Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 07:37 AM JST

PDB ID	:	5GTH / pdb_00005gth
Title	:	Native XFEL structure of photosystem II (dark dataset)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2016-08-20
Resolution	:	2.50 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:

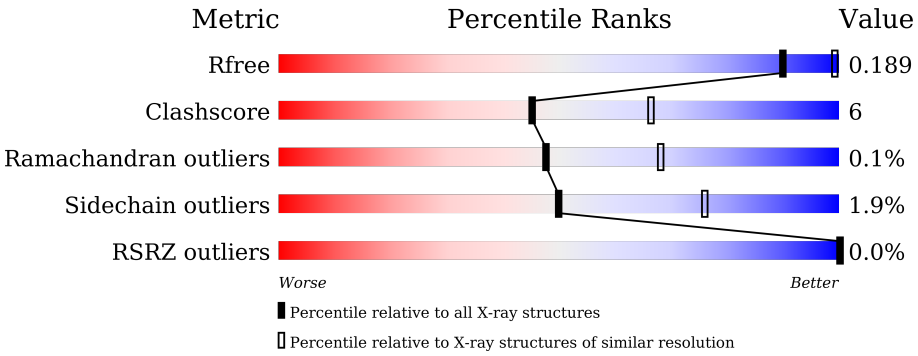
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	87% 10% ·
1	a	344	86% 11% ·
2	B	505	89% 10% ·
2	b	505	89% 10% ·
3	C	455	89% 9% ··
3	c	455	90% 10% ·

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Mol	Chain	Length	Quality of chain
4	D	342	93% 7%
4	d	342	93% 7%
5	E	84	80% 17%
5	e	84	79% 13% 6%
6	F	44	61% 16% 23%
6	f	44	64% 7% 30%
7	H	65	2% 92% 6%
7	h	65	85% 15%
8	I	38	82% 18%
8	i	38	76% 21%
9	J	39	85% 10%
9	j	39	85% 15%
10	K	37	84% 14%
10	k	37	70% 22% 8%
11	L	37	86% 11%
11	l	37	92% 5%
12	M	36	72% 19% 8%
12	m	36	69% 22% 6%
13	O	244	85% 14%
13	o	244	86% 13%
14	T	32	81% 6% 6% 6%
14	t	32	81% 9% 6%
15	U	104	78% 14% 8%
15	u	104	90% 7%
16	V	137	94% 6%

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Mol	Chain	Length	Quality of chain
16	v	137	93% 6%
17	X	40	90% 5% 5%
17	x	40	82% 12% 5%
18	Y	30	73% 20%
18	y	30	70% 27%
19	Z	62	85% 13%
19	z	62	85% 13%
20	R	34	85% 15%

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
40	HEC	V	202	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 52773 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
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	5	0
			2639	1732	431	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	5	0
			3537	2317	589	618	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 665	C 434	N 107	O 124	0	1	0
5	e	79	Total 648	C 424	N 105	O 119	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	31	Total 250	C 170	N 42	O 37	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total 514	C 344	N 84	O 84	S 2	0	1	0
7	h	65	Total 511	C 341	N 82	O 86	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total 272	C 182	N 42	O 47	S 1	0	0	0
9	j	39	Total 277	C 185	N 43	O 48	S 1	0	0	0

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total 301	C 202	N 47	O 52	0	1	0
11	l	36	Total 301	C 202	N 47	O 52	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 265	C 178	N 38	O 48	S 1	0	1	0
12	m	34	Total 269	C 179	N 40	O 49	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1889	C 1182	N 315	O 387	S 5	0	5	0
13	o	243	Total 1873	C 1171	N 315	O 382	S 5	0	2	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total 765	C 486	N 128	O 151	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

- 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		

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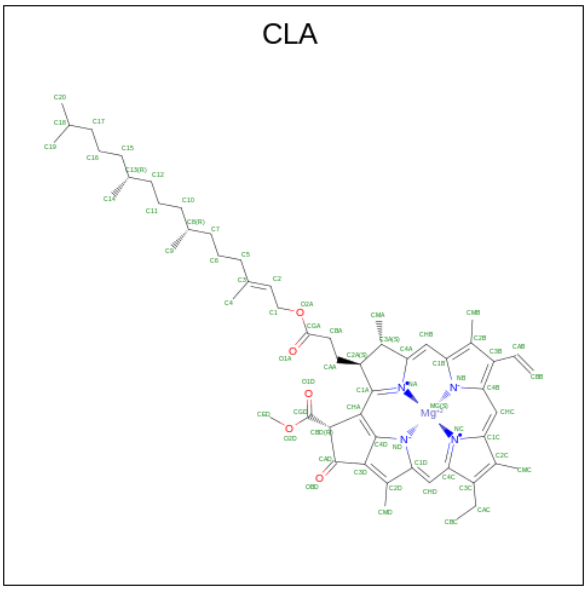
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

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

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

- 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 65 55 1 4 5	0	0
23	A	1	Total C Mg N O 65 55 1 4 5	0	0
23	A	1	Total C Mg N O 65 55 1 4 5	0	0
23	A	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0
23	B	1	Total C Mg N O 65 55 1 4 5	0	0

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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	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		

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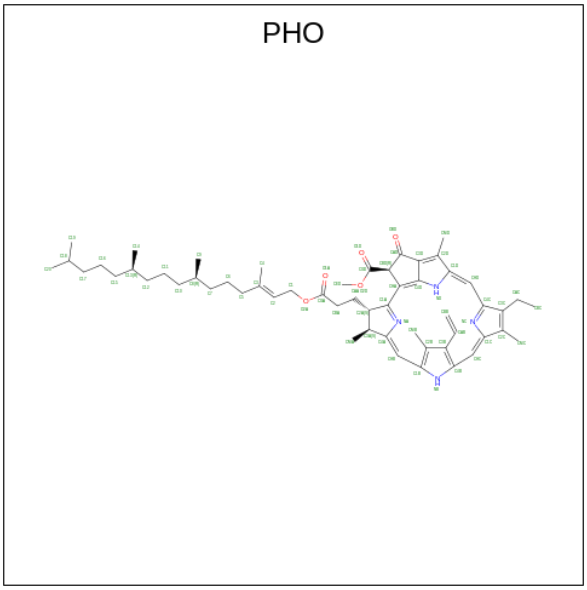
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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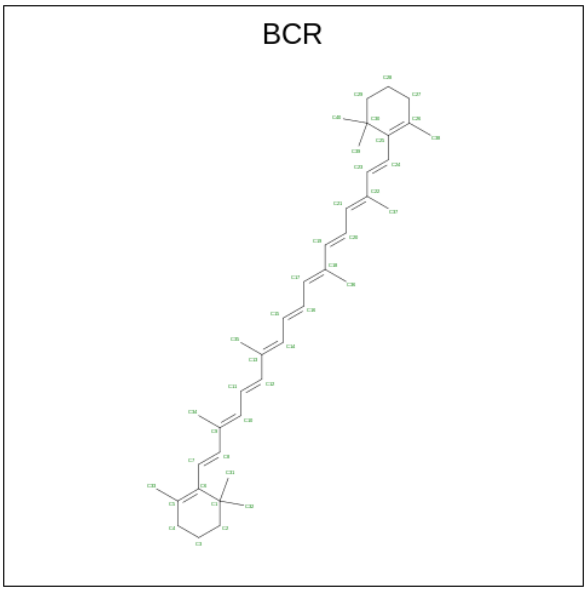
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	D	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: $C_{40}H_{56}$).



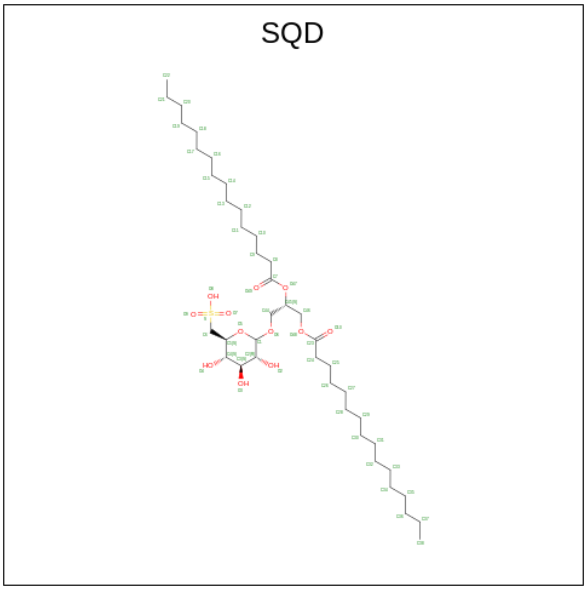
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	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

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



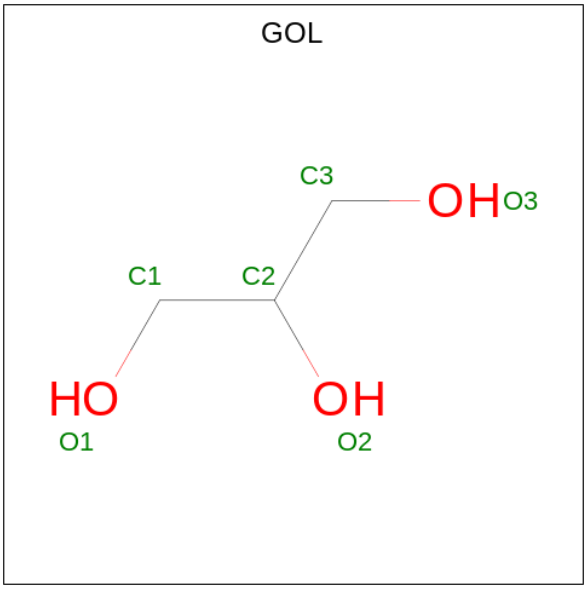
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total C O S 43 30 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	f	1	Total C O S 43 30 12 1	0	0

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



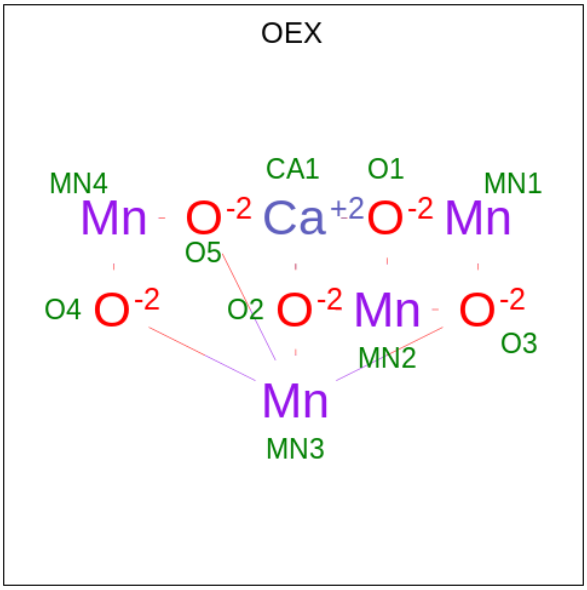
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0

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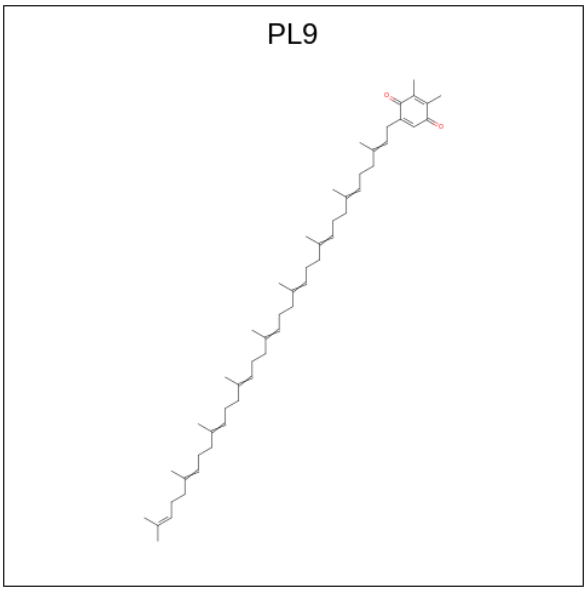
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	d	1	Total C O 6 3 3	0	0

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

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



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

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

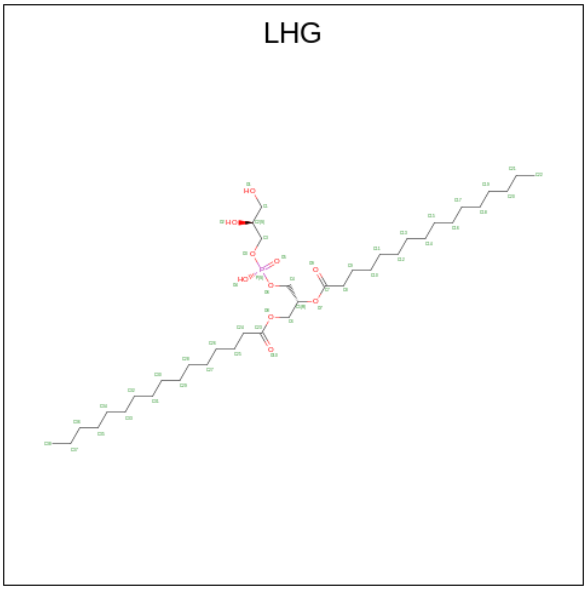
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 34 29 5	0	0
30	M	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	2	Total C O 69 59 10	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	1	Total C O 17 16 1	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



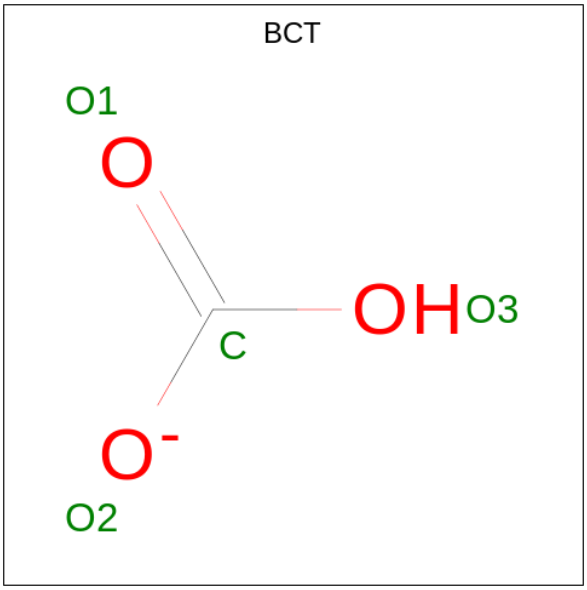
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O P 49 38 10 1	0	0
31	A	1	Total C O P 49 38 10 1	0	0
31	D	1	Total C O P 49 38 10 1	0	0

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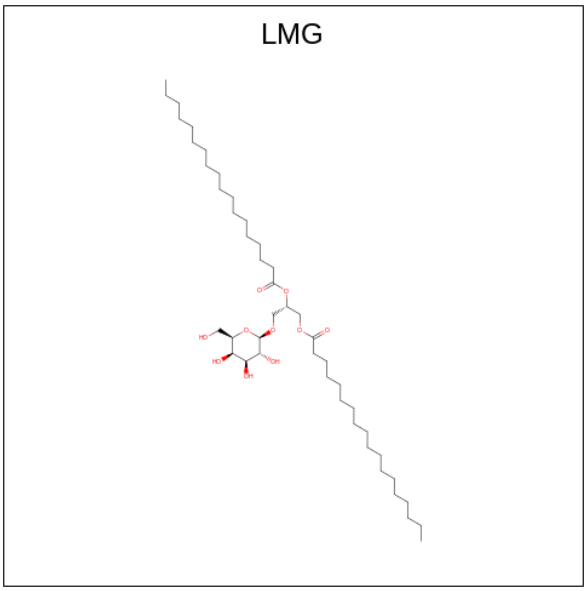
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

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



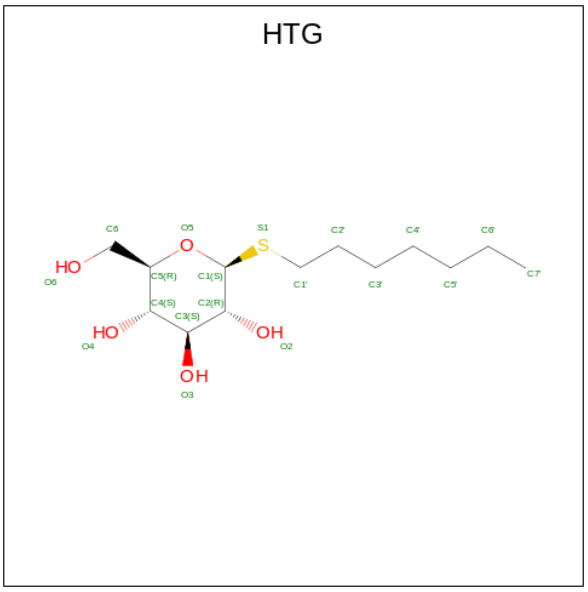
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	J	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 37 27 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	b	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	j	1	Total C O 51 41 10	0	0
33	z	1	Total C O 39 29 10	0	0

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



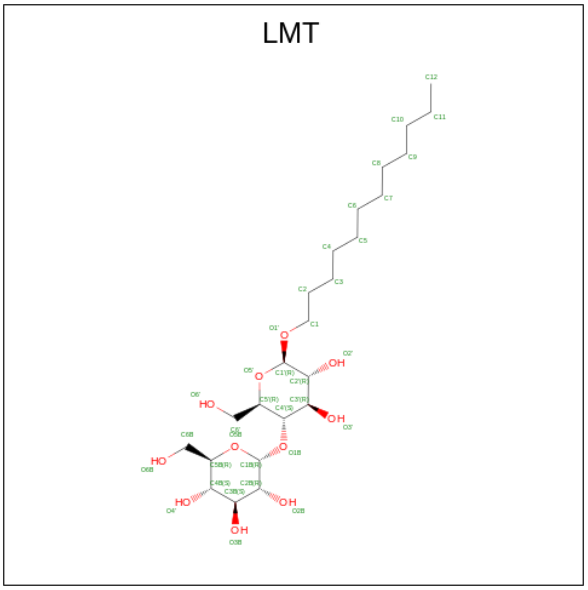
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	d	1	Total C O S 16 10 5 1	0	0

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



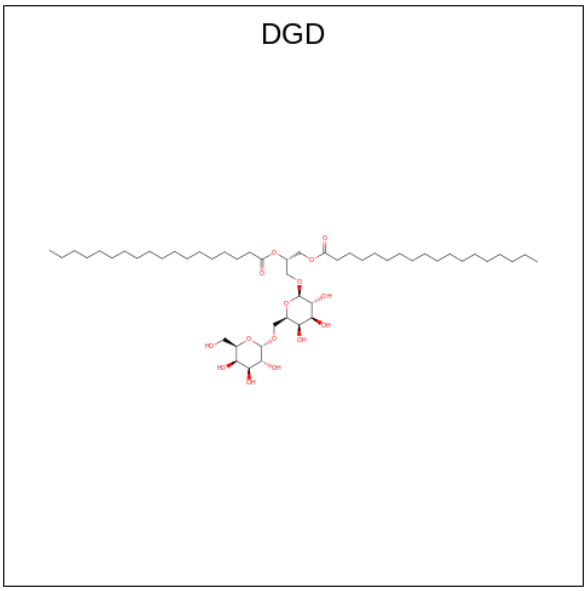
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total C O 25 19 6	0	0
35	B	1	Total C O 35 24 11	0	0
35	B	1	Total C O 26 19 7	0	0
35	D	1	Total C O 35 24 11	0	0
35	D	1	Total C O 35 24 11	0	0
35	E	1	Total C O 35 24 11	0	0
35	I	1	Total C O 35 24 11	0	0
35	M	1	Total C O 35 24 11	0	0
35	M	1	Total C O 35 24 11	0	0
35	a	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	b	1	Total C O 25 19 6	0	0
35	b	1	Total C O 25 19 6	0	0
35	e	1	Total C O 35 24 11	0	0
35	m	1	Total C O 35 24 11	0	0

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



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

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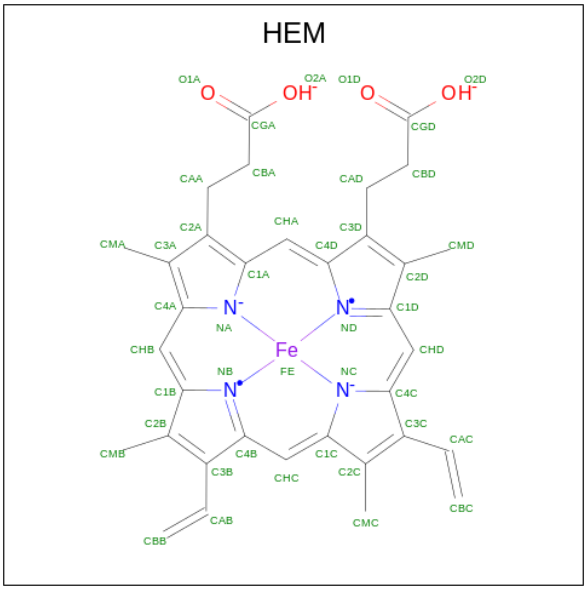
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	V	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0
37	o	1	Total Ca 1 1	0	0

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

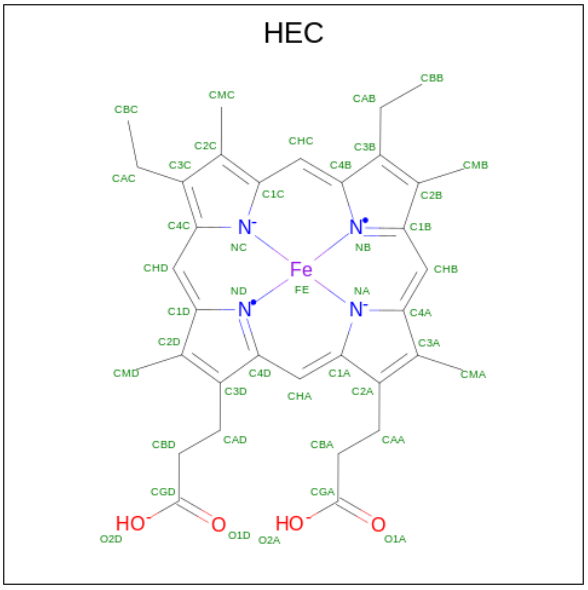


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	E	1	Total C Fe N O 43 34 1 4 4	0	0
38	e	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	127	Total O 127 127	0	0
41	B	175	Total O 175 175	0	0
41	C	148	Total O 148 148	0	0
41	D	111	Total O 111 111	0	0
41	E	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	5	Total O 5 5	0	0
41	H	19	Total O 19 19	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	6	Total O 6 6	0	0
41	L	9	Total O 9 9	0	0
41	M	14	Total O 14 14	0	0
41	O	100	Total O 100 100	0	0
41	T	10	Total O 10 10	0	0
41	U	46	Total O 46 46	0	0
41	V	78	Total O 79 79	0	1
41	X	3	Total O 3 3	0	0
41	Y	1	Total O 1 1	0	0
41	a	130	Total O 130 130	0	0
41	b	192	Total O 192 192	0	0
41	c	136	Total O 136 136	0	0
41	d	108	Total O 108 108	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	28	Total O 28 28	0	0
41	i	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	j	3	Total O 3 3	0	0
41	k	4	Total O 4 4	0	0
41	l	7	Total O 7 7	0	0
41	m	11	Total O 11 11	0	0
41	o	109	Total O 109 109	0	0
41	t	7	Total O 7 7	0	0
41	u	64	Total O 64 64	0	0
41	v	71	Total O 71 71	0	0
41	x	4	Total O 4 4	0	0
41	y	2	Total O 2 2	0	0

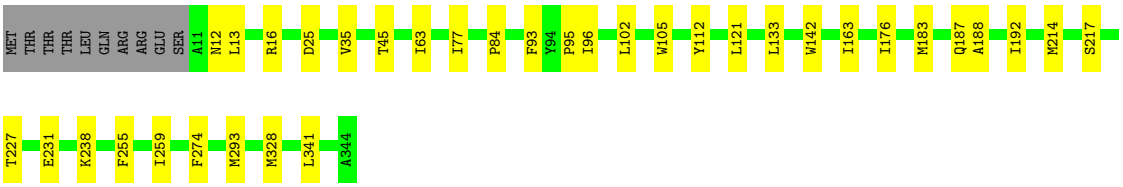
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

Chain A:

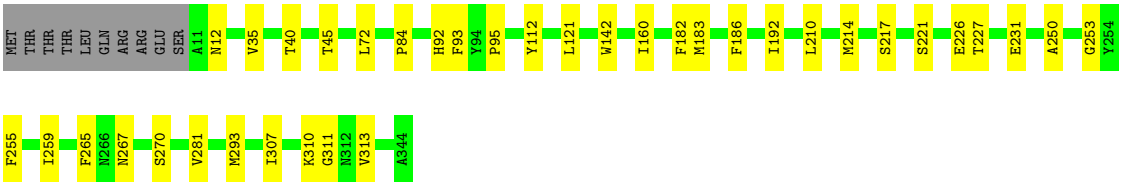




• Molecule 1: Photosystem II protein D1

Chain a:

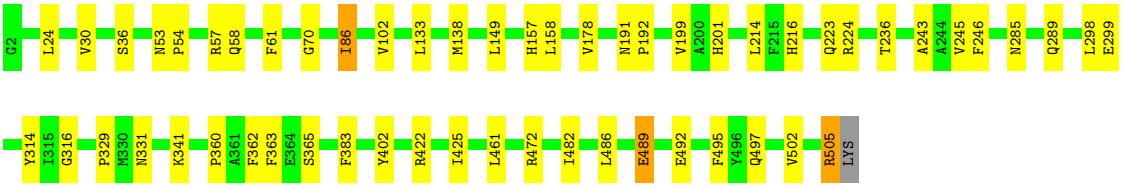




• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

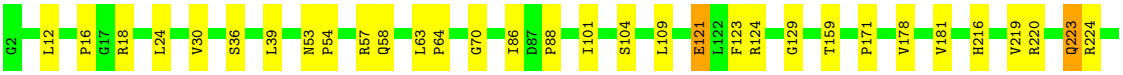




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



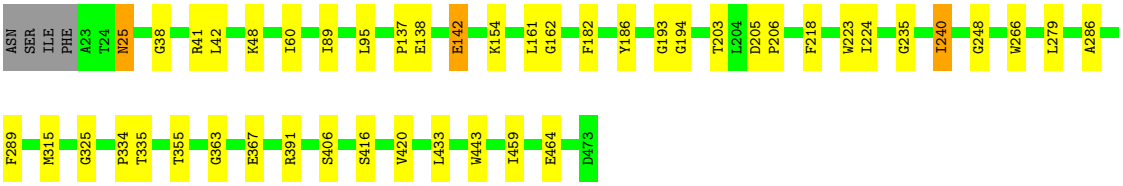




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

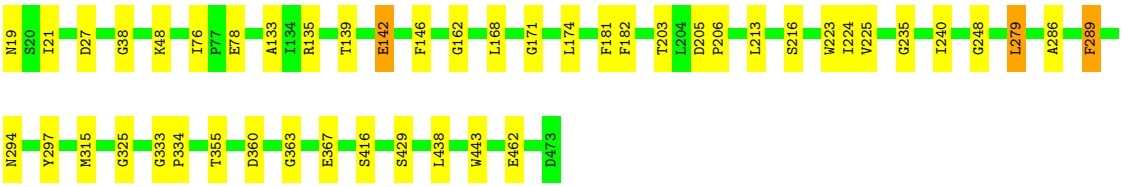




• Molecule 3: Photosystem II CP43 reaction center protein

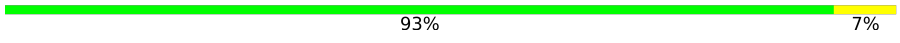
Chain c:





• Molecule 4: Photosystem II D2 protein

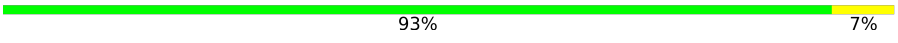
Chain D:

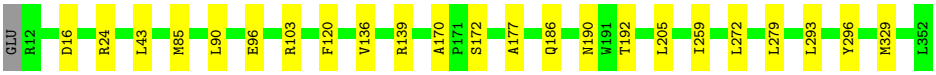




• Molecule 4: Photosystem II D2 protein

Chain d:

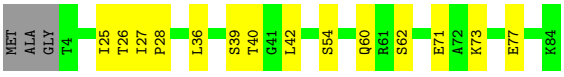




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

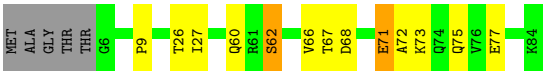




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta





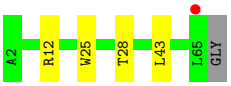
• Molecule 6: Cytochrome b559 subunit beta



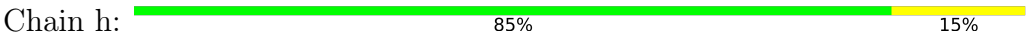


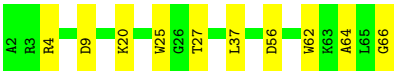
• Molecule 7: Photosystem II reaction center protein H



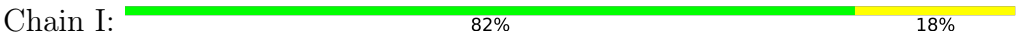


• Molecule 7: Photosystem II reaction center protein H





• Molecule 8: Photosystem II reaction center protein I



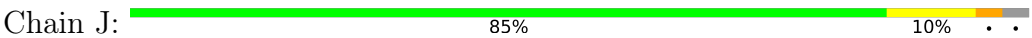


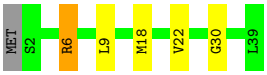
• Molecule 8: Photosystem II reaction center protein I





• Molecule 9: Photosystem II reaction center protein J

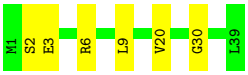




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

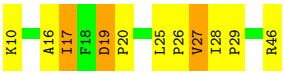




• Molecule 10: Photosystem II reaction center protein K

Chain k:

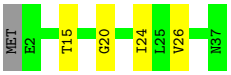




• Molecule 11: Photosystem II reaction center protein L

Chain L:

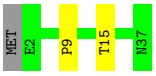




• Molecule 11: Photosystem II reaction center protein L

Chain l:

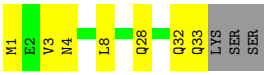




• Molecule 12: Photosystem II reaction center protein M

Chain M:





• Molecule 12: Photosystem II reaction center protein M

Chain m:

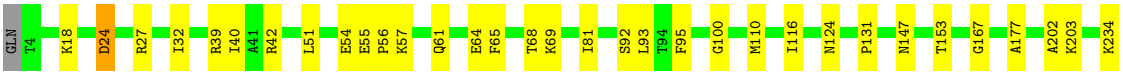




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:







• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

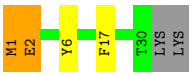




• Molecule 14: Photosystem II reaction center protein T

Chain T:

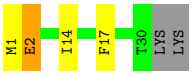




• Molecule 14: Photosystem II reaction center protein T

Chain t:

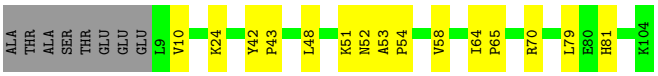




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

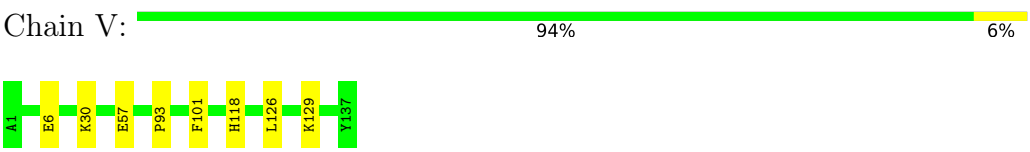
Chain u:





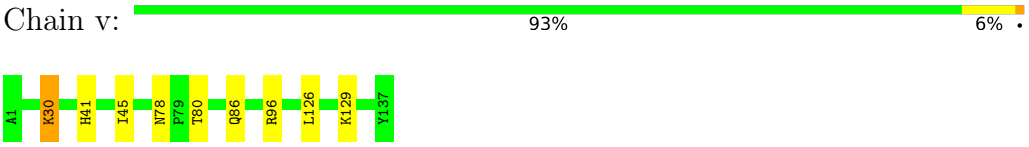
• Molecule 16: Cytochrome c-550

Chain V:



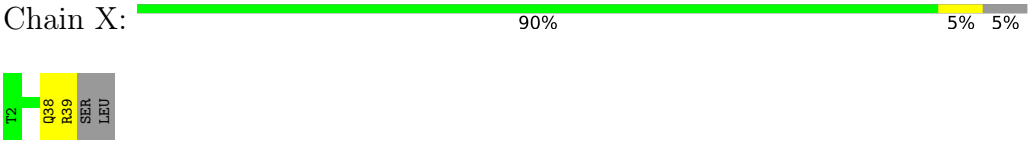
• Molecule 16: Cytochrome c-550

Chain v:



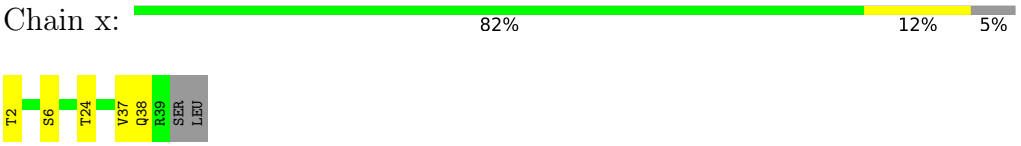
• Molecule 17: Photosystem II reaction center protein X

Chain X:



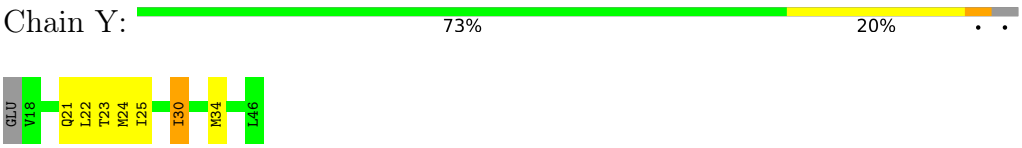
• Molecule 17: Photosystem II reaction center protein X

Chain x:



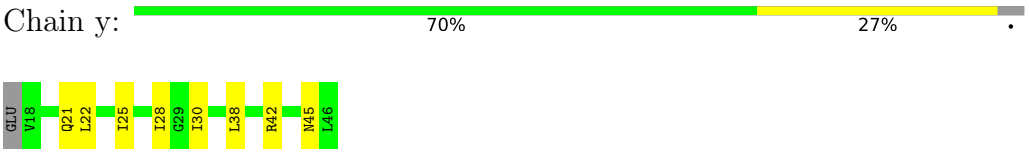
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



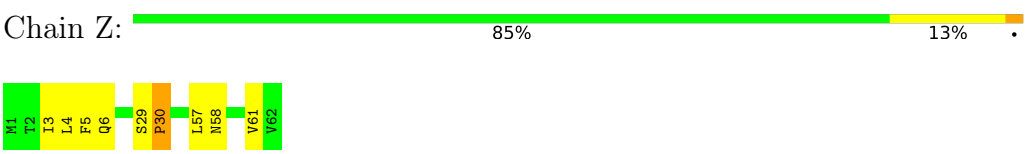
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 19: Photosystem II reaction center protein Z

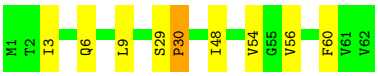
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

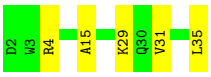




• Molecule 20: Photosystem II protein Y

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 99.7 (19.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.186 0.145 , 0.189	Depositor DCC
R_{free} test set	14615 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.57	0/2728	0.86	2/3719 (0.1%)
1	a	0.57	0/2739	0.84	1/3735 (0.0%)
2	B	0.52	0/4171	0.82	0/5683
2	b	0.52	0/4138	0.82	0/5640
3	C	0.50	1/3626 (0.0%)	0.84	1/4936 (0.0%)
3	c	0.51	0/3670	0.83	4/4996 (0.1%)
4	D	0.56	0/2827	0.84	4/3852 (0.1%)
4	d	0.56	0/2818	0.82	2/3840 (0.1%)
5	E	0.46	0/687	0.84	0/936
5	e	0.43	0/667	0.80	0/908
6	F	0.51	0/284	0.75	0/387
6	f	0.45	0/257	0.77	0/349
7	H	0.47	0/530	0.80	0/723
7	h	0.42	0/524	0.78	0/713
8	I	0.46	0/311	0.79	0/419
8	i	0.47	0/311	0.80	0/419
9	J	0.43	0/278	0.74	0/376
9	j	0.48	0/283	0.78	0/383
10	K	0.49	0/303	0.85	0/416
10	k	0.47	0/303	0.91	0/416
11	L	0.50	0/311	0.71	0/423
11	l	0.46	0/311	0.73	0/423
12	M	0.59	0/261	0.85	0/357
12	m	0.56	0/262	0.99	2/357 (0.6%)
13	O	0.46	0/1935	0.82	2/2623 (0.1%)
13	o	0.45	0/1910	0.82	2/2589 (0.1%)
14	T	0.58	0/257	0.75	0/349
14	t	0.58	0/257	0.80	0/349
15	U	0.48	0/776	0.81	0/1052
15	u	0.50	0/785	0.78	0/1064
16	V	0.51	0/1085	0.80	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.48	0/1085	0.81	0/1473
17	X	0.45	0/284	0.80	0/384
17	x	0.40	0/284	0.82	0/384
18	Y	0.42	0/216	0.78	0/289
18	y	0.44	0/216	0.83	0/289
19	Z	0.45	0/490	0.84	1/669 (0.1%)
19	z	0.42	0/490	0.85	0/669
20	R	0.44	0/279	0.75	0/383
All	All	0.51	1/42949 (0.0%)	0.82	21/58445 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	ILE	CA-CB	5.02	1.56	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	17	VAL	CA-C-N	-6.40	112.41	119.19
12	m	17	VAL	C-N-CA	-6.40	112.41	119.19
1	A	142	TRP	N-CA-C	6.33	120.62	113.02
3	C	193	GLY	N-CA-C	-6.25	104.77	112.33
3	c	333	GLY	CA-C-N	6.25	126.72	119.47
3	c	333	GLY	C-N-CA	6.25	126.72	119.47
4	D	170	ALA	CA-C-N	-6.23	113.56	119.85
4	D	170	ALA	C-N-CA	-6.23	113.56	119.85
4	D	94	GLY	CA-C-N	6.01	126.12	119.87
4	D	94	GLY	C-N-CA	6.01	126.12	119.87
13	o	55	GLU	CA-C-N	5.69	125.62	119.76
13	o	55	GLU	C-N-CA	5.69	125.62	119.76
19	Z	61	VAL	N-CA-C	-5.57	107.85	113.20
1	A	176	ILE	N-CA-C	5.50	115.64	110.30
3	c	76	ILE	CA-C-N	5.47	125.81	119.47
3	c	76	ILE	C-N-CA	5.47	125.81	119.47
4	d	170	ALA	CA-C-N	-5.11	114.69	119.85
4	d	170	ALA	C-N-CA	-5.11	114.69	119.85
1	a	142	TRP	N-CA-C	5.09	119.12	113.02
13	O	55	GLU	CA-C-N	5.08	125.01	119.78
13	O	55	GLU	C-N-CA	5.08	125.01	119.78

