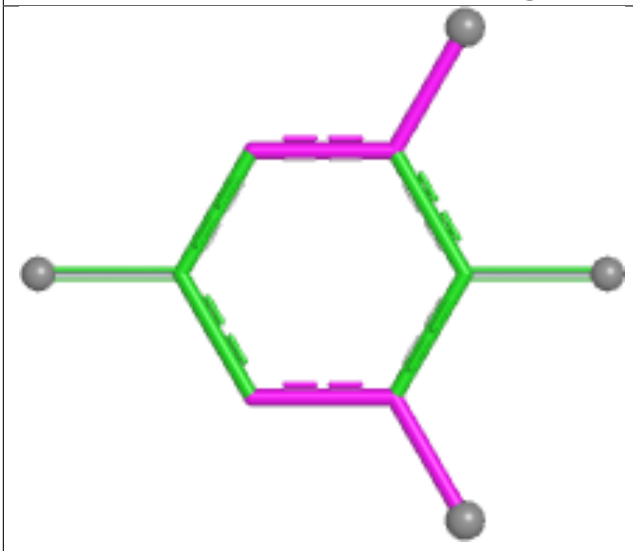


Rings

Ligand JOX a 2617



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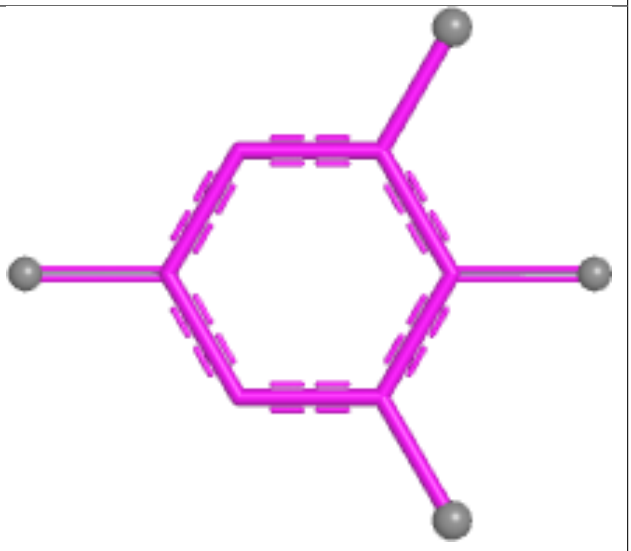
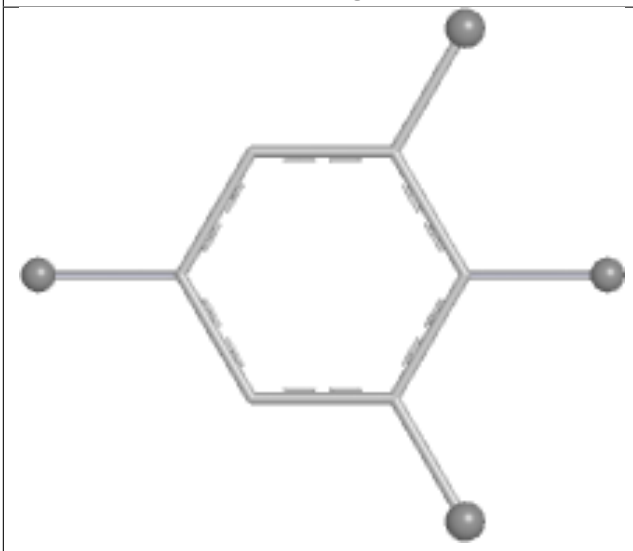


Bond angles



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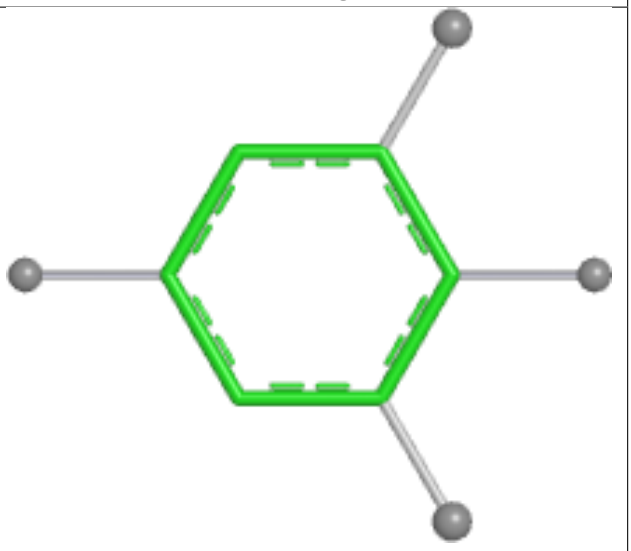
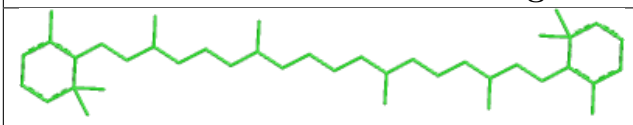


Rings

Ligand BCR z 101



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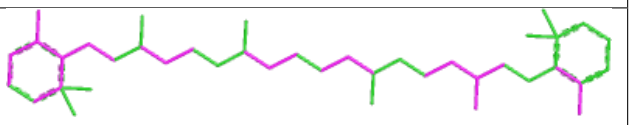
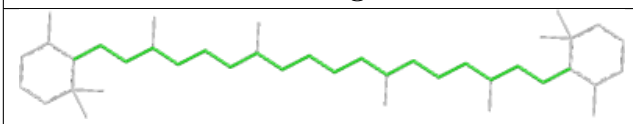


Bond angles



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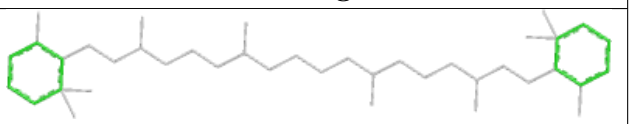
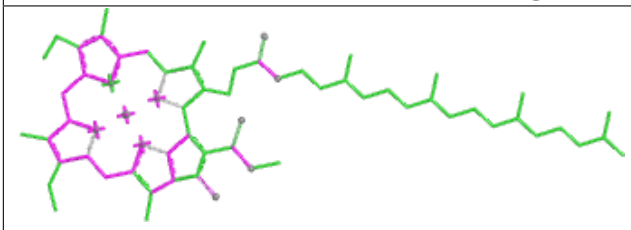


Rings

Ligand CLA b 618



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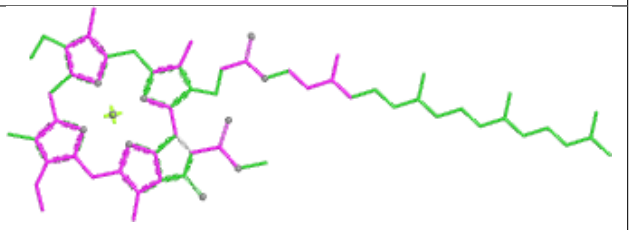
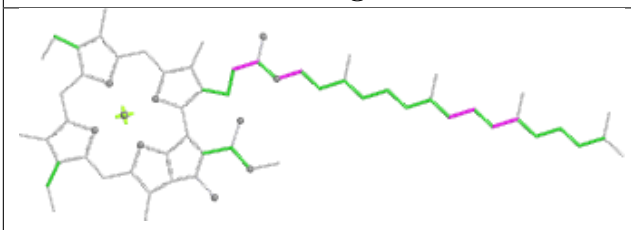


Bond angles



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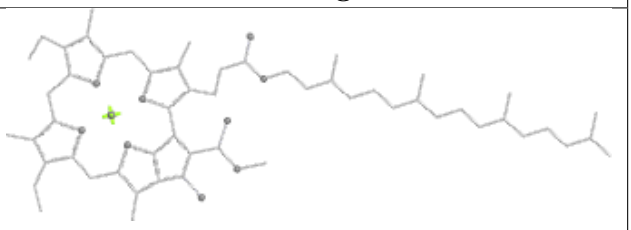
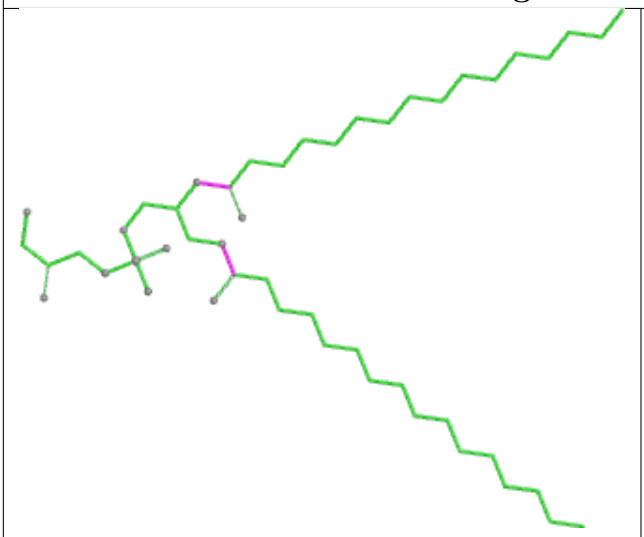


Rings

Ligand LHG D 2310



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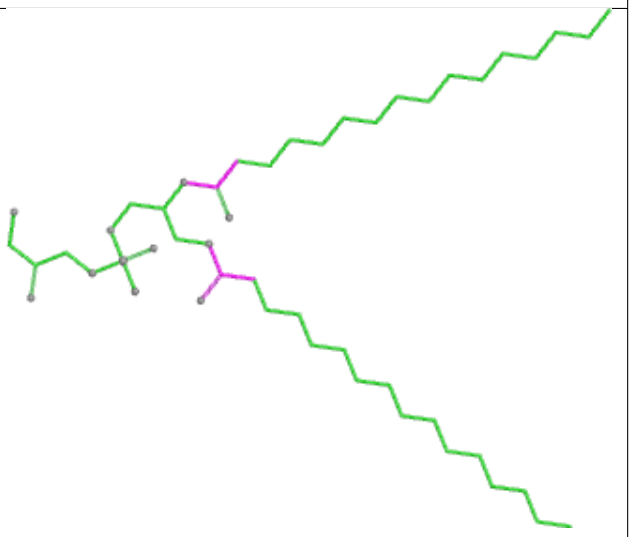
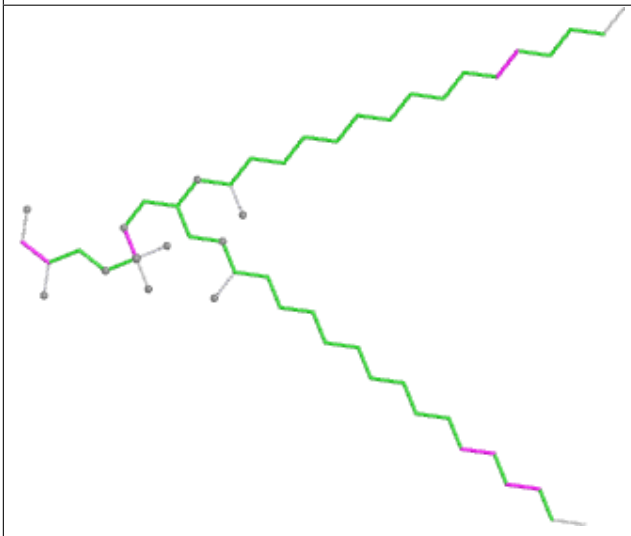


Bond angles



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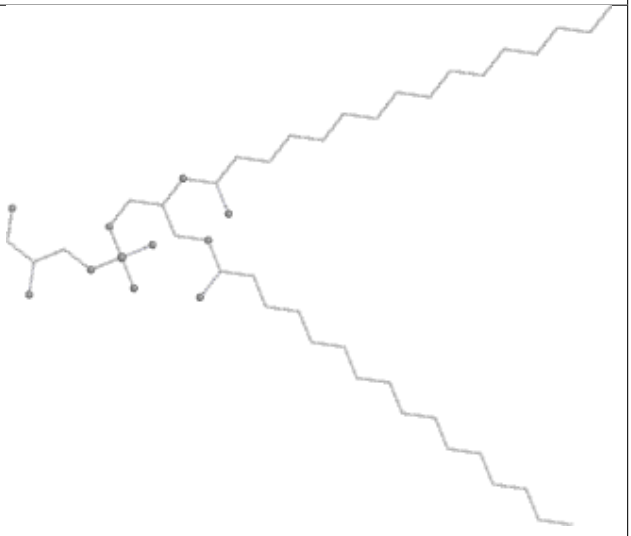
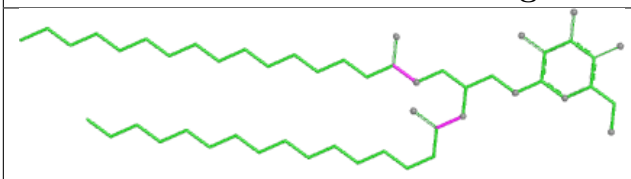
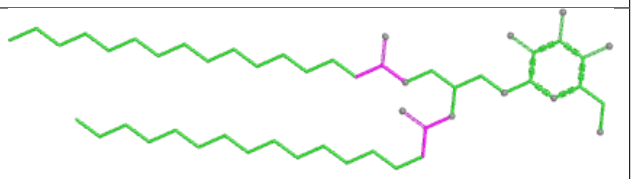


Rings

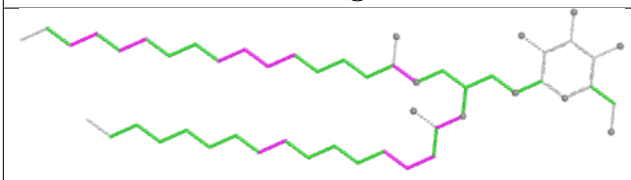
Ligand LMG C 520



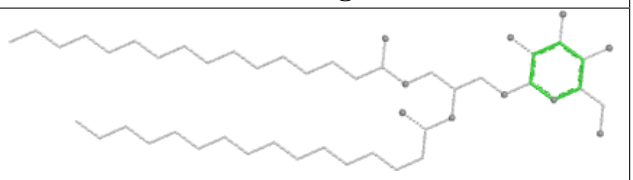
Bond lengths



Bond angles

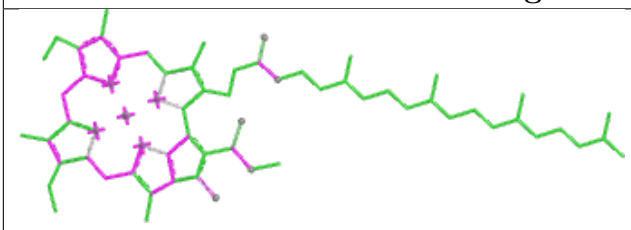


Torsions



Rings

Ligand CLA B 612



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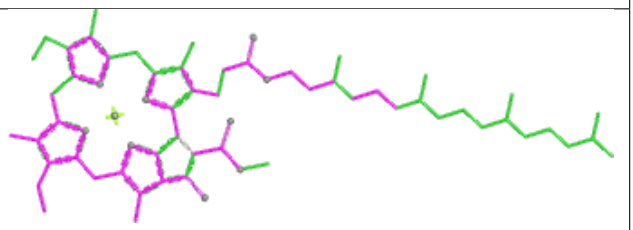
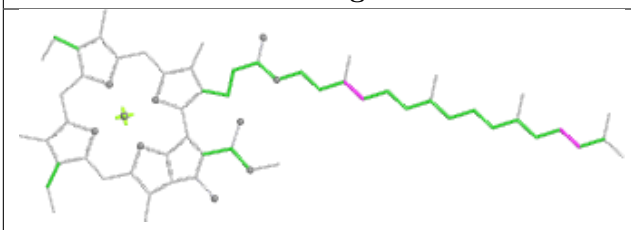
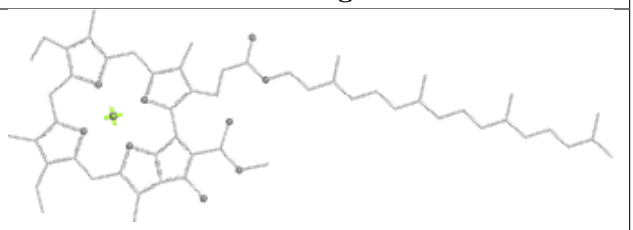


Bond angles

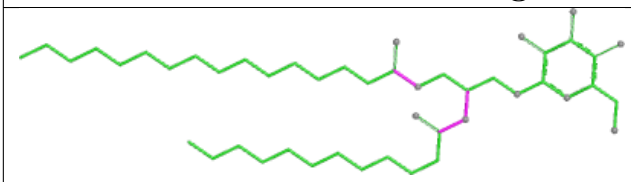


Torsions

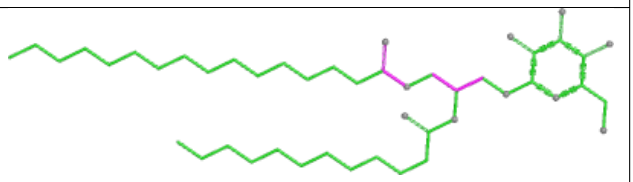


Rings

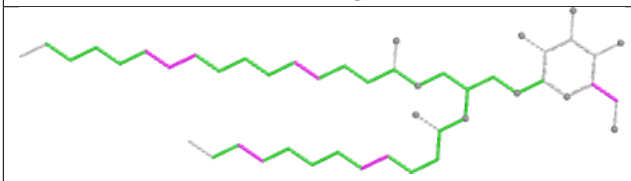
Ligand LMG D 2312



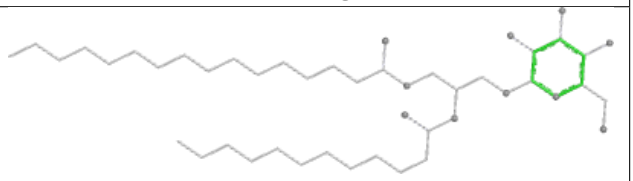
Bond lengths



Bond angles

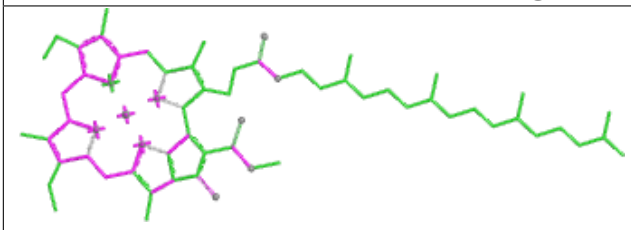


Torsions

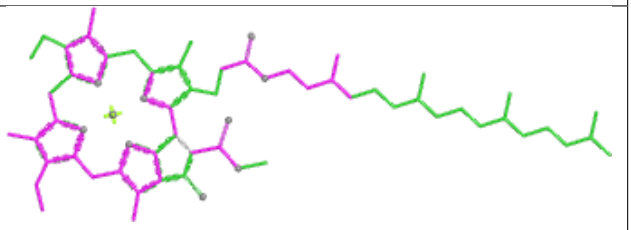


Rings

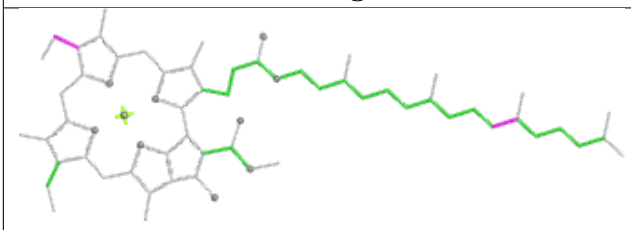
Ligand CLA c 514



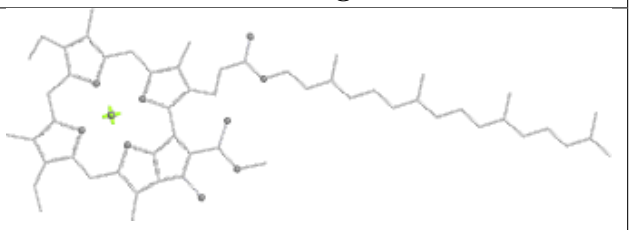
Bond lengths



Bond angles

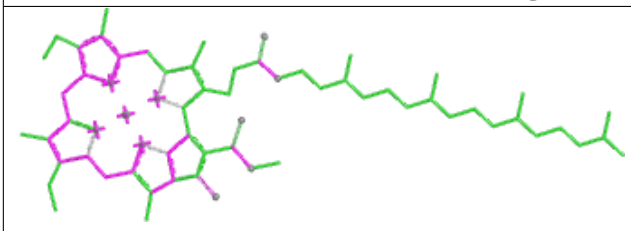


Torsions



Rings

Ligand CLA C 509



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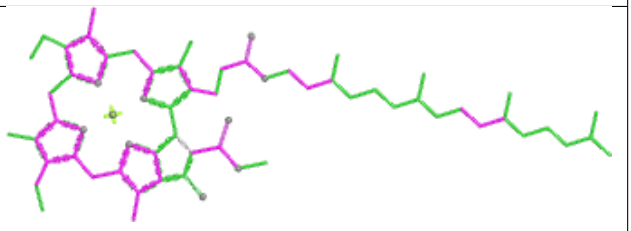
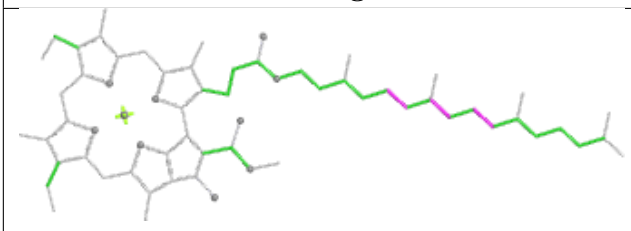
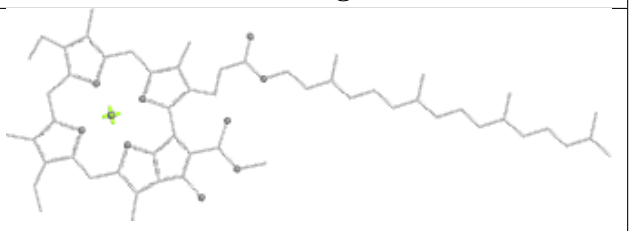


Bond angles

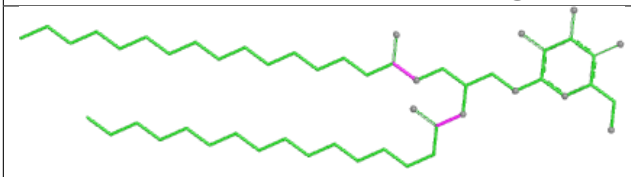


Torsions



Rings

Ligand LMG m 2802



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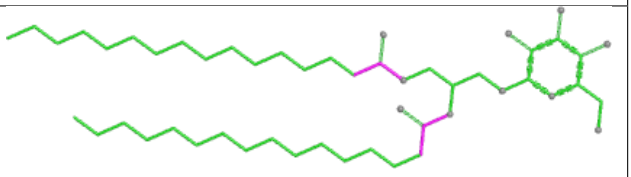
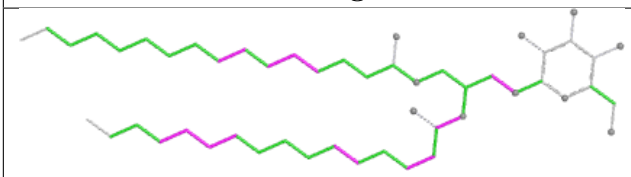


Bond angles



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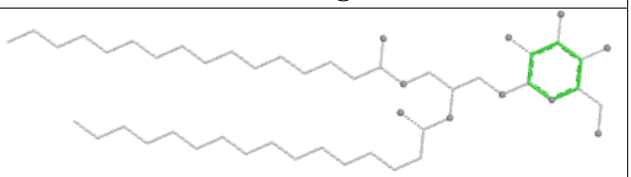
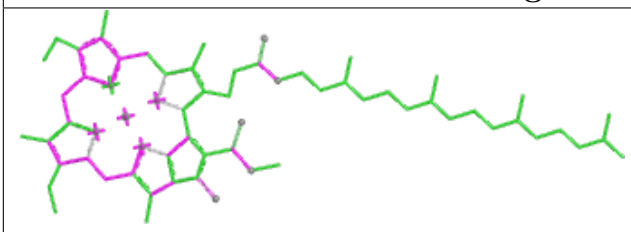
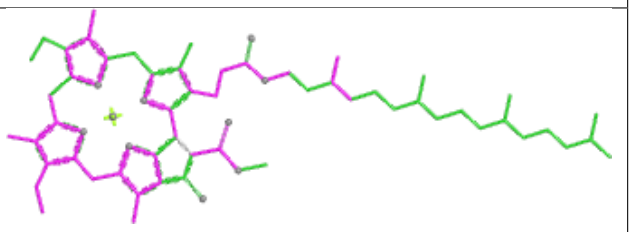


Rings

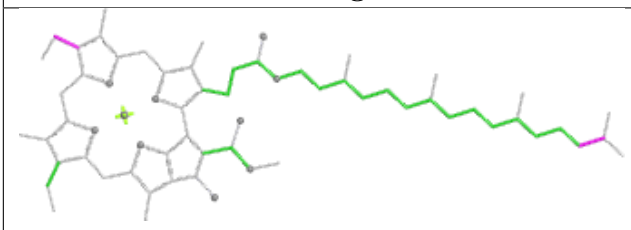
Ligand CLA B 608



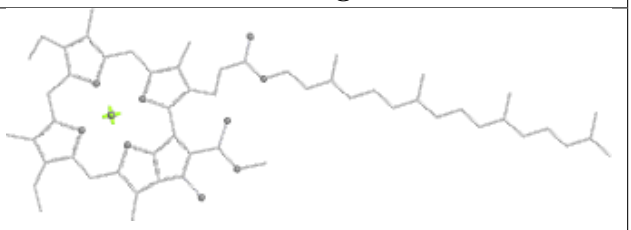
Bond lengths



Bond angles

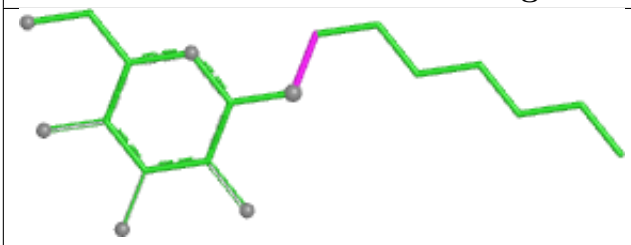


Torsions



Rings

Ligand HTG B 627



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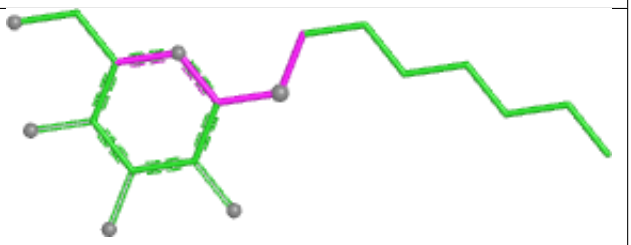
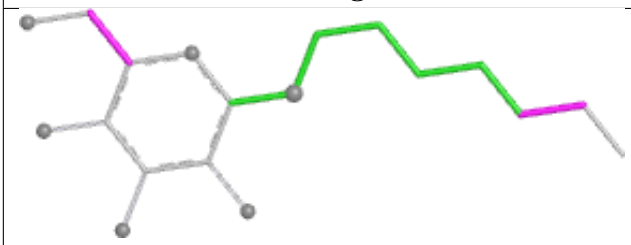


Bond angles



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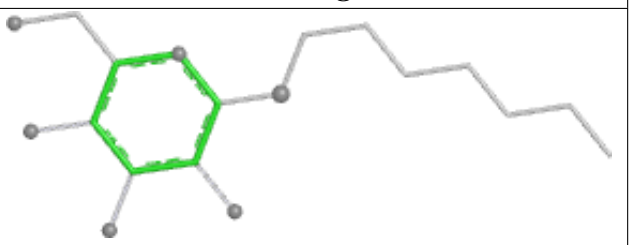
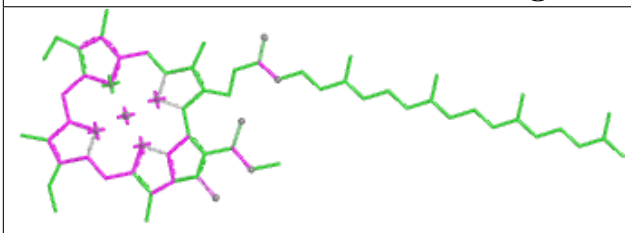


Rings

Ligand CLA c 506



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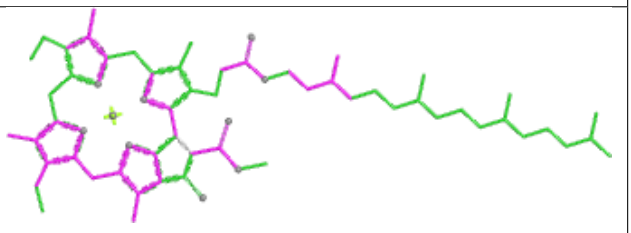
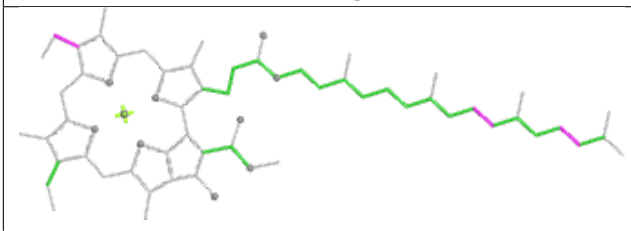


Bond angles



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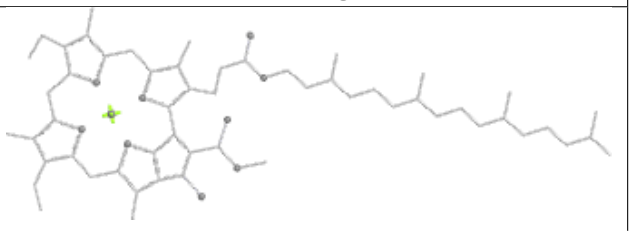
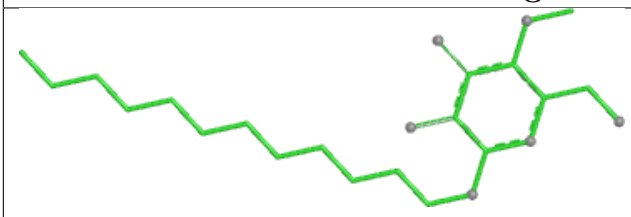


Rings

Ligand LMT d 404



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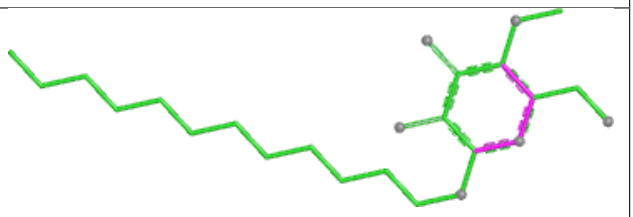
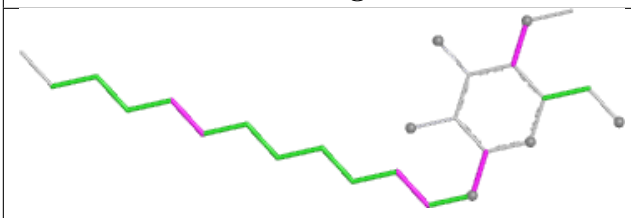


Bond angles



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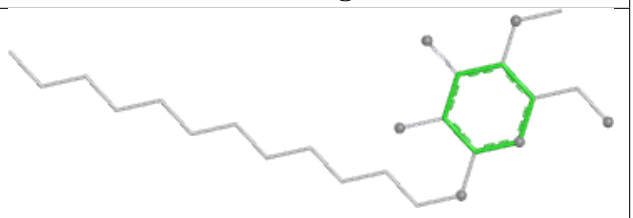
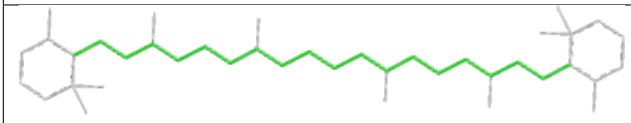


Rings

Ligand BCR B 619

Bond lengths

Bond angles



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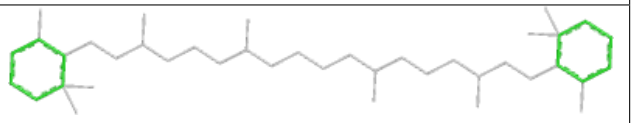
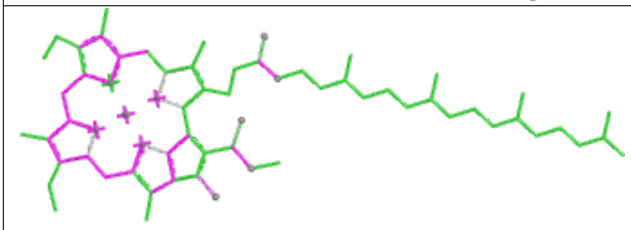
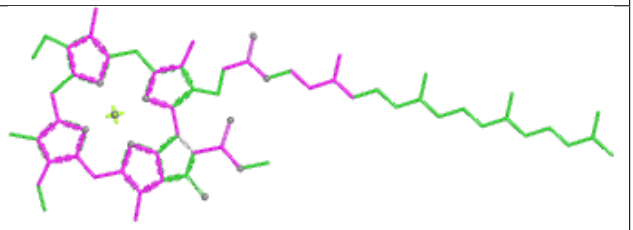


Rings

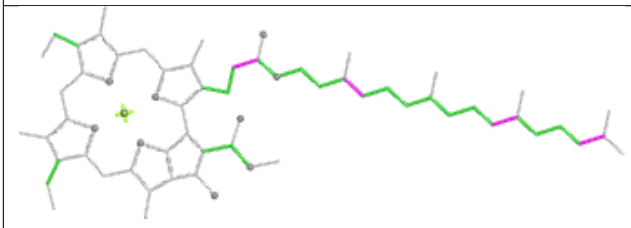
Ligand CLA C 506



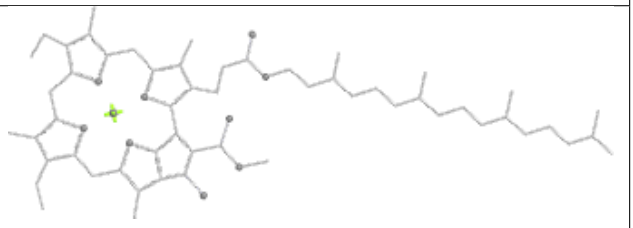
Bond lengths



Bond angles

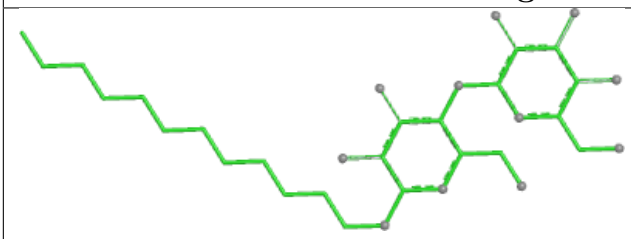


Torsions



Rings

Ligand LMT M 101



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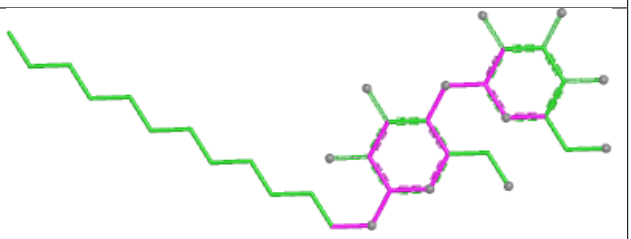

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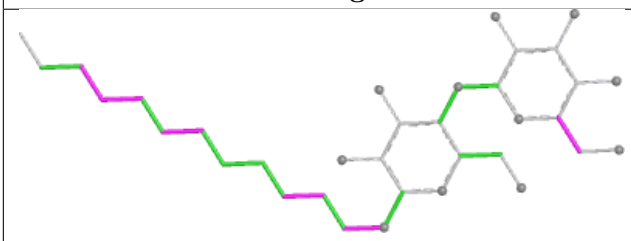

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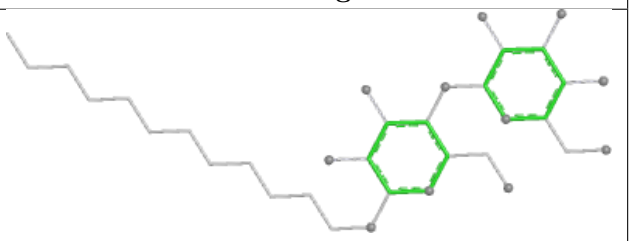
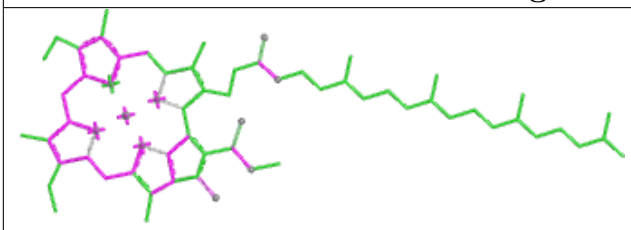


Rings

Ligand CLA c 512



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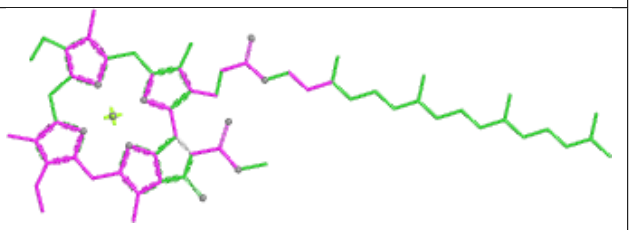
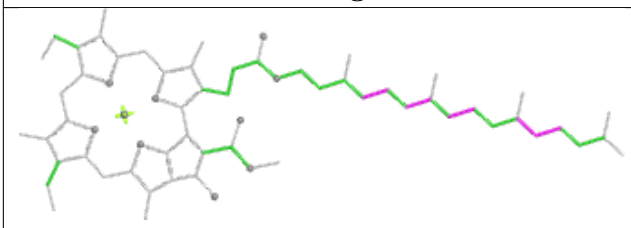


Bond angles



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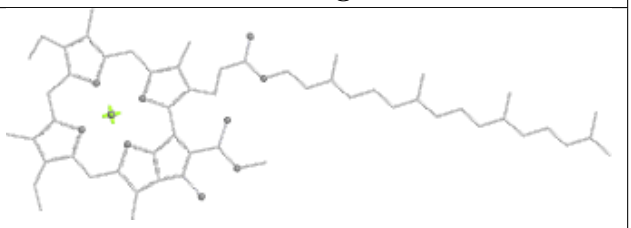
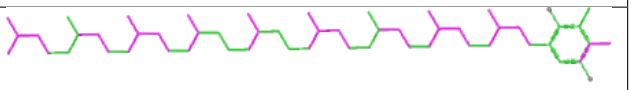


Rings

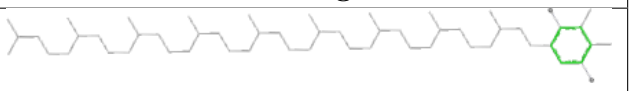
Ligand PL9 D 2306

Bond lengths



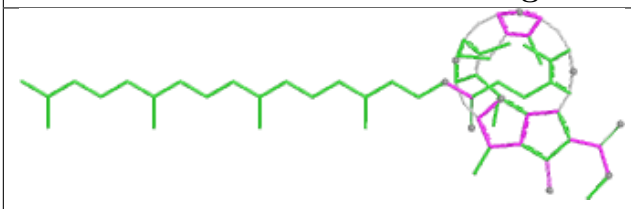
Bond angles

Torsions



Rings

Ligand PHO A 408



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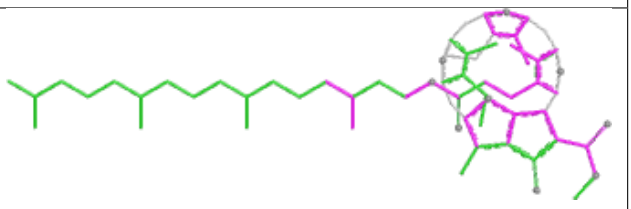
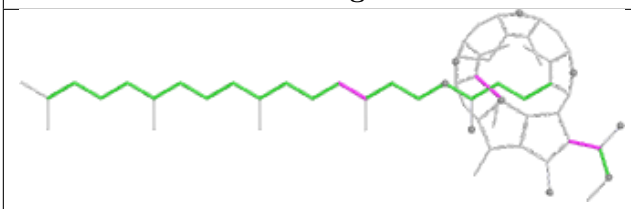
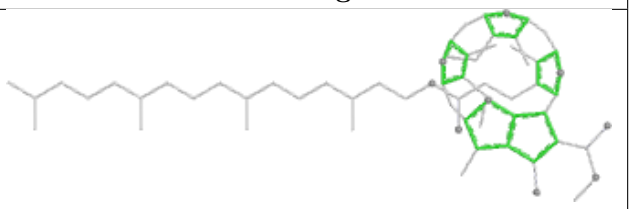


Bond angles

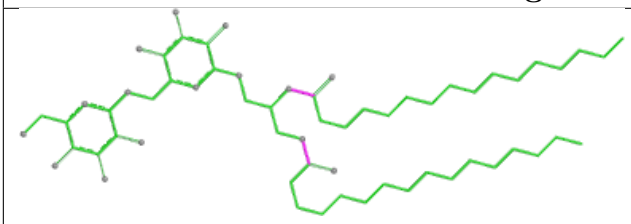


Torsions

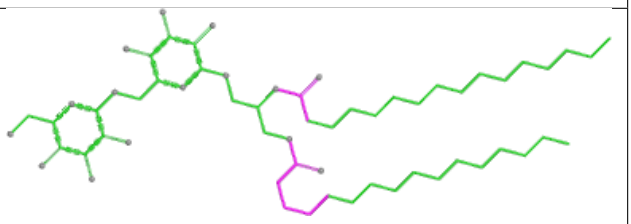


Rings

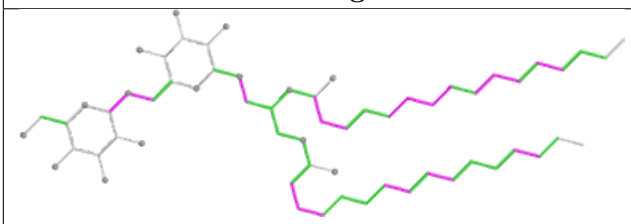
Ligand DGD c 519



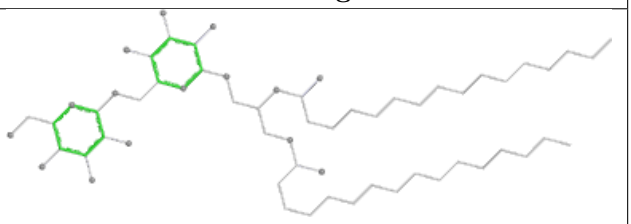
Bond lengths



Bond angles

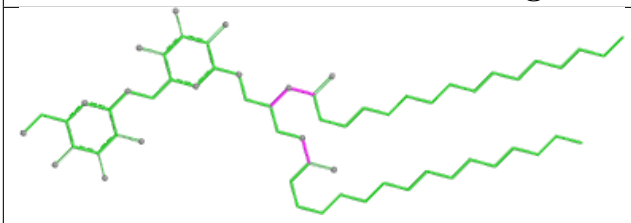


Torsions



Rings

Ligand DGD c 520



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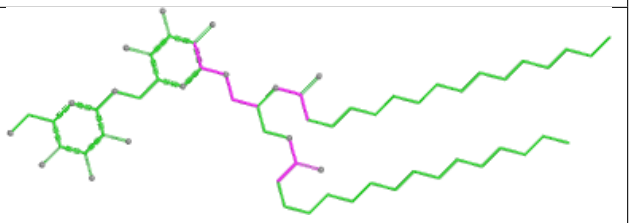
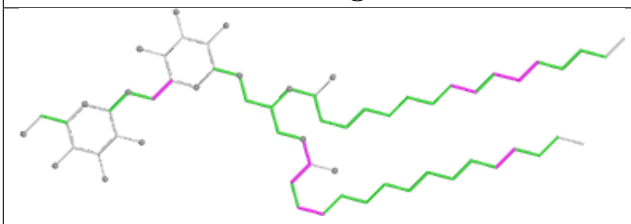
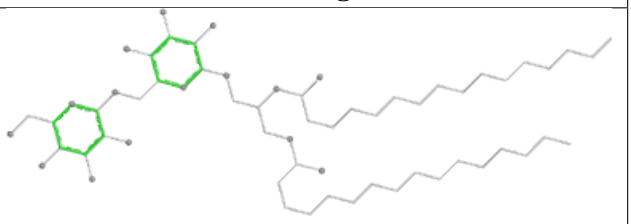


Bond angles

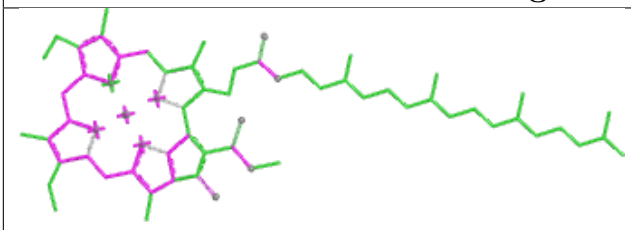


Torsions

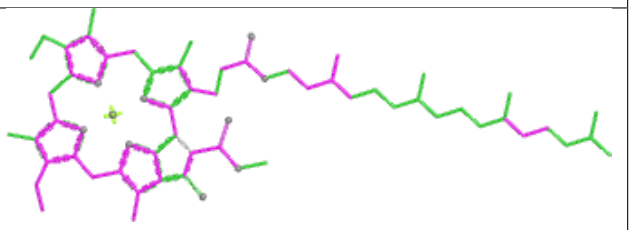


Rings

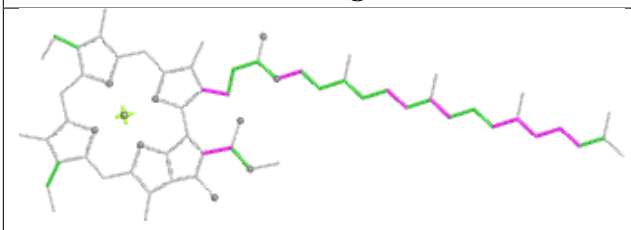
Ligand CLA c 509



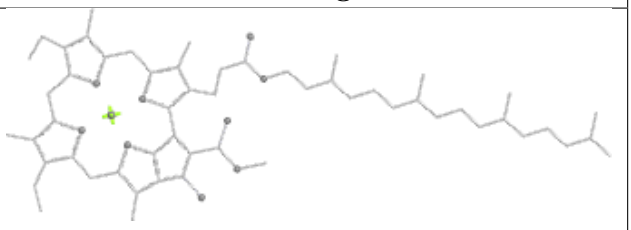
Bond lengths



Bond angles

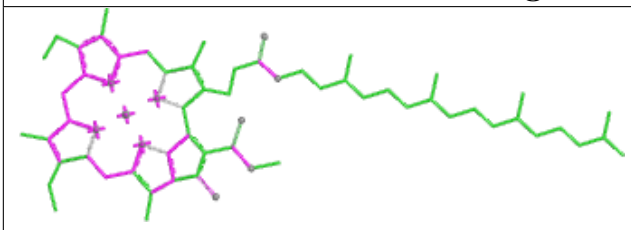


Torsions



Rings

Ligand CLA C 513



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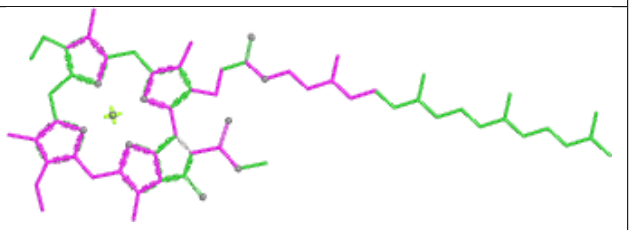
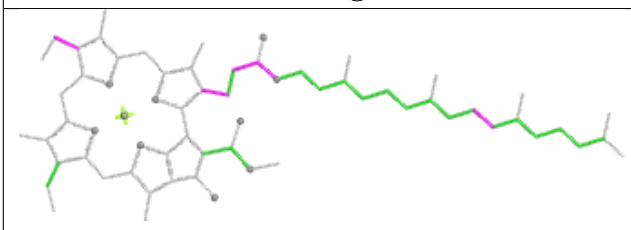
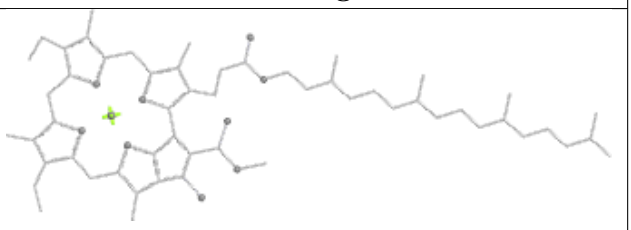


Bond angles

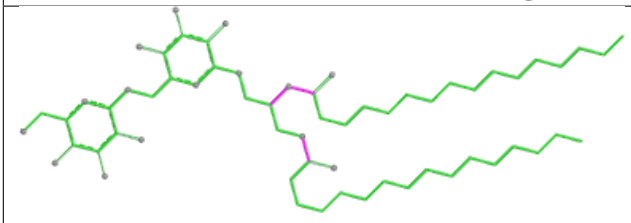


Torsions



Rings

Ligand DGD C 517



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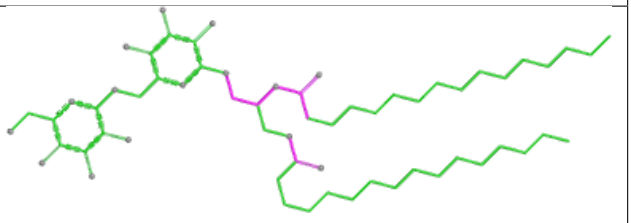
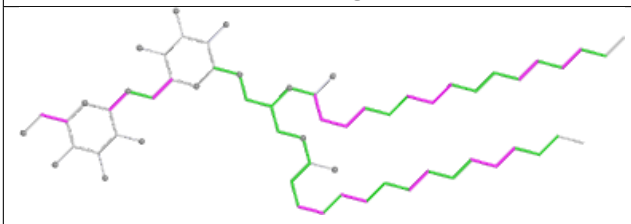


Bond angles



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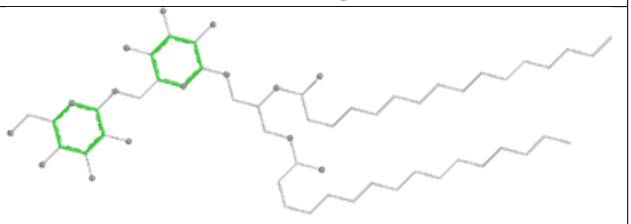
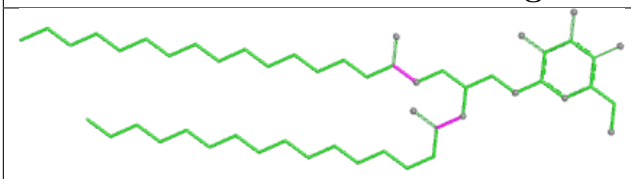


Rings

Ligand LMG c 501



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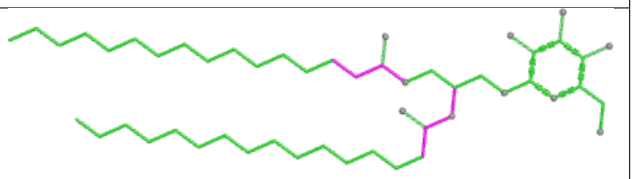
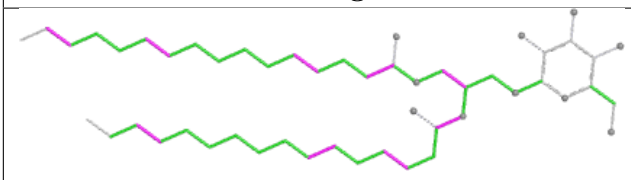


Bond angles



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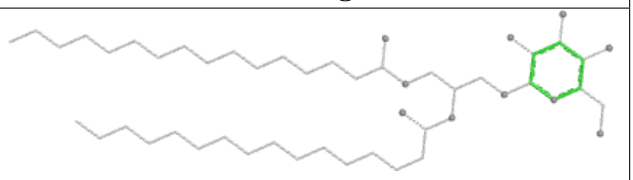
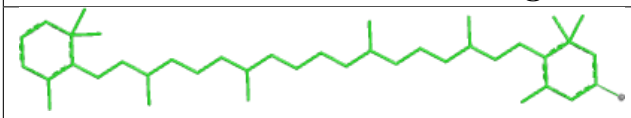


Rings

Ligand RRX h 101



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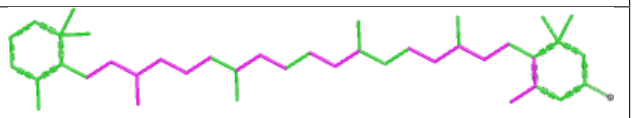
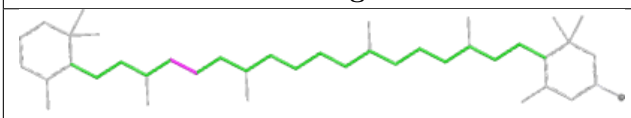


Bond angles



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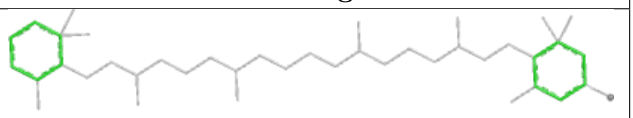
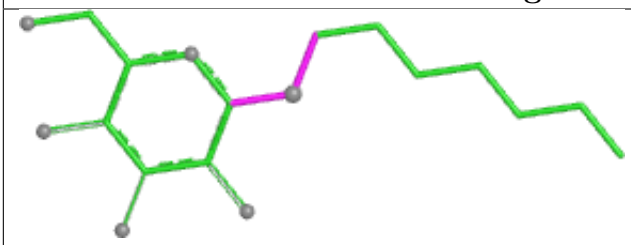


Rings

Ligand HTG b 626



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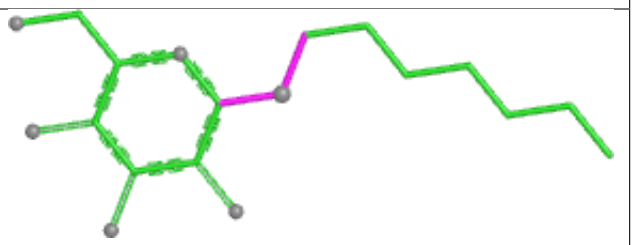
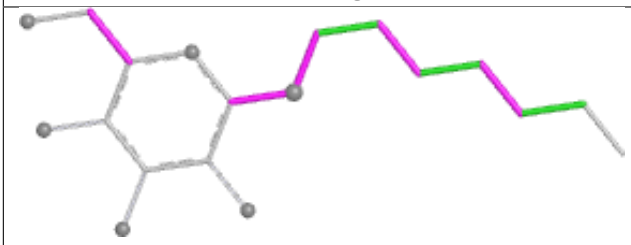
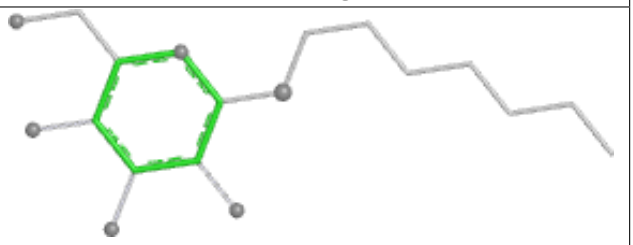


Bond angles

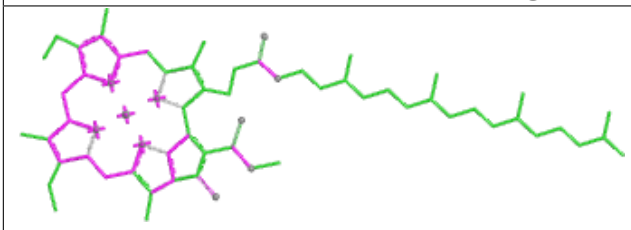


Torsions



Rings

Ligand CLA C 514



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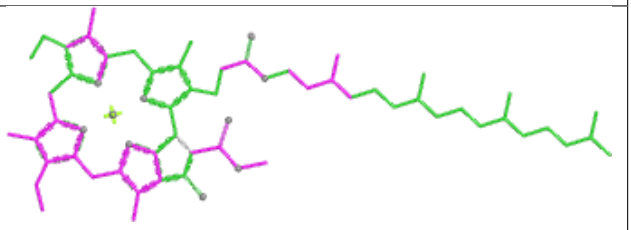
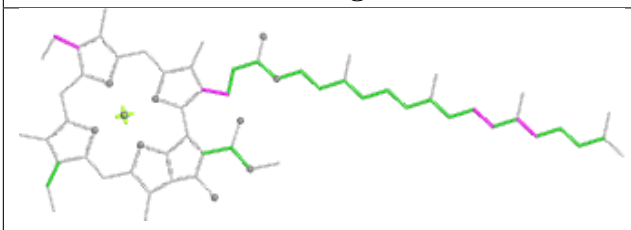


Bond angles



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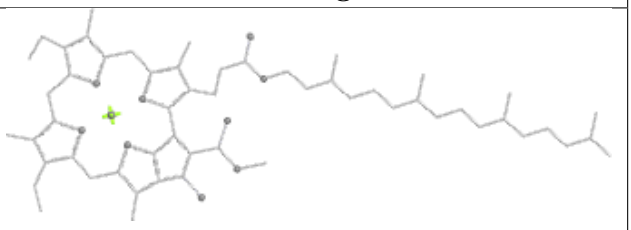
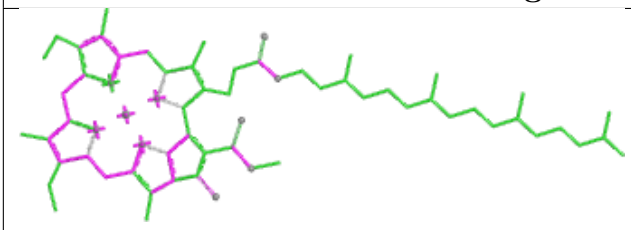


Rings

Ligand CLA B 607



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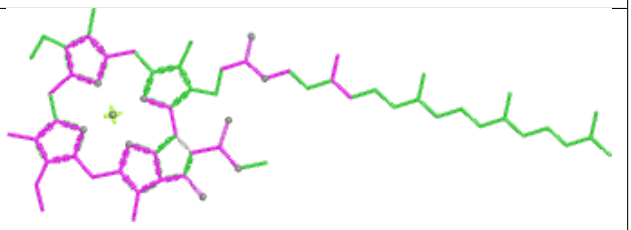
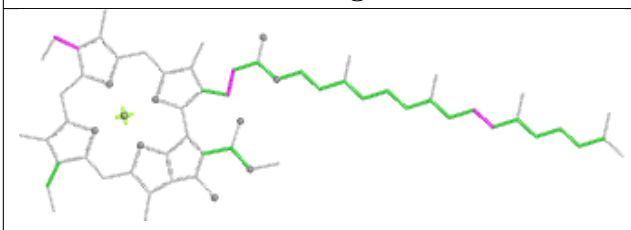


Bond angles



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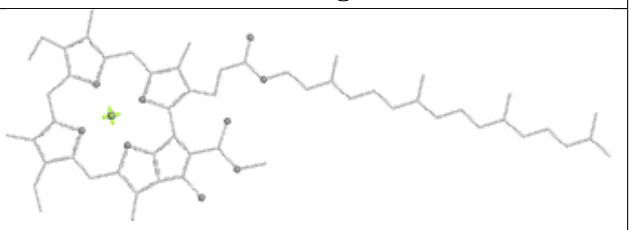
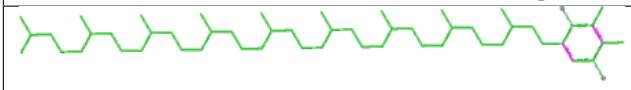


Rings

Ligand PL9 d 411



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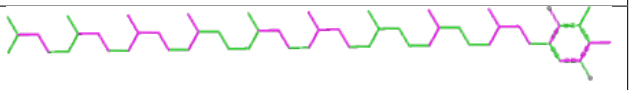
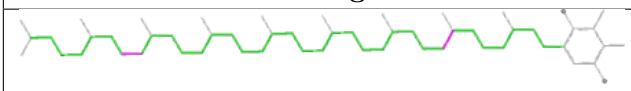
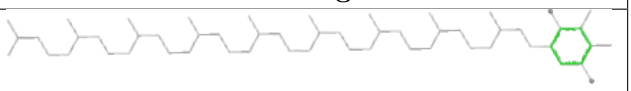


Bond angles

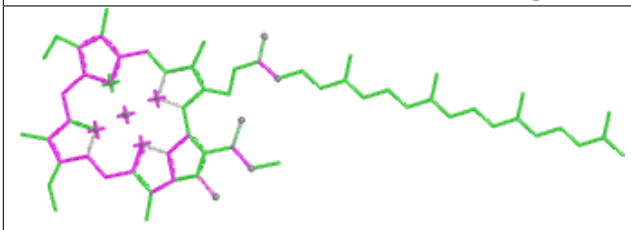


Torsions



Rings

Ligand CLA d 409



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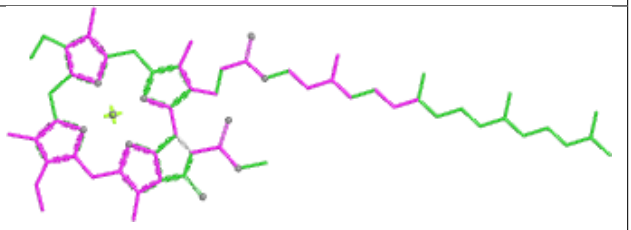
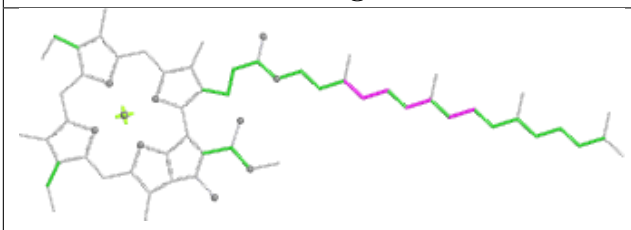


Bond angles



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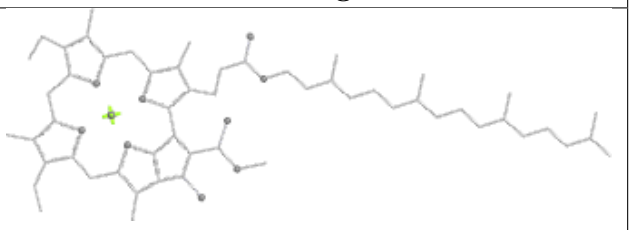
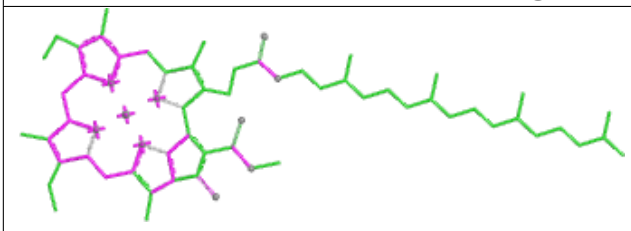


Rings

Ligand CLA c 516



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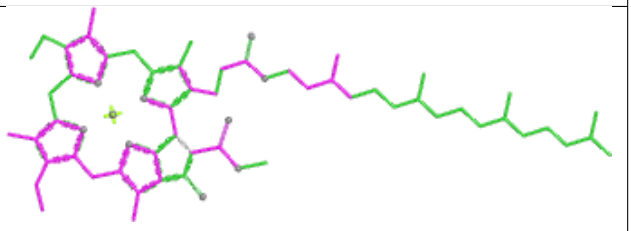
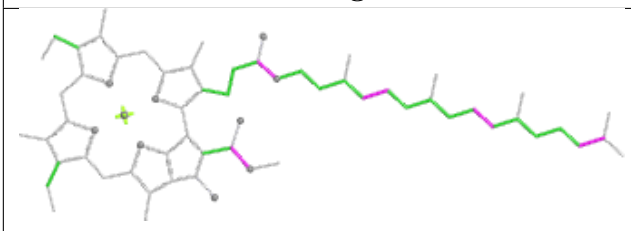


Bond angles



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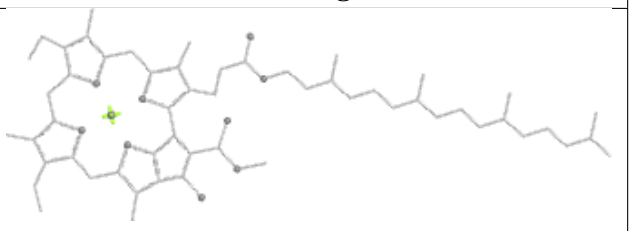
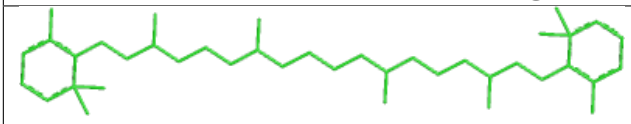


Rings

Ligand BCR c 517



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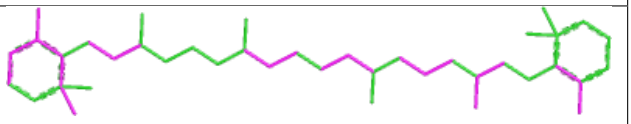
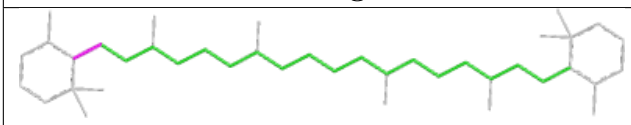
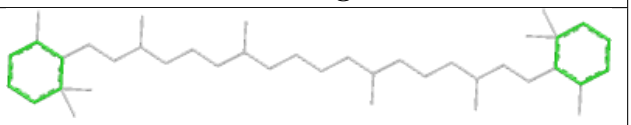


Bond angles

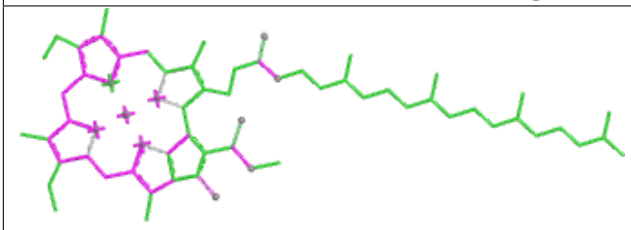


Torsions

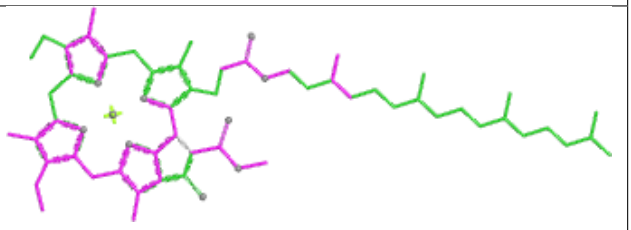


Rings

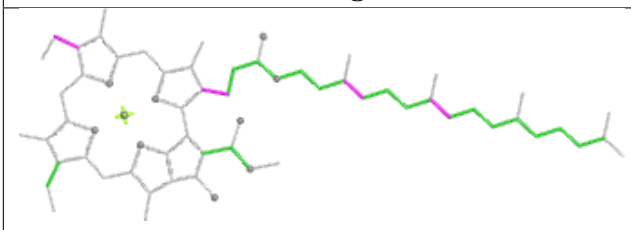
Ligand CLA b 614



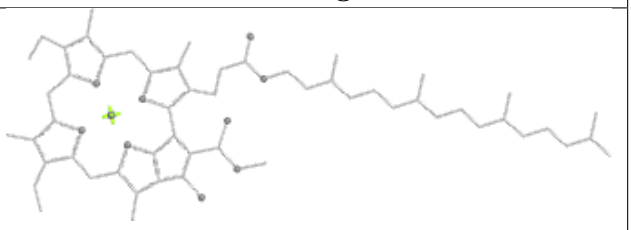
Bond lengths



Bond angles

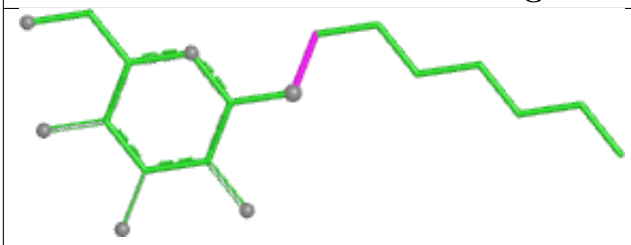


Torsions

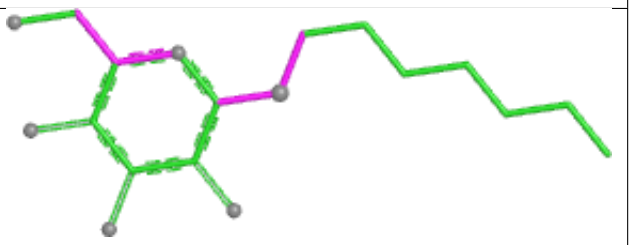


Rings

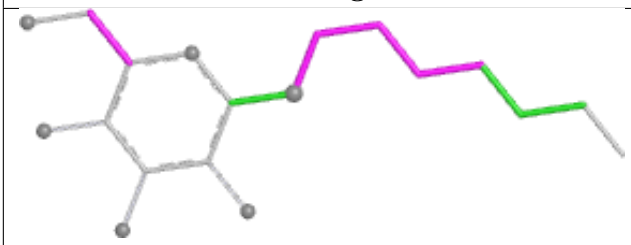
Ligand HTG o 301



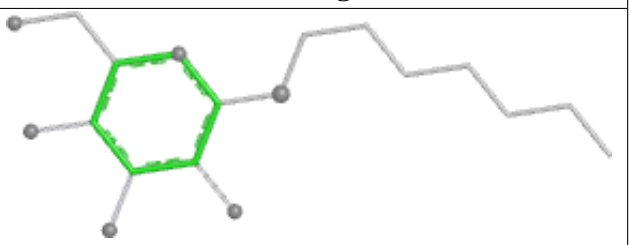
Bond lengths



Bond angles

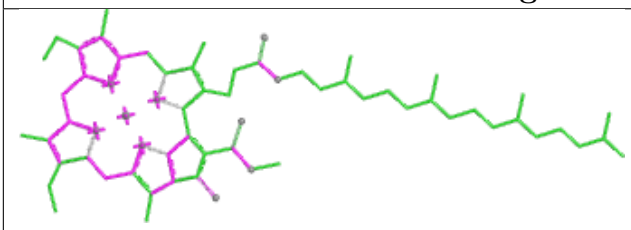


Torsions

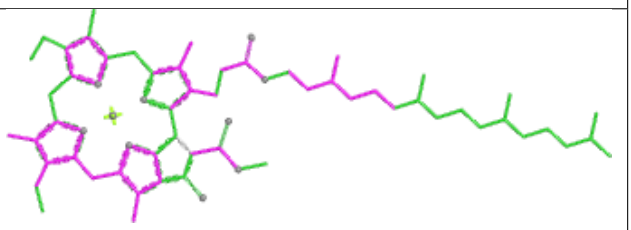


Rings

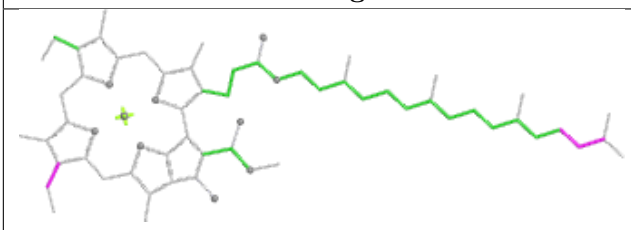
Ligand CLA a 2609



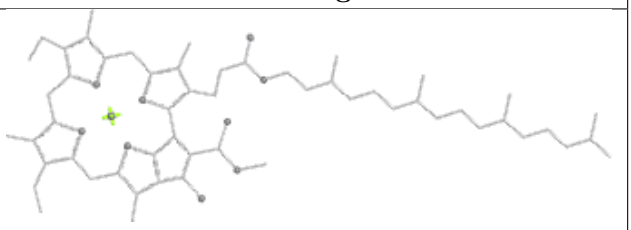
Bond lengths



Bond angles

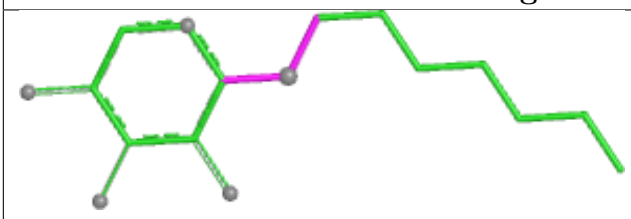


Torsions

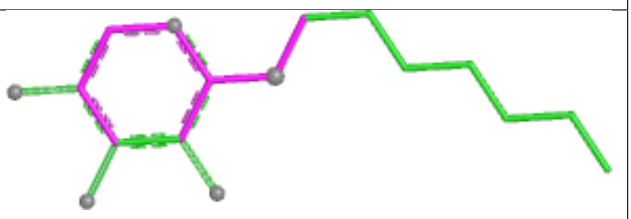


Rings

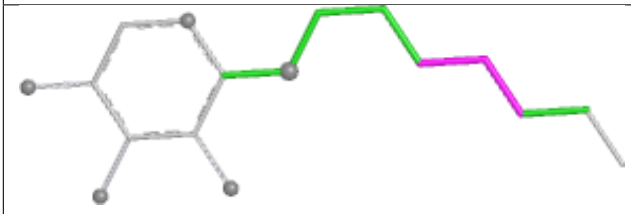
Ligand HTG H 101



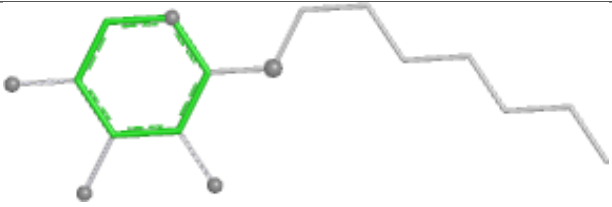
Bond lengths



Bond angles

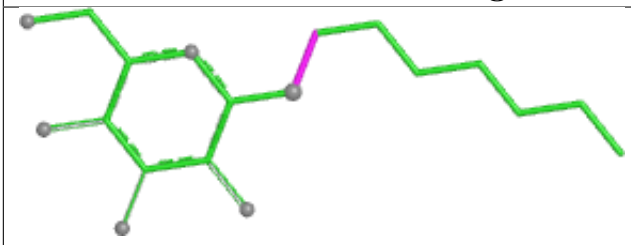


Torsions

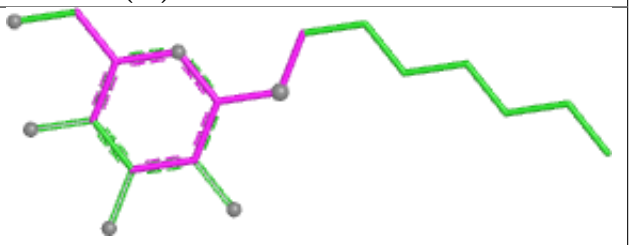


Rings

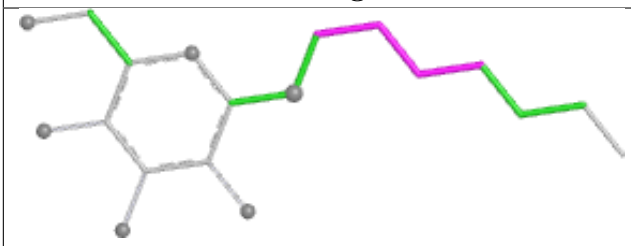
Ligand HTG B 624 (B)