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	2634	0	2546	24	0
1	a	2639	0	2554	26	0
2	B	4007	0	3879	42	0
2	b	3986	0	3855	44	0
3	C	3501	0	3428	31	0
3	c	3537	0	3471	31	0
4	D	2729	0	2632	18	0
4	d	2720	0	2626	17	0
5	E	665	0	653	11	0
5	e	648	0	634	14	0
6	F	275	0	282	6	0
6	f	250	0	261	2	0
7	H	514	0	542	4	0
7	h	511	0	532	11	0
8	I	314	0	328	3	0
8	i	314	0	328	4	0
9	J	272	0	279	3	0
9	j	277	0	284	4	0
10	K	293	0	305	4	0
10	k	293	0	305	8	0
11	L	301	0	315	3	0
11	l	301	0	315	2	0
12	M	265	0	286	4	0
12	m	269	0	288	7	0
13	O	1889	0	1871	22	0
13	o	1873	0	1852	18	0
14	T	258	0	261	5	0
14	t	258	0	261	3	0
15	U	765	0	767	7	0
15	u	774	0	773	2	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	5	0
17	X	281	0	312	2	0
17	x	281	0	312	6	0
18	Y	215	0	246	5	0
18	y	215	0	246	4	0
19	Z	479	0	516	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	479	0	516	4	0
20	R	273	0	305	5	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	12	0
23	B	1040	0	1152	40	0
23	C	845	0	936	42	0
23	D	130	0	144	3	0
23	a	195	0	216	9	0
23	b	1040	0	1152	37	0
23	c	845	0	936	45	0
23	d	195	0	216	12	0
24	A	64	0	74	2	0
24	D	64	0	74	1	0
24	a	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	80	0	112	5	0
25	D	40	0	56	2	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	T	40	0	56	5	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	7	0
25	c	80	0	112	10	0
25	d	40	0	56	5	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	3	0
25	y	40	0	56	1	0
26	A	108	0	156	6	0
26	B	54	0	78	2	0
26	D	43	0	53	1	0
26	L	54	0	78	5	0
26	a	108	0	156	4	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	12	0	16	2	0
27	C	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	a	6	0	8	1	0
27	b	6	0	8	0	0
27	d	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	6	0
29	D	55	0	80	3	0
29	a	55	0	80	4	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	32	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	98	0	148	5	0
31	D	98	0	148	6	0
31	E	42	0	57	1	0
31	d	147	0	222	10	0
31	e	42	0	57	2	0
31	l	49	0	74	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	51	0	72	1	0
33	C	102	0	144	7	0
33	J	51	0	72	3	0
33	Z	88	0	116	3	0
33	a	51	0	72	4	0
33	b	51	0	72	1	0
33	c	102	0	144	2	0
33	j	51	0	72	2	0
33	z	39	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	76	0	104	6	0
34	C	38	0	52	1	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	76	0	104	4	0
34	c	38	0	52	2	0
34	d	16	0	17	1	0
35	B	86	0	116	4	0
35	D	70	0	92	4	0
35	E	35	0	46	1	0
35	I	35	0	46	1	0
35	M	70	0	92	3	0
35	a	35	0	46	0	0
35	b	50	0	70	1	0
35	e	35	0	46	0	0
35	m	35	0	46	0	0
36	C	186	0	246	8	0
36	H	62	0	82	1	0
36	c	186	0	246	8	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
38	E	43	0	30	3	0
38	e	43	0	30	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	127	0	0	2	0
41	B	175	0	0	1	0
41	C	148	0	0	1	0
41	D	111	0	0	0	0
41	E	18	0	0	1	0
41	F	5	0	0	0	0
41	H	19	0	0	0	0
41	I	6	0	0	1	0
41	J	5	0	0	1	0
41	K	6	0	0	0	0
41	L	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	M	14	0	0	1	0
41	O	100	0	0	1	0
41	T	10	0	0	0	0
41	U	46	0	0	0	0
41	V	79	0	0	1	0
41	X	3	0	0	0	0
41	Y	1	0	0	0	0
41	a	130	0	0	2	0
41	b	192	0	0	5	0
41	c	136	0	0	1	0
41	d	108	0	0	1	0
41	e	15	0	0	0	0
41	f	5	0	0	0	0
41	h	28	0	0	0	0
41	i	4	0	0	0	0
41	j	3	0	0	0	0
41	k	4	0	0	0	0
41	l	7	0	0	0	0
41	m	11	0	0	1	0
41	o	109	0	0	0	0
41	t	7	0	0	1	0
41	u	64	0	0	0	0
41	v	71	0	0	2	0
41	x	4	0	0	0	0
41	y	2	0	0	0	0
All	All	52773	0	52080	604	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 6.

All (604) 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)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.46	0.95
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.52	0.91
2:b:224:ARG:HH11	35:b:621:LMT:H12	1.41	0.84
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.27	0.81
34:B:622:HTG:H1	35:B:630:LMT:H21	1.60	0.81
4:d:192:THR:HG23	23:d:403:CLA:HBC2	1.66	0.76
26:A:410:SQD:H251	31:D:409:LHG:H131	1.66	0.75
5:e:67:THR:H	5:e:75:GLN:HE22	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD1	41:A:501:HOH:O	2.05	0.75
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.69	0.75
5:e:9:PRO:HA	31:e:101:LHG:HC31	1.70	0.74
41:M:205:HOH:O	14:T:1:FME:SD	2.45	0.74
13:O:54:GLU:HG2	13:O:64:GLU:H	1.53	0.73
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.70	0.72
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.71	0.72
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.35	0.72
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.20	0.72
23:c:503:CLA:HBB1	23:c:512:CLA:H41	1.71	0.71
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.71	0.71
23:c:508:CLA:HBC3	23:c:510:CLA:H71	1.73	0.70
23:c:513:CLA:HBB1	25:c:514:BCR:H371	1.73	0.70
5:E:40:THR:HB	20:R:4:ARG:HG2	1.72	0.70
3:c:279:LEU:HD22	23:c:509:CLA:HED2	1.74	0.70
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.73	0.69
16:v:30:LYS:NZ	41:v:301:HOH:O	2.25	0.69
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.26	0.69
6:F:30:THR:HG21	33:J:101:LMG:H412	1.74	0.69
3:c:168:LEU:HD21	23:c:509:CLA:H61	1.75	0.68
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.75	0.67
25:B:618:BCR:H363	25:t:101:BCR:H19C	1.76	0.67
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.77	0.66
8:I:37:LEU:O	41:I:201:HOH:O	2.14	0.66
12:m:5:GLN:H	12:m:5:GLN:HE21	1.42	0.66
29:A:414:PL9:H253	23:D:404:CLA:H141	1.78	0.66
31:D:409:LHG:H132	31:D:409:LHG:H372	1.78	0.66
23:c:510:CLA:HBC3	23:c:510:CLA:H192	1.79	0.65
8:i:36:ASP:OD1	8:i:36:ASP:N	2.29	0.65
2:b:497:GLN:HB2	2:b:504:THR:HB	1.79	0.65
4:D:205:LEU:HD13	24:D:401:PHO:HAB	1.79	0.65
23:B:601:CLA:H12	23:B:601:CLA:H71	1.79	0.64
24:A:407:PHO:H3A	23:D:404:CLA:H142	1.80	0.63
23:A:408:CLA:H172	36:C:517:DGD:HAF1	1.79	0.63
13:o:124:ASN:ND2	13:o:147:ASN:HD22	1.96	0.63
23:A:408:CLA:H171	23:C:507:CLA:H142	1.81	0.63
8:i:35:LYS:O	8:i:37:LEU:N	2.32	0.63
3:C:286:ALA:HB2	23:C:503:CLA:HMD1	1.81	0.63
31:d:409:LHG:H372	31:d:409:LHG:H142	1.80	0.63
13:O:27:ARG:NH1	13:O:202:ALA:O	2.32	0.62
33:C:501:LMG:H211	36:C:517:DGD:HA82	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:513:CLA:HBB1	25:c:514:BCR:H24C	1.82	0.62
23:c:501:CLA:C4D	23:c:503:CLA:H2	2.30	0.62
23:C:506:CLA:HMD3	23:C:508:CLA:HAB	1.81	0.62
23:b:604:CLA:H42	23:b:605:CLA:H2	1.81	0.62
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.82	0.61
1:a:40:THR:HG23	23:a:408:CLA:HBB1	1.81	0.61
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.82	0.61
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.31	0.61
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.61
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.83	0.61
3:c:182:PHE:HA	34:c:521:HTG:H61	1.83	0.61
16:V:118:HIS:ND1	41:V:301:HOH:O	2.31	0.61
23:A:406:CLA:H152	29:A:414:PL9:H252	1.82	0.60
3:C:218:PHE:HE2	33:C:501:LMG:H111	1.67	0.60
2:B:285:ASN:O	2:B:289:GLN:HG2	2.01	0.60
23:d:404:CLA:H162	7:h:37:LEU:HD21	1.84	0.59
31:D:408:LHG:HC62	11:L:15:THR:HG23	1.85	0.59
13:O:124:ASN:ND2	13:O:147:ASN:HD22	1.97	0.59
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.38	0.59
34:B:623:HTG:O6	13:O:177:ALA:O	2.21	0.59
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.84	0.59
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.15	0.58
5:e:60:GLN:HG3	5:e:62:SER:H	1.68	0.58
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.32	0.58
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.69	0.58
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.86	0.57
5:e:27:ILE:HD11	38:e:103:HEM:HBC2	1.85	0.57
25:t:101:BCR:H321	25:t:101:BCR:HC8	1.84	0.57
33:Z:102:LMG:O5	33:Z:102:LMG:O4	2.23	0.57
12:M:8:LEU:HD11	35:M:103:LMT:H91	1.85	0.57
3:c:438:LEU:HD11	23:c:505:CLA:HBB1	1.86	0.57
26:L:101:SQD:O9	2:b:18:ARG:NH2	2.28	0.57
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.85	0.57
31:A:417:LHG:H201	11:L:26:VAL:HG11	1.87	0.56
13:O:92:SER:HB3	13:O:131:PRO:HA	1.88	0.56
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.70	0.56
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.88	0.56
2:b:24:LEU:HD21	23:b:616:CLA:HAB	1.86	0.56
3:c:286:ALA:HB2	23:c:502:CLA:HMD1	1.87	0.56
26:a:410:SQD:H301	23:c:508:CLA:H71	1.88	0.56
3:c:213[B]:LEU:HD11	25:c:515:BCR:H373	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.87	0.56
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.88	0.56
7:h:56:ASP:OD1	17:x:2:THR:OG1	2.23	0.56
23:c:501:CLA:HHC	23:c:501:CLA:HBB1	1.87	0.55
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.88	0.55
31:A:417:LHG:H191	29:D:407:PL9:H201	1.88	0.55
8:i:2:GLU:O	8:i:6:ILE:HG12	2.06	0.55
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.89	0.55
3:C:182:PHE:HA	34:C:521:HTG:H61	1.87	0.55
1:a:310:LYS:NZ	41:a:507:HOH:O	2.40	0.55
1:a:45:THR:HG23	23:d:401:CLA:H201	1.89	0.55
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.55
23:c:509:CLA:H192	23:c:512:CLA:HHD	1.89	0.55
1:A:187:GLN:HB2	23:A:404:CLA:HAC2	1.88	0.55
23:b:601:CLA:HAC1	25:h:101:BCR:H383	1.89	0.55
4:d:24:ARG:HD3	17:x:37:VAL:HG22	1.89	0.55
25:d:405:BCR:H383	33:j:101:LMG:H171	1.90	0.54
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.89	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.54
16:V:6:GLU:N	16:V:6:GLU:OE2	2.40	0.54
1:a:160:ILE:HD11	36:c:516:DGD:HBT2	1.89	0.54
23:B:604:CLA:HBB1	23:B:604:CLA:HMB1	1.89	0.54
23:C:513:CLA:O2D	23:C:514:CLA:HBB2	2.08	0.54
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.70	0.54
23:b:602:CLA:H101	23:b:609:CLA:H193	1.90	0.54
2:B:57:ARG:HH21	2:B:331:ASN:HD22	1.56	0.54
5:e:60:GLN:NE2	5:e:62:SER:HB3	2.22	0.54
3:c:174:LEU:HB3	23:c:502:CLA:H152	1.90	0.53
23:C:507:CLA:H71	35:I:101:LMT:H111	1.89	0.53
2:b:171:PRO:HD3	7:h:66:GLY:HA2	1.89	0.53
23:c:506:CLA:H71	25:c:515:BCR:H10C	1.90	0.53
23:b:612:CLA:H171	23:b:613:CLA:HBB2	1.90	0.53
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.39	0.53
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.91	0.53
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.91	0.53
23:A:408:CLA:H152	36:C:517:DGD:HAW2	1.91	0.52
25:D:406:BCR:H383	33:J:101:LMG:H171	1.90	0.52
14:T:2:GLU:H	14:T:2:GLU:CD	2.17	0.52
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.44	0.52
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.43	0.52
3:c:181:PHE:HE2	34:c:522:HTG:H7'3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.75	0.52
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.40	0.52
25:d:405:BCR:H391	9:j:20:VAL:HG13	1.91	0.52
23:B:614:CLA:H43	26:B:620:SQD:H111	1.91	0.52
33:b:620:LMG:O2	41:b:701:HOH:O	2.19	0.52
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.09	0.52
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.45	0.52
3:C:223:TRP:CG	3:C:224:ILE:H	2.28	0.52
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.91	0.52
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.92	0.52
3:c:223:TRP:CG	3:c:224:ILE:H	2.28	0.52
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.74	0.52
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.92	0.52
2:b:299:GLU:HG3	41:b:879:HOH:O	2.09	0.52
5:E:27:ILE:CD1	38:E:103:HEM:HBC2	2.40	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.09	0.51
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.92	0.51
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.10	0.51
23:c:504:CLA:H42	36:c:517:DGD:HB42	1.91	0.51
26:A:410:SQD:H192	31:D:409:LHG:H201	1.92	0.51
1:a:227:THR:HB	1:a:231:GLU:HG3	1.91	0.51
23:c:512:CLA:H143	23:c:513:CLA:H142	1.92	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
4:D:49:LEU:HD13	25:D:406:BCR:C15	2.41	0.51
12:m:5:GLN:H	12:m:5:GLN:NE2	2.08	0.51
23:c:505:CLA:HMD3	23:c:507:CLA:HAB	1.93	0.51
23:b:601:CLA:H72	23:b:601:CLA:H2	1.93	0.51
33:c:519:LMG:H181	10:k:27:VAL:HG11	1.93	0.51
13:o:42:ARG:O	13:o:241:ALA:HA	2.11	0.51
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.76	0.51
23:A:406:CLA:HED1	36:C:519:DGD:HAE2	1.92	0.51
3:c:429:SER:HA	36:c:517:DGD:HBW1	1.92	0.51
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.91	0.51
2:b:341:LYS:HE2	2:b:431:GLU:HG3	1.93	0.51
23:c:508:CLA:HMB3	23:c:508:CLA:HBB1	1.93	0.51
31:d:409:LHG:H122	31:d:409:LHG:C38	2.41	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.50
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.50
3:c:363:GLY:O	3:c:367:GLU:HG2	2.11	0.50
23:c:512:CLA:O2D	23:c:513:CLA:HBB2	2.11	0.50
13:O:81:ILE:HA	13:O:100:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:408:CLA:H151	23:C:507:CLA:H13	1.93	0.50
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.93	0.50
5:e:60:GLN:HE21	5:e:62:SER:HB3	1.77	0.50
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	1.93	0.50
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.93	0.50
3:c:325:GLY:O	15:u:51:LYS:NZ	2.39	0.50
9:J:18:MET:O	9:J:22:VAL:HG23	2.12	0.49
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.93	0.49
1:a:226:GLU:OE2	41:a:501:HOH:O	2.18	0.49
3:C:186:TYR:OH	3:C:194:GLY:HA3	2.13	0.49
35:D:402:LMT:H21	34:b:628:HTG:H1	1.93	0.49
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.47	0.49
10:k:17:ILE:HD13	10:k:17:ILE:H	1.77	0.49
23:B:614:CLA:H62	23:B:614:CLA:H41	1.56	0.49
29:a:414:PL9:H262	31:e:101:LHG:H201	1.94	0.49
23:b:614:CLA:H162	23:b:614:CLA:H122	1.53	0.49
3:c:443:TRP:CE2	23:c:508:CLA:HMD2	2.47	0.49
26:D:413:SQD:H241	6:F:18:VAL:HG22	1.94	0.49
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.95	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.13	0.48
31:d:409:LHG:H122	31:d:409:LHG:H382	1.95	0.48
33:B:621:LMG:O10	12:M:4:ASN:ND2	2.45	0.48
10:K:17:ILE:H	10:K:17:ILE:HD13	1.77	0.48
2:b:423:LYS:NZ	41:b:709:HOH:O	2.45	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.48	0.48
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.14	0.48
33:a:416:LMG:H222	36:c:516:DGD:HAT2	1.95	0.48
23:b:604:CLA:H143	23:b:615:CLA:HMA3	1.95	0.48
25:d:405:BCR:H391	9:j:20:VAL:CG1	2.43	0.48
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.42	0.48
23:b:605:CLA:H41	23:b:605:CLA:H62	1.62	0.48
3:c:78:GLU:HB3	41:v:321:HOH:O	2.12	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.48
23:c:504:CLA:H151	23:c:508:CLA:H143	1.94	0.48
23:d:404:CLA:H142	23:d:404:CLA:H112	1.75	0.48
23:B:602:CLA:H101	23:B:609:CLA:H193	1.95	0.48
23:b:610:CLA:HHC	23:b:610:CLA:HBB1	1.96	0.48
23:c:511:CLA:H72	25:k:101:BCR:H282	1.96	0.48
2:B:245:VAL:HG22	23:B:612:CLA:H202	1.95	0.48
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:497:GLN:HE22	17:x:38:GLN:HB2	1.79	0.48
13:o:210:GLU:OE2	13:o:240:TYR:OH	2.22	0.48
23:A:408:CLA:H171	23:C:507:CLA:H112	1.95	0.48
34:B:622:HTG:H61	35:B:630:LMT:H6E	1.95	0.48
25:c:514:BCR:H341	25:c:514:BCR:H11C	1.73	0.48
33:c:520:LMG:H232	33:c:520:LMG:H391	1.96	0.48
1:A:227:THR:HB	1:A:231:GLU:HG3	1.96	0.47
2:B:299:GLU:HG2	2:B:402:TYR:HD1	1.79	0.47
23:c:512:CLA:HHC	23:c:512:CLA:HBB1	1.96	0.47
23:c:513:CLA:H8	25:c:514:BCR:H23C	1.96	0.47
26:L:101:SQD:H462	26:L:101:SQD:H1	1.97	0.47
1:a:183:MET:HA	23:a:404:CLA:HMD1	1.96	0.47
3:c:174:LEU:HD22	23:c:502:CLA:H203	1.96	0.47
5:e:26:THR:HB	38:e:103:HEM:HAB	1.96	0.47
4:D:12:ARG:HH12	17:X:39:ARG:NH1	2.13	0.47
1:a:214:MET:HG2	29:a:414:PL9:H103	1.96	0.47
2:b:58:GLN:C	2:b:329:PRO:HB3	2.39	0.47
5:e:67:THR:N	5:e:75:GLN:HE22	2.09	0.47
12:m:5:GLN:HE21	12:m:5:GLN:N	2.11	0.47
1:A:217:SER:HA	4:D:272:LEU:HD12	1.97	0.47
23:C:507:CLA:H2	25:C:516:BCR:H10C	1.95	0.47
5:e:68:ASP:OD1	5:e:71:GLU:HB2	2.15	0.47
31:A:416:LHG:H361	23:B:613:CLA:H51	1.96	0.47
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.95	0.47
3:C:391:ARG:HD3	41:C:715:HOH:O	2.14	0.47
31:D:408:LHG:H192	14:T:17:PHE:HZ	1.80	0.47
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.49	0.47
33:a:416:LMG:HC71	3:c:216:SER:HB2	1.96	0.47
2:b:283:GLU:OE2	2:b:287:ARG:NH1	2.45	0.47
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.97	0.47
1:A:238[A]:LYS:NZ	41:A:504:HOH:O	2.47	0.47
29:A:414:PL9:H151	29:A:414:PL9:H171	1.57	0.47
26:a:410:SQD:H271	31:d:409:LHG:H141	1.96	0.47
3:c:213[A]:LEU:HG	23:c:506:CLA:H193	1.97	0.47
4:d:85:MET:HE2	4:d:90:LEU:HD21	1.96	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.51	0.46
3:c:146:PHE:HZ	23:c:512:CLA:HBB2	1.80	0.46
23:c:505:CLA:HBD	23:c:505:CLA:HAA1	1.96	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.39	0.46
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.82	0.46
3:C:325:GLY:O	15:U:51:LYS:NZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:341:LYS:NZ	34:b:622:HTG:S1	2.75	0.46
2:b:357:ARG:HB3	41:b:746:HOH:O	2.15	0.46
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.81	0.46
23:B:608:CLA:H191	4:D:89:LEU:HD13	1.98	0.46
6:F:21:VAL:O	6:F:25:THR:HG23	2.16	0.46
35:M:101:LMT:H6D	11:l:9:PRO:HA	1.97	0.46
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.97	0.46
23:d:404:CLA:H61	23:d:404:CLA:H41	1.59	0.46
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.97	0.46
23:B:615:CLA:H152	23:B:615:CLA:H112	1.56	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.96	0.46
23:b:608:CLA:H102	4:d:120:PHE:CE1	2.51	0.46
23:C:514:CLA:H152	33:Z:101:LMG:H412	1.96	0.46
23:C:505:CLA:H62	23:C:505:CLA:H41	1.68	0.46
2:B:36[A]:SER:OG	25:B:618:BCR:H362	2.16	0.46
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.97	0.46
25:B:619:BCR:H331	25:B:619:BCR:C8	2.46	0.46
7:H:25:TRP:O	7:H:28:THR:OG1	2.28	0.46
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.97	0.46
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.50	0.46
24:a:407:PHO:HBC3	4:d:279:LEU:HD22	1.97	0.46
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.49	0.46
23:C:507:CLA:H91	23:C:507:CLA:H111	1.80	0.46
12:M:28:GLN:O	12:M:32:GLN:HG3	2.16	0.46
23:a:408:CLA:H152	23:c:506:CLA:H101	1.98	0.46
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.51	0.46
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.80	0.45
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.99	0.45
26:a:410:SQD:H141	31:d:409:LHG:H152	1.97	0.45
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.78	0.45
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.96	0.45
36:c:518:DGD:HBH2	31:d:409:LHG:H211	1.98	0.45
1:a:92:HIS:HE2	3:c:360:ASP:CG	2.24	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.16	0.45
2:B:489:GLU:HB3	2:B:495:PHE:CG	2.51	0.45
35:M:101:LMT:H101	23:b:614:CLA:H92	1.98	0.45
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.97	0.45
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.75	0.45
11:L:20:GLY:O	11:L:24[A]:ILE:HG12	2.16	0.45
2:b:30:VAL:HG12	23:b:605:CLA:HHD	1.99	0.45
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.99	0.45
1:A:163:ILE:HD11	36:C:517:DGD:HA22	1.99	0.45
23:B:603:CLA:C4D	23:B:605:CLA:H43	2.47	0.45
33:C:501:LMG:H152	36:C:517:DGD:HA91	1.99	0.45
23:C:514:CLA:H172	33:Z:101:LMG:H402	1.98	0.45
2:b:86:ILE:HD12	2:b:88:PRO:HD3	1.98	0.45
25:d:405:BCR:H15C	25:d:405:BCR:H351	1.82	0.45
13:o:39:ARG:NH2	13:o:98:GLU:OE1	2.50	0.45
1:A:12:ASN:O	1:A:16:ARG:HG3	2.17	0.45
2:B:54:PRO:HB3	27:B:626:GOL:H11	1.99	0.45
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	1.99	0.45
26:L:101:SQD:H302	26:L:101:SQD:H332	1.80	0.45
2:b:490:GLN:HG3	2:b:496:TYR:HE2	1.80	0.45
41:d:576:HOH:O	17:x:6:SER:HA	2.16	0.45
26:B:620:SQD:H351	26:B:620:SQD:H383	1.84	0.45
4:D:186:GLN:HB2	23:D:404:CLA:HBC1	1.99	0.45
25:H:101:BCR:H331	25:H:101:BCR:C8	2.47	0.45
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.68	0.45
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.99	0.45
23:b:616:CLA:H92	23:b:616:CLA:H62	1.68	0.45
13:o:54:GLU:HG2	13:o:64:GLU:H	1.82	0.45
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
23:A:408:CLA:H143	23:C:506:CLA:H192	2.00	0.44
2:B:299:GLU:HG3	41:B:800:HOH:O	2.17	0.44
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.78	0.44
38:E:103:HEM:HAC	6:F:27:ALA:HB1	1.98	0.44
2:b:497:GLN:NE2	17:x:38:GLN:O	2.51	0.44
23:c:508:CLA:H93	31:d:409:LHG:H162	2.00	0.44
26:A:412:SQD:H292	26:A:412:SQD:H262	1.72	0.44
31:A:416:LHG:H312	31:A:416:LHG:H282	1.74	0.44
23:b:614:CLA:H101	25:b:617:BCR:H362	1.98	0.44
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.99	0.44
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.99	0.44
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.99	0.44
23:c:509:CLA:H92	23:c:509:CLA:H62	1.75	0.44
31:d:408:LHG:H192	14:t:17:PHE:HZ	1.83	0.44
5:e:66:VAL:HA	5:e:75:GLN:NE2	2.32	0.44
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.99	0.44
34:B:622:HTG:O5	27:a:411:GOL:H11	2.18	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
23:C:507:CLA:HMC2	23:C:508:CLA:H102	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:121[B]:LEU:HD23	33:a:416:LMG:H212	2.00	0.44
23:a:404:CLA:H191	31:d:408:LHG:H321	2.00	0.44
23:c:510:CLA:H61	23:c:510:CLA:H102	1.69	0.44
2:B:497:GLN:NE2	17:X:38:GLN:O	2.46	0.44
23:a:408:CLA:H152	23:c:506:CLA:H142	2.00	0.44
23:b:615:CLA:H92	23:b:615:CLA:H61	1.76	0.44
25:c:514:BCR:H371	25:c:514:BCR:H24C	1.74	0.44
31:d:408:LHG:HC62	11:l:15:THR:HG23	2.00	0.44
23:B:604:CLA:H62	23:B:604:CLA:H41	1.74	0.44
23:B:616:CLA:H11	23:B:616:CLA:H51	1.81	0.44
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.99	0.44
3:C:154:LYS:HG2	3:C:266:TRP:CE3	2.53	0.44
23:C:504:CLA:HBB2	23:C:513:CLA:H92	2.00	0.44
23:C:508:CLA:H62	23:C:508:CLA:H41	1.75	0.44
23:b:603:CLA:H141	23:b:603:CLA:H161	1.84	0.44
35:B:630:LMT:H52	1:a:72:LEU:HD11	1.99	0.44
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.99	0.44
23:C:514:CLA:HAB	25:C:515:BCR:H24C	1.99	0.44
35:E:102:LMT:O6'	41:E:201:HOH:O	2.21	0.44
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.99	0.44
1:A:214:MET:HG2	29:A:414:PL9:C10	2.48	0.44
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.88	0.44
9:J:6:ARG:HG3	41:J:201:HOH:O	2.17	0.44
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	2.00	0.44
1:a:307[A]:ILE:CG2	1:a:311:GLY:HA2	2.48	0.44
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	2.00	0.44
23:c:509:CLA:HMB1	23:c:511:CLA:HBB1	1.99	0.44
12:m:34:LYS:O	41:m:201:HOH:O	2.21	0.44
13:O:124:ASN:HD22	13:O:147:ASN:ND2	2.05	0.44
15:U:48:LEU:O	15:U:52:ASN:ND2	2.41	0.44
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.99	0.44
23:b:604:CLA:H62	23:b:604:CLA:H41	1.71	0.44
3:c:171:GLY:O	3:c:174:LEU:HB2	2.17	0.44
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.53	0.43
1:A:183:MET:HA	23:A:404:CLA:HMD1	2.00	0.43
23:C:507:CLA:H41	23:C:507:CLA:H62	1.83	0.43
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.88	0.43
29:a:414:PL9:H503	17:x:24:THR:OG1	2.17	0.43
12:m:28:GLN:O	12:m:32:GLN:HG3	2.18	0.43
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.00	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PRO:HB3	27:B:625:GOL:H32	1.99	0.43
33:C:501:LMG:H161	33:C:501:LMG:H191	1.80	0.43
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.43
13:O:110[B]:MET:HE2	13:O:116:ILE:HD11	2.00	0.43
23:a:405:CLA:HED1	36:c:518:DGD:HAE2	1.99	0.43
25:a:409:BCR:H11C	25:a:409:BCR:H341	1.88	0.43
23:c:513:CLA:H203	23:c:513:CLA:H161	1.75	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.00	0.43
3:C:142:GLU:CD	3:C:142:GLU:H	2.25	0.43
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.48	0.43
1:A:341:LEU:HD13	27:C:523:GOL:H31	1.99	0.43
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.85	0.43
5:E:26:THR:HA	20:R:15:ALA:HB1	2.00	0.43
13:O:18:LYS:HD3	41:O:460:HOH:O	2.17	0.43
2:b:219:VAL:O	41:b:702:HOH:O	2.21	0.43
38:e:103:HEM:CAC	6:f:27:ALA:HB1	2.49	0.43
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.43
34:B:622:HTG:H6'2	34:B:622:HTG:H3'1	1.94	0.43
25:H:101:BCR:H11C	25:H:101:BCR:H341	1.79	0.43
26:L:101:SQD:H211	25:T:101:BCR:H351	1.99	0.43
23:C:514:CLA:H141	23:C:514:CLA:H162	1.82	0.43
33:C:501:LMG:H232	23:C:506:CLA:H92	2.00	0.43
23:C:509:CLA:H142	23:C:509:CLA:H111	1.71	0.43
35:D:402:LMT:H51	2:b:39:LEU:HD22	2.00	0.43
25:H:101:BCR:H331	25:H:101:BCR:HC8	2.00	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.43
1:a:217:SER:HA	4:d:272:LEU:HD12	2.00	0.43
23:a:405:CLA:HAB	23:d:403:CLA:H72	2.01	0.43
13:o:32:ILE:HG21	13:o:93:LEU:HD21	2.00	0.43
1:A:214:MET:HG2	29:A:414:PL9:H103	2.00	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.43
24:a:407:PHO:H112	24:a:407:PHO:H72	1.75	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.43
2:B:102:VAL:HA	25:B:618:BCR:C40	2.49	0.43
3:C:60:ILE:HG22	23:C:504:CLA:HHD	1.99	0.43
36:C:518:DGD:HAF2	36:C:518:DGD:HAE2	1.86	0.43
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.88	0.43
3:c:294:ASN:HA	3:c:297:TYR:O	2.18	0.43
23:c:508:CLA:H162	23:c:508:CLA:H122	1.74	0.43
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.53	0.43
33:j:101:LMG:H341	33:j:101:LMG:H242	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:404:CLA:CBD	23:d:401:CLA:HAC2	2.48	0.42
2:b:101:ILE:O	2:b:104:SER:HB3	2.19	0.42
2:B:61:PHE:CZ	23:B:607:CLA:HBB1	2.54	0.42
23:B:606:CLA:H192	23:B:616:CLA:H101	2.01	0.42
3:C:443:TRP:CZ2	23:C:509:CLA:HMD1	2.54	0.42
8:I:2:GLU:O	8:I:6:ILE:HG12	2.19	0.42
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.00	0.42
23:b:609:CLA:C3B	25:h:101:BCR:H323	2.49	0.42
23:c:505:CLA:H112	23:c:505:CLA:H72	1.75	0.42
34:d:411:HTG:H5	7:h:25:TRP:NE1	2.33	0.42
19:z:29:SER:HA	19:z:30:PRO:HD3	1.91	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.62	0.42
23:B:602:CLA:H203	23:B:602:CLA:H162	1.75	0.42
13:O:57:LYS:HE3	2:b:338:GLN:HA	2.02	0.42
20:R:29:LYS:HB3	20:R:29:LYS:HE2	1.79	0.42
3:c:48:LYS:HG2	3:c:133:ALA:O	2.20	0.42
36:c:516:DGD:HAW2	36:c:516:DGD:HAN1	1.88	0.42
35:B:629:LMT:H2'	41:t:203:HOH:O	2.19	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.18	0.42
31:E:101:LHG:H261	31:E:101:LHG:H291	1.71	0.42
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.54	0.42
23:b:603:CLA:HBB2	23:b:605:CLA:H193	2.01	0.42
23:A:405:CLA:HED1	29:D:407:PL9:H362	2.01	0.42
2:B:133:LEU:HB3	2:B:138:MET:SD	2.59	0.42
35:D:403:LMT:O2B	30:D:411:UNL:O6	2.37	0.42
23:a:404:CLA:H161	23:a:404:CLA:H193	1.65	0.42
2:b:124:ARG:HD2	2:b:129:GLY:O	2.19	0.42
23:B:616:CLA:H152	23:B:616:CLA:H111	1.68	0.42
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.89	0.42
23:c:506:CLA:H162	23:c:506:CLA:H122	1.64	0.42
2:B:341:LYS:NZ	34:B:623:HTG:O2	2.37	0.42
23:B:602:CLA:H92	36:H:102:DGD:HB71	2.00	0.42
23:B:614:CLA:H92	23:B:614:CLA:H61	1.67	0.42
35:D:403:LMT:H91	35:D:403:LMT:H62	1.81	0.42
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.84	0.42
25:b:619:BCR:H331	25:b:619:BCR:C8	2.49	0.42
25:h:101:BCR:C8	25:h:101:BCR:H331	2.50	0.42
18:y:38:LEU:O	18:y:42:ARG:HG2	2.19	0.42
19:z:56:VAL:HG12	19:z:60:PHE:HE1	1.84	0.42
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.89	0.42
23:B:610:CLA:H122	23:B:615:CLA:HAA1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:30:ILE:HD12	18:Y:30:ILE:HA	1.86	0.42
10:k:16:ALA:O	10:k:19:ASP:HB2	2.20	0.42
25:k:101:BCR:H11C	25:k:101:BCR:H341	1.94	0.42
1:A:274:PHE:HD1	26:A:410:SQD:H101	1.85	0.42
31:A:416:LHG:O4	4:D:141:TYR:OH	2.28	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.42
23:B:602:CLA:H91	23:B:602:CLA:H111	1.84	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.02	0.42
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.51	0.42
25:b:618:BCR:H20C	25:b:618:BCR:H361	1.92	0.42
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.82	0.42
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.85	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.88	0.41
3:C:161:LEU:HD11	23:C:507:CLA:HBB1	2.02	0.41
23:C:508:CLA:H92	23:C:508:CLA:H61	1.88	0.41
6:F:34:LEU:HD23	6:F:34:LEU:HA	1.93	0.41
25:c:515:BCR:H24C	25:c:515:BCR:H371	1.83	0.41
2:B:502:VAL:O	2:B:505:ARG:HG3	2.20	0.41
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.88	0.41
26:L:101:SQD:H212	26:L:101:SQD:H181	1.86	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.41
36:c:517:DGD:HA91	36:c:518:DGD:HBF2	2.02	0.41
4:d:43:LEU:HD22	25:d:405:BCR:H323	2.02	0.41
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.01	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.90	0.41
10:k:20:PRO:HB3	18:y:21:GLN:HG3	2.03	0.41
13:o:51:LEU:HD23	13:o:67:PRO:HA	2.03	0.41
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.81	0.41
2:B:149:LEU:HG	23:B:606:CLA:HBB2	2.02	0.41
23:B:601:CLA:H42	23:B:601:CLA:OBD	2.20	0.41
23:B:605:CLA:H92	23:B:605:CLA:H61	1.75	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.55	0.41
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.02	0.41
3:C:433:LEU:HD13	23:C:503:CLA:CHC	2.51	0.41
1:a:281:VAL:HG12	26:a:410:SQD:H201	2.02	0.41
23:c:513:CLA:C4A	23:c:513:CLA:HBA1	2.49	0.41
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	2.01	0.41
23:C:509:CLA:H91	23:C:509:CLA:H112	1.82	0.41
31:D:409:LHG:H372	31:D:409:LHG:C13	2.50	0.41
1:a:265:PHE:HE2	29:a:414:PL9:H111	1.84	0.41
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:506:CLA:H101	23:C:506:CLA:H61	1.79	0.41
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.85	0.41
15:U:24:LYS:HB3	15:U:81:HIS:O	2.21	0.41
23:b:604:CLA:H91	23:b:604:CLA:H111	1.81	0.41
23:B:604:CLA:HAB	23:B:611:CLA:H191	2.02	0.41
23:B:611:CLA:H92	23:B:611:CLA:H62	1.91	0.41
33:C:501:LMG:H121	23:C:506:CLA:H201	2.02	0.41
15:U:64:ILE:HA	15:U:65:PRO:HD3	1.85	0.41
20:R:31:VAL:O	20:R:35:LEU:HG	2.21	0.41
9:j:3:GLU:O	9:j:6:ARG:HG2	2.20	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.90	0.41
5:E:25:ILE:O	5:E:28:PRO:HD2	2.21	0.41
5:E:42:LEU:HA	20:R:4:ARG:HH21	1.85	0.41
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.56	0.41
1:a:182:PHE:O	1:a:186:PHE:HB2	2.20	0.41
2:b:305:ILE:HA	2:b:306:PRO:HD3	1.84	0.41
23:d:401:CLA:C4A	23:d:401:CLA:HBA1	2.50	0.41
10:k:26:PRO:O	10:k:29:PRO:HD2	2.20	0.41
25:C:516:BCR:H24C	25:C:516:BCR:H371	1.82	0.41
2:b:16:PRO:HG2	2:b:123:PHE:HB3	2.03	0.41
23:b:608:CLA:H3A	23:b:608:CLA:HBA2	1.88	0.41
23:c:507:CLA:H142	23:c:507:CLA:H112	1.89	0.41
13:o:140:THR:O	13:o:201:VAL:HB	2.20	0.41
1:A:121[A]:LEU:HG	33:C:501:LMG:H182	2.02	0.41
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.56	0.41
23:B:616:CLA:H91	23:B:616:CLA:H112	1.80	0.41
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.80	0.41
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.21	0.41
23:C:506:CLA:H111	23:C:506:CLA:H93	1.87	0.41
13:O:56:PRO:HB3	13:O:61:GLN:CD	2.45	0.41
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.86	0.41
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.97	0.41
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.21	0.41
33:a:416:LMG:H211	33:a:416:LMG:H241	1.68	0.41
23:b:605:CLA:H111	23:b:605:CLA:H91	1.87	0.41
23:b:611:CLA:H172	23:b:613:CLA:ND	2.36	0.41
23:b:613:CLA:H203	23:b:613:CLA:H161	1.86	0.41
41:c:609:HOH:O	10:k:25:LEU:HB2	2.20	0.41
23:d:403:CLA:HBD	23:d:403:CLA:HAA2	2.02	0.41
25:h:101:BCR:H371	25:h:101:BCR:H24C	1.86	0.41
13:o:30:TYR:HA	13:o:31:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:80:THR:HA	16:v:86:GLN:O	2.21	0.41
1:A:45:THR:HG21	26:A:412:SQD:H202	2.03	0.41
2:B:157:HIS:HE1	23:B:606:CLA:NA	2.19	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.55	0.41
4:D:223:PHE:CZ	4:D:245:SER:HB2	2.56	0.41
33:J:101:LMG:H191	33:J:101:LMG:H231	2.03	0.41
10:K:15:TYR:CE1	19:Z:5:PHE:HZ	2.39	0.41
2:b:12:LEU:HB2	23:b:612:CLA:HMC2	2.03	0.41
2:b:223:GLN:HA	2:b:223:GLN:HE21	1.86	0.41
23:b:615:CLA:HBA1	23:b:615:CLA:H3A	1.88	0.41
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.94	0.41
23:d:401:CLA:H162	23:d:401:CLA:H203	1.85	0.41
12:m:6:LEU:HD23	12:m:6:LEU:HA	1.91	0.41
1:A:102:LEU:HD12	34:b:625:HTG:H61	2.03	0.40
2:B:191:ASN:HA	2:B:192:PRO:HD2	1.96	0.40
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.03	0.40
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.03	0.40
1:a:210:LEU:HG	24:a:407:PHO:NC	2.35	0.40
24:a:406:PHO:HAB	4:d:205:LEU:HD13	2.03	0.40
23:b:609:CLA:C2B	25:h:101:BCR:H323	2.50	0.40
23:d:404:CLA:H62	23:d:404:CLA:H92	1.75	0.40
5:e:66:VAL:HA	5:e:75:GLN:HE22	1.86	0.40
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.40
14:t:14:ILE:HG22	25:t:101:BCR:H10C	2.02	0.40
24:A:407:PHO:HHD	24:A:407:PHO:HBC2	2.04	0.40
3:C:137:PRO:HG3	23:C:514:CLA:HED3	2.02	0.40
2:b:159:THR:HA	2:b:181:VAL:O	2.21	0.40
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.83	0.40
23:b:604:CLA:HBD	23:b:604:CLA:HAA1	2.04	0.40
3:c:135:ARG:HA	3:c:135:ARG:HD2	1.96	0.40
3:c:334:PRO:HA	13:o:153:THR:OG1	2.21	0.40
4:d:186:GLN:HB2	23:d:403:CLA:HBC1	2.03	0.40
13:o:39:ARG:HH22	13:o:98:GLU:CD	2.29	0.40
23:A:405:CLA:H92	23:A:405:CLA:H62	1.89	0.40
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.51	0.40
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	2.02	0.40
36:C:518:DGD:HAE2	36:C:518:DGD:HA81	1.80	0.40
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.57	0.40
16:V:57:GLU:H	16:V:57:GLU:CD	2.30	0.40
2:b:63:LEU:N	2:b:64:PRO:HD2	2.36	0.40
7:h:4:ARG:HH11	7:h:9:ASP:CG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:28:ILE:HD11	18:y:28:ILE:HD13	2.03	0.40
19:z:48:ILE:HD11	33:z:101:LMG:H192	2.02	0.40
26:A:412:SQD:H261	2:b:109:LEU:HD13	2.02	0.40
29:A:414:PL9:H272	29:A:414:PL9:H251	1.91	0.40
23:C:513:CLA:HMB2	23:C:513:CLA:H202	2.02	0.40
4:D:202:ALA:HB2	29:D:407:PL9:H353	2.04	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.87	0.40
18:Y:34:MET:HE2	18:Y:34:MET:HB2	1.99	0.40
2:b:24:LEU:HD21	23:b:616:CLA:CAB	2.50	0.40
2:b:432:PHE:H	34:b:622:HTG:HO3	1.65	0.40
23:b:612:CLA:H122	23:b:612:CLA:H162	1.86	0.40
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.25	0.40
5:e:68:ASP:O	5:e:72:ALA:HB2	2.21	0.40
16:v:41:HIS:HA	16:v:45:ILE:O	2.22	0.40
2:B:482:ILE:HD12	2:B:486:LEU:HD22	2.04	0.40
3:C:25:ASN:O	3:C:41:ARG:HD3	2.20	0.40
23:C:513:CLA:H101	23:C:514:CLA:H141	2.02	0.40
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.84	0.40
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.03	0.40
23:b:612:CLA:HBD	23:b:612:CLA:HAA1	2.04	0.40
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.92	0.40
23:c:507:CLA:H62	23:c:507:CLA:H41	1.73	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%)	328 (98%)	6 (2%)	1 (0%)	36	55
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	36	55
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	30	49
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	30	49
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	6
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
13	o	243/244 (100%)	234 (96%)	9 (4%)	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	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100 100
18	y	27/30 (90%)	24 (89%)	3 (11%)	0	100 100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	7 13
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 13
20	R	32/34 (94%)	32 (100%)	0	0	100 100
All	All	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	48 63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	Z	30	PRO
19	z	30	PRO
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	272/279 (98%)	270 (99%)	2 (1%)	76 89
1	a	274/279 (98%)	272 (99%)	2 (1%)	76 89
2	B	410/403 (102%)	401 (98%)	9 (2%)	45 73
2	b	406/403 (101%)	398 (98%)	8 (2%)	48 75
3	C	356/356 (100%)	350 (98%)	6 (2%)	53 78
3	c	361/356 (101%)	351 (97%)	10 (3%)	38 66
4	D	278/277 (100%)	277 (100%)	1 (0%)	84 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	d	277/277 (100%)	274 (99%)	3 (1%)	65 84
5	E	73/73 (100%)	71 (97%)	2 (3%)	39 67
5	e	70/73 (96%)	68 (97%)	2 (3%)	37 65
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	25/38 (66%)	24 (96%)	1 (4%)	28 54
7	H	55/54 (102%)	53 (96%)	2 (4%)	31 58
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37 65
8	i	34/34 (100%)	32 (94%)	2 (6%)	18 37
9	J	26/27 (96%)	24 (92%)	2 (8%)	12 25
9	j	26/27 (96%)	24 (92%)	2 (8%)	12 25
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 8
10	k	30/30 (100%)	26 (87%)	4 (13%)	4 8
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	35/35 (100%)	35 (100%)	0	100 100
12	M	30/32 (94%)	29 (97%)	1 (3%)	33 61
12	m	30/32 (94%)	28 (93%)	2 (7%)	15 31
13	O	211/207 (102%)	208 (99%)	3 (1%)	59 81
13	o	208/207 (100%)	205 (99%)	3 (1%)	59 81
14	T	26/28 (93%)	25 (96%)	1 (4%)	29 56
14	t	26/28 (93%)	25 (96%)	1 (4%)	29 56
15	U	83/89 (93%)	81 (98%)	2 (2%)	43 70
15	u	84/89 (94%)	83 (99%)	1 (1%)	63 83
16	V	117/117 (100%)	116 (99%)	1 (1%)	70 87
16	v	117/117 (100%)	116 (99%)	1 (1%)	70 87
17	X	31/33 (94%)	31 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24 49
18	y	22/23 (96%)	20 (91%)	2 (9%)	9 19
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 56
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4360/4403 (99%)	4274 (98%)	86 (2%)	50 75