Bond lengths



Bond angles



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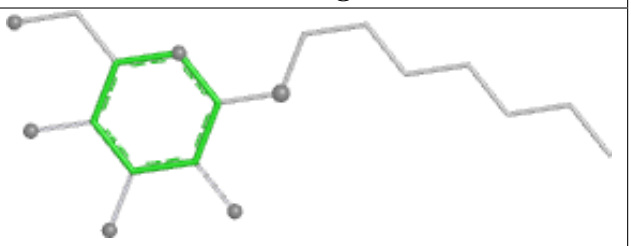

Rings

Ligand BCR C 516

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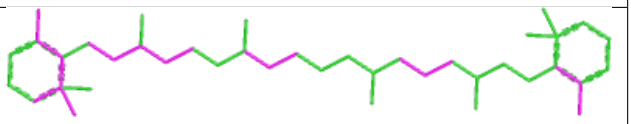
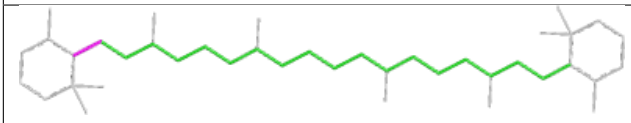
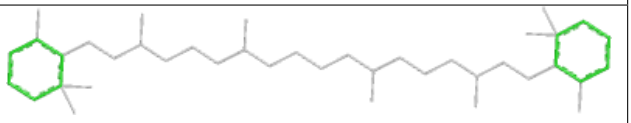


Bond angles

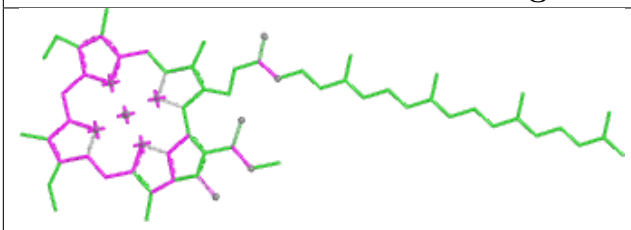


Torsions



Rings

Ligand CLA c 513



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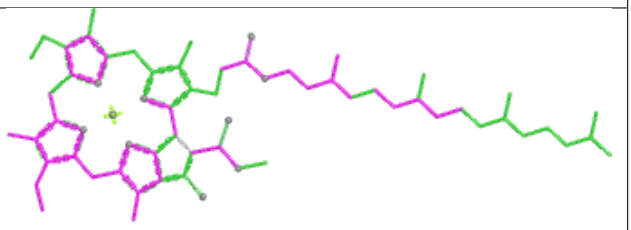
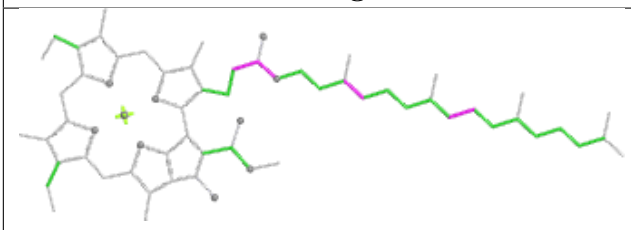


Bond angles



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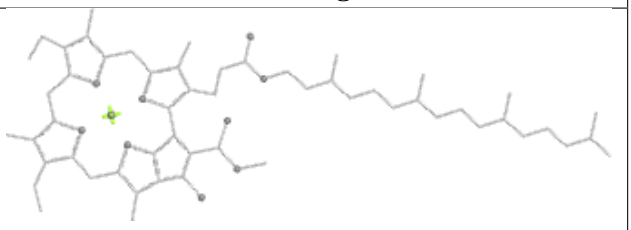
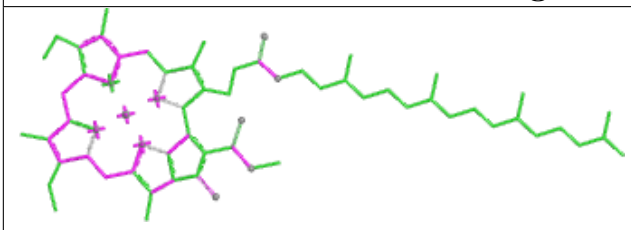


Rings

Ligand CLA c 507



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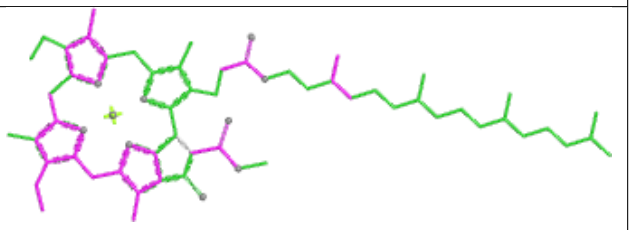
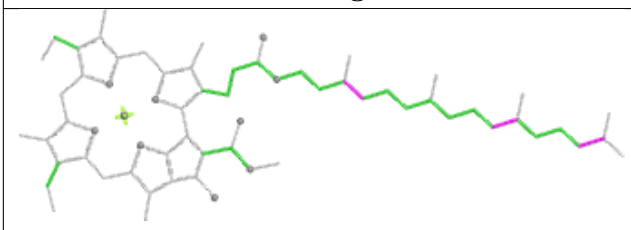


Bond angles



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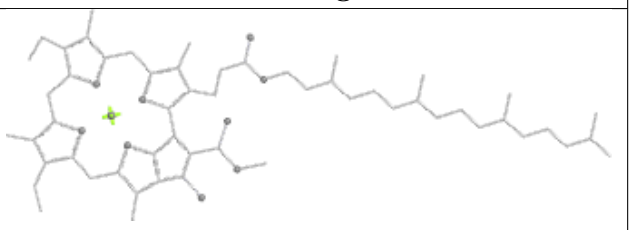
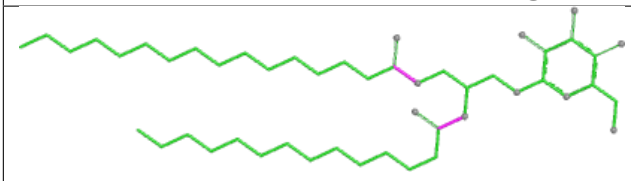


Rings

Ligand LMG c 521



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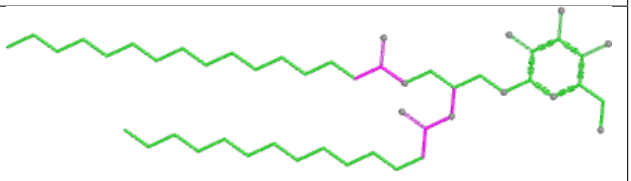
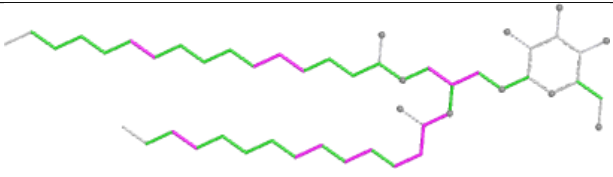


Bond angles



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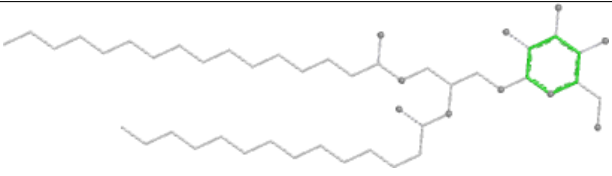
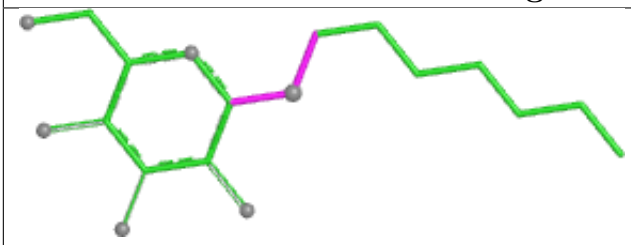


Rings

Ligand HTG c 523



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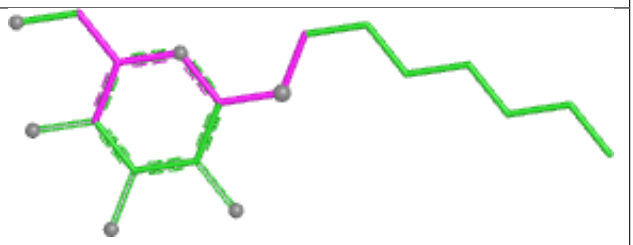
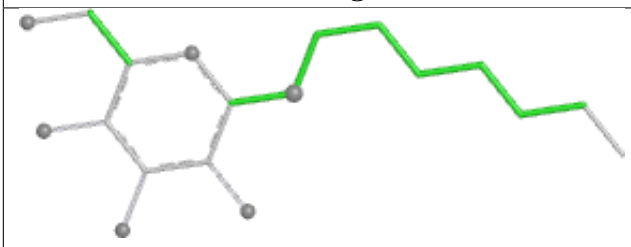


Bond angles



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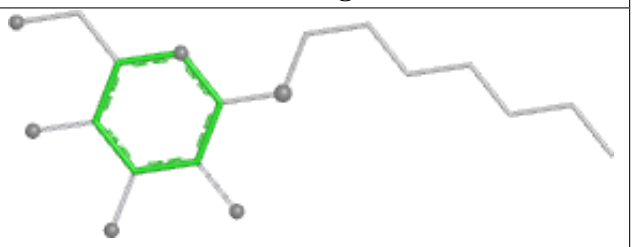
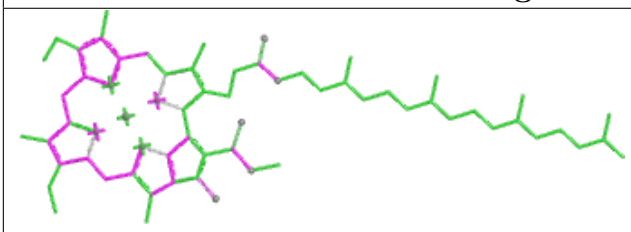


Rings

Ligand CLA D 2303



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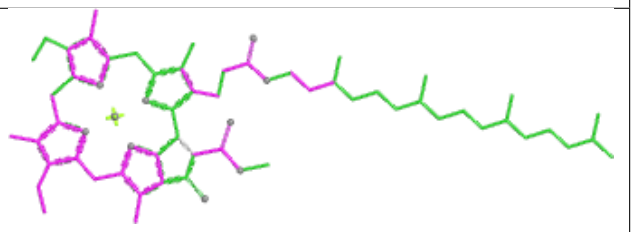
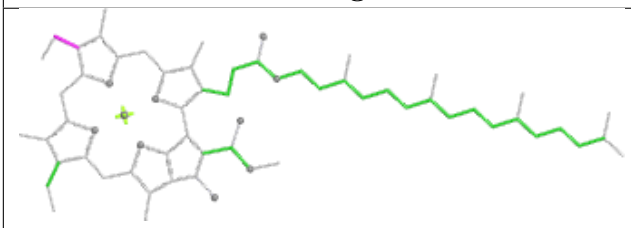


Bond angles



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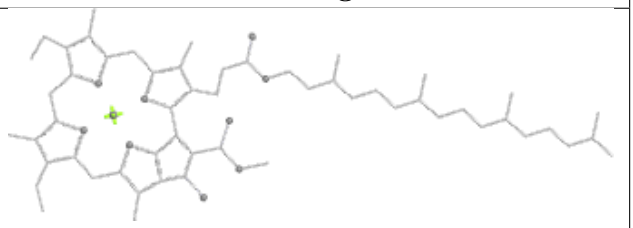


Rings

Ligand PL9 A 422

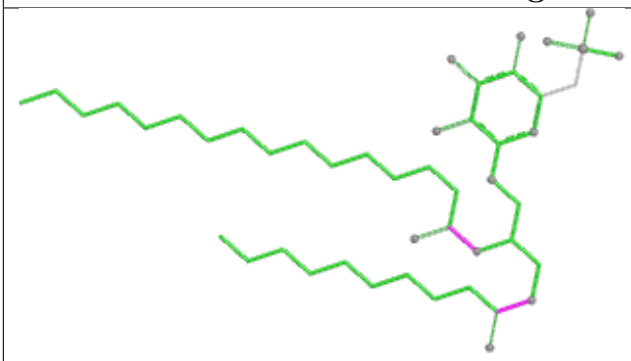
Bond lengths

Bond angles

Torsions

Rings

Ligand SQD b 601



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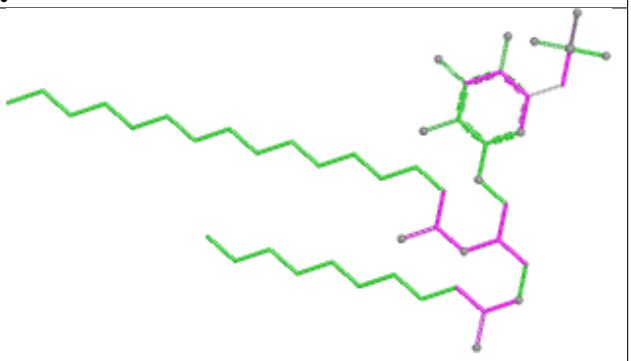
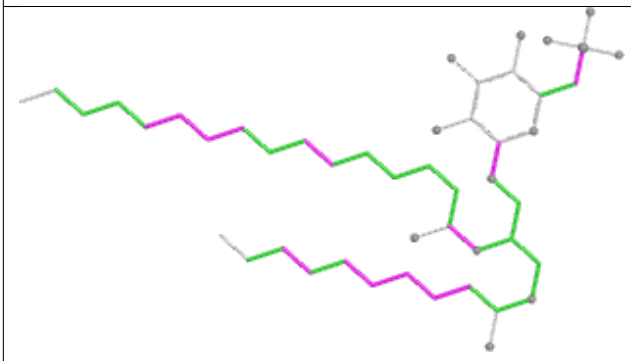


Bond angles



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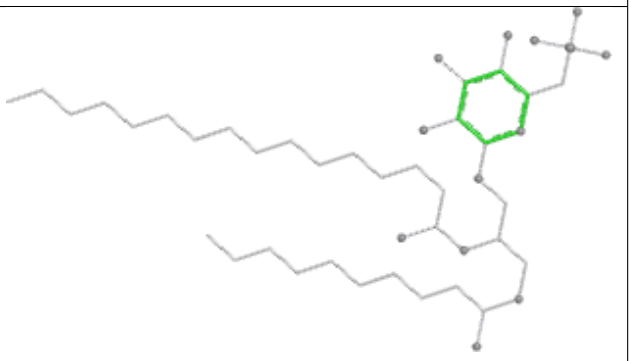
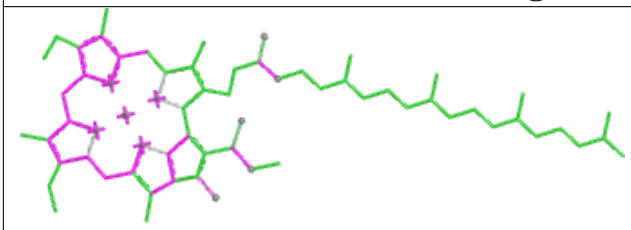


Rings

Ligand CLA b 619



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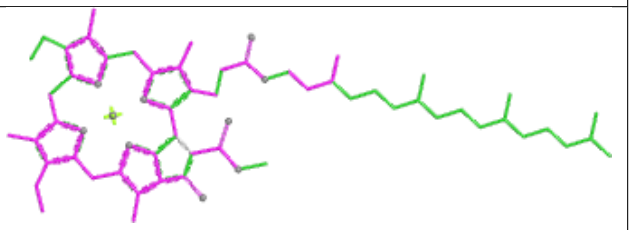
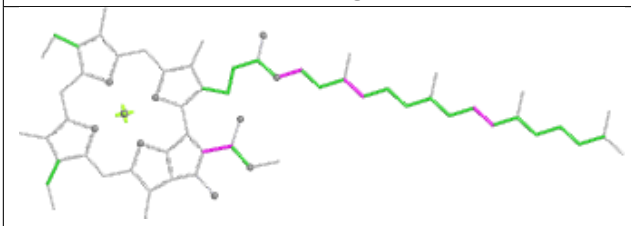


Bond angles



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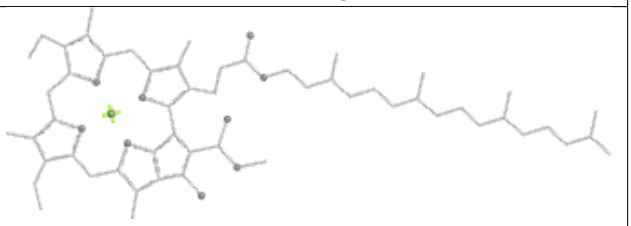
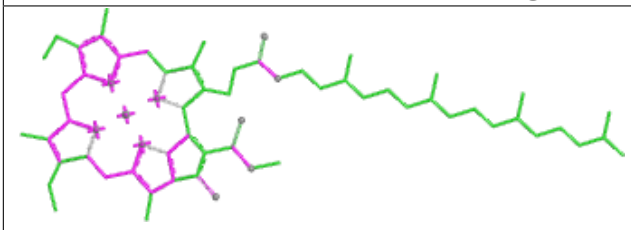


Rings

Ligand CLA C 502



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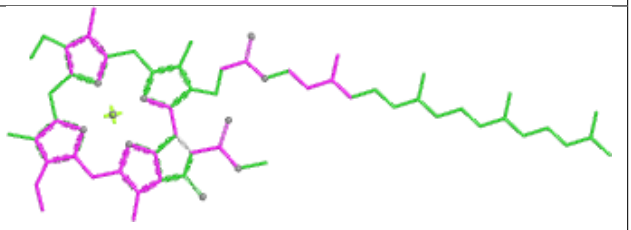
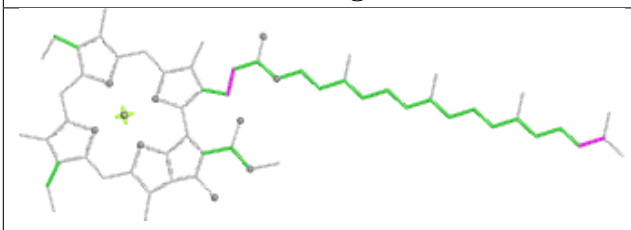
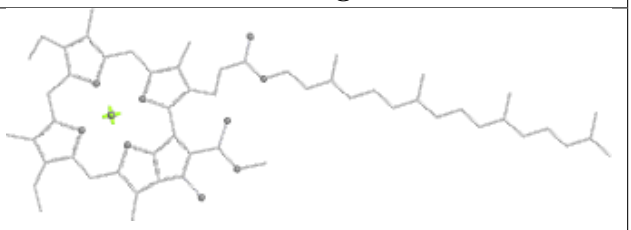


Bond angles

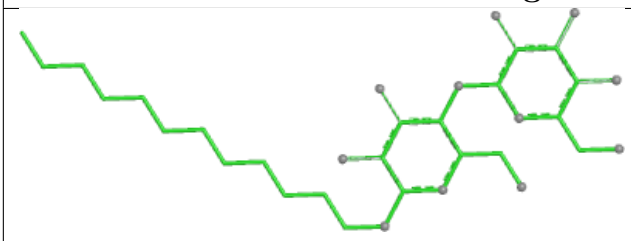


Torsions



Rings

Ligand LMT Z 101



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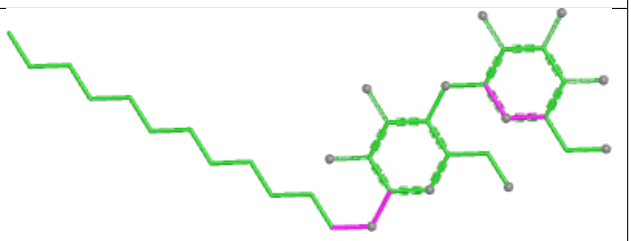
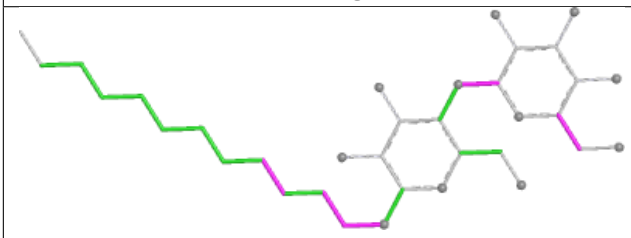
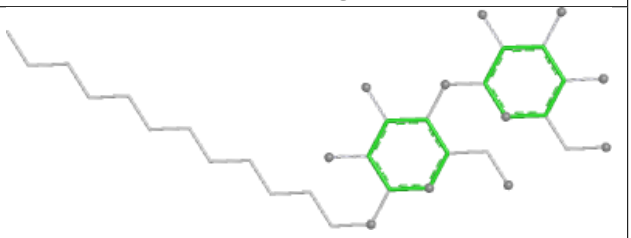


Bond angles

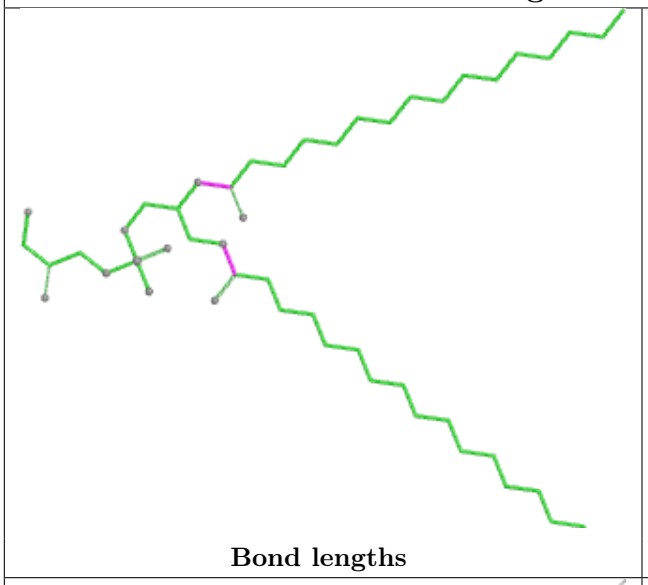


Torsions



Rings

Ligand LHG d 412



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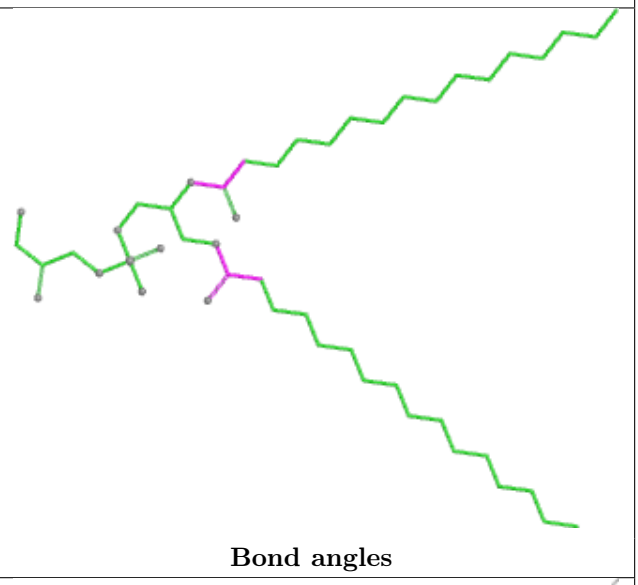
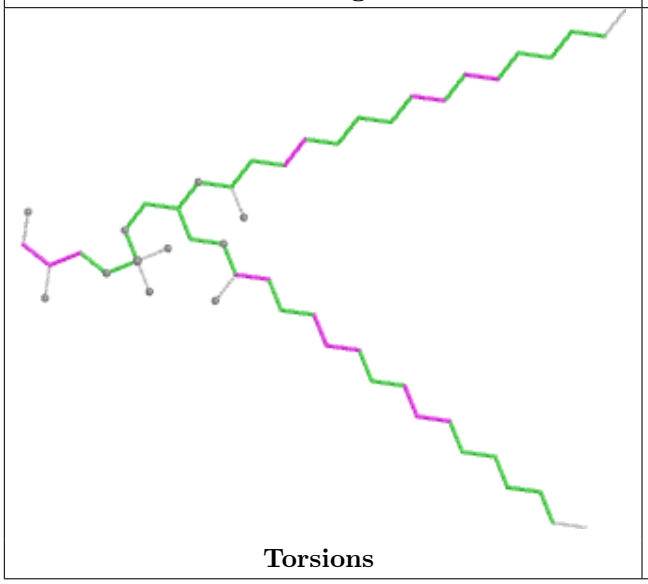
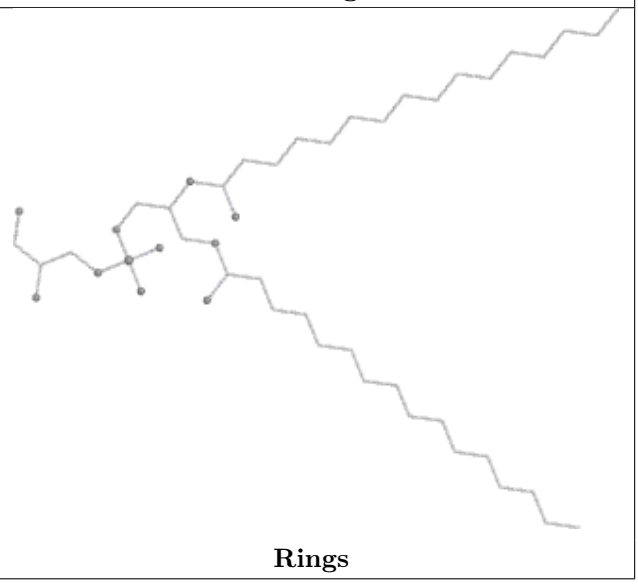


Bond angles

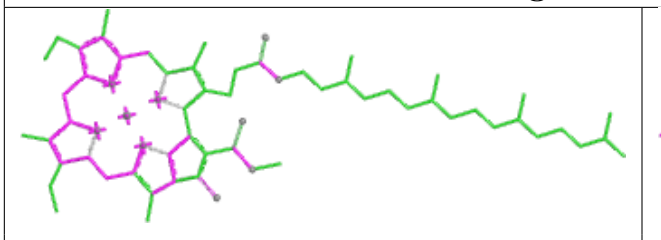


Torsions

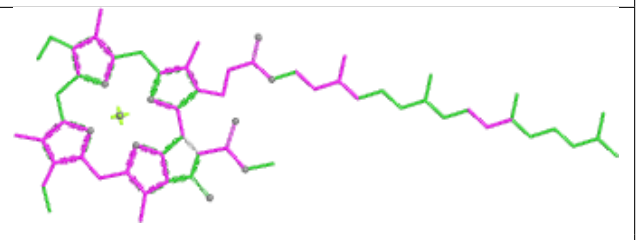


Rings

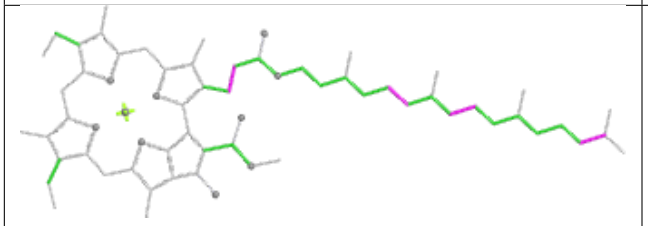
Ligand CLA b 615



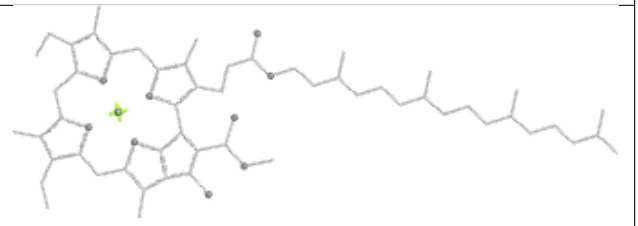
Bond lengths



Bond angles

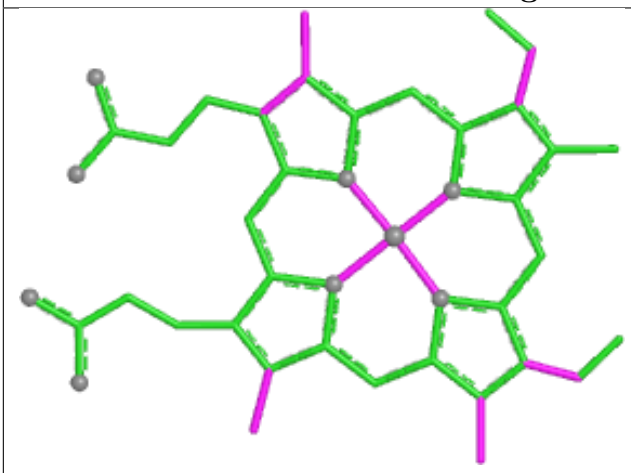


Torsions

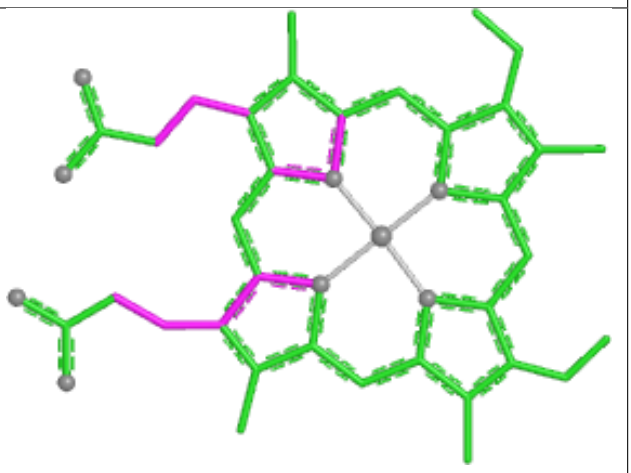


Rings

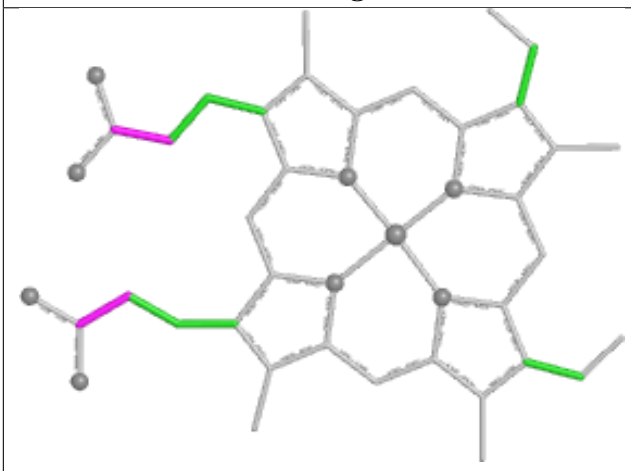
Ligand HEM F 101



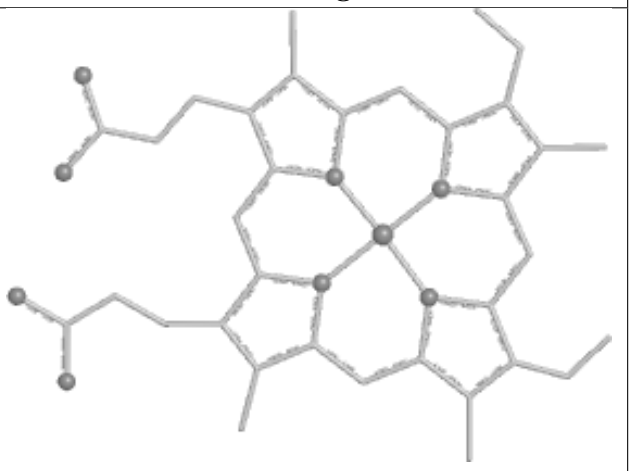
Bond lengths



Bond angles

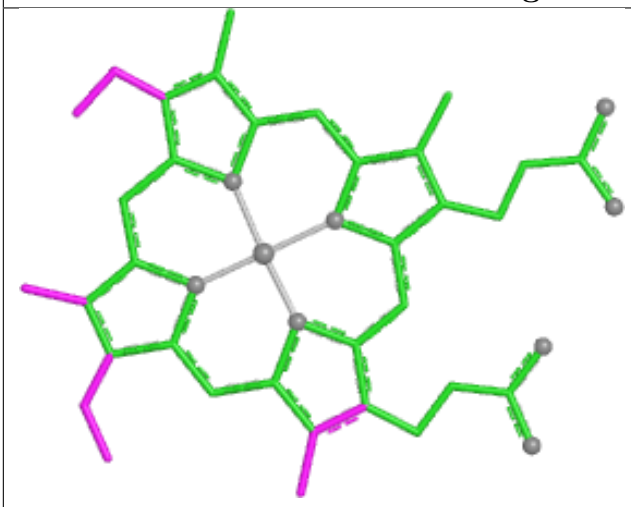


Torsions

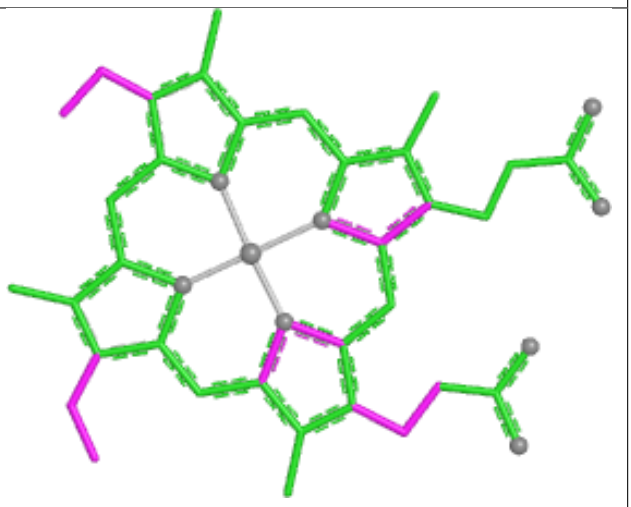


Rings

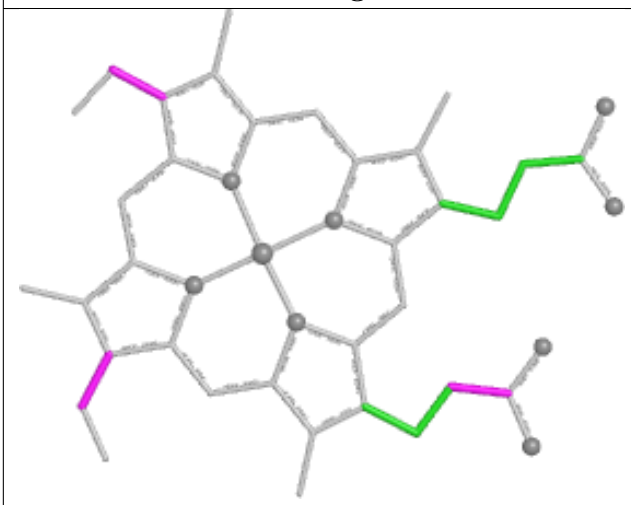
Ligand HEC V 201



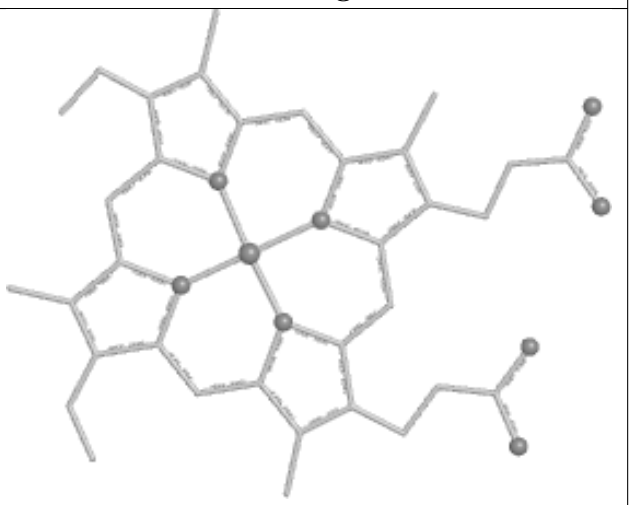
Bond lengths



Bond angles

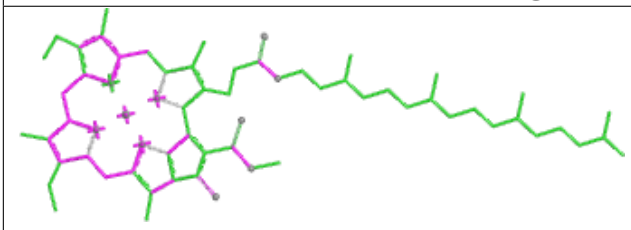


Torsions



Rings

Ligand CLA b 609



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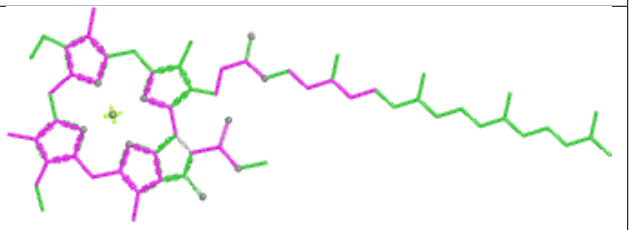
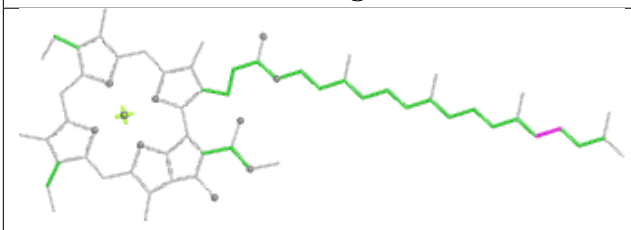
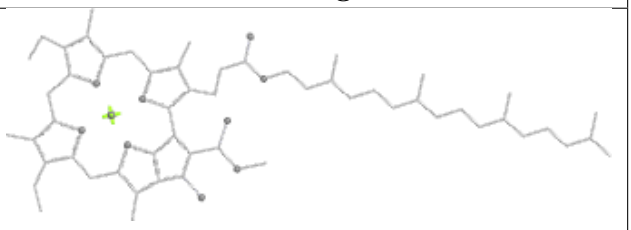


Bond angles

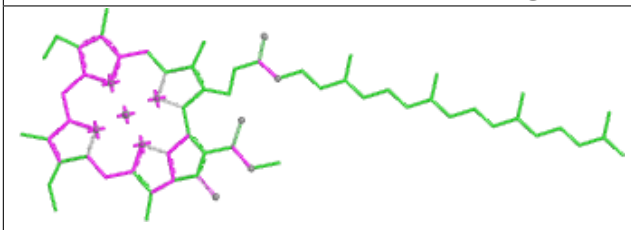


Torsions



Rings

Ligand CLA B 609



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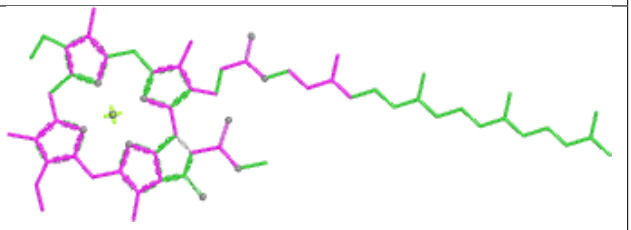
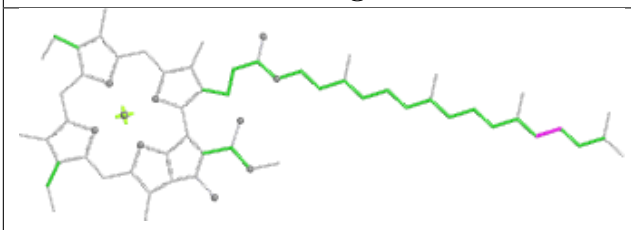
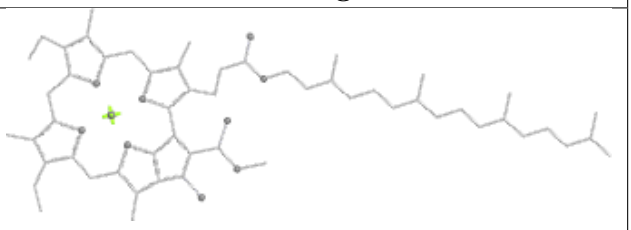


Bond angles

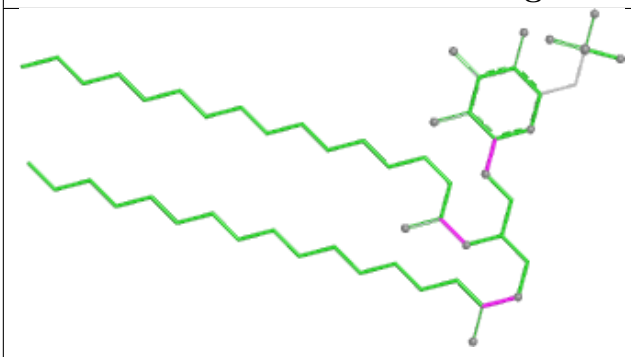


Torsions



Rings

Ligand SQD B 621



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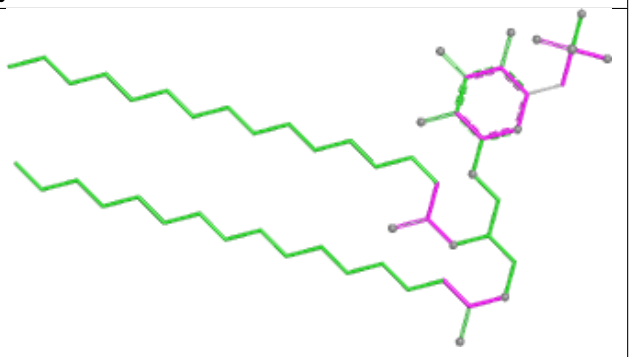
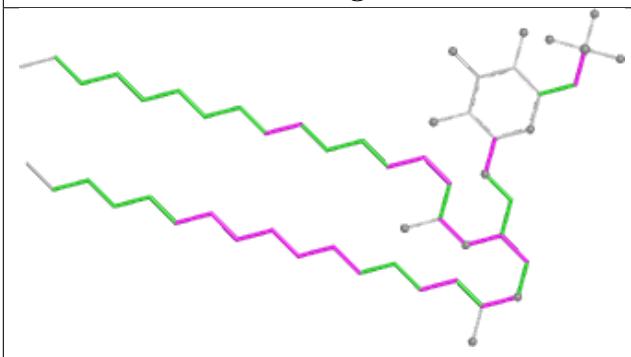
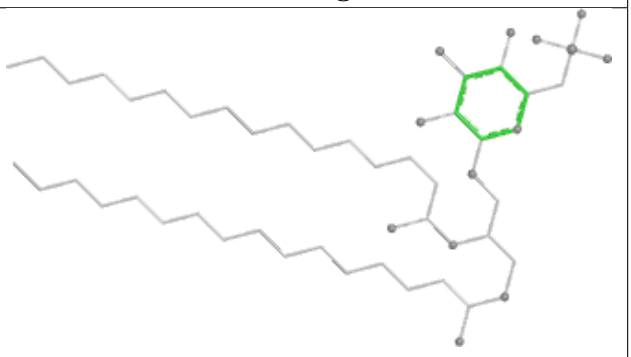


Bond angles

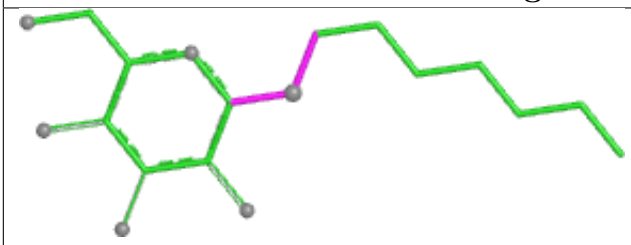


Torsions

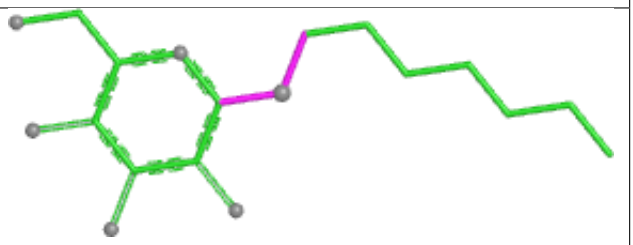


Rings

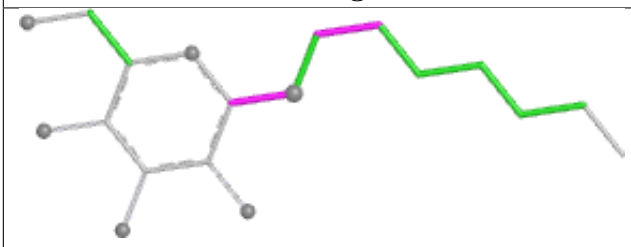
Ligand HTG d 415



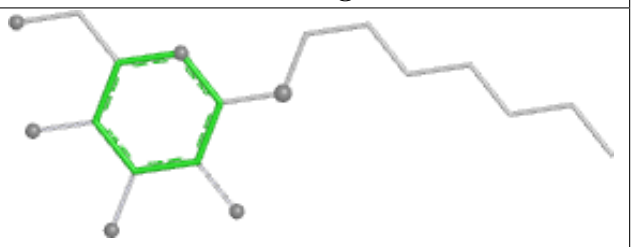
Bond lengths



Bond angles

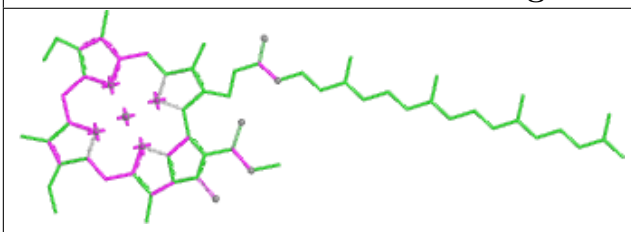


Torsions



Rings

Ligand CLA d 402



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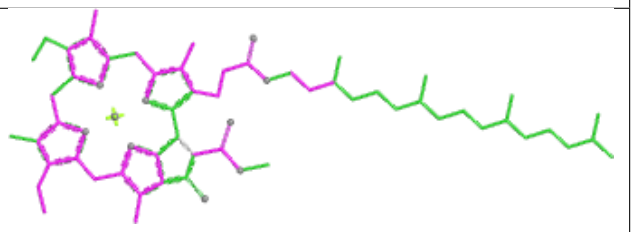
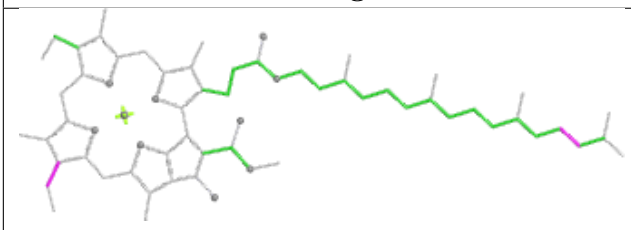
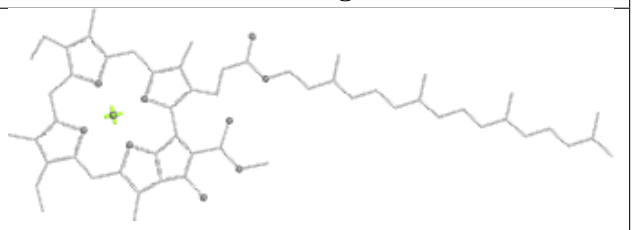


Bond angles

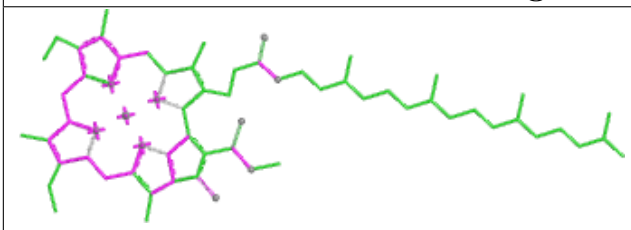


Torsions

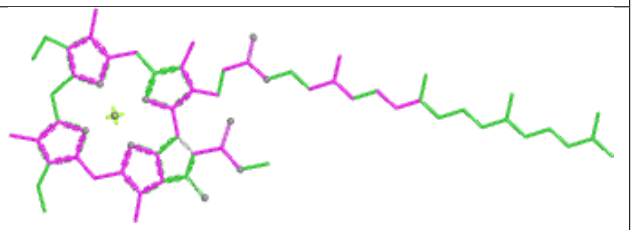


Rings

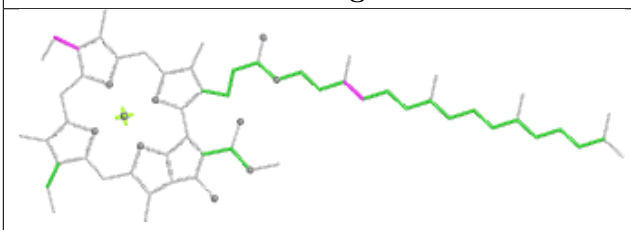
Ligand CLA b 608



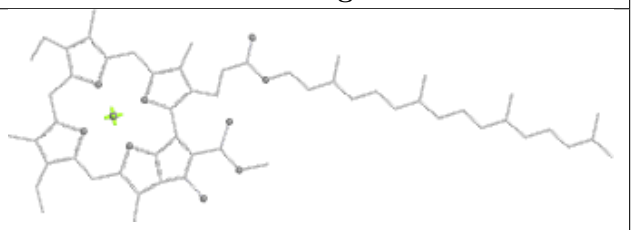
Bond lengths



Bond angles

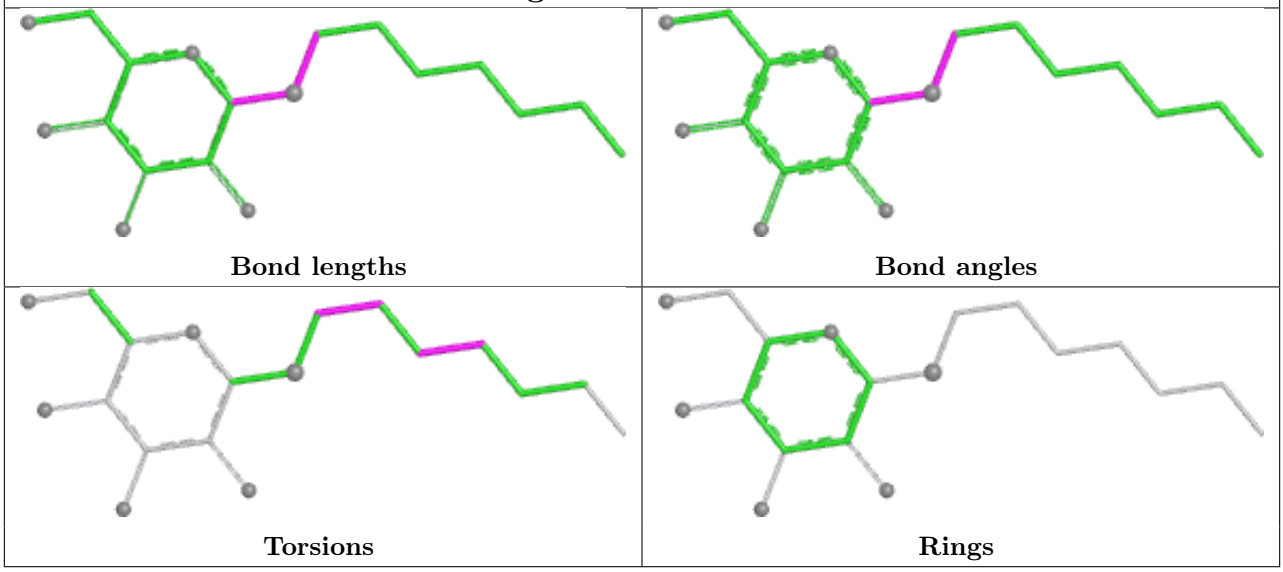


Torsions

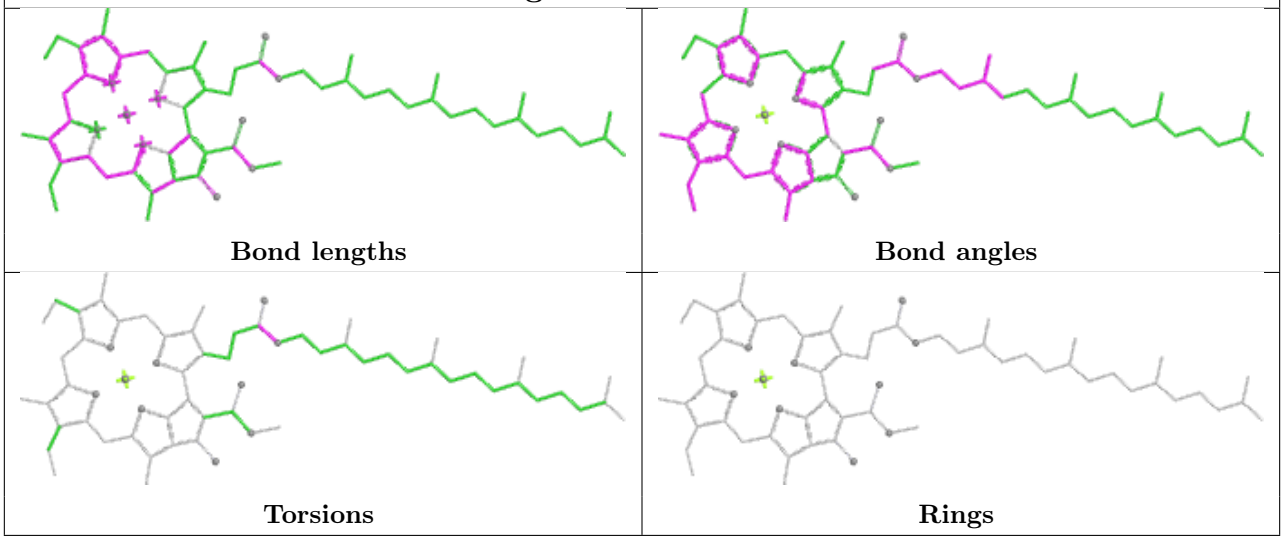


Rings

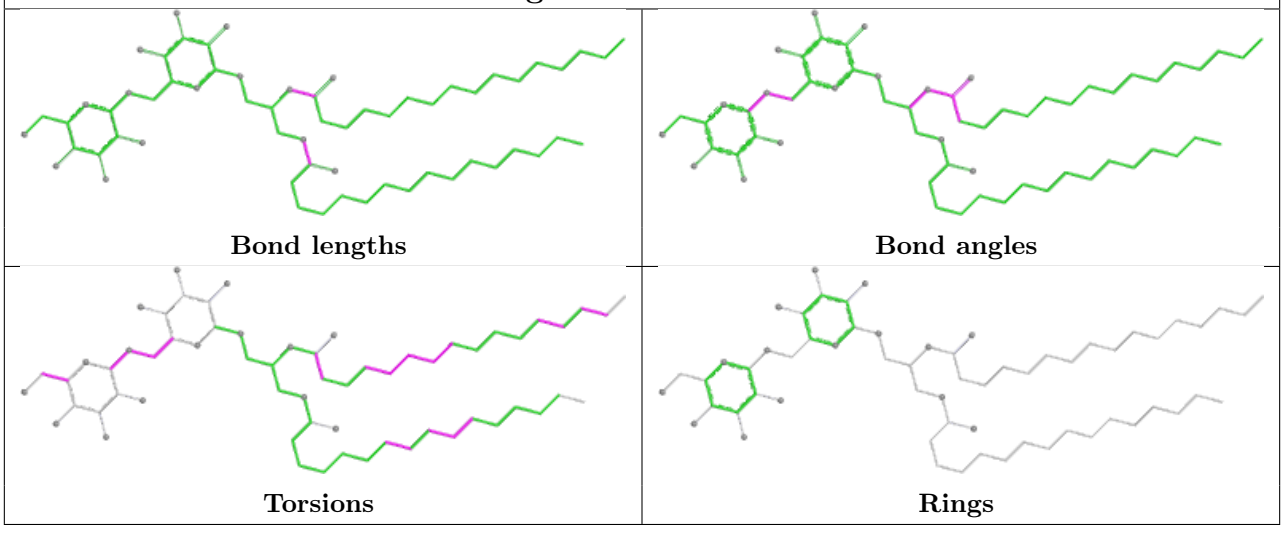
Ligand HTG c 526



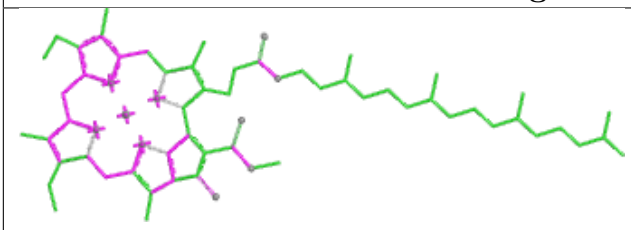
Ligand CLA C 512



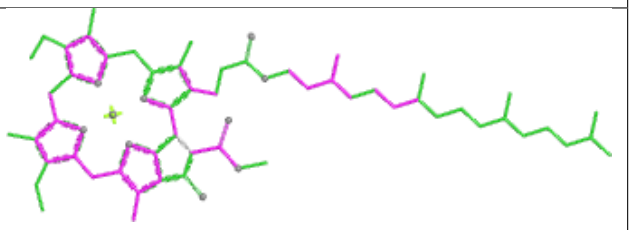
Ligand DGD c 518



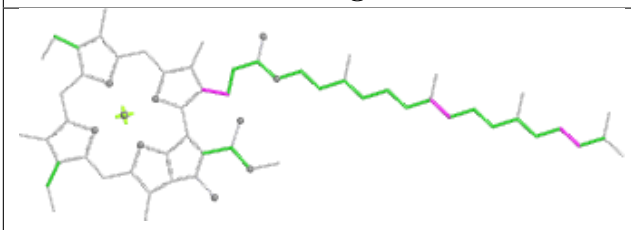
Ligand CLA c 511



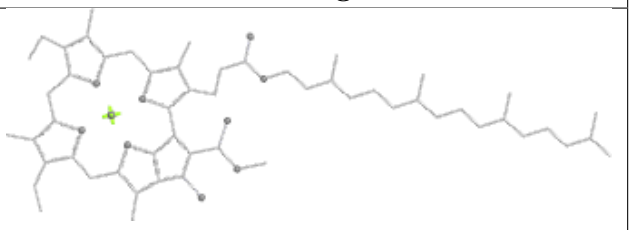
Bond lengths



Bond angles

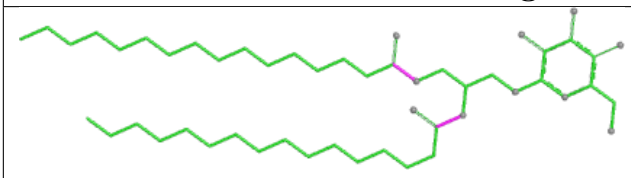


Torsions

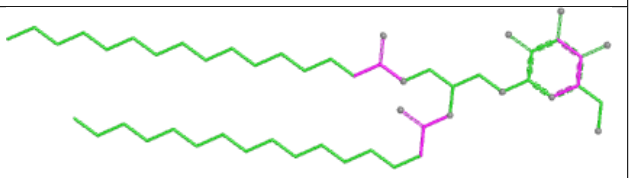


Rings

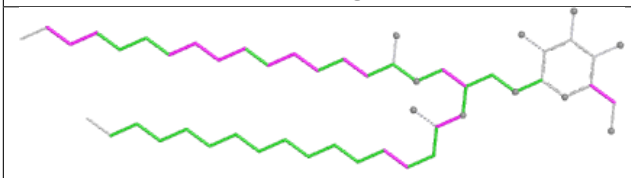
Ligand LMG C 527



Bond lengths



Bond angles



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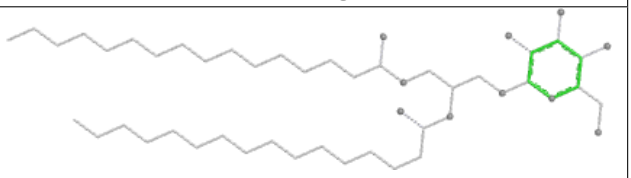
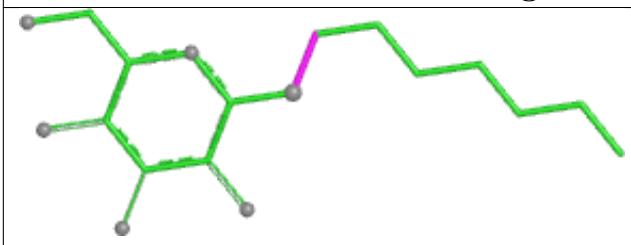
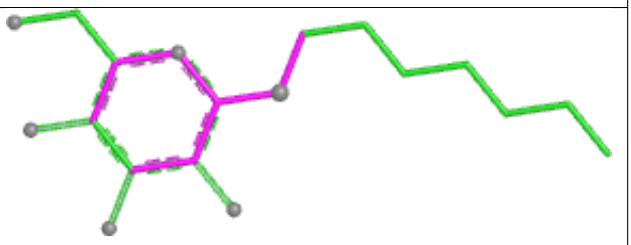


Rings

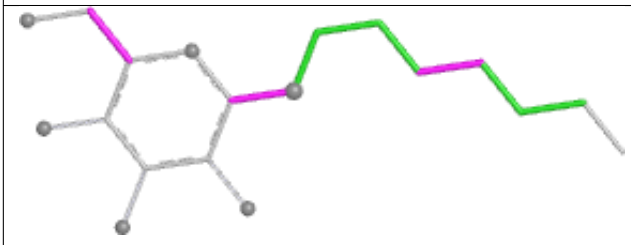
Ligand HTG V 204



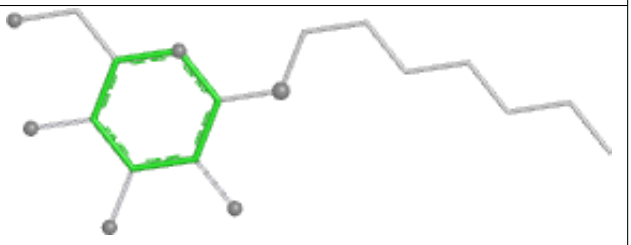
Bond lengths



Bond angles

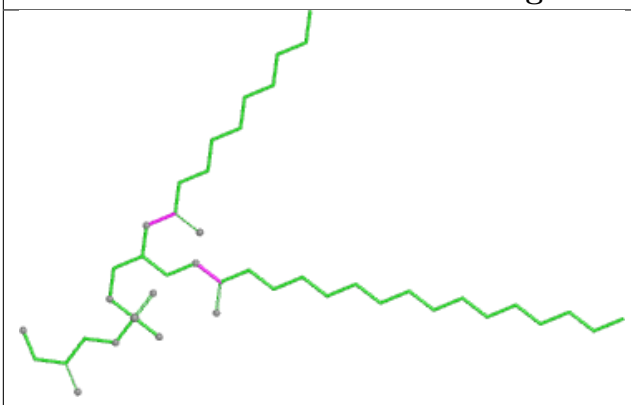


Torsions

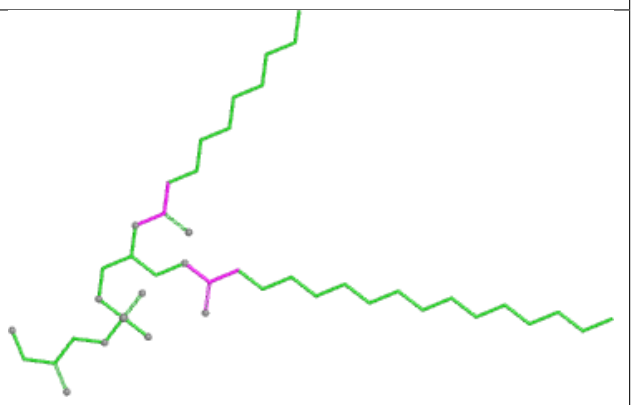


Rings

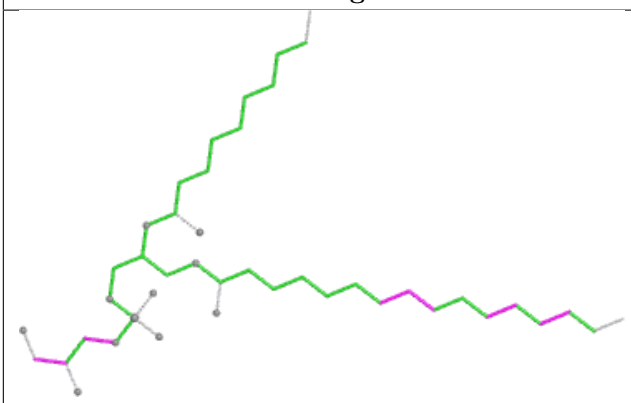
Ligand LHG d 403



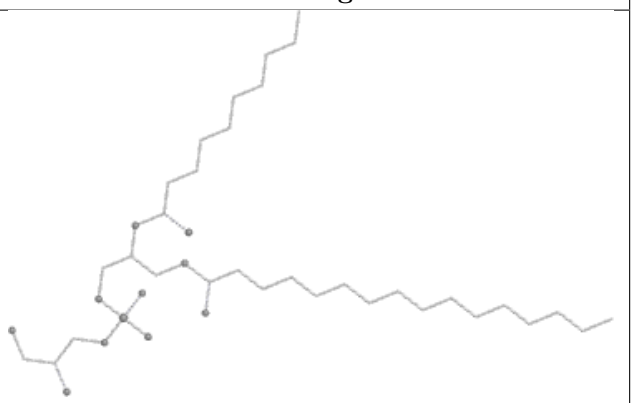
Bond lengths



Bond angles

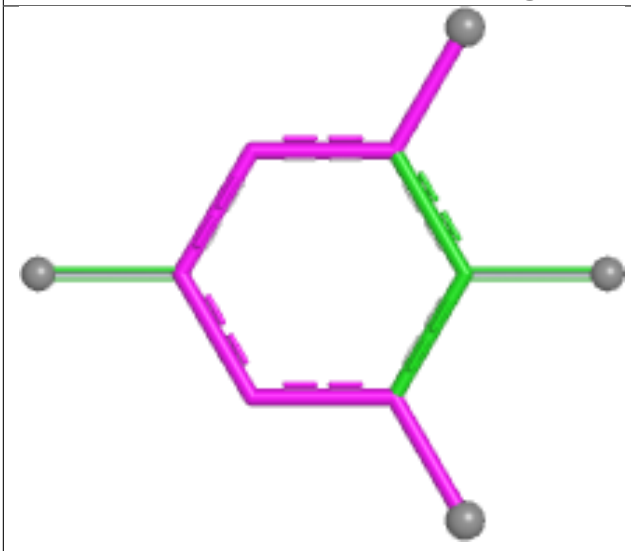


Torsions

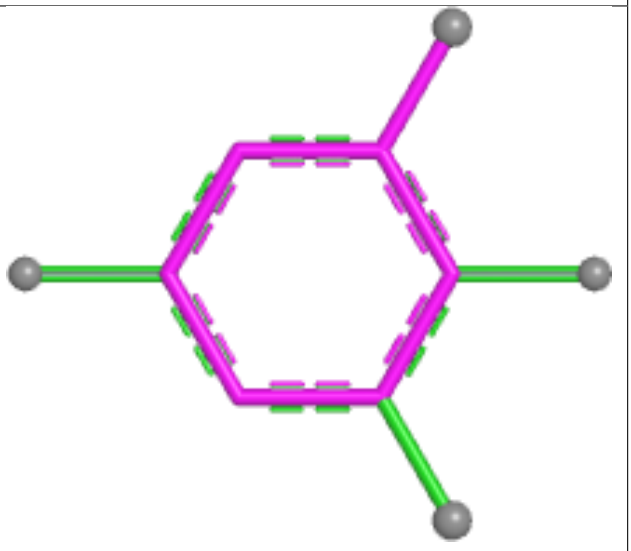


Rings

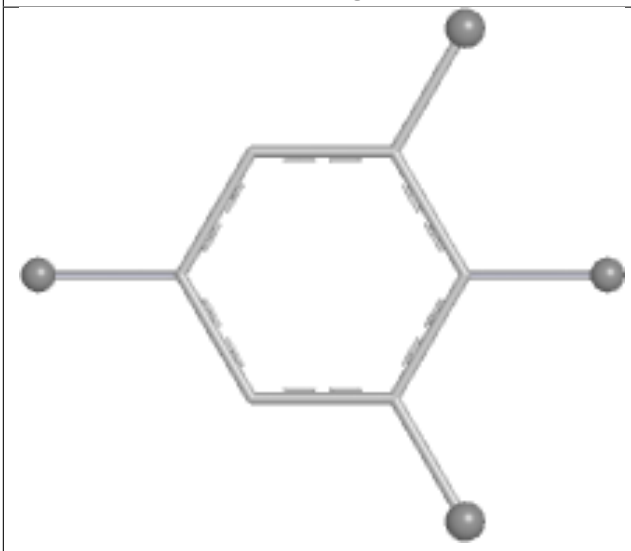
Ligand JOX a 2619



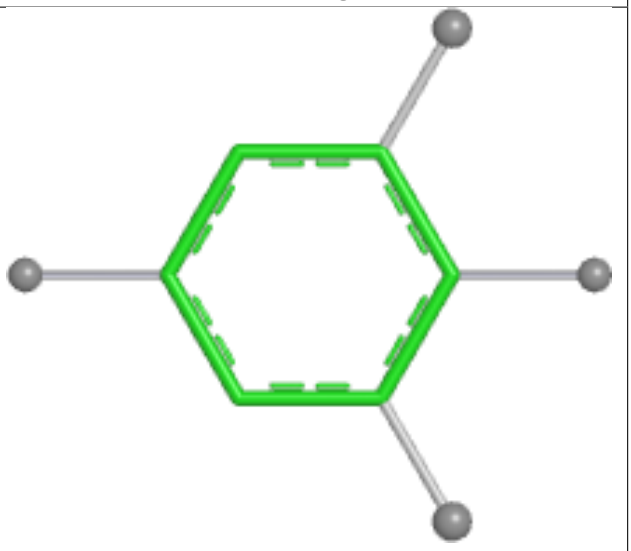
Bond lengths



Bond angles

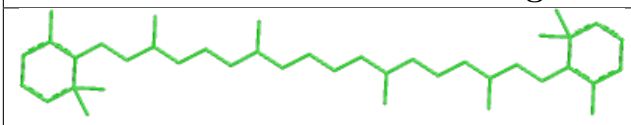


Torsions



Rings

Ligand BCR y 101



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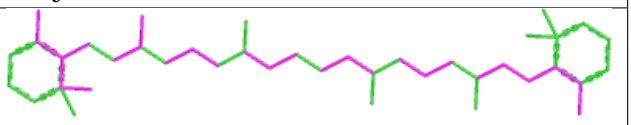