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	35	VAL
2	B	53	ASN
2	B	86	ILE
2	B	223	GLN
2	B	236	THR
2	B	362	PHE
2	B	472	ARG
2	B	489	GLU
2	B	492	GLU
2	B	505	ARG
3	C	25	ASN
3	C	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	136	VAL
5	E	54	SER
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
8	I	33	LYS
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	33	GLN
13	O	24	ASP
13	O	69	LYS
13	O	234	LYS
14	T	2	GLU
15	U	10	VAL
15	U	70	ARG

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Mol	Chain	Res	Type
16	V	30	LYS
18	Y	30	ILE
19	Z	3	ILE
19	Z	6	GLN
1	a	12	ASN
1	a	35	VAL
2	b	36	SER
2	b	53	ASN
2	b	121	GLU
2	b	223	GLN
2	b	245	VAL
2	b	431	GLU
2	b	472	ARG
2	b	485	GLU
3	c	19	ASN
3	c	21	ILE
3	c	142	GLU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	136	VAL
4	d	259	ILE
4	d	329	MET
5	e	62	SER
5	e	71	GLU
6	f	15	ILE
8	i	33	LYS
8	i	36	ASP
9	j	2	SER
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
10	k	27	VAL
12	m	5	GLN
12	m	20	VAL
13	o	69	LYS
13	o	118	LEU

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Mol	Chain	Res	Type
13	o	132	ASN
14	t	2	GLU
15	u	10	VAL
16	v	30	LYS
18	y	30	ILE
18	y	45	ASN
19	z	3	ILE
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	53	ASN
2	B	331	ASN
2	B	338	GLN
3	C	28	GLN
3	C	415	ASN
4	D	61	HIS
4	D	186	GLN
4	D	255	GLN
5	E	60	GLN
6	F	44	GLN
12	M	5	GLN
12	M	28	GLN
13	O	124	ASN
13	O	130	GLN
15	U	73	GLN
15	U	81	HIS
19	Z	58	ASN
1	a	12	ASN
1	a	165	GLN
1	a	234	ASN
2	b	53	ASN
2	b	223	GLN
2	b	289	GLN
2	b	331	ASN
2	b	374	ASN
3	c	19	ASN
3	c	28	GLN
3	c	201	ASN
5	e	60	GLN

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Mol	Chain	Res	Type
5	e	75	GLN
6	f	44	GLN
12	m	5	GLN
13	o	124	ASN
15	u	78	ASN
15	u	81	HIS
16	v	25	GLN
19	z	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	0.62	0	7,9,11	1.31	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.37	1 (14%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.85	3 (42%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.09	1 (14%)
12	FME	m	1	12	8,9,10	0.58	0	7,9,11	1.38	2 (28%)
12	FME	M	1	12	8,9,10	0.58	0	7,9,11	1.50	2 (28%)

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
14	FME	T	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O-C-CA	-2.73	117.62	124.78
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82
12	M	1	FME	CA-N-CN	-2.31	119.27	122.82
8	I	1	FME	O-C-CA	-2.29	118.77	124.78
14	T	1	FME	O-C-CA	-2.25	118.88	124.78
12	M	1	FME	O-C-CA	-2.22	118.95	124.78
12	m	1	FME	CA-N-CN	-2.19	119.45	122.82
8	i	1	FME	O-C-CA	-2.13	119.18	124.78
12	m	1	FME	O1-CN-N	-2.09	119.77	125.27
14	t	1	FME	O1-CN-N	-2.07	119.81	125.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 214 ligands modelled in this entry, 14 are monoatomic and 18 are unknown - leaving 182 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	$\#\|Z\| > 2$
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
23	CLA	B	613	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	31 (37%)
23	CLA	a	405	41	69,73,73	2.03	20 (28%)	83,113,113	2.85	32 (38%)
34	HTG	b	622	-	19,19,19	0.96	1 (5%)	23,24,24	1.52	3 (13%)
23	CLA	c	513	3	69,73,73	2.09	20 (28%)	83,113,113	2.90	29 (34%)
35	LMT	B	631	-	26,26,36	0.50	0	31,31,47	0.81	1 (3%)
35	LMT	b	627	-	25,25,36	0.56	1 (4%)	30,30,47	1.07	3 (10%)
23	CLA	b	604	2	69,73,73	2.00	18 (26%)	83,113,113	2.82	29 (34%)
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	83,113,113	2.77	29 (34%)
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
32	BCT	a	418	21	2,3,3	0.61	0	2,3,3	1.00	0
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.77	1 (2%)
23	CLA	B	614	2	69,73,73	2.03	21 (30%)	83,113,113	2.89	33 (39%)
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.95	2 (4%)
24	PHO	A	407	-	58,69,69	2.82	14 (24%)	56,99,99	2.97	18 (32%)
23	CLA	a	408	1	69,73,73	2.06	20 (28%)	83,113,113	2.82	34 (40%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.77	1 (2%)
23	CLA	C	504	3	69,73,73	2.02	18 (26%)	83,113,113	2.88	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.96	3 (5%)
23	CLA	B	616	2	69,73,73	2.06	20 (28%)	83,113,113	2.84	27 (32%)
23	CLA	b	605	2	69,73,73	2.05	22 (31%)	83,113,113	2.84	29 (34%)
36	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	c	509	3	69,73,73	2.11	20 (28%)	83,113,113	2.79	29 (34%)
36	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.99	6 (7%)
25	BCR	a	409	-	41,41,41	0.95	1 (2%)	56,56,56	1.51	12 (21%)
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.39	10 (17%)
26	SQD	A	410	-	53,54,54	0.97	3 (5%)	62,65,65	1.86	12 (19%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.10	6 (9%)
38	HEM	e	103	5,6	50,50,50	1.50	7 (14%)	66,82,82	1.75	11 (16%)
34	HTG	c	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	C	503	3	69,73,73	2.05	19 (27%)	83,113,113	2.70	28 (33%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.29	0
28	OEX	A	413	1,41,3	0,14,14	-	-	-		
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	6 (7%)
23	CLA	C	505	41	69,73,73	2.05	20 (28%)	83,113,113	2.81	32 (38%)
29	PL9	A	414	-	55,55,55	0.65	2 (3%)	68,69,69	1.95	21 (30%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.32	7 (14%)
23	CLA	c	511	3	69,73,73	2.10	21 (30%)	83,113,113	2.89	29 (34%)
34	HTG	B	623	-	19,19,19	0.84	1 (5%)	23,24,24	1.67	1 (4%)
36	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.16	6 (7%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.07	3 (6%)
23	CLA	c	506	3	69,73,73	2.05	20 (28%)	83,113,113	2.74	32 (38%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.92	2 (4%)
23	CLA	b	616	2	69,73,73	2.07	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	D	404	4	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	C	514	3	69,73,73	2.08	21 (30%)	83,113,113	2.89	29 (34%)
23	CLA	C	509	3	69,73,73	2.06	21 (30%)	83,113,113	2.78	28 (33%)
23	CLA	b	613	2	69,73,73	2.05	20 (28%)	83,113,113	2.75	31 (37%)
25	BCR	c	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	13 (23%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	13 (23%)
33	LMG	b	620	-	51,51,55	0.86	2 (3%)	59,59,63	1.26	8 (13%)
26	SQD	L	101	-	53,54,54	1.02	3 (5%)	62,65,65	1.53	9 (14%)
23	CLA	B	605	2	69,73,73	2.07	20 (28%)	83,113,113	2.91	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.52	11 (19%)
33	LMG	c	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	3 (5%)
23	CLA	c	510	3	69,73,73	1.98	20 (28%)	83,113,113	2.88	34 (40%)
31	LHG	A	416	-	48,48,48	0.90	3 (6%)	51,54,54	1.10	4 (7%)
35	LMT	b	621	-	25,25,36	0.46	0	30,30,47	0.66	0
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	6 (7%)
23	CLA	b	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.81	30 (36%)
23	CLA	b	603	2	69,73,73	2.09	20 (28%)	83,113,113	2.93	29 (34%)
23	CLA	c	508	3	69,73,73	2.07	20 (28%)	83,113,113	2.81	28 (33%)
23	CLA	c	512	3	69,73,73	2.05	19 (27%)	83,113,113	2.92	30 (36%)
23	CLA	B	607	41	69,73,73	2.04	20 (28%)	83,113,113	2.83	30 (36%)
25	BCR	d	405	-	41,41,41	1.09	1 (2%)	56,56,56	1.86	14 (25%)
34	HTG	B	622	-	19,19,19	1.01	1 (5%)	23,24,24	1.44	4 (17%)
23	CLA	B	603	2	69,73,73	2.03	19 (27%)	83,113,113	2.80	30 (36%)
40	HEC	V	202	16	50,50,50	1.73	10 (20%)	68,82,82	1.82	17 (25%)
25	BCR	b	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.69	13 (23%)
23	CLA	C	508	41	69,73,73	2.06	19 (27%)	83,113,113	2.80	29 (34%)
31	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	5 (9%)
31	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.91	3 (5%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.70	17 (30%)
23	CLA	b	611	2	69,73,73	2.05	20 (28%)	83,113,113	2.78	28 (33%)
23	CLA	C	510	3	69,73,73	2.08	20 (28%)	83,113,113	2.83	30 (36%)
23	CLA	b	610	41	69,73,73	2.12	20 (28%)	83,113,113	2.82	30 (36%)
34	HTG	b	623	-	19,19,19	1.07	2 (10%)	23,24,24	1.81	3 (13%)
29	PL9	d	406	-	55,55,55	0.63	1 (1%)	68,69,69	1.82	20 (29%)
23	CLA	C	502	3	69,73,73	1.97	20 (28%)	83,113,113	2.86	31 (37%)
33	LMG	Z	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.27	5 (8%)
36	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.09	6 (7%)
35	LMT	D	402	-	36,36,36	0.64	1 (2%)	47,47,47	1.26	4 (8%)
34	HTG	D	412	-	16,16,19	1.04	2 (12%)	20,21,24	1.45	1 (5%)
23	CLA	b	607	41	69,73,73	1.96	19 (27%)	83,113,113	2.83	28 (33%)
23	CLA	B	601	41	69,73,73	2.09	20 (28%)	83,113,113	2.80	29 (34%)
34	HTG	V	203	-	11,11,19	0.25	0	15,15,24	1.12	2 (13%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	11 (19%)
31	LHG	d	409	-	48,48,48	0.97	2 (4%)	51,54,54	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
26	SQD	D	413	-	42,43,54	1.15	3 (7%)	51,54,65	1.78	12 (23%)
23	CLA	a	404	1	69,73,73	2.02	19 (27%)	83,113,113	2.81	32 (38%)
27	GOL	d	402	-	5,5,5	0.32	0	5,5,5	0.55	0
25	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	13 (23%)
27	GOL	C	523	-	5,5,5	0.40	0	5,5,5	0.25	0
23	CLA	b	606	2	69,73,73	2.01	19 (27%)	83,113,113	2.86	31 (37%)
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.02	2 (4%)
23	CLA	B	610	41	69,73,73	2.08	20 (28%)	83,113,113	2.82	31 (37%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.68	11 (19%)
34	HTG	B	627	-	19,19,19	0.97	2 (10%)	23,24,24	1.40	2 (8%)
23	CLA	c	507	41	69,73,73	2.06	19 (27%)	83,113,113	2.75	30 (36%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.72	3 (13%)
26	SQD	a	410	-	53,54,54	0.96	3 (5%)	62,65,65	1.73	12 (19%)
23	CLA	d	403	4	69,73,73	2.04	19 (27%)	83,113,113	2.77	31 (37%)
26	SQD	a	412	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	7 (11%)
23	CLA	C	506	3	69,73,73	2.01	20 (28%)	83,113,113	2.83	31 (37%)
33	LMG	j	101	39	51,51,55	0.88	2 (3%)	59,59,63	1.07	5 (8%)
23	CLA	c	501	3	69,73,73	2.06	20 (28%)	83,113,113	2.77	29 (34%)
34	HTG	B	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.74	3 (13%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.58	12 (21%)
40	HEC	v	201	16	50,50,50	1.69	10 (20%)	68,82,82	1.80	19 (27%)
24	PHO	a	406	-	58,69,69	2.73	12 (20%)	56,99,99	2.88	17 (30%)
23	CLA	B	604	2	69,73,73	2.00	19 (27%)	83,113,113	2.75	30 (36%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
23	CLA	C	511	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	31 (37%)
27	GOL	a	411	-	5,5,5	0.38	0	5,5,5	0.41	0
25	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	16 (28%)
35	LMT	B	630	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
31	LHG	A	417	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	2 (3%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.67	13 (23%)
23	CLA	b	608	2	69,73,73	2.06	20 (28%)	83,113,113	2.78	27 (32%)
25	BCR	b	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
28	OEX	a	413	1,41,3	0,14,14	-	-	-		
32	BCT	A	418	21	2,3,3	0.60	0	2,3,3	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	611	2	69,73,73	2.04	20 (28%)	83,113,113	2.75	30 (36%)
24	PHO	a	407	-	58,69,69	2.81	12 (20%)	56,99,99	2.80	14 (25%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
33	LMG	Z	102	-	37,37,55	1.01	3 (8%)	45,45,63	1.64	9 (20%)
23	CLA	b	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.83	34 (40%)
23	CLA	C	513	3	69,73,73	2.05	20 (28%)	83,113,113	2.79	34 (40%)
26	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.38	7 (13%)
23	CLA	A	405	41	69,73,73	2.07	20 (28%)	83,113,113	2.95	32 (38%)
23	CLA	B	606	2	69,73,73	2.06	18 (26%)	83,113,113	2.89	29 (34%)
33	LMG	J	101	39	51,51,55	0.91	2 (3%)	59,59,63	0.98	5 (8%)
25	BCR	B	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	10 (17%)
25	BCR	D	406	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
23	CLA	b	615	2	69,73,73	2.00	18 (26%)	83,113,113	2.83	28 (33%)
23	CLA	c	502	3	69,73,73	2.03	20 (28%)	83,113,113	2.74	30 (36%)
23	CLA	B	602	2	69,73,73	2.10	21 (30%)	83,113,113	2.81	33 (39%)
23	CLA	c	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.88	29 (34%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.84	0
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	4 (7%)
23	CLA	c	504	41	69,73,73	2.06	20 (28%)	83,113,113	2.89	32 (38%)
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.81	2 (4%)
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.37	0
33	LMG	a	416	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	3 (5%)
34	HTG	c	522	-	19,19,19	0.96	2 (10%)	23,24,24	1.49	3 (13%)
23	CLA	A	406	41	69,73,73	2.06	20 (28%)	83,113,113	2.93	33 (39%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.48	10 (16%)
27	GOL	B	626	-	5,5,5	0.52	0	5,5,5	0.40	0
33	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	C	512	3	69,73,73	2.06	20 (28%)	83,113,113	2.87	31 (37%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	c	505	3	69,73,73	2.05	19 (27%)	83,113,113	2.76	30 (36%)
24	PHO	D	401	-	58,69,69	2.74	13 (22%)	56,99,99	3.02	18 (32%)
23	CLA	A	408	1	69,73,73	2.06	21 (30%)	83,113,113	2.91	29 (34%)
23	CLA	C	507	3	69,73,73	2.07	21 (30%)	83,113,113	2.79	33 (39%)
34	HTG	C	521	-	19,19,19	0.92	1 (5%)	23,24,24	1.44	3 (13%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.07	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PL9	a	414	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	20 (29%)
23	CLA	D	405	4	69,73,73	2.06	18 (26%)	83,113,113	2.97	32 (38%)
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.57	10 (17%)
23	CLA	B	615	2	69,73,73	2.01	18 (26%)	83,113,113	2.78	29 (34%)
23	CLA	b	612	2	69,73,73	2.07	20 (28%)	83,113,113	2.71	27 (32%)
29	PL9	D	407	-	55,55,55	0.65	1 (1%)	68,69,69	1.74	21 (30%)
38	HEM	E	103	5,6	50,50,50	1.54	7 (14%)	66,82,82	1.79	17 (25%)
35	LMT	B	629	-	25,25,36	0.46	0	30,30,47	0.70	0
23	CLA	A	404	1	69,73,73	2.09	21 (30%)	83,113,113	2.81	34 (40%)
31	LHG	l	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.11	5 (11%)
34	HTG	b	628	-	19,19,19	1.01	1 (5%)	23,24,24	1.83	4 (17%)
23	CLA	B	608	2	69,73,73	1.99	19 (27%)	83,113,113	2.85	30 (36%)
23	CLA	b	614	2	69,73,73	2.00	20 (28%)	83,113,113	2.86	31 (37%)
34	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.89	5 (21%)
33	LMG	c	520	-	51,51,55	0.97	3 (5%)	59,59,63	1.24	6 (10%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	B	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.75	30 (36%)
34	HTG	d	411	-	16,16,19	1.12	2 (12%)	20,21,24	1.50	1 (5%)
23	CLA	d	401	41	69,73,73	2.07	20 (28%)	83,113,113	2.95	33 (39%)
23	CLA	d	404	4	69,73,73	2.08	20 (28%)	83,113,113	2.89	34 (40%)
27	GOL	b	624	-	5,5,5	0.33	0	5,5,5	0.45	0
23	CLA	B	609	2	69,73,73	2.03	18 (26%)	83,113,113	2.78	28 (33%)

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
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
23	CLA	B	613	2	-	6/39/115/115	-
23	CLA	a	405	41	-	7/39/115/115	-
34	HTG	b	622	-	-	2/10/30/30	0/1/1/1
23	CLA	c	513	3	-	2/39/115/115	-
35	LMT	B	631	-	-	7/17/38/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	b	627	-	-	6/17/37/61	0/1/1/2
23	CLA	b	604	2	-	15/39/115/115	-
23	CLA	b	601	41	-	17/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	LMT	M	103	-	-	11/21/61/61	0/2/2/2
23	CLA	B	614	2	-	13/39/115/115	-
31	LHG	e	101	-	-	14/46/46/53	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	a	408	1	-	10/39/115/115	-
35	LMT	a	417	-	-	4/21/61/61	0/2/2/2
23	CLA	C	504	3	-	2/39/115/115	-
31	LHG	D	408	-	-	15/53/53/53	-
23	CLA	B	616	2	-	10/39/115/115	-
23	CLA	b	605	2	-	10/39/115/115	-
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	c	509	3	-	12/39/115/115	-
36	DGD	c	517	-	-	14/51/91/95	0/2/2/2
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	13/49/69/69	0/1/1/1
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
38	HEM	e	103	5,6	-	8/14/54/54	-
34	HTG	c	521	-	-	7/10/30/30	0/1/1/1
23	CLA	C	503	3	-	9/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
36	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	505	41	-	7/39/115/115	-
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1
35	LMT	D	403	-	-	9/21/61/61	0/2/2/2
23	CLA	c	511	3	-	3/39/115/115	-
34	HTG	B	623	-	-	6/10/30/30	0/1/1/1
36	DGD	c	516	-	-	13/51/91/95	0/2/2/2
35	LMT	I	101	-	-	10/21/61/61	0/2/2/2
23	CLA	c	506	3	-	8/39/115/115	-
35	LMT	m	102	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	616	2	-	15/39/115/115	-
23	CLA	D	404	4	-	2/39/115/115	-
23	CLA	C	514	3	-	13/39/115/115	-
23	CLA	C	509	3	-	5/39/115/115	-
23	CLA	b	613	2	-	10/39/115/115	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LMG	b	620	-	-	14/46/66/70	0/1/1/1
26	SQD	L	101	-	-	23/49/69/69	0/1/1/1
23	CLA	B	605	2	-	9/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
33	LMG	c	519	-	-	13/46/66/70	0/1/1/1
23	CLA	c	510	3	-	10/39/115/115	-
31	LHG	A	416	-	-	11/53/53/53	-
35	LMT	b	621	-	-	7/17/37/61	0/1/1/2
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
23	CLA	b	609	2	-	6/39/115/115	-
23	CLA	b	603	2	-	12/39/115/115	-
23	CLA	c	508	3	-	6/39/115/115	-
23	CLA	c	512	3	-	12/39/115/115	-
23	CLA	B	607	41	-	4/39/115/115	-
40	HEC	V	202	16	1/1/3/7	4/14/54/54	-
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
23	CLA	B	603	2	-	6/39/115/115	-
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	C	508	41	-	8/39/115/115	-
31	LHG	d	407	-	-	14/53/53/53	-
31	LHG	d	408	-	-	20/53/53/53	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	b	611	2	-	6/39/115/115	-
23	CLA	C	510	3	-	6/39/115/115	-
23	CLA	b	610	41	-	5/39/115/115	-
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	502	3	-	8/39/115/115	-
33	LMG	Z	101	-	-	9/46/66/70	0/1/1/1
36	DGD	c	518	-	-	5/51/91/95	0/2/2/2
35	LMT	D	402	-	-	6/21/61/61	0/2/2/2
34	HTG	D	412	-	-	0/7/27/30	0/1/1/1
23	CLA	b	607	41	-	6/39/115/115	-
23	CLA	B	601	41	-	13/39/115/115	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	y	101	-	-	7/29/63/63	0/2/2/2
31	LHG	d	409	-	-	16/53/53/53	-
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
23	CLA	a	404	1	-	10/39/115/115	-
27	GOL	d	402	-	-	2/4/4/4	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	b	606	2	-	12/39/115/115	-
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
23	CLA	B	610	41	-	8/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
34	HTG	B	627	-	-	2/10/30/30	0/1/1/1
23	CLA	c	507	41	-	9/39/115/115	-
34	HTG	b	625	-	-	6/10/30/30	0/1/1/1
26	SQD	a	410	-	-	12/49/69/69	0/1/1/1
23	CLA	d	403	4	-	5/39/115/115	-
26	SQD	a	412	-	-	11/49/69/69	0/1/1/1
23	CLA	C	506	3	-	10/39/115/115	-
33	LMG	j	101	39	-	12/46/66/70	0/1/1/1
23	CLA	c	501	3	-	6/39/115/115	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
25	BCR	A	409	-	-	2/29/63/63	0/2/2/2
40	HEC	v	201	16	1/1/3/7	4/14/54/54	-
24	PHO	a	406	-	-	2/37/103/103	0/5/6/6
23	CLA	B	604	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	520	-	-	15/46/66/70	0/1/1/1
23	CLA	C	511	3	-	14/39/115/115	-
27	GOL	a	411	-	-	2/4/4/4	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
35	LMT	B	630	-	-	7/21/61/61	0/2/2/2
31	LHG	A	417	-	-	21/53/53/53	-
33	LMG	B	621	-	-	13/46/66/70	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	608	2	-	4/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	2	-	3/39/115/115	-
24	PHO	a	407	-	-	3/37/103/103	0/5/6/6
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
33	LMG	Z	102	-	-	14/31/51/70	0/1/1/1
23	CLA	b	602	2	-	6/39/115/115	-
23	CLA	C	513	3	-	10/39/115/115	-
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
23	CLA	A	405	41	-	7/39/115/115	-
23	CLA	B	606	2	-	7/39/115/115	-
33	LMG	J	101	39	-	9/46/66/70	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
23	CLA	b	615	2	-	6/39/115/115	-
23	CLA	c	502	3	-	8/39/115/115	-
23	CLA	B	602	2	-	8/39/115/115	-
23	CLA	c	503	3	-	2/39/115/115	-
35	LMT	E	102	-	-	11/21/61/61	0/2/2/2
31	LHG	D	409	-	-	15/53/53/53	-
23	CLA	c	504	41	-	7/39/115/115	-
35	LMT	e	102	-	-	9/21/61/61	0/2/2/2
27	GOL	B	625	-	-	3/4/4/4	-
33	LMG	a	416	-	-	15/46/66/70	0/1/1/1
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
23	CLA	A	406	41	-	13/39/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	B	626	-	-	3/4/4/4	-
33	LMG	C	501	-	-	9/46/66/70	0/1/1/1
23	CLA	C	512	3	-	4/39/115/115	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	c	505	3	-	10/39/115/115	-
24	PHO	D	401	-	-	7/37/103/103	0/5/6/6
23	CLA	A	408	1	-	13/39/115/115	-
23	CLA	C	507	3	-	15/39/115/115	-
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
29	PL9	a	414	-	-	13/53/73/73	0/1/1/1
23	CLA	D	405	4	-	11/39/115/115	-
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
23	CLA	B	615	2	-	12/39/115/115	-
23	CLA	b	612	2	-	8/39/115/115	-
29	PL9	D	407	-	-	11/53/73/73	0/1/1/1
38	HEM	E	103	5,6	-	6/14/54/54	-
35	LMT	B	629	-	-	10/17/37/61	0/1/1/2
23	CLA	A	404	1	-	6/39/115/115	-
31	LHG	l	101	-	-	19/53/53/53	-
31	LHG	E	101	-	-	20/46/46/53	-
34	HTG	b	628	-	-	6/10/30/30	0/1/1/1
23	CLA	B	608	2	-	5/39/115/115	-
23	CLA	b	614	2	-	16/39/115/115	-
34	HTG	C	522	-	-	2/10/30/30	0/1/1/1
33	LMG	c	520	-	-	7/46/66/70	0/1/1/1
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	612	2	-	9/39/115/115	-
34	HTG	d	411	-	-	3/7/27/30	0/1/1/1
23	CLA	d	401	41	-	6/39/115/115	-
23	CLA	d	404	4	-	14/39/115/115	-
27	GOL	b	624	-	-	1/4/4/4	-
23	CLA	B	609	2	-	6/39/115/115	-