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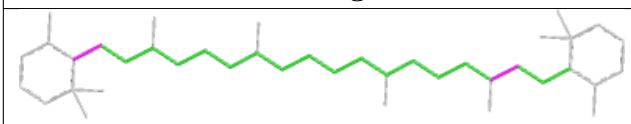

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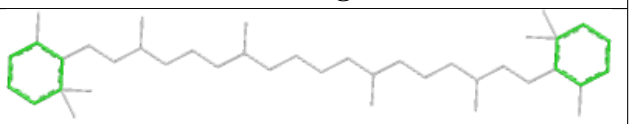
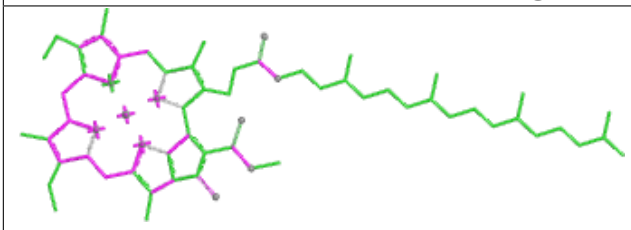


Rings

Ligand CLA c 510



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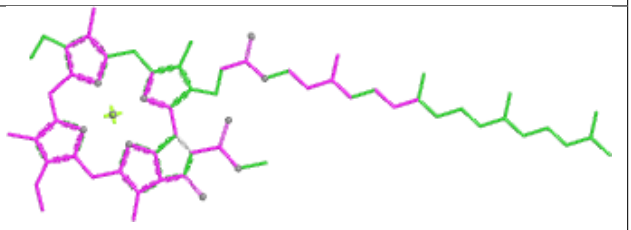

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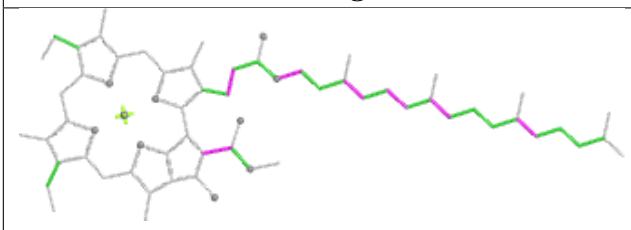

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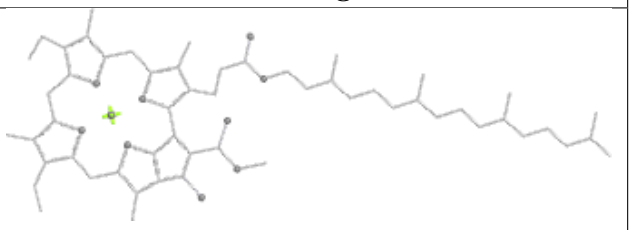

Rings

Ligand PHO a 2611

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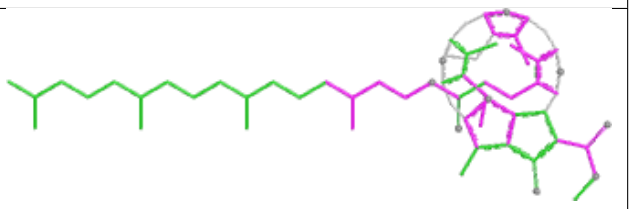

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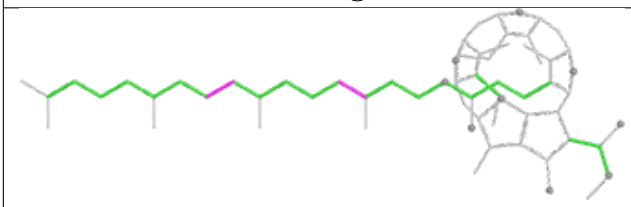

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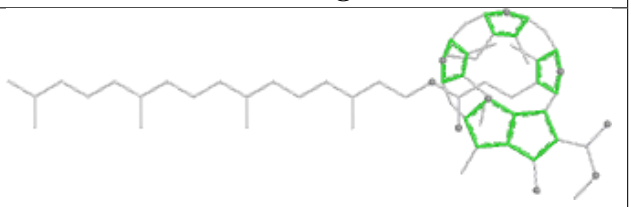
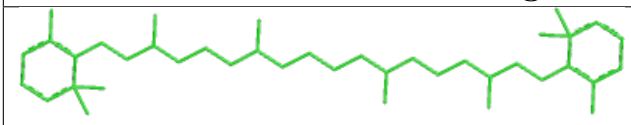


Rings

Ligand BCR C 515



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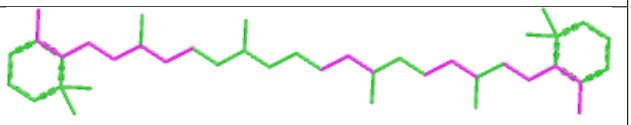
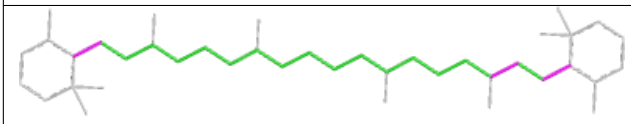


Bond angles



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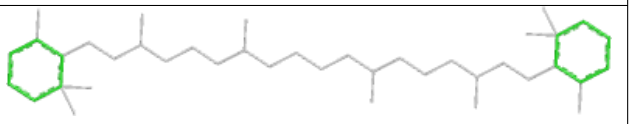
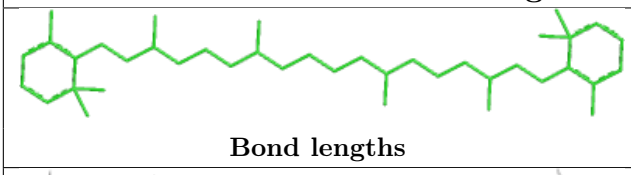


Rings

Ligand BCR d 410



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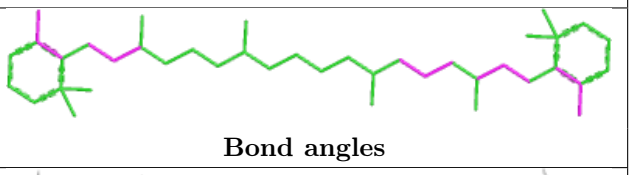

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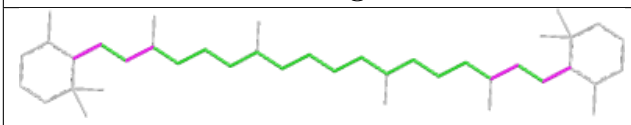

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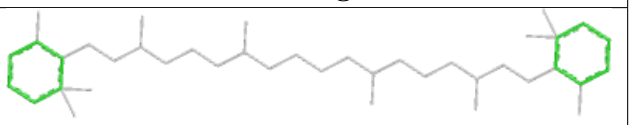
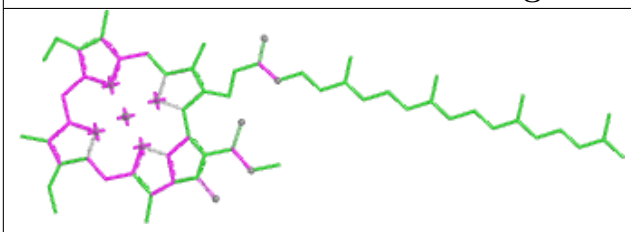


Rings

Ligand CLA A 407



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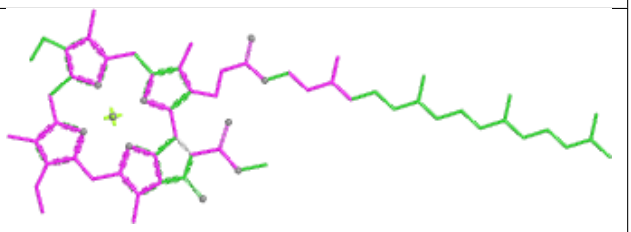
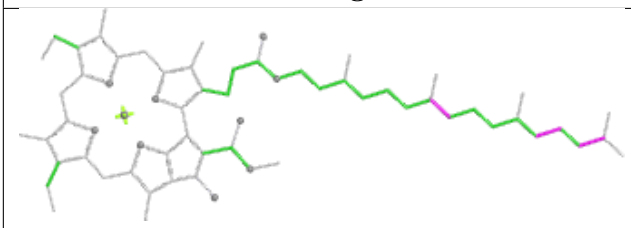


Bond angles



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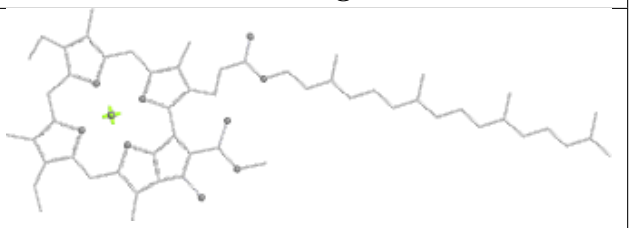
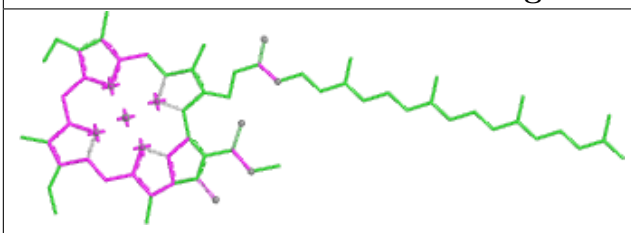


Rings

Ligand CLA B 611



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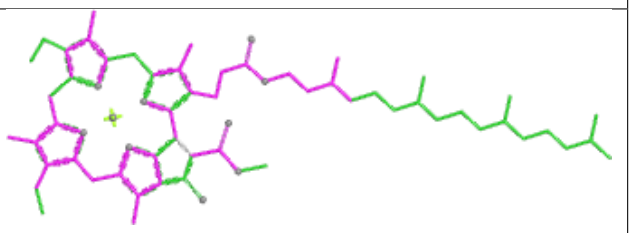

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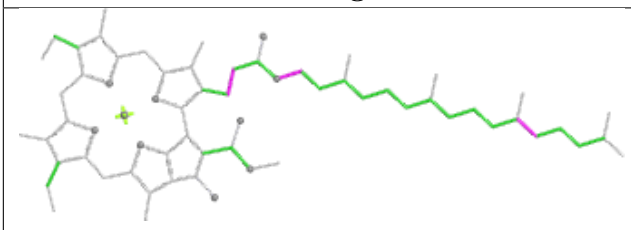

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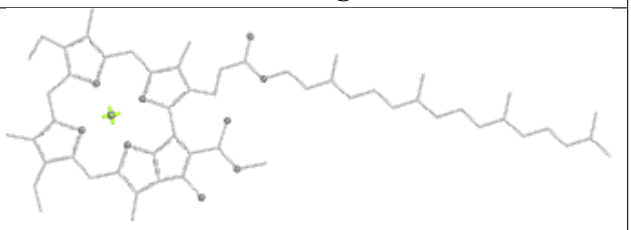
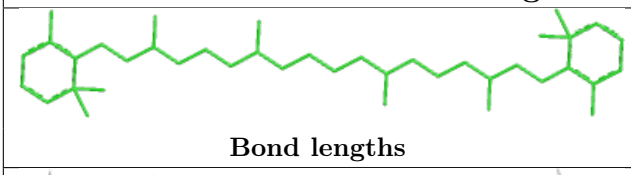


Rings

Ligand BCR B 620



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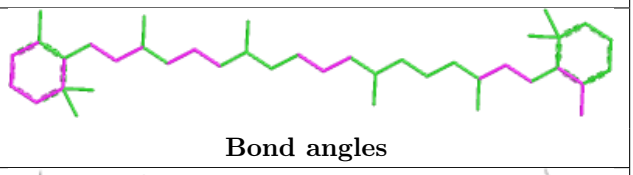
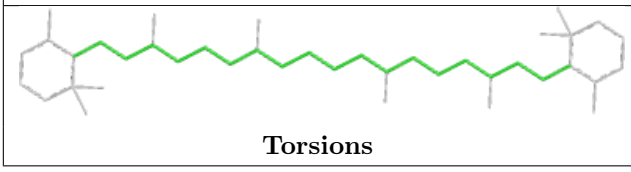


Bond angles



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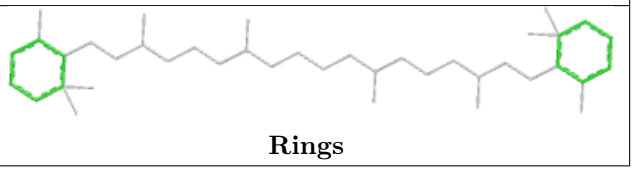
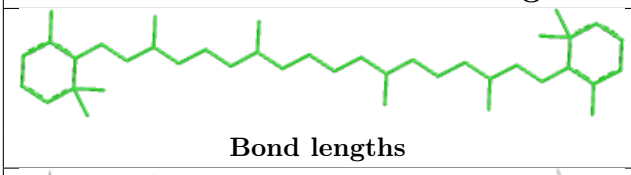


Rings

Ligand BCR B 633



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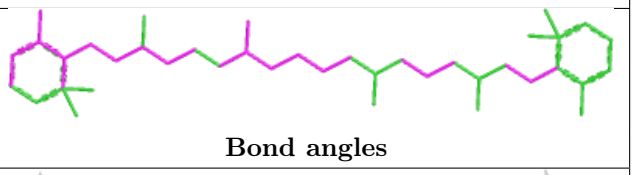
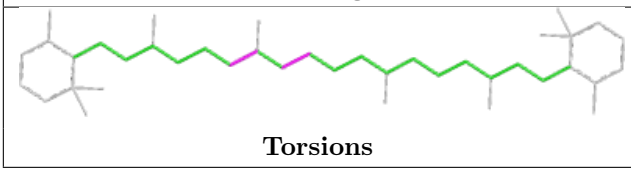


Bond angles



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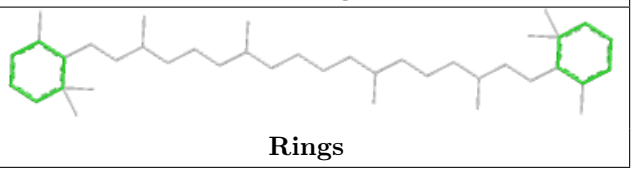
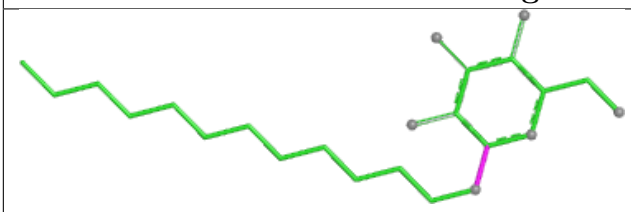


Rings

Ligand LMT T 103



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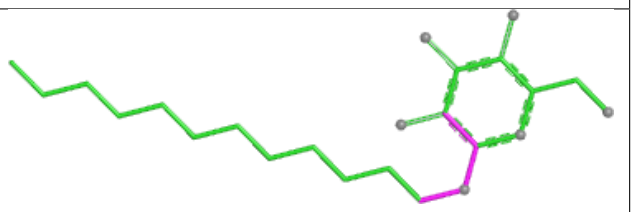
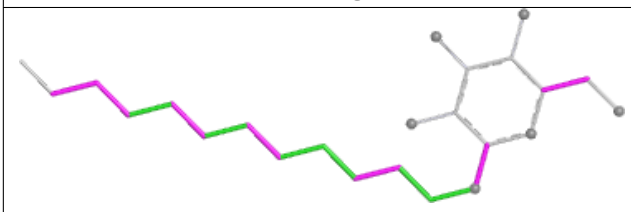


Bond angles



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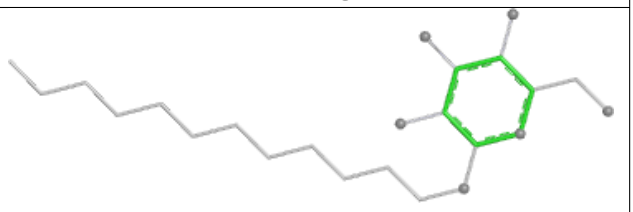
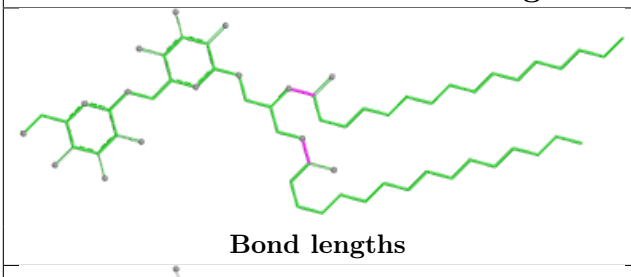


Rings

Ligand DGD h 102



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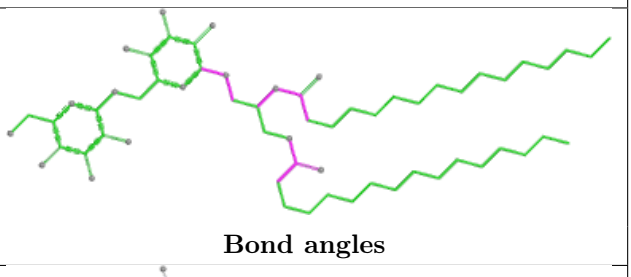
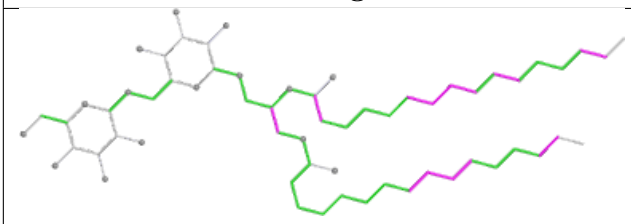


Bond angles



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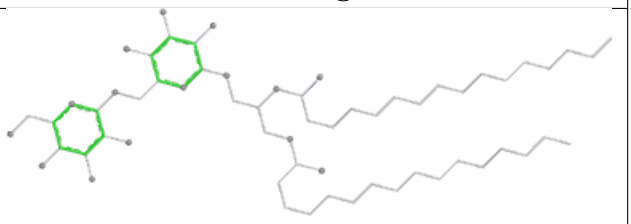
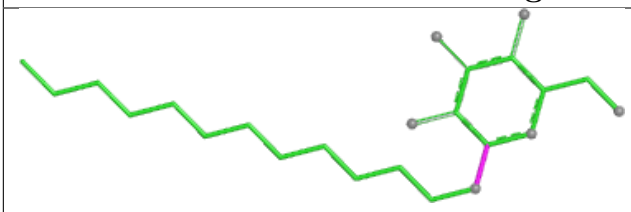


Rings

Ligand LMT J 303



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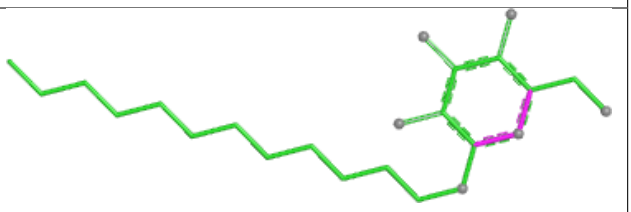
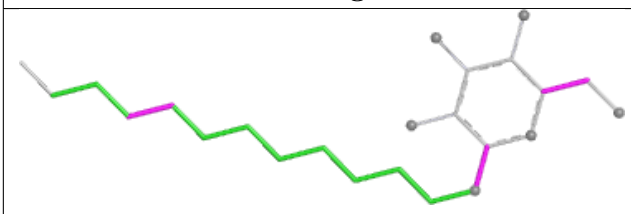


Bond angles



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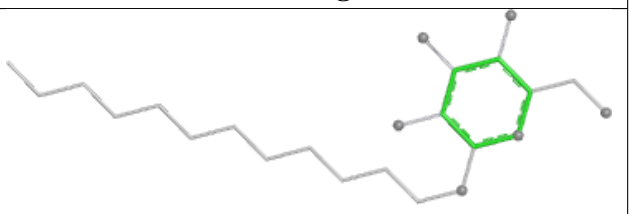
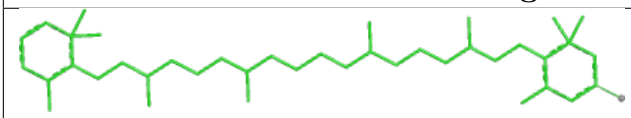


Rings

Ligand RRX H 102



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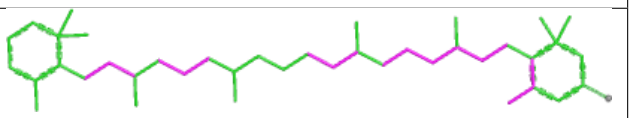
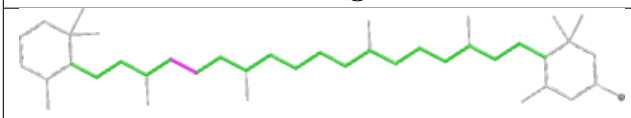


Bond angles



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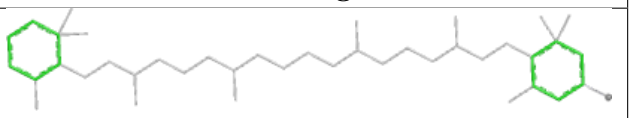
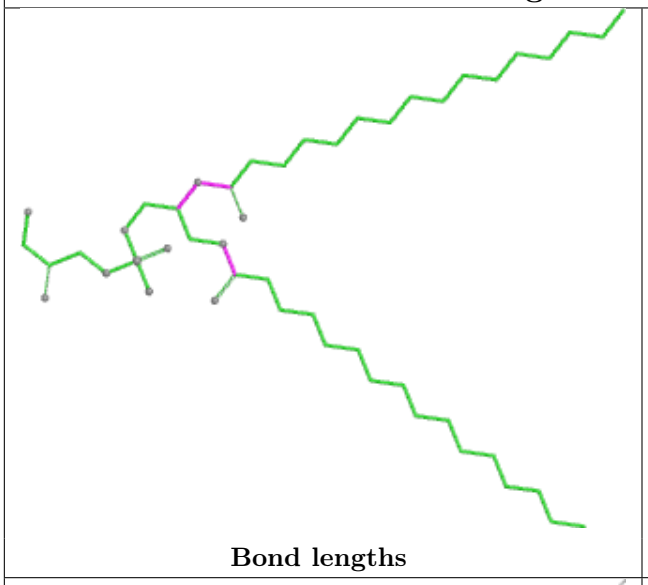
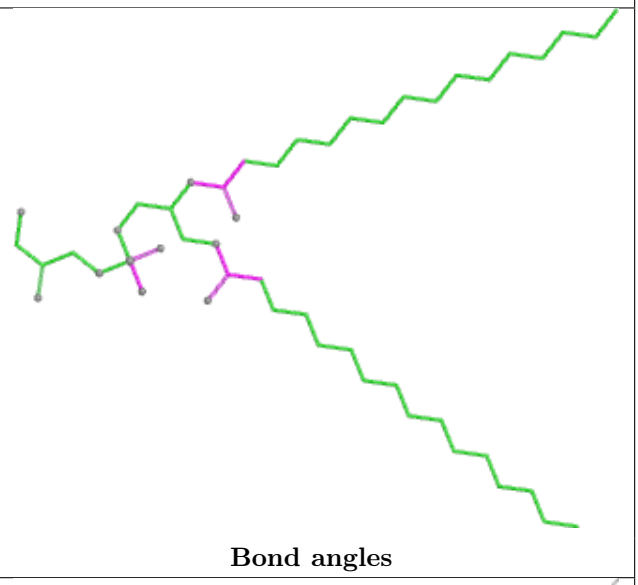


Rings

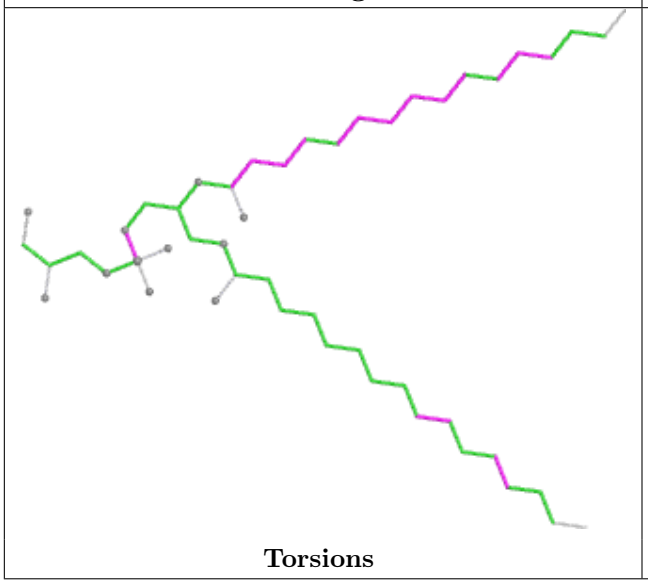
Ligand LHG L 101



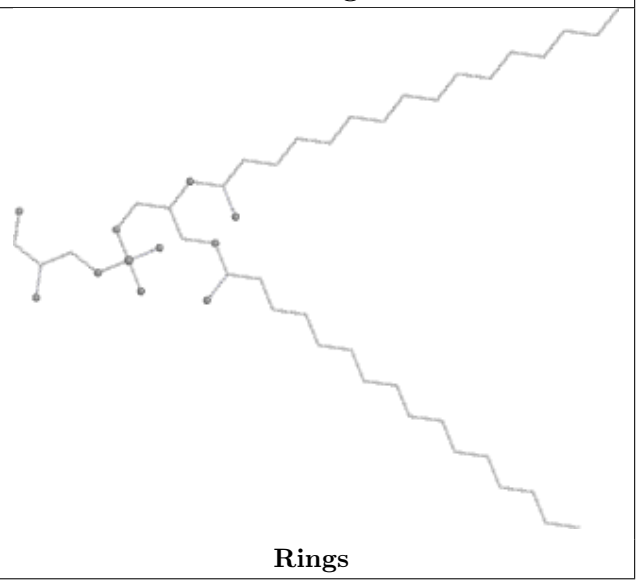
Bond lengths



Bond angles

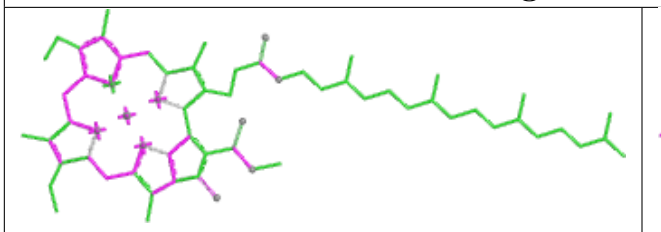


Torsions



Rings

Ligand CLA a 2613



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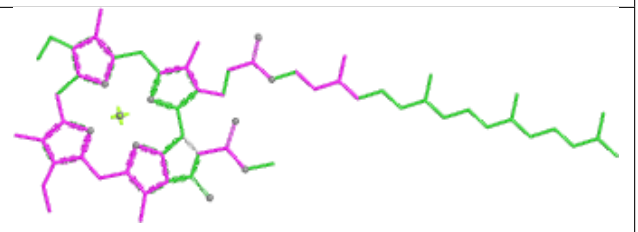
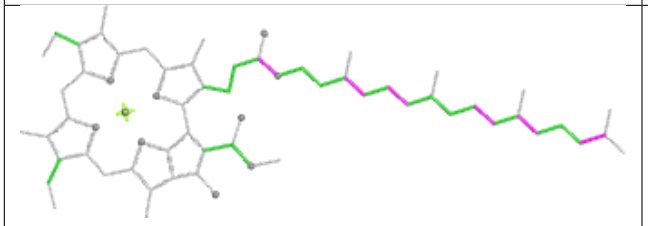


Bond angles



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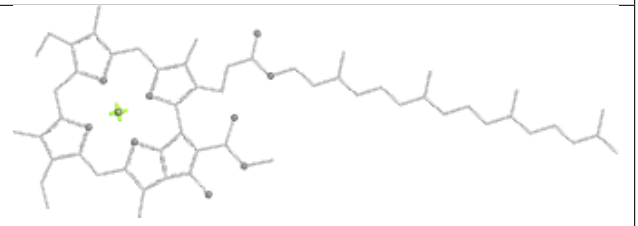
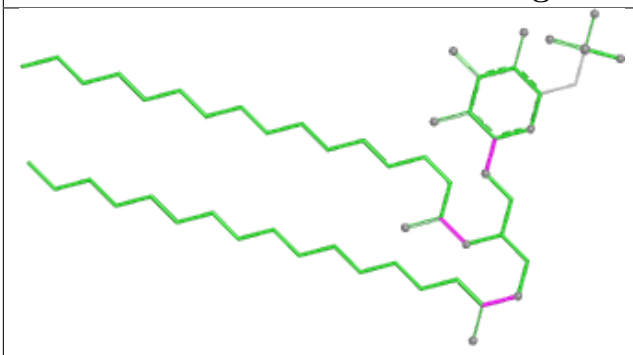


Rings

Ligand SQD l 101



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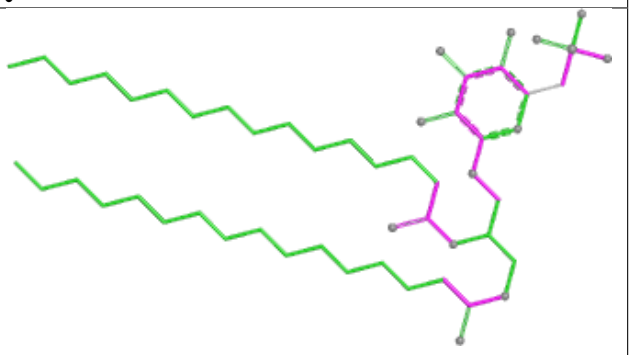
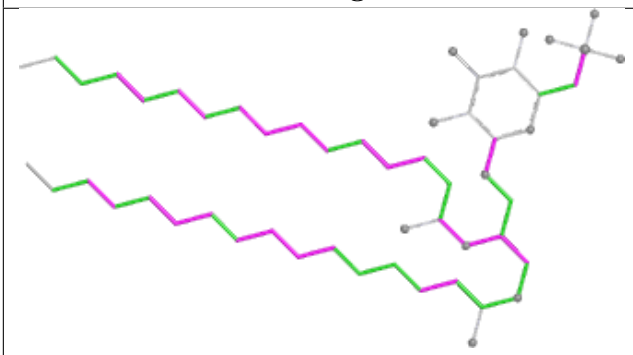


Bond angles



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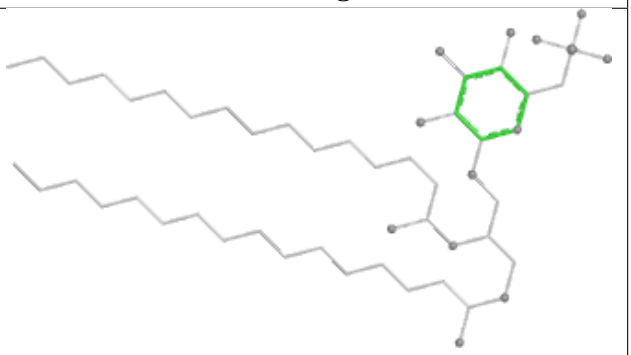
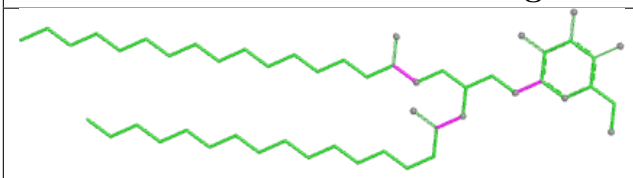


Rings

Ligand LMG c 522



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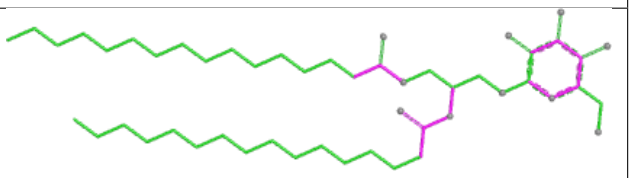
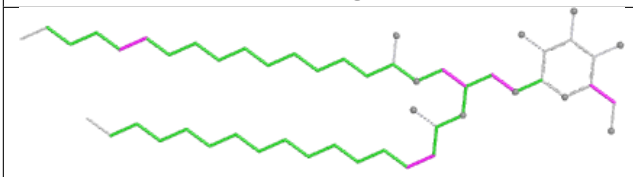


Bond angles



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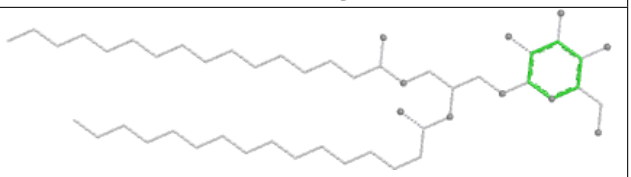
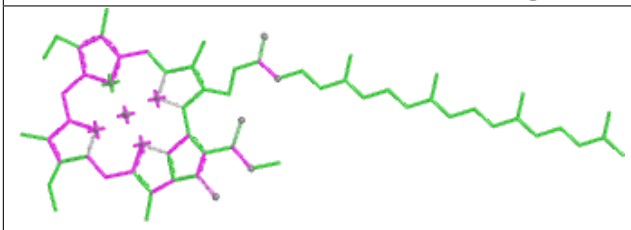


Rings

Ligand CLA C 504



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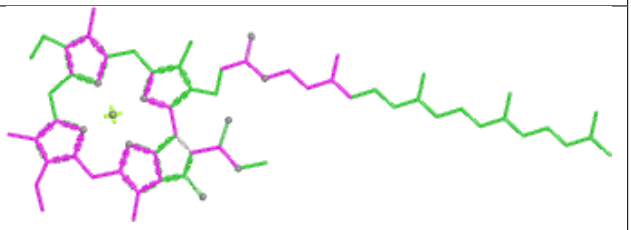
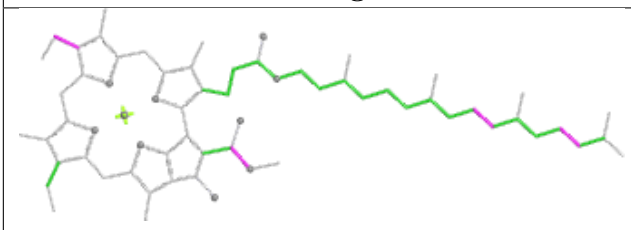


Bond angles



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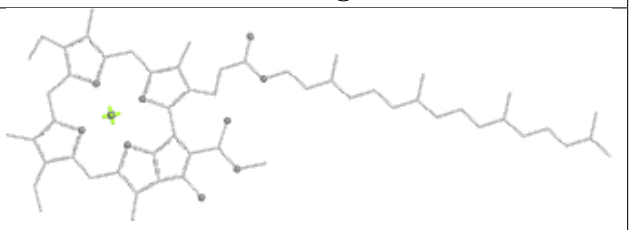
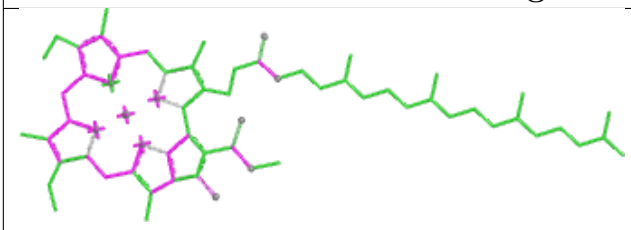


Rings

Ligand CLA b 610



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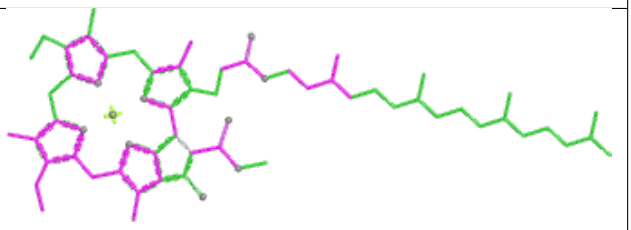
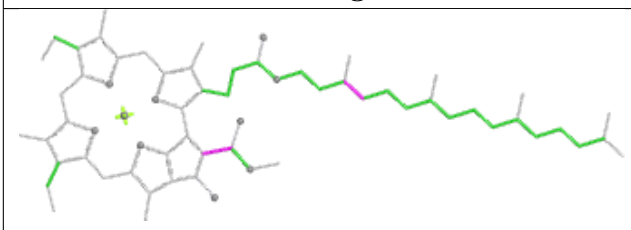


Bond angles



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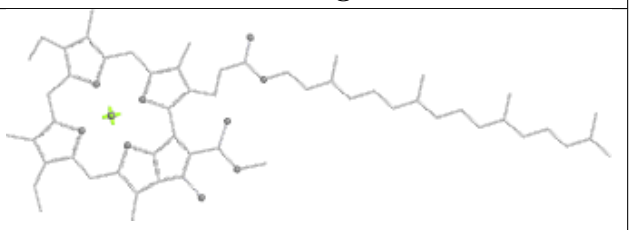
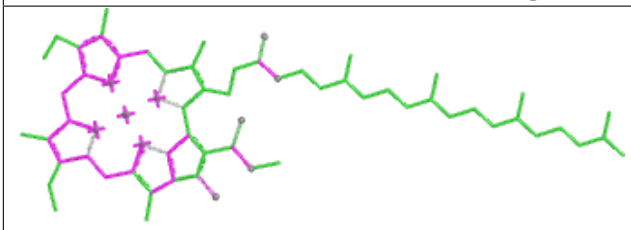


Rings

Ligand CLA C 510



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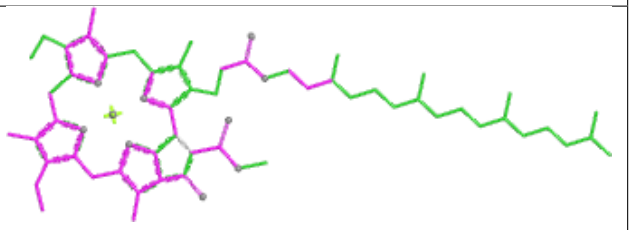
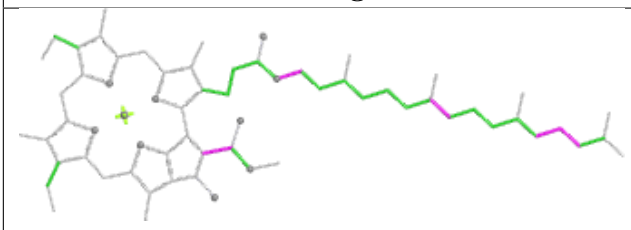


Bond angles



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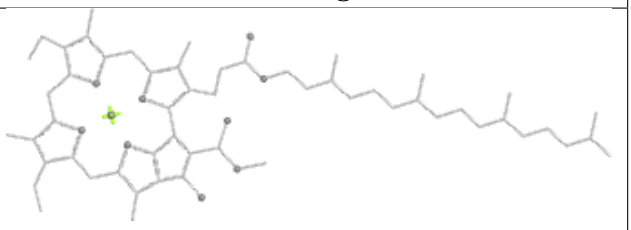
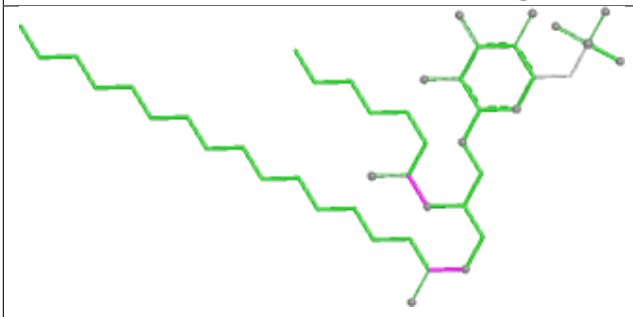


Rings

Ligand SQD D 2308



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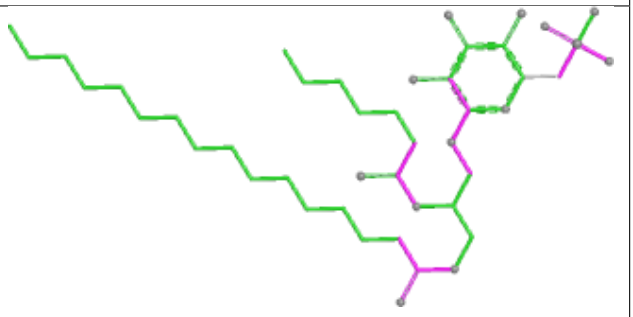
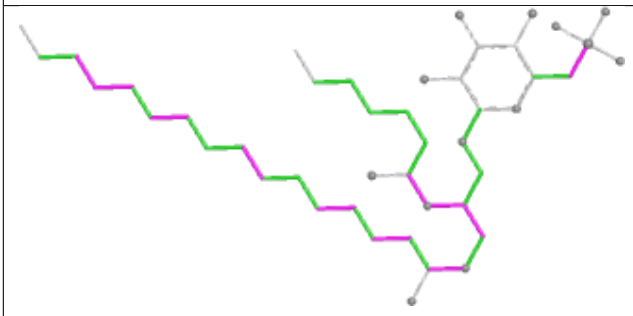


Bond angles



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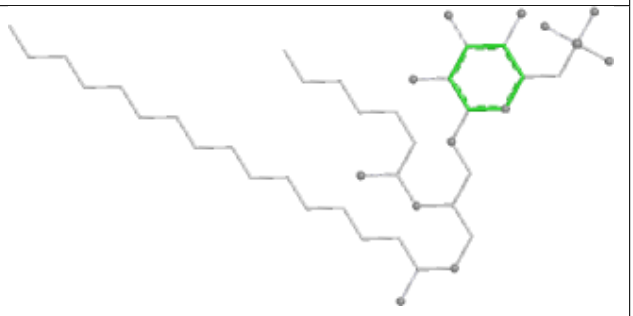
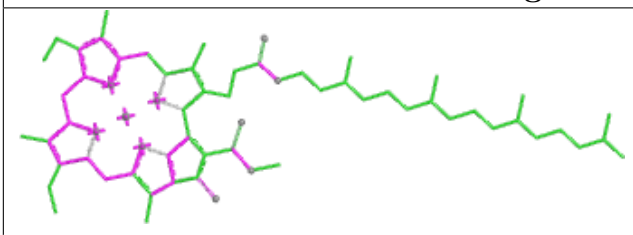
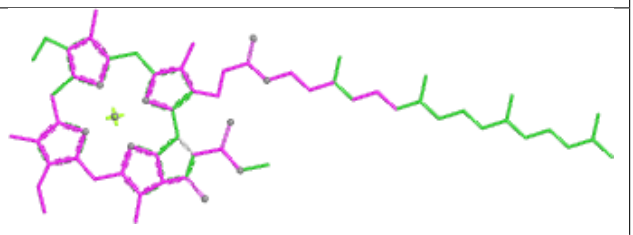


Rings

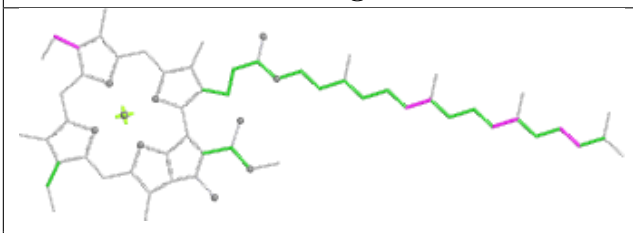
Ligand CLA C 505



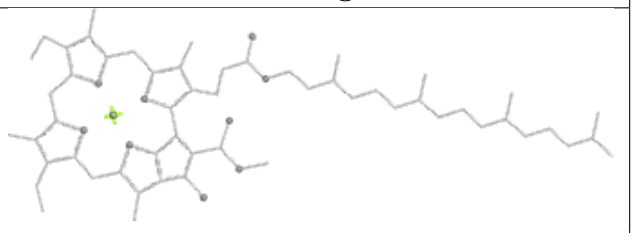
Bond lengths



Bond angles

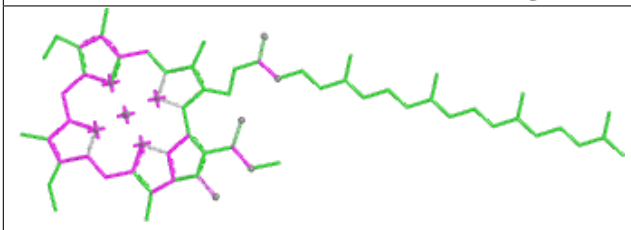


Torsions



Rings

Ligand CLA C 508



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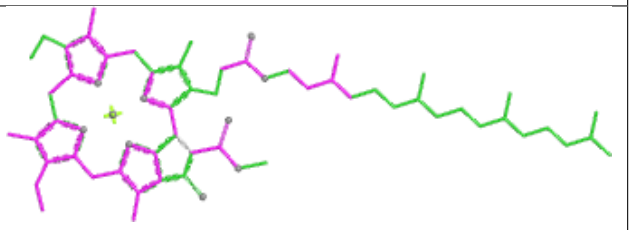
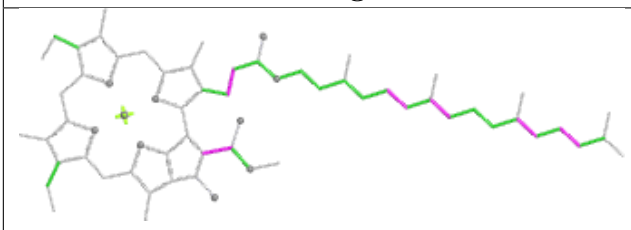


Bond angles



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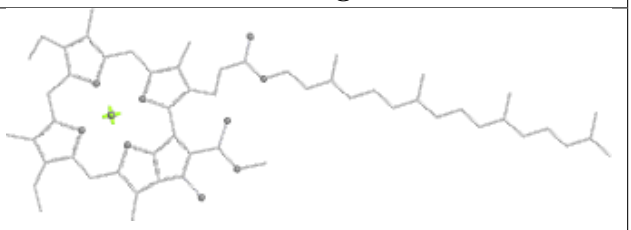
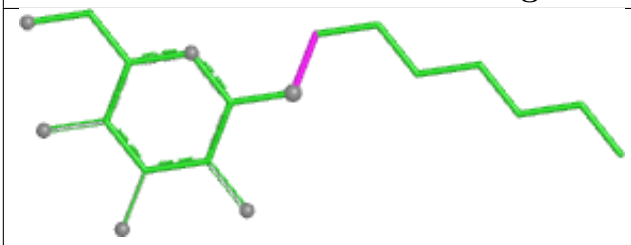


Rings

Ligand HTG C 522



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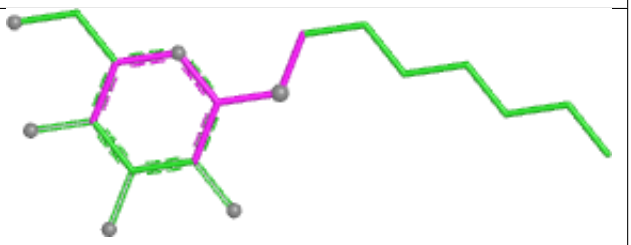
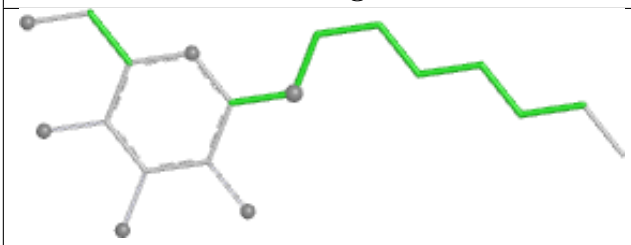
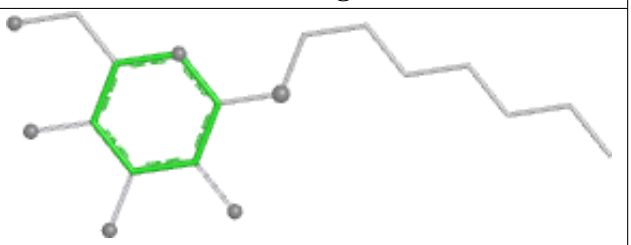


Bond angles

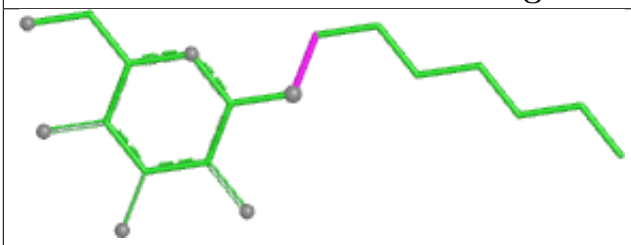


Torsions



Rings

Ligand HTG b 603



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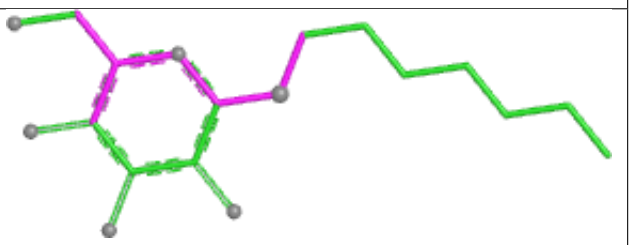
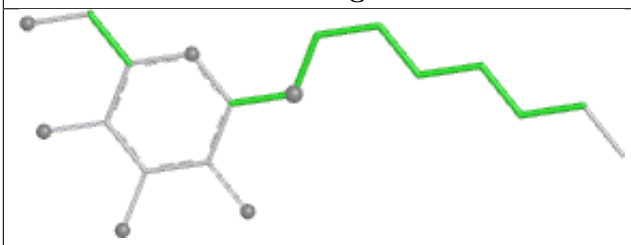
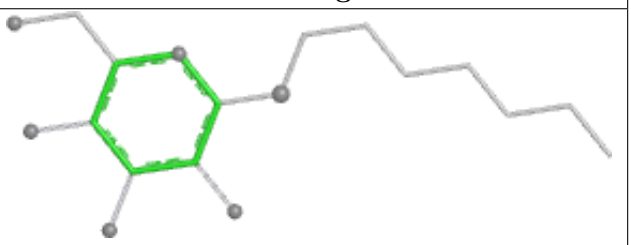


Bond angles

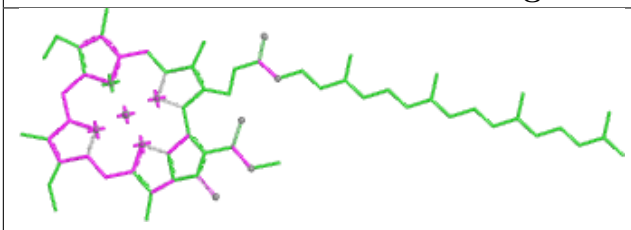


Torsions



Rings

Ligand CLA A 405



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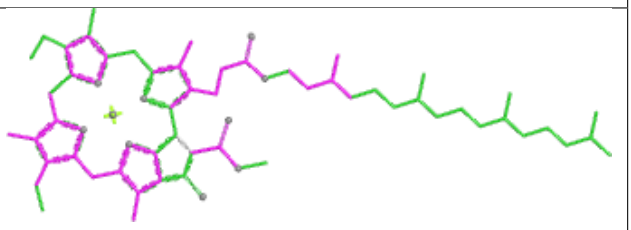
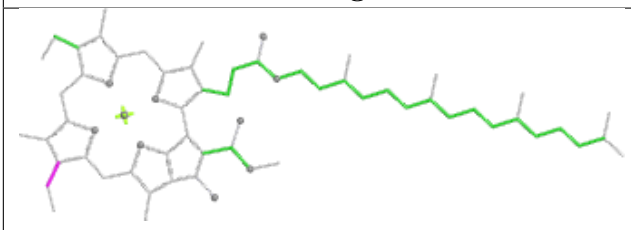
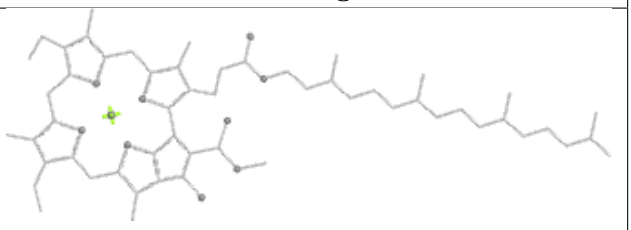


Bond angles

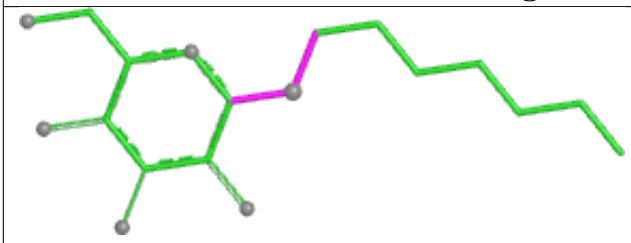


Torsions



Rings

Ligand HTG C 525



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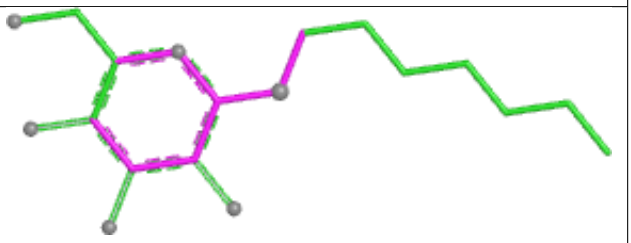
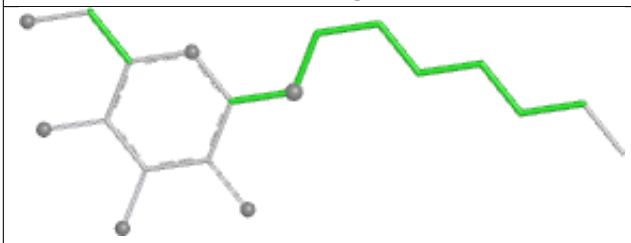
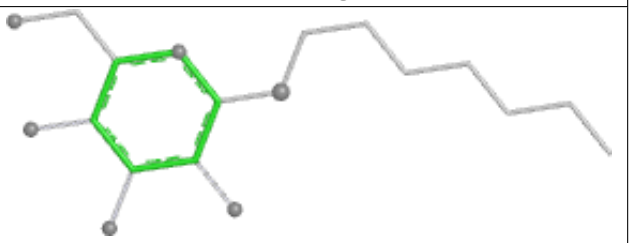


Bond angles

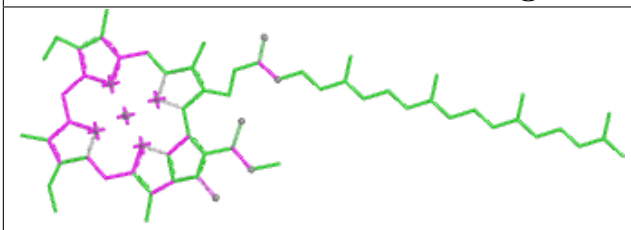


Torsions

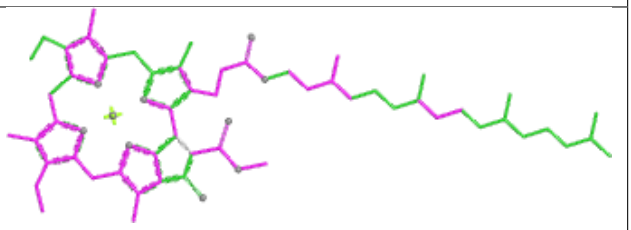


Rings

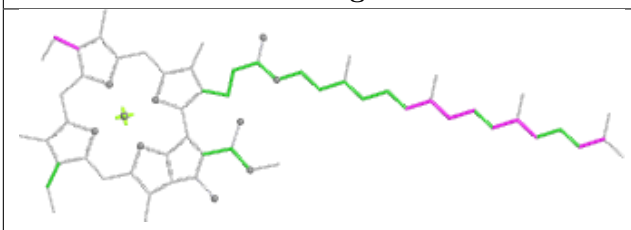
Ligand CLA a 2610



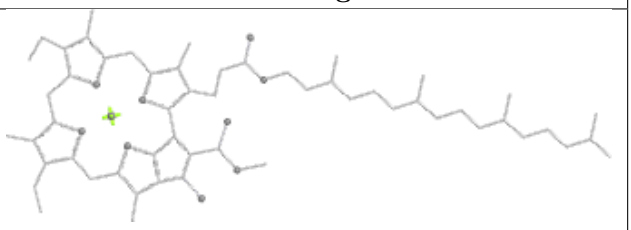
Bond lengths



Bond angles

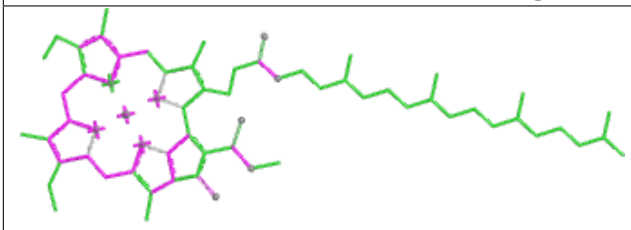


Torsions



Rings

Ligand CLA c 508



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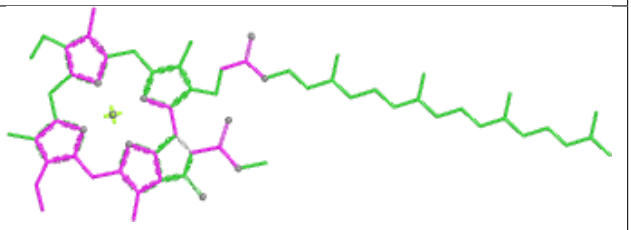
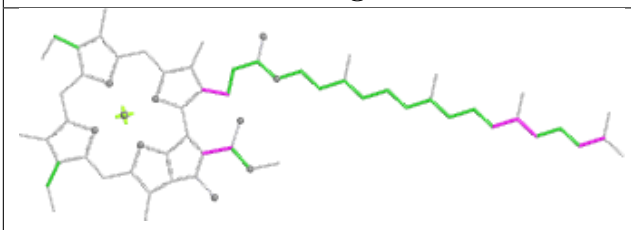
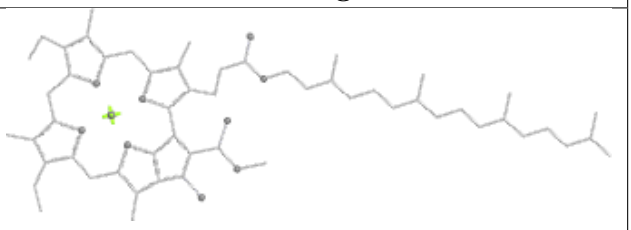


Bond angles

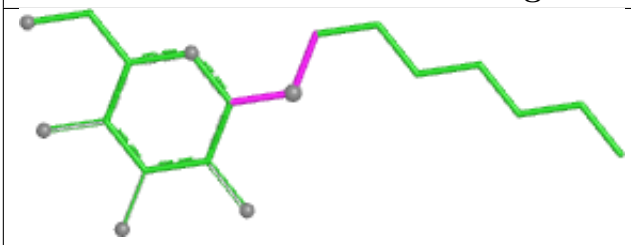


Torsions



Rings

Ligand HTG d 407



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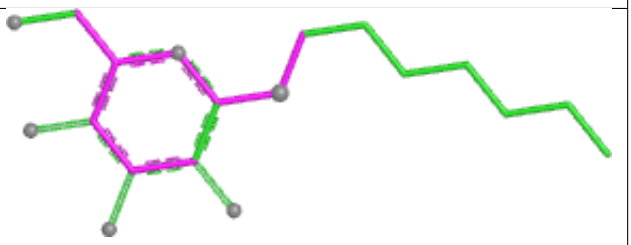
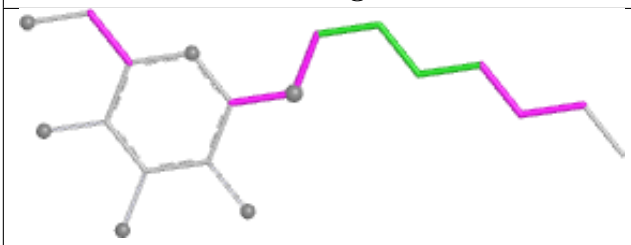
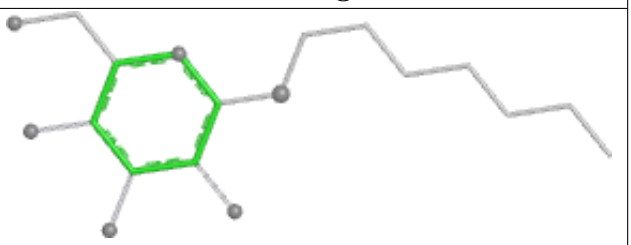


Bond angles

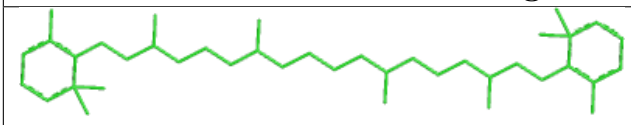


Torsions



Rings

Ligand BCR T 102



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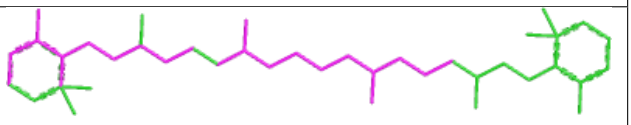
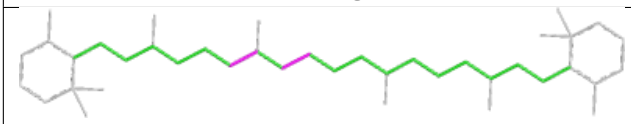
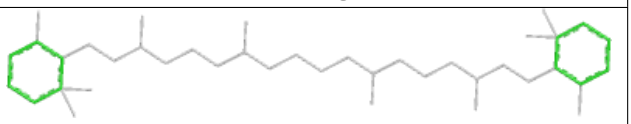


Bond angles

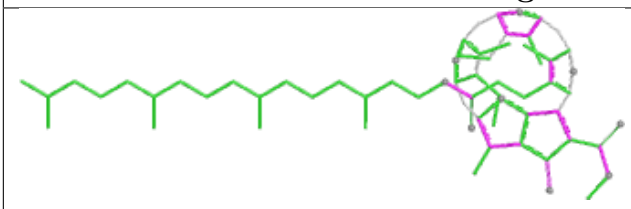


Torsions



Rings

Ligand PHO a 2612



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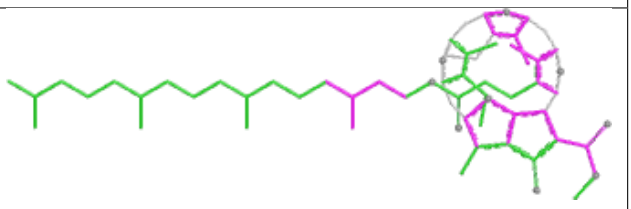
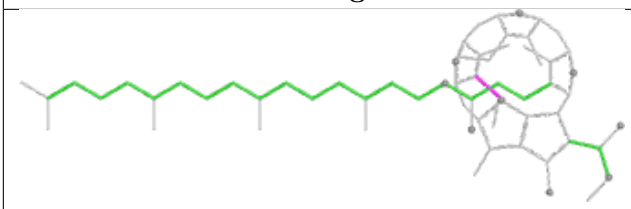


Bond angles



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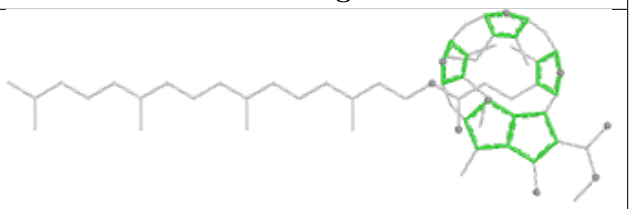
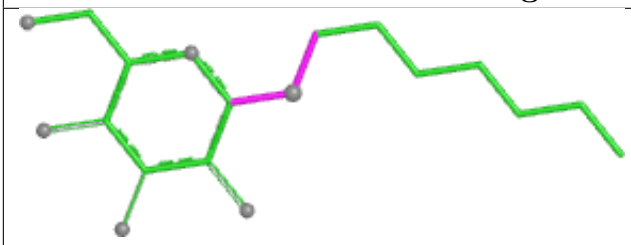


Rings

Ligand HTG B 626



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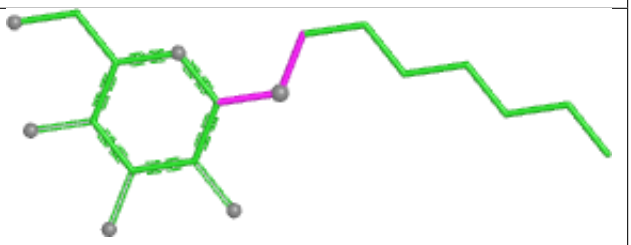
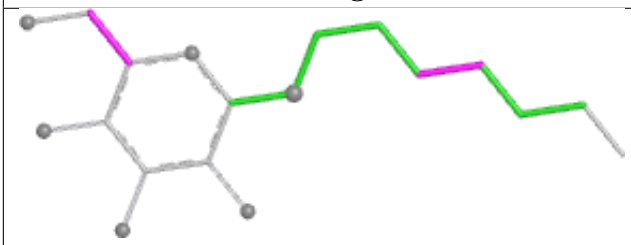


Bond angles



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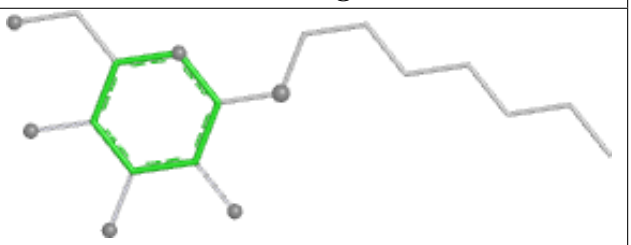
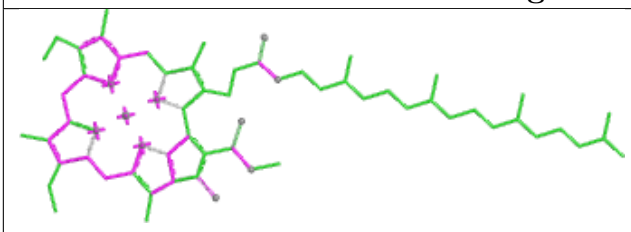
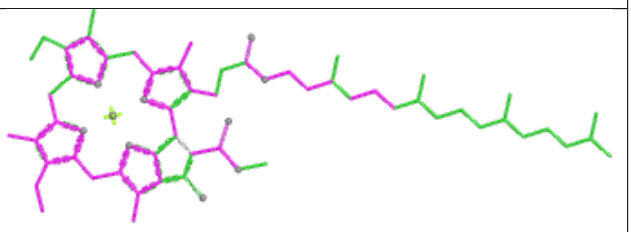