All (1614) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	C1D-C2D	9.58	1.50	1.39
24	a	407	PHO	C1D-C2D	9.19	1.49	1.39
24	A	407	PHO	C1D-C2D	9.14	1.49	1.39
24	A	407	PHO	C1B-C2B	8.96	1.49	1.39
24	a	406	PHO	C1D-C2D	8.75	1.49	1.39
24	a	406	PHO	C1B-C2B	8.67	1.49	1.39
24	D	401	PHO	C1B-C2B	8.57	1.49	1.39
24	a	407	PHO	C1B-C2B	8.50	1.49	1.39
24	a	407	PHO	C3B-C4B	7.40	1.50	1.41
24	A	407	PHO	C3B-C4B	7.36	1.49	1.41
24	D	401	PHO	C3B-C2B	6.66	1.49	1.40
24	a	406	PHO	C4D-CHA	6.63	1.50	1.39
24	a	406	PHO	C3B-C2B	6.55	1.49	1.40
24	a	407	PHO	C3B-C2B	6.45	1.49	1.40
24	A	407	PHO	C4D-CHA	6.29	1.49	1.39
24	D	401	PHO	C4D-CHA	6.22	1.49	1.39
24	a	406	PHO	C3B-C4B	6.18	1.48	1.41
24	A	407	PHO	C3B-C2B	6.16	1.48	1.40
24	A	407	PHO	C3C-C2C	5.83	1.49	1.36
24	a	407	PHO	C3C-C2C	5.82	1.49	1.36
23	d	401	CLA	C1D-ND	5.81	1.44	1.37
24	a	406	PHO	C3C-C2C	5.79	1.49	1.36
23	b	610	CLA	C3C-C2C	5.77	1.49	1.36
23	c	512	CLA	C3C-C2C	5.77	1.49	1.36
24	a	407	PHO	C4D-CHA	5.71	1.48	1.39
23	b	603	CLA	C3C-C2C	5.69	1.48	1.36
23	C	509	CLA	C3C-C2C	5.64	1.48	1.36
23	C	508	CLA	C3C-C2C	5.63	1.48	1.36
23	c	511	CLA	C1D-ND	5.61	1.44	1.37
23	A	408	CLA	C3C-C2C	5.59	1.48	1.36
23	B	601	CLA	C3C-C2C	5.58	1.48	1.36
23	A	404	CLA	C1D-ND	5.56	1.44	1.37
23	B	602	CLA	C3C-C2C	5.54	1.48	1.36
23	b	613	CLA	C3C-C2C	5.53	1.48	1.36
24	D	401	PHO	C3B-C4B	5.52	1.47	1.41
23	B	611	CLA	C1D-ND	5.52	1.44	1.37
23	B	605	CLA	C1D-ND	5.51	1.44	1.37
23	C	513	CLA	C3C-C2C	5.51	1.48	1.36
23	B	616	CLA	C3C-C2C	5.51	1.48	1.36
23	c	508	CLA	C3C-C2C	5.51	1.48	1.36
23	B	610	CLA	C3C-C2C	5.51	1.48	1.36
23	B	608	CLA	C3C-C2C	5.50	1.48	1.36
23	b	605	CLA	C3C-C2C	5.49	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	PHO	C3D-C2D	5.47	1.49	1.39
23	B	602	CLA	C1D-ND	5.47	1.44	1.37
23	B	603	CLA	C3C-C2C	5.47	1.48	1.36
23	A	406	CLA	C3C-C2C	5.46	1.48	1.36
24	D	401	PHO	C3D-C2D	5.46	1.49	1.39
23	C	504	CLA	C3C-C2C	5.44	1.48	1.36
23	b	615	CLA	C3C-C2C	5.44	1.48	1.36
23	C	507	CLA	O2D-CGD	5.43	1.46	1.33
24	a	407	PHO	C3D-C2D	5.40	1.49	1.39
23	b	606	CLA	C3C-C2C	5.39	1.48	1.36
23	B	607	CLA	C3C-C2C	5.39	1.48	1.36
23	a	405	CLA	C3C-C2C	5.39	1.48	1.36
23	b	616	CLA	C1D-ND	5.39	1.44	1.37
23	C	514	CLA	C1D-ND	5.38	1.44	1.37
23	b	612	CLA	C3C-C2C	5.37	1.48	1.36
23	c	501	CLA	C3C-C2C	5.36	1.48	1.36
23	D	404	CLA	C3C-C2C	5.35	1.48	1.36
23	c	507	CLA	C1D-ND	5.35	1.44	1.37
23	B	614	CLA	C3C-C2C	5.35	1.48	1.36
23	d	404	CLA	C3C-C2C	5.35	1.48	1.36
23	d	401	CLA	C3C-C2C	5.35	1.48	1.36
23	c	509	CLA	C3C-C2C	5.34	1.48	1.36
23	b	616	CLA	C3C-C2C	5.34	1.48	1.36
23	A	405	CLA	C3C-C2C	5.34	1.48	1.36
23	b	602	CLA	C3C-C2C	5.33	1.48	1.36
24	A	407	PHO	C3D-C2D	5.33	1.49	1.39
23	C	503	CLA	C3C-C2C	5.33	1.48	1.36
23	C	511	CLA	C3C-C2C	5.32	1.48	1.36
23	a	404	CLA	C1D-ND	5.32	1.44	1.37
23	c	501	CLA	C1D-ND	5.32	1.44	1.37
23	B	606	CLA	C3C-C2C	5.30	1.48	1.36
23	C	505	CLA	C3C-C2C	5.29	1.48	1.36
23	D	405	CLA	C3C-C2C	5.28	1.48	1.36
23	b	601	CLA	O2D-CGD	5.28	1.46	1.33
23	d	404	CLA	C1D-ND	5.28	1.44	1.37
23	c	505	CLA	C3C-C2C	5.27	1.47	1.36
23	b	601	CLA	C3C-C2C	5.27	1.47	1.36
23	a	408	CLA	C3C-C2C	5.27	1.47	1.36
23	b	616	CLA	CHC-C1C	5.27	1.49	1.38
23	A	406	CLA	CHC-C1C	5.27	1.49	1.38
23	C	512	CLA	O2D-CGD	5.26	1.46	1.33
23	b	604	CLA	C3C-C2C	5.26	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	102	BCR	C23-C22	-5.26	1.34	1.45
23	b	603	CLA	O2D-CGD	5.25	1.46	1.33
23	C	510	CLA	C3C-C2C	5.25	1.47	1.36
23	b	601	CLA	C1D-ND	5.24	1.44	1.37
23	C	505	CLA	O2D-CGD	5.24	1.46	1.33
25	C	515	BCR	C23-C22	-5.24	1.34	1.45
23	B	606	CLA	C1D-ND	5.23	1.44	1.37
23	A	404	CLA	C3C-C2C	5.23	1.47	1.36
23	c	509	CLA	C1D-ND	5.23	1.44	1.37
23	B	612	CLA	C3C-C2C	5.23	1.47	1.36
40	V	202	HEC	FE-NB	5.22	2.11	1.94
23	c	506	CLA	O2D-CGD	5.22	1.45	1.33
23	C	514	CLA	C3C-C2C	5.21	1.47	1.36
23	b	608	CLA	C3C-C2C	5.21	1.47	1.36
23	b	602	CLA	O2D-CGD	5.21	1.45	1.33
23	b	611	CLA	C3C-C2C	5.21	1.47	1.36
23	c	504	CLA	C1D-ND	5.21	1.44	1.37
23	B	610	CLA	C1D-ND	5.21	1.44	1.37
23	c	513	CLA	C3C-C2C	5.20	1.47	1.36
23	D	405	CLA	CHC-C1C	5.20	1.49	1.38
23	c	511	CLA	C3C-C2C	5.20	1.47	1.36
23	C	502	CLA	C3C-C2C	5.20	1.47	1.36
23	c	503	CLA	C1D-ND	5.19	1.44	1.37
24	a	407	PHO	O2D-CGD	5.19	1.45	1.33
23	c	503	CLA	C3C-C2C	5.19	1.47	1.36
23	B	605	CLA	C3C-C2C	5.18	1.47	1.36
23	c	507	CLA	C3C-C2C	5.18	1.47	1.36
23	c	502	CLA	C3C-C2C	5.18	1.47	1.36
23	B	614	CLA	C1D-ND	5.17	1.44	1.37
23	b	602	CLA	C1D-ND	5.17	1.44	1.37
23	C	507	CLA	C1D-ND	5.17	1.44	1.37
38	e	103	HEM	FE-NB	5.16	2.10	1.94
23	c	513	CLA	C1D-ND	5.16	1.44	1.37
24	D	401	PHO	C3C-C2C	5.15	1.47	1.36
23	b	611	CLA	O2D-CGD	5.15	1.45	1.33
23	c	509	CLA	O2D-CGD	5.14	1.45	1.33
25	k	101	BCR	C23-C22	-5.14	1.34	1.45
23	B	601	CLA	O2D-CGD	5.14	1.45	1.33
23	b	605	CLA	C1D-ND	5.14	1.44	1.37
23	c	506	CLA	C3C-C2C	5.14	1.47	1.36
23	B	615	CLA	O2D-CGD	5.14	1.45	1.33
25	b	619	BCR	C23-C22	-5.13	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	O2D-CGD	5.12	1.45	1.33
23	d	403	CLA	C3C-C2C	5.12	1.47	1.36
23	B	602	CLA	O2D-CGD	5.12	1.45	1.33
23	b	609	CLA	C1D-ND	5.12	1.44	1.37
23	c	513	CLA	O2D-CGD	5.12	1.45	1.33
23	B	609	CLA	O2D-CGD	5.12	1.45	1.33
38	E	103	HEM	FE-NB	5.11	2.10	1.94
23	B	611	CLA	O2D-CGD	5.11	1.45	1.33
23	B	603	CLA	C1D-ND	5.11	1.44	1.37
23	c	504	CLA	O2D-CGD	5.11	1.45	1.33
23	B	615	CLA	C1D-ND	5.10	1.44	1.37
23	B	615	CLA	C3C-C2C	5.09	1.47	1.36
23	b	603	CLA	CHC-C1C	5.08	1.48	1.38
23	b	613	CLA	O2D-CGD	5.08	1.45	1.33
23	b	606	CLA	C1D-ND	5.08	1.44	1.37
23	B	616	CLA	CHC-C1C	5.08	1.48	1.38
23	A	406	CLA	O2D-CGD	5.08	1.45	1.33
23	D	405	CLA	C1D-ND	5.07	1.44	1.37
23	b	609	CLA	O2D-CGD	5.07	1.45	1.33
23	c	510	CLA	O2D-CGD	5.07	1.45	1.33
23	b	612	CLA	C1D-ND	5.07	1.44	1.37
23	c	506	CLA	C1D-ND	5.07	1.44	1.37
23	B	613	CLA	C1D-ND	5.06	1.44	1.37
23	B	614	CLA	O2D-CGD	5.06	1.45	1.33
25	d	405	BCR	C23-C22	-5.06	1.35	1.45
23	b	611	CLA	C1D-ND	5.06	1.44	1.37
23	C	503	CLA	C1D-ND	5.05	1.44	1.37
23	d	404	CLA	CHC-C1C	5.05	1.48	1.38
24	a	407	PHO	OBD-CAD	5.05	1.29	1.22
23	c	502	CLA	C1D-ND	5.05	1.44	1.37
23	B	613	CLA	C3C-C2C	5.04	1.47	1.36
23	b	603	CLA	C1D-ND	5.04	1.44	1.37
23	A	408	CLA	C1D-ND	5.04	1.44	1.37
23	C	506	CLA	C3C-C2C	5.04	1.47	1.36
23	b	607	CLA	C3C-C2C	5.04	1.47	1.36
23	B	609	CLA	CHC-C1C	5.03	1.48	1.38
23	B	616	CLA	C1D-ND	5.03	1.44	1.37
23	a	404	CLA	C3C-C2C	5.03	1.47	1.36
23	B	608	CLA	O2D-CGD	5.03	1.45	1.33
23	C	512	CLA	C3C-C2C	5.02	1.47	1.36
25	D	406	BCR	C23-C22	-5.02	1.35	1.45
24	A	407	PHO	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	O2D-CGD	5.02	1.45	1.33
23	B	604	CLA	C3C-C2C	5.02	1.47	1.36
23	C	510	CLA	O2D-CGD	5.02	1.45	1.33
23	c	502	CLA	O2D-CGD	5.00	1.45	1.33
23	C	506	CLA	CHC-C1C	5.00	1.48	1.38
23	b	608	CLA	O2D-CGD	4.99	1.45	1.33
23	b	614	CLA	O2D-CGD	4.99	1.45	1.33
23	C	510	CLA	C1D-ND	4.98	1.43	1.37
23	C	514	CLA	CHC-C1C	4.98	1.48	1.38
23	B	601	CLA	C1D-ND	4.98	1.43	1.37
23	d	403	CLA	O2D-CGD	4.97	1.45	1.33
23	c	510	CLA	C3C-C2C	4.97	1.47	1.36
23	C	502	CLA	C1D-ND	4.97	1.43	1.37
25	c	514	BCR	C23-C22	-4.96	1.35	1.45
23	b	616	CLA	O2D-CGD	4.96	1.45	1.33
23	c	504	CLA	C3C-C2C	4.96	1.47	1.36
23	C	508	CLA	C1D-ND	4.95	1.43	1.37
23	A	405	CLA	C1D-ND	4.95	1.43	1.37
23	C	513	CLA	C1D-ND	4.95	1.43	1.37
23	c	512	CLA	O2D-CGD	4.94	1.45	1.33
23	c	505	CLA	C1D-ND	4.94	1.43	1.37
23	b	607	CLA	O2D-CGD	4.94	1.45	1.33
25	t	101	BCR	C23-C22	-4.94	1.35	1.45
23	B	611	CLA	C3C-C2C	4.94	1.47	1.36
23	B	605	CLA	O2D-CGD	4.93	1.45	1.33
23	C	507	CLA	C3C-C2C	4.93	1.47	1.36
23	C	504	CLA	C1D-ND	4.93	1.43	1.37
23	B	609	CLA	C3C-C2C	4.93	1.47	1.36
23	D	404	CLA	O2D-CGD	4.92	1.45	1.33
23	b	608	CLA	C1D-ND	4.92	1.43	1.37
23	b	604	CLA	C1D-ND	4.92	1.43	1.37
23	B	610	CLA	CHC-C1C	4.92	1.48	1.38
23	b	612	CLA	O2D-CGD	4.92	1.45	1.33
23	A	405	CLA	CHC-C1C	4.92	1.48	1.38
25	C	516	BCR	C23-C22	-4.92	1.35	1.45
24	D	401	PHO	O2D-CGD	4.91	1.45	1.33
23	c	505	CLA	CHC-C1C	4.91	1.48	1.38
23	a	405	CLA	C1D-ND	4.91	1.43	1.37
40	v	201	HEC	FE-NB	4.91	2.10	1.94
23	b	610	CLA	CHC-C1C	4.90	1.48	1.38
23	D	404	CLA	C1D-ND	4.90	1.43	1.37
23	C	506	CLA	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C1D-ND	4.90	1.43	1.37
23	b	610	CLA	C1D-ND	4.90	1.43	1.37
23	b	615	CLA	C1D-ND	4.89	1.43	1.37
23	c	508	CLA	C1D-ND	4.89	1.43	1.37
23	b	613	CLA	C1D-ND	4.88	1.43	1.37
23	c	507	CLA	O2D-CGD	4.88	1.45	1.33
25	b	618	BCR	C23-C22	-4.88	1.35	1.45
23	c	513	CLA	CHC-C1C	4.88	1.48	1.38
23	B	604	CLA	CHC-C1C	4.88	1.48	1.38
23	C	513	CLA	CHC-C1C	4.88	1.48	1.38
23	C	508	CLA	O2D-CGD	4.88	1.45	1.33
23	c	510	CLA	C1D-ND	4.87	1.43	1.37
23	B	604	CLA	O2D-CGD	4.87	1.45	1.33
25	B	619	BCR	C23-C22	-4.87	1.35	1.45
23	A	404	CLA	CHC-C1C	4.87	1.48	1.38
23	c	507	CLA	CHC-C1C	4.87	1.48	1.38
25	A	409	BCR	C23-C22	-4.86	1.35	1.45
23	D	405	CLA	O2D-CGD	4.86	1.45	1.33
23	b	604	CLA	O2D-CGD	4.86	1.45	1.33
23	a	408	CLA	O2D-CGD	4.86	1.45	1.33
23	B	610	CLA	O2D-CGD	4.86	1.45	1.33
23	C	512	CLA	C1D-ND	4.86	1.43	1.37
23	b	614	CLA	C3C-C2C	4.86	1.47	1.36
23	C	511	CLA	C1D-ND	4.85	1.43	1.37
23	B	606	CLA	O2D-CGD	4.85	1.45	1.33
23	b	605	CLA	O2D-CGD	4.85	1.45	1.33
23	C	509	CLA	O2D-CGD	4.84	1.45	1.33
23	b	612	CLA	CHC-C1C	4.84	1.48	1.38
25	H	101	BCR	C23-C22	-4.84	1.35	1.45
23	B	606	CLA	CHC-C1C	4.83	1.48	1.38
23	b	609	CLA	CHC-C1C	4.82	1.48	1.38
23	a	408	CLA	CHC-C1C	4.81	1.48	1.38
23	a	404	CLA	O2D-CGD	4.81	1.44	1.33
25	y	101	BCR	C23-C22	-4.81	1.35	1.45
25	b	617	BCR	C23-C22	-4.80	1.35	1.45
23	b	609	CLA	C3C-C2C	4.80	1.46	1.36
25	T	101	BCR	C23-C22	-4.80	1.35	1.45
23	d	401	CLA	O2D-CGD	4.80	1.44	1.33
23	A	408	CLA	CHD-C1D	4.80	1.47	1.38
23	b	615	CLA	O2D-CGD	4.79	1.44	1.33
23	c	503	CLA	O2D-CGD	4.79	1.44	1.33
23	B	602	CLA	CHD-C1D	4.79	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	CHC-C1C	4.79	1.48	1.38
23	C	503	CLA	CHD-C1D	4.78	1.47	1.38
23	A	404	CLA	O2D-CGD	4.77	1.44	1.33
23	C	503	CLA	CHC-C1C	4.77	1.48	1.38
23	B	605	CLA	CHC-C1C	4.77	1.48	1.38
23	C	511	CLA	CHC-C1C	4.77	1.48	1.38
23	c	511	CLA	CHC-C1C	4.77	1.48	1.38
23	c	508	CLA	CHC-C1C	4.77	1.48	1.38
23	a	405	CLA	O2D-CGD	4.76	1.44	1.33
23	C	511	CLA	O2D-CGD	4.76	1.44	1.33
23	C	514	CLA	O2D-CGD	4.74	1.44	1.33
23	B	609	CLA	C1D-ND	4.74	1.43	1.37
23	c	503	CLA	CHC-C1C	4.74	1.48	1.38
23	B	609	CLA	O2A-CGA	4.74	1.47	1.33
23	B	616	CLA	O2D-CGD	4.73	1.44	1.33
23	B	612	CLA	O2D-CGD	4.72	1.44	1.33
23	c	505	CLA	O2D-CGD	4.72	1.44	1.33
23	B	607	CLA	C1D-ND	4.72	1.43	1.37
25	c	515	BCR	C23-C22	-4.72	1.35	1.45
23	A	408	CLA	CHC-C1C	4.72	1.48	1.38
23	c	508	CLA	O2D-CGD	4.71	1.44	1.33
23	b	602	CLA	CHC-C1C	4.70	1.48	1.38
23	d	403	CLA	CHC-C1C	4.70	1.48	1.38
23	c	511	CLA	O2D-CGD	4.69	1.44	1.33
23	b	601	CLA	CHC-C1C	4.69	1.48	1.38
23	d	401	CLA	CHC-C1C	4.68	1.48	1.38
25	h	101	BCR	C23-C22	-4.68	1.35	1.45
23	c	501	CLA	CHD-C1D	4.68	1.47	1.38
23	B	608	CLA	C1D-ND	4.68	1.43	1.37
23	C	504	CLA	CHC-C1C	4.68	1.48	1.38
23	B	603	CLA	O2D-CGD	4.68	1.44	1.33
23	C	507	CLA	CHD-C1D	4.67	1.47	1.38
23	C	513	CLA	O2D-CGD	4.67	1.44	1.33
23	A	405	CLA	O2D-CGD	4.67	1.44	1.33
23	A	405	CLA	CHC-C4B	4.67	1.49	1.39
23	a	405	CLA	CHC-C1C	4.66	1.48	1.38
23	c	512	CLA	CHC-C1C	4.66	1.48	1.38
23	b	610	CLA	CHD-C1D	4.66	1.47	1.38
23	B	607	CLA	CHC-C1C	4.65	1.48	1.38
23	b	606	CLA	O2D-CGD	4.65	1.44	1.33
24	A	407	PHO	OBD-CAD	4.64	1.28	1.22
23	C	505	CLA	C1D-ND	4.64	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	O2D-CGD	4.63	1.44	1.33
23	C	509	CLA	C1D-ND	4.62	1.43	1.37
23	c	509	CLA	CHC-C1C	4.62	1.47	1.38
23	c	501	CLA	CHC-C1C	4.62	1.47	1.38
23	d	404	CLA	O2D-CGD	4.62	1.44	1.33
23	b	608	CLA	CHC-C1C	4.62	1.47	1.38
23	B	607	CLA	O2D-CGD	4.61	1.44	1.33
23	b	607	CLA	CHC-C1C	4.60	1.47	1.38
23	C	506	CLA	C1D-ND	4.60	1.43	1.37
23	b	614	CLA	C1D-ND	4.60	1.43	1.37
24	a	406	PHO	O2D-CGD	4.59	1.44	1.33
25	Y	101	BCR	C23-C22	-4.59	1.36	1.45
23	C	507	CLA	CHC-C1C	4.58	1.47	1.38
23	A	406	CLA	C1D-ND	4.57	1.43	1.37
23	B	601	CLA	CHC-C1C	4.56	1.47	1.38
23	C	502	CLA	O2D-CGD	4.56	1.44	1.33
33	z	101	LMG	O8-C28	4.56	1.46	1.33
23	b	601	CLA	CHD-C1D	4.56	1.47	1.38
23	d	403	CLA	C1B-NB	-4.55	1.32	1.37
23	B	602	CLA	CHC-C1C	4.55	1.47	1.38
23	B	601	CLA	O2A-CGA	4.54	1.46	1.33
23	C	510	CLA	CHC-C1C	4.54	1.47	1.38
23	C	512	CLA	CHC-C1C	4.54	1.47	1.38
23	b	615	CLA	CHC-C1C	4.54	1.47	1.38
23	b	602	CLA	CHD-C1D	4.54	1.47	1.38
25	B	617	BCR	C23-C22	-4.53	1.36	1.45
23	B	613	CLA	CHC-C1C	4.53	1.47	1.38
23	B	608	CLA	CHC-C1C	4.53	1.47	1.38
23	C	503	CLA	O2D-CGD	4.53	1.44	1.33
23	C	508	CLA	CHD-C1D	4.53	1.47	1.38
23	C	510	CLA	CHD-C1D	4.51	1.47	1.38
24	D	401	PHO	OBD-CAD	4.51	1.28	1.22
23	C	508	CLA	CHC-C1C	4.51	1.47	1.38
23	C	513	CLA	CHD-C1D	4.51	1.47	1.38
26	D	413	SQD	O47-C7	4.51	1.47	1.34
23	B	603	CLA	CHD-C1D	4.50	1.47	1.38
23	C	502	CLA	CHC-C1C	4.50	1.47	1.38
23	C	503	CLA	O2A-CGA	4.50	1.46	1.33
23	C	514	CLA	CHD-C1D	4.49	1.47	1.38
23	b	606	CLA	CHC-C1C	4.49	1.47	1.38
26	a	412	SQD	O48-C23	4.49	1.46	1.33
23	B	612	CLA	C1B-NB	-4.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E	101	LHG	O8-C23	4.48	1.46	1.33
24	a	406	PHO	OBD-CAD	4.48	1.28	1.22
23	c	504	CLA	CHC-C1C	4.48	1.47	1.38
23	B	603	CLA	CHC-C1C	4.48	1.47	1.38
23	d	404	CLA	CHD-C1D	4.48	1.47	1.38
26	f	101	SQD	O47-C7	4.47	1.46	1.34
23	c	508	CLA	O2A-CGA	4.46	1.46	1.33
23	B	611	CLA	CHC-C1C	4.46	1.47	1.38
23	b	613	CLA	CHC-C1C	4.45	1.47	1.38
23	d	401	CLA	O2A-CGA	4.45	1.46	1.33
26	B	620	SQD	O47-C7	4.44	1.46	1.34
23	b	605	CLA	CHD-C1D	4.44	1.47	1.38
23	c	501	CLA	O2D-CGD	4.43	1.44	1.33
23	C	504	CLA	O2D-CGD	4.43	1.44	1.33
23	b	601	CLA	O2A-CGA	4.43	1.46	1.33
23	b	609	CLA	CHD-C1D	4.43	1.47	1.38
23	b	611	CLA	CHC-C1C	4.42	1.47	1.38
23	d	401	CLA	CHD-C1D	4.42	1.47	1.38
23	d	404	CLA	O2A-CGA	4.41	1.46	1.33
23	C	508	CLA	O2A-CGA	4.41	1.46	1.33
23	b	611	CLA	O2A-CGA	4.41	1.46	1.33
23	B	607	CLA	CHD-C1D	4.40	1.46	1.38
36	c	517	DGD	O1G-C1A	4.40	1.46	1.33
40	V	202	HEC	FE-NC	4.40	2.10	1.95
23	a	404	CLA	CHC-C1C	4.40	1.47	1.38
23	c	507	CLA	CHD-C1D	4.40	1.46	1.38
23	d	403	CLA	O2A-CGA	4.40	1.46	1.33
25	a	409	BCR	C23-C22	-4.40	1.36	1.45
23	b	612	CLA	O2A-CGA	4.39	1.46	1.33
26	A	412	SQD	O47-C7	4.39	1.46	1.34
33	Z	101	LMG	O7-C10	4.39	1.46	1.34
23	B	601	CLA	CHD-C1D	4.39	1.46	1.38
23	C	512	CLA	CHD-C1D	4.38	1.46	1.38
31	d	409	LHG	O7-C7	4.38	1.46	1.34
23	a	408	CLA	CHD-C1D	4.38	1.46	1.38
23	B	610	CLA	OBD-CAD	4.38	1.30	1.22
23	B	614	CLA	CHD-C1D	4.38	1.46	1.38
23	B	612	CLA	CHC-C1C	4.36	1.47	1.38
23	c	503	CLA	CHD-C1D	4.36	1.46	1.38
23	C	511	CLA	CHD-C1D	4.36	1.46	1.38
23	a	404	CLA	CHD-C1D	4.36	1.46	1.38
23	c	513	CLA	CHD-C1D	4.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	O2A-CGA	4.35	1.46	1.33
23	c	506	CLA	CHC-C1C	4.35	1.47	1.38
23	b	616	CLA	CHD-C1D	4.35	1.46	1.38
23	C	512	CLA	O2A-CGA	4.35	1.46	1.33
23	C	505	CLA	O2A-CGA	4.35	1.46	1.33
23	c	506	CLA	CHD-C1D	4.35	1.46	1.38
23	b	608	CLA	O2A-CGA	4.35	1.46	1.33
23	c	512	CLA	O2A-CGA	4.35	1.46	1.33
26	B	620	SQD	O48-C23	4.34	1.46	1.33
33	C	501	LMG	O8-C28	4.34	1.46	1.33
33	Z	101	LMG	O8-C28	4.34	1.46	1.33
26	A	412	SQD	O48-C23	4.34	1.46	1.33
23	B	604	CLA	C1D-ND	4.33	1.43	1.37
23	c	510	CLA	CHC-C1C	4.33	1.47	1.38
23	B	612	CLA	CHD-C1D	4.33	1.46	1.38
23	B	615	CLA	CHC-C1C	4.33	1.47	1.38
23	C	509	CLA	CHD-C1D	4.33	1.46	1.38
23	b	614	CLA	CHC-C1C	4.33	1.47	1.38
23	C	505	CLA	CHC-C1C	4.32	1.47	1.38
31	l	101	LHG	O8-C23	4.31	1.45	1.33
23	D	404	CLA	CHC-C1C	4.31	1.47	1.38
23	C	506	CLA	O2A-CGA	4.30	1.45	1.33
23	c	502	CLA	CHD-C1D	4.30	1.46	1.38
31	e	101	LHG	O8-C23	4.30	1.45	1.33
23	A	405	CLA	O2A-CGA	4.30	1.45	1.33
23	C	514	CLA	O2A-CGA	4.30	1.45	1.33
26	L	101	SQD	O48-C23	4.29	1.45	1.33
23	B	607	CLA	O2A-CGA	4.29	1.45	1.33
23	b	613	CLA	CHD-C1D	4.29	1.46	1.38
23	c	509	CLA	O2A-CGA	4.28	1.45	1.33
33	c	520	LMG	O7-C10	4.28	1.46	1.34
23	B	615	CLA	O2A-CGA	4.28	1.45	1.33
33	c	520	LMG	O8-C28	4.27	1.45	1.33
26	A	410	SQD	O48-C23	4.27	1.45	1.33
23	c	502	CLA	O2A-CGA	4.27	1.45	1.33
31	A	417	LHG	O8-C23	4.26	1.45	1.33
23	B	615	CLA	CHD-C1D	4.26	1.46	1.38
23	C	504	CLA	CHD-C1D	4.26	1.46	1.38
23	b	606	CLA	CHD-C1D	4.25	1.46	1.38
23	c	504	CLA	O2A-CGA	4.25	1.45	1.33
23	c	513	CLA	O2A-CGA	4.25	1.45	1.33
33	Z	102	LMG	O7-C10	4.25	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	101	SQD	O47-C7	4.25	1.46	1.34
23	b	608	CLA	CHD-C1D	4.25	1.46	1.38
33	B	621	LMG	O8-C28	4.25	1.45	1.33
23	b	615	CLA	O2A-CGA	4.24	1.45	1.33
23	b	604	CLA	CHD-C1D	4.24	1.46	1.38
33	c	519	LMG	O8-C28	4.24	1.45	1.33
23	C	511	CLA	O2A-CGA	4.24	1.45	1.33
23	a	408	CLA	C1D-ND	4.24	1.43	1.37
23	C	504	CLA	CHD-C4C	4.24	1.48	1.39
23	B	606	CLA	O2A-CGA	4.23	1.45	1.33
26	f	101	SQD	O48-C23	4.23	1.45	1.33
33	a	416	LMG	O7-C10	4.23	1.46	1.34
23	c	510	CLA	CHD-C1D	4.23	1.46	1.38
23	b	611	CLA	CHB-C1B	4.22	1.48	1.39
33	C	501	LMG	O7-C10	4.22	1.46	1.34
23	B	602	CLA	CHD-C4C	4.22	1.48	1.39
23	C	502	CLA	O2A-CGA	4.22	1.45	1.33
23	c	512	CLA	CHD-C1D	4.21	1.46	1.38
23	b	601	CLA	CHD-C4C	4.21	1.48	1.39
23	c	502	CLA	CHC-C1C	4.21	1.47	1.38
23	C	509	CLA	CHC-C1C	4.21	1.47	1.38
40	v	201	HEC	FE-NC	4.20	2.09	1.95
23	C	513	CLA	O2A-CGA	4.20	1.45	1.33
23	c	511	CLA	CHD-C4C	4.20	1.48	1.39
23	a	405	CLA	CHD-C1D	4.20	1.46	1.38
23	c	511	CLA	CHD-C1D	4.20	1.46	1.38
23	b	616	CLA	CHC-C4B	4.20	1.48	1.39
23	c	509	CLA	CHD-C1D	4.20	1.46	1.38
23	b	611	CLA	CHD-C1D	4.20	1.46	1.38
23	B	611	CLA	CHD-C1D	4.19	1.46	1.38
23	C	502	CLA	CHD-C1D	4.19	1.46	1.38
23	b	614	CLA	CHD-C1D	4.19	1.46	1.38
31	e	101	LHG	O7-C7	4.19	1.46	1.34
23	d	401	CLA	C3D-C2D	4.18	1.50	1.39
23	A	406	CLA	O2A-CGA	4.18	1.45	1.33
23	c	511	CLA	CHB-C1B	4.18	1.48	1.39
23	A	404	CLA	CHD-C1D	4.18	1.46	1.38
23	c	505	CLA	CHB-C1B	4.17	1.48	1.39
24	a	407	PHO	O2A-CGA	4.17	1.45	1.33
23	B	609	CLA	CHD-C1D	4.17	1.46	1.38
23	c	504	CLA	CHD-C1D	4.16	1.46	1.38
23	a	405	CLA	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	CHC-C1C	4.16	1.47	1.38
23	D	404	CLA	CHD-C1D	4.15	1.46	1.38
23	c	508	CLA	CHD-C1D	4.15	1.46	1.38
23	c	506	CLA	O2A-CGA	4.15	1.45	1.33
23	B	605	CLA	CHC-C4B	4.15	1.48	1.39
23	C	507	CLA	O2A-CGA	4.15	1.45	1.33
23	c	511	CLA	O2A-CGA	4.15	1.45	1.33
33	C	520	LMG	O8-C28	4.15	1.45	1.33
31	d	409	LHG	O8-C23	4.14	1.45	1.33
23	C	511	CLA	CHD-C4C	4.14	1.48	1.39
23	c	505	CLA	O2A-CGA	4.14	1.45	1.33
23	B	616	CLA	O2A-CGA	4.14	1.45	1.33
31	D	409	LHG	O7-C7	4.14	1.46	1.34
23	B	606	CLA	CHD-C1D	4.14	1.46	1.38
23	C	507	CLA	CHD-C4C	4.14	1.48	1.39
23	c	503	CLA	CHC-C4B	4.14	1.48	1.39
33	J	101	LMG	O8-C28	4.14	1.45	1.33
23	C	508	CLA	C3D-C2D	4.14	1.50	1.39
24	D	401	PHO	O2A-CGA	4.13	1.45	1.33
23	B	607	CLA	CHD-C4C	4.13	1.48	1.39
23	B	604	CLA	O2A-CGA	4.13	1.45	1.33
23	b	612	CLA	CHD-C1D	4.12	1.46	1.38
23	C	510	CLA	O2A-CGA	4.12	1.45	1.33
33	c	519	LMG	O7-C10	4.12	1.45	1.34
23	c	503	CLA	O2A-CGA	4.11	1.45	1.33
23	B	604	CLA	CHD-C1D	4.11	1.46	1.38
23	b	610	CLA	CHC-C4B	4.11	1.48	1.39
33	a	416	LMG	O8-C28	4.11	1.45	1.33
23	C	513	CLA	CHD-C4C	4.11	1.48	1.39
23	c	508	CLA	C3D-C2D	4.11	1.50	1.39
23	B	612	CLA	C1D-ND	4.11	1.42	1.37
36	h	102	DGD	O2G-C1B	4.10	1.45	1.34
33	C	520	LMG	O7-C10	4.10	1.45	1.34
26	a	412	SQD	O47-C7	4.10	1.45	1.34
23	d	403	CLA	CHD-C1D	4.10	1.46	1.38
23	C	509	CLA	C3D-C2D	4.10	1.50	1.39
23	b	602	CLA	CHD-C4C	4.10	1.48	1.39
23	D	405	CLA	CHD-C1D	4.09	1.46	1.38
36	H	102	DGD	O2G-C1B	4.09	1.45	1.34
23	B	615	CLA	C3D-C2D	4.09	1.50	1.39
26	a	410	SQD	O48-C23	4.09	1.45	1.33
23	a	408	CLA	O2A-CGA	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C3D-C2D	4.08	1.50	1.39
23	b	608	CLA	C3D-C2D	4.08	1.50	1.39
36	H	102	DGD	O1G-C1A	4.08	1.45	1.33
33	j	101	LMG	O8-C28	4.08	1.45	1.33
23	b	603	CLA	CHD-C1D	4.08	1.46	1.38
23	C	504	CLA	O2A-CGA	4.08	1.45	1.33
23	c	501	CLA	CHB-C1B	4.07	1.48	1.39
31	l	101	LHG	O7-C7	4.07	1.45	1.34
23	b	601	CLA	C3D-C2D	4.07	1.50	1.39
38	e	103	HEM	FE-NC	4.06	2.08	1.95
23	b	615	CLA	CHD-C1D	4.06	1.46	1.38
23	d	404	CLA	C3D-C2D	4.06	1.50	1.39
23	c	513	CLA	CHD-C4C	4.06	1.48	1.39
23	A	404	CLA	CHD-C4C	4.06	1.48	1.39
23	b	613	CLA	C3D-C2D	4.06	1.50	1.39
23	D	404	CLA	O2A-CGA	4.06	1.45	1.33
26	D	413	SQD	O48-C23	4.06	1.45	1.33
23	B	611	CLA	CHB-C1B	4.05	1.48	1.39
23	B	602	CLA	C3D-C2D	4.05	1.50	1.39
23	C	510	CLA	CHD-C4C	4.05	1.48	1.39
23	c	502	CLA	C3D-C2D	4.05	1.50	1.39
23	B	614	CLA	CHC-C1C	4.05	1.46	1.38
33	z	101	LMG	O7-C10	4.05	1.45	1.34
33	b	620	LMG	O8-C28	4.05	1.45	1.33
23	b	605	CLA	C3D-C2D	4.05	1.50	1.39
23	A	406	CLA	CHD-C1D	4.05	1.46	1.38
23	B	615	CLA	OBD-CAD	4.04	1.29	1.22
23	c	509	CLA	CHD-C4C	4.04	1.48	1.39
23	c	510	CLA	CHD-C4C	4.04	1.48	1.39
23	B	601	CLA	C3D-C2D	4.04	1.50	1.39
23	b	613	CLA	O2A-CGA	4.04	1.45	1.33
36	c	518	DGD	O1G-C1A	4.04	1.45	1.33
23	c	501	CLA	CHD-C4C	4.04	1.48	1.39
23	B	608	CLA	CHD-C1D	4.04	1.46	1.38
40	V	202	HEC	CBC-CAC	-4.04	1.33	1.51
23	B	612	CLA	O2A-CGA	4.03	1.45	1.33
36	h	102	DGD	O1G-C1A	4.03	1.45	1.33
36	c	516	DGD	O1G-C1A	4.03	1.45	1.33
23	B	610	CLA	CHD-C1D	4.03	1.46	1.38
23	C	506	CLA	CHD-C1D	4.03	1.46	1.38
23	C	509	CLA	O2A-CGA	4.03	1.45	1.33
23	b	614	CLA	CHD-C4C	4.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CHD-C1D	4.03	1.46	1.38
23	C	514	CLA	CHD-C4C	4.03	1.48	1.39
23	D	404	CLA	CHD-C4C	4.02	1.48	1.39
23	B	613	CLA	CHD-C1D	4.02	1.46	1.38
23	B	611	CLA	O2A-CGA	4.02	1.45	1.33
25	B	618	BCR	C23-C22	-4.02	1.37	1.45
23	c	510	CLA	O2A-CGA	4.01	1.45	1.33
23	b	603	CLA	CHD-C4C	4.01	1.48	1.39
23	d	403	CLA	C1D-ND	4.01	1.42	1.37
23	B	603	CLA	CHD-C4C	4.00	1.48	1.39
23	a	408	CLA	CHD-C4C	4.00	1.48	1.39
23	c	511	CLA	OBD-CAD	4.00	1.29	1.22
38	E	103	HEM	FE-NC	4.00	2.08	1.95
23	B	613	CLA	O2A-CGA	4.00	1.45	1.33
23	c	501	CLA	CHC-C4B	4.00	1.48	1.39
23	C	509	CLA	CHB-C1B	4.00	1.48	1.39
31	E	101	LHG	O7-C7	3.99	1.45	1.34
23	b	609	CLA	CHD-C4C	3.99	1.48	1.39
26	a	410	SQD	O47-C7	3.99	1.45	1.34
23	C	508	CLA	CHD-C4C	3.99	1.48	1.39
23	C	509	CLA	OBD-CAD	3.99	1.29	1.22
23	C	503	CLA	CHD-C4C	3.98	1.48	1.39
23	B	610	CLA	CHC-C4B	3.98	1.48	1.39
23	B	615	CLA	CHD-C4C	3.98	1.48	1.39
23	c	501	CLA	O2A-CGA	3.98	1.45	1.33
23	A	405	CLA	C3D-C2D	3.98	1.50	1.39
23	b	608	CLA	CHC-C4B	3.98	1.48	1.39
23	b	605	CLA	CHD-C4C	3.98	1.48	1.39
23	B	616	CLA	C3D-C2D	3.98	1.50	1.39
23	A	408	CLA	CHD-C4C	3.98	1.48	1.39
23	B	616	CLA	CHD-C1D	3.98	1.46	1.38
23	b	602	CLA	O2A-CGA	3.98	1.45	1.33
40	v	201	HEC	CBC-CAC	-3.97	1.33	1.51
23	d	404	CLA	CHD-C4C	3.97	1.48	1.39
23	b	616	CLA	C3D-C2D	3.97	1.50	1.39
23	B	601	CLA	CHD-C4C	3.97	1.48	1.39
23	B	605	CLA	CHD-C4C	3.97	1.48	1.39
23	B	605	CLA	CHD-C1D	3.97	1.46	1.38
23	c	503	CLA	CHD-C4C	3.96	1.48	1.39
23	b	607	CLA	C3D-C2D	3.96	1.49	1.39
23	B	614	CLA	CHD-C4C	3.96	1.48	1.39
23	D	405	CLA	OBD-CAD	3.96	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	CHD-C4C	3.96	1.48	1.39
31	A	417	LHG	O7-C7	3.95	1.45	1.34
23	b	611	CLA	C3D-C2D	3.95	1.49	1.39
23	B	610	CLA	C3D-C2D	3.95	1.49	1.39
23	B	616	CLA	CHD-C4C	3.95	1.48	1.39
23	c	509	CLA	C3D-C2D	3.95	1.49	1.39
36	C	518	DGD	O2G-C1B	3.95	1.45	1.34
23	A	404	CLA	C1B-NB	-3.95	1.32	1.37
23	b	606	CLA	O2A-CGA	3.95	1.44	1.33
40	v	201	HEC	CBB-CAB	-3.95	1.33	1.51
23	d	404	CLA	CHC-C4B	3.94	1.48	1.39
23	b	609	CLA	OBD-CAD	3.94	1.29	1.22
23	c	502	CLA	CHD-C4C	3.94	1.48	1.39
23	b	606	CLA	CHD-C4C	3.94	1.48	1.39
31	d	408	LHG	O7-C7	3.94	1.45	1.34
23	B	605	CLA	CHB-C1B	3.94	1.48	1.39
23	b	605	CLA	O2A-CGA	3.94	1.44	1.33
31	D	408	LHG	O7-C7	3.94	1.45	1.34
23	B	602	CLA	O2A-CGA	3.94	1.44	1.33
40	V	202	HEC	CBB-CAB	-3.94	1.33	1.51
36	c	516	DGD	O2G-C1B	3.94	1.45	1.34
23	B	614	CLA	O2A-CGA	3.93	1.44	1.33
23	b	609	CLA	O2A-CGA	3.93	1.44	1.33
23	b	612	CLA	CHD-C4C	3.93	1.48	1.39
23	b	605	CLA	CHB-C1B	3.93	1.48	1.39
23	c	507	CLA	CHD-C4C	3.93	1.48	1.39
23	b	612	CLA	CHC-C4B	3.93	1.48	1.39
23	B	604	CLA	CHB-C1B	3.93	1.48	1.39
23	C	513	CLA	C3D-C2D	3.93	1.49	1.39
23	b	611	CLA	CHD-C4C	3.93	1.48	1.39
23	b	614	CLA	O2A-CGA	3.92	1.44	1.33
23	C	510	CLA	OBD-CAD	3.92	1.29	1.22
23	c	508	CLA	OBD-CAD	3.92	1.29	1.22
23	c	505	CLA	CHD-C4C	3.91	1.48	1.39
23	b	602	CLA	C3D-C2D	3.91	1.49	1.39
23	D	405	CLA	CHC-C4B	3.91	1.48	1.39
36	C	517	DGD	O2G-C1B	3.91	1.45	1.34
23	b	604	CLA	O2A-CGA	3.91	1.44	1.33
23	a	405	CLA	CHD-C4C	3.91	1.48	1.39
23	b	613	CLA	CHD-C4C	3.91	1.48	1.39
23	b	616	CLA	O2A-CGA	3.90	1.44	1.33
23	B	609	CLA	C3D-C2D	3.90	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHD-C1D	3.90	1.46	1.38
23	B	604	CLA	OBD-CAD	3.90	1.29	1.22
33	B	621	LMG	O7-C10	3.90	1.45	1.34
23	c	505	CLA	CHC-C4B	3.89	1.48	1.39
23	B	605	CLA	O2A-CGA	3.89	1.44	1.33
23	b	604	CLA	OBD-CAD	3.89	1.29	1.22
23	B	606	CLA	CHD-C4C	3.89	1.48	1.39
23	c	507	CLA	OBD-CAD	3.89	1.29	1.22
23	C	505	CLA	C3D-C2D	3.88	1.49	1.39
23	c	507	CLA	C3D-C2D	3.88	1.49	1.39
23	a	404	CLA	OBD-CAD	3.88	1.29	1.22
23	b	603	CLA	O2A-CGA	3.88	1.44	1.33
23	b	608	CLA	CHD-C4C	3.88	1.48	1.39
34	B	622	HTG	C1'-S1	-3.88	1.76	1.81
23	c	504	CLA	C3D-C2D	3.87	1.49	1.39
23	b	616	CLA	CHD-C4C	3.87	1.48	1.39
23	b	603	CLA	OBD-CAD	3.86	1.29	1.22
23	b	610	CLA	OBD-CAD	3.86	1.29	1.22
23	B	613	CLA	CHB-C1B	3.86	1.48	1.39
23	a	405	CLA	C3D-C2D	3.86	1.49	1.39
23	A	408	CLA	O2A-CGA	3.86	1.44	1.33
36	C	519	DGD	O1G-C1A	3.86	1.44	1.33
23	B	603	CLA	C3D-C2D	3.85	1.49	1.39
23	D	405	CLA	CHD-C4C	3.85	1.48	1.39
23	B	609	CLA	CHC-C4B	3.85	1.48	1.39
31	D	409	LHG	O8-C23	3.85	1.44	1.33
23	B	614	CLA	C3D-C2D	3.85	1.49	1.39
23	b	603	CLA	CHC-C4B	3.85	1.48	1.39
23	c	506	CLA	CHD-C4C	3.85	1.48	1.39
23	B	610	CLA	O2A-CGA	3.85	1.44	1.33
23	c	513	CLA	C3D-C2D	3.85	1.49	1.39
23	c	512	CLA	CHD-C4C	3.85	1.48	1.39
23	b	614	CLA	OBD-CAD	3.85	1.29	1.22
23	A	404	CLA	C3D-C2D	3.85	1.49	1.39
23	B	606	CLA	CHC-C4B	3.85	1.48	1.39
23	B	608	CLA	O2A-CGA	3.85	1.44	1.33
23	c	506	CLA	C3D-C2D	3.84	1.49	1.39
24	a	406	PHO	O2A-CGA	3.84	1.44	1.33
23	C	514	CLA	C3D-C2D	3.84	1.49	1.39
23	b	610	CLA	CHB-C1B	3.84	1.48	1.39
23	C	503	CLA	C3D-C2D	3.84	1.49	1.39
23	B	611	CLA	CHD-C4C	3.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CHD-C4C	3.83	1.48	1.39
36	C	518	DGD	O1G-C1A	3.83	1.44	1.33
23	d	403	CLA	CHD-C4C	3.83	1.48	1.39
23	b	602	CLA	CHC-C4B	3.83	1.48	1.39
23	c	508	CLA	CHD-C4C	3.83	1.48	1.39
23	C	506	CLA	CHB-C1B	3.83	1.48	1.39
23	d	401	CLA	CHD-C4C	3.83	1.48	1.39
36	C	519	DGD	O2G-C1B	3.83	1.45	1.34
23	B	613	CLA	CHC-C4B	3.83	1.48	1.39
23	a	404	CLA	CHD-C4C	3.83	1.48	1.39
23	b	611	CLA	CHC-C4B	3.83	1.48	1.39
23	c	506	CLA	OBD-CAD	3.83	1.29	1.22
23	B	609	CLA	CHD-C4C	3.83	1.48	1.39
23	b	610	CLA	O2A-CGA	3.82	1.44	1.33
23	c	510	CLA	CHB-C1B	3.82	1.48	1.39
34	b	628	HTG	C1'-S1	-3.82	1.76	1.81
36	c	518	DGD	O2G-C1B	3.82	1.45	1.34
23	B	614	CLA	CHB-C1B	3.82	1.48	1.39
23	B	610	CLA	CHB-C1B	3.82	1.48	1.39
23	a	404	CLA	C3D-C2D	3.82	1.49	1.39
36	c	517	DGD	O2G-C1B	3.82	1.45	1.34
23	b	607	CLA	CHD-C1D	3.81	1.45	1.38
23	b	609	CLA	C3D-C2D	3.81	1.49	1.39
23	C	505	CLA	CHC-C4B	3.81	1.48	1.39
23	b	610	CLA	C3D-C2D	3.81	1.49	1.39
23	C	511	CLA	OBD-CAD	3.81	1.29	1.22
31	d	407	LHG	O8-C23	3.81	1.44	1.33
23	b	601	CLA	CHC-C4B	3.80	1.47	1.39
23	B	611	CLA	C3D-C2D	3.80	1.49	1.39
23	A	405	CLA	CHB-C1B	3.80	1.47	1.39
23	B	604	CLA	C1B-NB	-3.80	1.33	1.37
34	b	623	HTG	C1'-S1	-3.80	1.76	1.81
23	B	612	CLA	C3D-C2D	3.80	1.49	1.39
23	c	502	CLA	CHB-C1B	3.80	1.47	1.39
23	b	605	CLA	OBD-CAD	3.79	1.29	1.22
23	A	406	CLA	C3D-C2D	3.79	1.49	1.39
23	a	405	CLA	OBD-CAD	3.79	1.29	1.22
23	b	609	CLA	CHB-C1B	3.79	1.47	1.39
23	b	612	CLA	C3D-C2D	3.79	1.49	1.39
23	b	601	CLA	OBD-CAD	3.78	1.29	1.22
31	A	416	LHG	O7-C7	3.78	1.45	1.34
23	c	512	CLA	C3D-C2D	3.78	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CHD-C4C	3.78	1.47	1.39
23	C	506	CLA	CHD-C4C	3.78	1.47	1.39
23	C	510	CLA	C3D-C2D	3.78	1.49	1.39
23	C	512	CLA	CHB-C1B	3.78	1.47	1.39
23	a	408	CLA	C1B-NB	-3.78	1.33	1.37
23	B	601	CLA	OBD-CAD	3.78	1.29	1.22
23	c	501	CLA	C3D-C2D	3.78	1.49	1.39
33	J	101	LMG	O7-C10	3.78	1.45	1.34
23	b	607	CLA	C1B-NB	-3.77	1.33	1.37
23	b	615	CLA	CHD-C4C	3.77	1.47	1.39
23	b	606	CLA	C3D-C2D	3.77	1.49	1.39
23	B	606	CLA	C3D-C2D	3.77	1.49	1.39
23	b	613	CLA	CHB-C1B	3.77	1.47	1.39
23	B	609	CLA	CHB-C1B	3.77	1.47	1.39
23	a	408	CLA	C3D-C2D	3.77	1.49	1.39
23	B	613	CLA	OBD-CAD	3.77	1.29	1.22
23	C	505	CLA	CHB-C1B	3.76	1.47	1.39
23	b	608	CLA	OBD-CAD	3.76	1.29	1.22
23	d	403	CLA	CHB-C1B	3.76	1.47	1.39
23	c	512	CLA	OBD-CAD	3.76	1.29	1.22
23	b	614	CLA	CHB-C1B	3.76	1.47	1.39
23	b	604	CLA	CHB-C1B	3.75	1.47	1.39
26	A	410	SQD	O47-C7	3.74	1.44	1.34
23	A	404	CLA	CHC-C4B	3.74	1.47	1.39
23	B	607	CLA	C3D-C2D	3.74	1.49	1.39
23	B	605	CLA	C3D-C2D	3.74	1.49	1.39
23	A	405	CLA	CHD-C1D	3.74	1.45	1.38
23	c	509	CLA	CHB-C1B	3.74	1.47	1.39
31	A	416	LHG	O8-C23	3.73	1.44	1.33
23	C	505	CLA	CHD-C4C	3.73	1.47	1.39
23	c	508	CLA	CHB-C1B	3.73	1.47	1.39
23	A	404	CLA	O2A-CGA	3.73	1.44	1.33
23	B	616	CLA	OBD-CAD	3.72	1.28	1.22
23	A	406	CLA	OBD-CAD	3.72	1.28	1.22
23	C	510	CLA	CHC-C4B	3.72	1.47	1.39
23	c	513	CLA	CHC-C4B	3.72	1.47	1.39
23	C	513	CLA	OBD-CAD	3.72	1.28	1.22
23	d	404	CLA	OBD-CAD	3.72	1.28	1.22
23	B	605	CLA	OBD-CAD	3.72	1.28	1.22
23	B	603	CLA	O2A-CGA	3.72	1.44	1.33
23	B	608	CLA	C3D-C2D	3.72	1.49	1.39
23	b	604	CLA	CHC-C4B	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	CHC-C4B	3.71	1.47	1.39
23	B	606	CLA	CHB-C1B	3.71	1.47	1.39
23	d	403	CLA	CHC-C4B	3.71	1.47	1.39
23	B	605	CLA	C4B-NB	-3.71	1.33	1.37
23	b	612	CLA	CHB-C1B	3.70	1.47	1.39
23	C	512	CLA	C3D-C2D	3.70	1.49	1.39
23	b	615	CLA	CHB-C1B	3.70	1.47	1.39
23	C	507	CLA	CHC-C4B	3.70	1.47	1.39
23	D	405	CLA	C3D-C2D	3.70	1.49	1.39
23	B	610	CLA	CHD-C4C	3.70	1.47	1.39
23	b	614	CLA	C3D-C2D	3.70	1.49	1.39
23	C	504	CLA	C3D-C2D	3.69	1.49	1.39
23	D	405	CLA	O2A-CGA	3.69	1.44	1.33
23	D	404	CLA	C3D-C2D	3.69	1.49	1.39
23	C	507	CLA	C3D-C2D	3.69	1.49	1.39
23	C	511	CLA	CHB-C1B	3.69	1.47	1.39
23	C	513	CLA	CHC-C4B	3.69	1.47	1.39
23	A	404	CLA	OBD-CAD	3.69	1.28	1.22
23	C	507	CLA	OBD-CAD	3.69	1.28	1.22
23	c	509	CLA	OBD-CAD	3.69	1.28	1.22
23	B	616	CLA	CHB-C1B	3.68	1.47	1.39
23	B	608	CLA	CHB-C1B	3.68	1.47	1.39
23	B	601	CLA	CHC-C4B	3.68	1.47	1.39
31	d	408	LHG	O8-C23	3.68	1.44	1.33
23	c	504	CLA	CHB-C1B	3.68	1.47	1.39
23	b	602	CLA	CHB-C1B	3.67	1.47	1.39
23	D	404	CLA	CHB-C1B	3.67	1.47	1.39
23	c	512	CLA	CHC-C4B	3.67	1.47	1.39
23	C	508	CLA	CHC-C4B	3.67	1.47	1.39
23	c	506	CLA	C1B-NB	-3.67	1.33	1.37
23	c	511	CLA	CHC-C4B	3.67	1.47	1.39
23	c	509	CLA	CHC-C4B	3.66	1.47	1.39
36	C	517	DGD	O1G-C1A	3.66	1.44	1.33
23	B	614	CLA	C4B-NB	-3.66	1.33	1.37
33	b	620	LMG	O7-C10	3.66	1.44	1.34
23	B	608	CLA	CHD-C4C	3.66	1.47	1.39
23	c	505	CLA	OBD-CAD	3.66	1.28	1.22
23	a	404	CLA	CHB-C1B	3.65	1.47	1.39
23	d	403	CLA	C3D-C2D	3.65	1.49	1.39
23	B	603	CLA	C1B-NB	-3.64	1.33	1.37
23	C	502	CLA	CHB-C1B	3.64	1.47	1.39
23	B	604	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3D-C2D	3.64	1.49	1.39
23	C	502	CLA	CHD-C4C	3.64	1.47	1.39
23	B	616	CLA	CHC-C4B	3.63	1.47	1.39
23	B	611	CLA	OBD-CAD	3.63	1.28	1.22
23	b	607	CLA	C1D-ND	3.63	1.42	1.37
23	a	408	CLA	OBD-CAD	3.63	1.28	1.22
23	b	608	CLA	C1B-NB	-3.63	1.33	1.37
23	b	609	CLA	CHC-C4B	3.62	1.47	1.39
23	c	504	CLA	OBD-CAD	3.62	1.28	1.22
23	b	607	CLA	OBD-CAD	3.62	1.28	1.22
23	C	512	CLA	OBD-CAD	3.62	1.28	1.22
23	B	613	CLA	CHD-C4C	3.62	1.47	1.39
23	C	514	CLA	CHB-C1B	3.61	1.47	1.39
23	b	613	CLA	CHC-C4B	3.61	1.47	1.39
23	C	514	CLA	OBD-CAD	3.61	1.28	1.22
23	c	502	CLA	OBD-CAD	3.61	1.28	1.22
23	A	408	CLA	C3D-C2D	3.61	1.49	1.39
34	C	522	HTG	C1'-S1	-3.61	1.76	1.81
34	d	411	HTG	C1'-S1	-3.61	1.76	1.81
23	b	603	CLA	C3D-C2D	3.61	1.49	1.39
23	A	405	CLA	CHD-C4C	3.60	1.47	1.39
23	C	505	CLA	OBD-CAD	3.60	1.28	1.22
23	c	503	CLA	C3D-C2D	3.60	1.48	1.39
23	B	612	CLA	CHB-C1B	3.60	1.47	1.39
23	d	403	CLA	OBD-CAD	3.60	1.28	1.22
23	D	405	CLA	C3B-C4B	3.60	1.51	1.42
23	A	408	CLA	CHC-C4B	3.60	1.47	1.39
23	c	513	CLA	OBD-CAD	3.59	1.28	1.22
23	c	507	CLA	CHC-C4B	3.59	1.47	1.39
23	b	615	CLA	C3D-C2D	3.59	1.48	1.39
23	b	607	CLA	O2A-CGA	3.58	1.43	1.33
23	b	616	CLA	OBD-CAD	3.58	1.28	1.22
23	b	606	CLA	CHB-C1B	3.58	1.47	1.39
23	C	512	CLA	CHC-C4B	3.58	1.47	1.39
24	A	407	PHO	O2A-CGA	3.58	1.43	1.33
23	B	612	CLA	OBD-CAD	3.58	1.28	1.22
23	D	405	CLA	CHB-C1B	3.58	1.47	1.39
23	C	506	CLA	CHC-C4B	3.57	1.47	1.39
23	C	510	CLA	CHB-C1B	3.57	1.47	1.39
23	b	607	CLA	CHB-C1B	3.57	1.47	1.39
23	c	504	CLA	CHC-C4B	3.57	1.47	1.39
23	c	513	CLA	CHB-C1B	3.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CHB-C1B	3.56	1.47	1.39
23	C	506	CLA	OBD-CAD	3.56	1.28	1.22
34	B	624	HTG	C1'-S1	-3.56	1.76	1.81
33	j	101	LMG	O7-C10	3.56	1.44	1.34
23	C	511	CLA	C3D-C2D	3.56	1.48	1.39
23	B	602	CLA	OBD-CAD	3.55	1.28	1.22
23	B	602	CLA	CHB-C1B	3.55	1.47	1.39
23	B	612	CLA	CHC-C4B	3.55	1.47	1.39
23	b	603	CLA	C1B-NB	-3.55	1.33	1.37
31	d	407	LHG	O7-C7	3.55	1.44	1.34
23	c	511	CLA	C3D-C2D	3.54	1.48	1.39
23	b	608	CLA	CHB-C1B	3.54	1.47	1.39
23	b	604	CLA	CHD-C4C	3.54	1.47	1.39
23	b	607	CLA	CHD-C4C	3.54	1.47	1.39
23	c	509	CLA	C1B-NB	-3.54	1.33	1.37
23	a	408	CLA	CHB-C1B	3.54	1.47	1.39
23	C	504	CLA	CHB-C1B	3.54	1.47	1.39
23	b	606	CLA	C1B-NB	-3.54	1.33	1.37
23	C	504	CLA	CHC-C4B	3.53	1.47	1.39
23	C	509	CLA	CHD-C4C	3.53	1.47	1.39
23	b	606	CLA	CHC-C4B	3.53	1.47	1.39
23	a	404	CLA	CHC-C4B	3.52	1.47	1.39
23	c	512	CLA	CHB-C1B	3.52	1.47	1.39
23	c	504	CLA	C4B-NB	-3.51	1.33	1.37
23	A	406	CLA	CHD-C4C	3.51	1.47	1.39
23	B	607	CLA	CHC-C4B	3.50	1.47	1.39
23	a	408	CLA	CHC-C4B	3.50	1.47	1.39
23	b	602	CLA	OBD-CAD	3.50	1.28	1.22
23	C	503	CLA	OBD-CAD	3.49	1.28	1.22
23	C	504	CLA	OBD-CAD	3.49	1.28	1.22
23	B	604	CLA	CHC-C4B	3.49	1.47	1.39
23	A	408	CLA	C1B-NB	-3.49	1.33	1.37
23	c	513	CLA	C1B-NB	-3.49	1.33	1.37
23	c	508	CLA	CHC-C4B	3.49	1.47	1.39
23	C	508	CLA	OBD-CAD	3.48	1.28	1.22
23	B	611	CLA	CHC-C4B	3.48	1.47	1.39
23	b	616	CLA	CHB-C1B	3.48	1.47	1.39
23	b	614	CLA	CHC-C4B	3.48	1.47	1.39
23	c	507	CLA	CHB-C1B	3.48	1.47	1.39
23	b	613	CLA	C4B-NB	-3.47	1.33	1.37
23	a	405	CLA	CHB-C1B	3.47	1.47	1.39
23	B	603	CLA	CHC-C4B	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	OBD-CAD	3.46	1.28	1.22
23	C	514	CLA	CHC-C4B	3.46	1.47	1.39
23	B	601	CLA	CHB-C1B	3.46	1.47	1.39
23	b	615	CLA	CHC-C4B	3.46	1.47	1.39
23	B	608	CLA	CHC-C4B	3.45	1.47	1.39
23	c	505	CLA	C3D-C2D	3.45	1.48	1.39
23	C	509	CLA	C4B-NB	-3.45	1.33	1.37
40	V	202	HEC	C4B-NB	-3.45	1.34	1.40
23	c	506	CLA	CHC-C4B	3.45	1.47	1.39
23	B	608	CLA	OBD-CAD	3.45	1.28	1.22
23	B	607	CLA	CHB-C1B	3.44	1.47	1.39
23	d	401	CLA	C1B-NB	-3.44	1.33	1.37
23	C	503	CLA	CHB-C1B	3.44	1.47	1.39
23	c	509	CLA	C4B-NB	-3.44	1.33	1.37
23	b	601	CLA	CHB-C1B	3.44	1.47	1.39
23	b	615	CLA	C1B-NB	-3.44	1.33	1.37
23	d	401	CLA	CHB-C1B	3.44	1.47	1.39
23	d	404	CLA	C1B-NB	-3.43	1.33	1.37
23	a	405	CLA	CHC-C4B	3.43	1.47	1.39
23	A	405	CLA	OBD-CAD	3.43	1.28	1.22
23	c	506	CLA	CHB-C1B	3.43	1.47	1.39
23	B	613	CLA	C1B-NB	-3.43	1.33	1.37
23	d	401	CLA	OBD-CAD	3.42	1.28	1.22
23	C	511	CLA	CHC-C4B	3.42	1.47	1.39
23	B	615	CLA	CHB-C1B	3.41	1.47	1.39
23	C	507	CLA	CHB-C1B	3.40	1.47	1.39
23	b	616	CLA	C3B-C4B	3.40	1.50	1.42
23	c	501	CLA	OBD-CAD	3.40	1.28	1.22
23	d	401	CLA	CHC-C4B	3.39	1.47	1.39
23	B	603	CLA	OBD-CAD	3.39	1.28	1.22
23	B	607	CLA	OBD-CAD	3.39	1.28	1.22
23	A	406	CLA	C3B-C4B	3.39	1.50	1.42
31	D	408	LHG	O8-C23	3.39	1.43	1.33
23	B	609	CLA	C1B-NB	-3.39	1.33	1.37
23	C	502	CLA	CHC-C4B	3.38	1.47	1.39
23	c	510	CLA	CHC-C4B	3.38	1.47	1.39
40	v	201	HEC	C1D-ND	-3.37	1.34	1.40
23	b	603	CLA	C3B-C4B	3.37	1.50	1.42
23	b	604	CLA	C3D-C2D	3.37	1.48	1.39
23	b	615	CLA	OBD-CAD	3.37	1.28	1.22
23	B	614	CLA	OBD-CAD	3.37	1.28	1.22
23	A	406	CLA	C4B-NB	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	CHC-C4B	3.36	1.46	1.39
23	B	606	CLA	C1B-NB	-3.36	1.33	1.37
23	b	607	CLA	CHC-C4B	3.36	1.46	1.39
23	A	406	CLA	C1B-NB	-3.35	1.33	1.37
34	B	627	HTG	C1'-S1	-3.35	1.77	1.81
34	b	622	HTG	C1'-S1	-3.35	1.77	1.81
23	c	503	CLA	OBD-CAD	3.34	1.28	1.22
23	A	406	CLA	CHC-C4B	3.34	1.46	1.39
23	c	506	CLA	C4B-NB	-3.33	1.33	1.37
23	A	408	CLA	C4B-NB	-3.33	1.33	1.37
23	a	404	CLA	O2A-CGA	3.33	1.43	1.33
23	B	613	CLA	C4B-NB	-3.33	1.33	1.37
23	A	405	CLA	C3B-C4B	3.33	1.50	1.42
23	a	404	CLA	C1B-NB	-3.33	1.33	1.37
23	c	510	CLA	OBD-CAD	3.32	1.28	1.22
23	B	601	CLA	C1B-NB	-3.32	1.33	1.37
38	E	103	HEM	C1B-NB	-3.31	1.34	1.40
38	e	103	HEM	C1B-NB	-3.31	1.34	1.40
40	V	202	HEC	C1D-ND	-3.31	1.34	1.40
23	A	408	CLA	CHB-C1B	3.31	1.46	1.39
23	c	510	CLA	C3D-C2D	3.31	1.48	1.39
34	c	522	HTG	C1'-S1	-3.30	1.77	1.81
23	C	509	CLA	CHC-C4B	3.30	1.46	1.39
23	C	506	CLA	C1B-NB	-3.29	1.33	1.37
23	B	612	CLA	CHD-C4C	3.29	1.46	1.39
23	A	406	CLA	CHB-C1B	3.29	1.46	1.39
23	B	603	CLA	CHB-C1B	3.28	1.46	1.39
40	v	201	HEC	C4B-NB	-3.28	1.34	1.40
23	B	602	CLA	CHC-C4B	3.28	1.46	1.39
38	E	103	HEM	C4D-ND	-3.28	1.34	1.40
23	b	611	CLA	C1B-NB	-3.27	1.33	1.37
23	B	604	CLA	C3D-C2D	3.27	1.48	1.39
23	a	404	CLA	C4B-NB	-3.27	1.33	1.37
23	A	405	CLA	C1B-NB	-3.27	1.33	1.37
23	b	610	CLA	C4B-NB	-3.26	1.33	1.37
23	C	513	CLA	CHB-C1B	3.26	1.46	1.39
23	C	511	CLA	C1B-NB	-3.26	1.33	1.37
23	C	514	CLA	C4B-NB	-3.26	1.33	1.37
23	B	609	CLA	C3B-C4B	3.25	1.50	1.42
23	d	403	CLA	C4B-NB	-3.25	1.33	1.37
23	C	505	CLA	C1B-NB	-3.25	1.33	1.37
23	C	506	CLA	C3D-C2D	3.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C1B-NB	-3.24	1.33	1.37
23	C	507	CLA	C1B-NB	-3.24	1.33	1.37
23	A	404	CLA	CHB-C1B	3.24	1.46	1.39
23	C	508	CLA	C1B-NB	-3.23	1.33	1.37
23	b	611	CLA	OBD-CAD	3.23	1.28	1.22
23	b	613	CLA	OBD-CAD	3.23	1.28	1.22
23	c	503	CLA	C1B-NB	-3.22	1.33	1.37
23	B	606	CLA	C3B-C4B	3.21	1.50	1.42
23	c	513	CLA	C3B-C4B	3.21	1.50	1.42
23	b	614	CLA	C1B-NB	-3.20	1.33	1.37
23	C	504	CLA	C3B-C4B	3.20	1.50	1.42
23	c	502	CLA	C1B-NB	-3.20	1.33	1.37
23	d	404	CLA	CHB-C1B	3.19	1.46	1.39
23	b	603	CLA	CHB-C1B	3.19	1.46	1.39
34	C	521	HTG	C1'-S1	-3.18	1.77	1.81
23	B	606	CLA	OBD-CAD	3.18	1.28	1.22
23	B	610	CLA	C1B-NB	-3.18	1.33	1.37
23	B	611	CLA	C1B-NB	-3.17	1.33	1.37
23	C	508	CLA	CHB-C1B	3.16	1.46	1.39
23	D	404	CLA	C4B-NB	-3.16	1.33	1.37
23	B	608	CLA	C1B-NB	-3.16	1.33	1.37
23	c	502	CLA	CHC-C4B	3.16	1.46	1.39
23	B	605	CLA	C3B-C4B	3.14	1.50	1.42
23	B	602	CLA	C4B-NB	-3.14	1.33	1.37
38	e	103	HEM	C4D-ND	-3.13	1.34	1.40
23	B	607	CLA	C1B-NB	-3.13	1.33	1.37
23	c	504	CLA	C1B-NB	-3.12	1.33	1.37
23	B	612	CLA	C4B-NB	-3.12	1.33	1.37
23	d	401	CLA	C4B-NB	-3.12	1.33	1.37
23	A	405	CLA	C1C-C2C	3.12	1.50	1.44
34	D	412	HTG	C1'-S1	-3.11	1.77	1.81
23	D	404	CLA	OBD-CAD	3.11	1.27	1.22
23	B	615	CLA	CHC-C4B	3.11	1.46	1.39
23	B	609	CLA	OBD-CAD	3.11	1.27	1.22
23	c	512	CLA	C1B-NB	-3.10	1.34	1.37
23	b	606	CLA	OBD-CAD	3.10	1.27	1.22
23	C	510	CLA	C4B-NB	-3.09	1.34	1.37
23	C	512	CLA	C1B-C2B	3.09	1.50	1.43
23	b	601	CLA	C4B-NB	-3.09	1.34	1.37
23	b	612	CLA	C4B-NB	-3.08	1.34	1.37
23	B	615	CLA	C1B-NB	-3.08	1.34	1.37
23	C	513	CLA	C1B-NB	-3.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C4B-NB	-3.08	1.34	1.37
23	C	512	CLA	C4B-NB	-3.07	1.34	1.37
23	c	512	CLA	C3B-C4B	3.07	1.49	1.42
23	B	616	CLA	C1B-NB	-3.06	1.34	1.37
23	B	614	CLA	CHC-C4B	3.06	1.46	1.39
23	b	610	CLA	C4C-C3C	3.06	1.50	1.45
23	c	507	CLA	C1B-NB	-3.05	1.34	1.37
23	C	513	CLA	C3B-C4B	3.05	1.49	1.42
23	c	505	CLA	C3B-C4B	3.05	1.49	1.42
34	c	521	HTG	C1'-S1	-3.05	1.77	1.81
23	c	501	CLA	C3B-C4B	3.03	1.49	1.42
23	c	503	CLA	C3B-C4B	3.03	1.49	1.42
23	A	404	CLA	C4B-NB	-3.03	1.34	1.37
23	C	511	CLA	C4B-NB	-3.03	1.34	1.37
23	b	610	CLA	C1B-NB	-3.03	1.34	1.37
23	b	606	CLA	C3B-C4B	3.03	1.49	1.42
23	b	614	CLA	C1B-C2B	3.02	1.50	1.43
23	D	404	CLA	C4C-C3C	3.02	1.50	1.45
23	c	502	CLA	C1B-C2B	3.01	1.50	1.43
23	b	602	CLA	C4B-NB	-3.01	1.34	1.37
23	B	608	CLA	C4B-NB	-3.00	1.34	1.37
23	b	609	CLA	C3B-C4B	3.00	1.49	1.42
23	a	408	CLA	C3B-C4B	3.00	1.49	1.42
23	d	404	CLA	C3B-C4B	2.98	1.49	1.42
23	B	604	CLA	C4B-NB	-2.97	1.34	1.37
23	c	502	CLA	C4B-NB	-2.97	1.34	1.37
23	A	404	CLA	C4C-C3C	2.97	1.50	1.45
23	b	601	CLA	C1B-NB	-2.97	1.34	1.37
23	b	613	CLA	C1B-NB	-2.97	1.34	1.37
23	c	501	CLA	C1B-NB	-2.97	1.34	1.37
23	C	512	CLA	C3B-C4B	2.96	1.49	1.42
23	b	605	CLA	C3B-C4B	2.96	1.49	1.42
23	C	510	CLA	C1C-C2C	2.96	1.50	1.44
23	c	505	CLA	C1B-C2B	2.96	1.50	1.43
23	C	502	CLA	OBD-CAD	2.96	1.27	1.22
23	C	508	CLA	C4B-NB	-2.95	1.34	1.37
34	B	623	HTG	C1'-S1	-2.94	1.77	1.81
23	B	601	CLA	C3B-C4B	2.94	1.49	1.42
23	C	506	CLA	C1C-C2C	2.94	1.50	1.44
23	c	508	CLA	C1B-NB	-2.94	1.34	1.37
23	c	505	CLA	C1C-C2C	2.94	1.50	1.44
23	c	513	CLA	C1C-C2C	2.93	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C4B-NB	-2.93	1.34	1.37
23	b	602	CLA	C1B-NB	-2.92	1.34	1.37
23	c	509	CLA	C4C-C3C	2.92	1.50	1.45
23	B	614	CLA	C1B-C2B	2.92	1.50	1.43
23	D	404	CLA	CHC-C4B	2.92	1.45	1.39
23	C	503	CLA	C4B-NB	-2.91	1.34	1.37
23	b	612	CLA	C3B-C4B	2.91	1.49	1.42
23	C	510	CLA	C3B-C4B	2.91	1.49	1.42
23	C	514	CLA	C3B-C4B	2.91	1.49	1.42
23	b	603	CLA	C1C-C2C	2.91	1.50	1.44
23	b	605	CLA	C1B-NB	-2.90	1.34	1.37
34	b	625	HTG	C1'-S1	-2.90	1.77	1.81
23	A	408	CLA	OBD-CAD	2.90	1.27	1.22
23	B	616	CLA	C3B-C4B	2.90	1.49	1.42
23	a	405	CLA	C4B-NB	-2.90	1.34	1.37
35	D	402	LMT	O1'-C1'	2.90	1.45	1.40
23	b	601	CLA	C3B-C4B	2.89	1.49	1.42
23	C	503	CLA	C1B-NB	-2.89	1.34	1.37
23	B	606	CLA	C4B-NB	-2.89	1.34	1.37
23	D	404	CLA	C1C-C2C	2.89	1.50	1.44
23	B	615	CLA	C3B-C4B	2.89	1.49	1.42
23	b	609	CLA	C1B-NB	-2.89	1.34	1.37
23	B	607	CLA	C4D-CHA	2.88	1.48	1.38
23	b	609	CLA	C4B-NB	-2.88	1.34	1.37
23	C	510	CLA	C1B-NB	-2.88	1.34	1.37
23	b	605	CLA	C1B-C2B	2.88	1.50	1.43
23	c	509	CLA	C3B-C4B	2.87	1.49	1.42
23	C	504	CLA	C4B-NB	-2.87	1.34	1.37
23	b	610	CLA	C1C-C2C	2.87	1.50	1.44
23	a	408	CLA	C1B-C2B	2.87	1.50	1.43
23	b	604	CLA	C1C-C2C	2.87	1.50	1.44
23	c	510	CLA	C4B-NB	-2.86	1.34	1.37