Rings

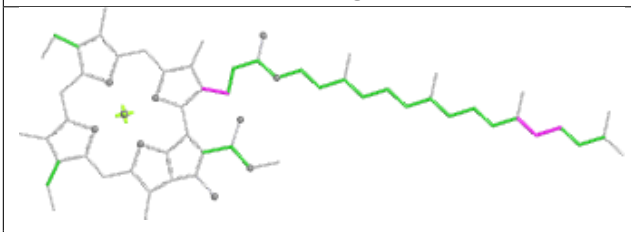
Ligand CLA b 616



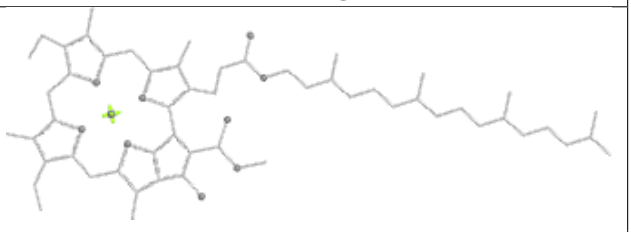
Bond lengths



Bond angles

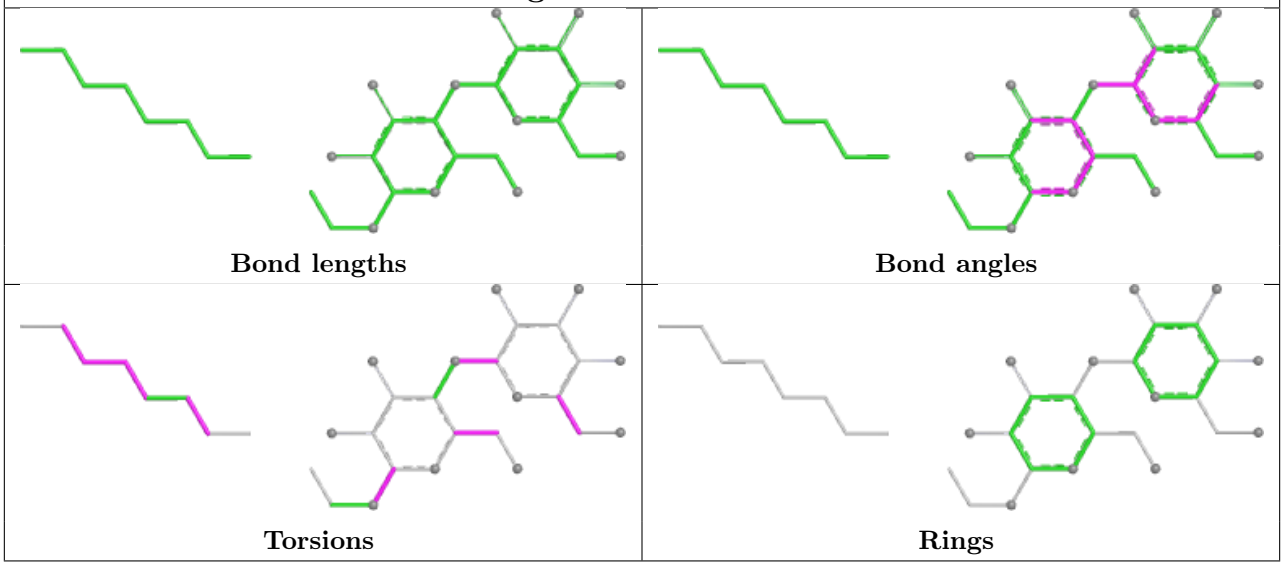


Torsions

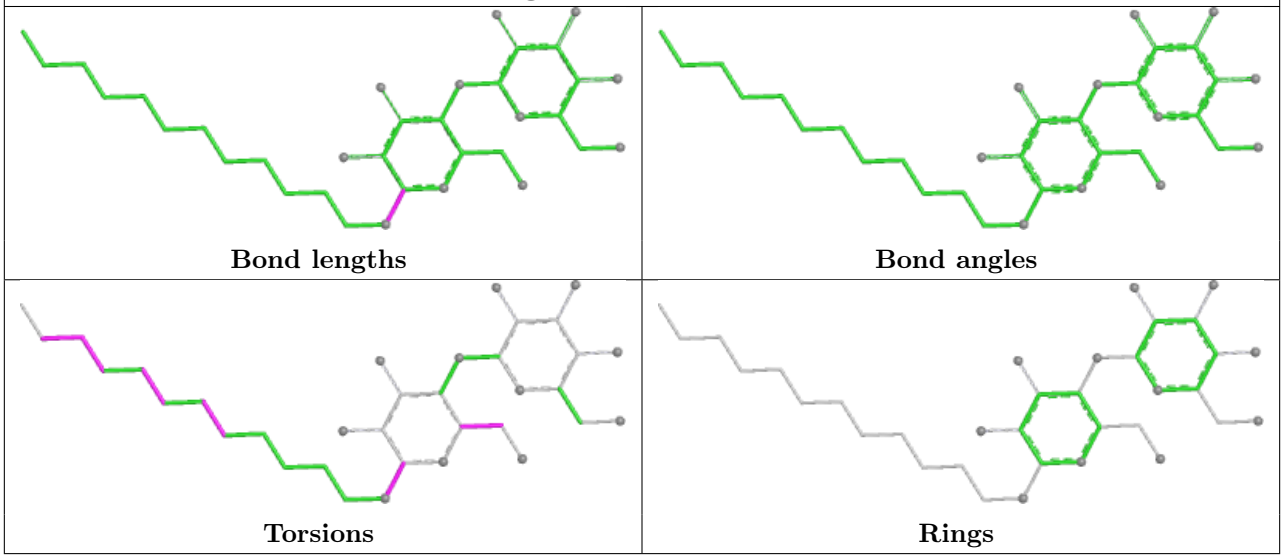


Rings

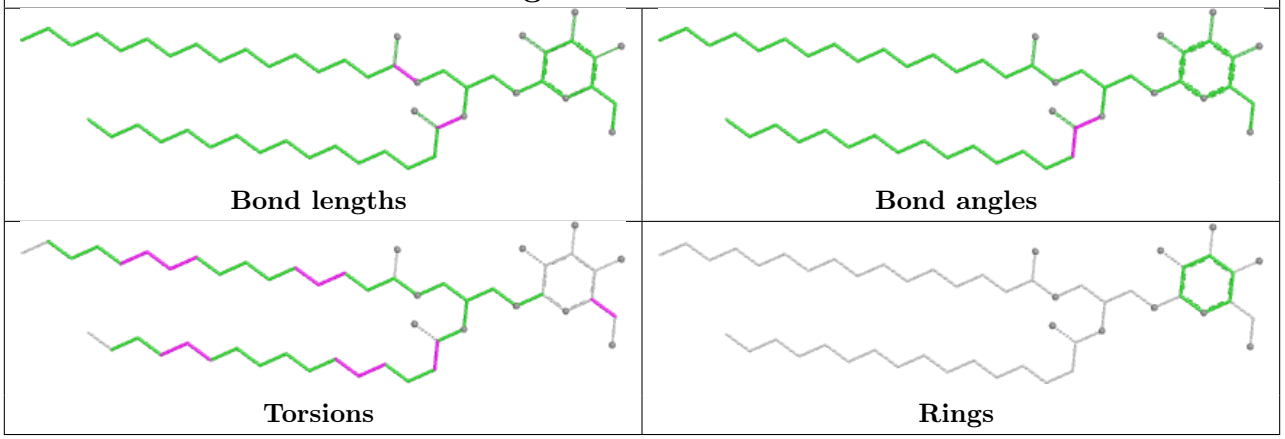
Ligand LMT z 102



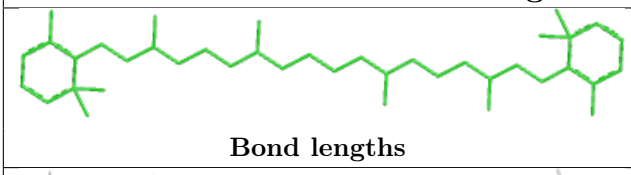
Ligand LMT B 634



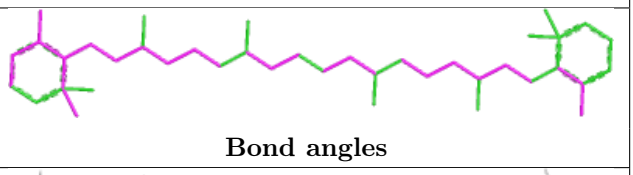
Ligand LMG d 414



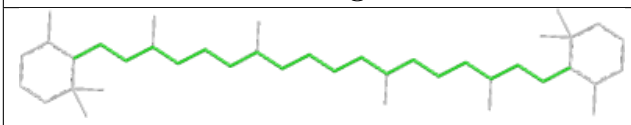
Ligand BCR k 302



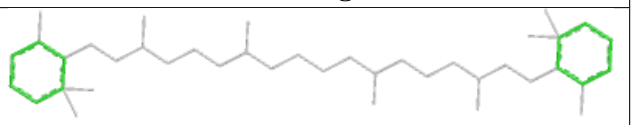
Bond lengths



Bond angles

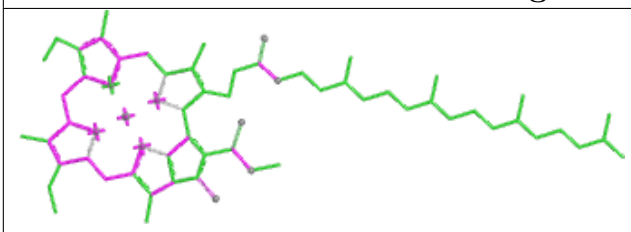


Torsions



Rings

Ligand CLA c 504



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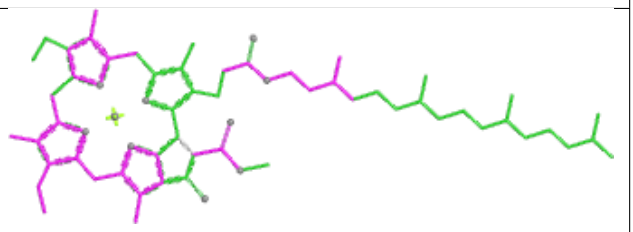
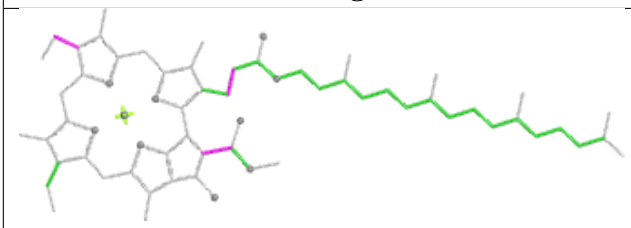
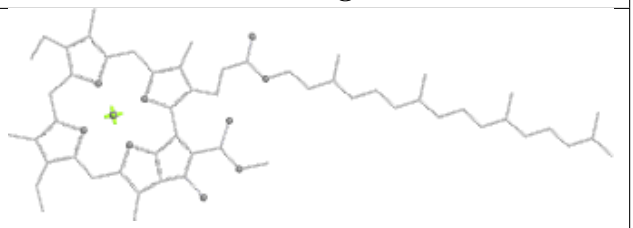


Bond angles

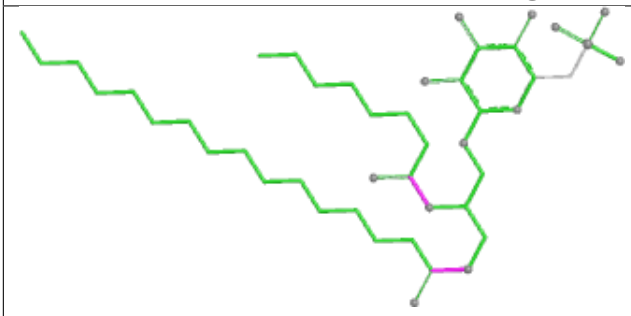


Torsions



Rings

Ligand SQD A 412



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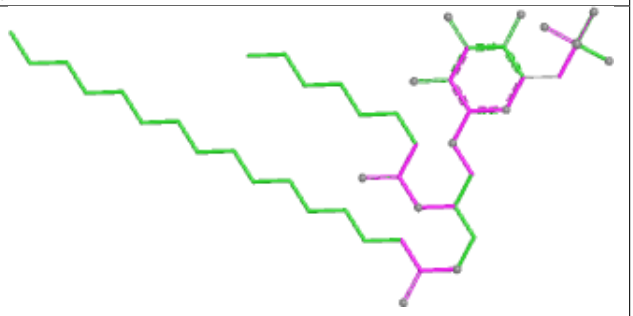
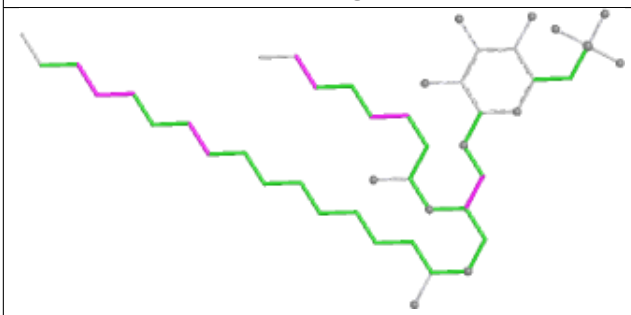


Bond angles



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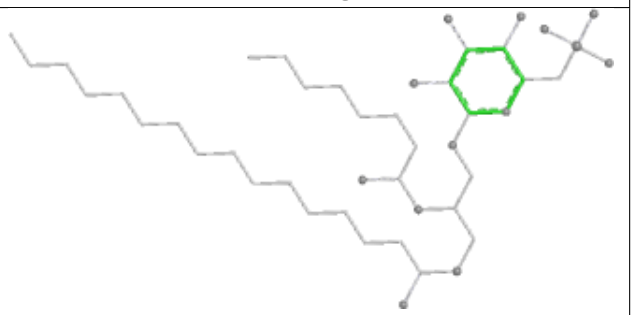
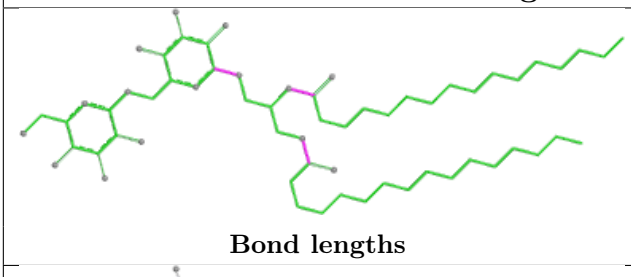
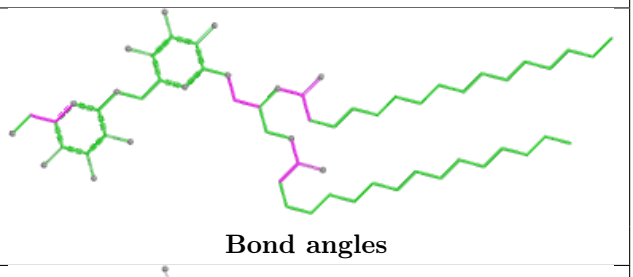


Rings

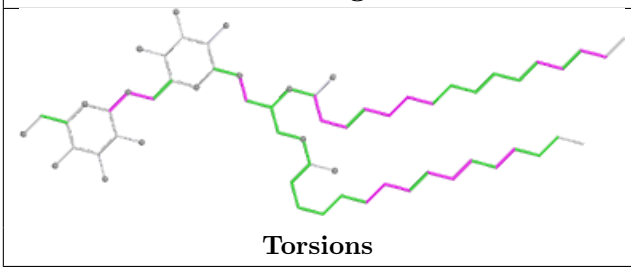
Ligand DGD C 518



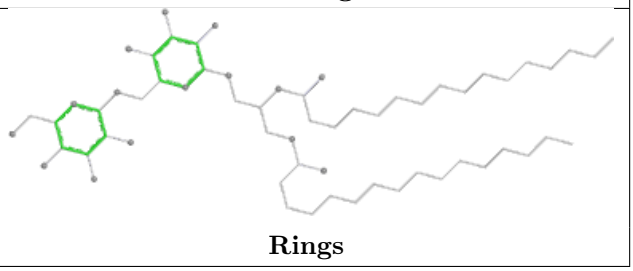
Bond lengths



Bond angles

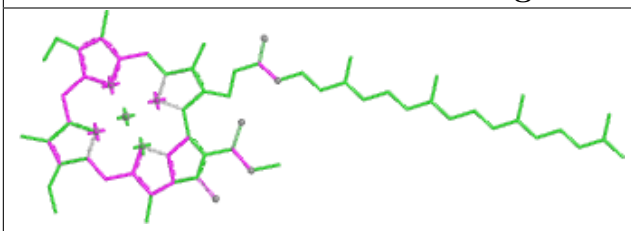


Torsions

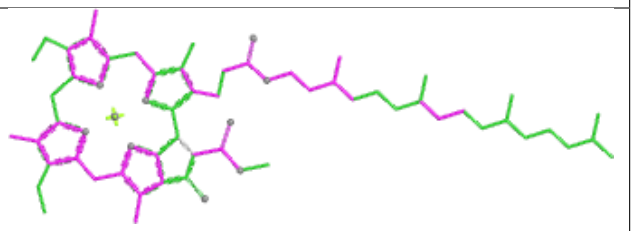


Rings

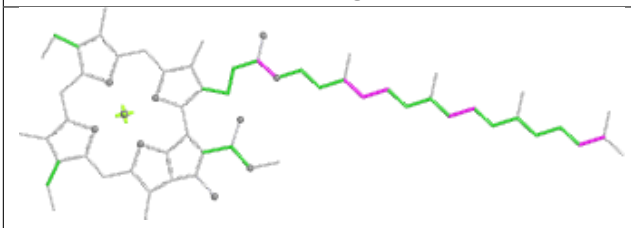
Ligand CLA D 2304



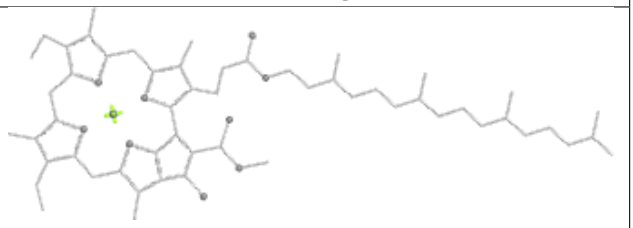
Bond lengths



Bond angles

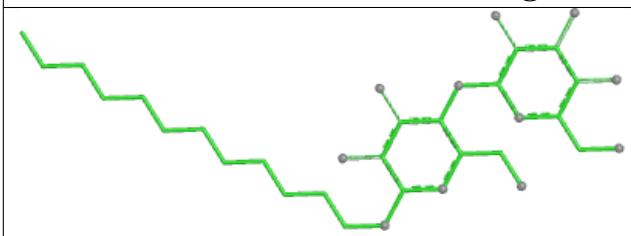


Torsions

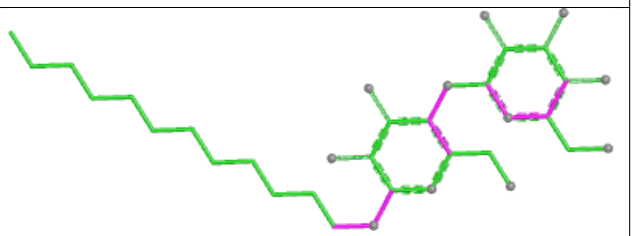


Rings

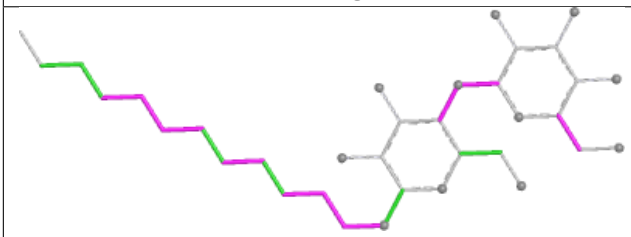
Ligand LMT B 623



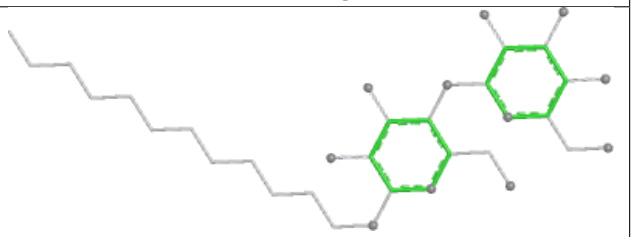
Bond lengths



Bond angles

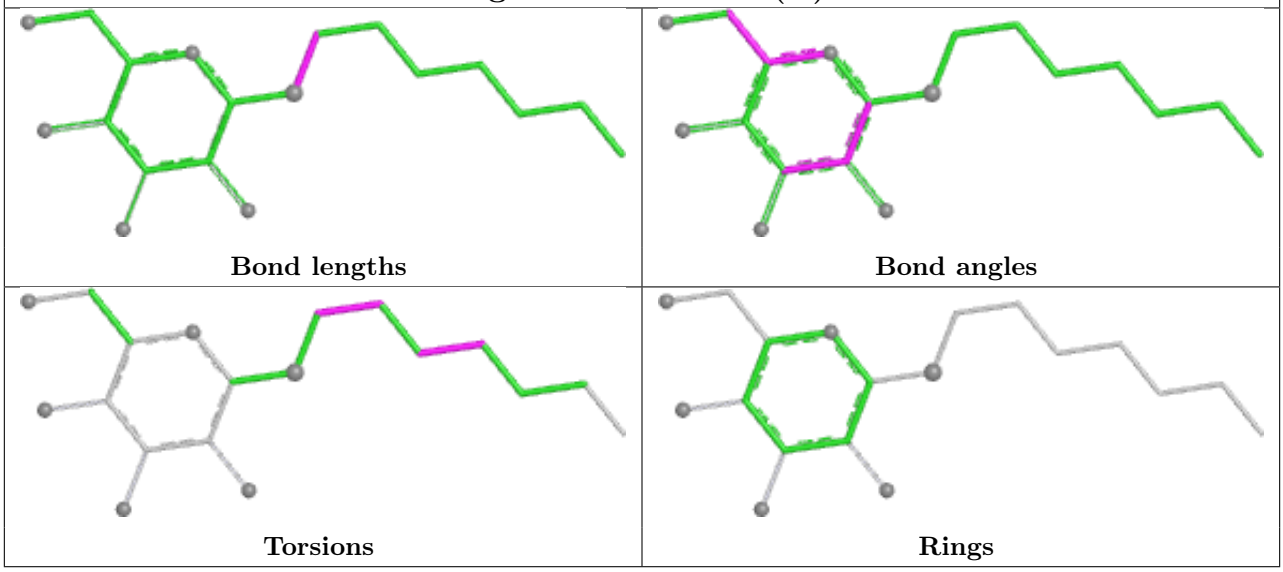


Torsions

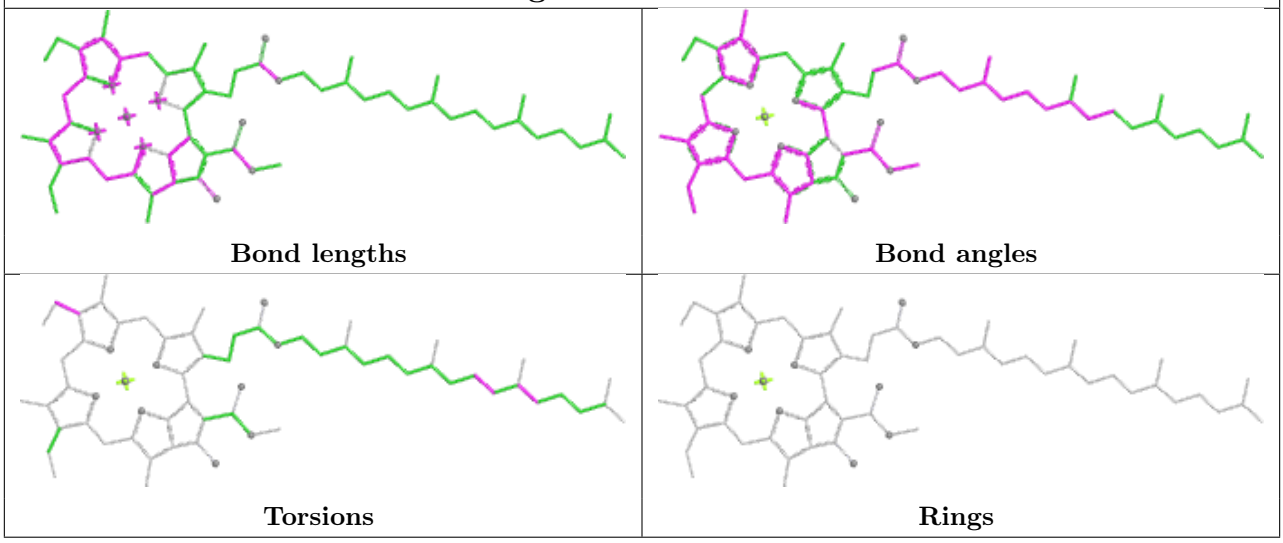


Rings

Ligand HTG B 624 (A)



Ligand CLA b 620



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

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

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	61	VAL	4.2
2	B	479	PHE	4.1
8	I	28	PRO	4.1
8	i	28	PRO	4.0
5	e	6	GLY	4.0
18	x	2	THR	3.9
8	I	32	PRO	3.9
8	i	29	ALA	3.8
1	a	246	TYR	3.6
2	B	84	THR	3.5
14	T	30	THR	3.5
5	e	65[A]	LEU	3.5
14	t	30	THR	3.4
1	A	11	ALA	3.4
19	z	3	ILE	3.3
1	A	229	GLU	3.3
8	i	32	PRO	3.3
18	X	2	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLY	3.2
5	e	79	PHE	3.2
5	E	76	VAL	3.2
1	a	235	TYR	3.2
5	E	79	PHE	3.1
2	b	484	PRO	3.1
3	c	19	ASN	3.1
1	A	14	TRP	3.1
4	D	12	ARG	3.1
7	H	64	ALA	3.1
8	I	29	ALA	3.1
6	f	15	ILE	3.1
7	H	63	LYS	3.0
5	E	4	THR	3.0
1	a	260	PHE	3.0
2	b	84	THR	3.0
3	C	24	THR	2.9
2	b	479	PHE	2.9
5	e	43	ALA	2.9
8	I	31	ASN	2.8
5	E	83	LEU	2.8
6	F	12	SER	2.8
1	a	251	ALA	2.8
11	L	1	MET	2.8
5	E	72	ALA	2.8
1	a	224	ILE	2.8
8	i	30	ARG	2.7
1	a	222[A]	SER	2.7
19	z	2	THR	2.7
2	B	487	SER	2.7
2	B	86	ILE	2.7
17	Y	18	VAL	2.7
3	C	23	ALA	2.6
6	F	15	ILE	2.6
1	A	230	THR	2.6
1	a	247	ASN	2.6
2	B	500	GLY	2.5
1	a	265	PHE	2.5
3	C	257	PHE	2.5
2	B	478	VAL	2.4
2	B	502	VAL	2.4
5	E	61	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
8	I	26	GLY	2.4
6	f	42	PHE	2.4
5	e	76	VAL	2.4
9	j	2	MET	2.4
7	h	64	ALA	2.4
1	A	19	ASN	2.4
13	O	58	ASN	2.4
13	o	58	ASN	2.4
6	f	16	PHE	2.4
19	Z	60	PHE	2.4
1	a	14	TRP	2.4
3	C	143	TYR	2.3
4	d	135	LEU	2.3
16	v	26	TYR	2.3
2	b	482	ILE	2.3
19	Z	62	VAL	2.2
8	I	27	ASP	2.2
17	y	25	ILE	2.2
7	H	58	VAL	2.2
3	c	183	GLY	2.2
15	U	9	LEU	2.2
13	O	60	ARG	2.2
15	U	8	GLU	2.1
12	m	33	GLN	2.1
5	E	65	LEU	2.1
19	z	5	PHE	2.1
18	x	35	ASP	2.0
6	f	14	PRO	2.0
4	D	341	PHE	2.0
9	J	5	GLY	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	0.84	0.11	114,129,141,143	0
19	FME	Z	1	10/11	0.90	0.12	96,112,117,118	0
14	FME	T	1	10/11	0.94	0.09	48,54,84,88	0

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	GOL	E	104	6/6	0.56	0.13	124,126,128,129	0
34	DMS	X	101	4/4	0.56	0.17	172,174,175,175	0
34	DMS	A	425	4/4	0.58	0.25	152,153,153,155	0
34	DMS	O	308	4/4	0.61	0.21	124,127,127,132	0
34	DMS	U	504	4/4	0.62	0.22	119,124,127,129	0
34	DMS	C	534	4/4	0.63	0.25	141,141,143,143	0
34	DMS	v	210	4/4	0.64	0.22	137,140,140,143	0
34	DMS	c	542	4/4	0.65	0.27	148,149,150,151	0
34	DMS	o	309	4/4	0.65	0.27	131,139,139,141	0
34	DMS	B	645	4/4	0.65	0.17	124,125,125,127	0
34	DMS	o	310	4/4	0.66	0.22	144,147,149,149	0
34	DMS	c	546	4/4	0.67	0.23	151,153,154,154	0
34	DMS	a	2624	4/4	0.67	0.25	79,105,106,109	0
34	DMS	B	642	4/4	0.68	0.24	95,106,108,114	0
34	DMS	c	541	4/4	0.68	0.29	121,128,129,132	0
34	DMS	c	549	4/4	0.68	0.20	124,126,128,128	0
34	DMS	H	104	4/4	0.69	0.17	129,131,133,133	0
30	UNL	j	2702	16/-	0.69	0.23	89,96,108,111	0
30	UNL	a	2616	27/-	0.70	0.19	86,103,140,149	0

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

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

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

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

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

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

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

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

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

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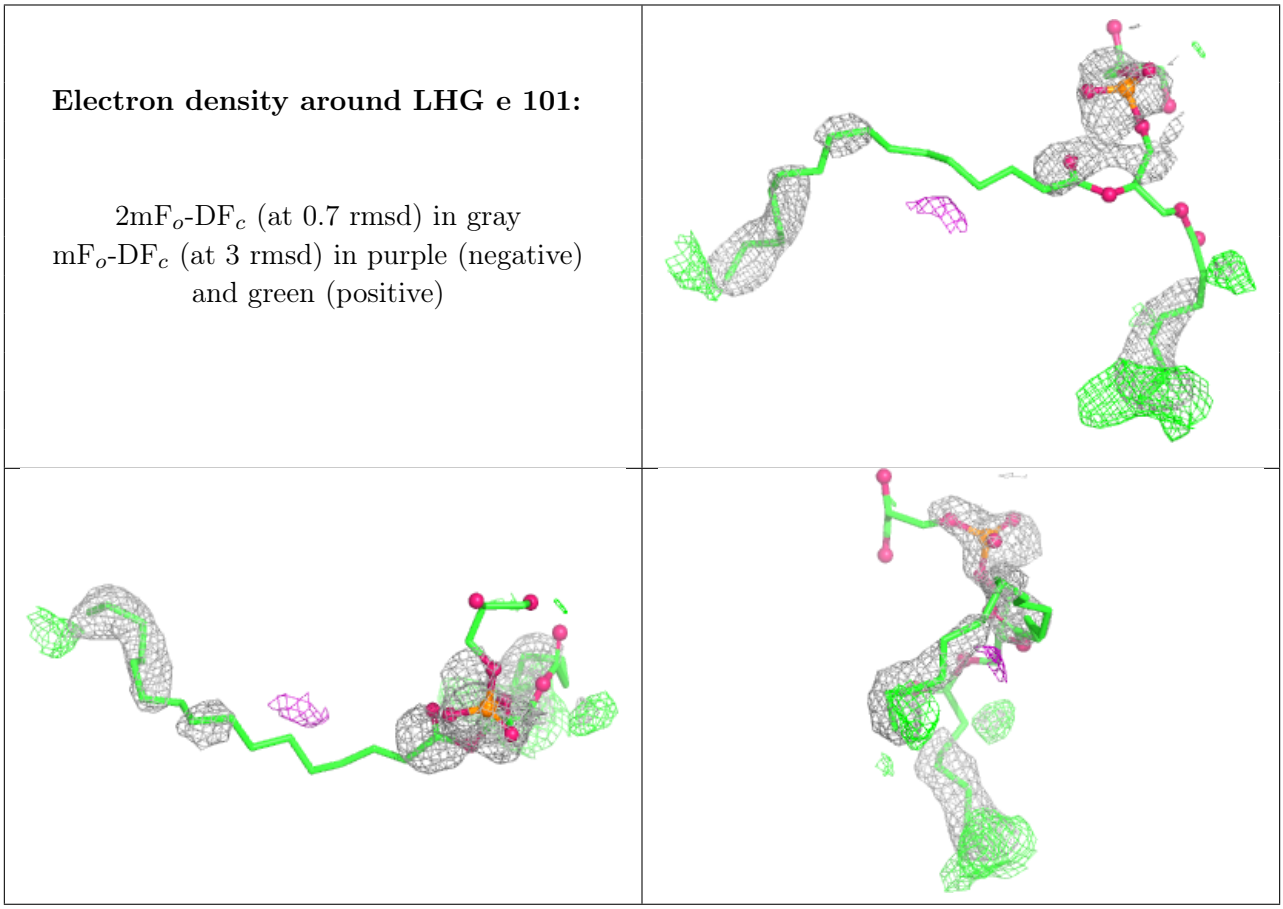
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CA	c	503	1/1	0.99	0.03	73,73,73,73	0
35	CA	o	302	1/1	0.99	0.03	74,74,74,74	0
34	DMS	b	633	4/4	0.99	0.06	45,50,52,61	0
42	HEC	V	201	43/43	0.99	0.06	41,46,52,56	0
20	OEX	A	401	10/10	0.99	0.03	41,46,50,52	0
22	CL	a	2607	1/1	1.00	0.03	46,46,46,46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

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

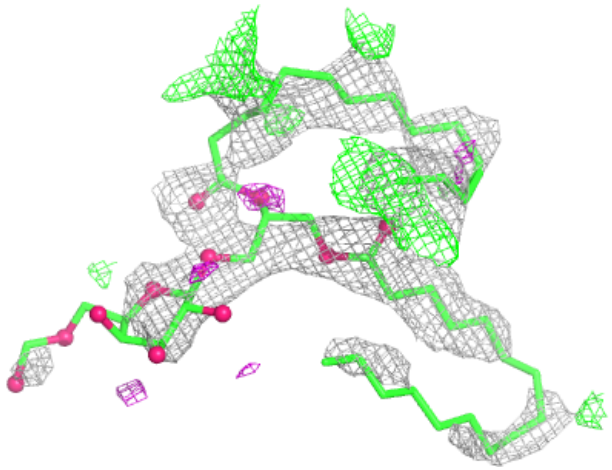
Electron density around LHG e 101:

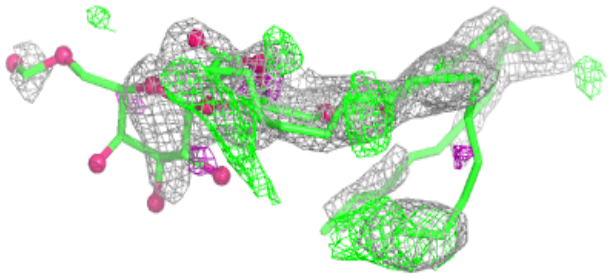
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD D 2307:

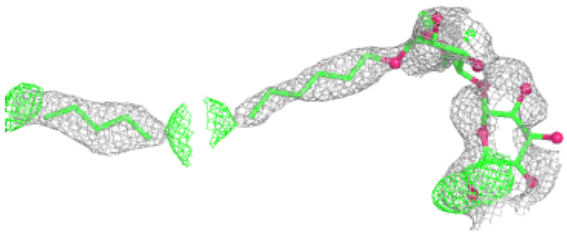
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

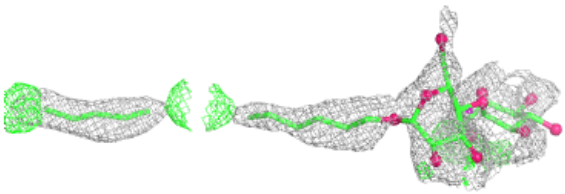


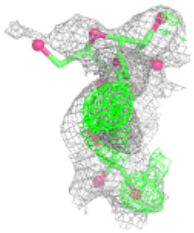


Electron density around LMT j 2701:

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

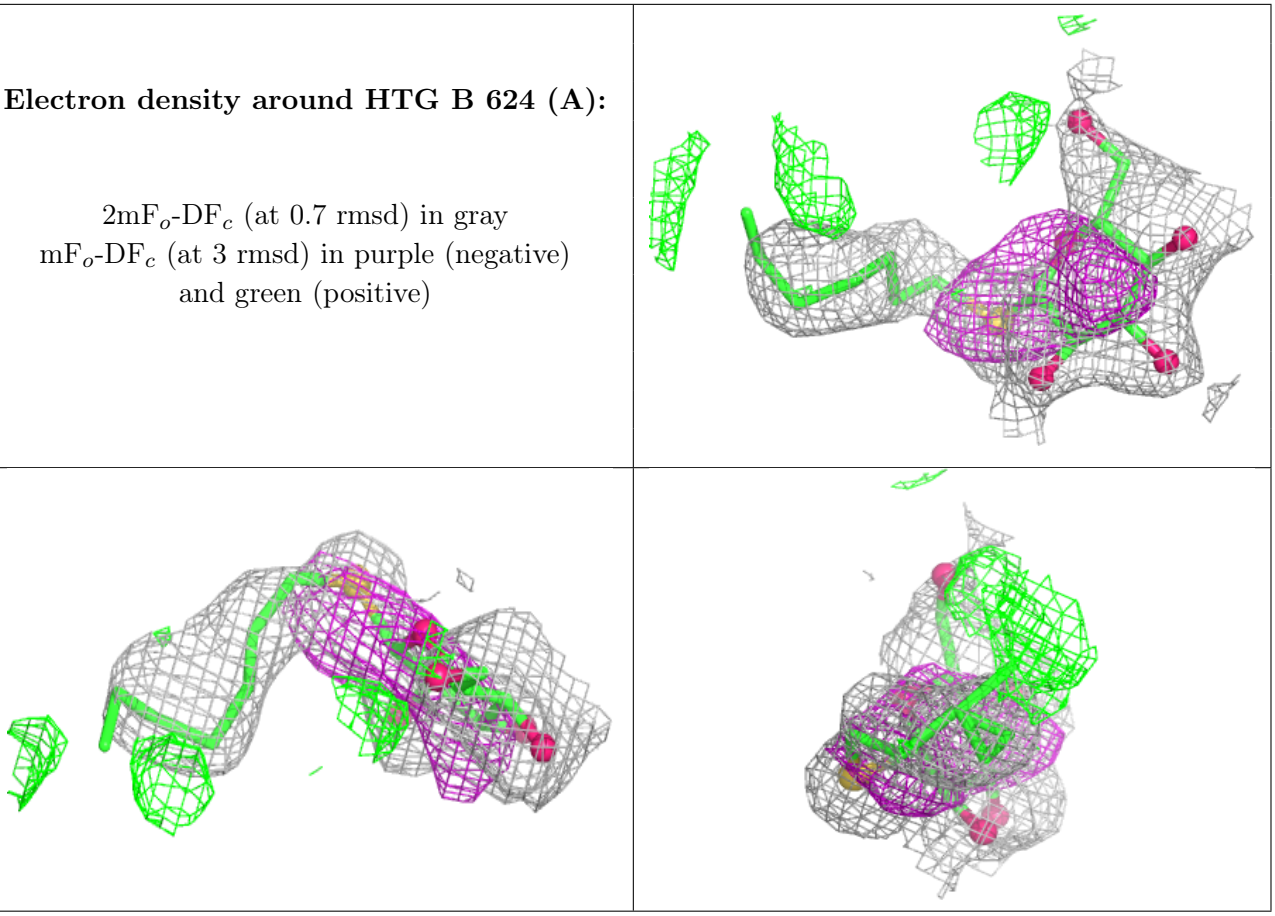






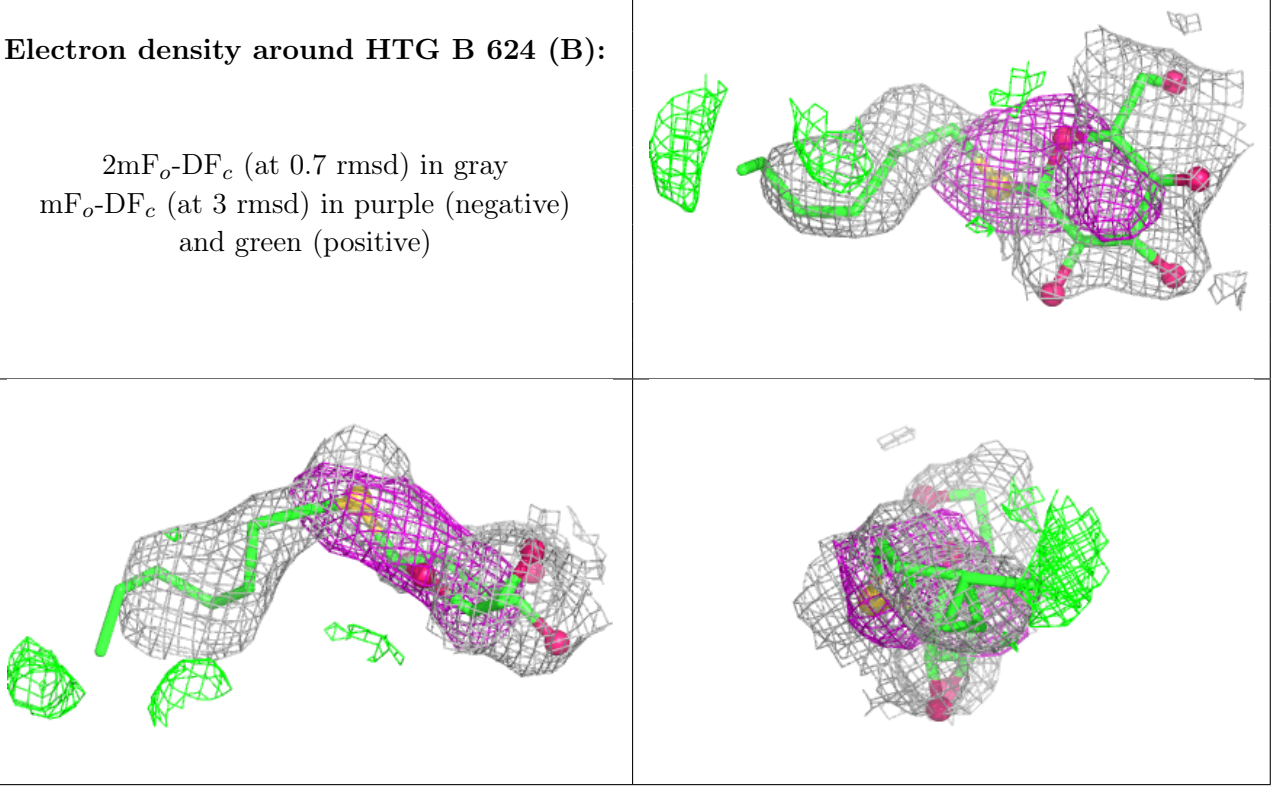
Electron density around HTG B 624 (A):

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



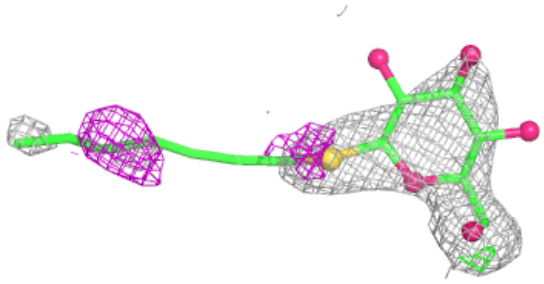
Electron density around HTG B 624 (B):

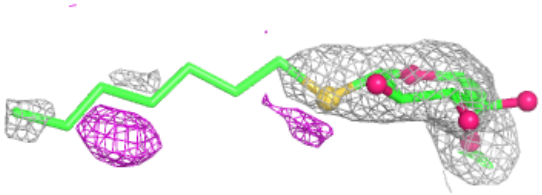
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

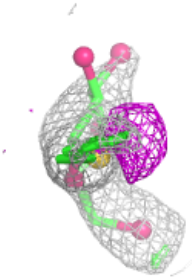


Electron density around HTG C 522:

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

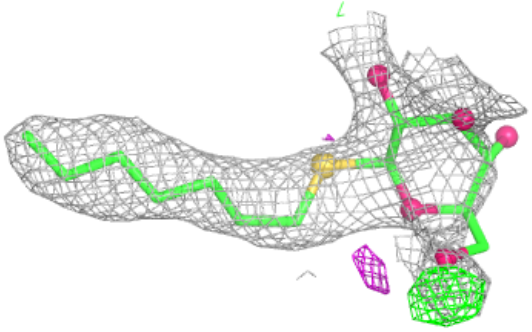


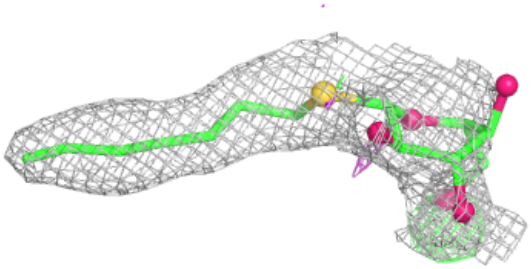


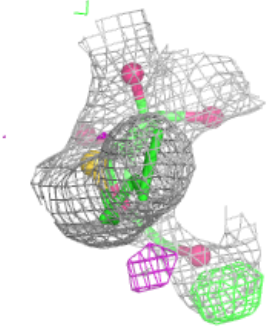


Electron density around HTG i 102:

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

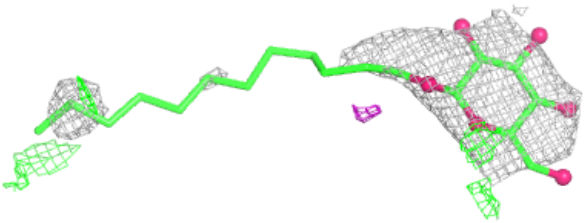


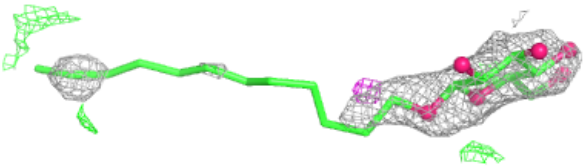


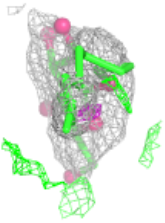


Electron density around LMT F 102:

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

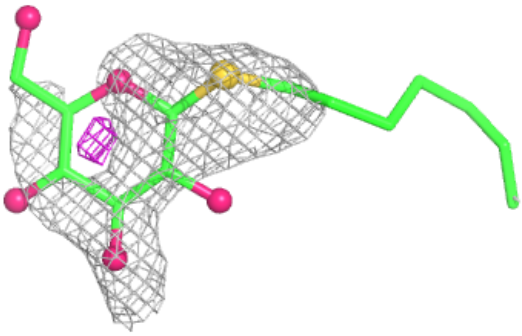


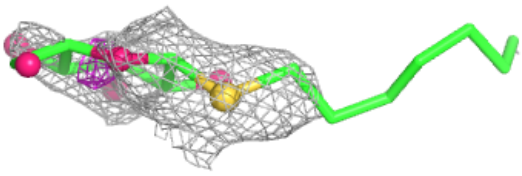


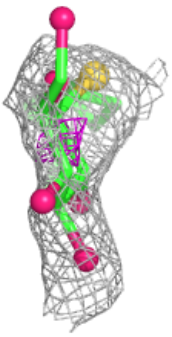


Electron density around HTG d 407:

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

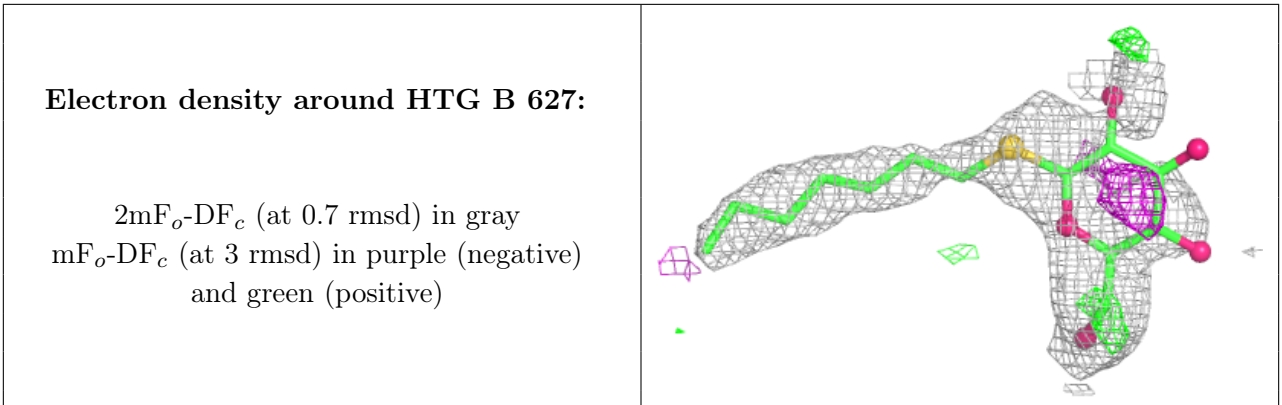






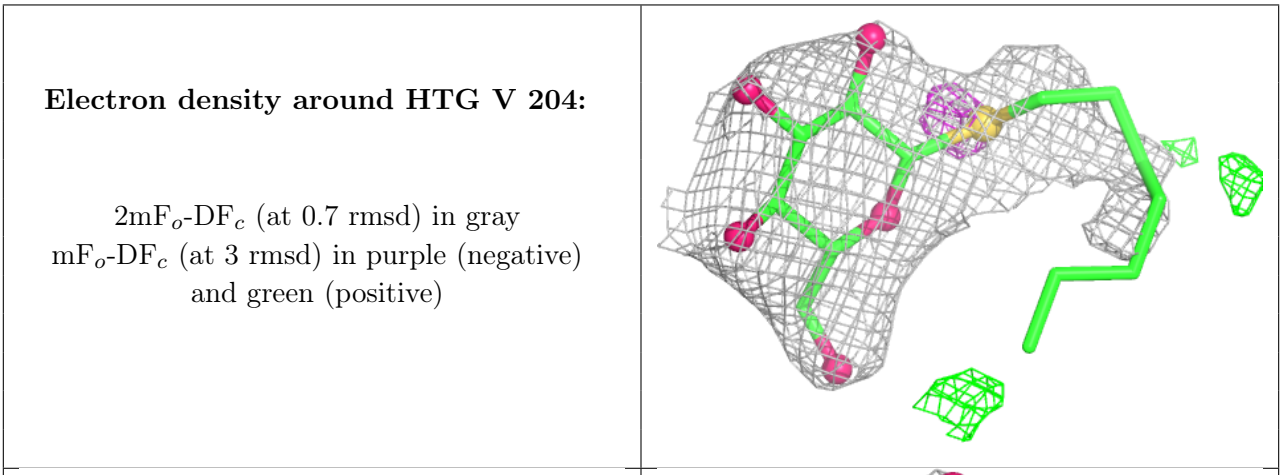
Electron density around HTG B 627:

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



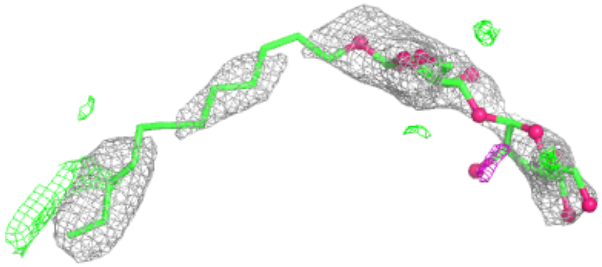
Electron density around HTG V 204:

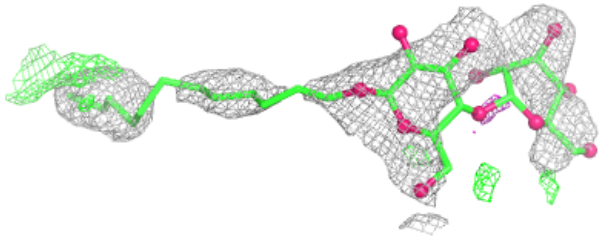
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

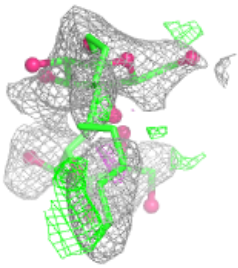


Electron density around LMT m 2804:

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

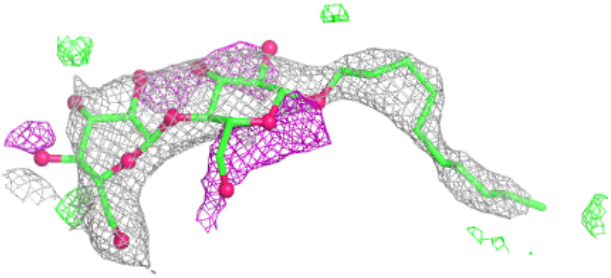


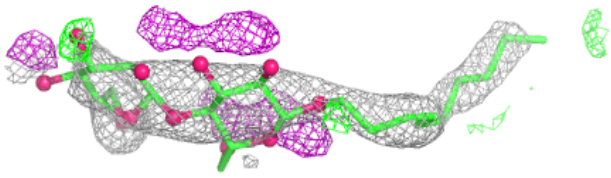


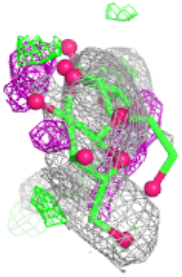


Electron density around LMT A 414:

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

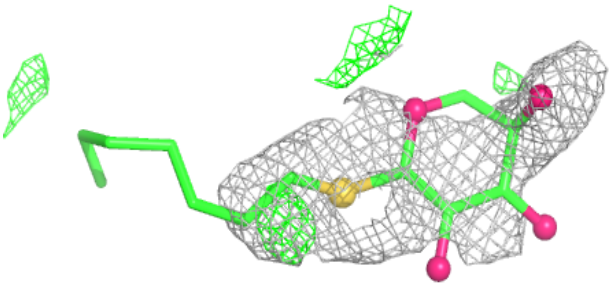


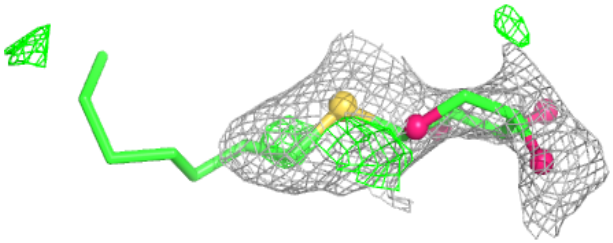


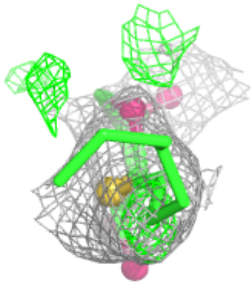


Electron density around HTG H 101:

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

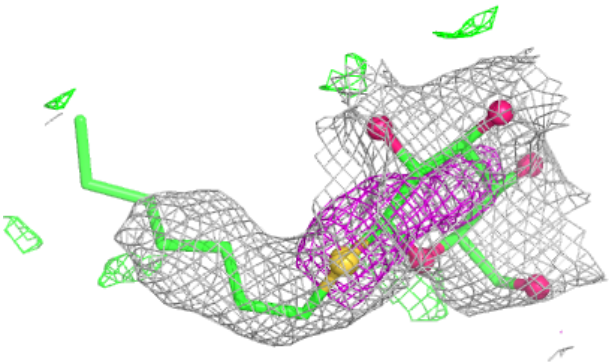


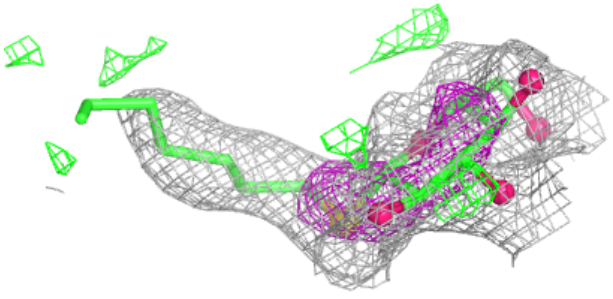


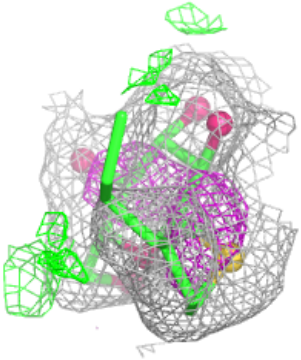


Electron density around HTG b 625:

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

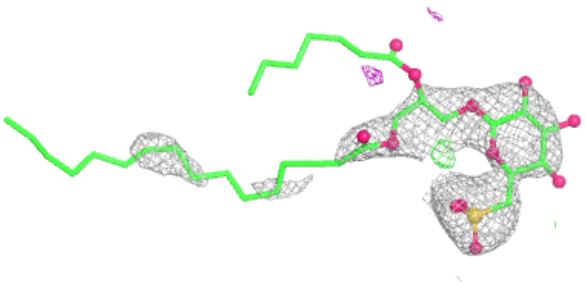


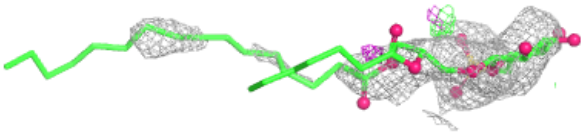


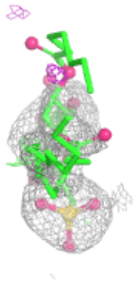


Electron density around SQD D 2308:

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

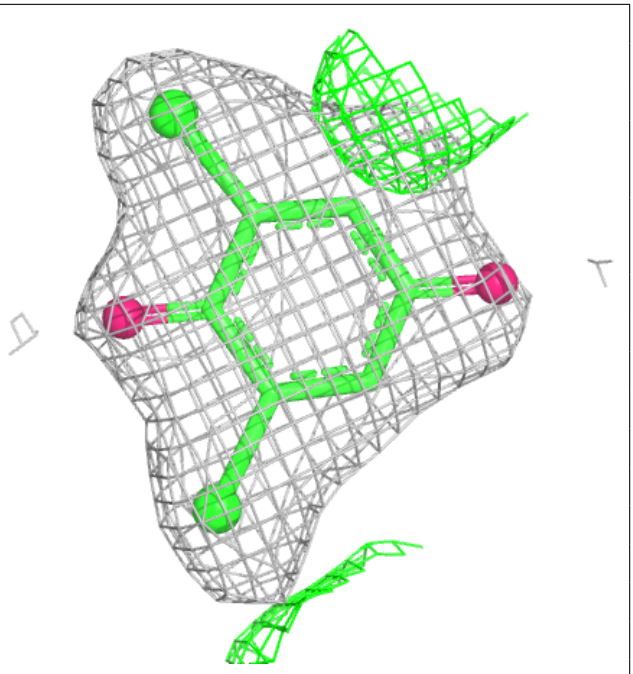


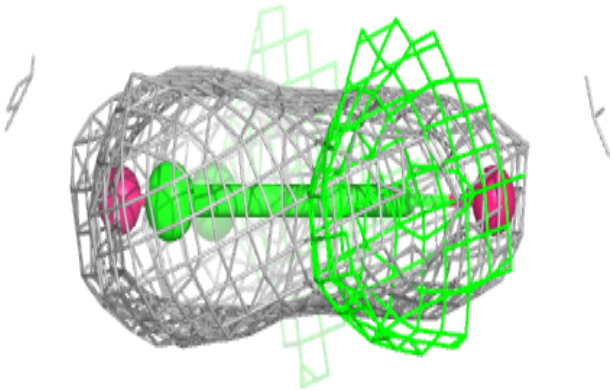


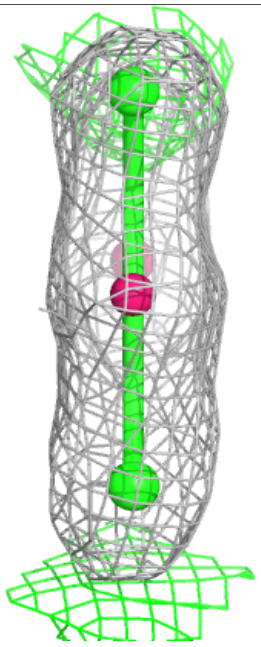


Electron density around JOX A 418:

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

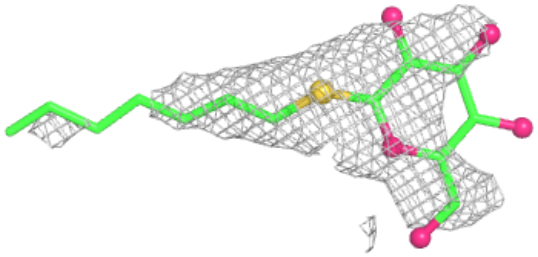


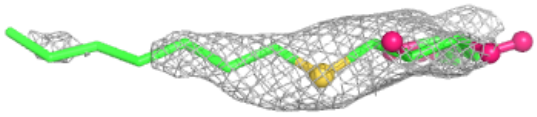


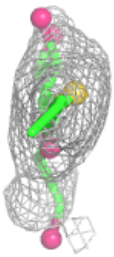


Electron density around HTG C 525:

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

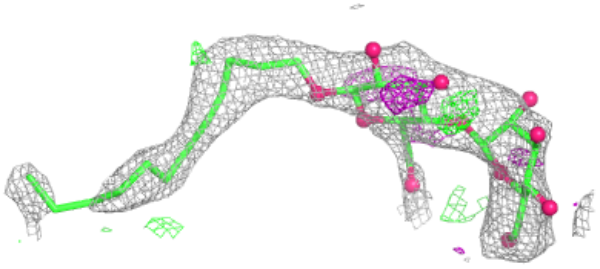


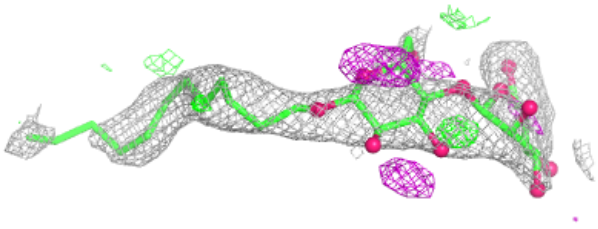


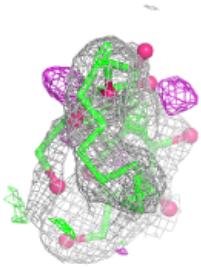


Electron density around LMT d 401:

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

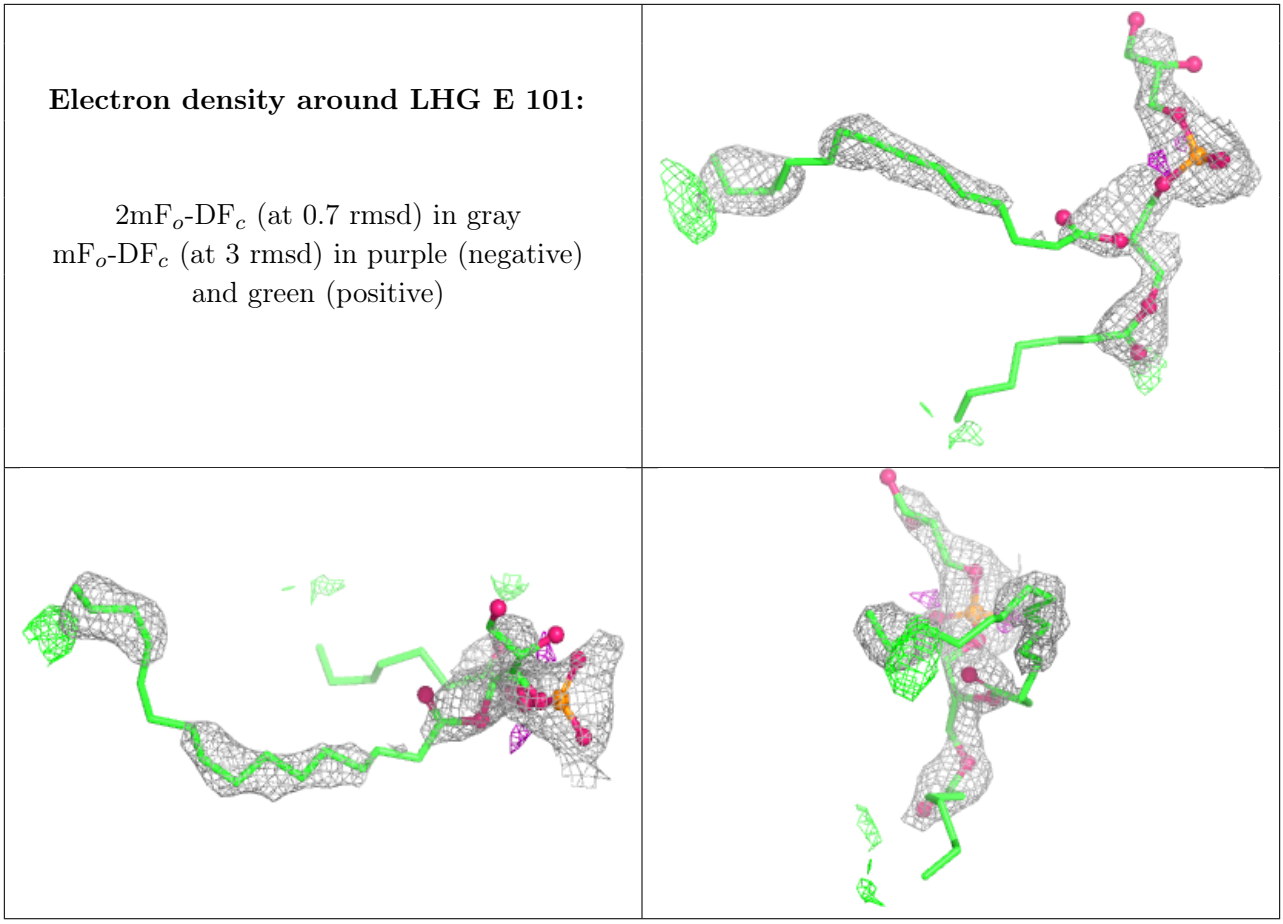






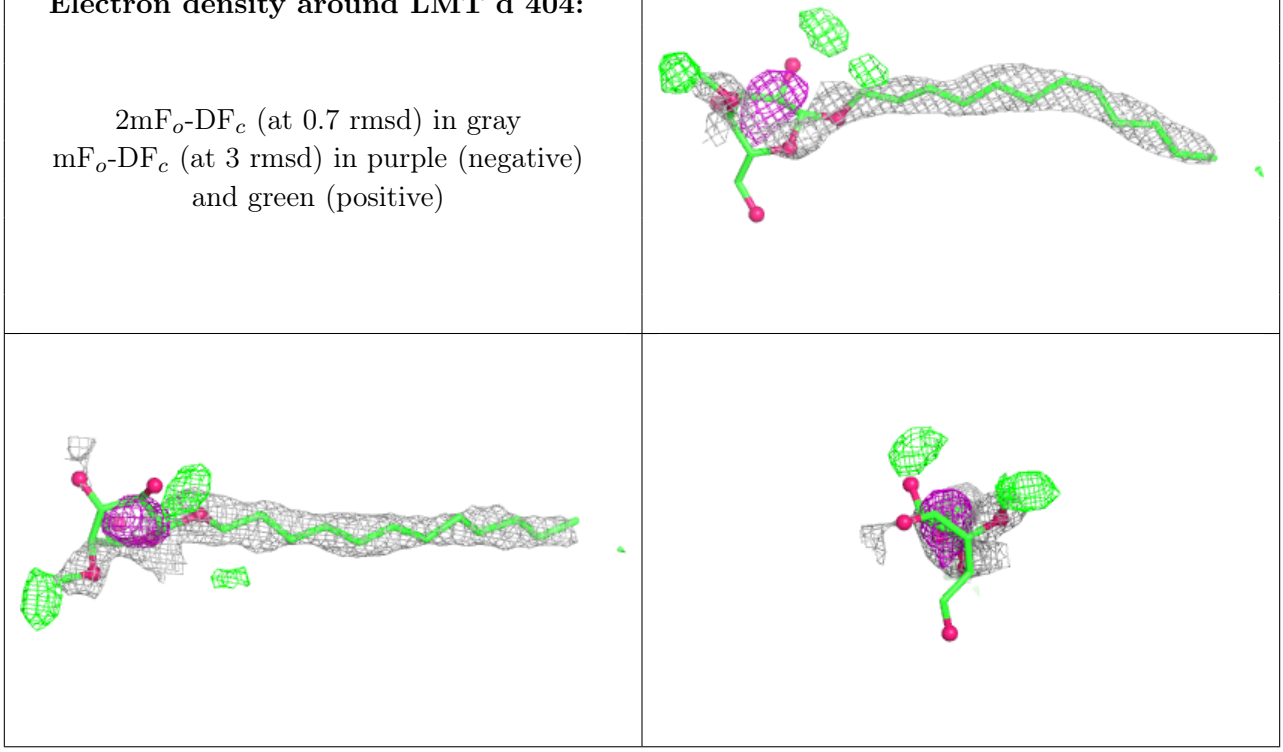
Electron density around LHG E 101:

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



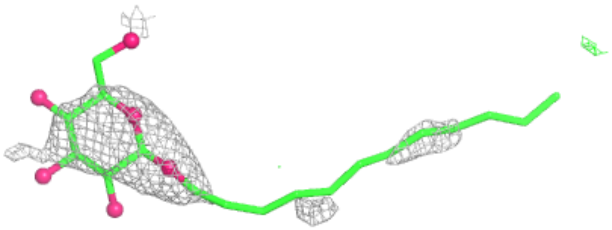
Electron density around LMT d 404:

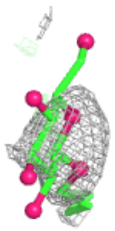
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT f 101:

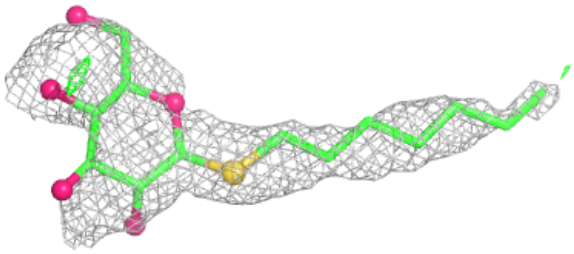
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

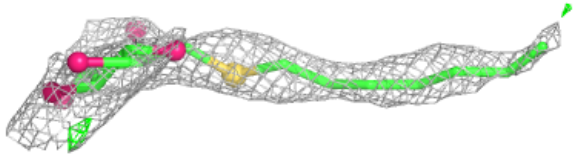


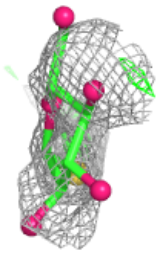


Electron density around HTG B 625:

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

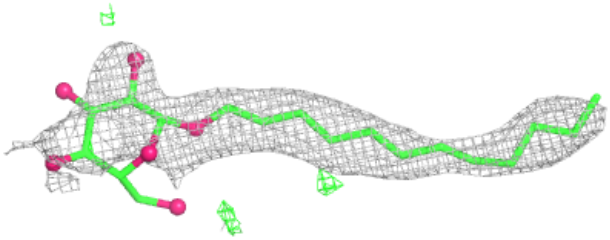


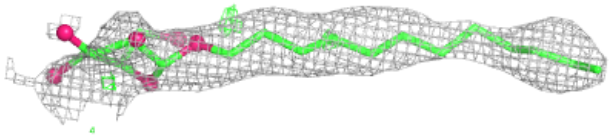


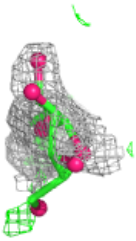


Electron density around LMT J 303:

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

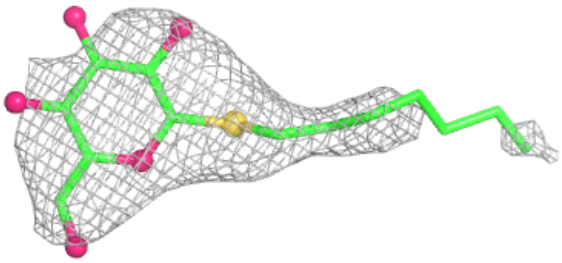


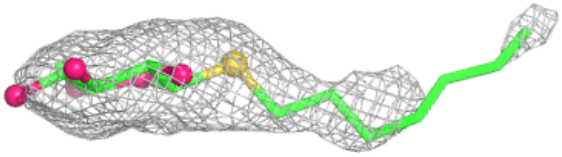


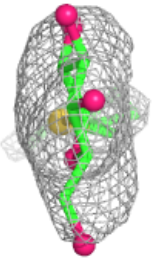


Electron density around HTG c 523:

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

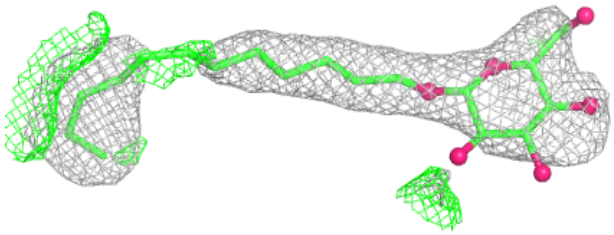


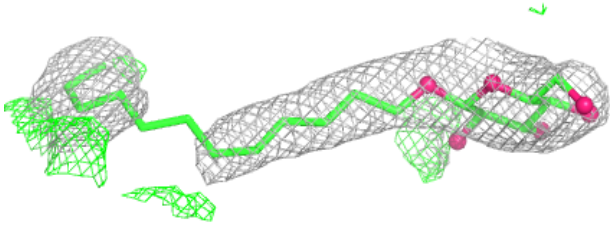


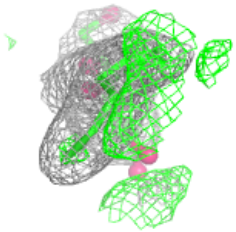


Electron density around LMT T 103:

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

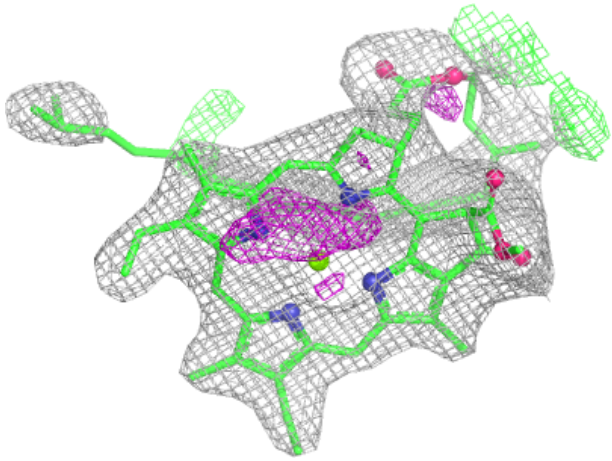


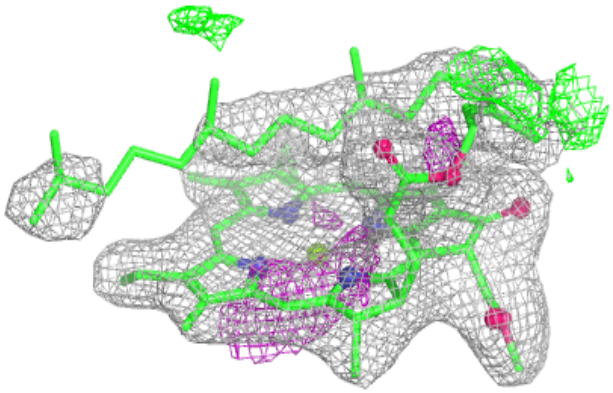


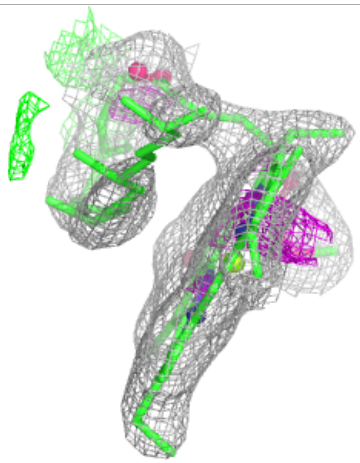


Electron density around CLA B 602:

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

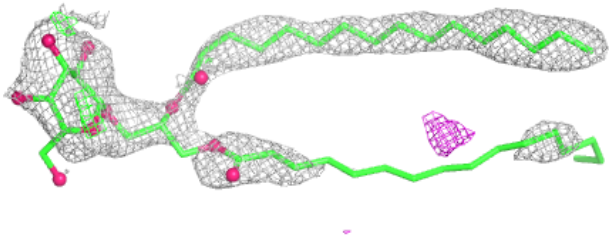


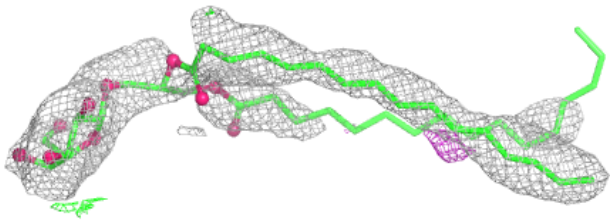


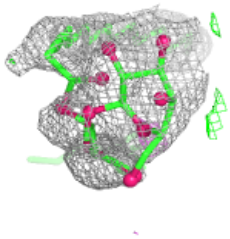


Electron density around LMG c 522:

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

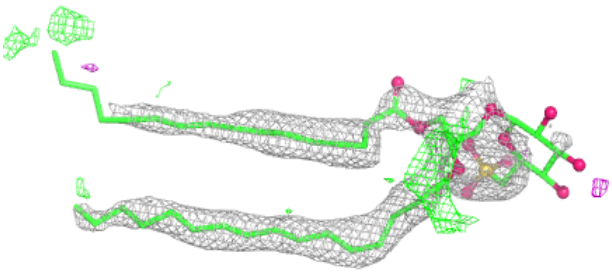


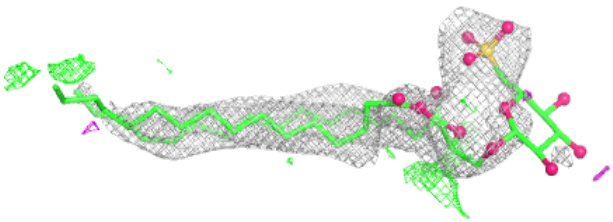


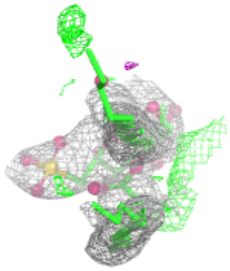


Electron density around SQD D 2302:

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

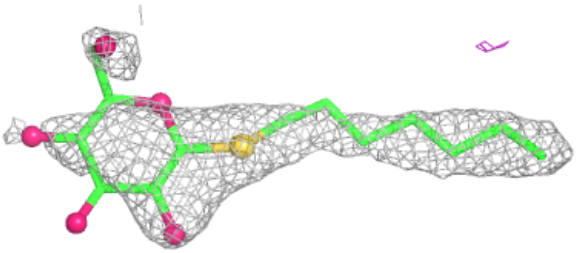


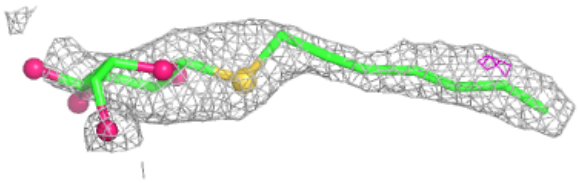


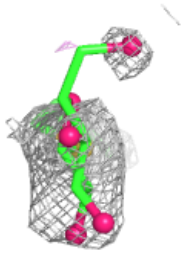


Electron density around HTG c 524:

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

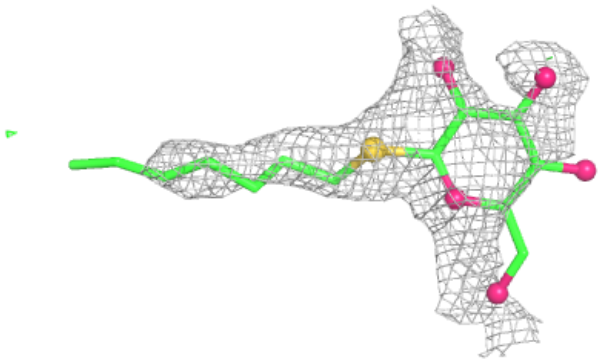


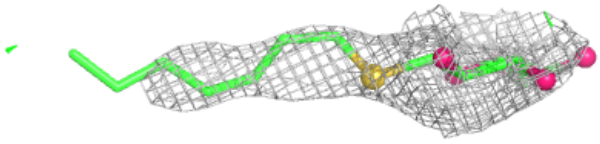


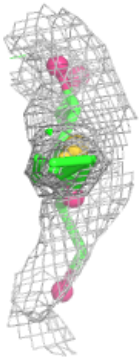


Electron density around HTG c 526:

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

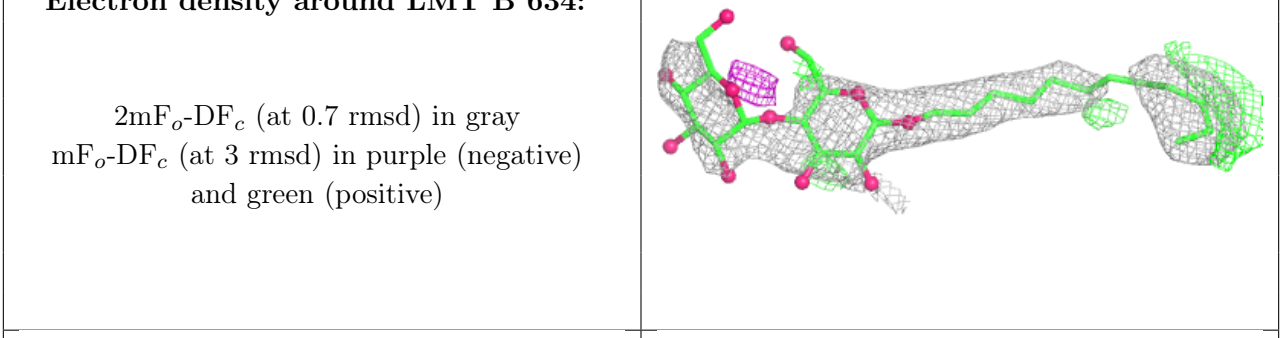


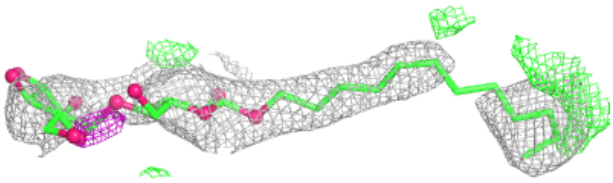


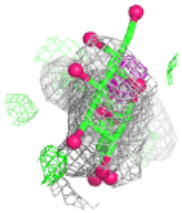


Electron density around LMT B 634:

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

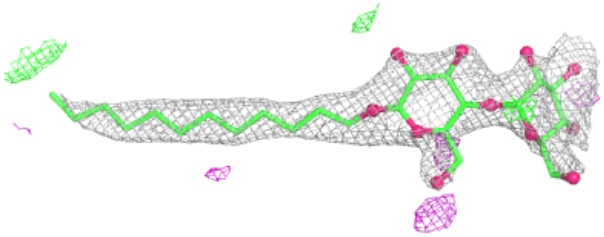


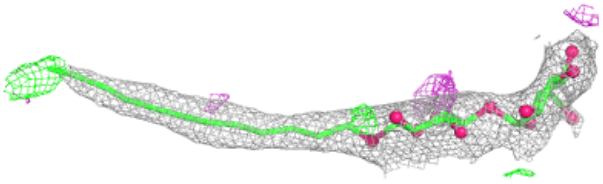


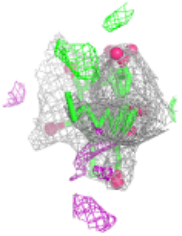


Electron density around LMT m 2803:

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

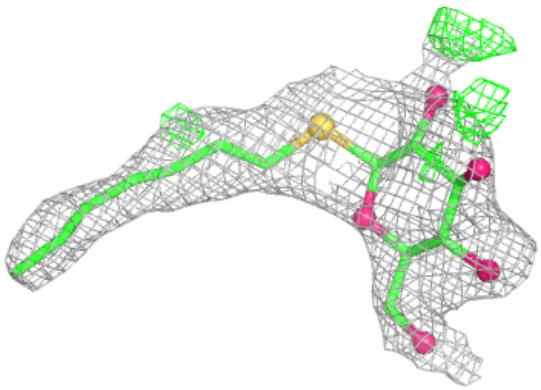


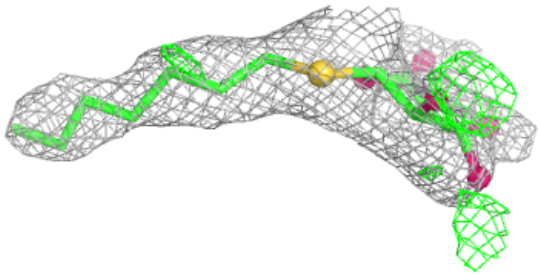


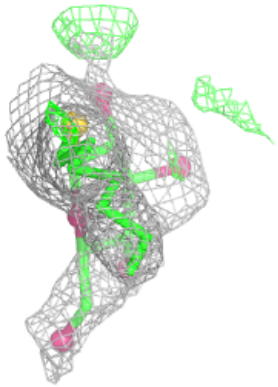


Electron density around HTG b 626:

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

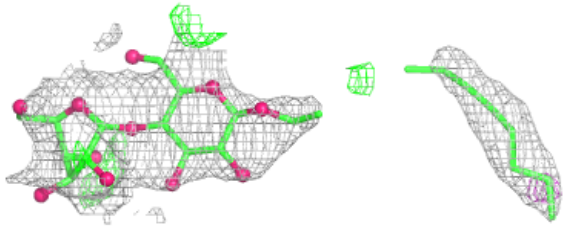


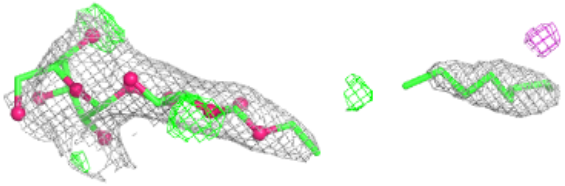


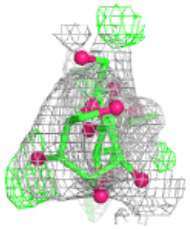


Electron density around LMT z 102:

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

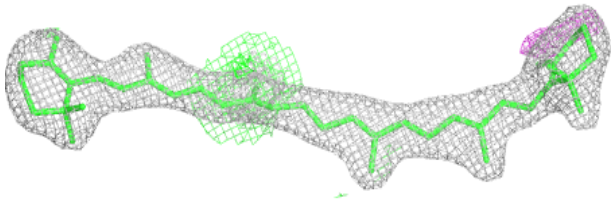


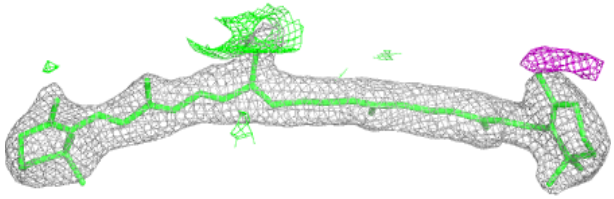


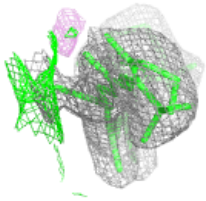


Electron density around BCR T 102:

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

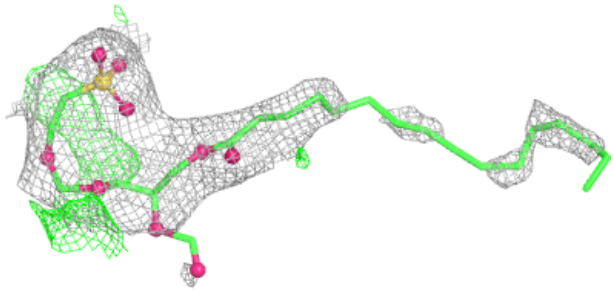


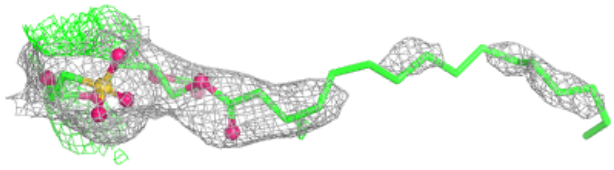


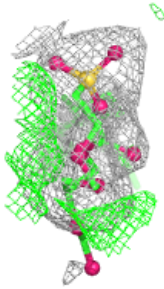


Electron density around SQD d 417:

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

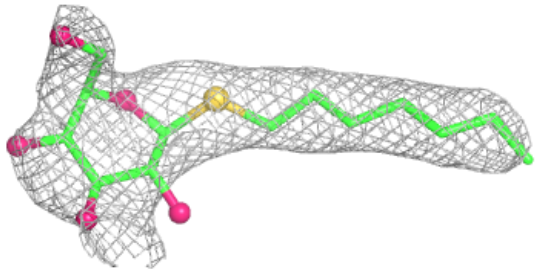


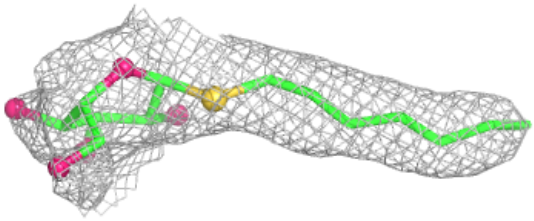


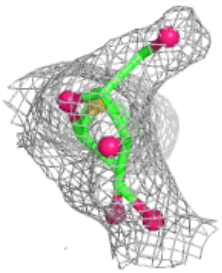


Electron density around HTG I 101:

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

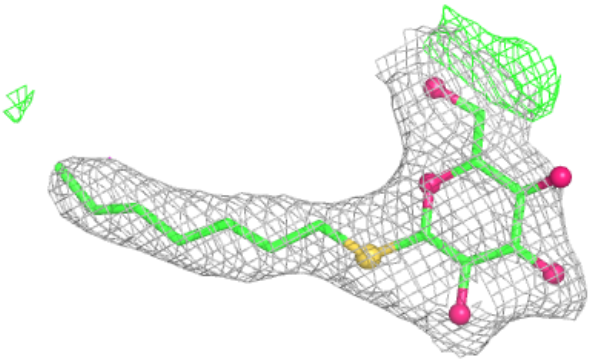


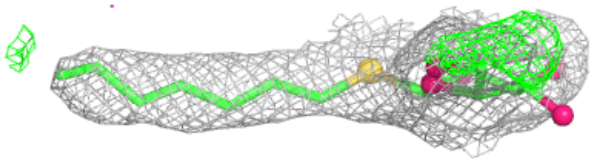


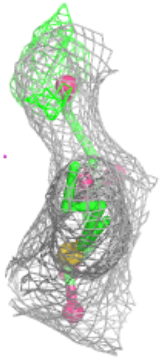


Electron density around HTG b 604:

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

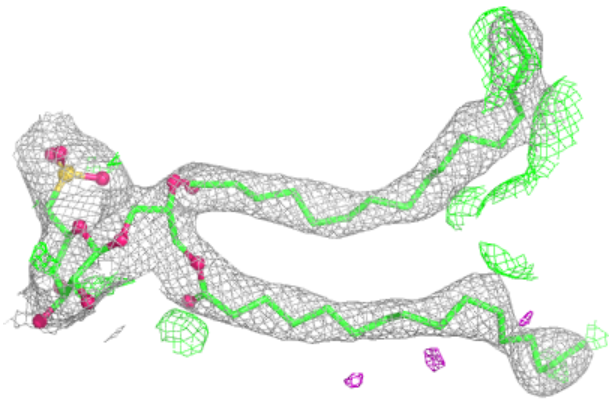


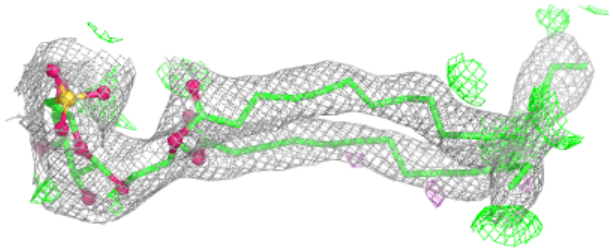


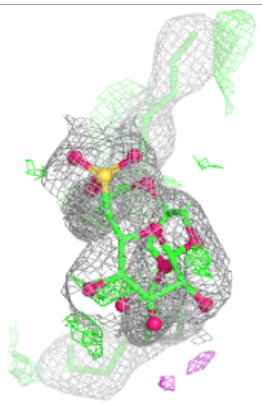


Electron density around SQD l 101:

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

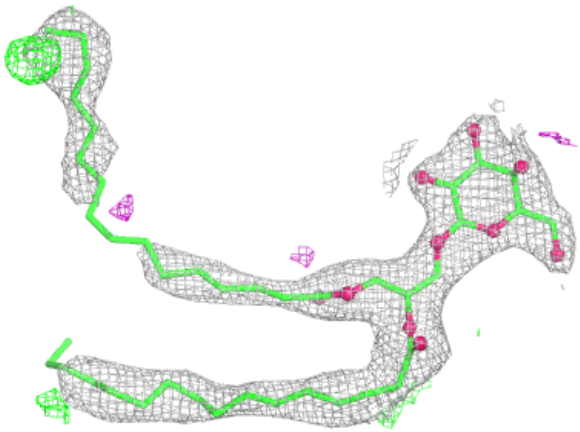


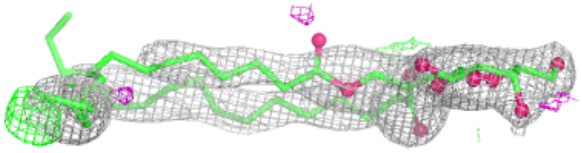


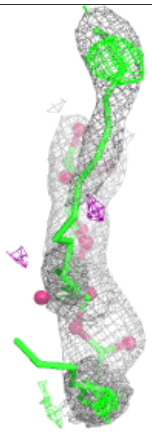


Electron density around LMG C 520:

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

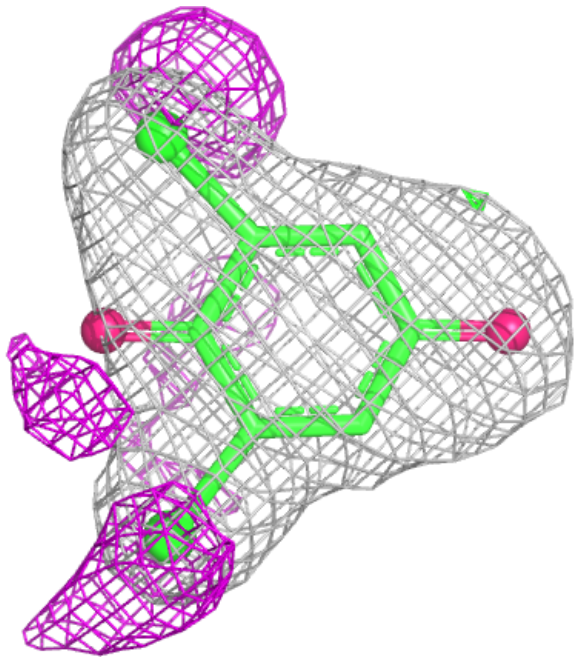


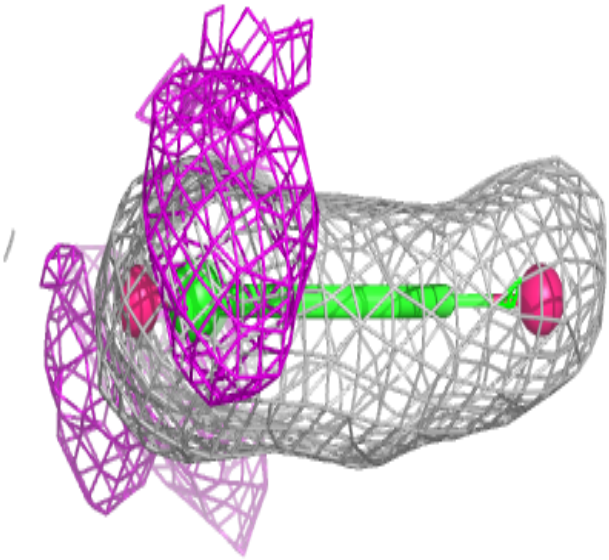


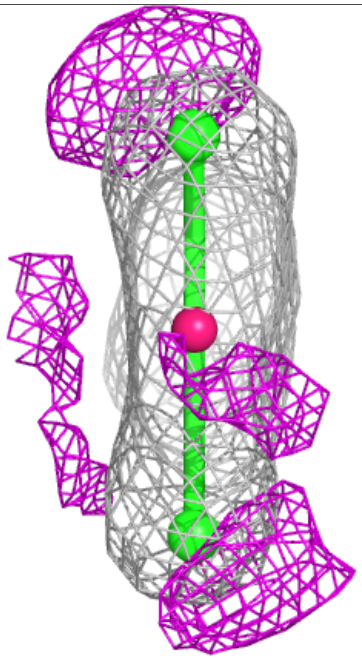


Electron density around JOX A 419:

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

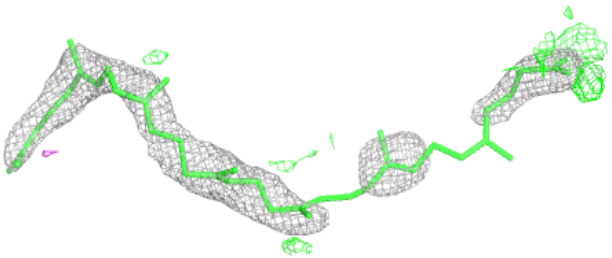


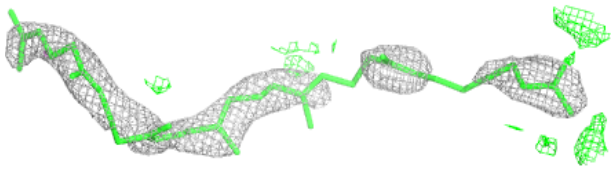


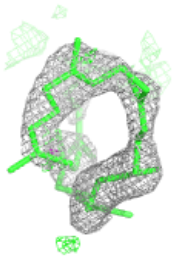


Electron density around PL9 A 422:

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

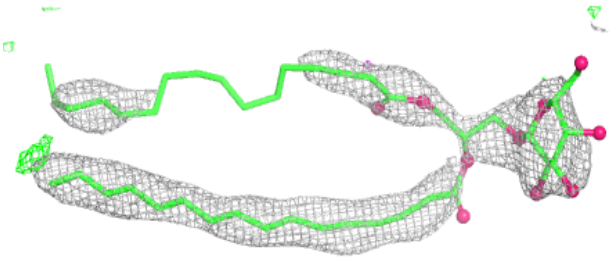


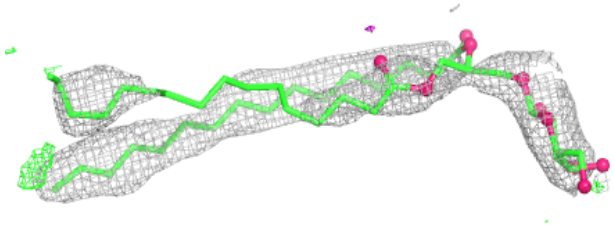


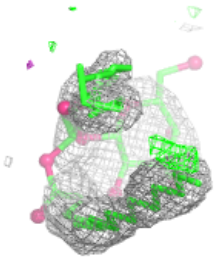


Electron density around LMG C 527:

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

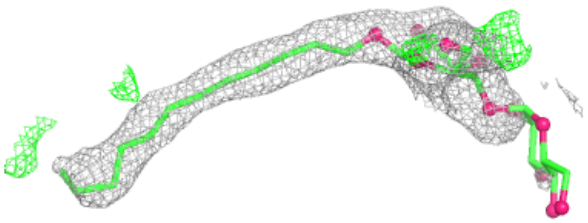


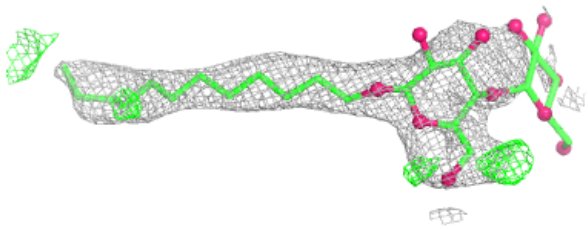


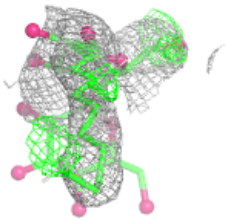


Electron density around LMT M 101:

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

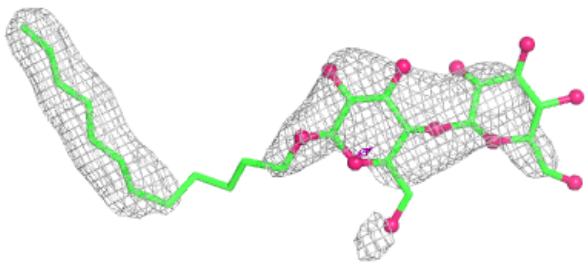


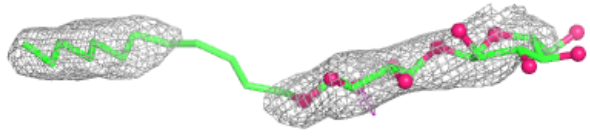


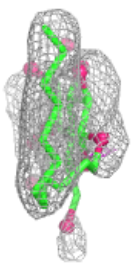


Electron density around LMT Z 101:

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

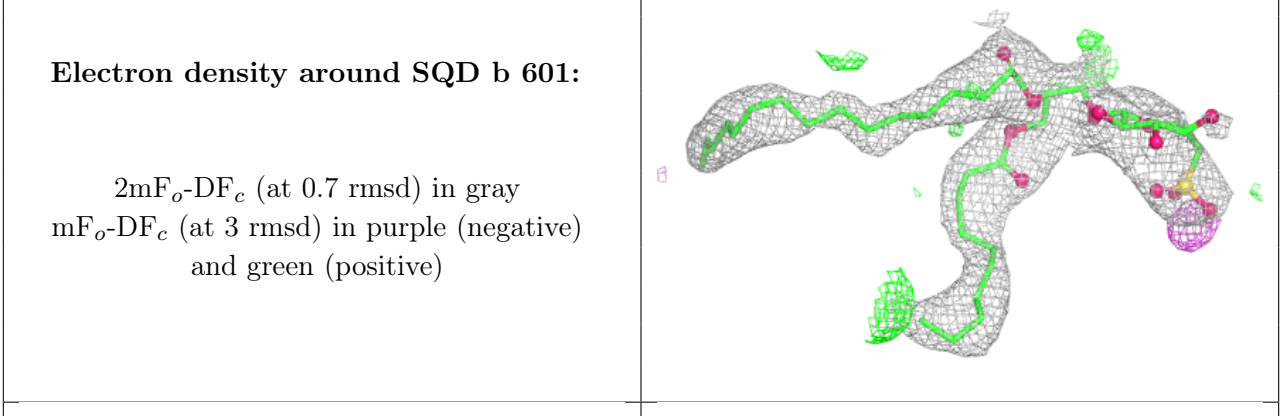






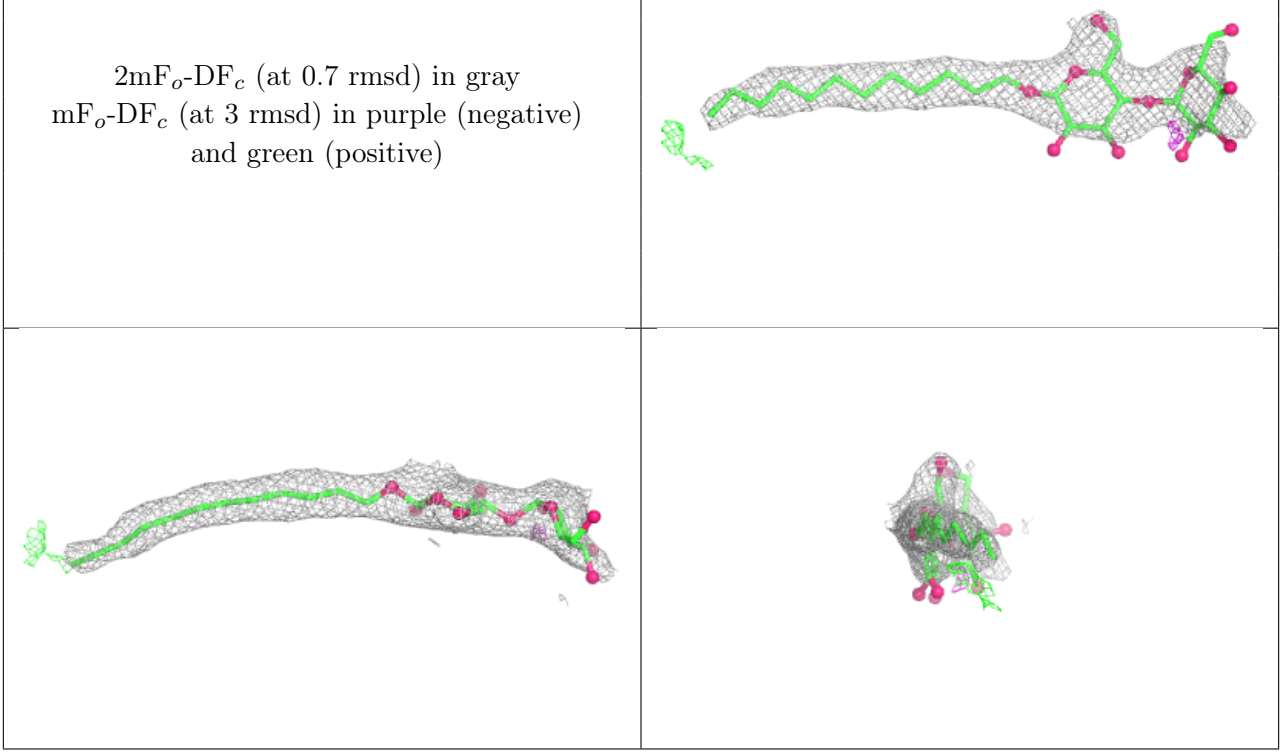
Electron density around SQD b 601:

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



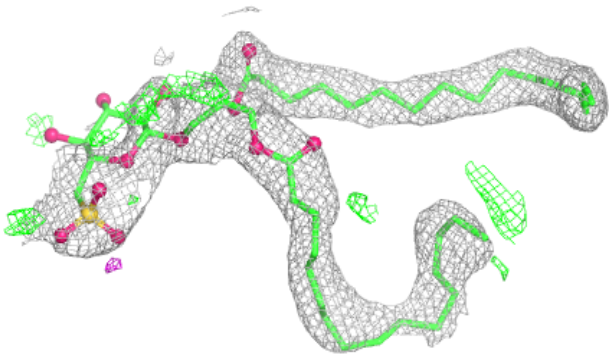
Electron density around LMT M 102:

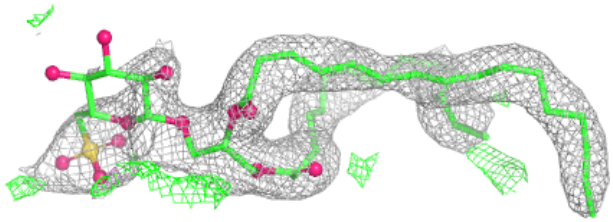
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

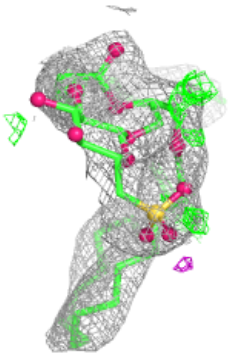


Electron density around SQD a 2603:

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

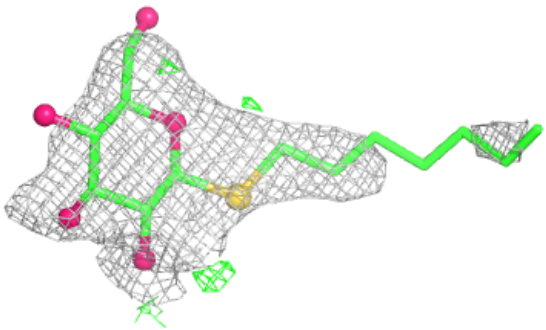


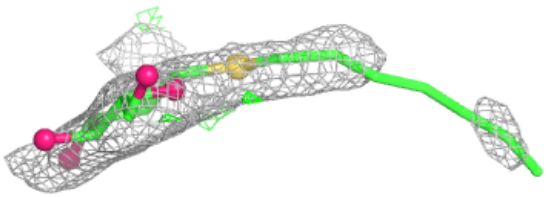


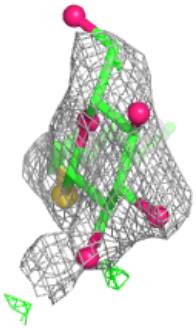


Electron density around HTG d 415:

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

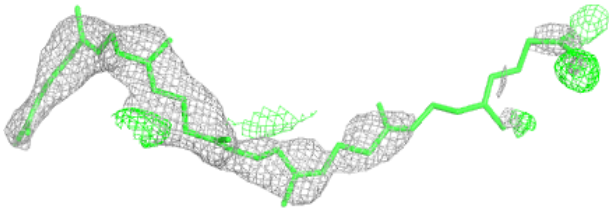


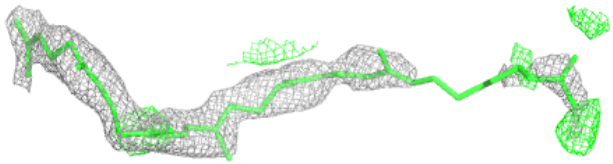


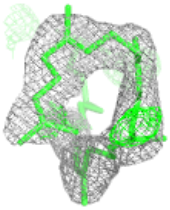


Electron density around PL9 x 1301:

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

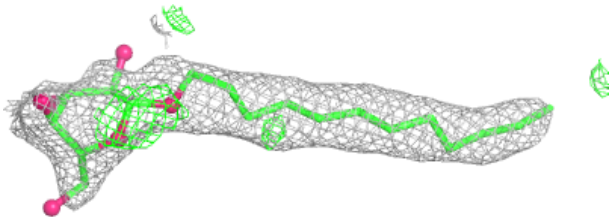


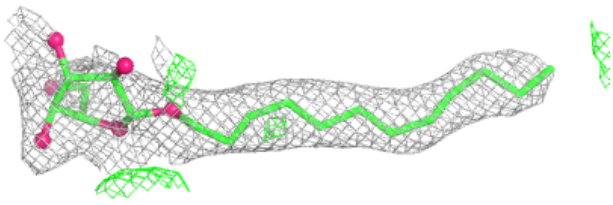


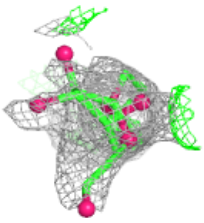


Electron density around LMT i 103:

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

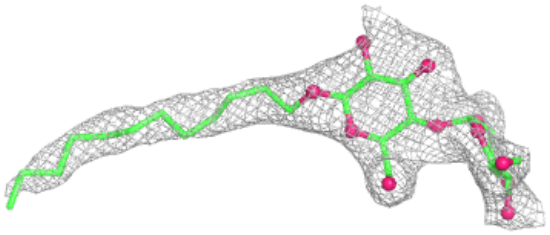


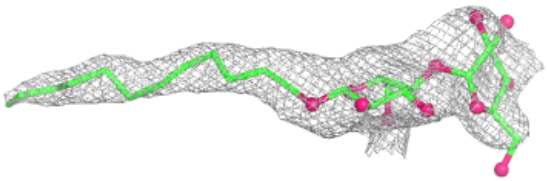


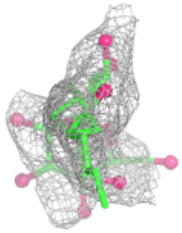


Electron density around LMT B 623:

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

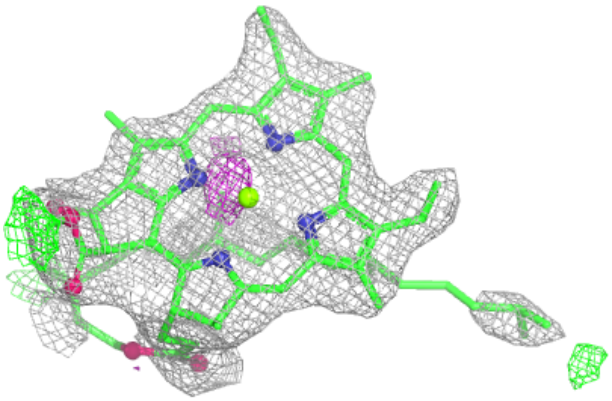


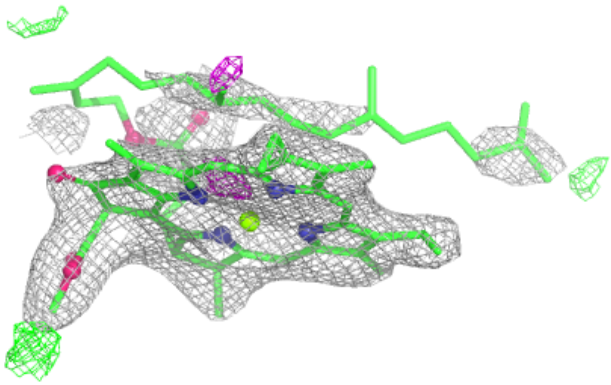


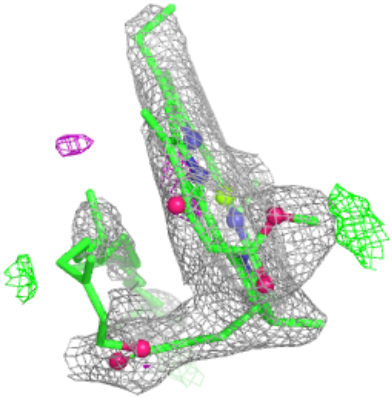


Electron density around CLA b 606:

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

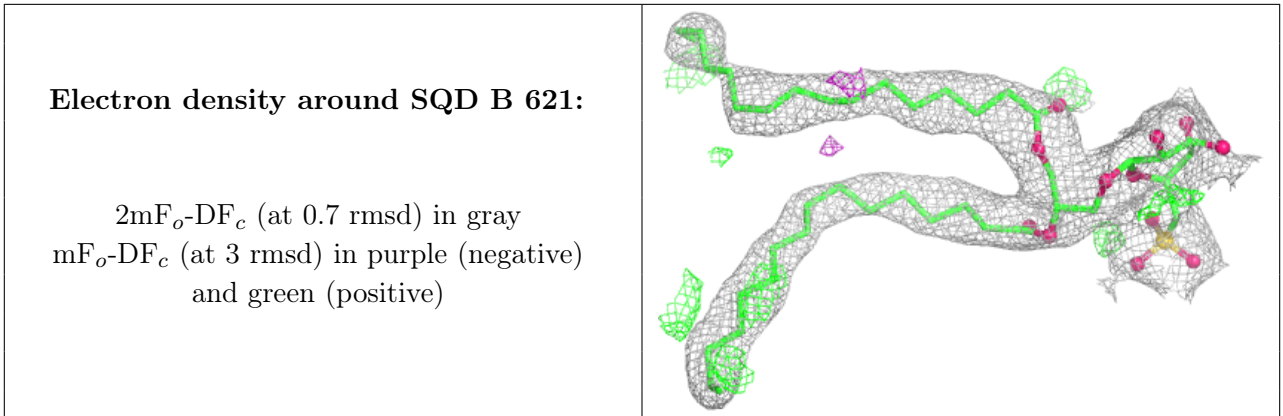






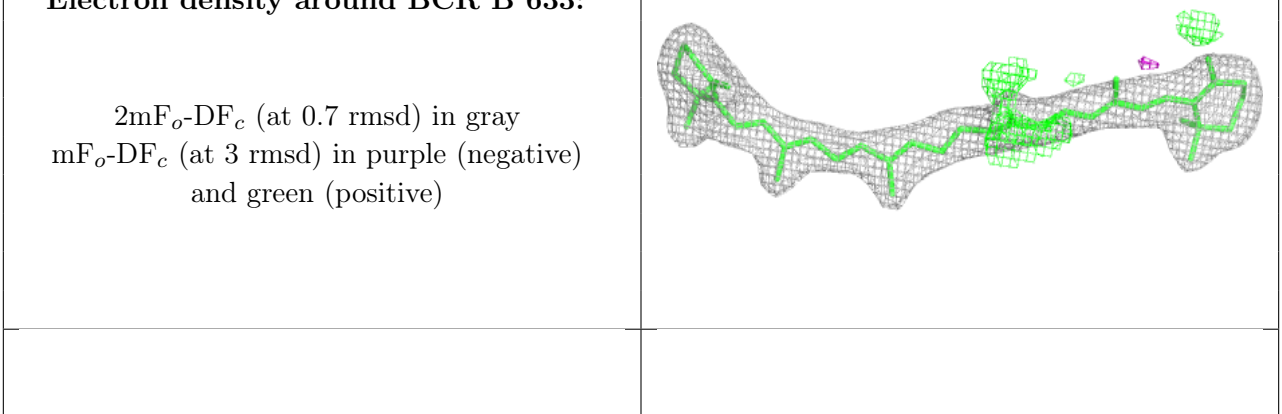
Electron density around SQD B 621:

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



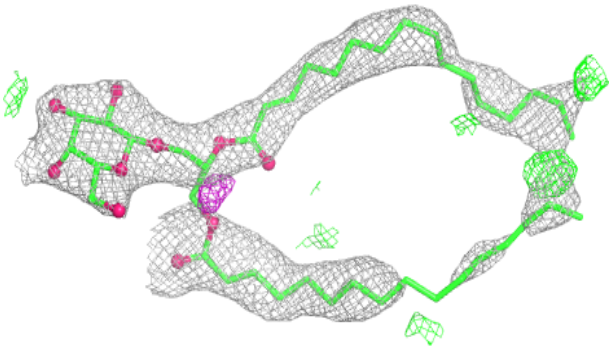
Electron density around BCR B 633:

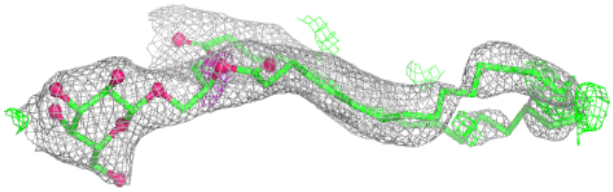
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

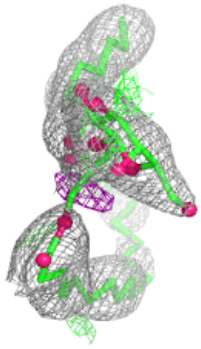


Electron density around LMG c 501:

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

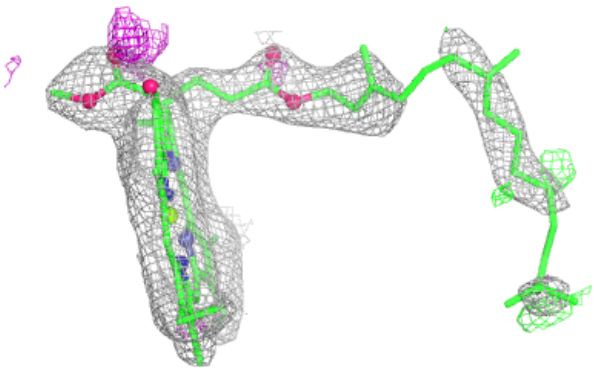


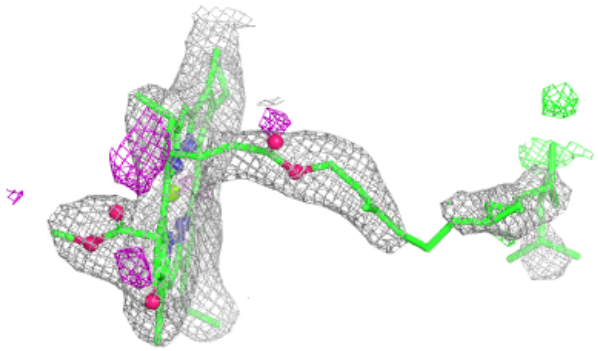


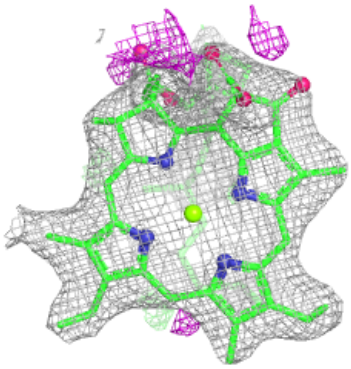


Electron density around CLA C 507:

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

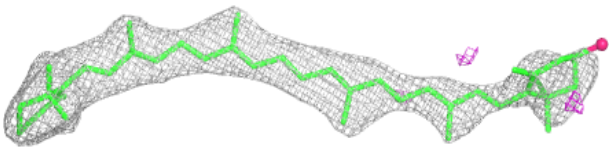


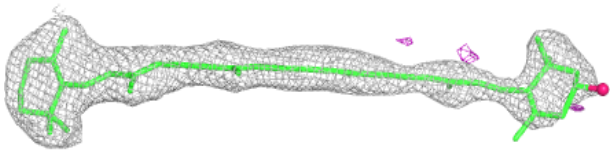


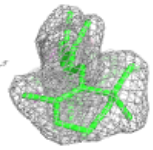


Electron density around RRX h 101:

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

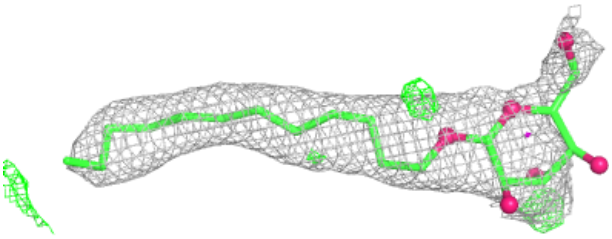


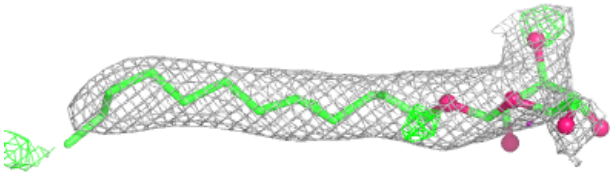


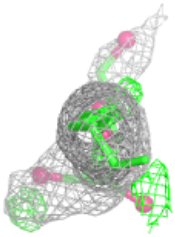


Electron density around LMT A 420:

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

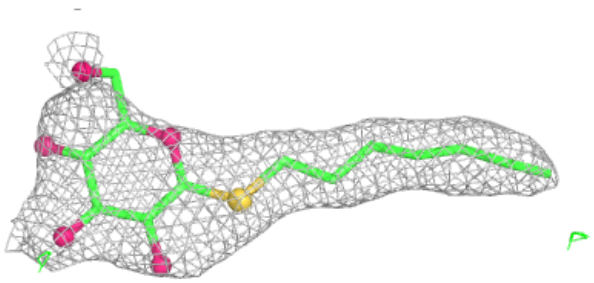


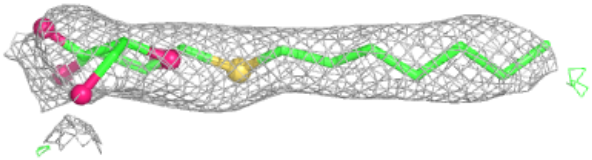


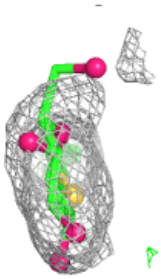


Electron density around HTG B 626:

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

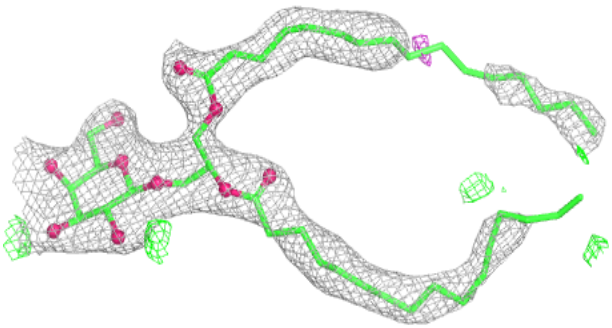


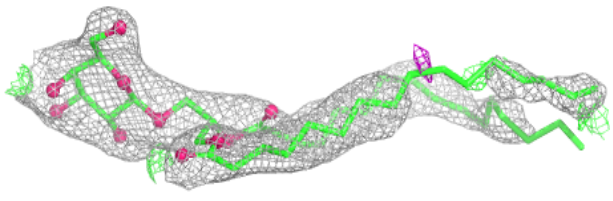


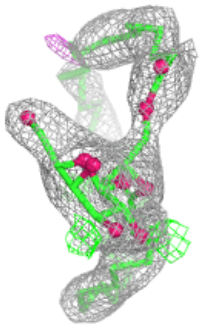


Electron density around LMG A 413:

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

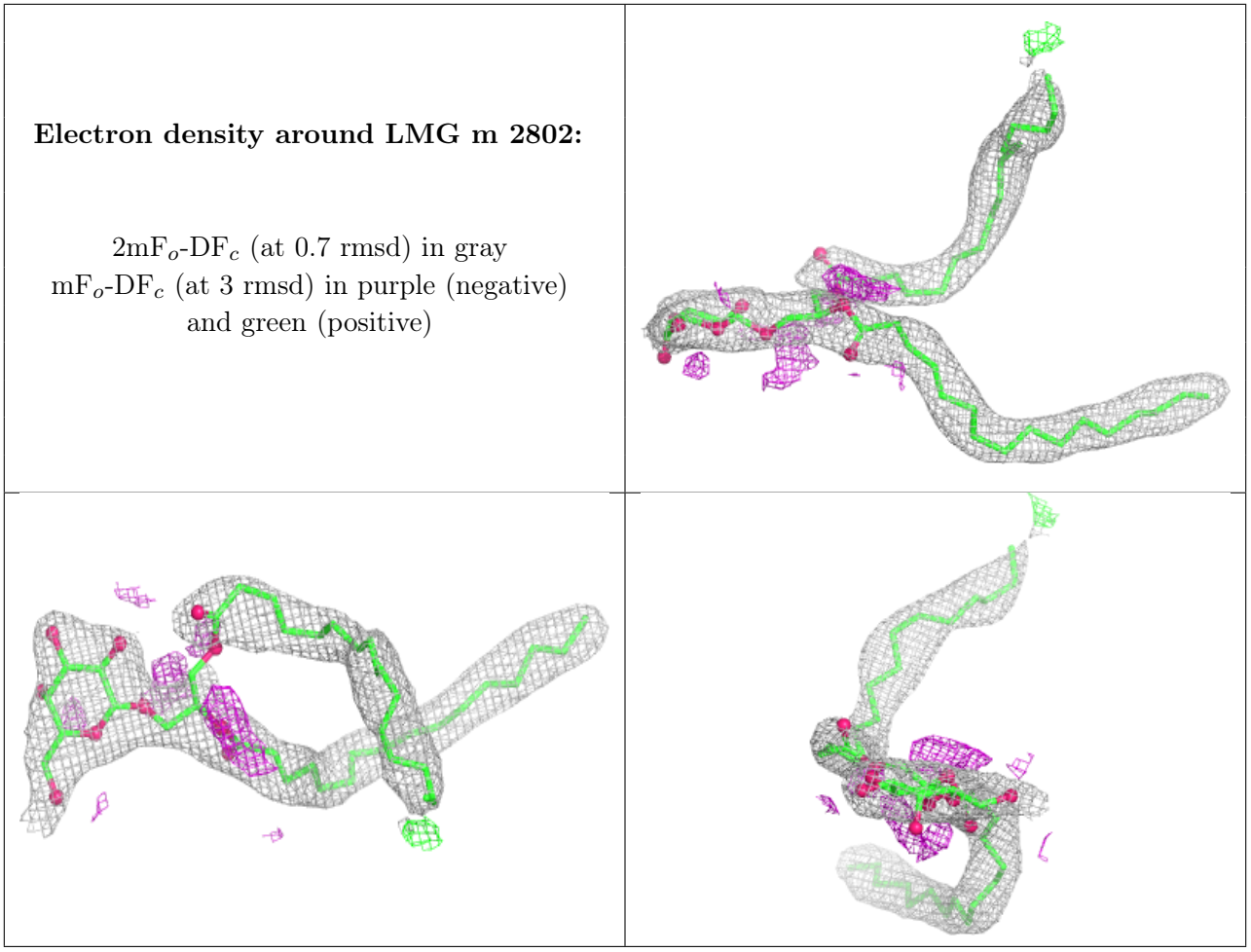






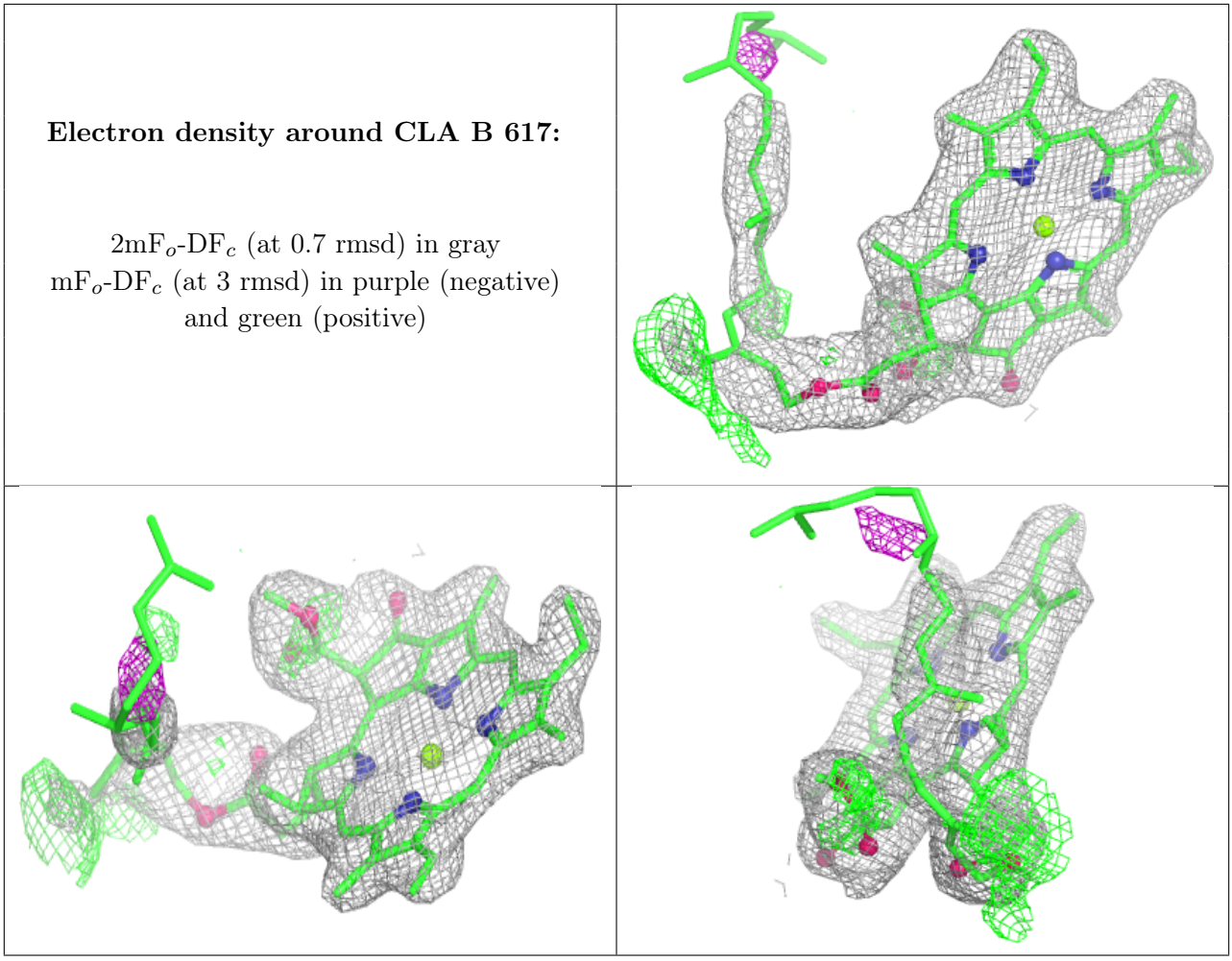
Electron density around LMG m 2802:

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



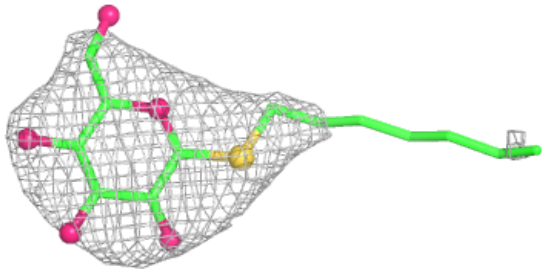
Electron density around CLA B 617:

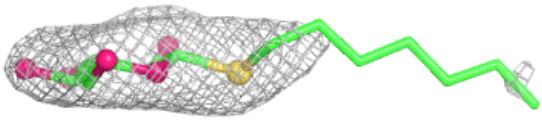
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

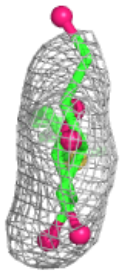


Electron density around HTG C 521:

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

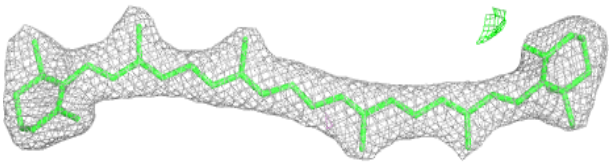


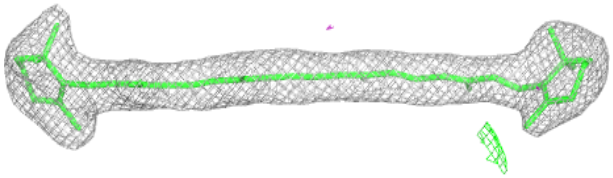


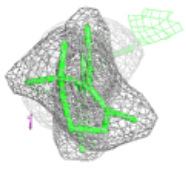


Electron density around BCR b 623:

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

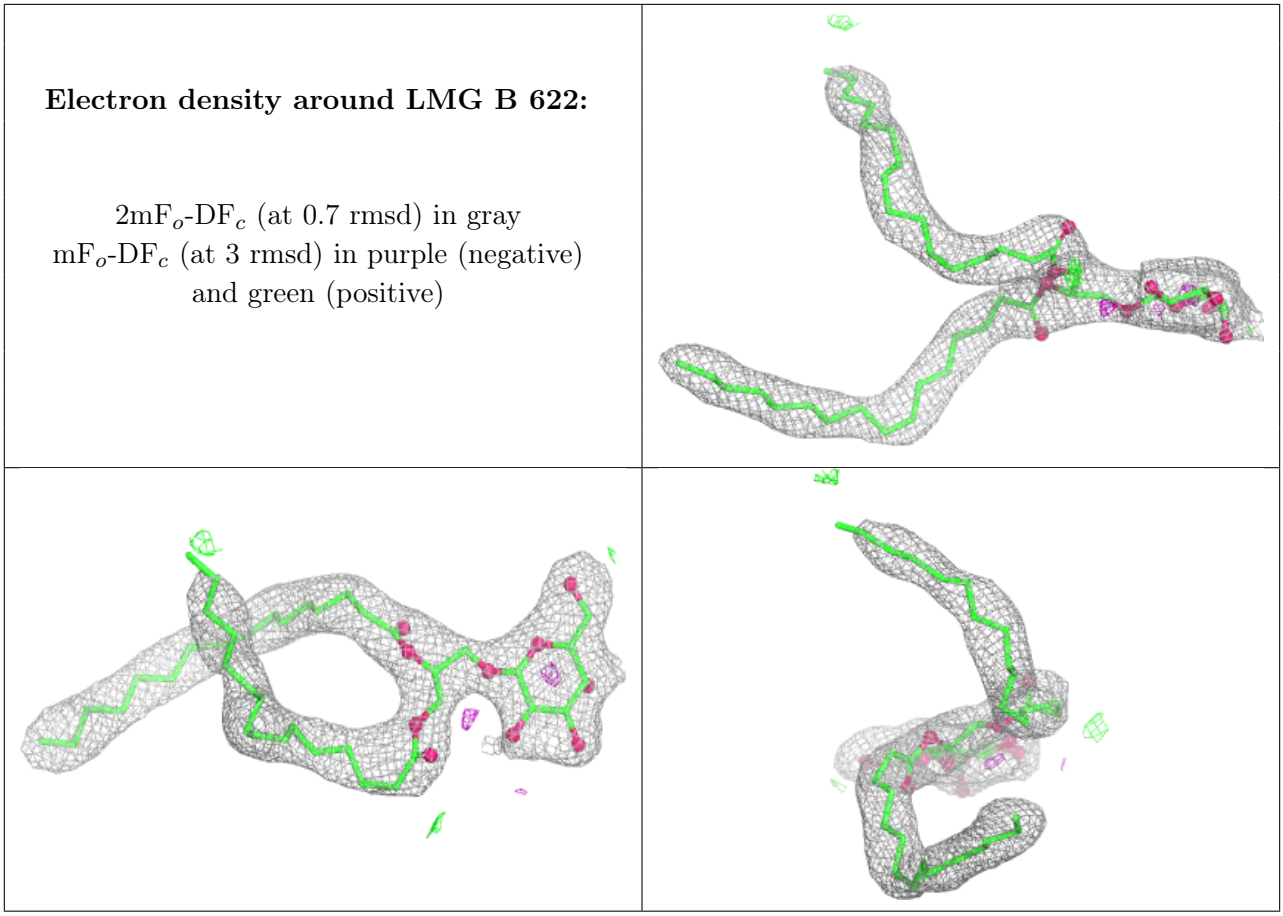






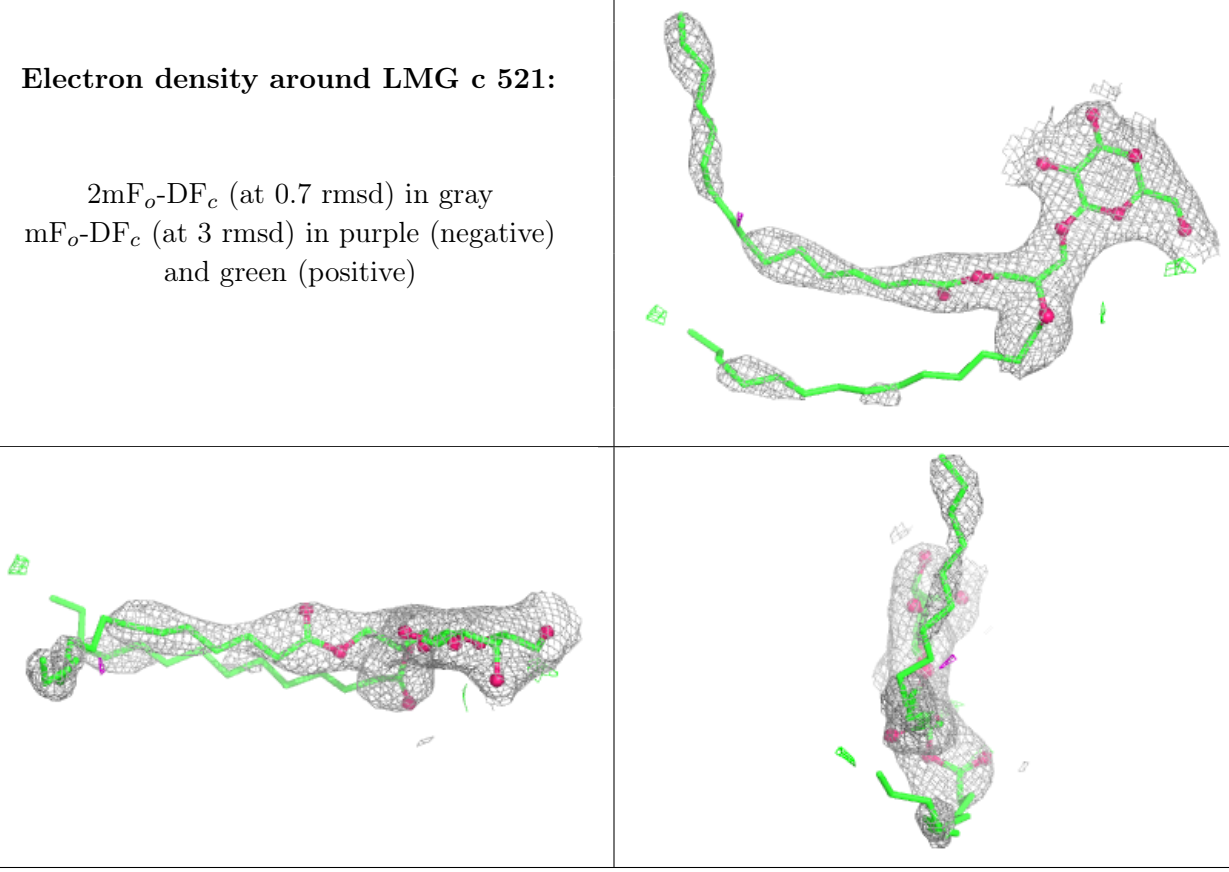
Electron density around LMG B 622:

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



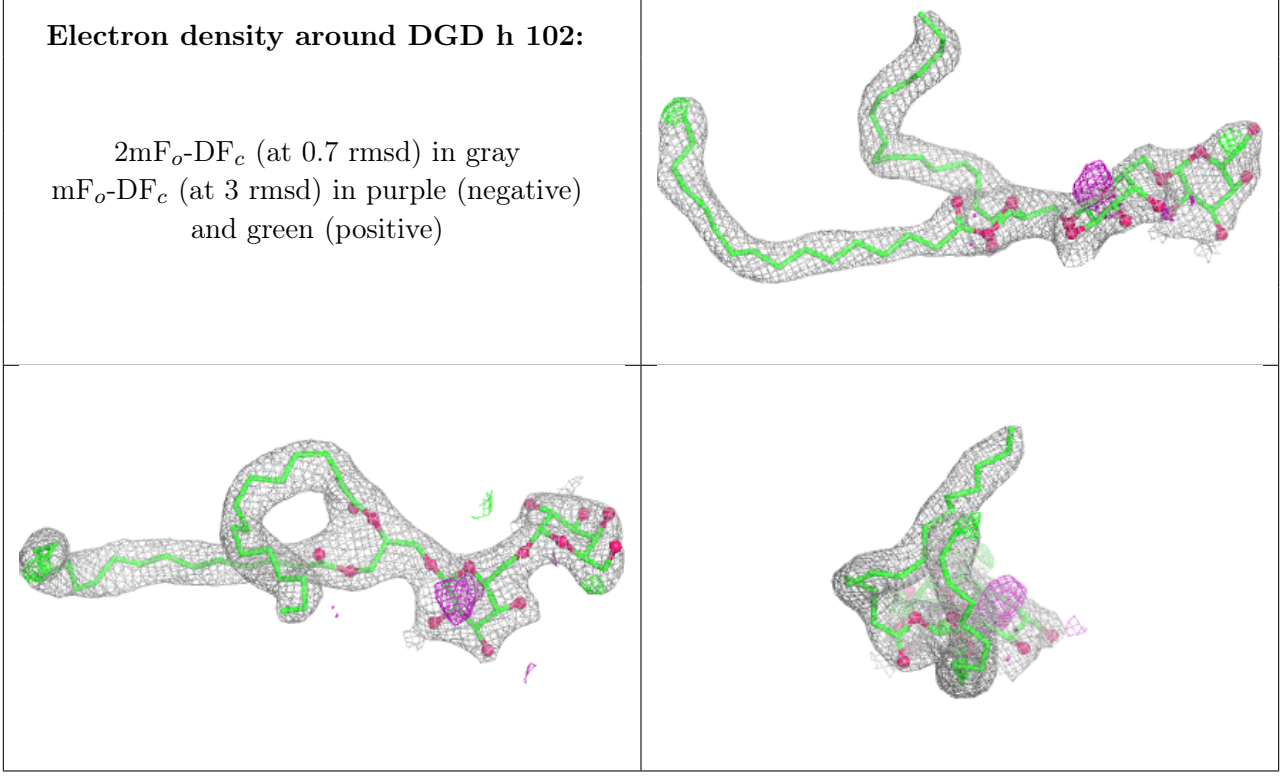
Electron density around LMG c 521:

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



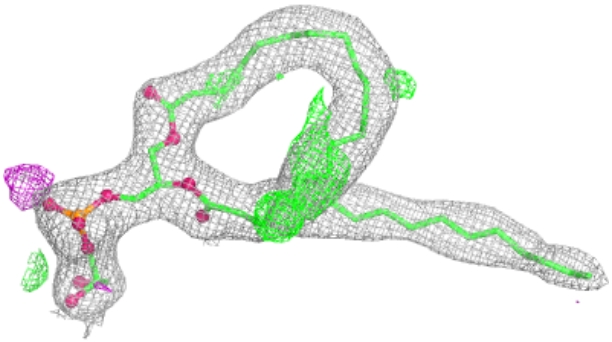
Electron density around DGD h 102:

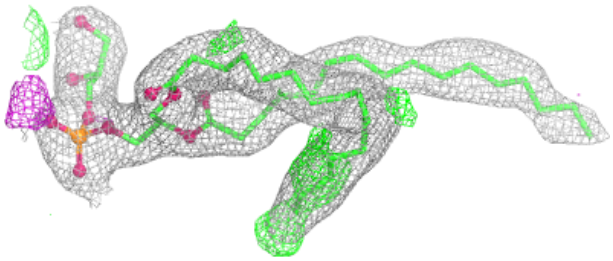
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG D 2309:

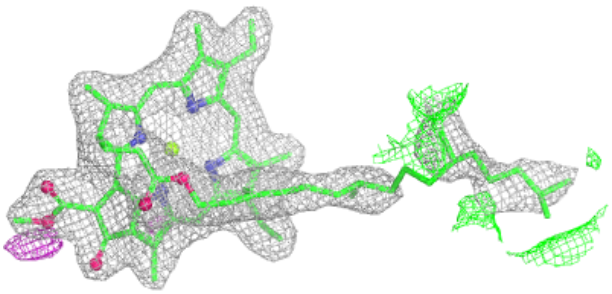
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

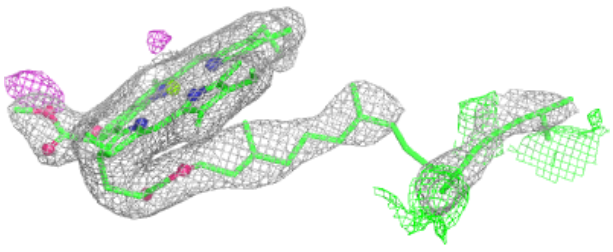


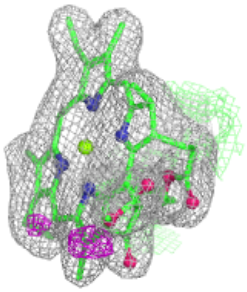


Electron density around CLA b 619:

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

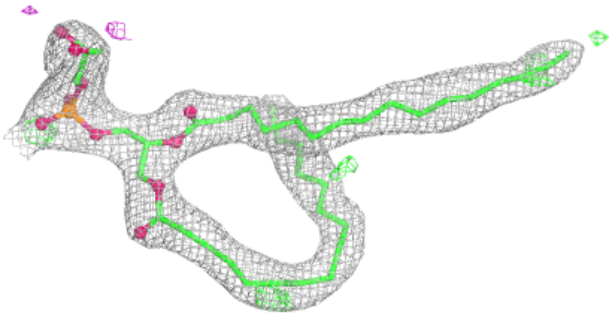


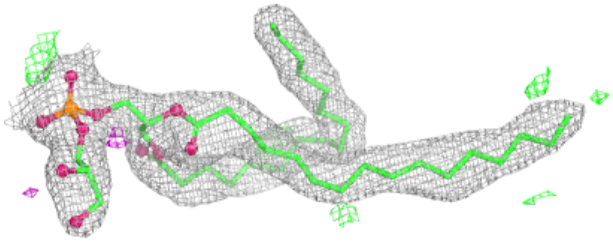


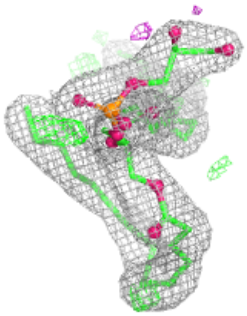


Electron density around LHG d 412:

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

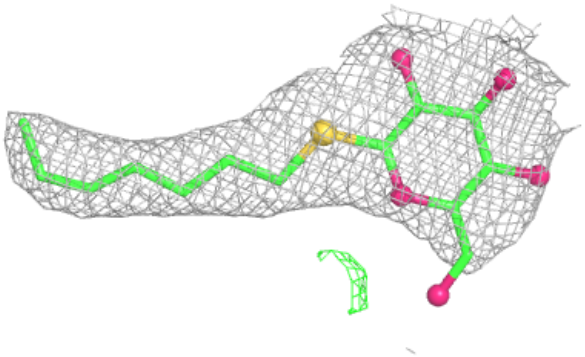


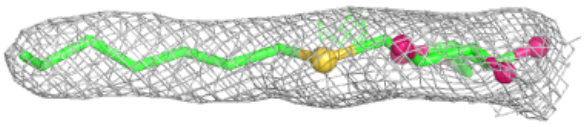


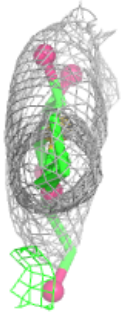


Electron density around HTG b 603:

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

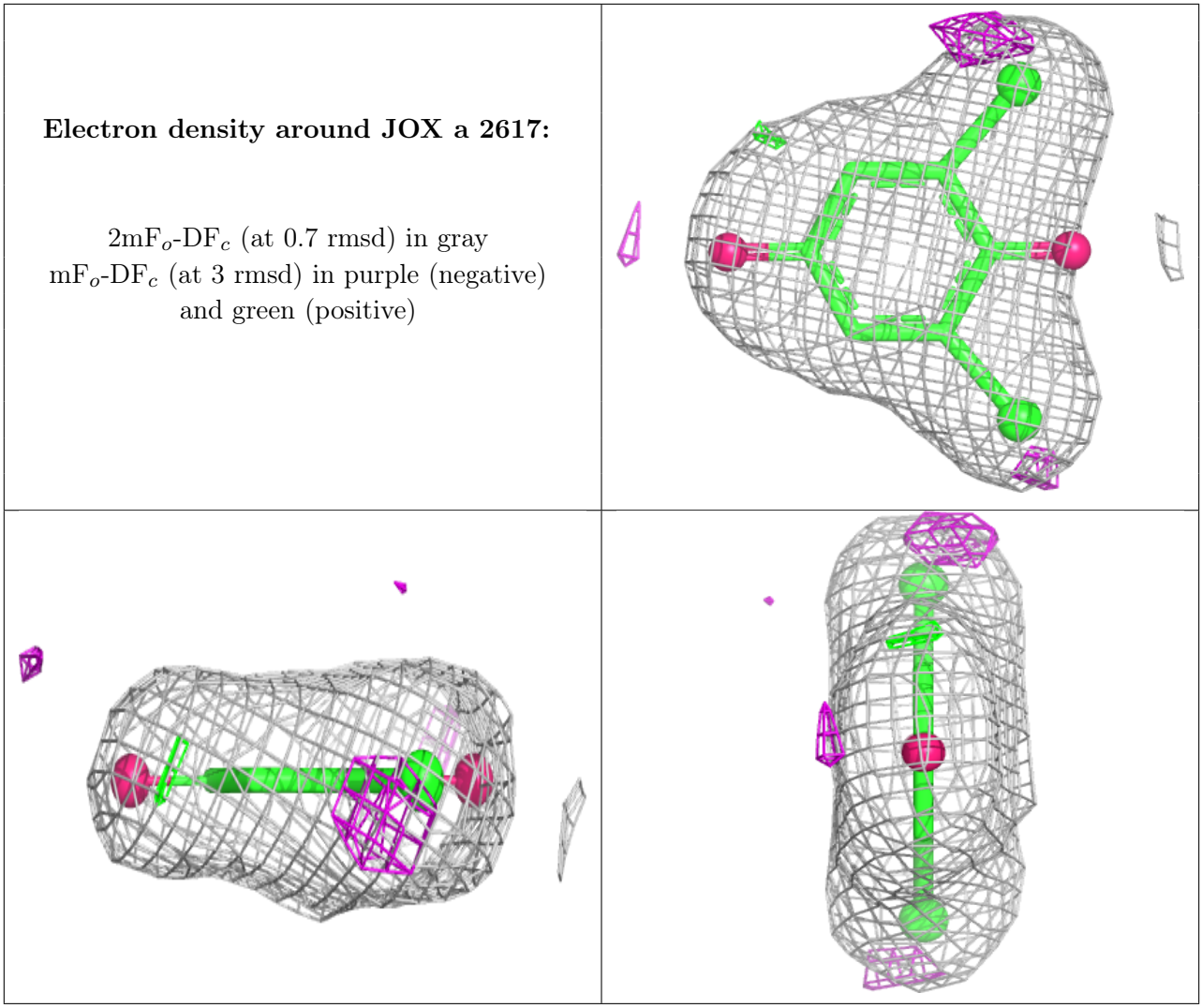






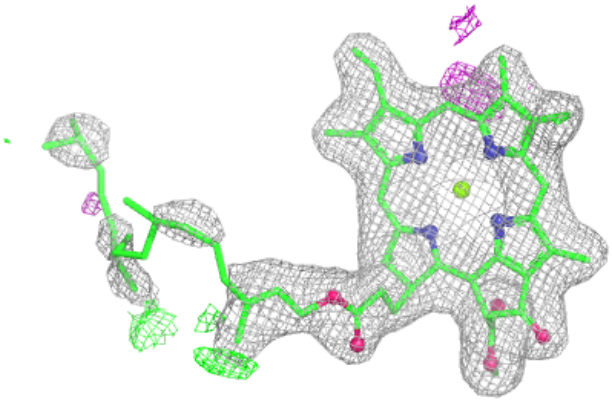
Electron density around JOX a 2617:

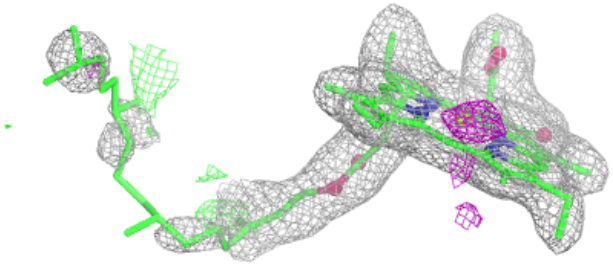
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

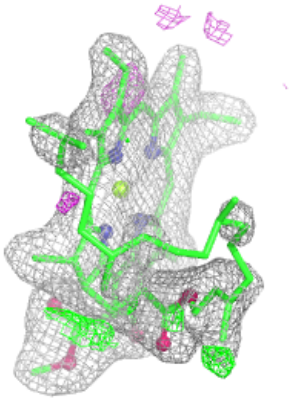


Electron density around CLA a 2613:

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

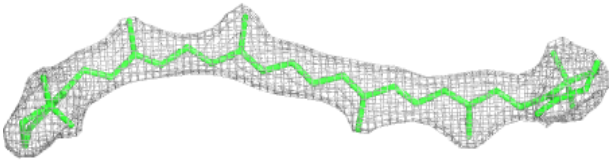


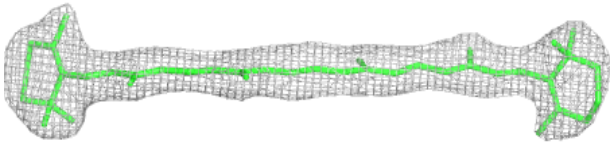


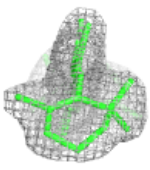


Electron density around BCR C 516:

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

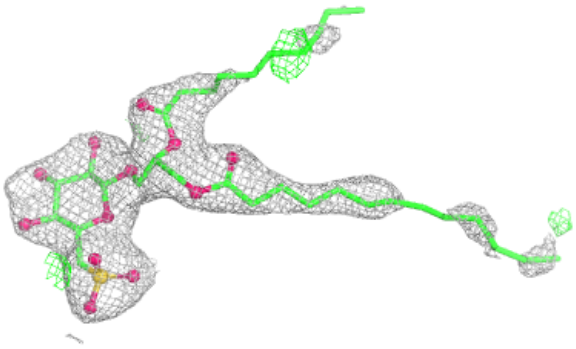


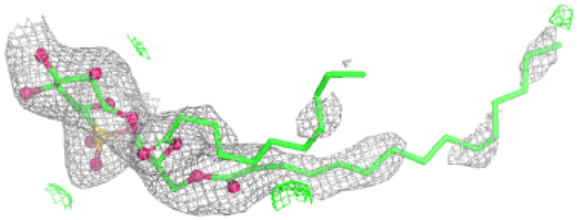


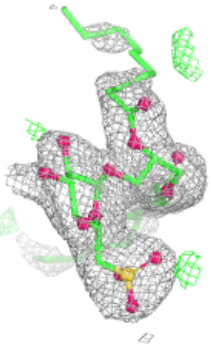


Electron density around SQD a 2615:

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

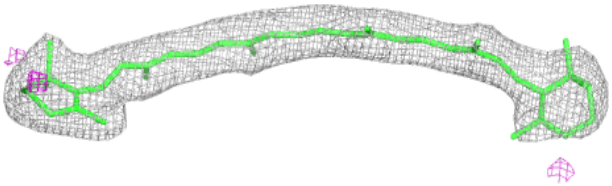


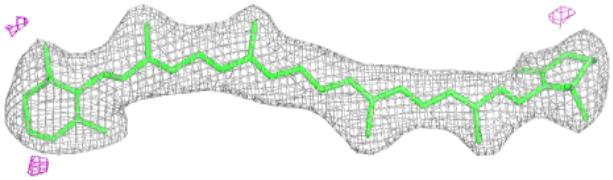


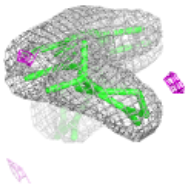


Electron density around BCR D 2305:

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

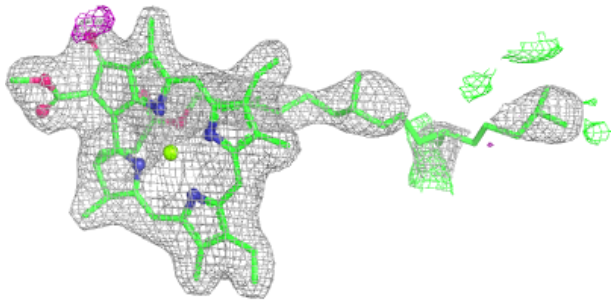


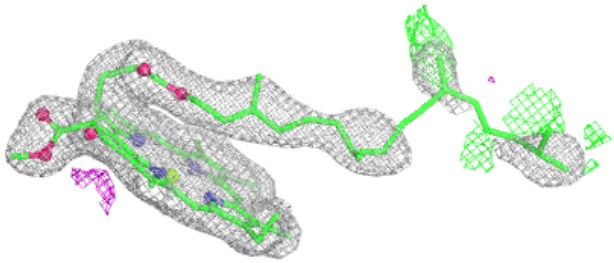


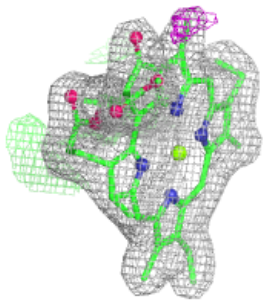


Electron density around CLA B 615:

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

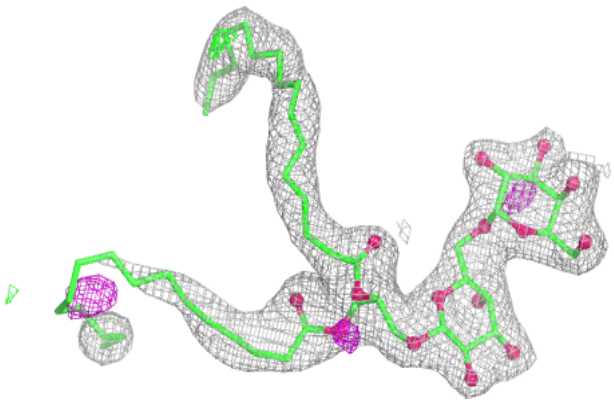


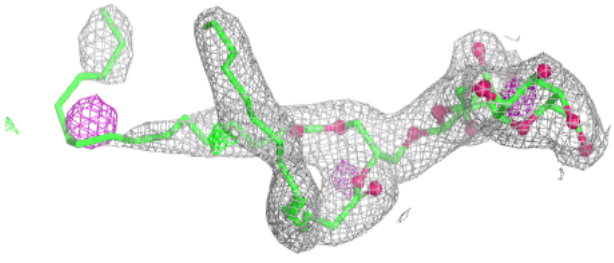


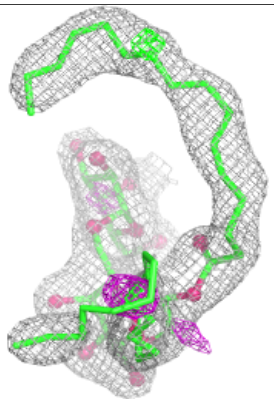


Electron density around DGD C 518:

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

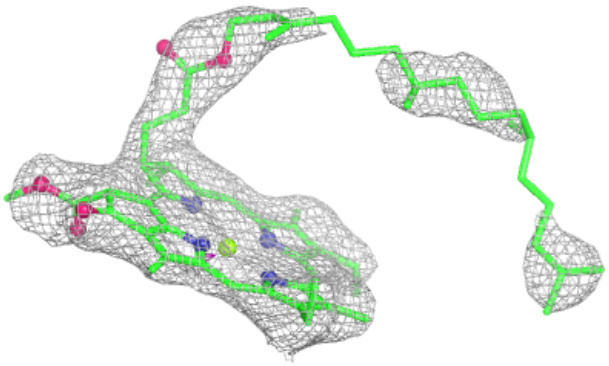


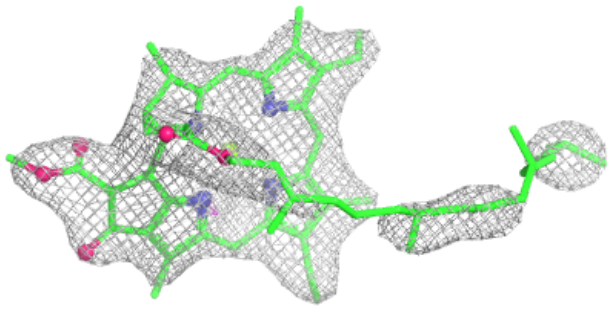


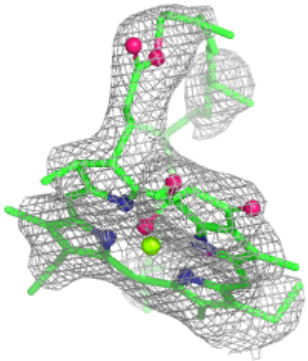


Electron density around CLA C 514:

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

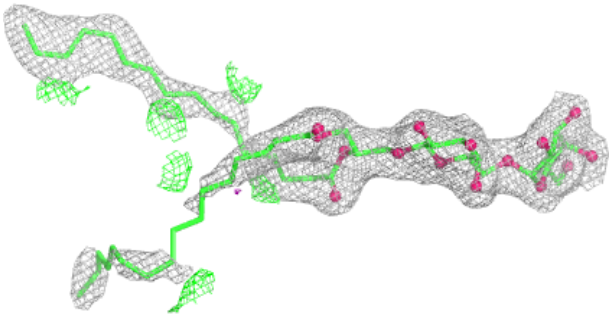


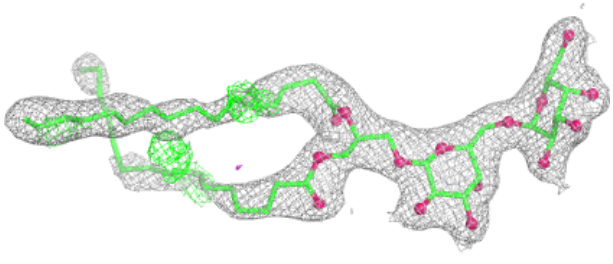


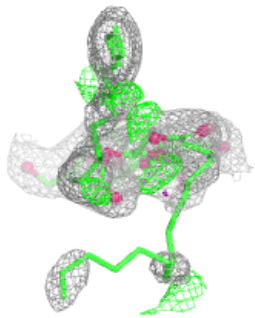


Electron density around DGD c 518:

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

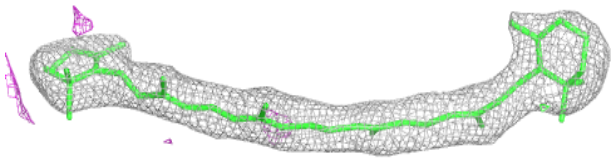


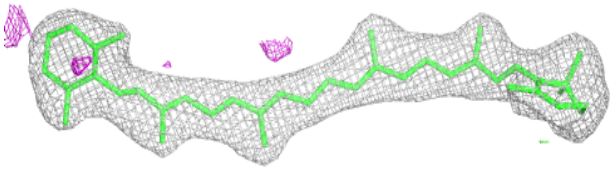


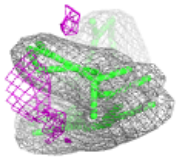


Electron density around BCR d 410:

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

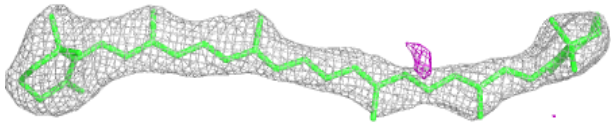


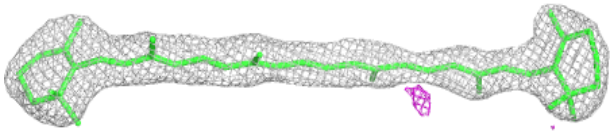


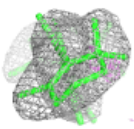


Electron density around BCR z 101:

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

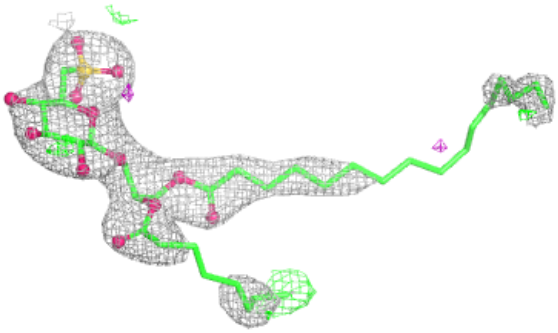


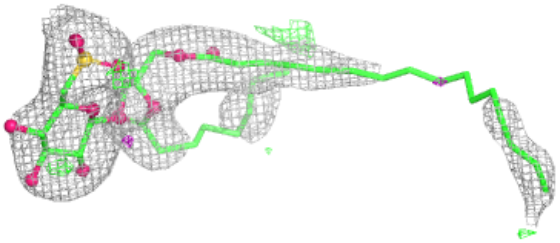


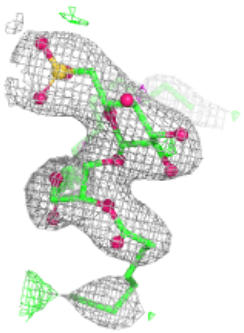


Electron density around SQD A 412:

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

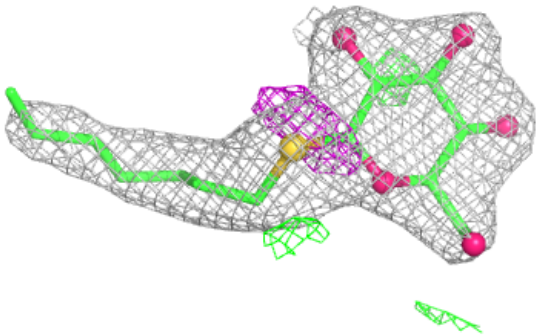


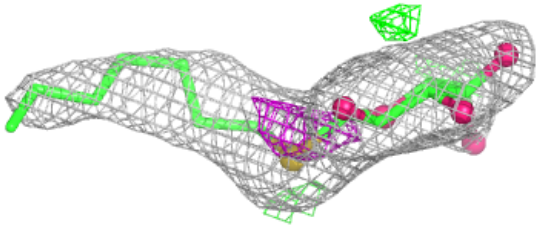


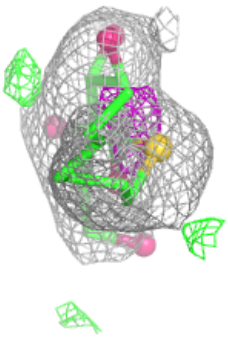


Electron density around HTG b 602:

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

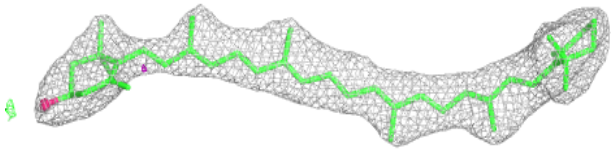


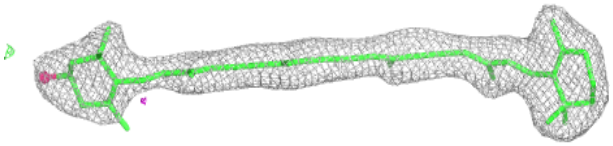


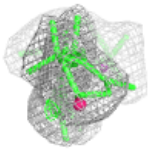


Electron density around RRX H 102:

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

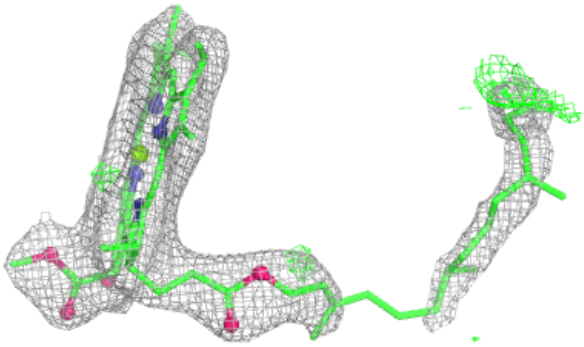


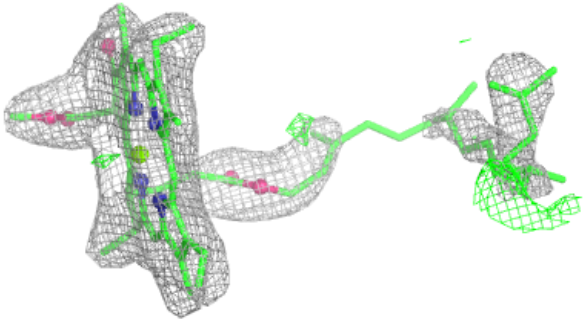


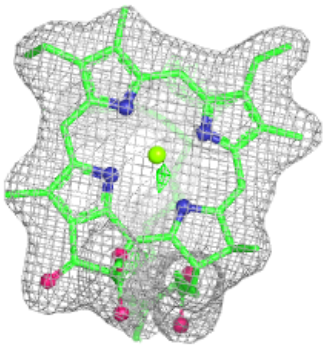


Electron density around CLA c 509:

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

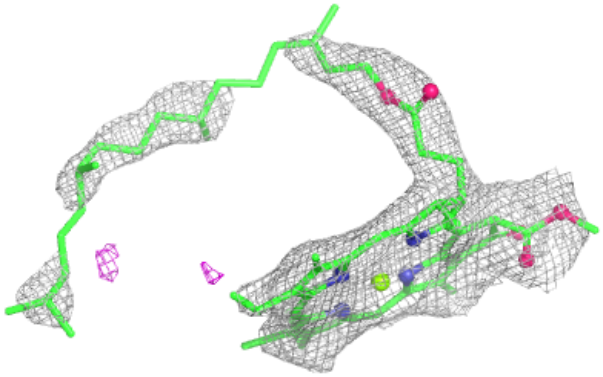


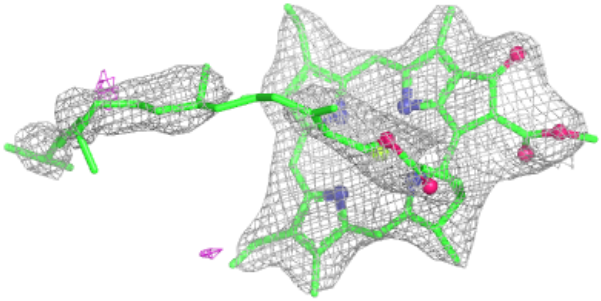


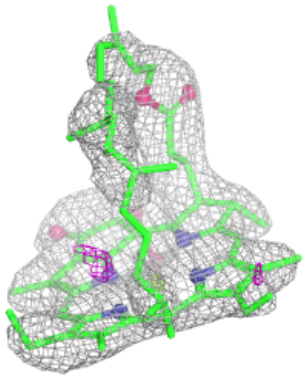


Electron density around CLA c 516:

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

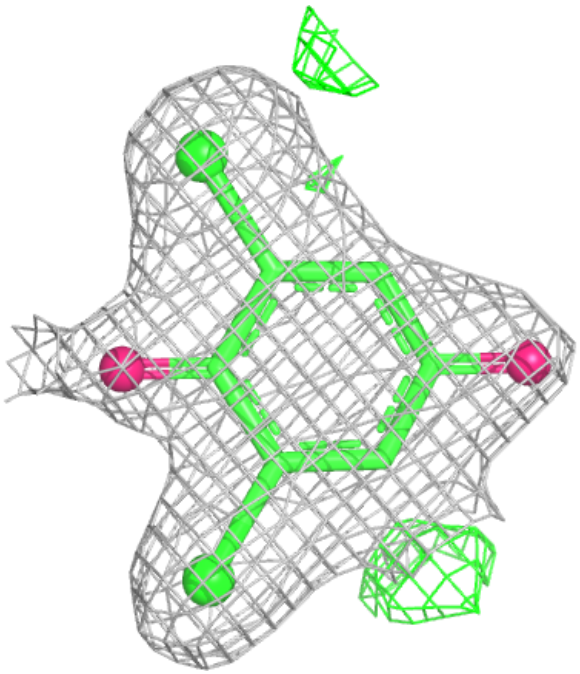


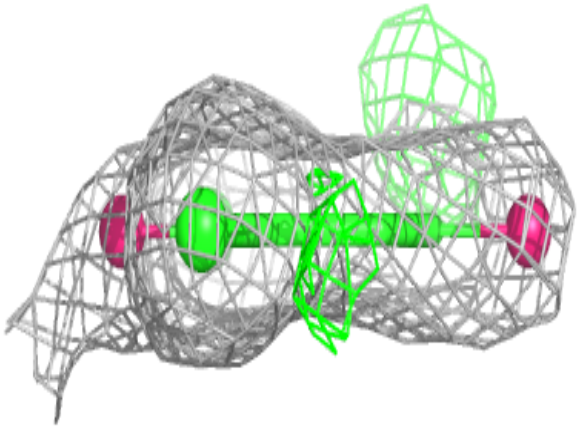


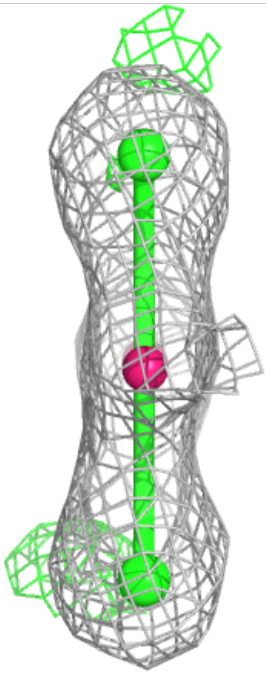


Electron density around JOX a 2619:

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

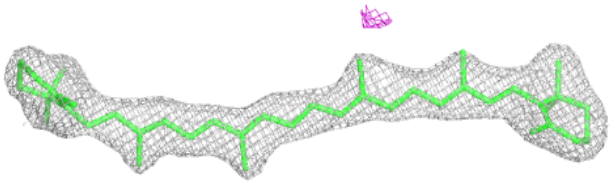


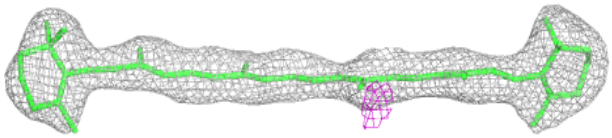


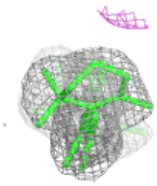


Electron density around BCR C 515:

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

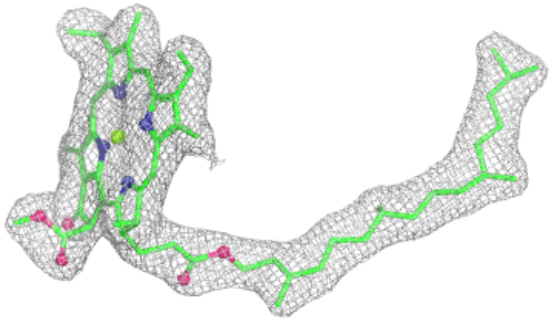


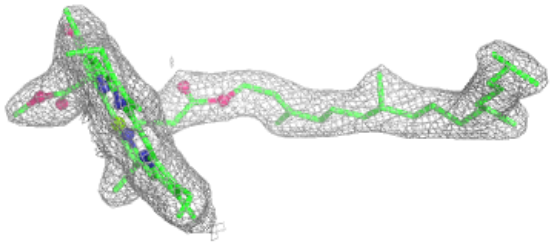


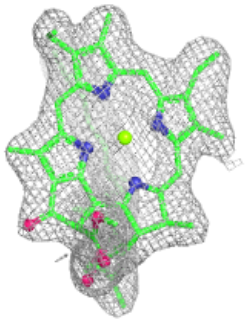


Electron density around CLA B 610:

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

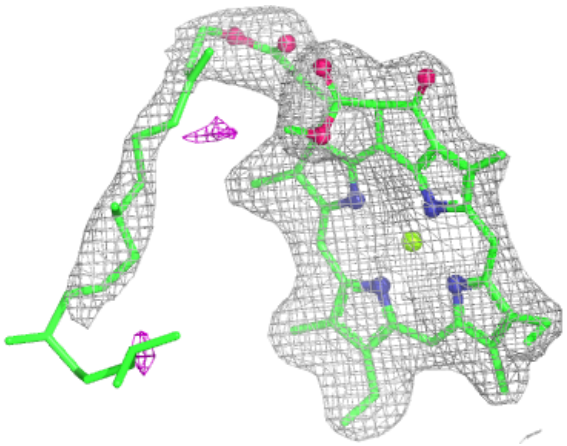


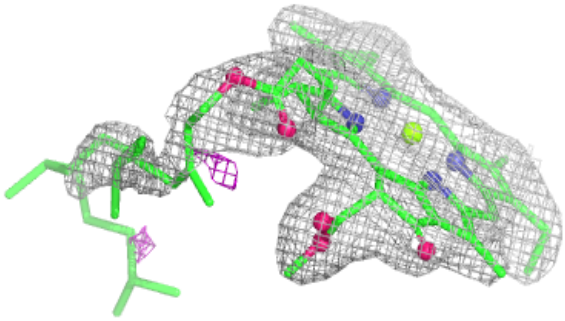


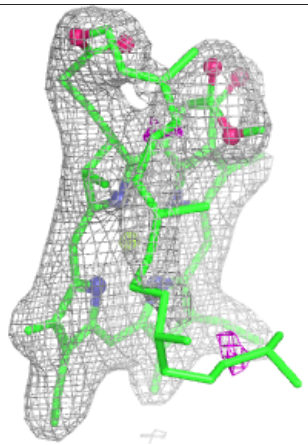


Electron density around CLA b 621:

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

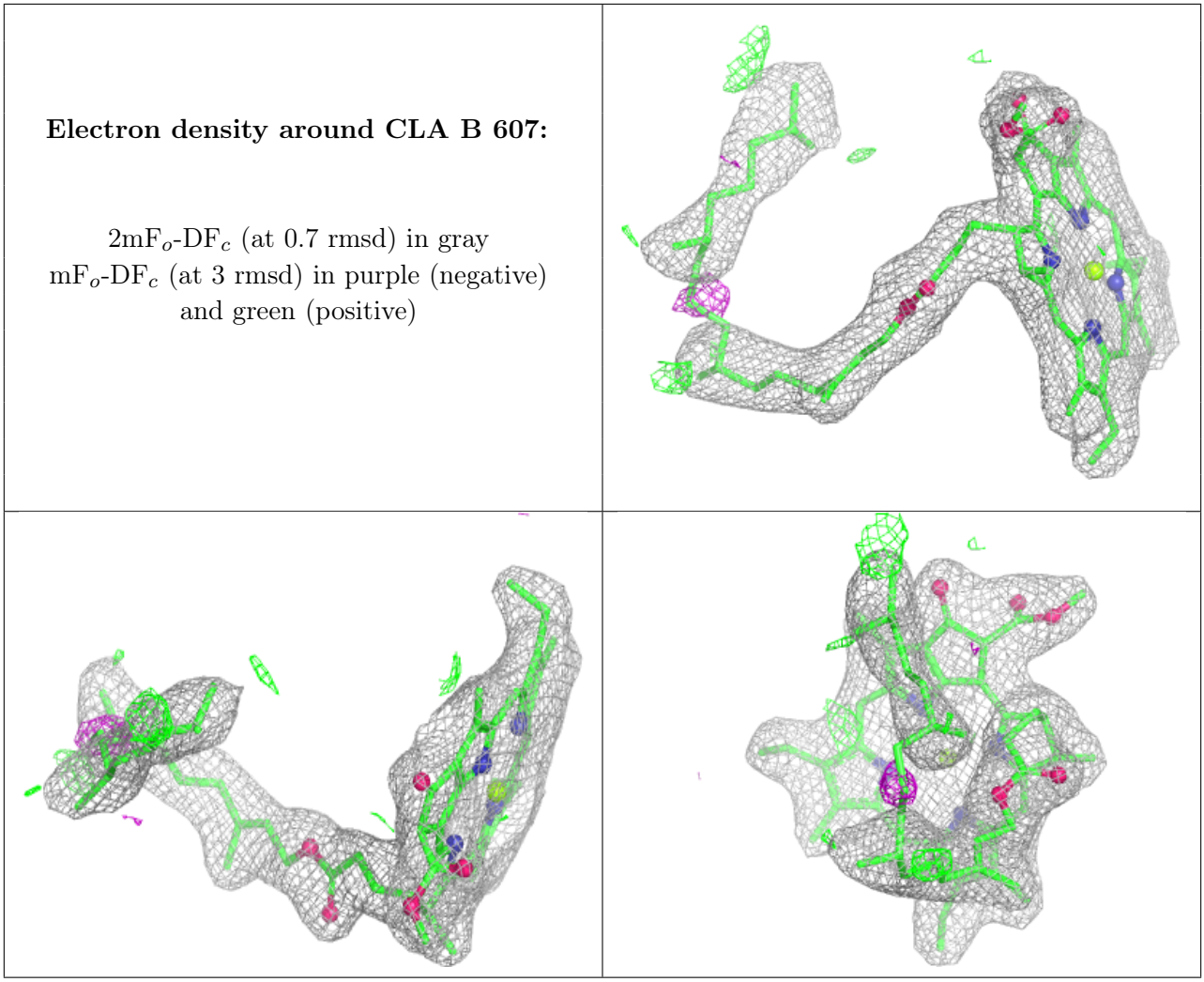






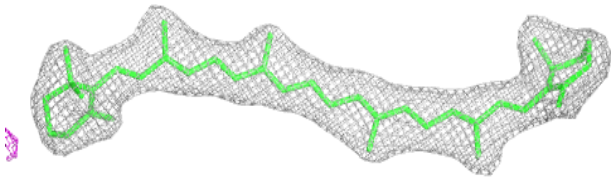
Electron density around CLA B 607:

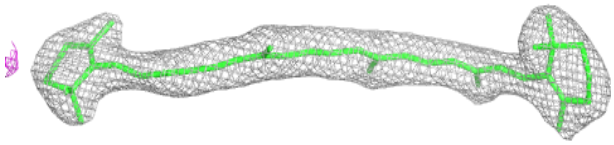
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

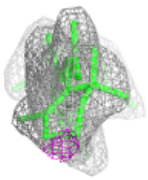


Electron density around BCR Y 302:

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

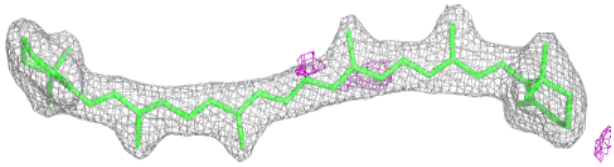


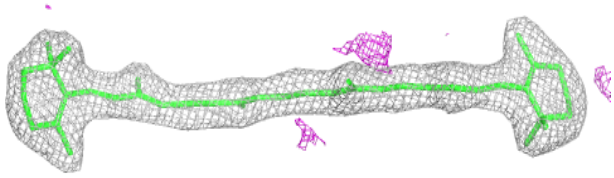


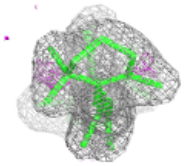


Electron density around BCR a 2614:

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

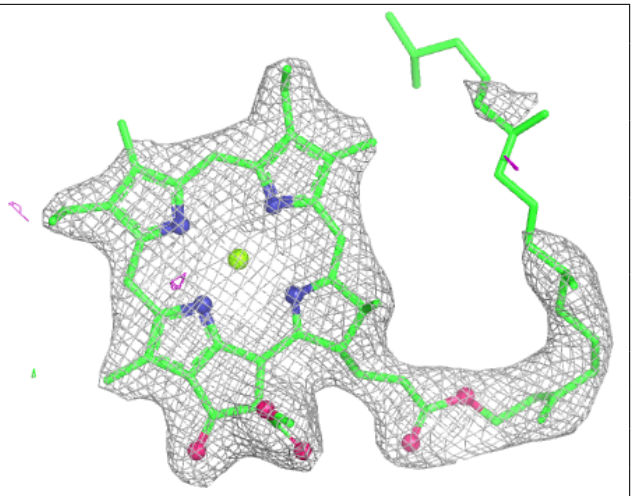


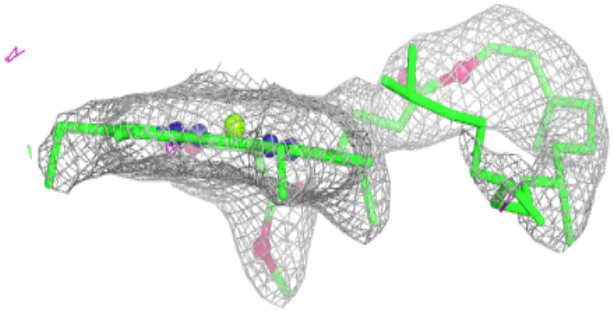


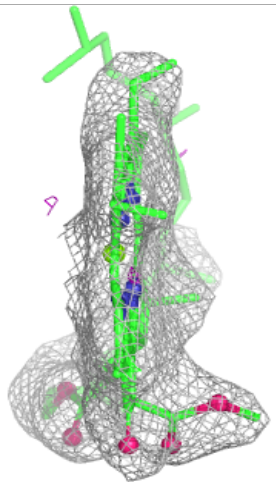


Electron density around CLA c 515:

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

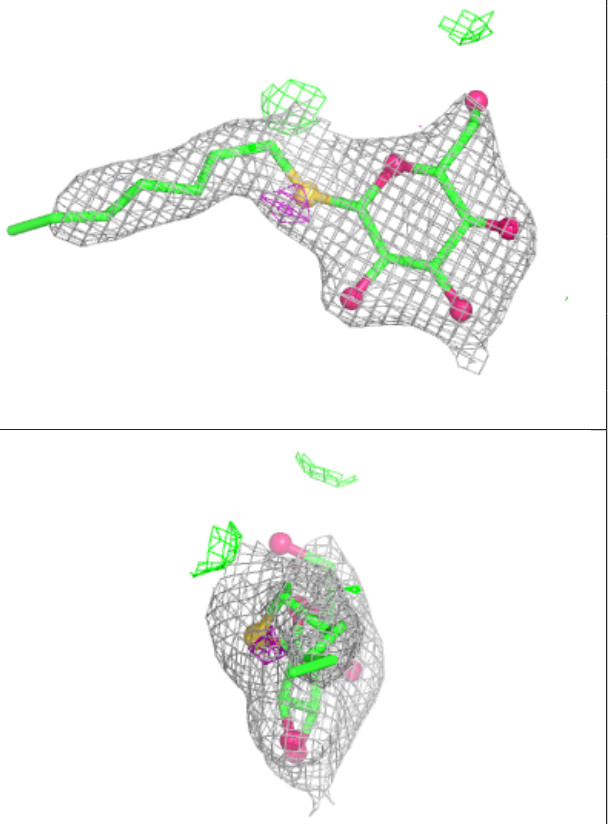






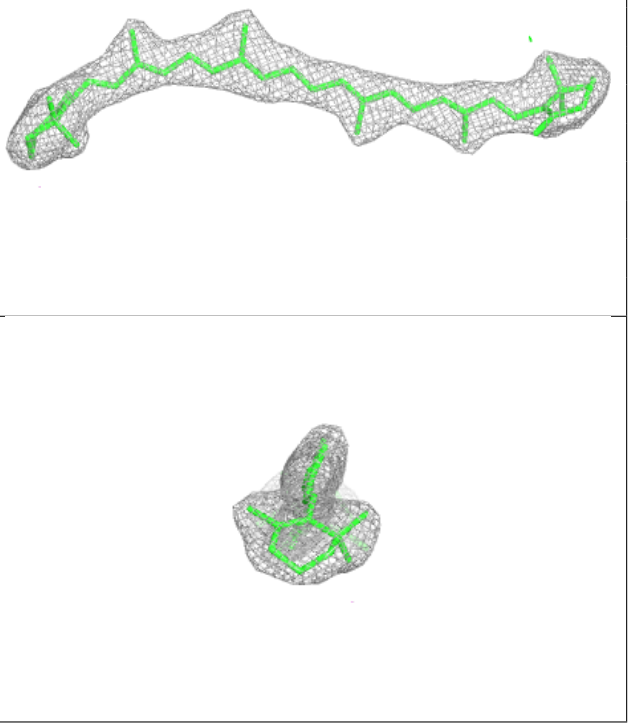
Electron density around HTG o 301:

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



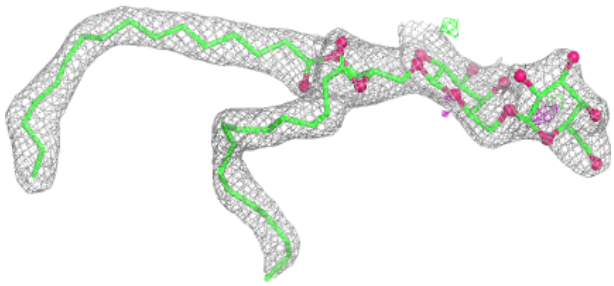
Electron density around BCR c 517:

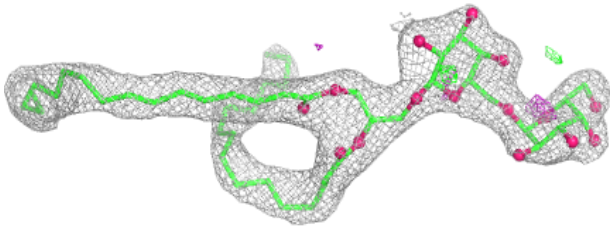
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD H 103:

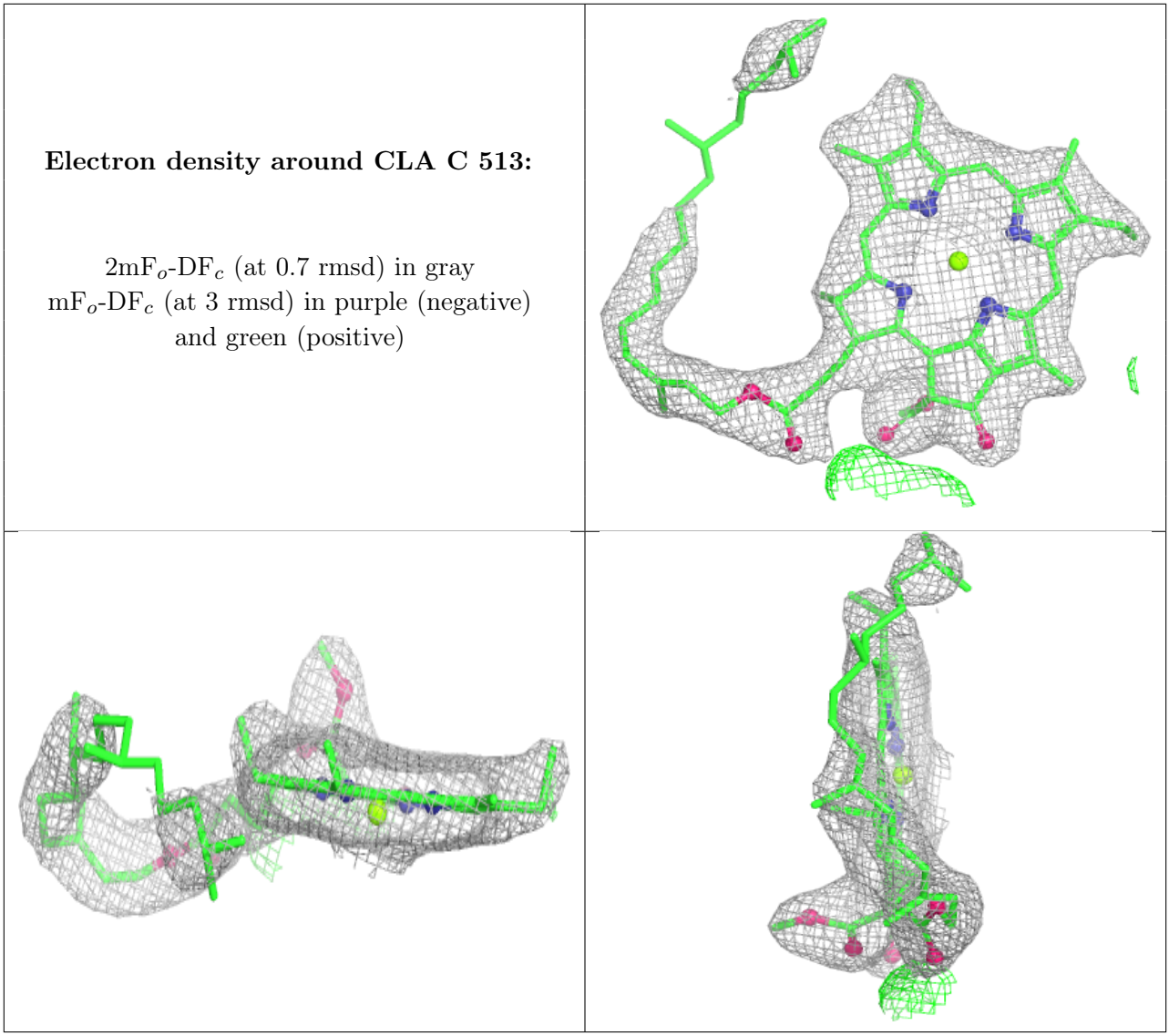
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





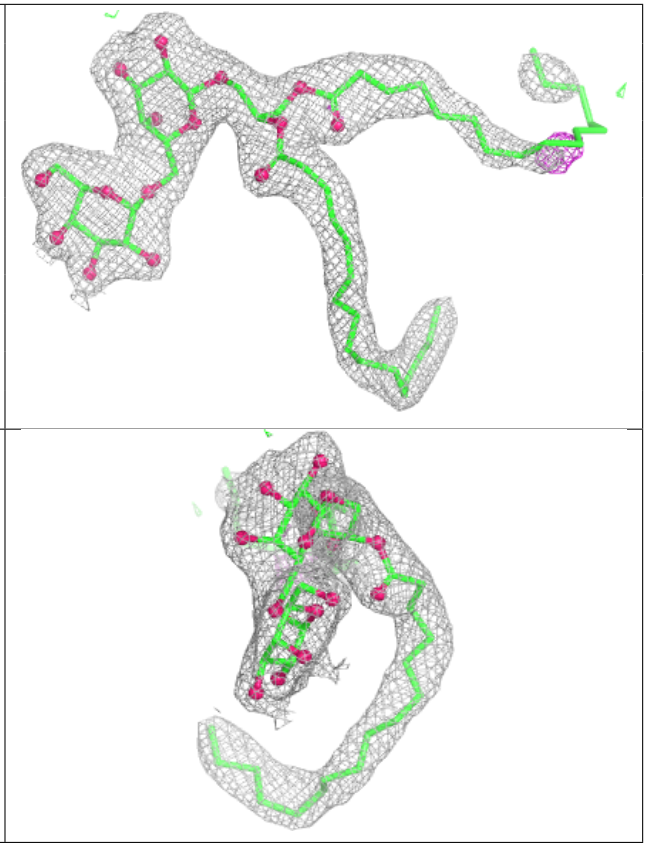
Electron density around CLA C 513:

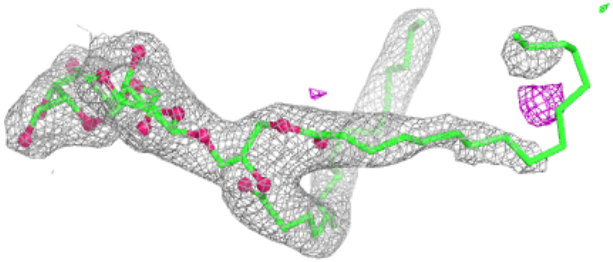
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD c 519:

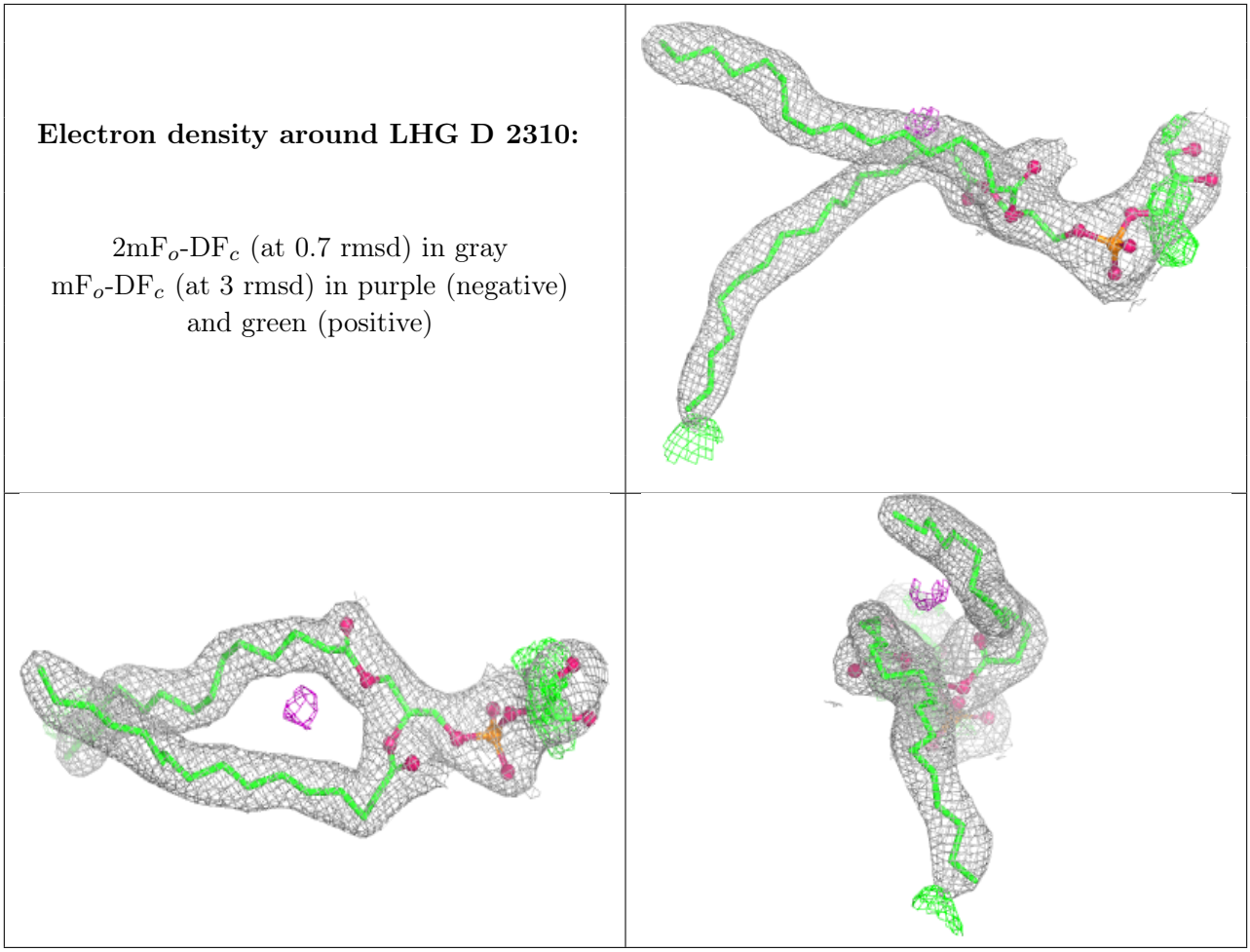
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





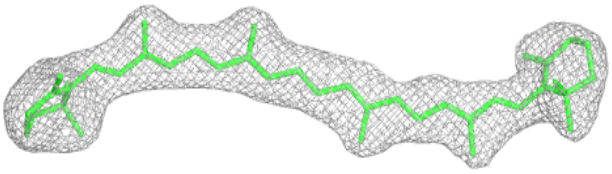
Electron density around LHG D 2310:

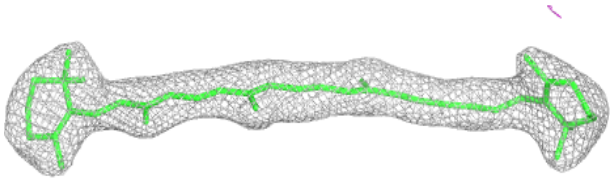
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

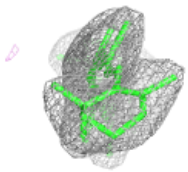


Electron density around BCR y 101:

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

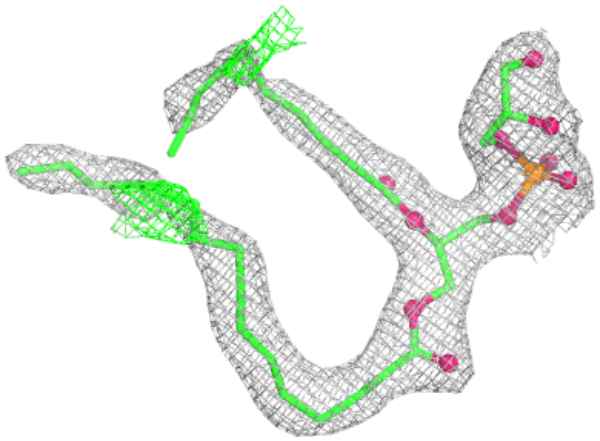


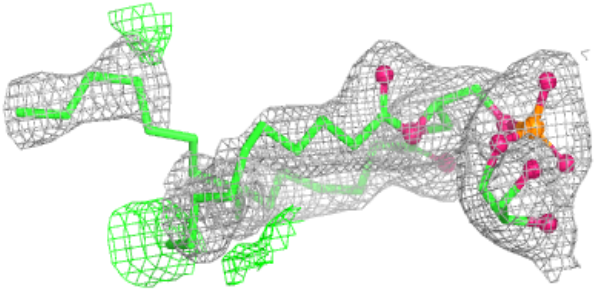


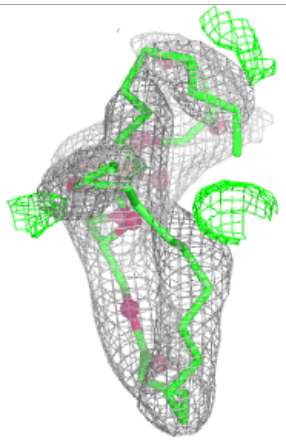


Electron density around LHG d 403:

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

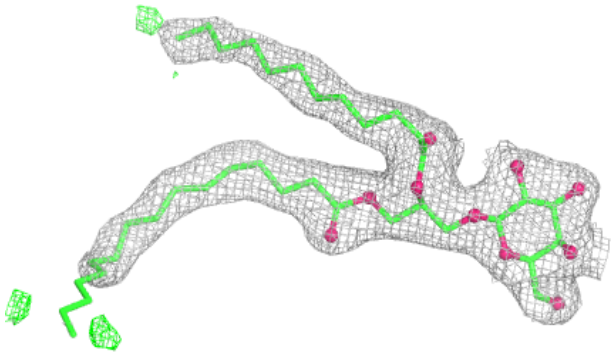


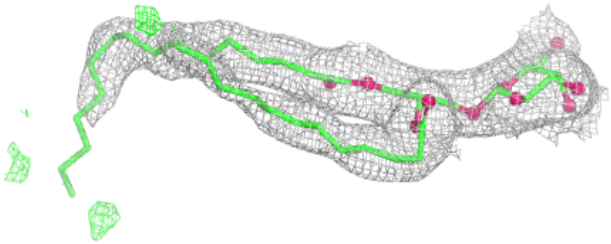


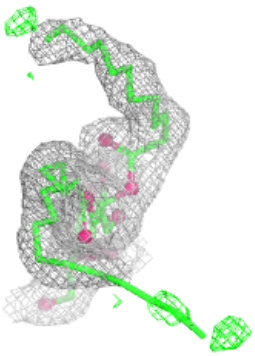


Electron density around LMG D 2312:

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

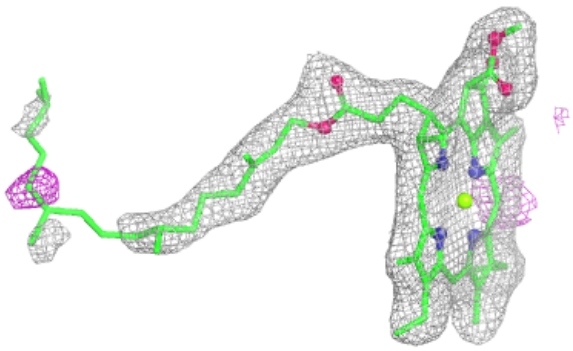


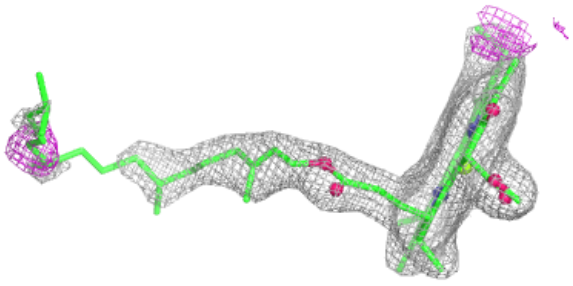


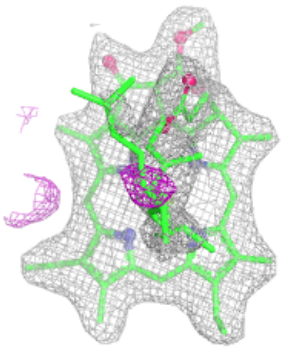


Electron density around CLA d 409:

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

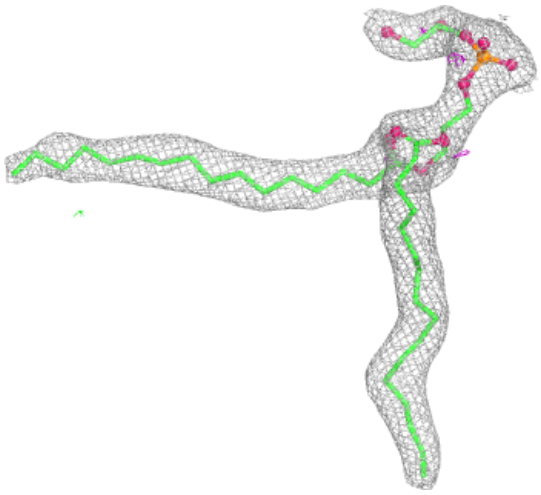


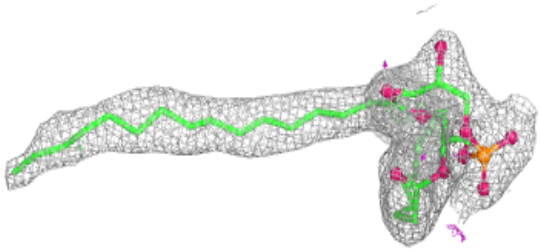


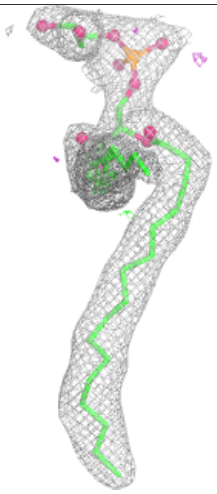


Electron density around LHG l 103:

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

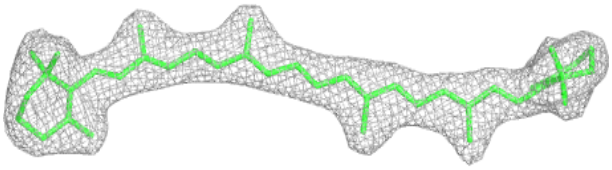


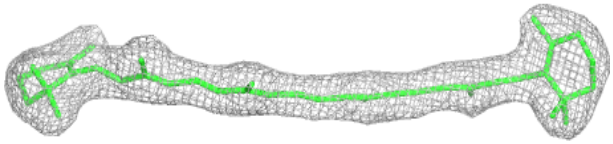


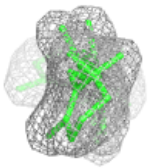


Electron density around BCR B 618:

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

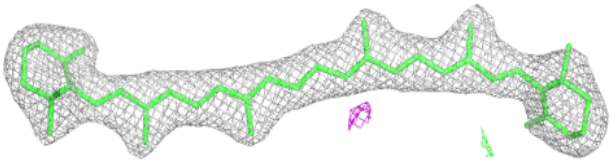


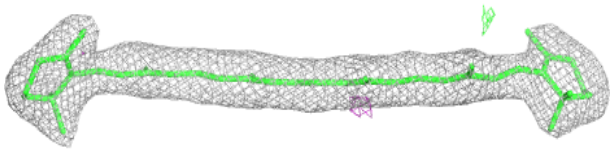


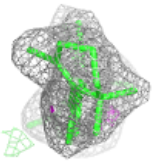


Electron density around BCR B 619:

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

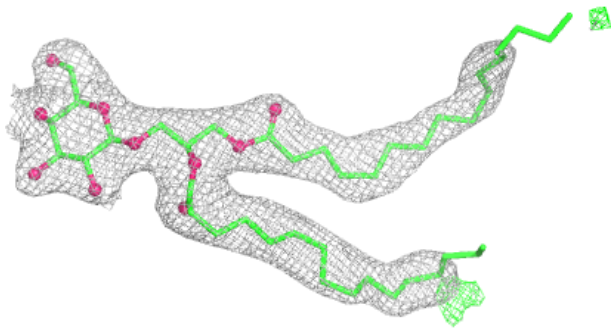


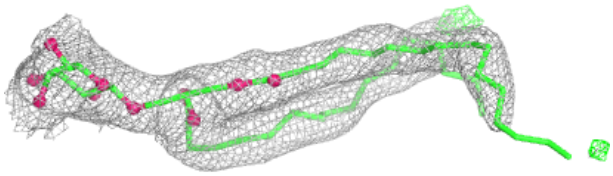




Electron density around LMG d 414:

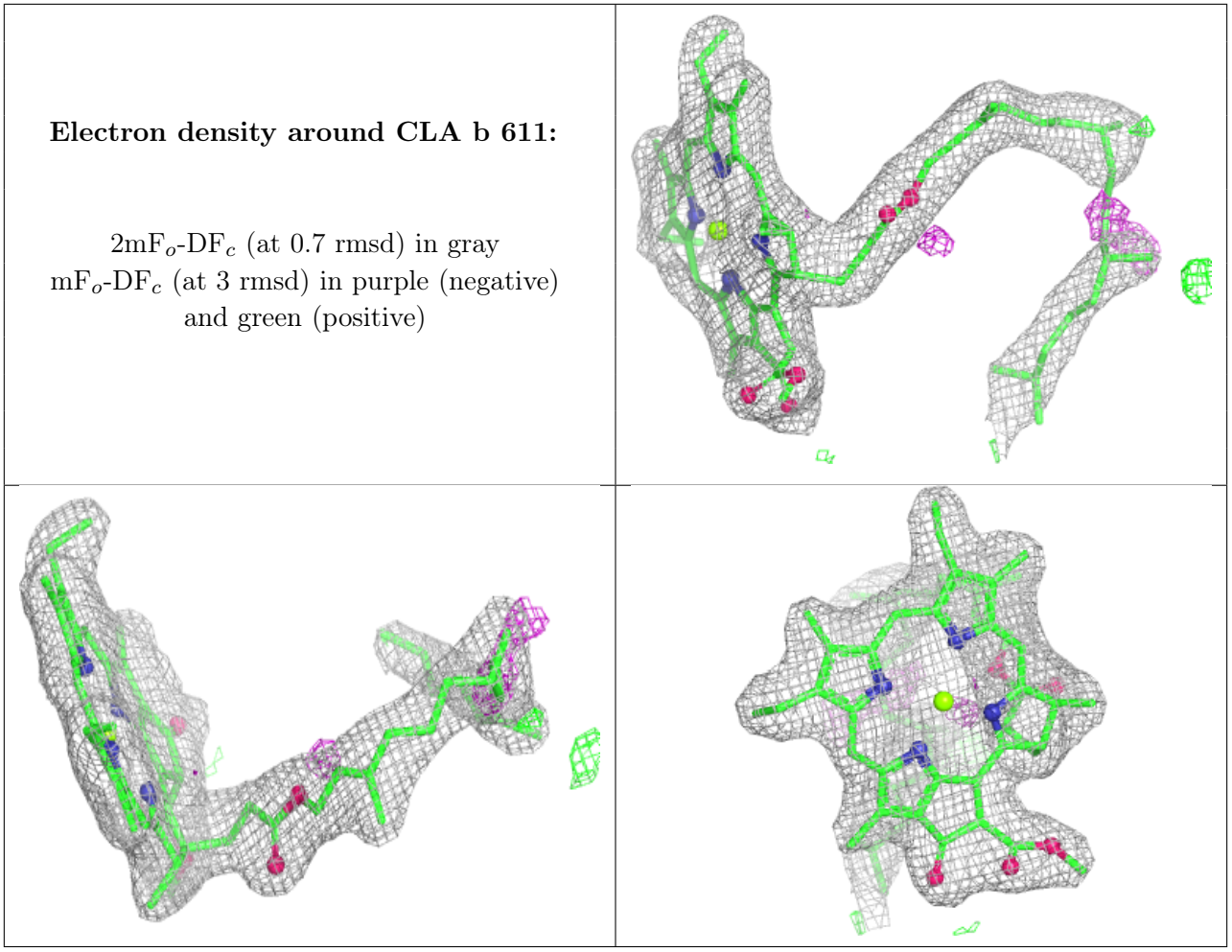
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