23	C	505	CLA	C1B-C2B	2.85	1.50	1.43
23	c	511	CLA	C4B-NB	-2.85	1.34	1.37
23	c	511	CLA	C1B-NB	-2.85	1.34	1.37
26	f	101	SQD	C6-S	-2.85	1.66	1.77
23	C	504	CLA	C1B-NB	-2.85	1.34	1.37
23	b	604	CLA	C1B-C2B	2.85	1.50	1.43
23	a	405	CLA	C3B-C4B	2.85	1.49	1.42
23	C	502	CLA	C4B-NB	-2.85	1.34	1.37
23	C	512	CLA	C1C-C2C	2.85	1.50	1.44
23	b	602	CLA	C3B-C4B	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C4D-CHA	2.85	1.48	1.38
23	C	508	CLA	C1B-C2B	2.85	1.50	1.43
23	c	505	CLA	C1B-NB	-2.85	1.34	1.37
23	C	514	CLA	C1C-C2C	2.84	1.50	1.44
38	E	103	HEM	C1C-C2C	-2.84	1.39	1.45
23	B	603	CLA	C1B-C2B	2.84	1.49	1.43
23	C	514	CLA	C1B-NB	-2.84	1.34	1.37
23	B	603	CLA	C4B-NB	-2.84	1.34	1.37
23	c	505	CLA	C4B-NB	-2.84	1.34	1.37
23	b	611	CLA	C1B-C2B	2.83	1.49	1.43
23	b	606	CLA	C4B-NB	-2.83	1.34	1.37
23	C	509	CLA	C1B-C2B	2.83	1.49	1.43
23	B	610	CLA	C3B-C4B	2.83	1.49	1.42
23	A	408	CLA	C3B-C4B	2.83	1.49	1.42
23	b	608	CLA	C3B-C4B	2.83	1.49	1.42
23	b	605	CLA	C4B-NB	-2.83	1.34	1.37
23	C	505	CLA	C1C-C2C	2.83	1.50	1.44
23	b	608	CLA	C4B-NB	-2.83	1.34	1.37
23	b	610	CLA	C3B-C4B	2.83	1.49	1.42
24	A	407	PHO	C3A-C2A	-2.82	1.52	1.54
23	B	616	CLA	C1B-C2B	2.82	1.49	1.43
26	A	412	SQD	C6-S	-2.82	1.67	1.77
23	c	513	CLA	C4B-NB	-2.82	1.34	1.37
23	c	510	CLA	C1B-NB	-2.81	1.34	1.37
23	c	511	CLA	C1B-C2B	2.81	1.49	1.43
23	C	508	CLA	C3B-C4B	2.81	1.49	1.42
23	c	512	CLA	C4B-NB	-2.81	1.34	1.37
23	c	510	CLA	C3B-C4B	2.81	1.49	1.42
23	b	612	CLA	C1B-NB	-2.81	1.34	1.37
23	D	405	CLA	C1C-C2C	2.81	1.50	1.44
23	b	604	CLA	C1B-NB	-2.80	1.34	1.37
23	B	608	CLA	C3B-C4B	2.80	1.49	1.42
23	D	404	CLA	C1B-NB	-2.80	1.34	1.37
23	B	610	CLA	C4B-NB	-2.80	1.34	1.37
23	c	504	CLA	C1C-C2C	2.80	1.50	1.44
23	B	611	CLA	C1C-C2C	2.78	1.50	1.44
23	b	611	CLA	C4C-C3C	2.78	1.49	1.45
23	d	401	CLA	C3B-C4B	2.78	1.49	1.42
29	a	414	PL9	C6-C5	2.78	1.49	1.35
23	C	502	CLA	C1B-C2B	2.77	1.49	1.43
23	A	404	CLA	C1B-C2B	2.77	1.49	1.43
23	D	405	CLA	C1B-NB	-2.77	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C3B-C4B	2.77	1.49	1.42
23	B	602	CLA	C1B-C2B	2.77	1.49	1.43
23	D	405	CLA	C1B-C2B	2.76	1.49	1.43
23	b	616	CLA	C1B-NB	-2.76	1.34	1.37
23	c	508	CLA	C1C-C2C	2.76	1.49	1.44
23	b	611	CLA	C4B-NB	-2.75	1.34	1.37
23	C	509	CLA	C1B-NB	-2.75	1.34	1.37
23	C	509	CLA	C4C-C3C	2.75	1.49	1.45
23	B	607	CLA	C3B-C4B	2.75	1.49	1.42
23	C	507	CLA	C3B-C4B	2.75	1.49	1.42
23	B	603	CLA	C4D-CHA	2.75	1.48	1.38
23	B	611	CLA	C4B-NB	-2.75	1.34	1.37
23	C	503	CLA	C3B-C4B	2.75	1.49	1.42
23	b	615	CLA	C4D-CHA	2.75	1.48	1.38
24	a	407	PHO	C3A-C2A	-2.75	1.52	1.54
26	B	620	SQD	C6-S	-2.74	1.67	1.77
26	a	412	SQD	C6-S	-2.74	1.67	1.77
23	c	508	CLA	C1B-C2B	2.74	1.49	1.43
23	b	613	CLA	C4D-CHA	2.74	1.48	1.38
23	C	505	CLA	C4D-CHA	2.74	1.48	1.38
23	B	604	CLA	C1B-C2B	2.74	1.49	1.43
23	C	506	CLA	C4B-NB	-2.74	1.34	1.37
23	C	508	CLA	C4D-CHA	2.73	1.48	1.38
23	c	508	CLA	C3B-C4B	2.73	1.49	1.42
23	B	607	CLA	C1C-C2C	2.73	1.49	1.44
23	b	615	CLA	C4B-NB	-2.73	1.34	1.37
29	A	414	PL9	C6-C5	2.73	1.49	1.35
23	d	404	CLA	C4B-NB	-2.73	1.34	1.37
23	A	408	CLA	C4D-CHA	2.73	1.48	1.38
26	D	413	SQD	C6-S	-2.72	1.67	1.77
23	C	511	CLA	C4C-C3C	2.72	1.49	1.45
23	c	509	CLA	C1B-C2B	2.72	1.49	1.43
23	B	602	CLA	C1B-NB	-2.71	1.34	1.37
23	a	405	CLA	C1B-NB	-2.71	1.34	1.37
23	b	602	CLA	C1C-C2C	2.71	1.49	1.44
23	C	509	CLA	C4D-CHA	2.71	1.48	1.38
23	c	511	CLA	C3B-C4B	2.71	1.49	1.42
23	b	613	CLA	C1B-C2B	2.71	1.49	1.43
23	c	506	CLA	C1B-C2B	2.71	1.49	1.43
23	c	510	CLA	C1B-C2B	2.71	1.49	1.43
23	B	608	CLA	C1B-C2B	2.71	1.49	1.43
23	B	607	CLA	C4B-NB	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3B-C4B	2.70	1.49	1.42
23	B	613	CLA	C1C-C2C	2.70	1.49	1.44
23	b	605	CLA	C4D-CHA	2.69	1.48	1.38
23	b	615	CLA	C3B-C4B	2.69	1.49	1.42
23	b	607	CLA	C4B-NB	-2.69	1.34	1.37
23	b	604	CLA	C3B-C4B	2.69	1.49	1.42
23	B	602	CLA	C4C-C3C	2.69	1.49	1.45
23	b	607	CLA	C1B-C2B	2.68	1.49	1.43
23	b	607	CLA	C4D-CHA	2.68	1.47	1.38
23	c	503	CLA	C1C-C2C	2.68	1.49	1.44
23	b	616	CLA	C1C-C2C	2.68	1.49	1.44
26	A	410	SQD	C6-S	-2.68	1.67	1.77
23	d	403	CLA	C4C-C3C	2.68	1.49	1.45
23	a	408	CLA	C4B-NB	-2.68	1.34	1.37
23	D	404	CLA	C1B-C2B	2.68	1.49	1.43
23	B	615	CLA	C1B-C2B	2.67	1.49	1.43
23	C	510	CLA	C4D-CHA	2.67	1.47	1.38
23	B	612	CLA	C1B-C2B	2.67	1.49	1.43
23	b	615	CLA	C1B-C2B	2.67	1.49	1.43
23	A	406	CLA	C1C-C2C	2.66	1.49	1.44
23	c	507	CLA	C1B-C2B	2.66	1.49	1.43
23	a	408	CLA	C4C-C3C	2.66	1.49	1.45
23	a	408	CLA	C4D-CHA	2.66	1.47	1.38
23	B	615	CLA	C4D-CHA	2.66	1.47	1.38
23	B	603	CLA	C4C-C3C	2.65	1.49	1.45
23	C	512	CLA	C4D-CHA	2.65	1.47	1.38
23	c	507	CLA	C1C-C2C	2.65	1.49	1.44
23	C	502	CLA	C4D-CHA	2.65	1.47	1.38
23	B	604	CLA	C4D-CHA	2.65	1.47	1.38
23	B	612	CLA	C1C-C2C	2.65	1.49	1.44
23	B	612	CLA	C4D-CHA	2.64	1.47	1.38
23	C	511	CLA	C4D-CHA	2.64	1.47	1.38
23	B	611	CLA	C1B-C2B	2.64	1.49	1.43
23	b	609	CLA	C1B-C2B	2.64	1.49	1.43
23	B	613	CLA	C4D-CHA	2.64	1.47	1.38
23	C	507	CLA	C4B-NB	-2.64	1.34	1.37
23	B	604	CLA	C3D-C4D	-2.63	1.38	1.44
26	L	101	SQD	C6-S	-2.63	1.67	1.77
23	c	501	CLA	C4D-CHA	2.63	1.47	1.38
23	B	601	CLA	C1B-C2B	2.63	1.49	1.43
23	C	507	CLA	C4D-CHA	2.63	1.47	1.38
23	b	604	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4D-CHA	2.63	1.47	1.38
23	b	614	CLA	C3B-C4B	2.63	1.48	1.42
23	B	614	CLA	C4D-CHA	2.62	1.47	1.38
23	c	507	CLA	C3B-C4B	2.62	1.48	1.42
23	B	614	CLA	C3B-C4B	2.62	1.48	1.42
23	c	512	CLA	C1B-C2B	2.62	1.49	1.43
23	b	607	CLA	C1C-C2C	2.61	1.49	1.44
23	c	509	CLA	C1C-C2C	2.61	1.49	1.44
23	C	504	CLA	C4D-CHA	2.61	1.47	1.38
33	Z	102	LMG	O8-C28	2.61	1.46	1.33
23	B	601	CLA	C4D-CHA	2.61	1.47	1.38
23	c	509	CLA	C4D-CHA	2.61	1.47	1.38
23	b	610	CLA	C4D-CHA	2.60	1.47	1.38
23	c	508	CLA	C4D-CHA	2.60	1.47	1.38
23	b	602	CLA	C4D-CHA	2.60	1.47	1.38
23	c	504	CLA	C4D-CHA	2.60	1.47	1.38
23	b	616	CLA	C4D-CHA	2.59	1.47	1.38
23	c	501	CLA	C4B-NB	-2.59	1.34	1.37
23	B	602	CLA	C3B-C4B	2.59	1.48	1.42
23	C	503	CLA	C3D-C4D	-2.59	1.38	1.44
23	a	408	CLA	C1C-C2C	2.59	1.49	1.44
26	a	410	SQD	C6-S	-2.59	1.67	1.77
23	c	503	CLA	C4D-CHA	2.59	1.47	1.38
23	A	405	CLA	C4D-CHA	2.59	1.47	1.38
23	C	513	CLA	C4D-CHA	2.58	1.47	1.38
23	B	613	CLA	C4C-C3C	2.58	1.49	1.45
23	d	401	CLA	C1B-C2B	2.58	1.49	1.43
23	B	606	CLA	C4D-CHA	2.58	1.47	1.38
24	A	407	PHO	CHA-CBD	-2.58	1.48	1.51
23	b	609	CLA	C4D-CHA	2.58	1.47	1.38
23	c	504	CLA	C4C-C3C	2.58	1.49	1.45
23	C	514	CLA	C1B-C2B	2.57	1.49	1.43
23	b	612	CLA	C4D-CHA	2.57	1.47	1.38
23	c	502	CLA	C3B-C4B	2.57	1.48	1.42
23	B	611	CLA	C4D-CHA	2.57	1.47	1.38
23	d	403	CLA	C3D-C4D	-2.57	1.38	1.44
23	B	609	CLA	C1C-C2C	2.57	1.49	1.44
23	B	605	CLA	C1C-C2C	2.57	1.49	1.44
23	c	511	CLA	C4D-CHA	2.57	1.47	1.38
23	c	504	CLA	C3B-C4B	2.57	1.48	1.42
23	c	502	CLA	C4D-CHA	2.56	1.47	1.38
23	B	601	CLA	C4B-NB	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C3D-C4D	-2.56	1.38	1.44
23	c	506	CLA	C3B-C4B	2.56	1.48	1.42
23	C	513	CLA	C1C-C2C	2.56	1.49	1.44
23	a	404	CLA	C1B-C2B	2.56	1.49	1.43
24	D	401	PHO	CHA-CBD	-2.55	1.48	1.51
23	b	601	CLA	C4D-CHA	2.55	1.47	1.38
23	C	505	CLA	C3B-C2B	2.55	1.49	1.41
23	b	603	CLA	C4B-NB	-2.55	1.34	1.37
23	b	602	CLA	C1B-C2B	2.55	1.49	1.43
23	A	405	CLA	C4B-NB	-2.55	1.34	1.37
23	B	608	CLA	C4D-CHA	2.55	1.47	1.38
23	c	512	CLA	C4D-CHA	2.54	1.47	1.38
23	B	616	CLA	C1C-C2C	2.54	1.49	1.44
23	B	616	CLA	C4D-CHA	2.54	1.47	1.38
23	c	505	CLA	C4D-CHA	2.54	1.47	1.38
29	d	406	PL9	C6-C5	2.54	1.48	1.35
23	C	507	CLA	C4C-C3C	2.54	1.49	1.45
23	b	606	CLA	C1B-C2B	2.54	1.49	1.43
23	b	614	CLA	C4D-CHA	2.53	1.47	1.38
23	b	613	CLA	C3B-C4B	2.53	1.48	1.42
23	C	504	CLA	C4C-C3C	2.53	1.49	1.45
23	c	503	CLA	C1B-C2B	2.53	1.49	1.43
23	C	510	CLA	C1B-C2B	2.53	1.49	1.43
23	C	503	CLA	C1B-C2B	2.53	1.49	1.43
23	c	510	CLA	C4D-CHA	2.52	1.47	1.38
23	c	504	CLA	C1B-C2B	2.52	1.49	1.43
23	B	606	CLA	C1C-C2C	2.52	1.49	1.44
23	B	607	CLA	C4C-C3C	2.52	1.49	1.45
23	B	603	CLA	C3B-C4B	2.52	1.48	1.42
23	d	401	CLA	C4D-CHA	2.52	1.47	1.38
23	b	612	CLA	C4C-C3C	2.52	1.49	1.45
23	C	512	CLA	C4C-C3C	2.52	1.49	1.45
23	D	404	CLA	C3D-C4D	-2.51	1.38	1.44
23	C	509	CLA	C3B-C2B	2.51	1.49	1.41
23	C	504	CLA	C1B-C2B	2.51	1.49	1.43
23	B	602	CLA	C4D-CHA	2.51	1.47	1.38
23	B	605	CLA	C1B-C2B	2.50	1.49	1.43
23	D	405	CLA	C4D-CHA	2.50	1.47	1.38
23	C	507	CLA	C3D-C4D	-2.50	1.38	1.44
23	d	403	CLA	C4D-CHA	2.50	1.47	1.38
23	b	612	CLA	C1C-C2C	2.50	1.49	1.44
23	B	615	CLA	C1C-C2C	2.50	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3D-C4D	-2.50	1.38	1.44
40	V	202	HEC	C4D-ND	-2.50	1.33	1.38
23	c	507	CLA	C4B-NB	-2.49	1.34	1.37
23	d	403	CLA	C1B-C2B	2.49	1.49	1.43
23	B	614	CLA	C1B-NB	-2.49	1.34	1.37
23	C	509	CLA	C1C-C2C	2.49	1.49	1.44
23	B	607	CLA	C1B-C2B	2.49	1.49	1.43
23	b	606	CLA	C1C-C2C	2.49	1.49	1.44
23	b	611	CLA	C4D-CHA	2.49	1.47	1.38
23	C	514	CLA	C4D-CHA	2.48	1.47	1.38
23	b	606	CLA	C4D-CHA	2.48	1.47	1.38
23	C	505	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	510	CLA	C3B-C2B	2.48	1.49	1.41
23	c	501	CLA	C1B-C2B	2.48	1.49	1.43
23	b	603	CLA	C1B-C2B	2.48	1.49	1.43
23	a	405	CLA	C3D-C4D	-2.48	1.38	1.44
23	A	404	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	602	CLA	C3D-C4D	-2.48	1.38	1.44
23	a	405	CLA	C1B-C2B	2.47	1.49	1.43
23	C	510	CLA	C4C-C3C	2.47	1.49	1.45
23	b	613	CLA	C1C-C2C	2.47	1.49	1.44
23	B	605	CLA	C4C-C3C	2.47	1.49	1.45
40	v	201	HEC	C1B-NB	-2.47	1.33	1.38
23	b	608	CLA	C1C-C2C	2.47	1.49	1.44
23	b	616	CLA	C4B-NB	-2.47	1.34	1.37
23	c	511	CLA	C1C-C2C	2.47	1.49	1.44
29	D	407	PL9	C6-C5	2.47	1.48	1.35
23	A	408	CLA	C3D-C4D	-2.46	1.38	1.44
23	B	606	CLA	C1B-C2B	2.46	1.49	1.43
23	b	612	CLA	C1B-C2B	2.46	1.49	1.43
23	D	405	CLA	C4B-NB	-2.46	1.34	1.37
23	c	501	CLA	C4C-C3C	2.46	1.49	1.45
23	B	610	CLA	C4D-CHA	2.45	1.47	1.38
23	C	511	CLA	C1B-C2B	2.45	1.49	1.43
23	C	508	CLA	C1C-C2C	2.45	1.49	1.44
23	B	611	CLA	C3D-C4D	-2.45	1.38	1.44
23	A	406	CLA	C1B-C2B	2.45	1.49	1.43
23	C	513	CLA	C1B-C2B	2.44	1.49	1.43
23	c	506	CLA	C4D-CHA	2.44	1.47	1.38
23	c	513	CLA	C4D-CHA	2.44	1.47	1.38
23	b	603	CLA	C4D-CHA	2.44	1.47	1.38
23	b	614	CLA	C4B-NB	-2.44	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C1B-C2B	2.44	1.49	1.43
23	a	404	CLA	C4D-CHA	2.44	1.47	1.38
23	B	613	CLA	C3B-C4B	2.44	1.48	1.42
23	C	512	CLA	C1B-NB	-2.44	1.34	1.37
23	A	404	CLA	C4D-CHA	2.44	1.47	1.38
23	C	502	CLA	C3B-C2B	2.44	1.49	1.41
23	b	612	CLA	C3B-C2B	2.43	1.49	1.41
23	B	609	CLA	C4D-CHA	2.43	1.47	1.38
23	c	510	CLA	C3D-C4D	-2.43	1.38	1.44
23	c	503	CLA	C4B-NB	-2.43	1.34	1.37
23	a	404	CLA	C3D-C4D	-2.43	1.38	1.44
23	b	616	CLA	C3D-C4D	-2.42	1.38	1.44
23	a	405	CLA	C4D-CHA	2.42	1.47	1.38
23	c	510	CLA	C4C-C3C	2.42	1.49	1.45
23	B	601	CLA	C4C-C3C	2.42	1.49	1.45
23	C	502	CLA	C4C-C3C	2.42	1.49	1.45
23	B	604	CLA	C3B-C4B	2.42	1.48	1.42
23	B	604	CLA	C1C-C2C	2.42	1.49	1.44
23	B	609	CLA	C1B-C2B	2.42	1.48	1.43
23	C	511	CLA	C3D-C4D	-2.41	1.38	1.44
23	A	408	CLA	C1C-C2C	2.41	1.49	1.44
23	b	609	CLA	C1C-C2C	2.41	1.49	1.44
23	b	607	CLA	C4C-C3C	2.41	1.49	1.45
23	b	602	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	608	CLA	C4D-CHA	2.40	1.46	1.38
23	c	506	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	502	CLA	C3B-C4B	2.40	1.48	1.42
23	C	502	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	507	CLA	C1B-C2B	2.40	1.48	1.43
23	B	602	CLA	C1C-C2C	2.40	1.49	1.44
23	A	406	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	511	CLA	C3B-C4B	2.40	1.48	1.42
23	C	506	CLA	C1B-C2B	2.40	1.48	1.43
23	C	511	CLA	C1C-C2C	2.40	1.49	1.44
23	b	608	CLA	C3D-C4D	-2.40	1.38	1.44
23	c	508	CLA	C4C-C3C	2.39	1.49	1.45
23	B	612	CLA	C3B-C4B	2.39	1.48	1.42
23	d	404	CLA	C4D-CHA	2.39	1.46	1.38
23	D	404	CLA	C3B-C2B	2.39	1.49	1.41
23	B	601	CLA	C1C-C2C	2.39	1.49	1.44
23	C	508	CLA	C4C-C3C	2.39	1.49	1.45
23	B	605	CLA	C1B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C1B-C2B	2.38	1.48	1.43
23	b	613	CLA	C3B-C2B	2.38	1.49	1.41
23	d	404	CLA	C1C-C2C	2.38	1.49	1.44
23	a	405	CLA	C3B-C2B	2.38	1.49	1.41
23	b	614	CLA	C3B-C2B	2.37	1.49	1.41
23	B	613	CLA	C3B-C2B	2.37	1.49	1.41
23	c	504	CLA	C3B-C2B	2.37	1.49	1.41
23	B	605	CLA	C4D-CHA	2.37	1.46	1.38
23	b	614	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	611	CLA	C3B-C2B	2.37	1.49	1.41
23	D	405	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	610	CLA	C4C-C3C	2.36	1.49	1.45
23	C	502	CLA	C1C-C2C	2.36	1.49	1.44
23	C	506	CLA	C4D-CHA	2.36	1.46	1.38
23	B	607	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	612	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	601	CLA	C3D-C4D	-2.35	1.38	1.44
23	b	610	CLA	C3B-C2B	2.35	1.49	1.41
23	c	501	CLA	C1C-C2C	2.35	1.49	1.44
23	b	606	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	616	CLA	C1B-C2B	2.34	1.48	1.43
23	A	404	CLA	C3B-C4B	2.34	1.48	1.42
23	c	512	CLA	C4C-C3C	2.34	1.49	1.45
23	c	511	CLA	C3B-C2B	2.34	1.49	1.41
23	c	503	CLA	C4C-C3C	2.34	1.49	1.45
23	c	508	CLA	C3B-C2B	2.34	1.49	1.41
40	V	202	HEC	C1B-NB	-2.33	1.34	1.38
23	A	404	CLA	C3B-C2B	2.33	1.49	1.41
23	c	502	CLA	C3B-C2B	2.33	1.49	1.41
23	C	508	CLA	C3D-C4D	-2.33	1.38	1.44
23	b	605	CLA	C4C-C3C	2.33	1.49	1.45
36	c	518	DGD	O2G-C2G	-2.33	1.40	1.46
23	b	601	CLA	C1C-C2C	2.33	1.49	1.44
23	b	602	CLA	C3B-C2B	2.33	1.49	1.41
23	b	607	CLA	C3D-C4D	-2.33	1.38	1.44
23	B	616	CLA	C4B-NB	-2.33	1.34	1.37
23	B	611	CLA	C3B-C2B	2.33	1.49	1.41
23	A	408	CLA	C1B-C2B	2.32	1.48	1.43
34	b	625	HTG	C1-S1	-2.32	1.77	1.80
23	C	510	CLA	C3D-C4D	-2.32	1.38	1.44
23	c	509	CLA	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	C1B-NB	-2.32	1.34	1.38
23	b	607	CLA	C3B-C4B	2.32	1.48	1.42
23	a	405	CLA	C4C-C3C	2.32	1.49	1.45
23	A	404	CLA	C1C-C2C	2.32	1.49	1.44
23	b	608	CLA	C3B-C2B	2.32	1.49	1.41
23	b	609	CLA	C4C-C3C	2.32	1.49	1.45
24	a	406	PHO	C4B-NB	-2.31	1.34	1.38
23	C	509	CLA	C3B-C4B	2.31	1.48	1.42
23	c	501	CLA	C3D-C4D	-2.31	1.39	1.44
23	D	404	CLA	C4D-CHA	2.30	1.46	1.38
23	B	609	CLA	C3D-C4D	-2.30	1.39	1.44
23	B	614	CLA	C4C-C3C	2.30	1.49	1.45
23	A	405	CLA	C1B-C2B	2.30	1.48	1.43
23	b	611	CLA	C3B-C4B	2.30	1.48	1.42
23	b	605	CLA	C1C-C2C	2.29	1.49	1.44
23	b	610	CLA	C3D-C4D	-2.29	1.39	1.44
23	a	404	CLA	C3B-C2B	2.29	1.49	1.41
23	C	513	CLA	C4B-NB	-2.29	1.35	1.37
33	Z	102	LMG	O1-C1	2.29	1.44	1.40
34	B	627	HTG	C1-S1	-2.29	1.77	1.80
23	B	611	CLA	C3B-C4B	2.29	1.48	1.42
23	C	507	CLA	C1C-C2C	2.29	1.49	1.44
24	a	407	PHO	CHA-CBD	-2.29	1.48	1.51
23	c	511	CLA	C4C-C3C	2.29	1.49	1.45
23	b	610	CLA	C1B-C2B	2.29	1.48	1.43
23	b	604	CLA	C3B-C2B	2.29	1.48	1.41
23	c	502	CLA	C3D-C4D	-2.29	1.39	1.44
23	d	404	CLA	C1B-C2B	2.29	1.48	1.43
23	B	614	CLA	C1C-NC	-2.28	1.34	1.37
23	d	404	CLA	C3D-C4D	-2.28	1.39	1.44
38	e	103	HEM	C1C-C2C	-2.28	1.40	1.45
40	v	201	HEC	C4A-C3A	-2.28	1.40	1.45
23	B	616	CLA	C4C-C3C	2.27	1.49	1.45
23	c	505	CLA	C3D-C4D	-2.27	1.39	1.44
23	b	603	CLA	C4C-C3C	2.27	1.48	1.45
23	C	506	CLA	C4C-C3C	2.27	1.48	1.45
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	B	610	CLA	C3D-C4D	-2.26	1.39	1.44
34	D	412	HTG	C1-S1	-2.26	1.77	1.80
23	A	406	CLA	C4D-CHA	2.26	1.46	1.38
23	d	401	CLA	C3B-C2B	2.26	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1B-C2B	2.26	1.48	1.43
23	c	513	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	616	CLA	C3B-C2B	2.26	1.48	1.41
23	C	512	CLA	C3D-C4D	-2.25	1.39	1.44
38	e	103	HEM	C1D-ND	-2.25	1.34	1.38
23	c	503	CLA	C3D-C4D	-2.25	1.39	1.44
23	C	513	CLA	C3D-C4D	-2.25	1.39	1.44
23	a	408	CLA	C3D-C4D	-2.25	1.39	1.44
23	a	405	CLA	C1C-C2C	2.25	1.48	1.44
23	C	514	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	611	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	603	CLA	C3D-C4D	-2.24	1.39	1.44
23	c	511	CLA	C1D-C2D	2.24	1.49	1.45
23	B	608	CLA	C1C-C2C	2.24	1.48	1.44
23	C	512	CLA	C3B-C2B	2.24	1.48	1.41
23	B	613	CLA	C1B-C2B	2.24	1.48	1.43
23	B	610	CLA	C1C-C2C	2.24	1.48	1.44
23	d	401	CLA	C1D-C2D	2.24	1.49	1.45
23	b	609	CLA	C3D-C4D	-2.24	1.39	1.44
23	C	503	CLA	C1C-C2C	2.23	1.48	1.44
23	b	603	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	606	CLA	C3D-C4D	-2.23	1.39	1.44
23	d	403	CLA	C1C-C2C	2.23	1.48	1.44
23	b	608	CLA	C1B-C2B	2.23	1.48	1.43
23	c	509	CLA	C3B-C2B	2.22	1.48	1.41
23	c	513	CLA	C4C-C3C	2.22	1.48	1.45
23	A	405	CLA	C3B-C2B	2.22	1.48	1.41
23	A	405	CLA	C3D-C4D	-2.22	1.39	1.44
23	b	602	CLA	C4C-C3C	2.21	1.48	1.45
35	b	627	LMT	O1'-C1'	2.21	1.44	1.40
24	D	401	PHO	C4B-NB	-2.21	1.34	1.38
23	a	408	CLA	C1D-C2D	2.21	1.49	1.45
23	C	507	CLA	C1D-C2D	2.20	1.49	1.45
23	c	512	CLA	C1C-C2C	2.20	1.48	1.44
40	v	201	HEC	C4D-ND	-2.20	1.34	1.38
23	c	508	CLA	C3D-C4D	-2.20	1.39	1.44
23	C	503	CLA	C3B-C2B	2.20	1.48	1.41
23	c	502	CLA	C4C-C3C	2.20	1.48	1.45
23	B	601	CLA	C3B-C2B	2.20	1.48	1.41
23	a	404	CLA	C1C-C2C	2.20	1.48	1.44
24	A	407	PHO	C4B-NB	-2.19	1.34	1.38
26	B	620	SQD	O6-C1	2.19	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	C1D-C2D	2.19	1.49	1.45
23	c	502	CLA	C1C-C2C	2.19	1.48	1.44
23	c	510	CLA	C1C-C2C	2.19	1.48	1.44
23	c	506	CLA	C4C-C3C	2.19	1.48	1.45
23	c	512	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	612	CLA	C4C-C3C	2.19	1.48	1.45
23	b	614	CLA	C1C-C2C	2.19	1.48	1.44
23	B	612	CLA	C3B-C2B	2.18	1.48	1.41
23	B	614	CLA	C3D-C4D	-2.18	1.39	1.44
23	b	615	CLA	C4C-C3C	2.18	1.48	1.45
35	E	102	LMT	O1'-C1'	2.18	1.43	1.40
35	B	630	LMT	O1'-C1'	2.18	1.43	1.40
23	b	601	CLA	C3B-C2B	2.17	1.48	1.41
23	b	605	CLA	C1C-NC	-2.17	1.34	1.37
23	C	513	CLA	C3B-C2B	2.17	1.48	1.41
23	B	607	CLA	C3B-C2B	2.17	1.48	1.41
23	B	602	CLA	C3B-C2B	2.16	1.48	1.41
36	c	517	DGD	O3G-C1D	2.16	1.43	1.40
23	c	511	CLA	C3D-C4D	-2.16	1.39	1.44
24	a	406	PHO	C1D-ND	-2.16	1.34	1.38
23	b	611	CLA	C1C-C2C	2.16	1.48	1.44
23	C	506	CLA	C3B-C2B	2.15	1.48	1.41
23	B	608	CLA	C3D-C4D	-2.15	1.39	1.44
23	c	506	CLA	C1C-NC	-2.15	1.34	1.37
23	d	404	CLA	C3B-C2B	2.15	1.48	1.41
23	A	406	CLA	C1D-C2D	2.15	1.49	1.45
23	c	503	CLA	C3B-C2B	2.14	1.48	1.41
23	C	507	CLA	C3B-C2B	2.14	1.48	1.41
23	D	404	CLA	C3B-C4B	2.14	1.47	1.42
23	A	408	CLA	C1C-NC	-2.14	1.34	1.37
34	d	411	HTG	C1-S1	-2.13	1.77	1.80
23	B	614	CLA	C1C-C2C	2.13	1.48	1.44
36	h	102	DGD	O5D-C1E	2.13	1.43	1.40
23	b	601	CLA	C4C-C3C	2.13	1.48	1.45
23	C	514	CLA	C4C-C3C	2.13	1.48	1.45
23	b	605	CLA	C3B-C2B	2.12	1.48	1.41
23	C	504	CLA	C3D-C4D	-2.12	1.39	1.44
34	C	522	HTG	C1-S1	-2.12	1.77	1.80
23	b	613	CLA	C4C-C3C	2.11	1.48	1.45
23	C	509	CLA	C1C-NC	-2.11	1.34	1.37
23	C	511	CLA	C3B-C2B	2.11	1.48	1.41
23	c	504	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C4C-C3C	2.10	1.48	1.45
23	A	408	CLA	C4C-C3C	2.10	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.10	1.39	1.44
23	b	613	CLA	C3D-C4D	-2.10	1.39	1.44
23	A	408	CLA	C3B-C2B	2.10	1.48	1.41
23	b	606	CLA	C3B-C2B	2.10	1.48	1.41
23	B	602	CLA	C1D-C2D	2.10	1.49	1.45
23	c	513	CLA	C3B-C2B	2.09	1.48	1.41
23	B	610	CLA	C3B-C2B	2.09	1.48	1.41
23	c	506	CLA	C3B-C2B	2.09	1.48	1.41
23	d	401	CLA	C1C-C2C	2.09	1.48	1.44
23	c	510	CLA	C3B-C2B	2.08	1.48	1.41
24	A	407	PHO	C1B-NB	-2.08	1.34	1.38
35	I	101	LMT	O1'-C1'	2.08	1.43	1.40
23	b	614	CLA	C4C-C3C	2.08	1.48	1.45
23	C	514	CLA	C3B-C2B	2.08	1.48	1.41
34	c	522	HTG	C1-S1	-2.08	1.77	1.80
23	d	404	CLA	C1D-C2D	2.08	1.49	1.45
23	C	505	CLA	C4C-C3C	2.08	1.48	1.45
23	b	601	CLA	C3D-C4D	-2.07	1.39	1.44
23	B	615	CLA	C3D-C4D	-2.07	1.39	1.44
23	B	612	CLA	C3D-C4D	-2.07	1.39	1.44
23	B	613	CLA	C3D-C4D	-2.06	1.39	1.44
23	A	405	CLA	C1D-C2D	2.06	1.49	1.45
23	B	604	CLA	C3B-C2B	2.06	1.48	1.41
23	B	605	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	501	CLA	C1D-C2D	2.06	1.49	1.45
23	C	514	CLA	C1D-C2D	2.06	1.49	1.45
29	A	414	PL9	C2-C3	2.05	1.40	1.34
38	E	103	HEM	C1D-ND	-2.05	1.34	1.38
23	b	608	CLA	C4C-C3C	2.05	1.48	1.45
23	d	401	CLA	C3D-C4D	-2.05	1.39	1.44
23	B	608	CLA	C3B-C2B	2.05	1.48	1.41
36	H	102	DGD	O5D-C1E	2.05	1.43	1.40
31	A	416	LHG	O7-C5	-2.04	1.41	1.46
23	C	513	CLA	C4C-C3C	2.04	1.48	1.45
40	V	202	HEC	C4B-C3B	2.04	1.48	1.45
23	C	509	CLA	C3D-C4D	-2.04	1.39	1.44
23	B	614	CLA	C3B-C2B	2.04	1.48	1.41
29	a	414	PL9	C2-C3	2.03	1.40	1.34
23	c	505	CLA	C4C-C3C	2.03	1.48	1.45
23	b	616	CLA	C3B-C2B	2.03	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C4C-C3C	2.03	1.48	1.45
40	v	201	HEC	C4B-C3B	2.03	1.48	1.45
23	d	403	CLA	C3B-C2B	2.03	1.48	1.41
34	b	623	HTG	C1-S1	-2.02	1.77	1.80
33	c	520	LMG	O1-C1	2.02	1.43	1.40
23	B	615	CLA	C4B-NB	-2.02	1.35	1.37
40	V	202	HEC	C4A-C3A	-2.02	1.41	1.45
23	b	603	CLA	C1D-C2D	2.01	1.49	1.45
38	E	103	HEM	C4B-NB	-2.01	1.34	1.38
23	b	609	CLA	C1D-C2D	2.01	1.49	1.45
38	e	103	HEM	C3C-C4C	-2.01	1.42	1.46
23	c	507	CLA	C3D-C4D	-2.01	1.39	1.44
23	B	605	CLA	C1D-C2D	2.01	1.49	1.45
23	b	605	CLA	C1D-C2D	2.01	1.49	1.45
23	a	404	CLA	C3B-C4B	2.00	1.47	1.42
23	B	609	CLA	C1D-C2D	2.00	1.49	1.45
23	B	611	CLA	C4C-C3C	2.00	1.48	1.45

All (2878) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	401	PHO	C2D-C1D-ND	12.21	117.96	109.53
24	a	406	PHO	C2D-C1D-ND	12.16	117.92	109.53
24	A	407	PHO	C2D-C1D-ND	11.63	117.56	109.53
24	a	407	PHO	C2D-C1D-ND	10.64	116.87	109.53
23	B	605	CLA	C1D-ND-C4D	-10.55	98.84	106.33
23	A	405	CLA	C1D-ND-C4D	-10.48	98.89	106.33
23	A	406	CLA	C1D-ND-C4D	-10.39	98.95	106.33
23	C	514	CLA	C1D-ND-C4D	-10.23	99.06	106.33
23	B	608	CLA	C1D-ND-C4D	-9.93	99.28	106.33
23	D	405	CLA	C1D-ND-C4D	-9.91	99.29	106.33
23	C	504	CLA	C1D-ND-C4D	-9.85	99.33	106.33
23	d	401	CLA	C1D-ND-C4D	-9.83	99.35	106.33
23	a	405	CLA	C1D-ND-C4D	-9.83	99.35	106.33
23	b	603	CLA	C1D-ND-C4D	-9.83	99.35	106.33
23	c	503	CLA	C1D-ND-C4D	-9.81	99.37	106.33
23	c	511	CLA	C1D-ND-C4D	-9.80	99.38	106.33
23	c	504	CLA	C1D-ND-C4D	-9.55	99.55	106.33
23	C	512	CLA	C1D-ND-C4D	-9.53	99.56	106.33
23	C	510	CLA	C1D-ND-C4D	-9.50	99.59	106.33
23	c	513	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	c	512	CLA	C1D-ND-C4D	-9.45	99.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404	CLA	C1D-ND-C4D	-9.43	99.63	106.33
23	B	609	CLA	C1D-ND-C4D	-9.42	99.64	106.33
23	c	505	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	b	605	CLA	C1D-ND-C4D	-9.33	99.70	106.33
23	b	607	CLA	C2D-C1D-ND	9.27	116.93	110.10
23	b	607	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	a	408	CLA	C1D-ND-C4D	-9.23	99.77	106.33
23	B	606	CLA	C1D-ND-C4D	-9.18	99.81	106.33
23	b	615	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	C	511	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	B	610	CLA	C1D-ND-C4D	-9.11	99.86	106.33
23	b	608	CLA	C1D-ND-C4D	-9.10	99.87	106.33
23	c	510	CLA	C1D-ND-C4D	-9.10	99.87	106.33
23	b	606	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	A	405	CLA	C2D-C1D-ND	9.03	116.76	110.10
23	B	615	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	c	501	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	B	612	CLA	C1D-ND-C4D	-9.00	99.94	106.33
23	c	506	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	611	CLA	C1D-ND-C4D	-8.96	99.97	106.33
23	B	601	CLA	C1D-ND-C4D	-8.96	99.97	106.33
23	B	608	CLA	C2D-C1D-ND	8.95	116.70	110.10
23	b	610	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	c	509	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	B	616	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	B	607	CLA	C1D-ND-C4D	-8.90	100.01	106.33
23	B	614	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	C	506	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	b	609	CLA	C1D-ND-C4D	-8.87	100.04	106.33
23	A	408	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	b	604	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	c	508	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	b	616	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	b	612	CLA	C1D-ND-C4D	-8.77	100.11	106.33
23	d	403	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	b	614	CLA	C1D-ND-C4D	-8.74	100.13	106.33
23	B	605	CLA	C2D-C1D-ND	8.73	116.54	110.10
23	C	502	CLA	C1D-ND-C4D	-8.70	100.15	106.33
23	B	611	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	b	613	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	d	404	CLA	C2B-C1B-NB	8.67	116.04	110.23
23	C	509	CLA	C1D-ND-C4D	-8.65	100.19	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	C1D-ND-C4D	-8.65	100.19	106.33
23	b	601	CLA	C1D-ND-C4D	-8.64	100.19	106.33
23	B	603	CLA	C1D-ND-C4D	-8.63	100.20	106.33
23	C	503	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	B	602	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	c	512	CLA	C2B-C1B-NB	8.61	116.00	110.23
23	C	505	CLA	C1D-ND-C4D	-8.60	100.22	106.33
23	A	406	CLA	C2B-C1B-NB	8.60	116.00	110.23
23	c	502	CLA	C1D-ND-C4D	-8.59	100.24	106.33
23	C	513	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	B	613	CLA	C1D-ND-C4D	-8.49	100.31	106.33
23	C	509	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	504	CLA	C2D-C1D-ND	8.45	116.33	110.10
23	d	401	CLA	C2D-C1D-ND	8.45	116.33	110.10
23	b	602	CLA	C1D-ND-C4D	-8.44	100.34	106.33
23	B	613	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	D	404	CLA	C1D-ND-C4D	-8.42	100.36	106.33
23	A	406	CLA	C2D-C1D-ND	8.41	116.31	110.10
23	C	504	CLA	C2D-C1D-ND	8.40	116.30	110.10
23	C	508	CLA	C1D-ND-C4D	-8.34	100.41	106.33
23	B	610	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	C	504	CLA	C2B-C1B-NB	8.32	115.81	110.23
23	c	503	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	C	507	CLA	C1D-ND-C4D	-8.29	100.45	106.33
23	a	404	CLA	C1D-ND-C4D	-8.28	100.45	106.33
23	C	505	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	C	514	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	a	405	CLA	C2D-C1D-ND	8.25	116.19	110.10
23	A	408	CLA	C2B-C1B-NB	8.25	115.76	110.23
23	B	609	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	b	606	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	B	615	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	c	512	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	b	616	CLA	C2B-C1B-NB	8.20	115.73	110.23
23	b	613	CLA	C2D-C1D-ND	8.20	116.14	110.10
23	B	604	CLA	C1D-ND-C4D	-8.19	100.51	106.33
23	D	405	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	B	614	CLA	C2D-C1D-ND	8.14	116.10	110.10
23	A	404	CLA	C1D-ND-C4D	-8.14	100.55	106.33
23	B	612	CLA	C2D-C1D-ND	8.13	116.10	110.10
23	C	512	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	A	408	CLA	C2D-C1D-ND	8.11	116.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	B	607	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	b	608	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	b	606	CLA	C2B-C1B-NB	8.07	115.64	110.23
23	B	606	CLA	C2D-C1D-ND	8.05	116.04	110.10
23	b	603	CLA	C2B-C1B-NB	8.02	115.61	110.23
23	c	511	CLA	C2D-C1D-ND	7.98	115.99	110.10
24	D	401	PHO	O2D-CGD-CBD	7.97	121.10	111.00
23	b	611	CLA	C2D-C1D-ND	7.95	115.96	110.10
23	c	508	CLA	C2D-C1D-ND	7.95	115.96	110.10
23	C	510	CLA	C2D-C1D-ND	7.95	115.96	110.10
23	C	513	CLA	C2B-C1B-NB	7.94	115.56	110.23
23	b	605	CLA	C2D-C1D-ND	7.93	115.95	110.10
23	B	616	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	c	513	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	d	404	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	b	603	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	c	513	CLA	C2B-C1B-NB	7.86	115.50	110.23
23	d	401	CLA	C2B-C1B-NB	7.84	115.49	110.23
23	A	404	CLA	CMD-C2D-C1D	7.82	138.49	124.71
23	B	611	CLA	C2D-C1D-ND	7.79	115.84	110.10
23	b	614	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	a	408	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	c	507	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	c	506	CLA	C2D-C1D-ND	7.77	115.83	110.10
23	b	614	CLA	C2B-C1B-NB	7.77	115.44	110.23
23	D	405	CLA	C2B-C1B-NB	7.75	115.43	110.23
23	c	504	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	B	601	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	a	404	CLA	C2B-C1B-NB	7.71	115.40	110.23
23	b	616	CLA	C2D-C1D-ND	7.71	115.79	110.10
23	A	405	CLA	C2B-C1B-NB	7.71	115.40	110.23
23	C	505	CLA	C2B-C1B-NB	7.70	115.39	110.23
23	C	512	CLA	C2B-C1B-NB	7.68	115.38	110.23
24	a	407	PHO	O2D-CGD-CBD	7.61	120.64	111.00
24	a	406	PHO	O2D-CGD-CBD	7.61	120.63	111.00
23	C	502	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	b	601	CLA	C2B-C1B-NB	7.59	115.32	110.23
23	C	508	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	c	502	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	b	604	CLA	C2D-C1D-ND	7.52	115.64	110.10
23	c	511	CLA	CMD-C2D-C1D	7.51	137.94	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C2B-C1B-NB	7.50	115.26	110.23
23	B	613	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	C	510	CLA	C2B-C1B-NB	7.46	115.23	110.23
23	a	405	CLA	C2B-C1B-NB	7.46	115.23	110.23
23	c	501	CLA	C2D-C1D-ND	7.44	115.59	110.10
23	D	404	CLA	C2D-C1D-ND	7.44	115.58	110.10
23	C	506	CLA	CMD-C2D-C1D	7.43	137.81	124.71
23	B	601	CLA	C2D-C1D-ND	7.43	115.58	110.10
23	c	509	CLA	C2D-C1D-ND	7.41	115.57	110.10
23	c	509	CLA	C2B-C1B-NB	7.41	115.20	110.23
23	b	608	CLA	C2B-C1B-NB	7.40	115.19	110.23
24	A	407	PHO	C2B-C1B-NB	7.40	114.64	109.53
23	B	606	CLA	C4A-NA-C1A	-7.40	103.38	106.71
23	c	510	CLA	CMD-C2D-C1D	7.40	137.75	124.71
23	B	603	CLA	C2D-C1D-ND	7.38	115.54	110.10
23	c	505	CLA	C2D-C1D-ND	7.38	115.54	110.10
23	B	616	CLA	C2B-C1B-NB	7.38	115.18	110.23
23	a	408	CLA	C2B-C1B-NB	7.36	115.17	110.23
23	b	601	CLA	C2D-C1D-ND	7.36	115.53	110.10
23	C	507	CLA	CMD-C2D-C1D	7.33	137.64	124.71
23	b	609	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	B	603	CLA	C2B-C1B-NB	7.31	115.13	110.23
23	C	511	CLA	CMD-C2D-C1D	7.30	137.58	124.71
23	A	404	CLA	C2B-C1B-NB	7.30	115.12	110.23
23	c	508	CLA	C2B-C1B-NB	7.30	115.12	110.23
23	B	602	CLA	C2B-C1B-NB	7.30	115.12	110.23
23	C	514	CLA	C2B-C1B-NB	7.29	115.12	110.23
23	C	511	CLA	C2B-C1B-NB	7.27	115.11	110.23
23	C	513	CLA	C2D-C1D-ND	7.26	115.46	110.10
23	C	508	CLA	C2B-C1B-NB	7.26	115.10	110.23
23	B	606	CLA	C2B-C1B-NB	7.25	115.09	110.23
23	b	602	CLA	C2B-C1B-NB	7.25	115.09	110.23
23	B	614	CLA	C2B-C1B-NB	7.22	115.07	110.23
23	b	610	CLA	C2B-C1B-NB	7.21	115.07	110.23
23	B	604	CLA	C2D-C1D-ND	7.20	115.41	110.10
24	A	407	PHO	C4D-ND-C1D	-7.19	101.52	108.83
23	C	504	CLA	C4A-NA-C1A	-7.18	103.48	106.71
23	b	604	CLA	CMD-C2D-C1D	7.17	137.35	124.71
23	b	602	CLA	C2D-C1D-ND	7.17	115.39	110.10
23	C	503	CLA	C2D-C1D-ND	7.17	115.39	110.10
23	c	510	CLA	C2B-C1B-NB	7.16	115.03	110.23
23	B	605	CLA	C2B-C1B-NB	7.16	115.03	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	CMD-C2D-C1D	7.14	137.29	124.71
23	b	615	CLA	CMD-C2D-C1D	7.13	137.27	124.71
23	b	610	CLA	C2D-C1D-ND	7.12	115.35	110.10
23	C	511	CLA	C2D-C1D-ND	7.11	115.35	110.10
23	A	408	CLA	C4A-NA-C1A	-7.10	103.51	106.71
23	C	502	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	c	510	CLA	C2D-C1D-ND	7.08	115.32	110.10
23	b	613	CLA	C2B-C1B-NB	7.08	114.98	110.23
23	C	506	CLA	C2D-C1D-ND	7.05	115.30	110.10
23	b	616	CLA	C4A-NA-C1A	-7.05	103.54	106.71
23	b	615	CLA	C2B-C1B-NB	7.03	114.94	110.23
23	d	403	CLA	C2D-C1D-ND	7.00	115.26	110.10
23	b	603	CLA	CMD-C2D-C1D	6.99	137.04	124.71
23	b	612	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	B	607	CLA	C4A-NA-C1A	-6.99	103.56	106.71
23	D	404	CLA	C4A-NA-C1A	-6.96	103.58	106.71
23	B	615	CLA	C2B-C1B-NB	6.96	114.90	110.23
24	D	401	PHO	C4D-ND-C1D	-6.95	101.76	108.83
23	C	503	CLA	C2B-C1B-NB	6.92	114.87	110.23
23	d	403	CLA	C2B-C1B-NB	6.91	114.87	110.23
24	D	401	PHO	C1C-C2C-C3C	-6.91	102.87	108.61
23	C	509	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	B	604	CLA	CMD-C2D-C1D	6.89	136.85	124.71
23	A	405	CLA	CHD-C1D-ND	-6.88	118.13	124.45
23	C	504	CLA	CHD-C1D-ND	-6.86	118.15	124.45
23	C	514	CLA	CHD-C1D-ND	-6.86	118.15	124.45
34	B	624	HTG	C1'-S1-C1	6.85	112.91	100.09
23	A	405	CLA	CHD-C4C-C3C	-6.85	114.77	124.84
23	c	502	CLA	C2B-C1B-NB	6.85	114.83	110.23
23	b	605	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	b	609	CLA	C2B-C1B-NB	6.82	114.80	110.23
23	b	612	CLA	C2D-C1D-ND	6.81	115.13	110.10
23	B	608	CLA	C2B-C1B-NB	6.80	114.79	110.23
23	B	602	CLA	CMD-C2D-C1D	6.78	136.67	124.71
23	c	513	CLA	C4A-NA-C1A	-6.77	103.66	106.71
34	b	623	HTG	C1'-S1-C1	6.76	112.73	100.09
23	B	612	CLA	C2B-C1B-NB	6.76	114.76	110.23
23	B	610	CLA	C2B-C1B-NB	6.76	114.76	110.23
24	a	406	PHO	C4D-ND-C1D	-6.74	101.97	108.83
23	c	507	CLA	C2B-C1B-NB	6.74	114.75	110.23
24	a	407	PHO	C2B-C1B-NB	6.74	114.18	109.53
23	b	607	CLA	C2B-C1B-NB	6.73	114.75	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	401	CLA	CHD-C1D-ND	-6.72	118.28	124.45
23	c	501	CLA	CMD-C2D-C1D	6.72	136.56	124.71
23	D	404	CLA	C2C-C1C-NC	6.72	116.26	109.97
23	C	507	CLA	C2B-C1B-NB	6.71	114.73	110.23
23	c	511	CLA	C2B-C1B-NB	6.71	114.73	110.23
23	D	405	CLA	CMD-C2D-C1D	6.68	136.49	124.71
23	b	614	CLA	CMD-C2D-C1D	6.67	136.47	124.71
23	B	602	CLA	C2D-C1D-ND	6.66	115.02	110.10
23	C	512	CLA	CMD-C2D-C1D	6.66	136.44	124.71
23	B	607	CLA	CMD-C2D-C1D	6.65	136.43	124.71
23	A	408	CLA	CMD-C2D-C1D	6.65	136.43	124.71
24	A	407	PHO	O2D-CGD-CBD	6.64	119.41	111.00
23	c	513	CLA	CHD-C1D-ND	-6.64	118.35	124.45
34	B	623	HTG	C1'-S1-C1	6.64	112.50	100.09
23	B	606	CLA	CMD-C2D-C1D	6.62	136.39	124.71
23	B	609	CLA	CHD-C4C-C3C	-6.58	115.16	124.84
23	C	514	CLA	CMD-C2D-C1D	6.57	136.29	124.71
23	C	511	CLA	C4A-NA-C1A	-6.55	103.76	106.71
24	a	407	PHO	C4D-ND-C1D	-6.55	102.17	108.83
23	c	511	CLA	CHD-C1D-ND	-6.54	118.44	124.45
23	C	504	CLA	CMD-C2D-C1D	6.53	136.22	124.71
23	a	404	CLA	CMD-C2D-C1D	6.52	136.21	124.71
23	c	501	CLA	C2B-C1B-NB	6.51	114.60	110.23
23	c	505	CLA	C2B-C1B-NB	6.50	114.59	110.23
23	a	404	CLA	C2D-C1D-ND	6.49	114.89	110.10
23	a	405	CLA	CMD-C2D-C1D	6.49	136.15	124.71
23	b	616	CLA	CHD-C4C-C3C	-6.49	115.31	124.84
23	c	505	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
23	c	504	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	D	405	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
24	A	407	PHO	C1C-C2C-C3C	-6.47	103.23	108.61
24	a	406	PHO	C2B-C1B-NB	6.47	114.00	109.53
23	c	504	CLA	CMD-C2D-C1D	6.47	136.12	124.71
23	C	502	CLA	CMD-C2D-C1D	6.47	136.11	124.71
23	C	511	CLA	CHD-C1D-ND	-6.46	118.51	124.45
23	B	608	CLA	CHD-C4C-C3C	-6.46	115.34	124.84
23	C	506	CLA	C2B-C1B-NB	6.46	114.56	110.23
26	A	410	SQD	O6-C1-C2	6.46	118.38	108.30
23	D	404	CLA	CMD-C2D-C1D	6.45	136.09	124.71
23	b	603	CLA	CHD-C1D-ND	-6.45	118.53	124.45
23	B	616	CLA	C4A-NA-C1A	-6.44	103.81	106.71
23	C	507	CLA	C4A-NA-C1A	-6.43	103.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C2D-C1D-ND	6.42	114.84	110.10
23	B	604	CLA	C2B-C1B-NB	6.41	114.53	110.23
23	d	403	CLA	C4A-NA-C1A	-6.41	103.83	106.71
23	A	406	CLA	CMD-C2D-C1D	6.40	136.00	124.71
23	b	616	CLA	CMD-C2D-C1D	6.40	135.98	124.71
23	c	513	CLA	CMD-C2D-C1D	6.39	135.97	124.71
23	B	606	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	c	507	CLA	CMD-C2D-C1D	6.38	135.96	124.71
23	B	607	CLA	C2B-C1B-NB	6.38	114.51	110.23
23	B	605	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	C	506	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
23	D	405	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	B	616	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
23	c	510	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	C	512	CLA	CHD-C1D-ND	-6.35	118.62	124.45
23	b	609	CLA	CMD-C2D-C1D	6.35	135.90	124.71
23	c	503	CLA	CMD-C2D-C1D	6.34	135.89	124.71
23	d	404	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	c	508	CLA	O2D-CGD-CBD	6.31	122.48	111.27
23	c	506	CLA	C2B-C1B-NB	6.31	114.46	110.23
23	C	507	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	B	614	CLA	CMD-C2D-C1D	6.30	135.82	124.71
23	a	404	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	D	404	CLA	C2B-C1B-NB	6.29	114.45	110.23
23	C	508	CLA	O2D-CGD-CBD	6.29	122.45	111.27
23	B	612	CLA	CHD-C4C-C3C	-6.28	115.60	124.84
23	b	604	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	a	405	CLA	CHD-C1D-ND	-6.28	118.69	124.45
23	C	509	CLA	C2C-C1C-NC	6.27	115.85	109.97
23	b	602	CLA	CMD-C2D-C1D	6.27	135.77	124.71
23	B	616	CLA	O2D-CGD-CBD	6.27	122.41	111.27
23	c	502	CLA	C2C-C1C-NC	6.27	115.84	109.97
23	b	615	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	c	503	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	b	610	CLA	CMD-C2D-C1D	6.26	135.74	124.71
23	A	404	CLA	C2D-C1D-ND	6.25	114.71	110.10
23	A	404	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	b	605	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	C	513	CLA	C4A-NA-C1A	-6.24	103.90	106.71
23	B	615	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
23	B	609	CLA	CMD-C2D-C1D	6.23	135.69	124.71
23	B	606	CLA	CHD-C4C-C3C	-6.23	115.69	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
23	C	506	CLA	O2D-CGD-CBD	6.22	122.33	111.27
23	B	604	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	610	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	d	401	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	c	505	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	b	602	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	B	608	CLA	CHD-C1D-ND	-6.21	118.75	124.45
23	c	501	CLA	CHD-C1D-ND	-6.20	118.75	124.45
23	B	607	CLA	CHD-C1D-ND	-6.19	118.76	124.45
23	B	601	CLA	CMD-C2D-C1D	6.19	135.63	124.71
23	B	602	CLA	CHD-C1D-ND	-6.19	118.76	124.45
23	B	609	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	A	406	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	b	611	CLA	C2B-C1B-NB	6.18	114.37	110.23
23	c	509	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	B	605	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	b	607	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	B	616	CLA	CMD-C2D-C1D	6.17	135.58	124.71
23	b	604	CLA	O2D-CGD-CBD	6.17	122.22	111.27
24	D	401	PHO	C2B-C1B-NB	6.16	113.78	109.53
23	b	612	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	b	608	CLA	CHD-C4C-C3C	-6.15	115.81	124.84
23	b	606	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	d	401	CLA	CHD-C4C-C3C	-6.13	115.84	124.84
23	c	503	CLA	C4A-NA-C1A	-6.12	103.95	106.71
23	d	403	CLA	C2C-C1C-NC	6.12	115.71	109.97
24	a	406	PHO	C1C-C2C-C3C	-6.11	103.53	108.61
23	b	601	CLA	C4A-NA-C1A	-6.10	103.96	106.71
23	C	505	CLA	C2C-C1C-NC	6.10	115.69	109.97
23	b	603	CLA	C4A-NA-C1A	-6.10	103.97	106.71
23	b	610	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	b	602	CLA	O2D-CGD-CBD	6.09	122.09	111.27
23	b	613	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	c	503	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	C	510	CLA	CMD-C2D-C1D	6.08	135.43	124.71
23	d	403	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	A	408	CLA	CHD-C1D-ND	-6.07	118.88	124.45
23	d	404	CLA	CMD-C2D-C1D	6.07	135.40	124.71
23	c	506	CLA	CMD-C2D-C1D	6.06	135.40	124.71
23	D	405	CLA	O2D-CGD-CBD	6.06	122.04	111.27
23	C	506	CLA	C4A-NA-C1A	-6.06	103.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	b	606	CLA	C4A-NA-C1A	-6.06	103.98	106.71
23	b	601	CLA	CMD-C2D-C1D	6.06	135.39	124.71
23	C	512	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	b	605	CLA	CMD-C2D-C1D	6.04	135.36	124.71
23	B	614	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	b	601	CLA	CHD-C1D-ND	-6.03	118.91	124.45
23	B	602	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	c	506	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	B	609	CLA	C2B-C1B-NB	6.02	114.27	110.23
23	C	503	CLA	CMD-C2D-C1D	6.02	135.32	124.71
23	c	512	CLA	O2D-CGD-CBD	6.02	121.96	111.27
23	C	510	CLA	CHD-C1D-ND	-6.01	118.93	124.45
23	a	405	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	b	601	CLA	O2D-CGD-CBD	5.98	121.89	111.27
23	c	507	CLA	O2D-CGD-CBD	5.97	121.88	111.27
23	b	602	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	B	605	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	C	510	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	c	511	CLA	CHD-C4C-C3C	-5.94	116.10	124.84
23	B	610	CLA	CMD-C2D-C1D	5.94	135.19	124.71
23	b	614	CLA	O2D-CGD-CBD	5.93	121.81	111.27
34	c	521	HTG	C1'-S1-C1	5.93	111.18	100.09
23	d	404	CLA	C4A-NA-C1A	-5.93	104.04	106.71
23	b	606	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	d	403	CLA	CHD-C1D-ND	-5.92	119.01	124.45
23	B	601	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	C	502	CLA	C2C-C1C-NC	5.91	115.51	109.97
23	c	507	CLA	CHD-C1D-ND	-5.90	119.03	124.45
23	B	615	CLA	CMD-C2D-C1D	5.89	135.09	124.71
23	A	406	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
23	B	614	CLA	O2D-CGD-CBD	5.89	121.73	111.27
23	b	604	CLA	C2B-C1B-NB	5.88	114.17	110.23
23	A	405	CLA	CMD-C2D-C1D	5.87	135.07	124.71
26	D	413	SQD	O47-C7-C8	5.87	124.15	111.50
23	C	514	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
25	D	406	BCR	C7-C8-C9	-5.86	117.38	126.23
23	C	505	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	B	613	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	b	611	CLA	CMD-C2D-C1D	5.85	135.02	124.71
23	b	613	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	b	603	CLA	CHD-C4C-C3C	-5.84	116.26	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	CHD-C1D-ND	-5.83	119.09	124.45
23	d	404	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
23	B	615	CLA	CHD-C1D-ND	-5.82	119.10	124.45
23	C	508	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	B	612	CLA	O2D-CGD-CBD	5.82	121.61	111.27
23	c	507	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	b	616	CLA	O2D-CGD-CBD	5.81	121.59	111.27
34	D	412	HTG	C1'-S1-C1	5.81	110.95	100.09
23	A	408	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	C	502	CLA	CHD-C1D-ND	-5.80	119.12	124.45
23	B	613	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	C	513	CLA	O2D-CGD-CBD	5.80	121.57	111.27
23	B	604	CLA	O2D-CGD-CBD	5.79	121.56	111.27
23	B	611	CLA	CHD-C1D-ND	-5.79	119.13	124.45
23	B	611	CLA	C2B-C1B-NB	5.79	114.11	110.23
23	B	603	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	c	512	CLA	CHD-C4C-C3C	-5.79	116.34	124.84
23	c	512	CLA	CMD-C2D-C1D	5.78	134.91	124.71
23	c	508	CLA	C4A-NA-C1A	-5.78	104.11	106.71
23	C	513	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	b	611	CLA	C2C-C1C-NC	5.78	115.38	109.97
23	B	614	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	A	404	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	b	611	CLA	O2D-CGD-CBD	5.75	121.49	111.27
23	b	601	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	D	404	CLA	CHD-C1D-ND	-5.73	119.19	124.45
34	d	411	HTG	C1'-S1-C1	5.73	110.80	100.09
23	c	501	CLA	C4A-NA-C1A	-5.73	104.13	106.71
23	C	508	CLA	CMD-C2D-C1D	5.72	134.80	124.71
23	c	506	CLA	CHD-C1D-ND	-5.72	119.20	124.45
23	c	508	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	B	609	CLA	C4A-NA-C1A	-5.72	104.14	106.71
23	B	602	CLA	C2C-C1C-NC	5.72	115.33	109.97
34	b	625	HTG	C1'-S1-C1	5.72	110.78	100.09
23	b	604	CLA	CHD-C1D-ND	-5.71	119.20	124.45
23	c	506	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	B	601	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	b	615	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	b	614	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	b	609	CLA	C4A-NA-C1A	-5.70	104.14	106.71
23	C	506	CLA	CHD-C1D-ND	-5.70	119.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C2C-C1C-NC	5.69	115.31	109.97
23	B	603	CLA	CMD-C2D-C1D	5.69	134.74	124.71
23	b	612	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	C	505	CLA	CMD-C2D-C1D	5.68	134.72	124.71
23	c	513	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	b	603	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	C	503	CLA	CHD-C4C-C3C	-5.66	116.51	124.84
23	b	609	CLA	CHD-C1D-ND	-5.66	119.26	124.45
23	c	512	CLA	CHD-C1D-ND	-5.65	119.26	124.45
23	C	502	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	b	610	CLA	CHD-C1D-ND	-5.65	119.27	124.45
23	c	501	CLA	O2D-CGD-CBD	5.64	121.29	111.27
23	C	502	CLA	O2D-CGD-CBD	5.64	121.29	111.27
23	b	607	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	a	408	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	C	507	CLA	C2C-C1C-NC	5.62	115.24	109.97
23	B	606	CLA	O2D-CGD-CBD	5.62	121.25	111.27
23	b	615	CLA	C2C-C1C-NC	5.62	115.23	109.97
25	Y	101	BCR	C33-C5-C6	-5.61	118.22	124.53
23	c	504	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
23	B	603	CLA	C2C-C1C-NC	5.59	115.21	109.97
23	c	509	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	b	610	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
23	c	502	CLA	CHD-C1D-ND	-5.58	119.32	124.45
23	C	502	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	B	610	CLA	O2D-CGD-CBD	5.57	121.17	111.27
23	B	607	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	C	513	CLA	CMD-C2D-C1D	5.55	134.50	124.71
23	C	503	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	B	614	CLA	CHD-C1D-ND	-5.54	119.36	124.45
23	d	401	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	B	607	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	C	503	CLA	O2D-CGD-CBD	5.53	121.10	111.27
26	D	413	SQD	O6-C1-C2	5.53	116.94	108.30
23	b	607	CLA	CMD-C2D-C1D	5.53	134.45	124.71
23	C	513	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	C	508	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
23	b	608	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	b	607	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	B	608	CLA	CMD-C2D-C1D	5.50	134.40	124.71
23	b	614	CLA	CHD-C1D-ND	-5.49	119.41	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	b	606	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	b	604	CLA	C4A-NA-C1A	-5.48	104.24	106.71
23	c	508	CLA	C2C-C1C-NC	5.48	115.10	109.97
23	b	611	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	c	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	C	509	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
23	c	509	CLA	C2C-C1C-NC	5.45	115.07	109.97
23	b	605	CLA	O2D-CGD-CBD	5.44	120.94	111.27
23	b	611	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	B	612	CLA	C3C-C4C-NC	5.42	116.65	110.57
23	c	510	CLA	C2C-C1C-NC	5.41	115.04	109.97
23	B	603	CLA	CHD-C1D-ND	-5.41	119.49	124.45
29	a	414	PL9	C7-C3-C4	5.40	121.27	116.88
23	C	511	CLA	O2D-CGD-CBD	5.40	120.86	111.27
23	C	511	CLA	C2C-C1C-NC	5.39	115.03	109.97
23	b	610	CLA	C2C-C1C-NC	5.39	115.03	109.97
23	B	613	CLA	C4A-NA-C1A	-5.39	104.28	106.71
23	a	408	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	A	404	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	b	608	CLA	CMD-C2D-C1D	5.38	134.19	124.71
23	b	610	CLA	O2D-CGD-CBD	5.38	120.82	111.27
23	B	605	CLA	O2D-CGD-CBD	5.37	120.82	111.27
23	B	615	CLA	C4A-NA-C1A	-5.37	104.29	106.71
23	c	512	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	c	503	CLA	O2D-CGD-CBD	5.36	120.79	111.27
23	C	514	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	C	503	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	C	509	CLA	O2D-CGD-CBD	5.34	120.76	111.27
23	B	611	CLA	C2C-C1C-NC	5.34	114.97	109.97
24	a	407	PHO	C1C-C2C-C3C	-5.34	104.17	108.61
26	a	410	SQD	O47-C7-C8	5.33	122.99	111.50
23	b	605	CLA	C2C-C1C-NC	5.33	114.97	109.97
24	a	407	PHO	C3D-C4D-ND	5.33	114.98	107.72
23	c	510	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	c	510	CLA	C1-C2-C3	-5.32	116.84	126.04
23	a	408	CLA	CHD-C1D-ND	-5.32	119.56	124.45
23	b	613	CLA	CMD-C2D-C1D	5.32	134.09	124.71
23	b	609	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
23	b	616	CLA	CHD-C1D-ND	-5.31	119.58	124.45
23	b	606	CLA	O2D-CGD-CBD	5.30	120.69	111.27
23	C	508	CLA	C2C-C1C-NC	5.29	114.93	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	O2D-CGD-CBD	5.28	120.66	111.27
23	b	608	CLA	O2D-CGD-CBD	5.28	120.64	111.27
23	b	604	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	A	407	PHO	C3D-C4D-ND	5.27	114.90	107.72
23	c	501	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
23	c	508	CLA	CMD-C2D-C1D	5.25	133.97	124.71
23	c	511	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	c	502	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	a	408	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	B	610	CLA	CHD-C1D-ND	-5.25	119.63	124.45
23	b	612	CLA	CHD-C1D-ND	-5.25	119.63	124.45
23	C	508	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	a	404	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	c	503	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	C	506	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	c	509	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
23	C	505	CLA	CHD-C1D-ND	-5.22	119.65	124.45
23	B	612	CLA	C2C-C1C-NC	5.21	114.86	109.97
23	B	607	CLA	O2D-CGD-CBD	5.21	120.53	111.27
23	d	404	CLA	C3B-C2B-C1B	-5.21	100.87	107.16
23	A	408	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
23	B	610	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	b	609	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	C	512	CLA	C2C-C1C-NC	5.19	114.84	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
23	c	508	CLA	CHD-C1D-ND	-5.19	119.69	124.45
23	B	601	CLA	C2C-C1C-NC	5.18	114.83	109.97
23	a	404	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
23	A	406	CLA	C3D-C4D-ND	5.17	118.61	110.24
23	b	607	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
23	b	611	CLA	C4A-NA-C1A	-5.16	104.38	106.71
23	c	504	CLA	C3B-C2B-C1B	-5.16	100.93	107.16
23	C	504	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	b	608	CLA	C4A-NA-C1A	-5.16	104.39	106.71
23	b	602	CLA	C2C-C1C-NC	5.16	114.80	109.97
23	b	609	CLA	O2D-CGD-CBD	5.16	120.43	111.27
23	c	509	CLA	O2D-CGD-CBD	5.16	120.43	111.27
23	c	509	CLA	C4A-NA-C1A	-5.15	104.39	106.71
34	b	628	HTG	C1'-S1-C1	5.15	109.73	100.09
23	B	613	CLA	CMD-C2D-C1D	5.15	133.78	124.71
23	b	614	CLA	C2C-C1C-NC	5.15	114.79	109.97
23	a	408	CLA	C2C-C1C-NC	5.14	114.78	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	401	PHO	C3D-C4D-ND	5.14	114.72	107.72
23	C	503	CLA	C2C-C1C-NC	5.13	114.78	109.97
23	a	408	CLA	O2D-CGD-CBD	5.13	120.38	111.27
23	B	603	CLA	O2D-CGD-CBD	5.13	120.38	111.27
23	c	502	CLA	CMD-C2D-C1D	5.12	133.73	124.71
23	c	504	CLA	C2C-C1C-NC	5.12	114.76	109.97
34	C	522	HTG	C1'-S1-C1	5.11	109.65	100.09
23	d	404	CLA	O2D-CGD-CBD	5.11	120.35	111.27
23	D	404	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
23	a	404	CLA	CHD-C1D-ND	-5.09	119.78	124.45
23	C	508	CLA	C3B-C2B-C1B	-5.09	101.02	107.16
23	b	614	CLA	C3B-C2B-C1B	-5.08	101.02	107.16
23	A	406	CLA	C3B-C2B-C1B	-5.08	101.03	107.16
26	a	410	SQD	O6-C1-C2	5.07	116.22	108.30
34	b	622	HTG	C1'-S1-C1	5.07	109.57	100.09
23	c	512	CLA	C3B-C2B-C1B	-5.07	101.05	107.16
23	c	505	CLA	CHD-C1D-ND	-5.06	119.80	124.45
23	b	601	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	B	602	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
24	A	407	PHO	C1-C2-C3	-5.06	117.30	126.04
23	C	510	CLA	C4A-NA-C1A	-5.05	104.44	106.71
24	a	407	PHO	C1-C2-C3	-5.05	117.31	126.04
23	a	404	CLA	C3B-C2B-C1B	-5.05	101.07	107.16
23	B	603	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
23	a	405	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	b	612	CLA	C2C-C1C-NC	5.04	114.69	109.97
25	t	101	BCR	C33-C5-C6	-5.03	118.88	124.53
23	C	512	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
23	B	615	CLA	C2C-C1C-NC	5.01	114.66	109.97
23	B	613	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	C	504	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
26	L	101	SQD	O47-C7-C8	5.00	122.27	111.50
34	B	627	HTG	C1'-S1-C1	5.00	109.43	100.09
23	c	501	CLA	C2C-C1C-NC	4.99	114.65	109.97
26	f	101	SQD	O47-C7-C8	4.99	122.25	111.50
23	C	507	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
23	c	505	CLA	C3C-C4C-NC	4.99	116.16	110.57
23	b	604	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	c	505	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	d	401	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	C	509	CLA	C3C-C4C-NC	4.97	116.15	110.57
23	b	613	CLA	C3B-C2B-C1B	-4.96	101.17	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	O2D-CGD-CBD	4.96	120.08	111.27
23	b	601	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
23	B	611	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
38	E	103	HEM	CHC-C4B-NB	4.95	129.80	124.42
23	B	608	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	A	408	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
23	B	607	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	A	405	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	D	405	CLA	C4A-NA-C1A	-4.94	104.48	106.71
23	d	403	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
26	B	620	SQD	O6-C1-C2	4.94	116.01	108.30
23	C	511	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
34	C	522	HTG	C1-O5-C5	4.94	121.68	112.58
23	c	512	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	b	612	CLA	O2D-CGD-CBD	4.93	120.03	111.27
25	c	515	BCR	C7-C8-C9	-4.93	118.79	126.23
23	B	614	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
23	B	601	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	b	615	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	C	510	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
23	c	504	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
23	c	505	CLA	C2C-C1C-NC	4.91	114.58	109.97
23	b	612	CLA	C4A-NA-C1A	-4.91	104.50	106.71
23	B	602	CLA	C3B-C2B-C1B	-4.91	101.23	107.16
23	C	510	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	b	608	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	b	614	CLA	C4A-NA-C1A	-4.91	104.50	106.71
23	d	401	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
23	c	507	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	B	613	CLA	CHD-C1D-ND	-4.90	119.95	124.45
34	c	522	HTG	C1'-S1-C1	4.90	109.25	100.09
23	A	405	CLA	C3D-C4D-ND	4.90	118.16	110.24
23	A	408	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	C	514	CLA	C3B-C2B-C1B	-4.89	101.25	107.16
23	C	509	CLA	CMD-C2D-C1D	4.89	133.34	124.71
23	B	609	CLA	C2C-C1C-NC	4.89	114.55	109.97
23	b	610	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
23	B	614	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	C	505	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	c	513	CLA	O2D-CGD-CBD	4.89	119.95	111.27
23	B	608	CLA	C3D-C2D-C1D	-4.88	99.16	105.83
23	B	605	CLA	C3B-C2B-C1B	-4.88	101.27	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	521	HTG	C1'-S1-C1	4.87	109.21	100.09
23	B	610	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	A	404	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
23	B	605	CLA	C3D-C4D-ND	4.86	118.11	110.24
23	D	404	CLA	C1-C2-C3	-4.86	117.63	126.04
23	B	605	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	C	514	CLA	C3D-C4D-ND	4.86	118.11	110.24
23	B	603	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
23	C	504	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
33	C	501	LMG	O7-C10-C11	4.86	121.98	111.50
23	A	405	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	a	406	PHO	C3D-C4D-ND	4.86	114.34	107.72
23	C	510	CLA	C2C-C1C-NC	4.85	114.51	109.97
25	T	101	BCR	C15-C16-C17	-4.85	113.55	123.47
23	C	506	CLA	C3C-C4C-NC	4.84	116.00	110.57
23	a	405	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	C	505	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
23	B	604	CLA	C3C-C4C-NC	4.83	115.98	110.57
23	c	513	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	b	606	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	C	509	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	C	502	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
23	c	509	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
23	b	615	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	b	607	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	B	606	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	B	606	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	605	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	606	CLA	C3B-C2B-C1B	-4.79	101.39	107.16
23	b	616	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
23	c	509	CLA	C1-C2-C3	-4.78	117.78	126.04
23	D	404	CLA	O2D-CGD-CBD	4.77	119.75	111.27
23	B	613	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
23	b	602	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
23	c	511	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	a	405	CLA	C3D-C4D-ND	4.77	117.96	110.24
23	C	509	CLA	CHD-C1D-ND	-4.77	120.07	124.45
23	C	513	CLA	C2C-C1C-NC	4.76	114.43	109.97
23	b	607	CLA	O2D-CGD-CBD	4.76	119.72	111.27
23	B	616	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
23	C	509	CLA	C3B-C2B-C1B	-4.75	101.42	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	C	513	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
23	b	616	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
23	d	401	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
25	y	101	BCR	C33-C5-C6	-4.73	119.21	124.53
23	c	508	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
23	c	504	CLA	O2D-CGD-CBD	4.72	119.65	111.27
26	A	410	SQD	C1-C2-C3	-4.71	100.18	110.00