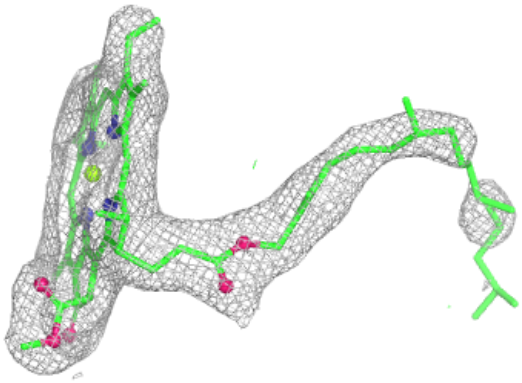
Electron density around CLA b 611:

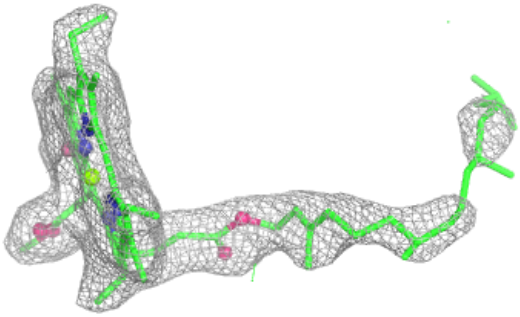
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

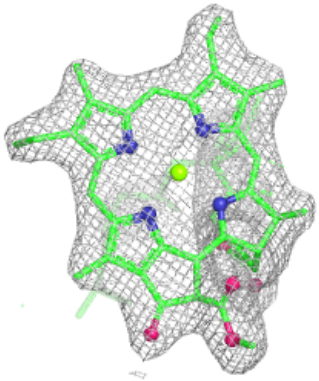


Electron density around CLA D 2304:

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

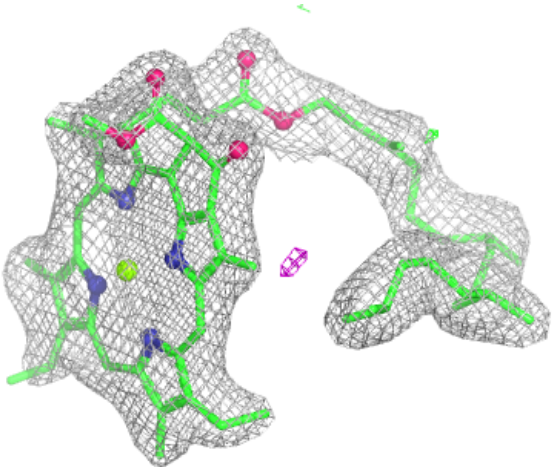


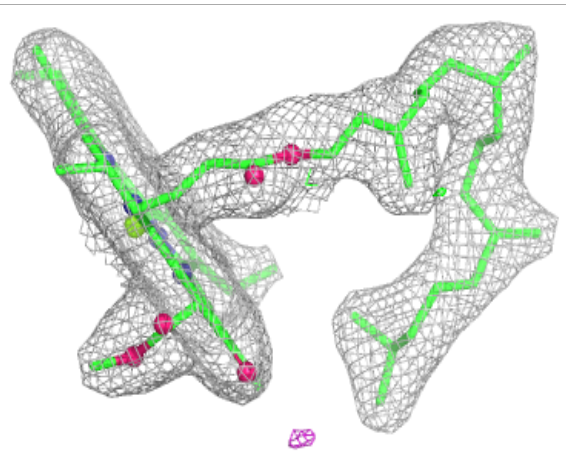


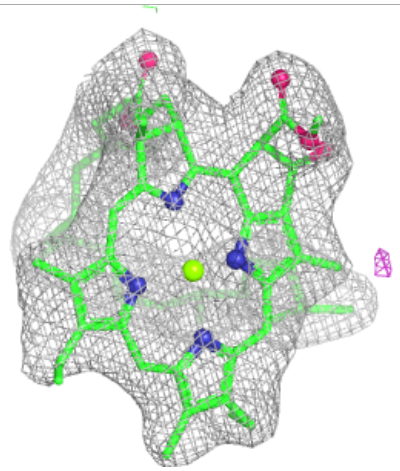


Electron density around CLA C 504:

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

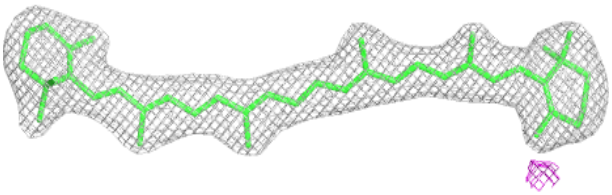


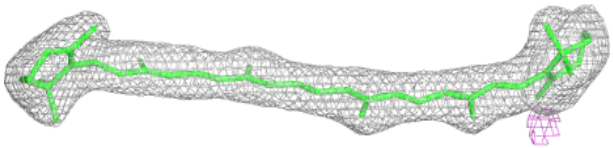


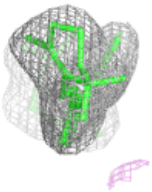


Electron density around BCR B 620:

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

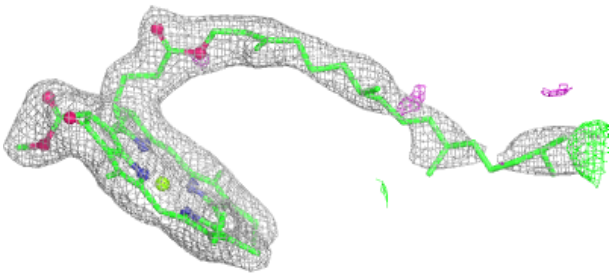


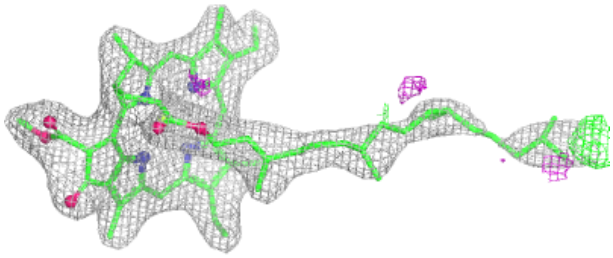


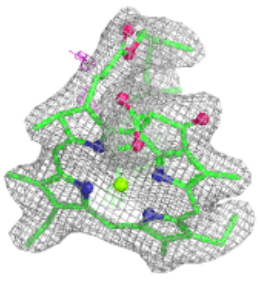


Electron density around CLA C 505:

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

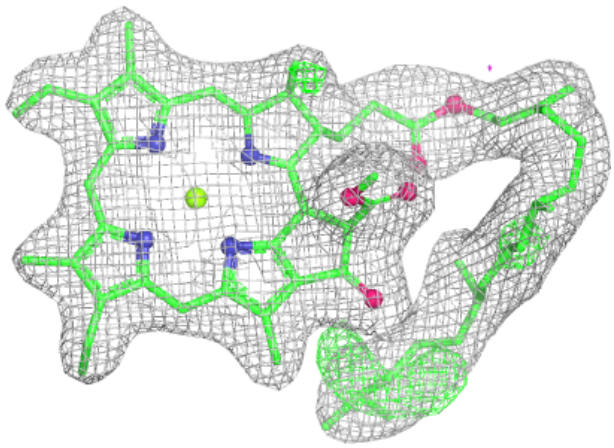


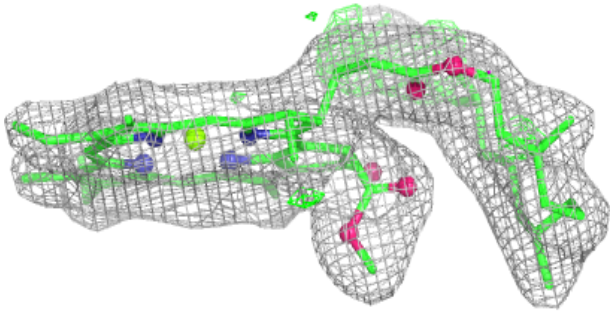


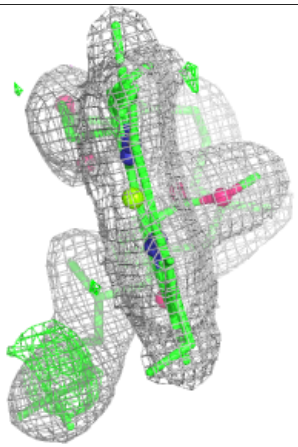


Electron density around CLA B 611:

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

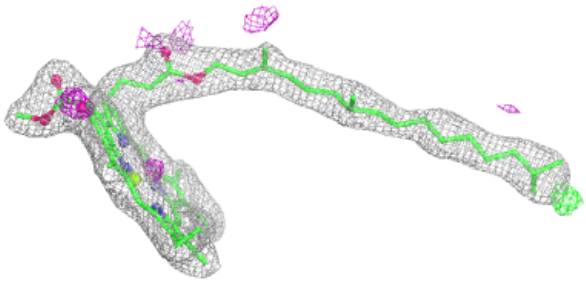


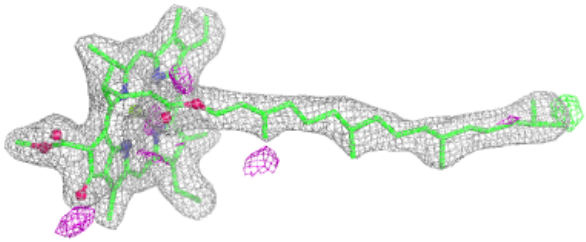


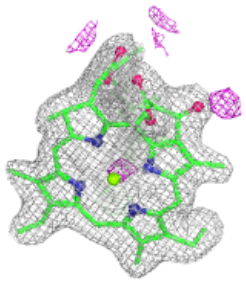


Electron density around CLA b 612:

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

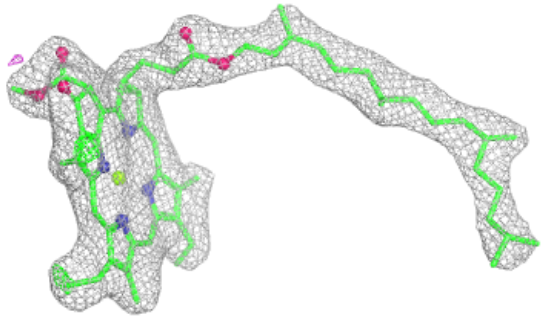


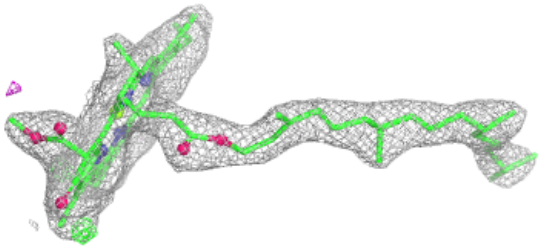


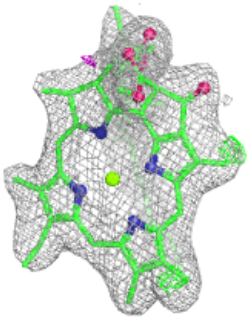


Electron density around CLA b 614:

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

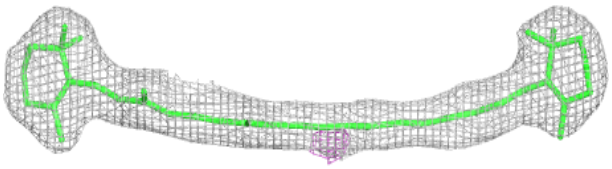


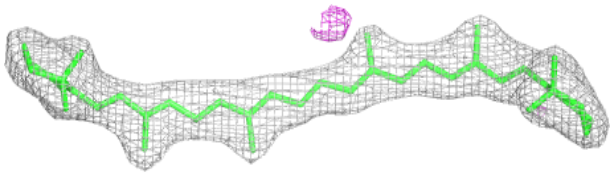


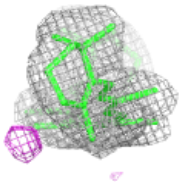


Electron density around BCR K 101:

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

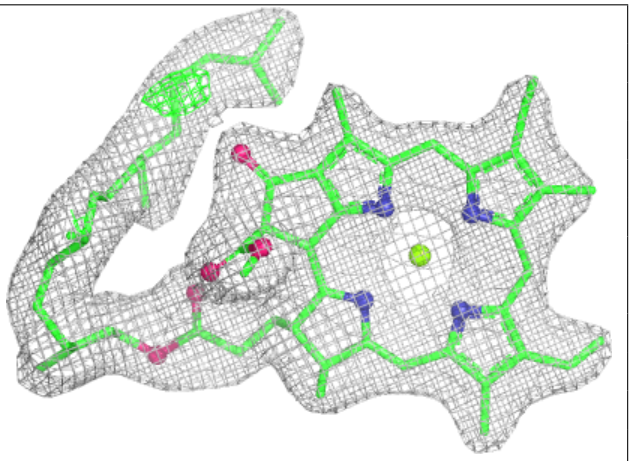


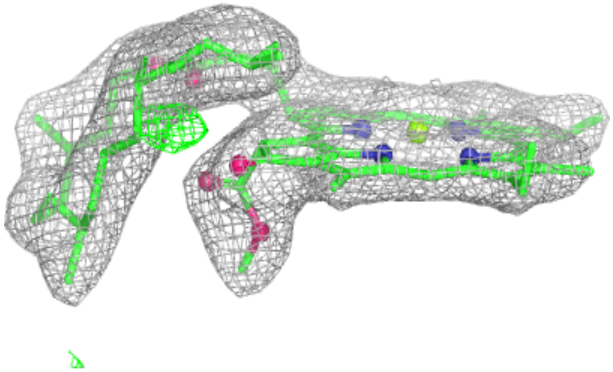


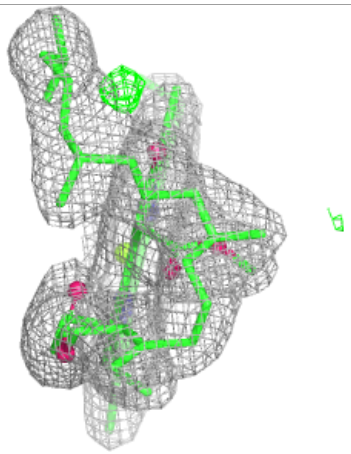


Electron density around CLA b 615:

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

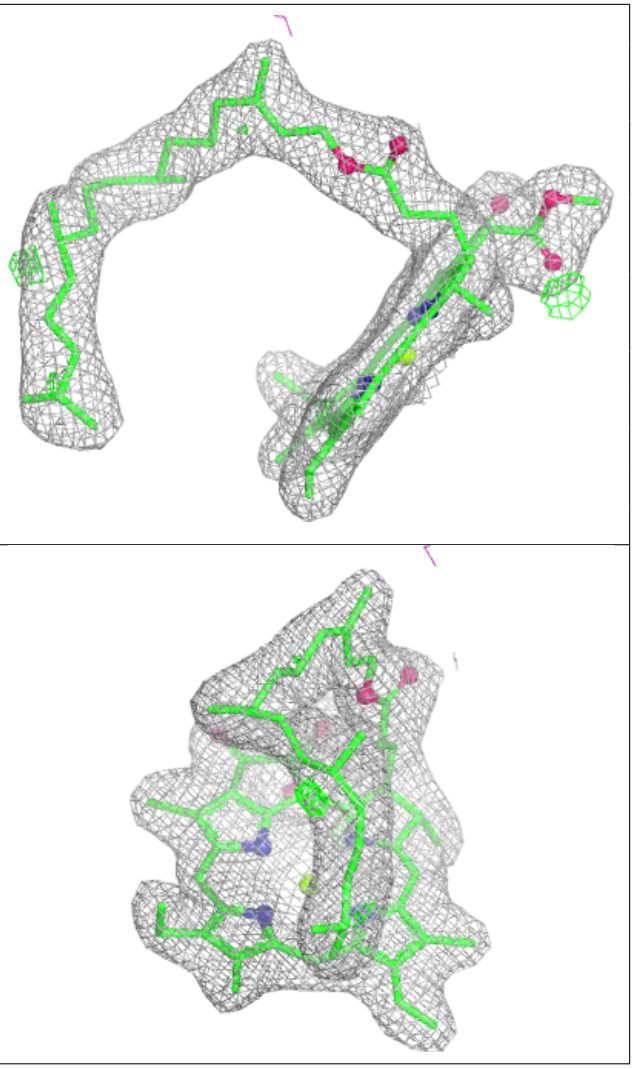






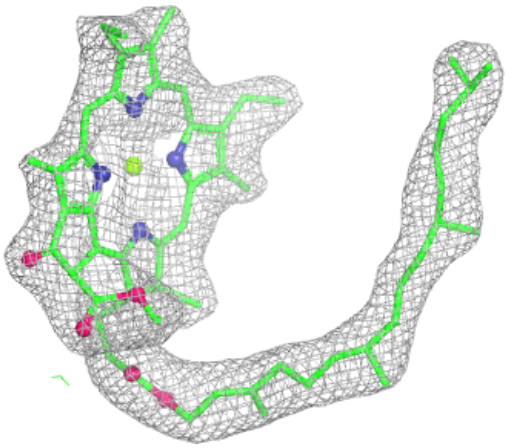
Electron density around CLA b 616:

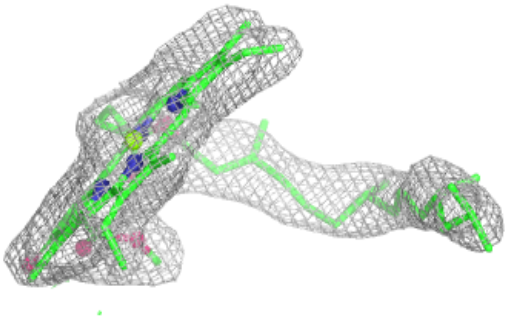
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

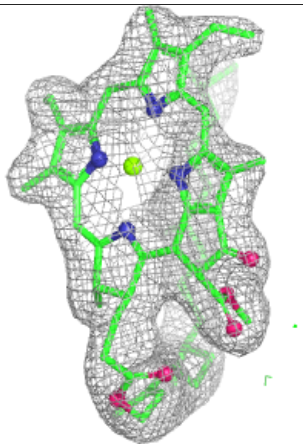


Electron density around CLA C 508:

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

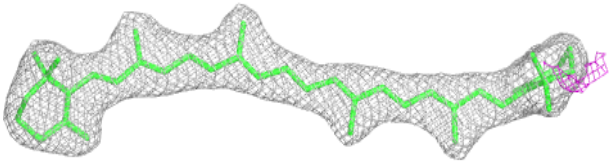


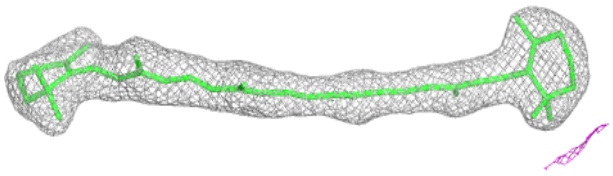


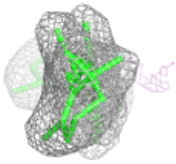


Electron density around BCR b 622:

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

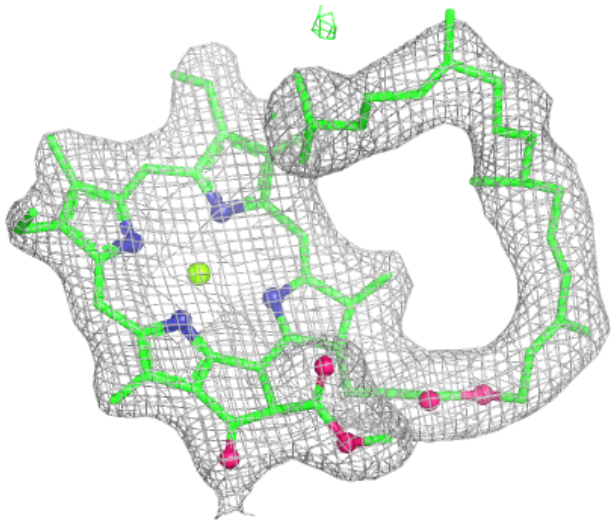


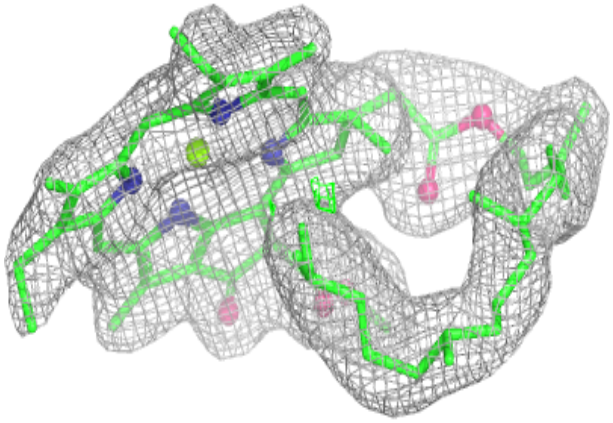


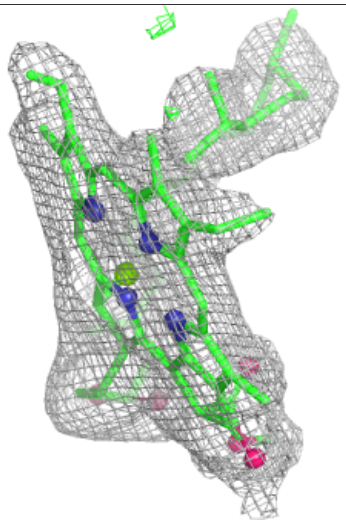


Electron density around CLA b 620:

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

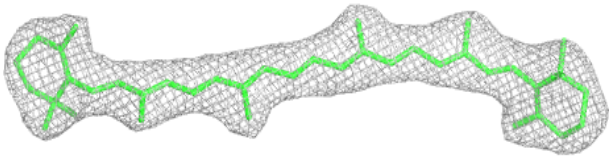


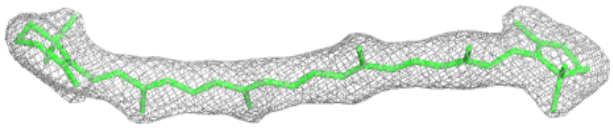


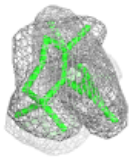


Electron density around BCR b 624:

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

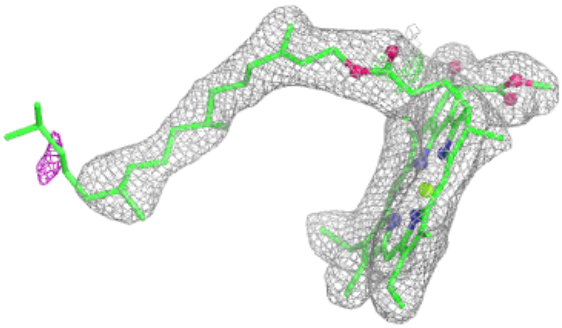


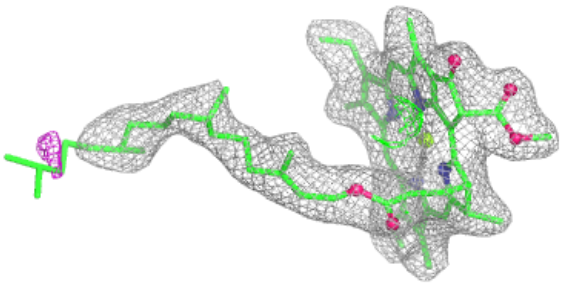


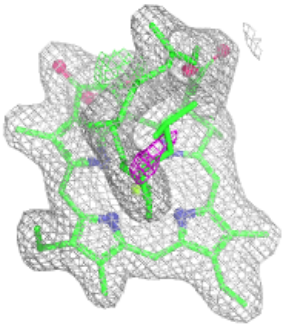


Electron density around CLA C 509:

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

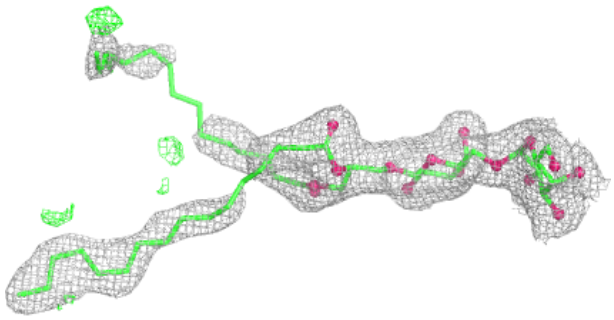


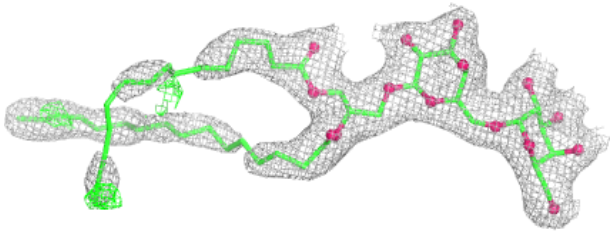


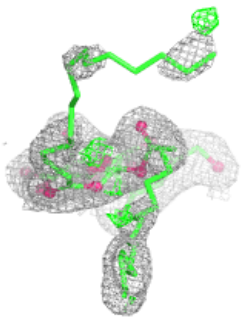


Electron density around DGD C 517:

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

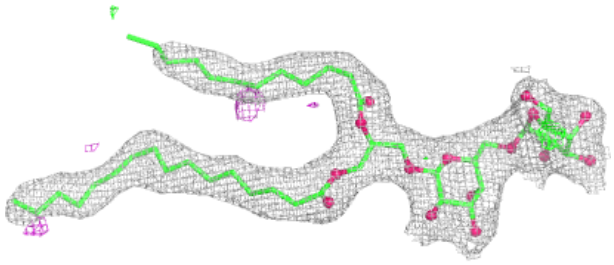


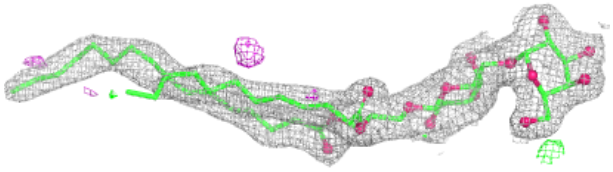


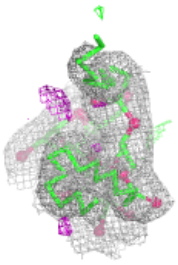


Electron density around DGD C 519:

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

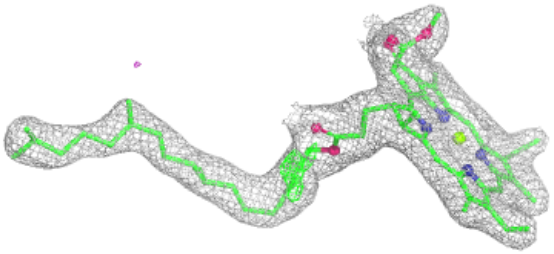


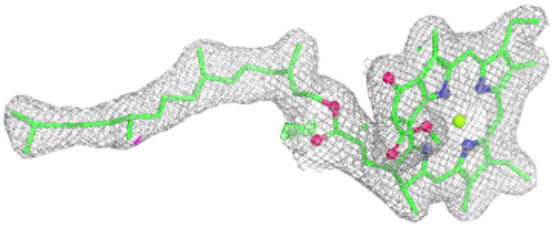


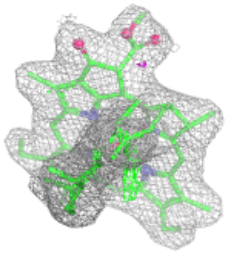


Electron density around CLA c 505:

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

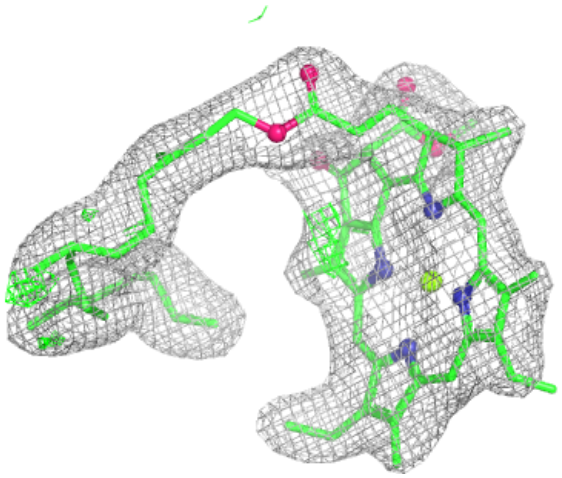


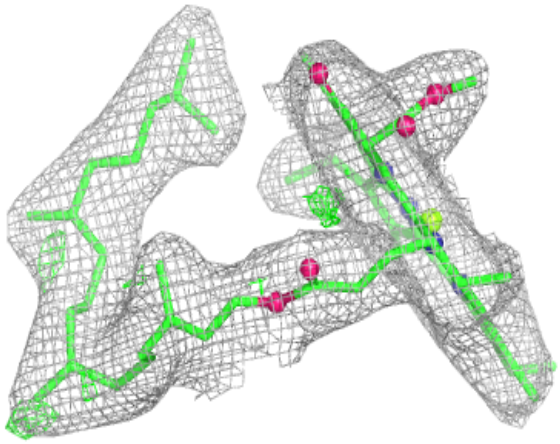


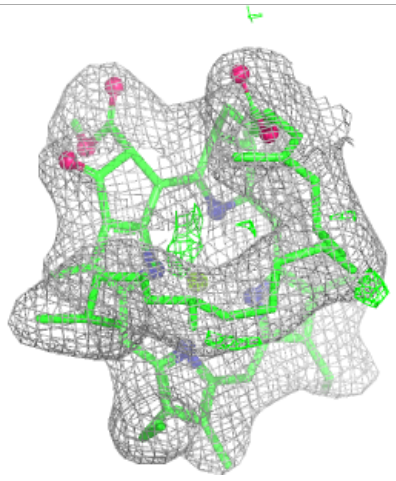


Electron density around CLA c 506:

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

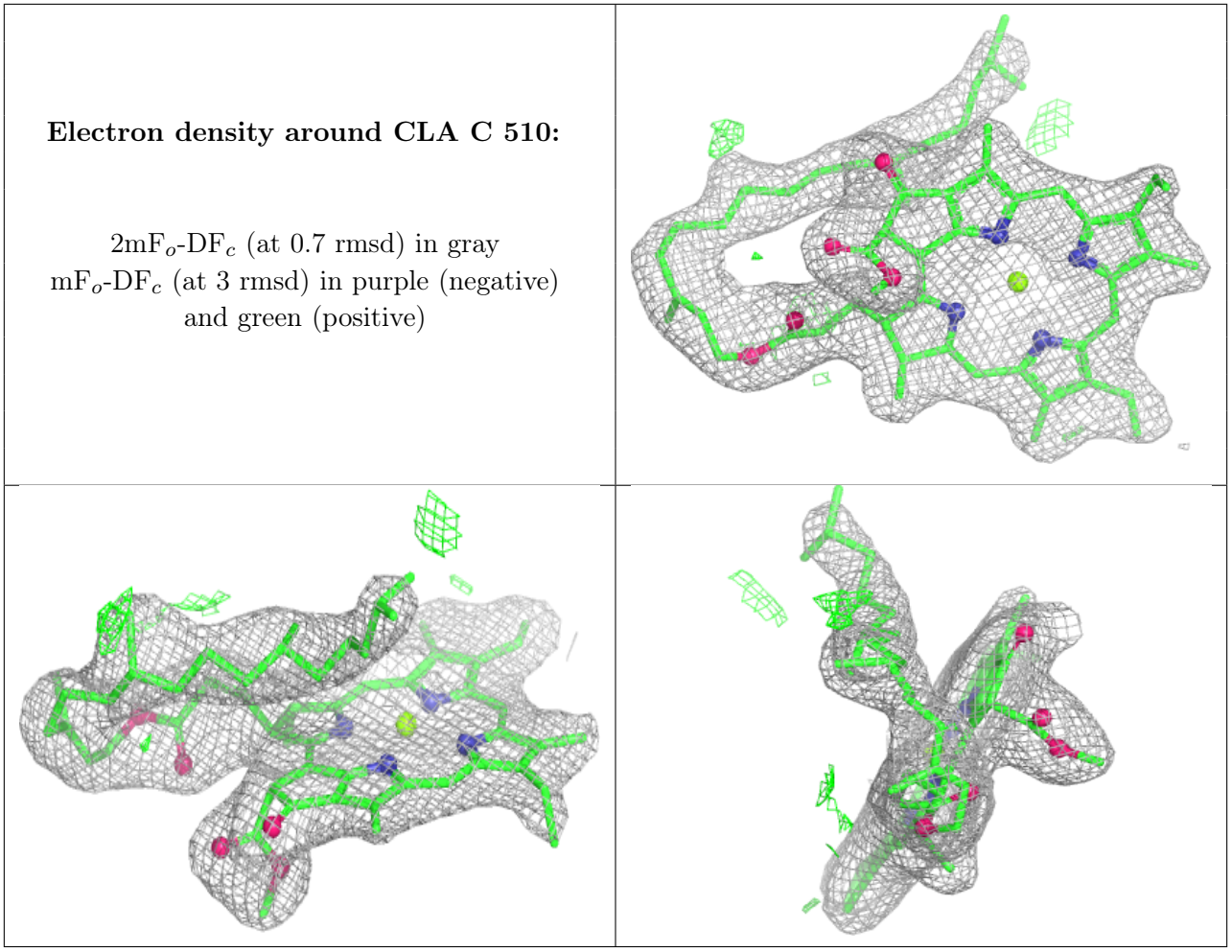






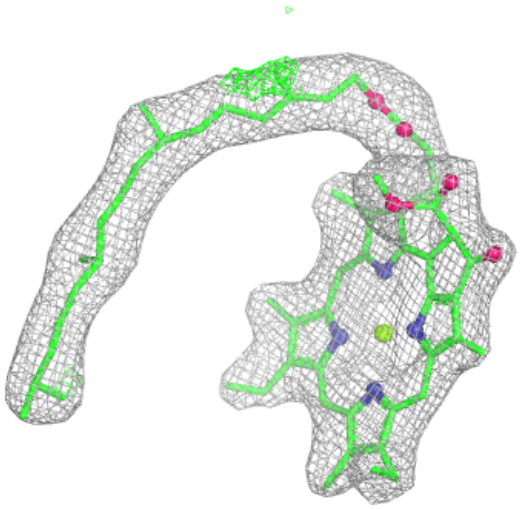
Electron density around CLA C 510:

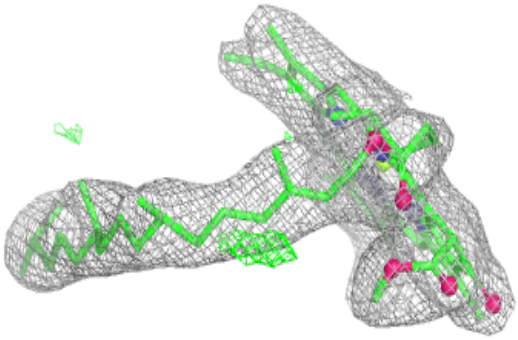
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

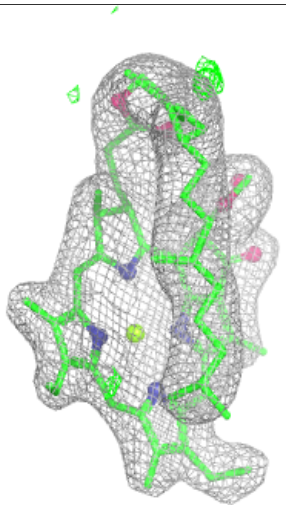


Electron density around CLA c 510:

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

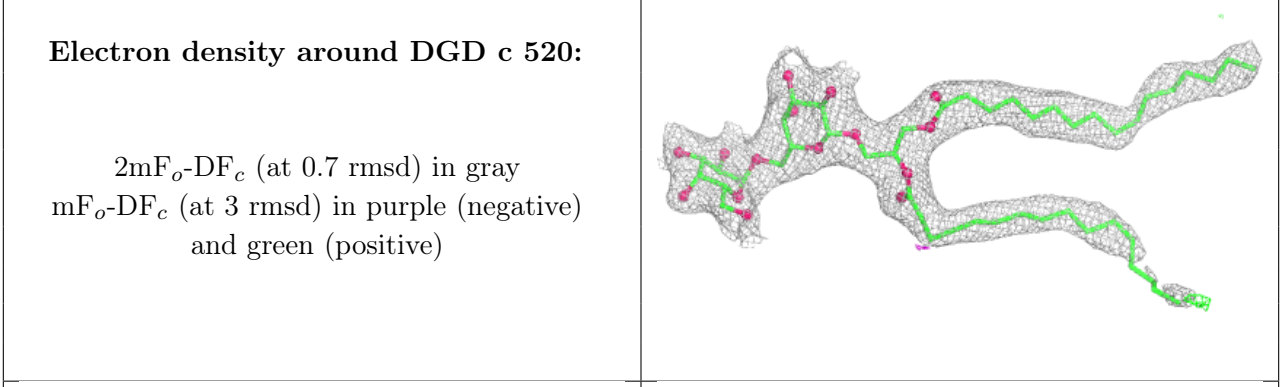






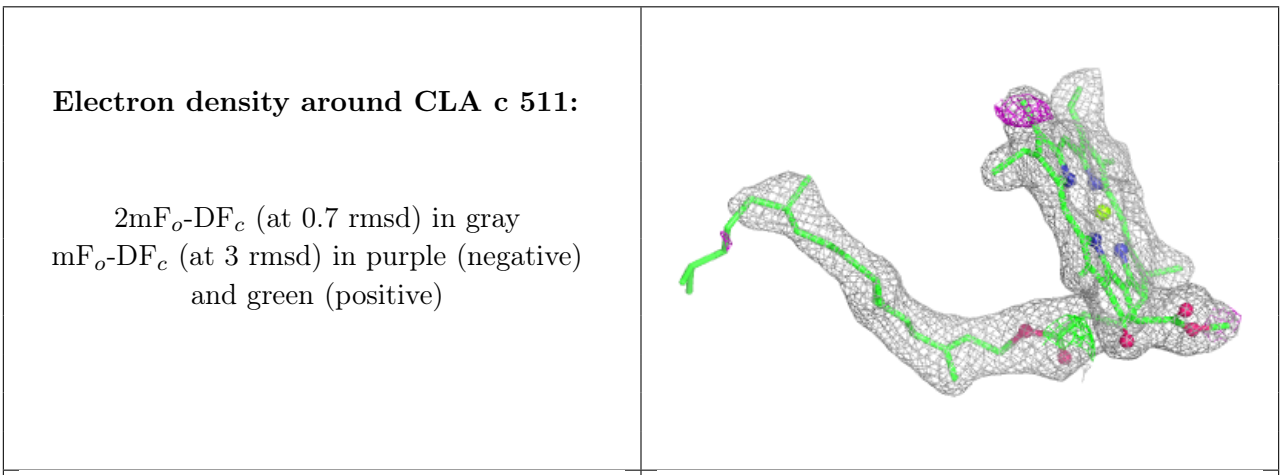
Electron density around DGD c 520:

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



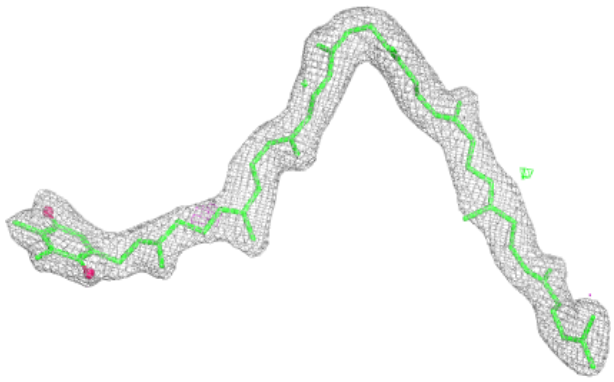
Electron density around CLA c 511:

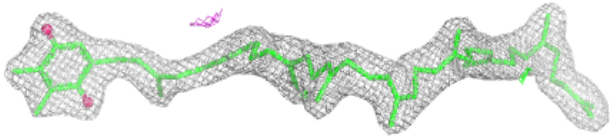
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PL9 D 2306:

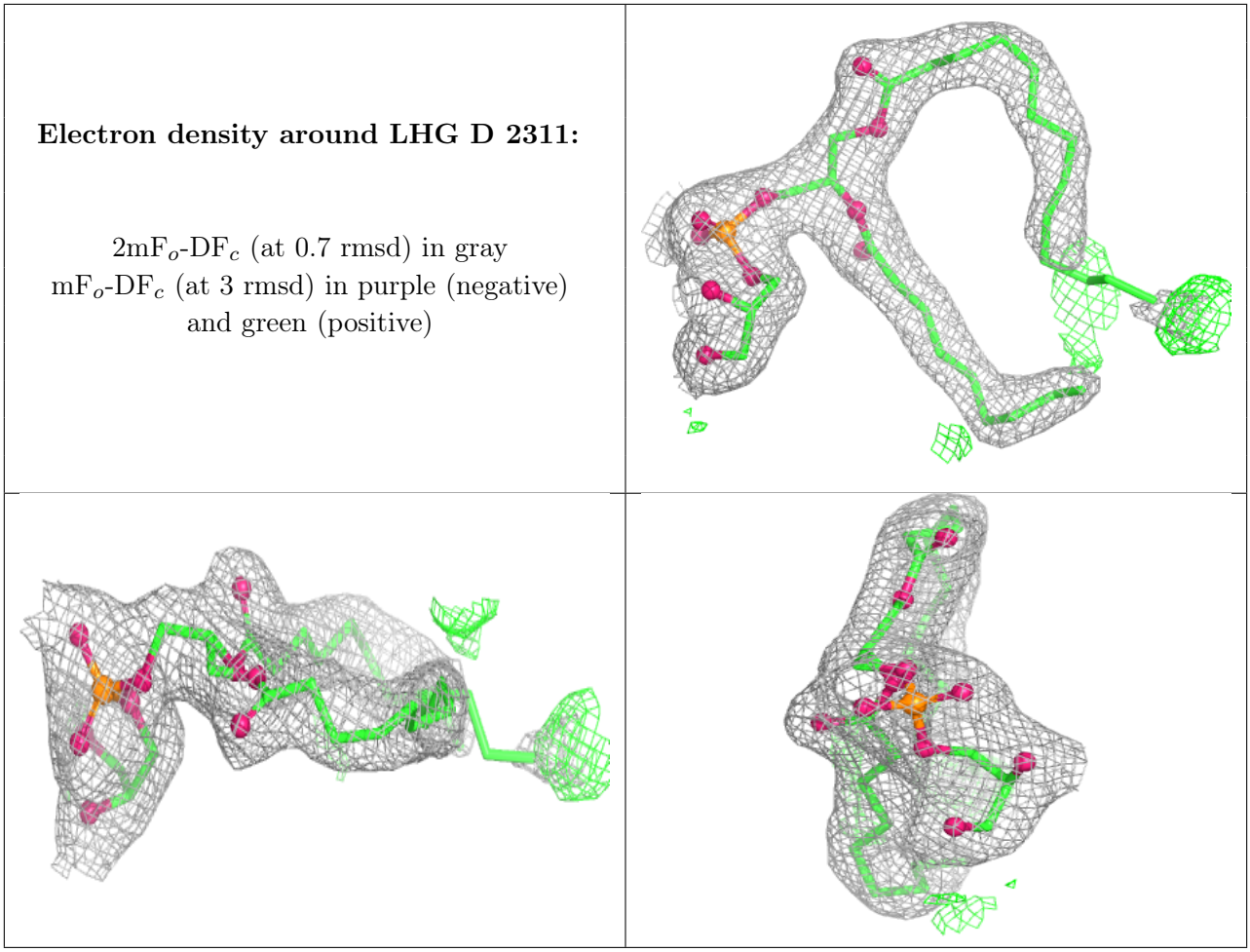
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





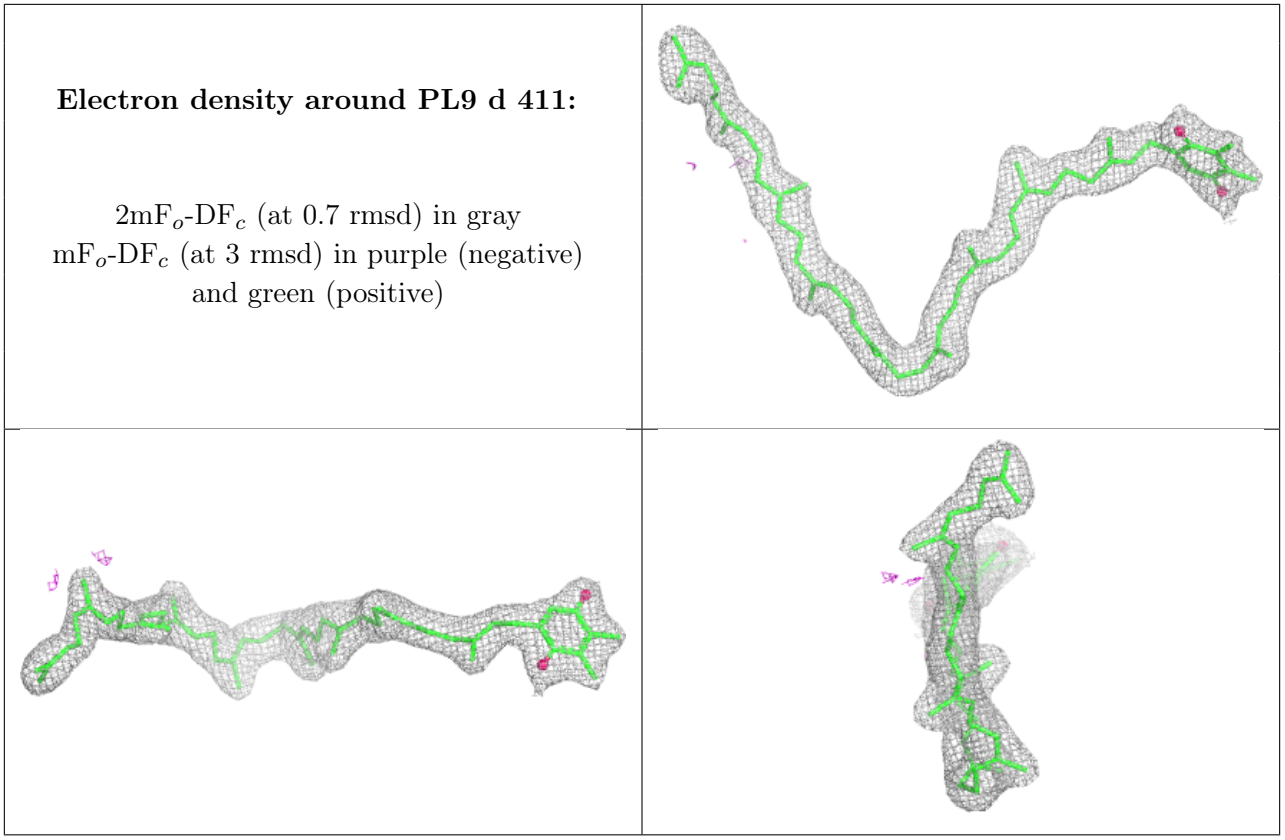
Electron density around LHG D 2311:

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



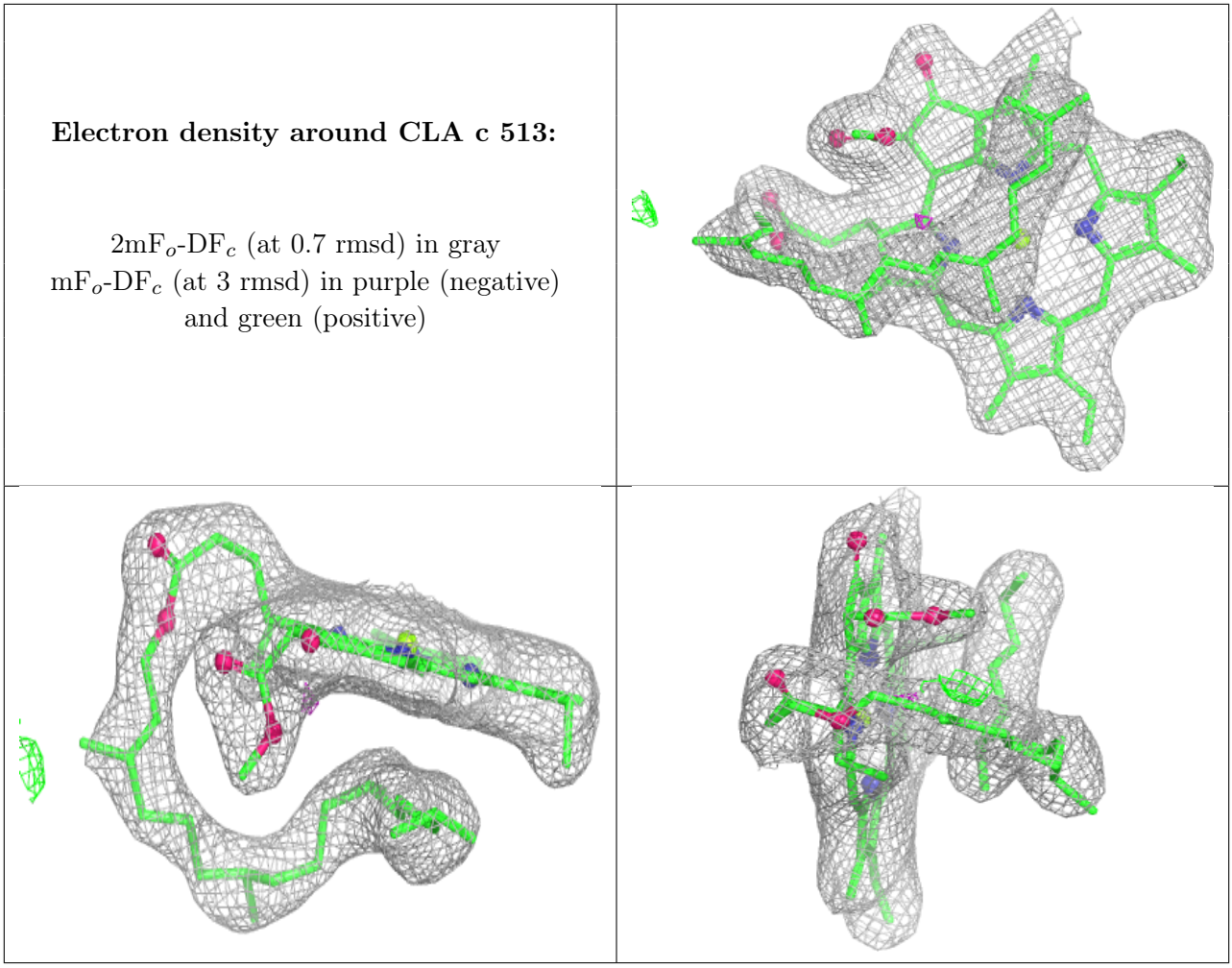
Electron density around PL9 d 411:

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



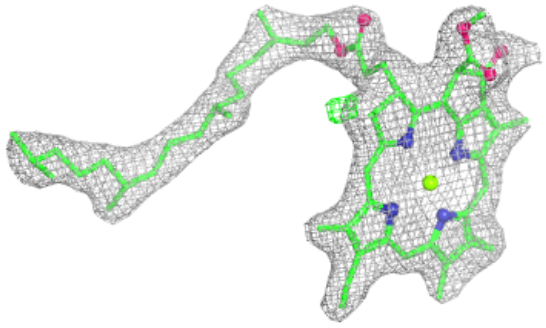
Electron density around CLA c 513:

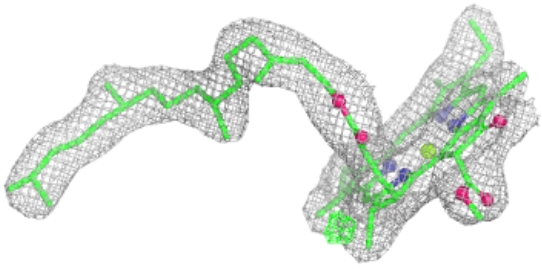
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

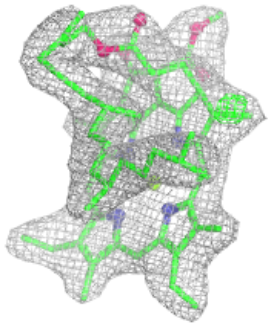


Electron density around CLA c 514:

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

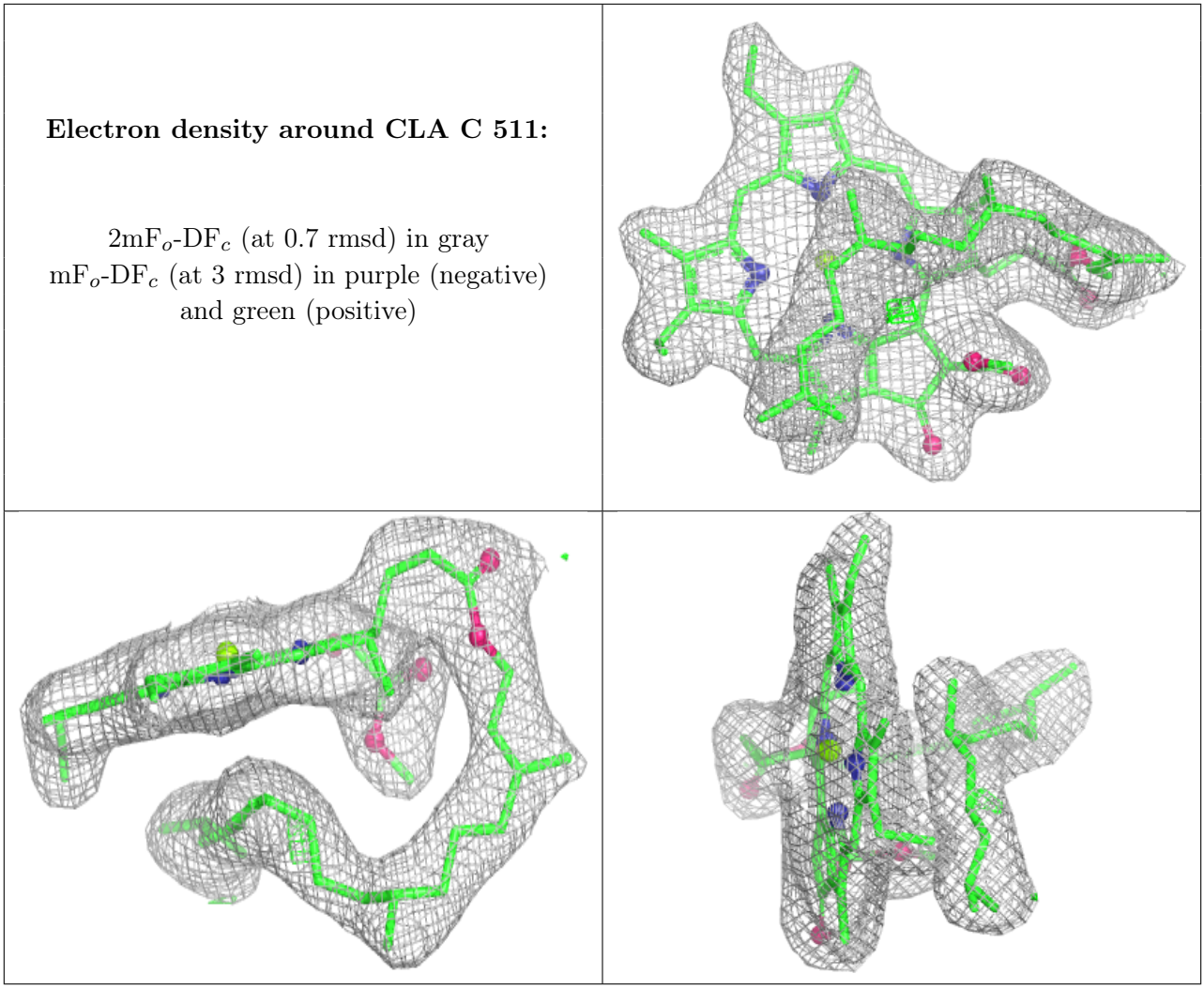






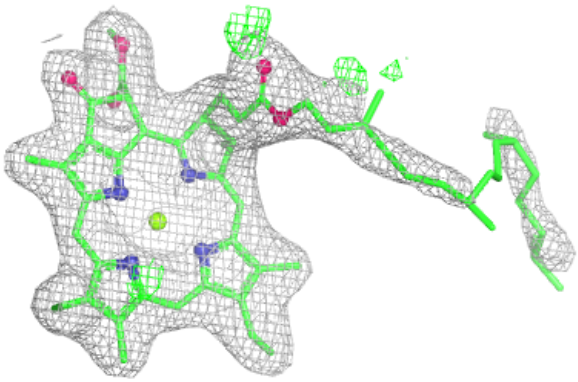
Electron density around CLA C 511:

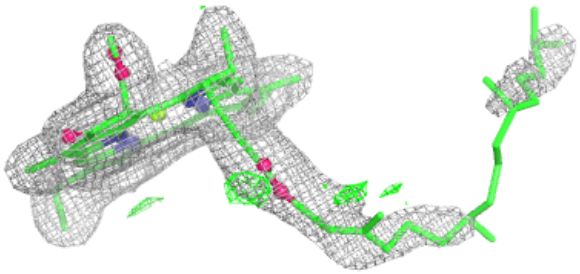
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

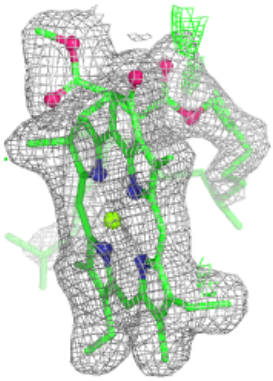


Electron density around CLA A 410:

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

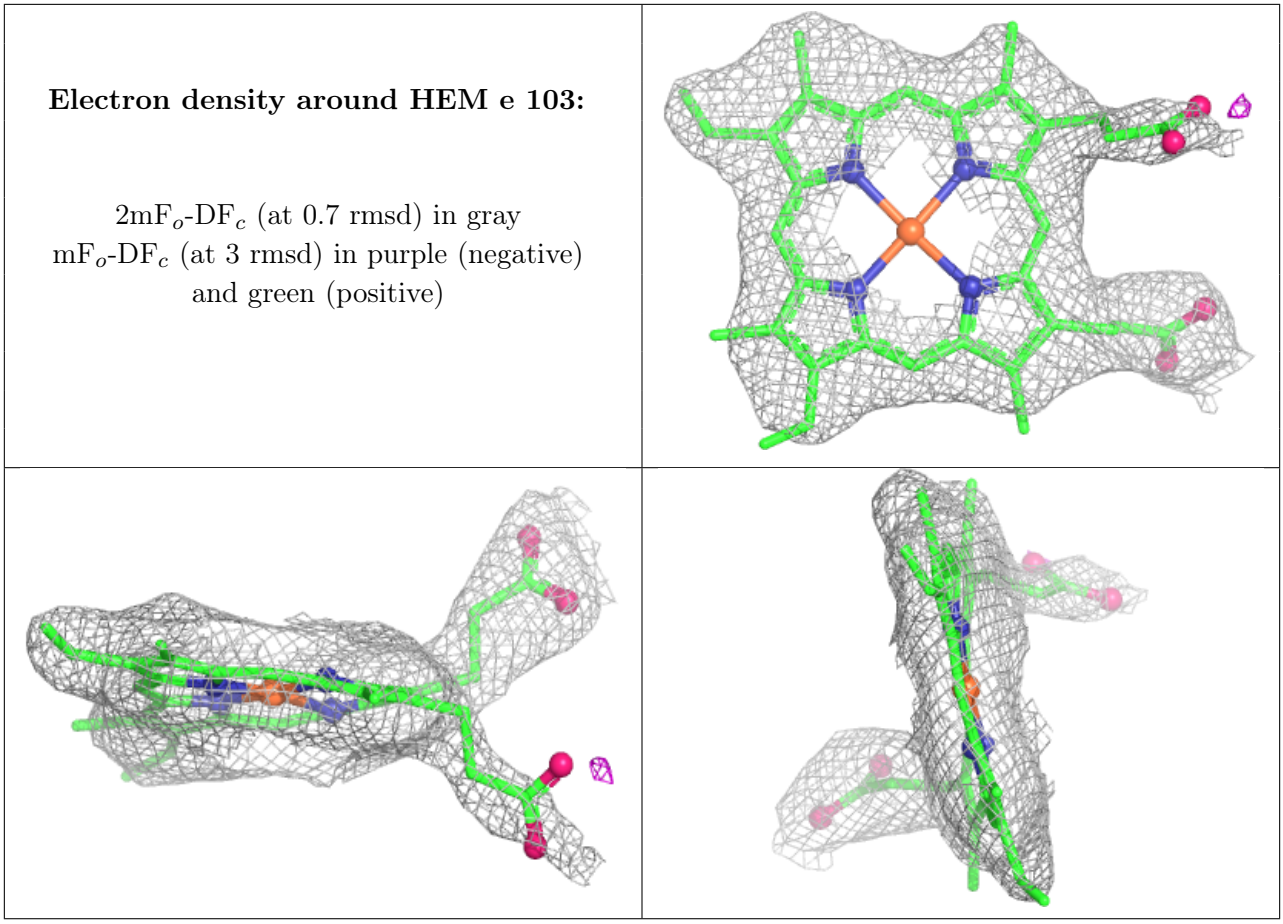






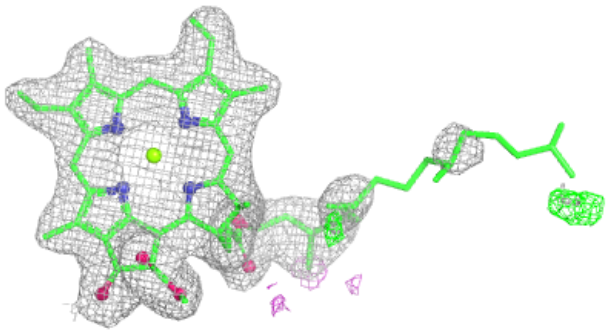
Electron density around HEM e 103:

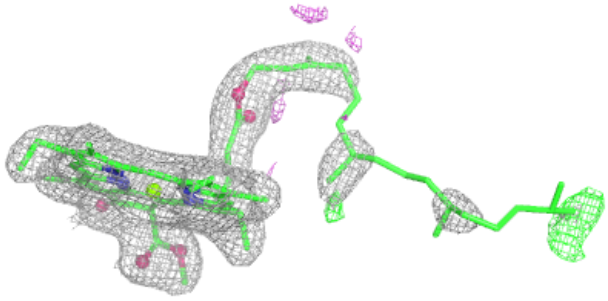
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

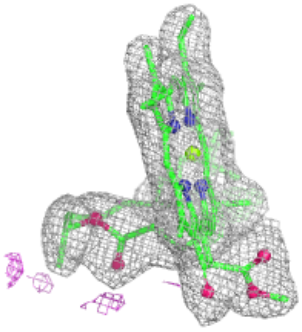


Electron density around CLA A 407:

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

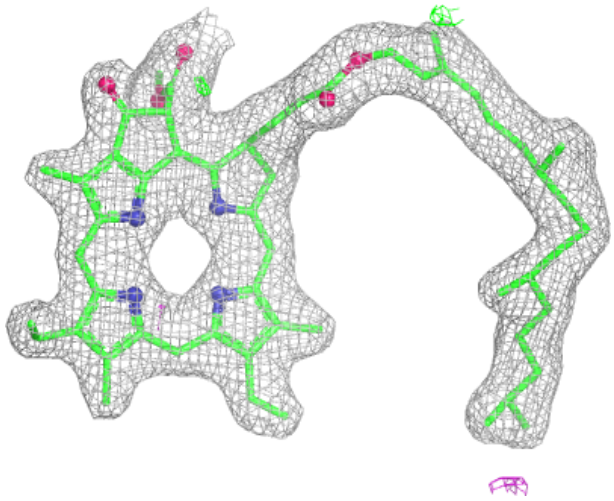


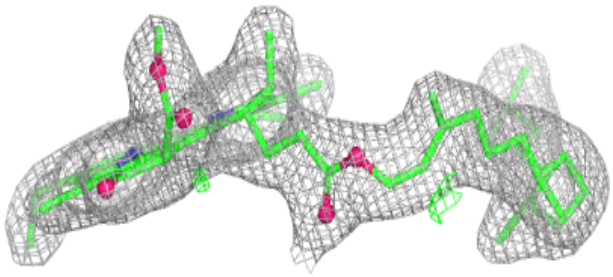


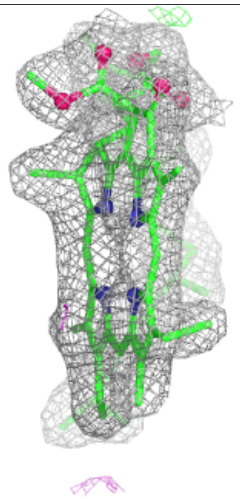


Electron density around PHO A 408:

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

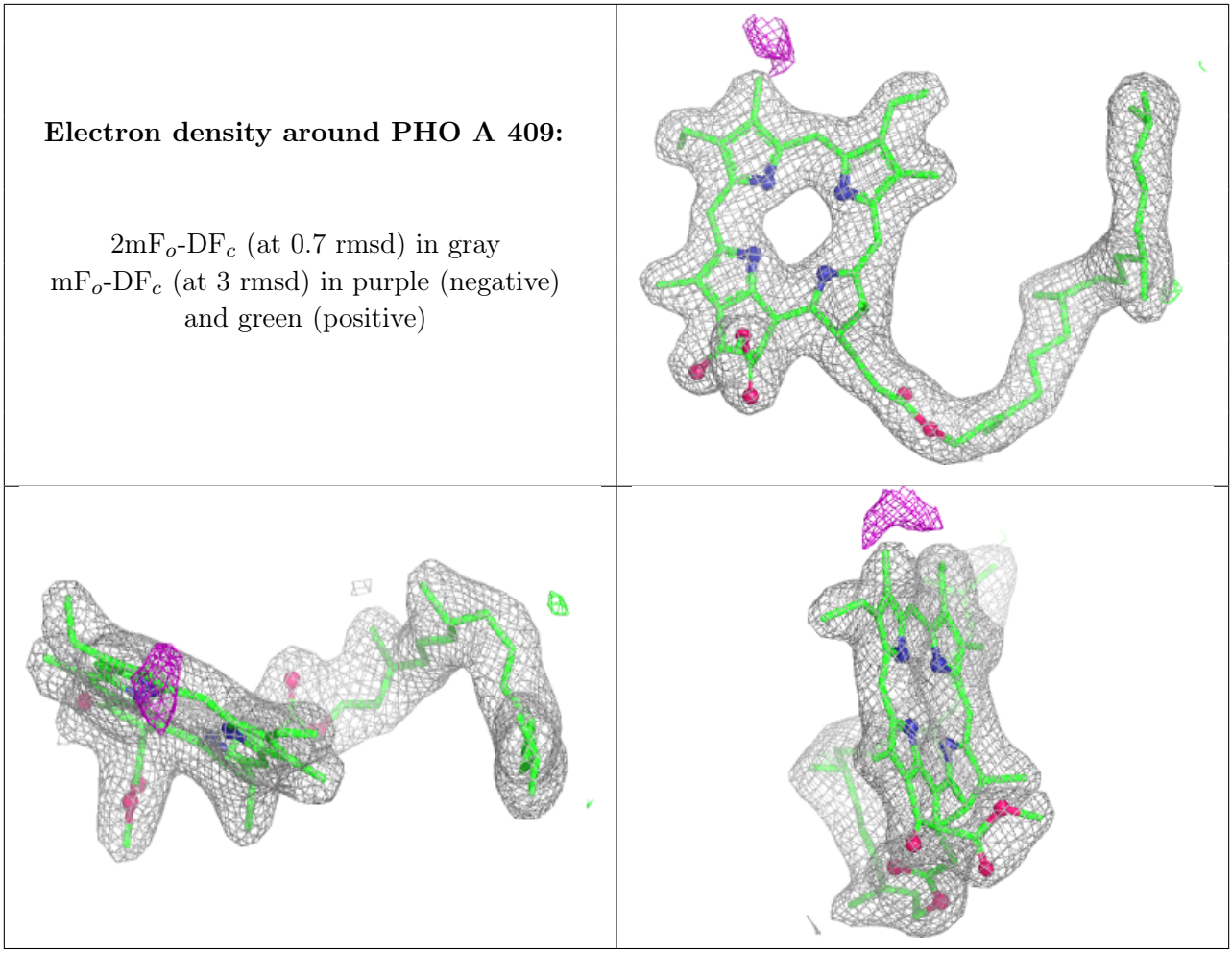






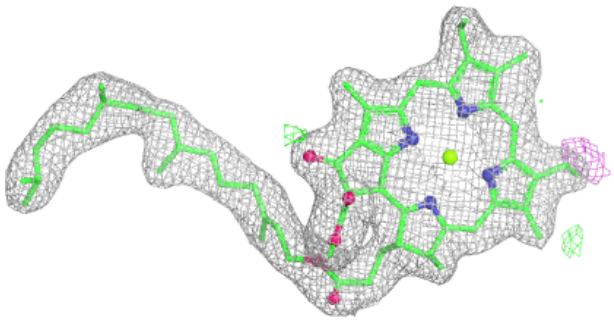
Electron density around PHO A 409:

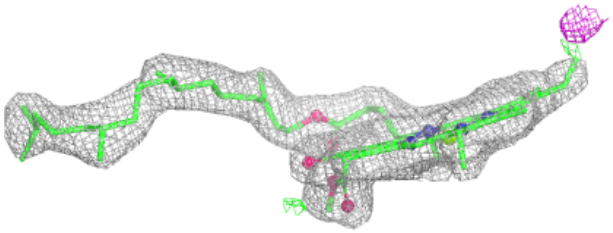
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

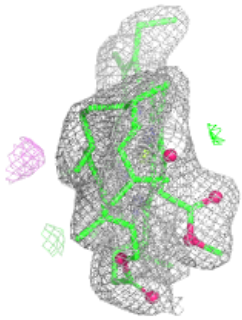


Electron density around CLA B 603:

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

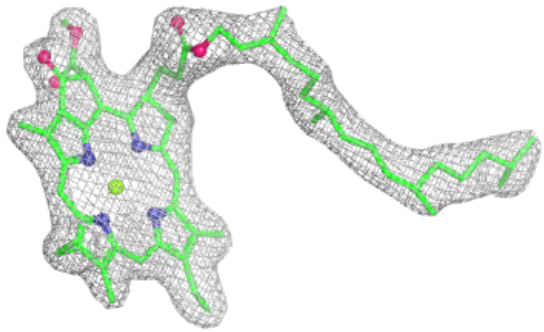


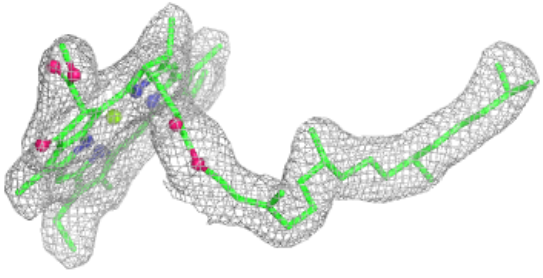


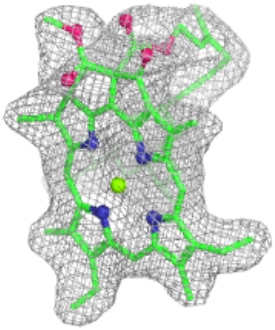


Electron density around CLA C 512:

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

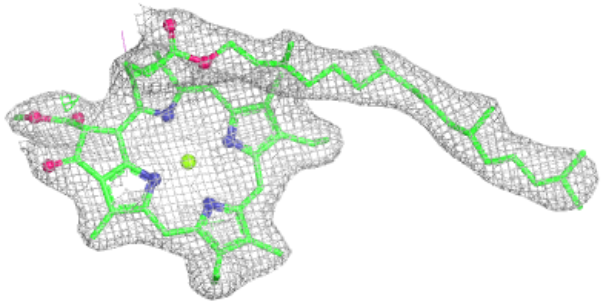


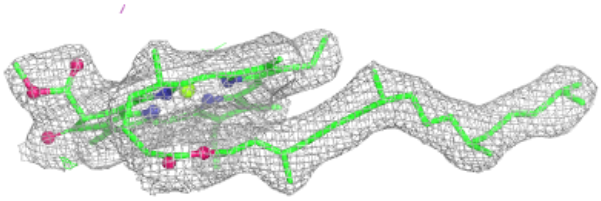


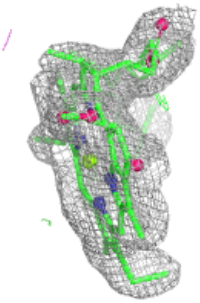


Electron density around CLA c 504:

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

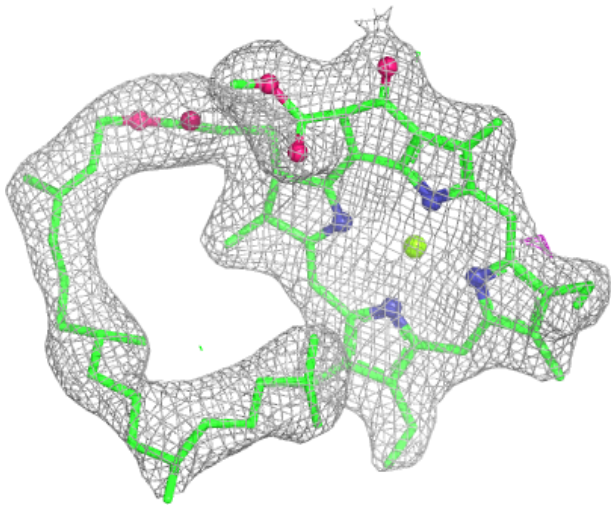


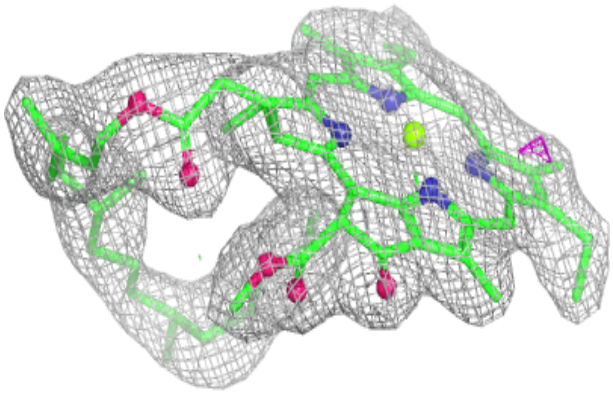


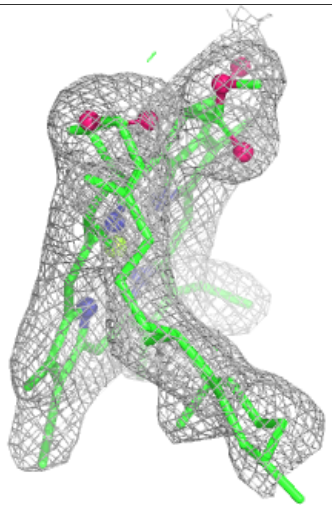


Electron density around CLA B 616:

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

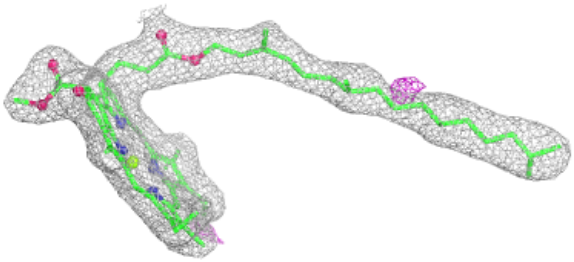


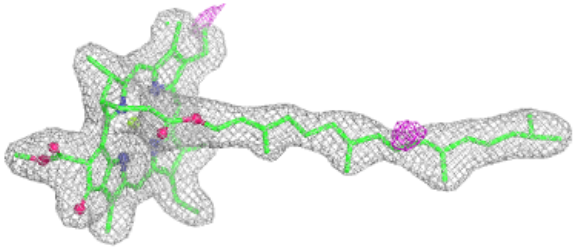


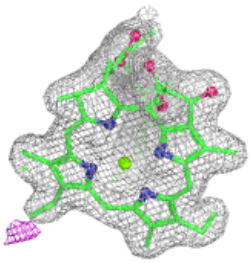


Electron density around CLA B 608:

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

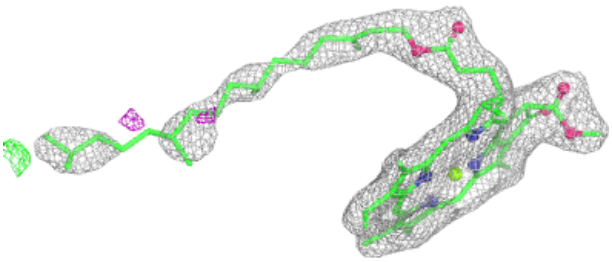


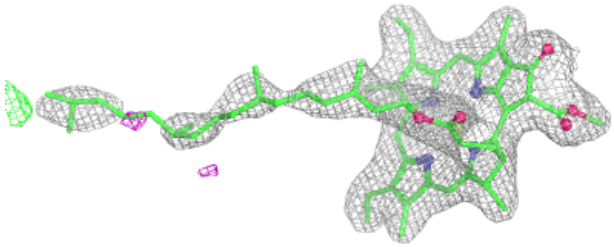


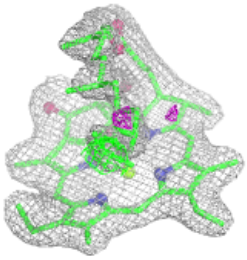


Electron density around CLA c 507:

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

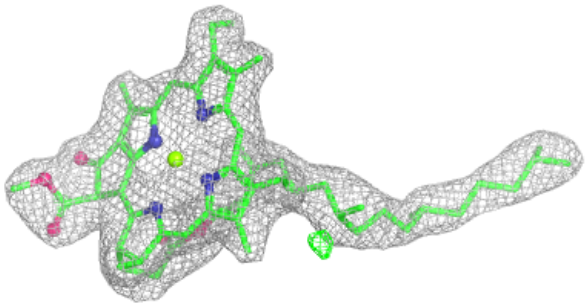


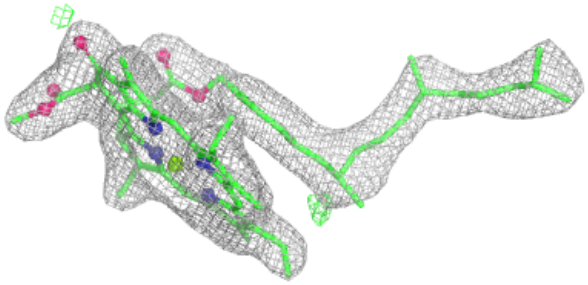


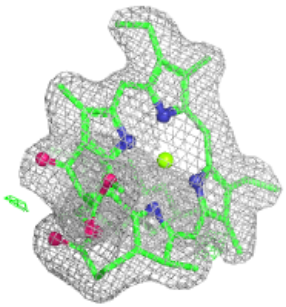


Electron density around CLA c 508:

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

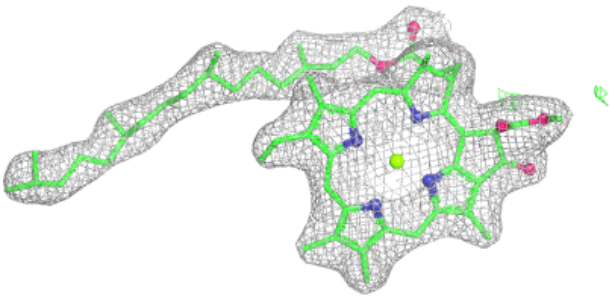


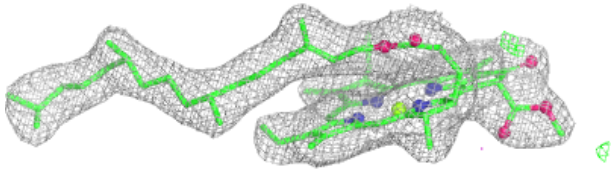


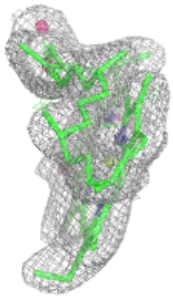


Electron density around CLA C 502:

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

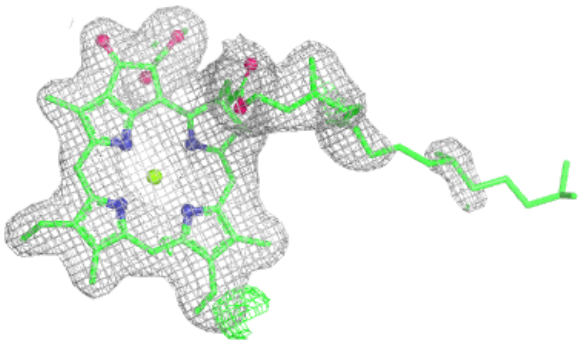


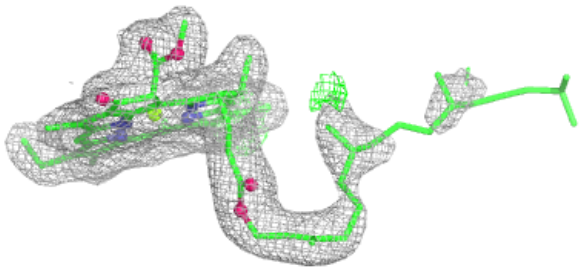


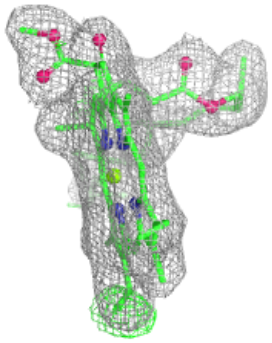


Electron density around CLA a 2610:

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

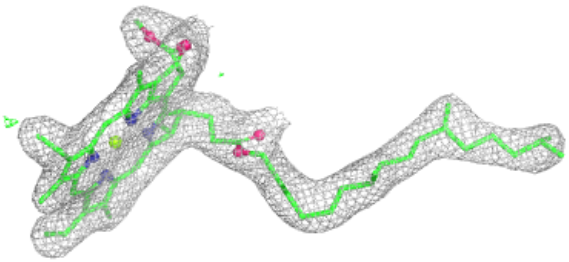


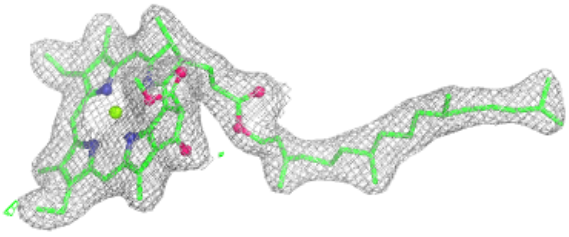


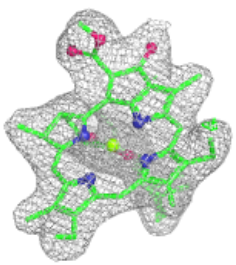


Electron density around CLA C 503:

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

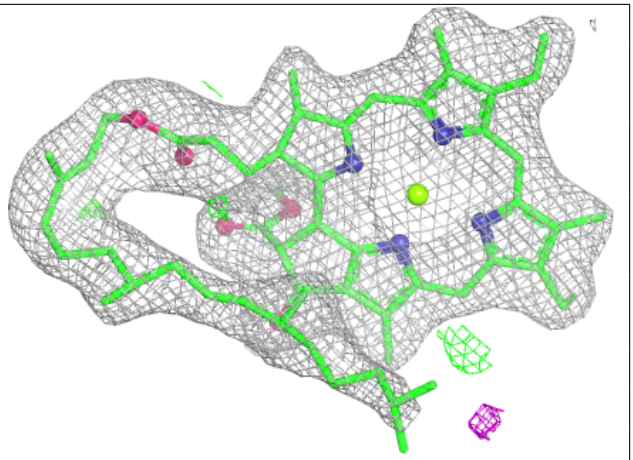


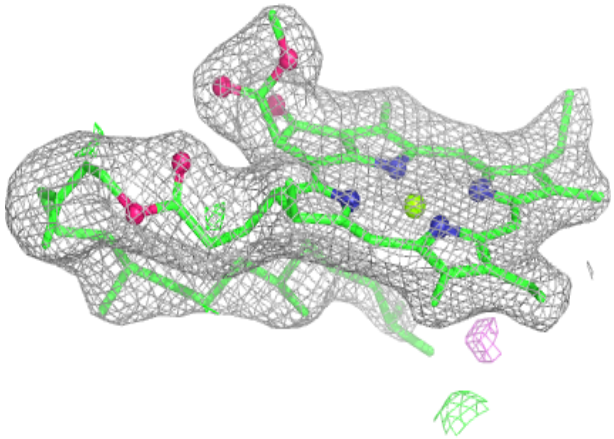


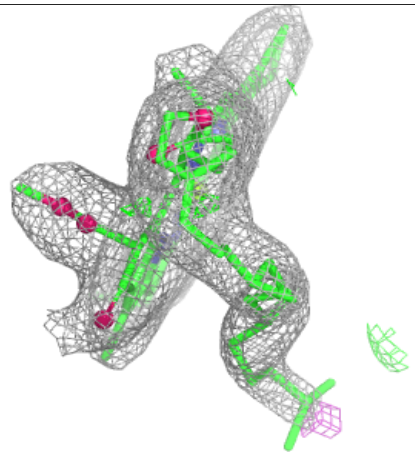


Electron density around CLA c 512:

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

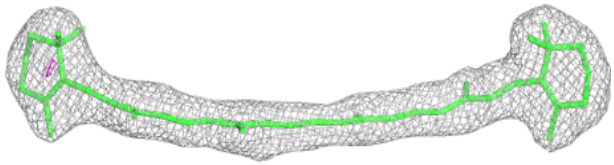


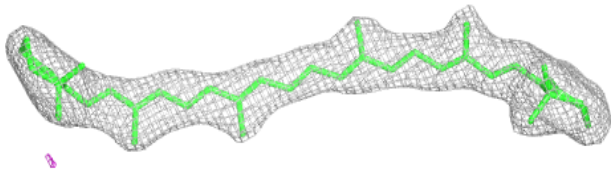


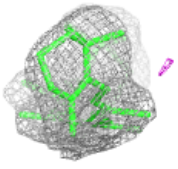


Electron density around BCR k 302:

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

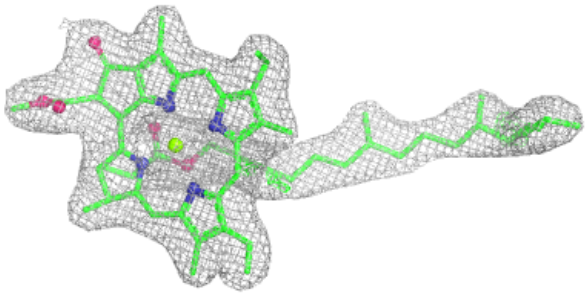


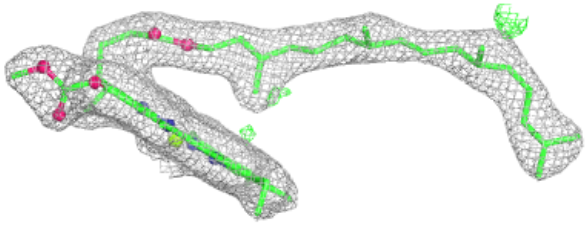


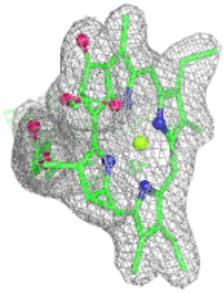


Electron density around CLA B 609:

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

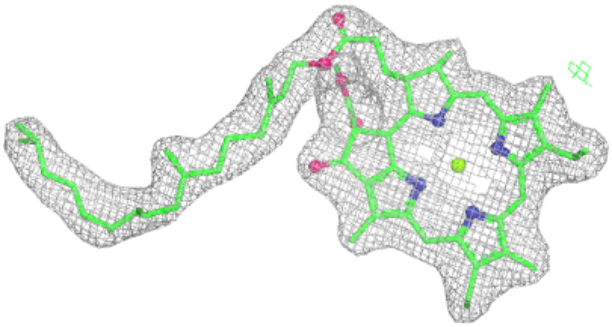


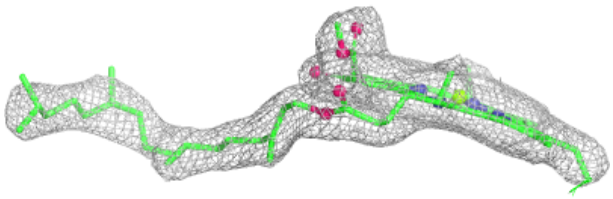




Electron density around CLA b 607:

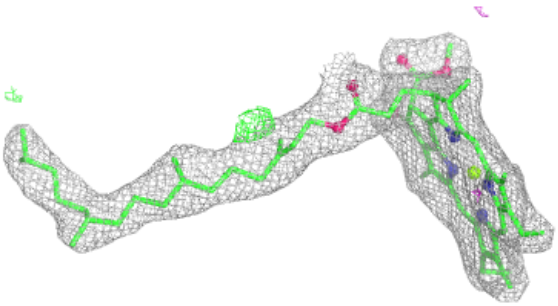
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

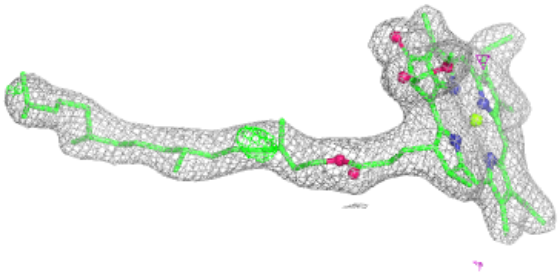


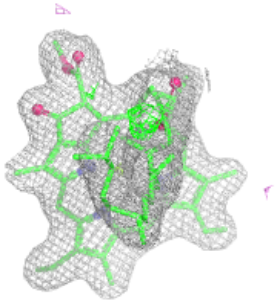


Electron density around CLA b 609:

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

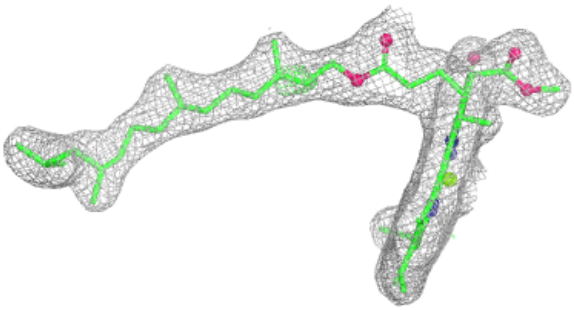


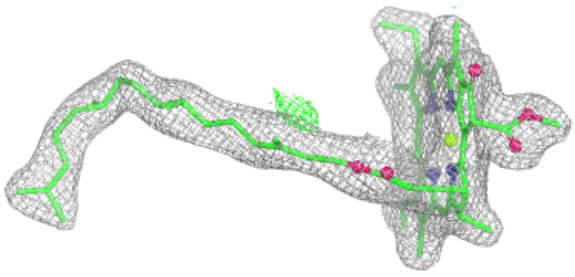


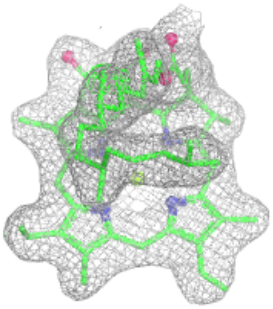


Electron density around CLA b 610:

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

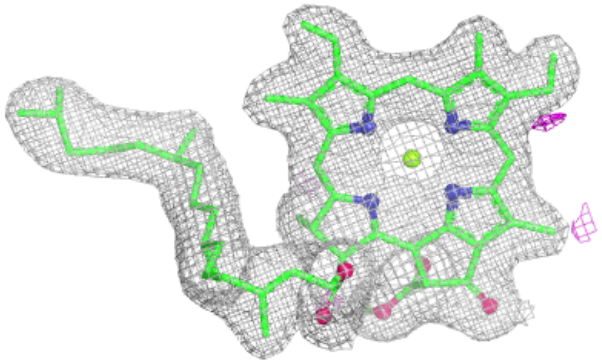


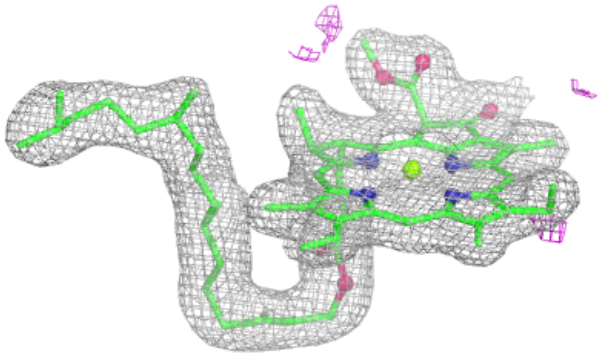


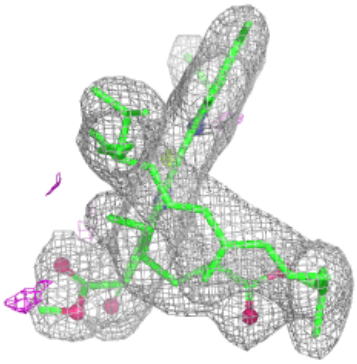


Electron density around CLA d 402:

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

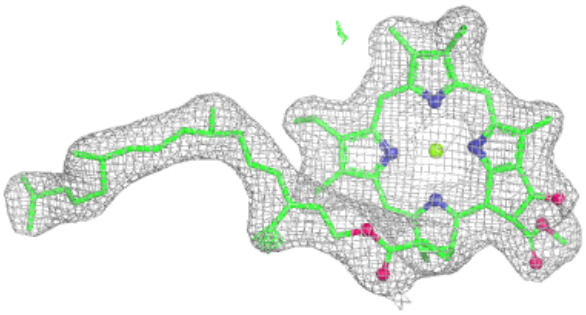


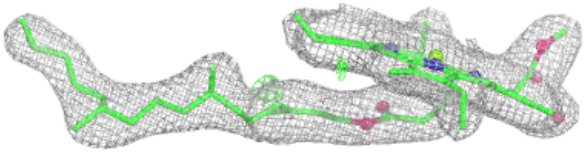




Electron density around CLA B 604:

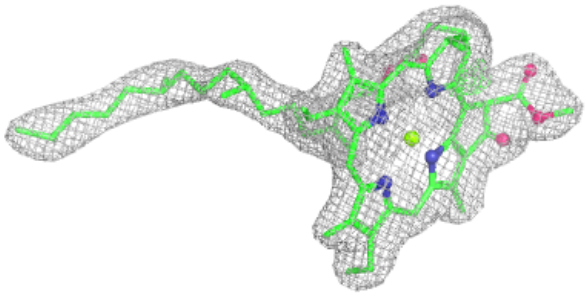
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

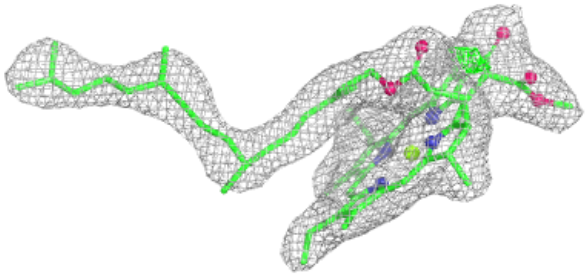


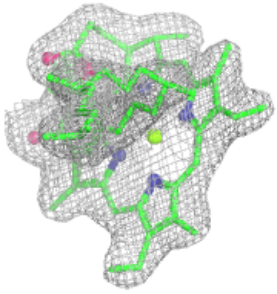


Electron density around CLA C 506:

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

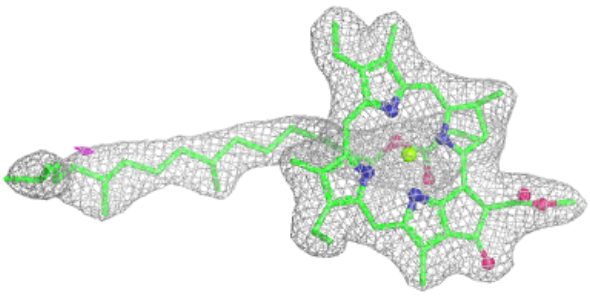


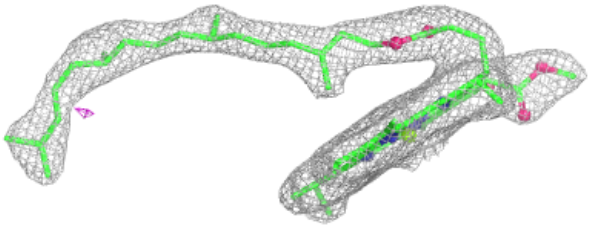


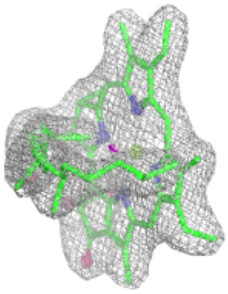


Electron density around CLA b 613:

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

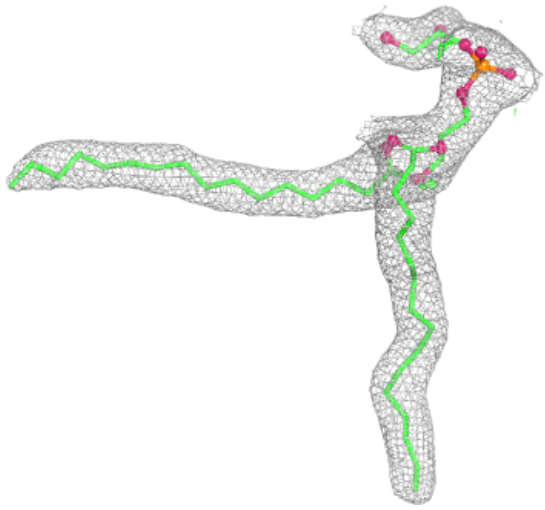


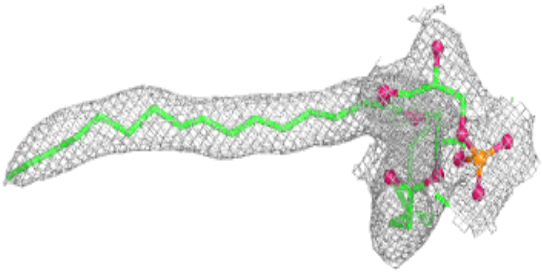


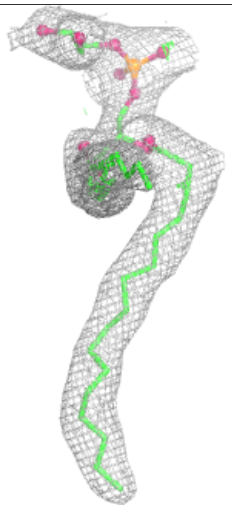


Electron density around LHG L 101:

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

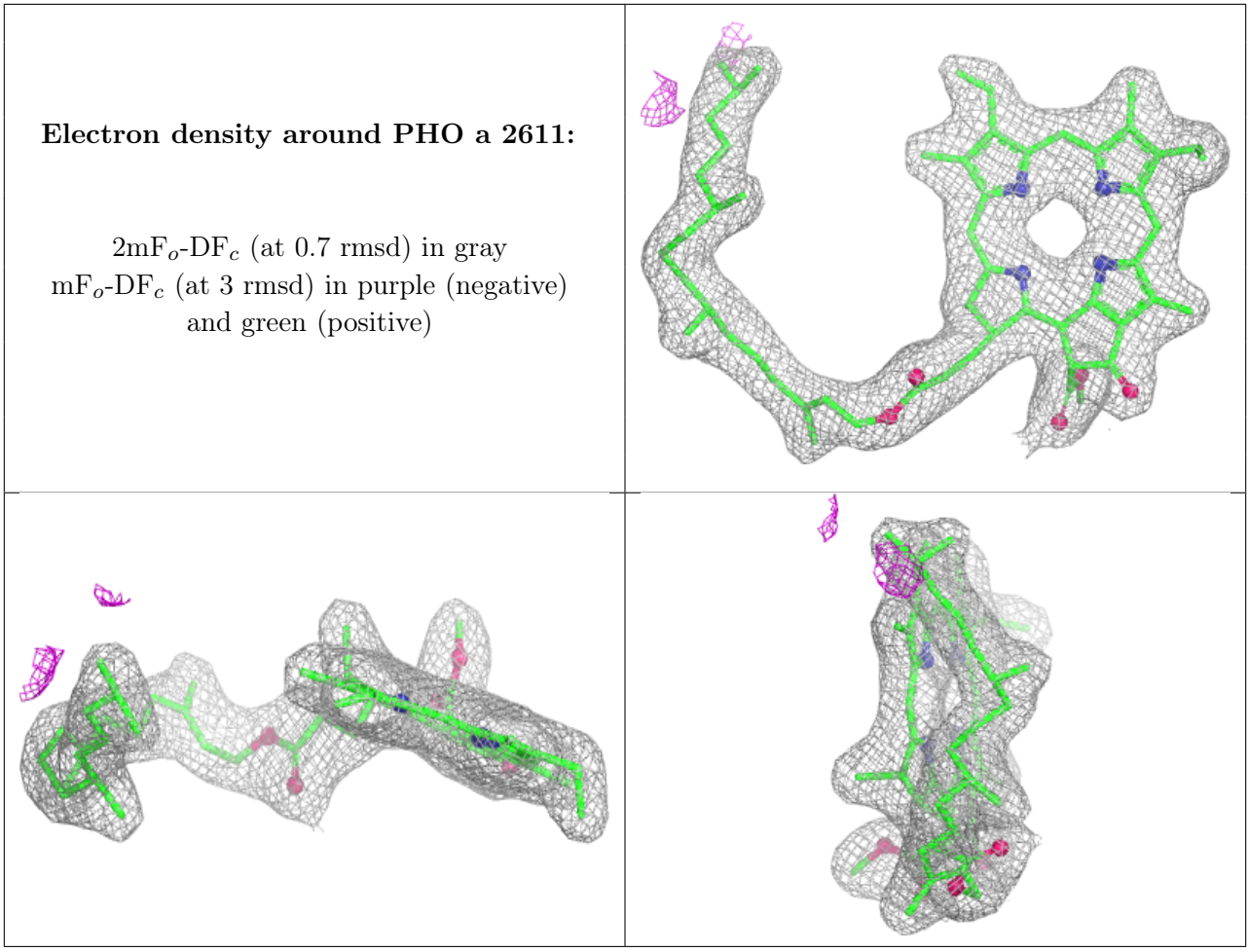






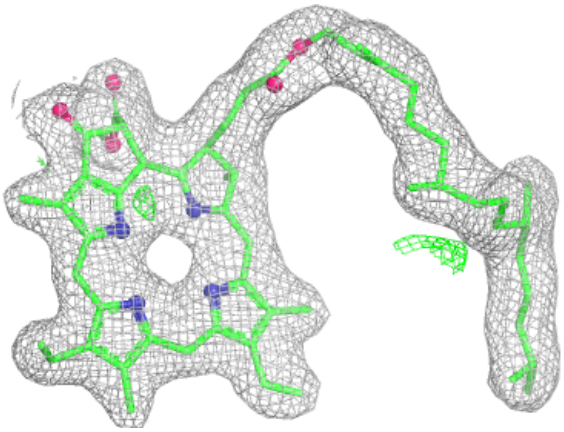
Electron density around PHO a 2611:

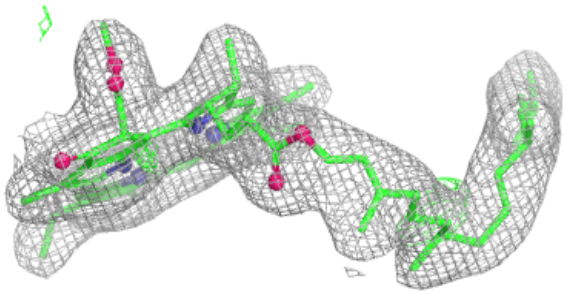
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

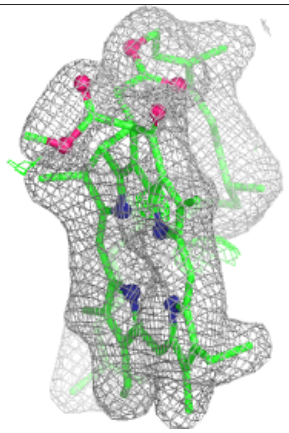


Electron density around PHO a 2612:

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

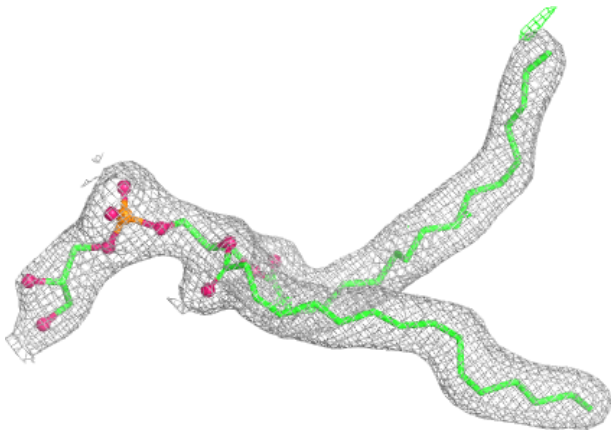


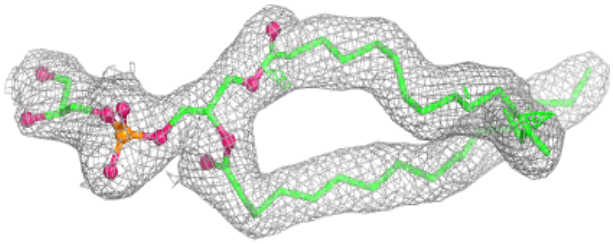


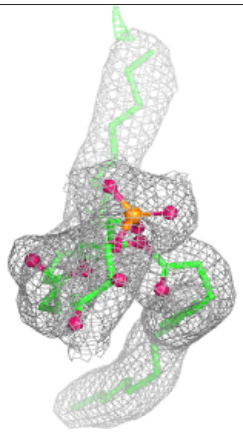


Electron density around LHG d 413:

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

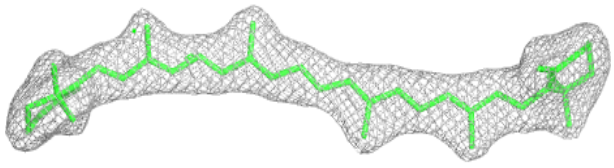


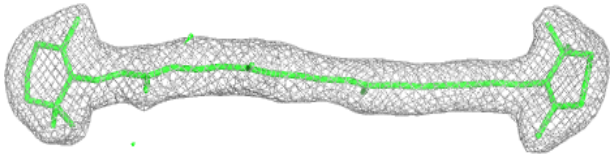


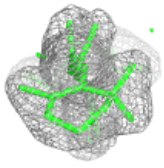


Electron density around BCR A 411:

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

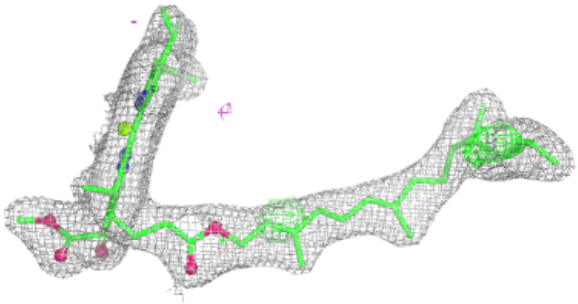


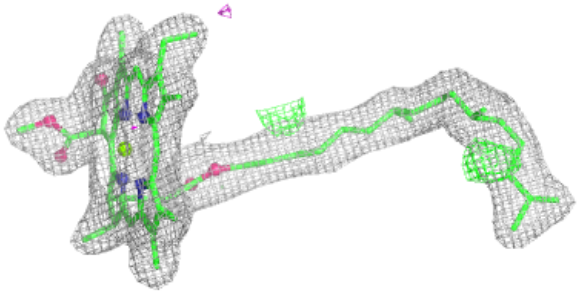


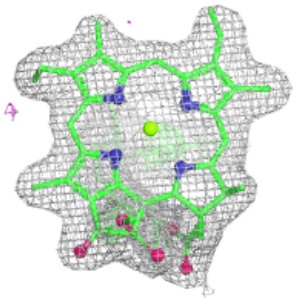


Electron density around CLA B 606:

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

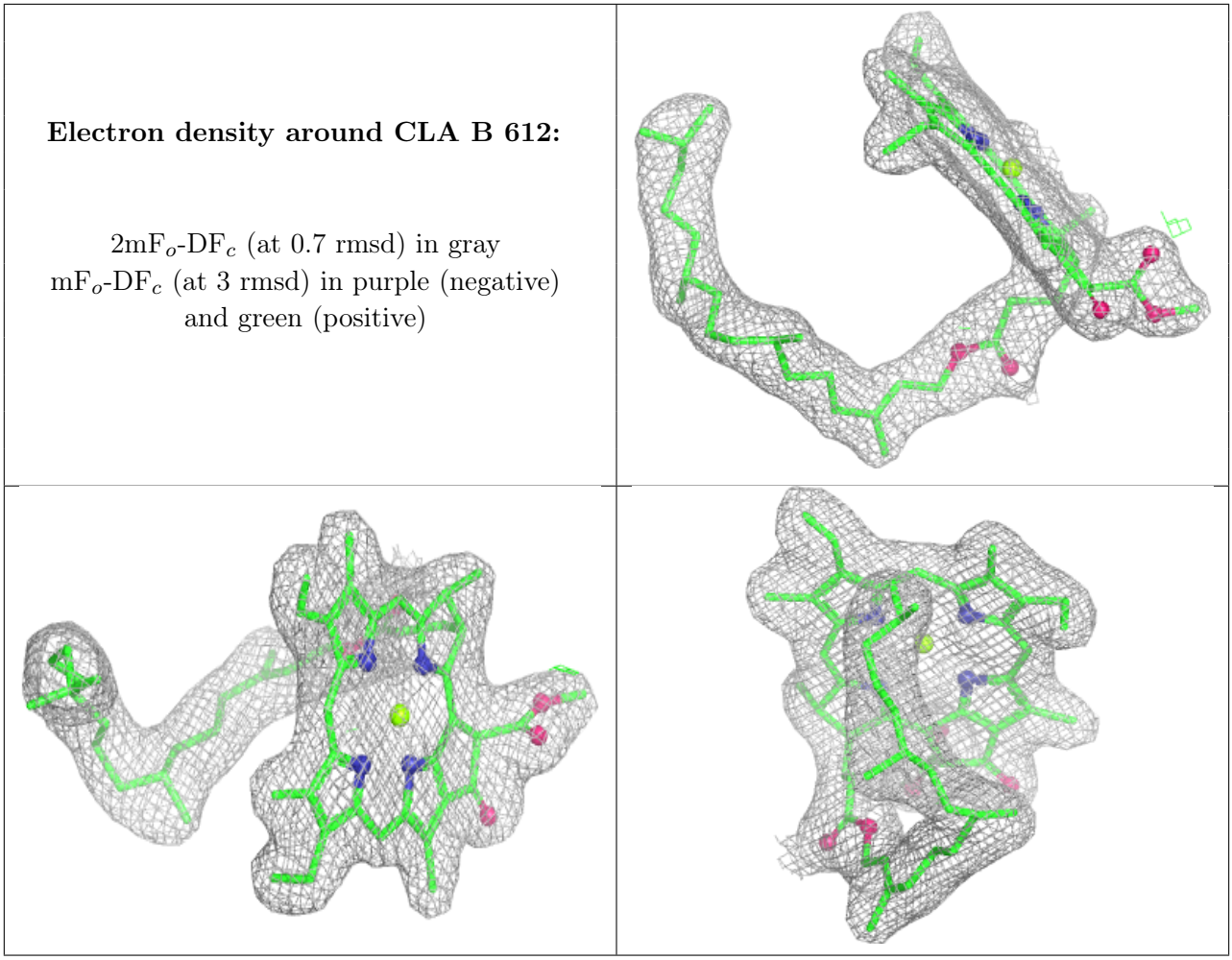






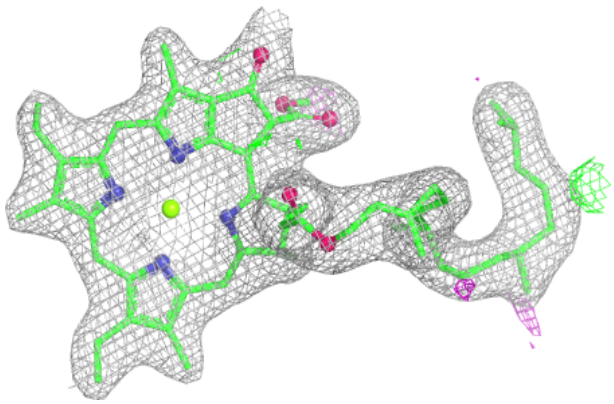
Electron density around CLA B 612:

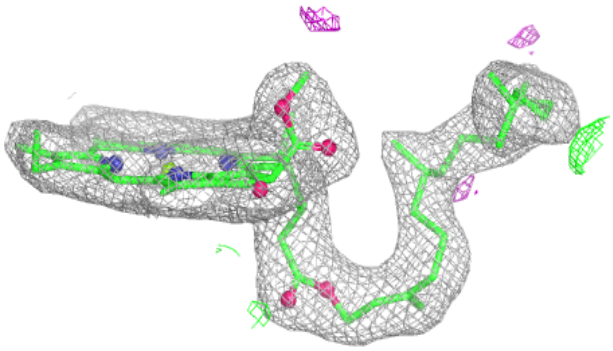
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

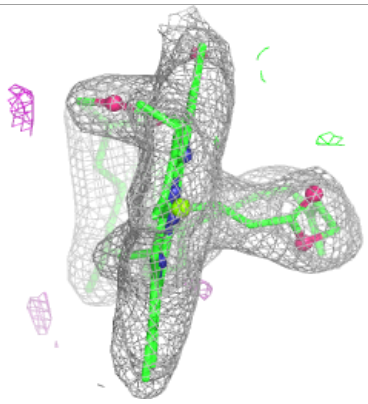


Electron density around CLA B 613:

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

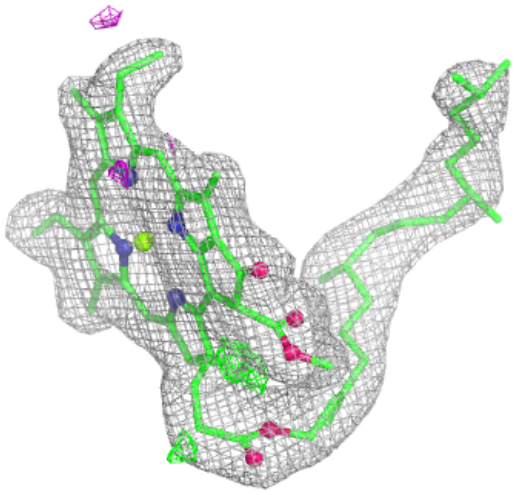


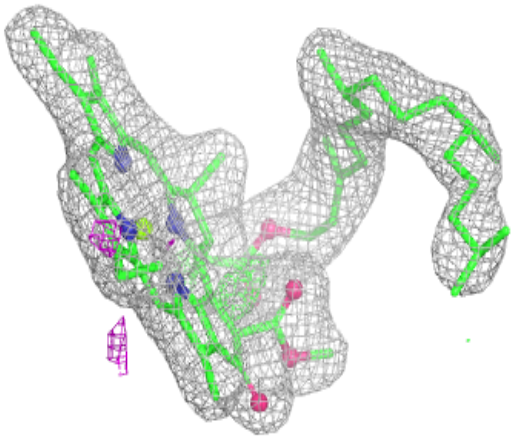


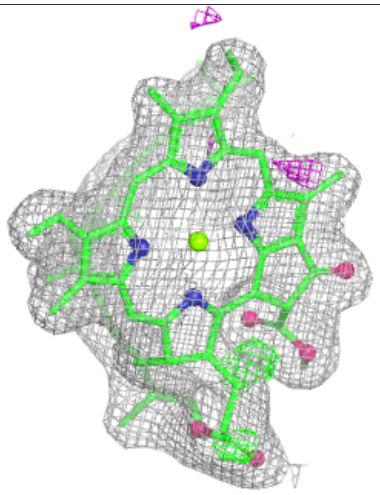


Electron density around CLA b 618:

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

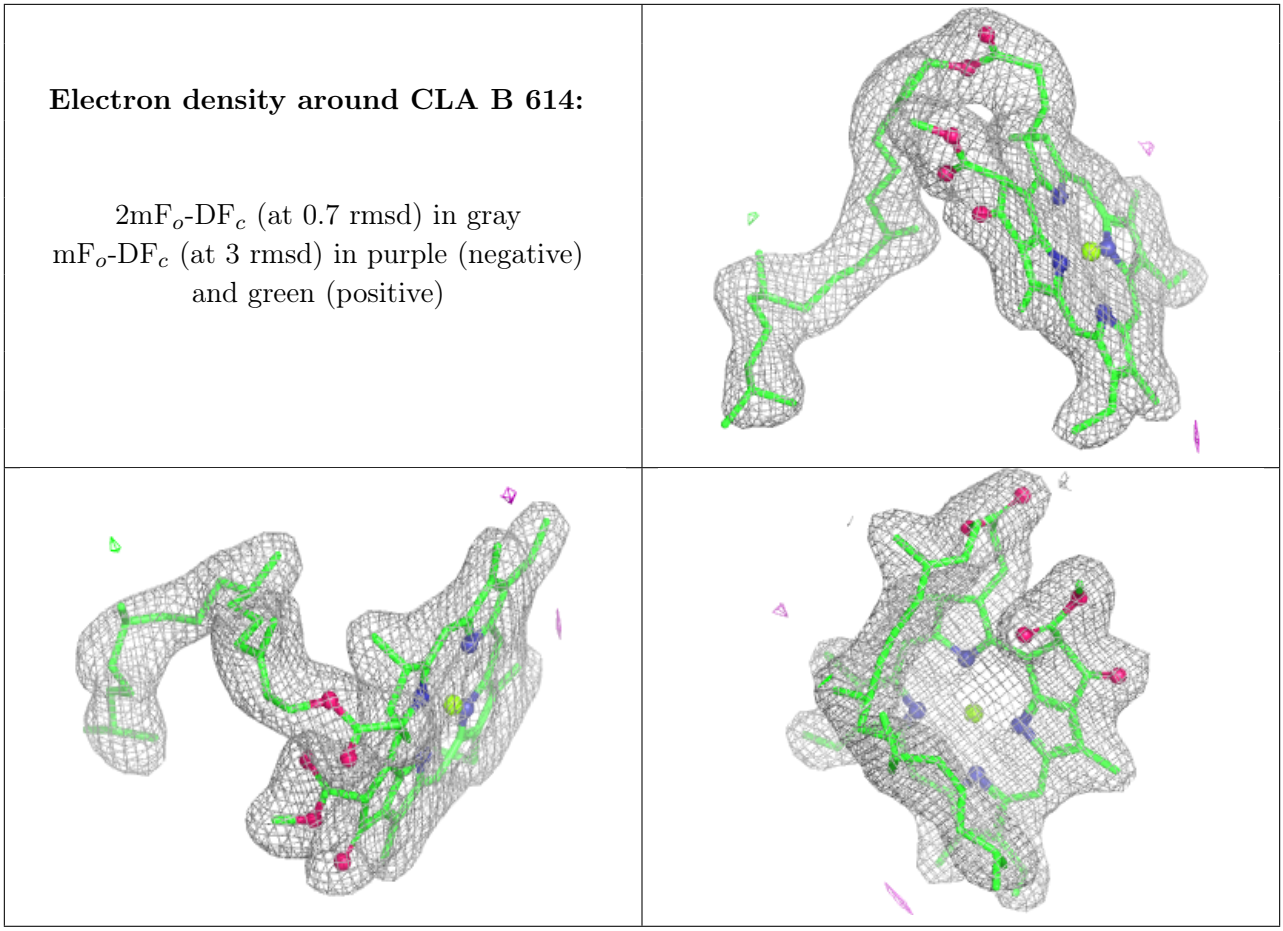






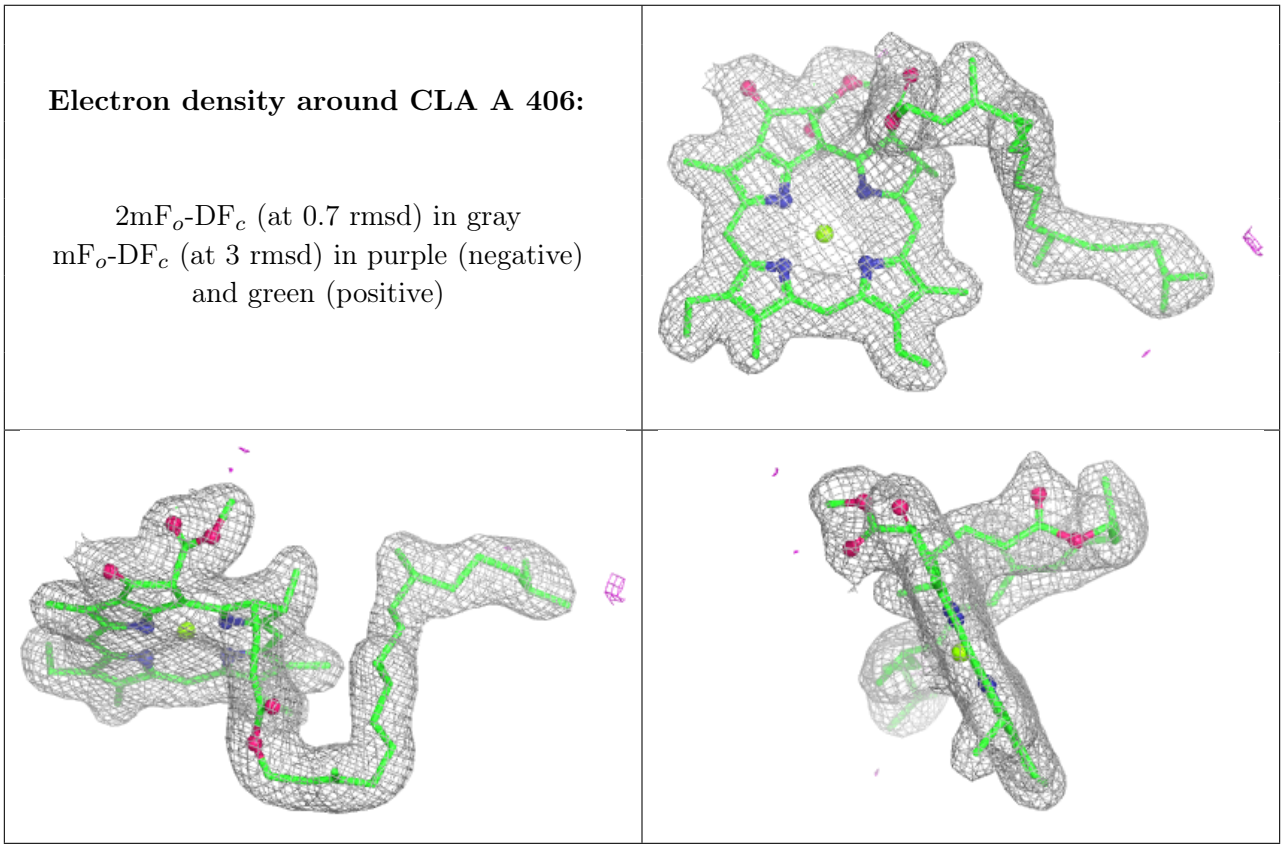
Electron density around CLA B 614:

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



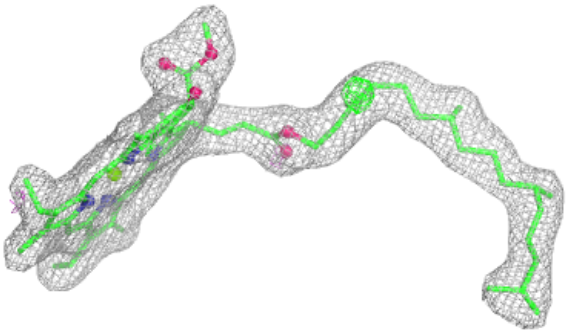
Electron density around CLA A 406:

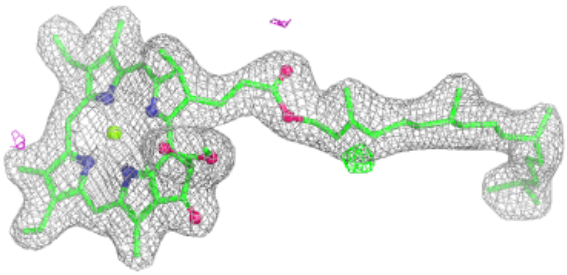
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

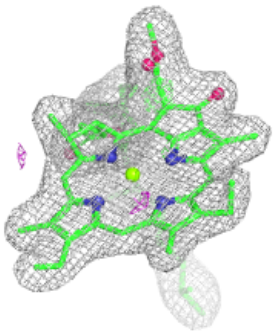


Electron density around CLA D 2303:

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

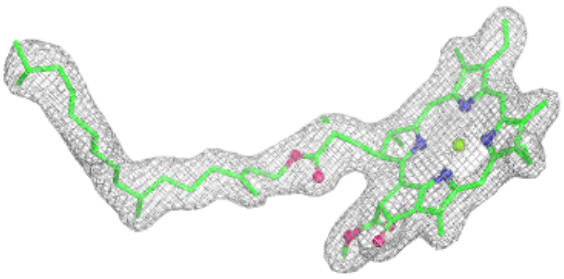


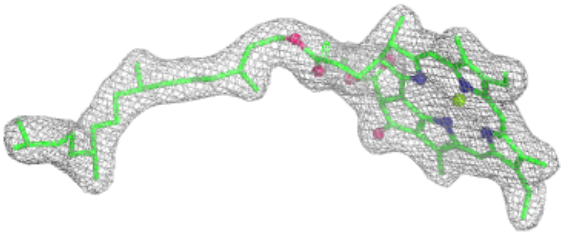


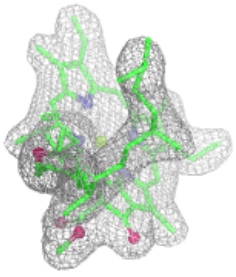


Electron density around CLA A 405:

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

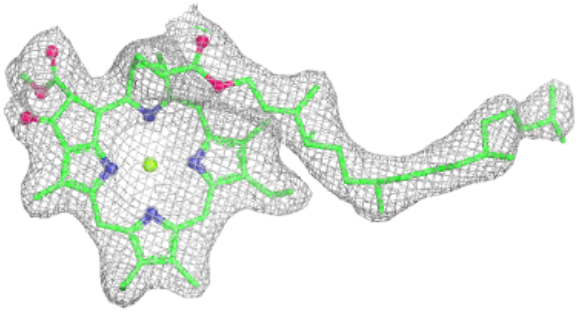


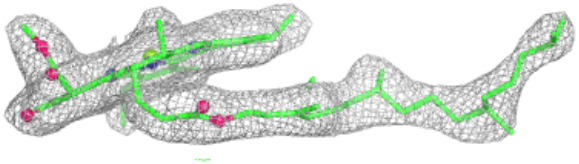


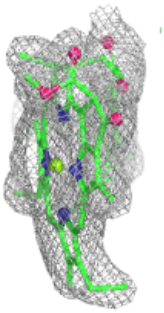


Electron density around CLA b 608:

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

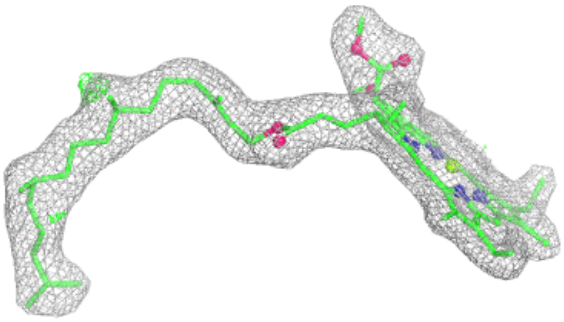


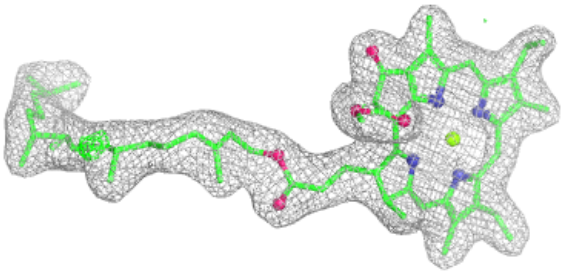


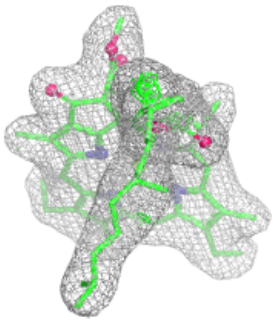


Electron density around CLA d 408:

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

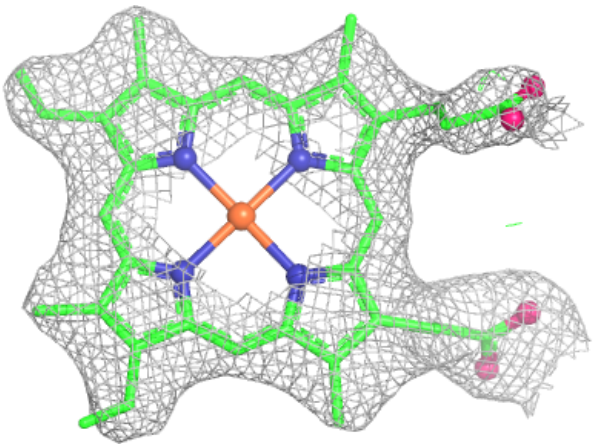


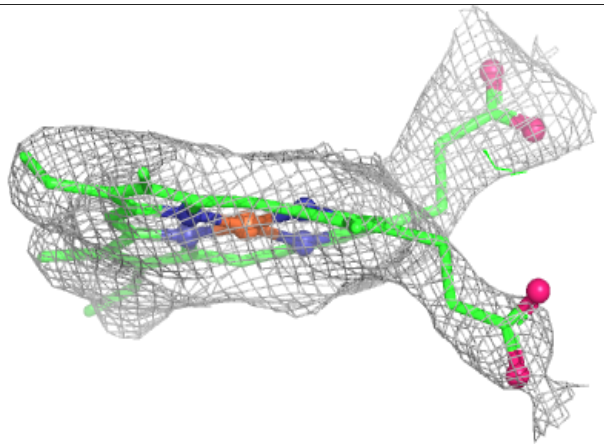


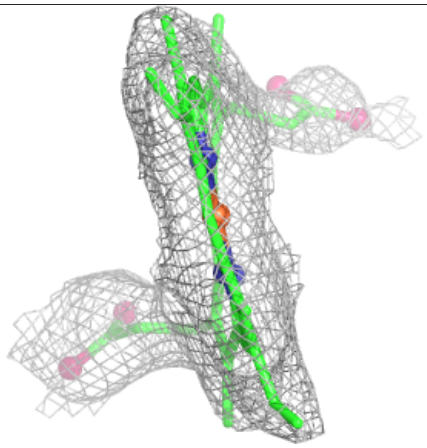


Electron density around HEM F 101:

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

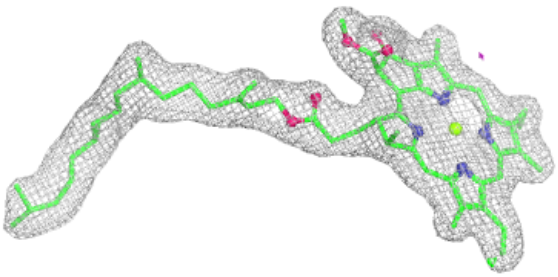


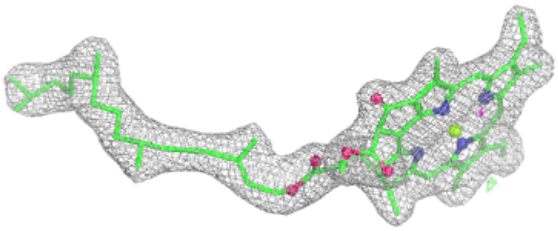


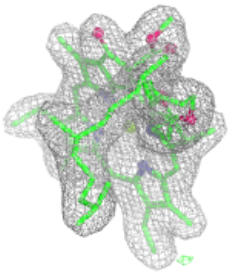


Electron density around CLA a 2609:

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

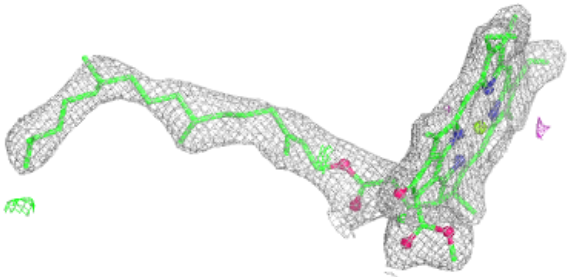


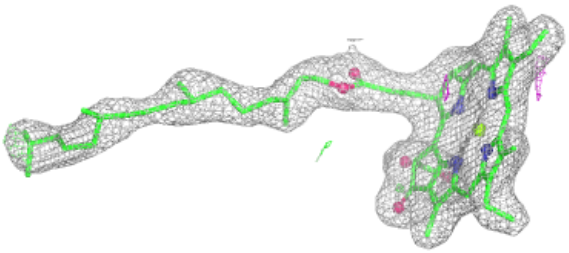


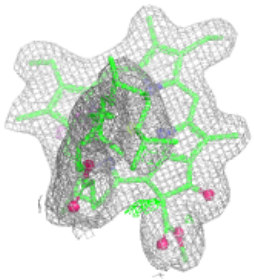


Electron density around CLA B 605:

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

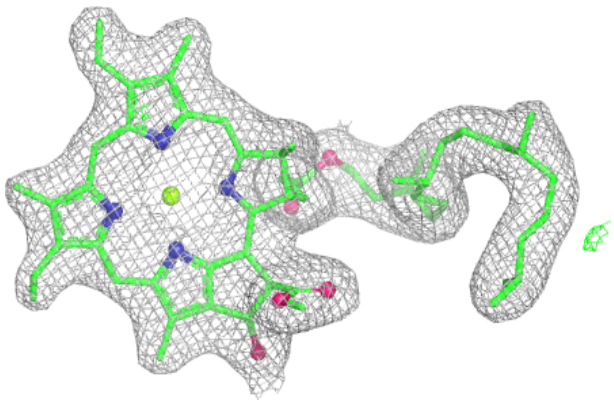


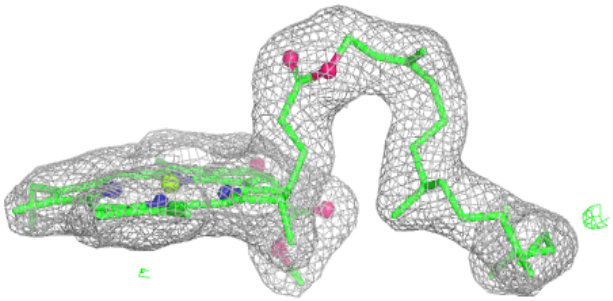


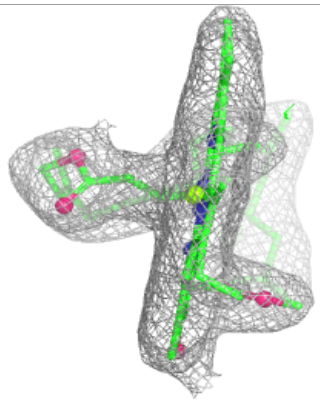


Electron density around CLA b 617:

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

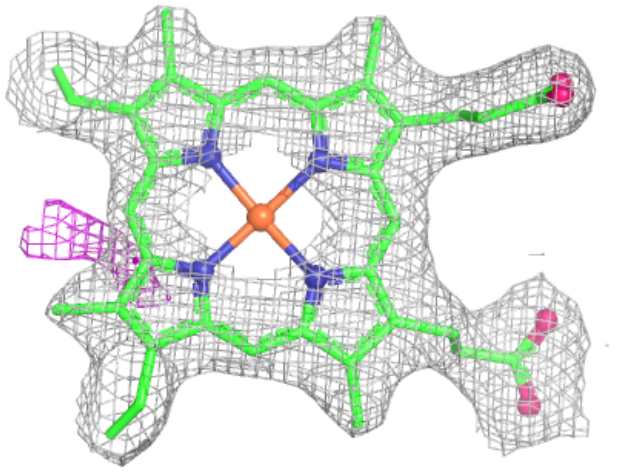


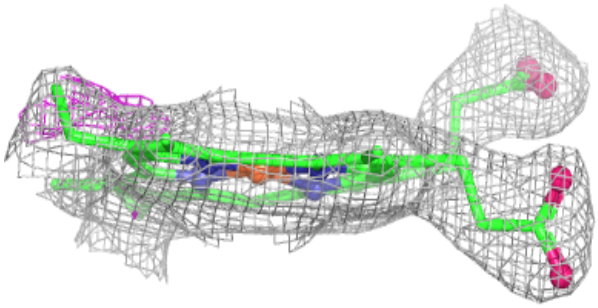




Electron density around HEC v 201:

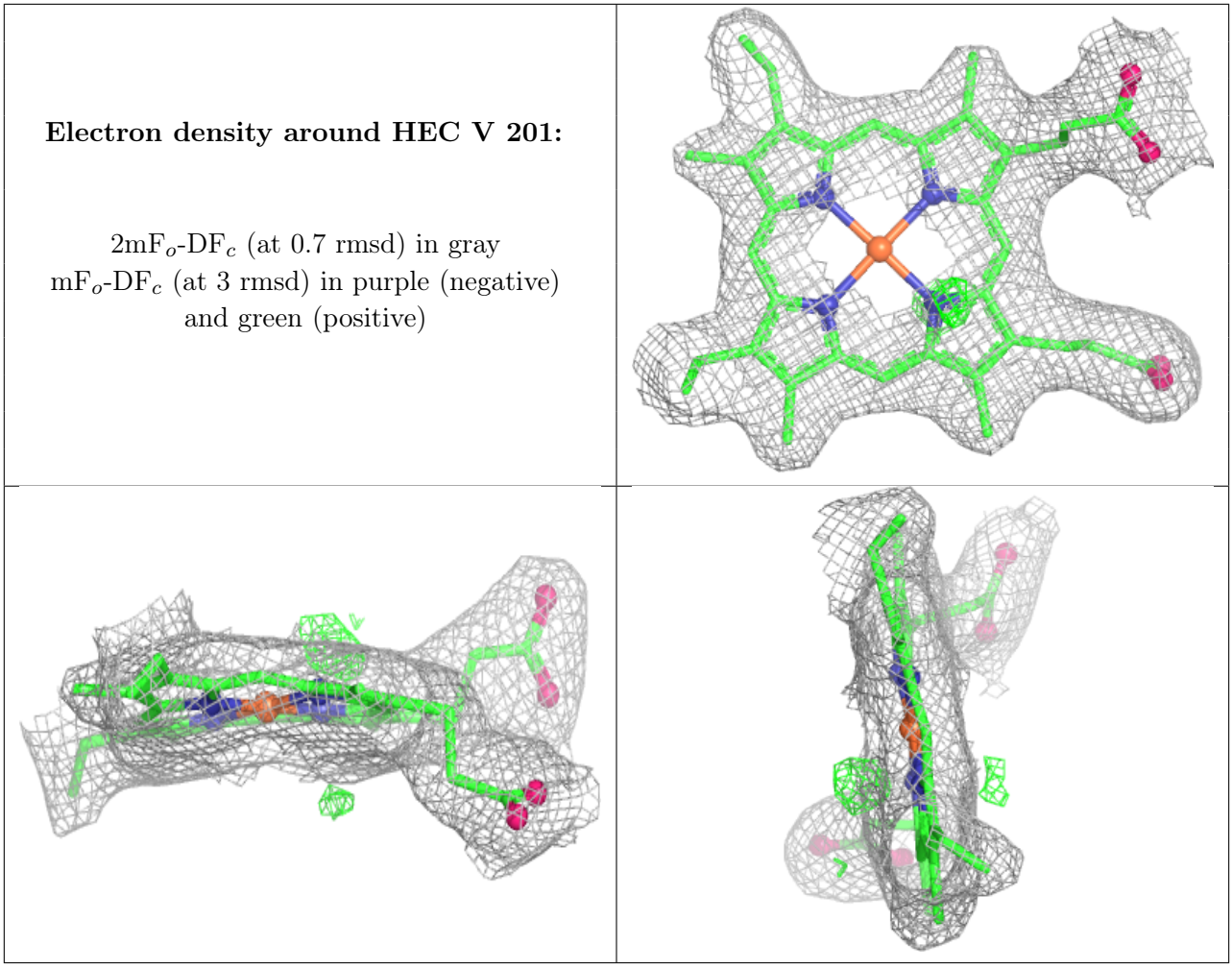
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC V 201:

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



6.5 Other polymers

There are no such residues in this entry.