23	A	405	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	D	404	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	B	616	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	a	405	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	c	511	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	b	613	CLA	CHD-C1D-ND	-4.70	120.13	124.45
23	d	401	CLA	C3D-C4D-ND	4.70	117.84	110.24
23	b	611	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	502	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	D	404	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
23	D	404	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	C	503	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
23	B	612	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
23	C	505	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
26	A	410	SQD	O47-C7-C8	4.67	121.56	111.50
23	d	404	CLA	C3D-C4D-ND	4.66	117.78	110.24
23	a	404	CLA	C1C-C2C-C3C	-4.66	102.05	106.96
23	B	601	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
23	A	406	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
38	e	103	HEM	CHC-C4B-NB	4.66	129.48	124.42
23	B	610	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	c	506	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	b	608	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	b	610	CLA	C1-C2-C3	-4.65	118.01	126.04
23	d	404	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	b	613	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	B	615	CLA	O2D-CGD-CBD	4.64	119.51	111.27
23	B	602	CLA	O2D-CGD-CBD	4.64	119.50	111.27
23	a	408	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	b	605	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	b	607	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	B	611	CLA	C4A-NA-C1A	-4.63	104.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
23	C	514	CLA	C2C-C1C-NC	4.62	114.30	109.97
38	E	103	HEM	CAD-CBD-CGD	4.62	123.55	113.60
23	b	609	CLA	C1-C2-C3	-4.62	118.05	126.04
23	b	606	CLA	C2C-C1C-NC	4.62	114.30	109.97
23	C	514	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	c	503	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
23	c	508	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
23	b	612	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
23	c	507	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
23	b	613	CLA	C4A-NA-C1A	-4.59	104.64	106.71
31	D	409	LHG	O7-C7-C8	4.59	121.39	111.50
23	D	405	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	b	603	CLA	C3D-C4D-ND	4.59	117.66	110.24
23	d	403	CLA	C3D-C4D-ND	4.58	117.66	110.24
23	C	504	CLA	C3D-C4D-ND	4.58	117.65	110.24
23	a	405	CLA	O2D-CGD-CBD	4.58	119.41	111.27
23	b	614	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	A	406	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	B	615	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
23	c	502	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
23	c	511	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
26	L	101	SQD	O6-C1-C2	4.57	115.43	108.30
23	C	504	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	C	509	CLA	C3B-C4B-NB	4.55	114.73	110.52
29	D	407	PL9	C42-C43-C44	-4.55	116.71	127.66
23	b	605	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	B	609	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	c	512	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	c	513	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	c	508	CLA	O2D-CGD-O1D	-4.53	114.98	123.84
23	C	508	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	B	608	CLA	C3D-C4D-ND	4.53	117.57	110.24
23	D	405	CLA	C3D-C4D-ND	4.53	117.57	110.24
23	B	610	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	C	512	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	c	502	CLA	C1C-C2C-C3C	-4.53	102.20	106.96
23	c	504	CLA	C4A-NA-C1A	-4.52	104.67	106.71
25	H	101	BCR	C11-C10-C9	-4.52	120.86	127.31
23	b	610	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	B	604	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	B	601	CLA	C3D-C4D-ND	4.52	117.55	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	O2D-CGD-CBD	4.52	119.30	111.27
23	B	605	CLA	C4A-NA-C1A	-4.52	104.67	106.71
25	c	514	BCR	C11-C10-C9	-4.52	120.86	127.31
23	c	513	CLA	C3D-C4D-ND	4.51	117.54	110.24
25	T	101	BCR	C33-C5-C6	-4.51	119.46	124.53
23	B	609	CLA	C3D-C4D-ND	4.51	117.54	110.24
25	d	405	BCR	C15-C14-C13	-4.50	120.89	127.31
23	b	604	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
23	c	501	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	b	608	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
23	b	603	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	C	510	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	B	608	CLA	O2D-CGD-CBD	4.49	119.24	111.27
23	C	503	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
23	c	510	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	b	602	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	C	510	CLA	C3D-C4D-ND	4.48	117.48	110.24
23	B	604	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	B	608	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
23	a	408	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	D	405	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	c	505	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	B	602	CLA	C3D-C4D-ND	4.46	117.45	110.24
23	C	511	CLA	C3D-C4D-ND	4.45	117.44	110.24
40	v	201	HEC	C4B-NB-C1B	4.45	109.67	105.07
23	a	405	CLA	C4A-NA-C1A	-4.45	104.70	106.71
23	B	613	CLA	C1-C2-C3	-4.45	118.35	126.04
23	B	613	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	b	611	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
23	b	609	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	b	608	CLA	C3D-C4D-ND	4.43	117.41	110.24
23	b	609	CLA	C3D-C4D-ND	4.43	117.40	110.24
23	c	508	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	b	616	CLA	C1D-CHD-C4C	-4.42	116.52	126.06
23	b	613	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	B	606	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	c	502	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	c	513	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
25	B	617	BCR	C33-C5-C6	-4.40	119.59	124.53
33	Z	102	LMG	O7-C10-C11	4.40	120.97	111.50
23	C	512	CLA	C3D-C4D-ND	4.40	117.35	110.24
40	V	202	HEC	C4B-NB-C1B	4.39	109.61	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	A	406	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	b	605	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	C	512	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	c	503	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	b	603	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
23	c	508	CLA	C3D-C4D-ND	4.39	117.33	110.24
23	b	603	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
23	B	606	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
23	b	615	CLA	O2D-CGD-CBD	4.38	119.04	111.27
23	A	405	CLA	C2C-C1C-NC	4.38	114.07	109.97
23	c	512	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	c	503	CLA	C3C-C4C-NC	4.37	115.47	110.57
23	b	609	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
26	A	410	SQD	C1-O5-C5	-4.36	105.12	113.69
26	L	101	SQD	O7-S-C6	4.36	112.12	106.94
23	c	511	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	B	616	CLA	C3C-C4C-NC	4.36	115.46	110.57
23	B	601	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
23	b	612	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	C	507	CLA	O2D-CGD-CBD	4.35	119.00	111.27
23	c	510	CLA	C3D-C4D-ND	4.35	117.27	110.24
23	b	601	CLA	C3D-C4D-ND	4.35	117.27	110.24
23	B	604	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
26	B	620	SQD	O47-C7-C8	4.34	120.86	111.50
23	b	613	CLA	O2D-CGD-CBD	4.34	118.97	111.27
23	b	601	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	C	514	CLA	O2D-CGD-CBD	4.33	118.97	111.27
23	b	615	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
23	C	505	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	C	502	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
40	V	202	HEC	CHC-C4B-NB	4.33	129.71	124.37
23	B	616	CLA	C2C-C1C-NC	4.33	114.03	109.97
23	b	607	CLA	C3D-C4D-ND	4.33	117.23	110.24
23	B	609	CLA	O2D-CGD-CBD	4.32	118.95	111.27
23	a	408	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
34	b	628	HTG	C1-O5-C5	4.32	120.54	112.58
23	b	605	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
23	c	509	CLA	C3D-C4D-ND	4.31	117.22	110.24
38	e	103	HEM	C4C-NC-C1C	4.31	109.57	105.35
23	d	403	CLA	O2D-CGD-CBD	4.31	118.93	111.27
23	b	611	CLA	C3D-C4D-ND	4.31	117.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	603	CLA	C3D-C2D-C1D	-4.31	99.96	105.83
23	C	505	CLA	C3B-C4B-NB	4.31	114.51	110.52
23	C	503	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	b	607	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	d	403	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	B	614	CLA	C1D-CHD-C4C	-4.29	116.79	126.06
23	D	404	CLA	C3C-C4C-NC	4.29	115.39	110.57
23	B	610	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
23	a	404	CLA	C3B-C4B-NB	4.29	114.49	110.52
38	E	103	HEM	C1B-NB-C4B	4.29	109.50	105.07
25	b	619	BCR	C3-C4-C5	-4.28	106.43	114.08
23	c	506	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	c	507	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	A	404	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
23	c	501	CLA	O2D-CGD-O1D	-4.27	115.49	123.84
23	B	607	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
23	B	611	CLA	O2D-CGD-CBD	4.27	118.85	111.27
23	c	502	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	A	408	CLA	C4-C3-C5	4.27	122.45	115.27
23	c	509	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
23	c	505	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	c	501	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	A	404	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	C	507	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
23	c	510	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	C	505	CLA	C1D-CHD-C4C	-4.24	116.90	126.06
25	d	405	BCR	C28-C27-C26	-4.24	106.50	114.08
23	B	615	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	C	513	CLA	C3D-C4D-ND	4.24	117.10	110.24
23	a	404	CLA	C1D-CHD-C4C	-4.24	116.91	126.06
23	c	513	CLA	C3C-C4C-NC	4.24	115.32	110.57
23	a	404	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	B	612	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	b	610	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	b	616	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	c	506	CLA	C3B-C4B-NB	4.23	114.44	110.52
35	D	402	LMT	C1'-O5'-C5'	4.22	121.98	113.69
23	B	615	CLA	CMB-C2B-C1B	4.22	131.80	125.37
23	c	506	CLA	O2D-CGD-CBD	4.22	118.77	111.27
23	C	508	CLA	C1D-CHD-C4C	-4.22	116.95	126.06
23	B	603	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	B	611	CLA	C3B-C2B-C1B	-4.22	102.07	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	BCR	C15-C14-C13	-4.22	121.29	127.31
23	b	602	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	C	506	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
23	C	507	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
25	B	617	BCR	C7-C8-C9	-4.21	119.88	126.23
23	c	501	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
23	b	604	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
23	b	606	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
23	C	513	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
33	Z	101	LMG	C3-C4-C5	4.19	117.72	110.24
23	C	507	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	c	509	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	B	605	CLA	CMB-C2B-C1B	4.18	131.74	125.37
23	c	502	CLA	C3B-C4B-NB	4.18	114.39	110.52
23	C	508	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	B	611	CLA	C3C-C4C-NC	4.18	115.26	110.57
38	e	103	HEM	C1B-NB-C4B	4.18	109.39	105.07
23	D	405	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
23	b	614	CLA	C3C-C4C-NC	4.17	115.25	110.57
23	B	603	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
23	c	510	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	c	503	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
23	C	502	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
23	B	610	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	B	615	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
23	B	602	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	C	508	CLA	CMB-C2B-C1B	4.15	131.69	125.37
23	B	616	CLA	C3D-C4D-ND	4.15	116.95	110.24
29	a	414	PL9	C32-C33-C34	-4.15	117.67	127.66
23	C	510	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	b	616	CLA	C3D-C4D-ND	4.15	116.94	110.24
23	B	615	CLA	C3D-C4D-ND	4.14	116.94	110.24
40	V	202	HEC	CHA-C4D-ND	4.14	128.92	124.42
23	C	511	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
23	b	606	CLA	C3C-C4C-NC	4.13	115.21	110.57
23	A	405	CLA	O2D-CGD-CBD	4.13	118.61	111.27
26	A	410	SQD	C44-O6-C1	-4.13	105.67	113.74
23	A	408	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	c	511	CLA	O2D-CGD-CBD	4.12	118.59	111.27
23	C	506	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
24	D	401	PHO	CBC-CAC-C3C	-4.12	106.85	112.88
23	A	405	CLA	C1C-C2C-C3C	-4.12	102.63	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
36	c	516	DGD	O2G-C1B-C2B	4.12	120.37	111.50
23	C	512	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	B	604	CLA	C4A-NA-C1A	-4.11	104.86	106.71
23	c	502	CLA	C4A-NA-C1A	-4.11	104.86	106.71
23	D	405	CLA	C3C-C4C-NC	4.11	115.18	110.57
23	b	612	CLA	C3C-C4C-NC	4.11	115.17	110.57
23	b	606	CLA	C3D-C4D-ND	4.10	116.88	110.24
23	C	506	CLA	C3D-C4D-ND	4.10	116.88	110.24
23	B	606	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	B	614	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
23	C	507	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
23	A	404	CLA	C3B-C4B-NB	4.09	114.31	110.52
25	b	617	BCR	C33-C5-C6	-4.09	119.93	124.53
23	B	614	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	B	612	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
29	A	414	PL9	C7-C3-C4	4.09	120.20	116.88
23	b	613	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	c	512	CLA	C3C-C4C-NC	4.09	115.15	110.57
23	a	404	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
35	D	402	LMT	O5'-C5'-C4'	4.08	118.36	109.75
23	B	612	CLA	CMD-C2D-C1D	4.08	131.91	124.71
23	b	614	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	B	607	CLA	C3D-C4D-ND	4.08	116.83	110.24
23	A	406	CLA	C2C-C1C-NC	4.07	113.79	109.97
23	B	614	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	b	611	CLA	C1-C2-C3	-4.07	119.01	126.04
23	C	508	CLA	C3D-C4D-ND	4.06	116.81	110.24
25	H	101	BCR	C7-C8-C9	-4.06	120.10	126.23
29	a	414	PL9	C15-C14-C16	4.06	122.10	115.27
25	b	619	BCR	C7-C8-C9	-4.06	120.10	126.23
23	C	509	CLA	C3D-C4D-ND	4.06	116.80	110.24
23	A	408	CLA	O2D-CGD-CBD	4.06	118.47	111.27
23	B	612	CLA	O2D-CGD-O1D	-4.05	115.91	123.84
25	k	101	BCR	C11-C10-C9	-4.05	121.53	127.31
23	B	604	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
23	d	404	CLA	C2C-C1C-NC	4.05	113.76	109.97
23	A	404	CLA	O2A-CGA-CBA	4.04	124.60	111.91
23	c	506	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
23	b	613	CLA	C3D-C4D-ND	4.04	116.77	110.24
23	B	613	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	c	506	CLA	C3C-C4C-NC	4.03	115.09	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	C1-C2-C3	-4.03	119.07	126.04
23	A	408	CLA	C3D-C4D-ND	4.03	116.75	110.24
33	c	520	LMG	O7-C10-C11	4.03	120.18	111.50
23	c	511	CLA	C4-C3-C5	4.02	122.04	115.27
23	C	502	CLA	C3D-C4D-ND	4.02	116.75	110.24
23	c	507	CLA	CMB-C2B-C1B	4.02	131.49	125.37
23	b	615	CLA	C3D-C4D-ND	4.02	116.74	110.24
23	d	401	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
34	b	625	HTG	C1-O5-C5	4.01	119.97	112.58
40	v	201	HEC	CHC-C4B-NB	4.01	129.31	124.37
31	E	101	LHG	O7-C7-C8	4.01	120.14	111.50
23	A	406	CLA	CMB-C2B-C1B	4.01	131.47	125.37
23	D	405	CLA	C2C-C1C-NC	4.01	113.72	109.97
23	b	603	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
23	A	406	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	B	611	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	608	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	607	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	D	404	CLA	C3D-C4D-ND	4.00	116.70	110.24
33	J	101	LMG	O7-C10-C11	4.00	120.11	111.50
25	c	514	BCR	C20-C21-C22	-4.00	121.61	127.31
23	D	405	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
23	C	514	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	B	616	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	B	608	CLA	C4A-NA-C1A	-3.99	104.91	106.71
23	b	605	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	B	606	CLA	C1D-CHD-C4C	-3.99	117.46	126.06
23	C	512	CLA	O2D-CGD-CBD	3.98	118.34	111.27
23	A	404	CLA	CAC-C3C-C4C	3.98	129.97	124.81
23	c	507	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	C	513	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
38	e	103	HEM	CAD-CBD-CGD	3.97	122.15	113.60
23	a	408	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	C	503	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	B	612	CLA	CHD-C1D-ND	-3.96	120.81	124.45
23	a	408	CLA	C1-C2-C3	-3.96	119.19	126.04
23	B	605	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	c	505	CLA	CMB-C2B-C1B	3.96	131.40	125.37
23	c	512	CLA	C1-C2-C3	-3.96	119.20	126.04
23	b	608	CLA	C3C-C4C-NC	3.96	115.01	110.57
35	I	101	LMT	C1'-O5'-C5'	3.95	121.45	113.69
23	B	604	CLA	C1C-C2C-C3C	-3.95	102.81	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	C	511	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
25	H	101	BCR	C16-C17-C18	-3.94	121.69	127.31
25	b	618	BCR	C7-C8-C9	-3.94	120.28	126.23
25	d	405	BCR	C29-C30-C25	3.94	116.54	110.48
23	B	607	CLA	C3C-C4C-NC	3.94	114.98	110.57
29	A	414	PL9	C7-C8-C9	-3.93	120.25	126.79
23	b	604	CLA	C3D-C4D-ND	3.93	116.60	110.24
23	B	613	CLA	CMC-C2C-C1C	3.93	131.02	125.04
23	B	615	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
29	a	414	PL9	C27-C28-C29	-3.92	118.21	127.66
24	D	401	PHO	C1-C2-C3	-3.92	119.26	126.04
23	b	606	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	D	405	CLA	C1-C2-C3	-3.92	119.26	126.04
23	B	608	CLA	C3C-C4C-NC	3.92	114.97	110.57
23	d	403	CLA	C3D-C2D-C1D	-3.92	100.49	105.83
36	H	102	DGD	O2G-C1B-C2B	3.92	119.94	111.50
23	C	507	CLA	C1-C2-C3	-3.91	119.28	126.04
33	Z	101	LMG	O7-C10-C11	3.90	119.92	111.50
23	D	405	CLA	CMB-C2B-C1B	3.90	131.31	125.37
23	b	613	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
23	c	507	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	a	404	CLA	O2D-CGD-CBD	3.90	118.20	111.27
23	b	614	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
23	b	601	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	c	504	CLA	C3C-C4C-NC	3.89	114.94	110.57
23	C	502	CLA	C1-C2-C3	-3.89	119.31	126.04
23	A	404	CLA	CAA-C2A-C3A	-3.89	102.12	112.78
38	E	103	HEM	C4C-NC-C1C	3.89	109.16	105.35
23	c	506	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	B	610	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
29	a	414	PL9	C7-C3-C2	-3.89	118.19	123.30
23	A	405	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	C	512	CLA	C3B-C4B-NB	3.89	114.12	110.52
23	c	513	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	c	506	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
23	B	613	CLA	C3D-C4D-ND	3.88	116.52	110.24
23	C	506	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
23	a	405	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
23	b	612	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
23	A	405	CLA	CHD-C4C-NC	3.87	130.30	124.20
23	C	502	CLA	C3C-C4C-NC	3.87	114.91	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	A	405	CLA	CMC-C2C-C1C	3.87	130.93	125.04
26	a	410	SQD	C45-O47-C7	-3.86	108.28	117.79
23	C	513	CLA	C3C-C4C-NC	3.86	114.90	110.57
23	b	615	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
23	b	605	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
23	d	403	CLA	C3C-C4C-NC	3.86	114.90	110.57
38	e	103	HEM	CHD-C4C-NC	3.86	128.61	124.44
23	C	507	CLA	CAC-C3C-C4C	3.85	129.81	124.81
29	a	414	PL9	C22-C23-C24	-3.85	118.39	127.66
26	a	410	SQD	O8-S-C6	3.85	111.87	105.74
23	a	404	CLA	CAA-C2A-C3A	-3.85	102.24	112.78
23	B	612	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
23	c	511	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
25	C	515	BCR	C16-C17-C18	-3.84	121.82	127.31
23	c	502	CLA	C3C-C4C-NC	3.84	114.88	110.57
23	B	605	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	b	602	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	c	505	CLA	C3D-C2D-C1D	-3.84	100.60	105.83
23	b	604	CLA	C1C-C2C-C3C	-3.83	102.92	106.96
23	b	615	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	C	505	CLA	C3D-C4D-ND	3.83	116.43	110.24
23	B	611	CLA	C3D-C4D-ND	3.83	116.43	110.24
23	b	602	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	b	612	CLA	C1-C2-C3	-3.83	119.42	126.04
23	b	611	CLA	C3C-C4C-NC	3.83	114.86	110.57
25	B	618	BCR	C15-C14-C13	-3.82	121.85	127.31
23	B	602	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	c	501	CLA	C3C-C4C-NC	3.82	114.85	110.57
23	b	604	CLA	CMB-C2B-C1B	3.82	131.18	125.37
23	d	401	CLA	C3B-C4B-NB	3.82	114.06	110.52
29	d	406	PL9	C10-C9-C11	3.81	121.68	115.27
23	c	505	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
33	B	621	LMG	O7-C10-C11	3.81	119.71	111.50
25	d	405	BCR	C7-C8-C9	-3.81	120.48	126.23
29	d	406	PL9	C42-C43-C44	-3.81	118.50	127.66
23	b	603	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	B	608	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
23	B	605	CLA	C1-C2-C3	-3.80	119.47	126.04
23	C	510	CLA	C1-C2-C3	-3.80	119.47	126.04
33	c	519	LMG	O7-C10-C11	3.80	119.68	111.50
29	d	406	PL9	C7-C8-C9	-3.79	120.48	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	618	BCR	C37-C22-C21	-3.78	117.63	122.92
23	B	604	CLA	C3D-C4D-ND	3.78	116.35	110.24
25	c	514	BCR	C15-C14-C13	-3.78	121.92	127.31
23	b	614	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
23	B	605	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	C	508	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
23	b	608	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	B	611	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	B	614	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	b	602	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	c	508	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	c	511	CLA	C1-C2-C3	-3.77	119.52	126.04
23	B	612	CLA	C4C-C3C-C2C	-3.77	101.41	106.90
23	C	503	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
23	a	405	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
23	B	601	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
23	A	408	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
31	A	417	LHG	O7-C7-C8	3.75	119.59	111.50
23	b	612	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
23	d	403	CLA	C3B-C4B-NB	3.75	114.00	110.52
23	c	511	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	C	514	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	A	404	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
23	b	611	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
25	b	619	BCR	C38-C26-C25	-3.74	120.32	124.53
33	j	101	LMG	O7-C10-C11	3.74	119.57	111.50
23	a	408	CLA	C3B-C4B-NB	3.74	113.99	110.52
23	b	605	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
23	b	601	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
23	B	612	CLA	C4A-NA-C1A	-3.74	105.03	106.71
23	c	510	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
33	c	520	LMG	O6-C5-C4	3.73	116.47	109.69
23	b	609	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
23	c	512	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
23	a	404	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	d	401	CLA	C4A-NA-C1A	-3.72	105.03	106.71
23	A	405	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
23	b	605	CLA	C3B-C4B-NB	3.72	113.97	110.52
23	B	609	CLA	CMB-C2B-C1B	3.72	131.03	125.37
25	c	514	BCR	C16-C17-C18	-3.71	122.01	127.31
23	B	610	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
23	a	405	CLA	C3C-C4C-NC	3.71	114.73	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
26	B	620	SQD	O7-S-C6	3.71	111.34	106.94
33	a	416	LMG	O7-C10-C11	3.71	119.49	111.50
23	c	506	CLA	C4A-NA-C1A	-3.70	105.04	106.71
23	C	505	CLA	C4A-NA-C1A	-3.70	105.04	106.71
23	d	401	CLA	O2D-CGD-CBD	3.70	117.84	111.27
23	B	601	CLA	C3C-C4C-NC	3.70	114.72	110.57
23	b	609	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
23	C	502	CLA	C3B-C4B-NB	3.69	113.94	110.52
34	C	522	HTG	O5-C5-C4	3.69	116.40	109.69
23	d	404	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	d	404	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	C	509	CLA	C4C-C3C-C2C	-3.68	101.53	106.90
23	b	607	CLA	C3B-C4B-NB	3.68	113.93	110.52
29	A	414	PL9	C7-C3-C2	-3.68	118.46	123.30
40	V	202	HEC	C4C-NC-C1C	3.68	108.95	105.35
23	c	502	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
23	B	601	CLA	C1-C2-C3	-3.68	119.68	126.04
23	C	509	CLA	O2D-CGD-O1D	-3.67	116.65	123.84
23	C	512	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
25	B	618	BCR	C29-C30-C25	3.67	116.13	110.48
25	Y	101	BCR	C15-C14-C13	-3.66	122.08	127.31
23	c	512	CLA	CMB-C2B-C1B	3.66	130.95	125.37
33	Z	102	LMG	C3-C4-C5	3.66	116.77	110.24
33	Z	101	LMG	O6-C5-C4	3.66	116.33	109.69
23	B	609	CLA	C1D-CHD-C4C	-3.65	118.17	126.06
23	C	504	CLA	O2D-CGD-CBD	3.65	117.76	111.27
23	B	614	CLA	CMB-C2B-C1B	3.65	130.93	125.37
23	c	510	CLA	C3B-C4B-NB	3.65	113.90	110.52
29	a	414	PL9	C37-C38-C39	-3.65	118.88	127.66
23	b	611	CLA	C3B-C4B-NB	3.64	113.89	110.52
24	A	407	PHO	C1A-C2A-C3A	-3.64	99.37	102.84
23	b	609	CLA	C3C-C4C-NC	3.64	114.65	110.57
25	C	516	BCR	C7-C8-C9	-3.64	120.73	126.23
23	b	609	CLA	CMB-C2B-C1B	3.64	130.91	125.37
23	B	607	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	C	511	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	B	613	CLA	CAC-C3C-C4C	3.64	129.53	124.81
23	c	504	CLA	CAC-C3C-C4C	3.63	129.53	124.81
23	B	603	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	C	509	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	C	502	CLA	O2D-CGD-O1D	-3.63	116.74	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	c	504	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
25	k	101	BCR	C24-C23-C22	-3.63	120.75	126.23
40	v	201	HEC	C4C-NC-C1C	3.63	108.90	105.35
23	B	608	CLA	C1-C2-C3	-3.62	119.78	126.04
25	h	101	BCR	C7-C8-C9	-3.62	120.77	126.23
23	d	404	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
23	b	608	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	A	408	CLA	C1-C2-C3	-3.61	119.80	126.04
23	B	610	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
23	B	616	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
29	A	414	PL9	C27-C28-C29	-3.60	118.98	127.66
23	c	508	CLA	C3B-C4B-NB	3.60	113.86	110.52
23	c	508	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
23	c	512	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	b	614	CLA	C3B-C4B-NB	3.60	113.86	110.52
24	D	401	PHO	C1A-C2A-C3A	-3.60	99.42	102.84
23	B	602	CLA	C3C-C4C-NC	3.59	114.60	110.57
23	B	601	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	b	607	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	C	510	CLA	CMC-C2C-C1C	3.59	130.50	125.04
23	C	510	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
23	C	503	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
23	b	604	CLA	C1-C2-C3	-3.59	119.84	126.04
23	d	403	CLA	O2A-CGA-CBA	3.58	123.16	111.91
23	B	603	CLA	O2A-CGA-O1A	-3.58	114.55	123.59
23	b	616	CLA	C2C-C1C-NC	3.58	113.33	109.97
26	a	410	SQD	C1-O5-C5	-3.58	106.66	113.69
23	c	513	CLA	CMC-C2C-C1C	3.58	130.49	125.04
25	H	101	BCR	C24-C23-C22	-3.58	120.83	126.23
36	C	518	DGD	O2G-C1B-C2B	3.58	119.21	111.50
29	D	407	PL9	C53-C6-C1	3.58	122.30	114.99
23	d	401	CLA	CHD-C4C-NC	3.57	129.83	124.20
33	z	101	LMG	O7-C10-C11	3.57	119.20	111.50
23	b	609	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
36	C	517	DGD	O2G-C1B-C2B	3.57	119.19	111.50
23	c	504	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
25	K	102	BCR	C7-C8-C9	-3.56	120.85	126.23
36	c	517	DGD	O2G-C1B-C2B	3.56	119.18	111.50
23	B	614	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	d	401	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
31	d	407	LHG	O7-C7-C8	3.56	119.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
23	B	604	CLA	C1-C2-C3	-3.56	119.89	126.04
26	D	413	SQD	O7-S-C6	3.55	111.16	106.94
40	V	202	HEC	C1D-ND-C4D	3.55	108.74	105.07
23	D	404	CLA	C3B-C4B-NB	3.55	113.81	110.52
23	B	602	CLA	C3B-C4B-NB	3.55	113.81	110.52
40	v	201	HEC	CHA-C4D-ND	3.55	128.27	124.42
23	b	611	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
23	C	504	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
31	l	101	LHG	O7-C7-C8	3.54	119.13	111.50
23	C	508	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
33	Z	102	LMG	C1-C2-C3	3.54	117.36	110.00
40	v	201	HEC	C1D-ND-C4D	3.53	108.72	105.07
23	A	406	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
23	b	609	CLA	CAC-C3C-C4C	3.53	129.39	124.81
25	A	409	BCR	C33-C5-C6	-3.53	120.57	124.53
23	b	603	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	b	608	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
25	h	101	BCR	C16-C17-C18	-3.52	122.28	127.31
23	a	408	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	B	604	CLA	C3B-C4B-NB	3.52	113.78	110.52
23	a	408	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
31	d	409	LHG	O7-C7-C8	3.51	119.07	111.50
23	B	614	CLA	CHC-C1C-C2C	-3.51	116.98	126.73
23	b	613	CLA	C3B-C4B-NB	3.51	113.77	110.52
23	c	507	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	C	513	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
40	V	202	HEC	CHB-C1B-NB	3.50	128.22	124.42
23	c	501	CLA	CAC-C3C-C4C	3.50	129.35	124.81
23	B	603	CLA	C3B-C4B-NB	3.50	113.76	110.52
23	B	603	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
23	C	504	CLA	C3C-C4C-NC	3.50	114.50	110.57
23	C	506	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
23	C	512	CLA	CMC-C2C-C1C	3.50	130.36	125.04
23	C	504	CLA	C4-C3-C5	3.49	121.15	115.27
23	B	609	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	b	615	CLA	C3B-C4B-NB	3.49	113.75	110.52
38	E	103	HEM	CHB-C1B-NB	3.49	128.68	124.37
25	C	516	BCR	C11-C10-C9	-3.49	122.33	127.31
23	c	513	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	C	512	CLA	CAC-C3C-C4C	3.48	129.33	124.81
23	B	608	CLA	CHD-C4C-NC	3.48	129.69	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	b	615	CLA	C11-C10-C8	-3.48	104.67	115.92
23	c	501	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
25	H	101	BCR	C38-C26-C25	-3.48	120.62	124.53
23	B	602	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
23	b	610	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
38	e	103	HEM	CHB-C1B-NB	3.48	128.66	124.37
38	E	103	HEM	CHD-C4C-NC	3.47	128.20	124.44
23	C	512	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	615	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	C	507	CLA	CBC-CAC-C3C	-3.47	102.86	112.43
23	C	502	CLA	CBC-CAC-C3C	-3.47	102.86	112.43
23	B	608	CLA	O2A-CGA-O1A	-3.47	114.84	123.59
23	B	603	CLA	C3C-C4C-NC	3.46	114.46	110.57
23	B	610	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	b	616	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
25	b	617	BCR	C7-C8-C9	-3.46	121.01	126.23
23	B	613	CLA	C3B-C4B-NB	3.46	113.72	110.52
23	b	605	CLA	CMB-C2B-C1B	3.46	130.63	125.37
23	A	404	CLA	C3C-C4C-NC	3.46	114.45	110.57
23	C	507	CLA	CMC-C2C-C1C	3.45	130.30	125.04
29	A	414	PL9	C22-C23-C24	-3.45	119.35	127.66
23	c	505	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
23	b	601	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	c	509	CLA	C3B-C4B-NB	3.45	113.71	110.52
23	b	613	CLA	O2A-CGA-CBA	3.44	122.72	111.91
23	b	605	CLA	C4-C3-C5	3.44	121.06	115.27
23	c	509	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	d	401	CLA	CBC-CAC-C3C	-3.44	102.95	112.43
23	c	511	CLA	C3B-C4B-NB	3.44	113.70	110.52
25	K	102	BCR	C24-C23-C22	-3.43	121.05	126.23
23	b	614	CLA	CAC-C3C-C4C	3.43	129.26	124.81
23	c	504	CLA	CMC-C2C-C1C	3.43	130.26	125.04
23	b	607	CLA	CMB-C2B-C1B	3.42	130.59	125.37
25	t	101	BCR	C37-C22-C23	3.42	123.47	118.08
26	A	410	SQD	O7-S-C6	3.42	111.01	106.94
23	C	506	CLA	CMC-C2C-C1C	3.42	130.25	125.04
23	C	509	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
25	k	101	BCR	C29-C30-C25	3.41	115.74	110.48
23	C	514	CLA	CMB-C2B-C1B	3.41	130.57	125.37
23	B	613	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
23	c	501	CLA	C1C-C2C-C3C	-3.41	103.37	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
29	a	414	PL9	C10-C9-C11	3.41	121.00	115.27
23	B	615	CLA	CED-O2D-CGD	3.41	123.64	115.94
26	a	410	SQD	C1-C2-C3	-3.40	102.91	110.00
23	a	408	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
23	B	607	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
23	b	606	CLA	C4-C3-C5	3.40	120.99	115.27
34	b	622	HTG	O5-C1-C2	3.40	114.59	110.31
25	d	405	BCR	C33-C5-C6	-3.40	120.71	124.53
23	C	510	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	B	603	CLA	C4-C3-C5	3.39	120.97	115.27
23	b	605	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	C	504	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
23	C	514	CLA	C1-C2-C3	-3.38	120.19	126.04
23	C	503	CLA	CMB-C2B-C1B	3.38	130.52	125.37
26	f	101	SQD	O7-S-C6	3.38	110.95	106.94
25	t	101	BCR	C11-C10-C9	-3.38	122.49	127.31
40	V	202	HEC	CBC-CAC-C3C	3.38	121.74	112.43
23	C	511	CLA	C1-C2-C3	-3.37	120.21	126.04
23	c	504	CLA	C3B-C4B-NB	3.37	113.64	110.52
23	c	509	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
23	B	614	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
23	b	615	CLA	CMB-C2B-C1B	3.37	130.50	125.37
23	C	514	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
23	b	607	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
23	D	405	CLA	CHD-C4C-NC	3.36	129.50	124.20
33	c	520	LMG	C3-C4-C5	3.36	116.24	110.24
23	C	507	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
29	d	406	PL9	C20-C19-C21	3.35	120.91	115.27
25	A	409	BCR	C24-C23-C22	-3.35	121.17	126.23
23	d	401	CLA	C3C-C4C-NC	3.35	114.33	110.57
23	c	502	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	B	614	CLA	C4A-NA-C1A	-3.35	105.20	106.71
25	D	406	BCR	C38-C26-C25	-3.35	120.77	124.53
31	A	416	LHG	O8-C23-C24	3.35	122.41	111.91
23	d	403	CLA	C1-C2-C3	-3.35	120.26	126.04
26	A	412	SQD	O48-C23-C24	3.34	122.40	111.91
29	A	414	PL9	C15-C14-C16	3.34	120.89	115.27
26	a	410	SQD	O9-S-C6	3.33	110.90	106.94
40	v	201	HEC	CHB-C1B-NB	3.33	128.04	124.42
38	e	103	HEM	CHA-C4D-ND	3.33	128.48	124.37
23	a	408	CLA	O2D-CGD-O1D	-3.33	117.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Z	102	LMG	C4-C3-C2	3.33	116.63	110.82
23	B	611	CLA	C3B-C4B-NB	3.33	113.60	110.52
25	D	406	BCR	C24-C23-C22	-3.32	121.22	126.23
29	A	414	PL9	C30-C29-C31	3.32	120.86	115.27
23	C	509	CLA	C1-C2-C3	-3.32	120.30	126.04
23	D	405	CLA	CMC-C2C-C1C	3.31	130.08	125.04
29	A	414	PL9	C32-C33-C34	-3.31	119.69	127.66
23	c	510	CLA	C4-C3-C5	3.31	120.84	115.27
25	h	101	BCR	C38-C26-C25	-3.31	120.81	124.53
23	C	507	CLA	C3C-C4C-NC	3.31	114.28	110.57
26	a	412	SQD	O47-C7-C8	3.31	118.63	111.50
23	A	408	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
23	b	610	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
25	y	101	BCR	C38-C26-C25	-3.31	120.81	124.53
26	f	101	SQD	C1-O5-C5	3.31	120.18	113.69
23	b	614	CLA	C1-C2-C3	-3.30	120.33	126.04
26	A	412	SQD	O8-S-C6	3.30	111.00	105.74
25	T	101	BCR	C7-C8-C9	-3.30	121.25	126.23
23	b	609	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
23	b	612	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
34	b	623	HTG	O5-C1-C2	3.29	114.46	110.31
29	a	414	PL9	C30-C29-C31	3.29	120.81	115.27
23	D	404	CLA	CAC-C3C-C4C	3.29	129.08	124.81
23	C	509	CLA	C4A-NA-C1A	-3.29	105.23	106.71
23	B	614	CLA	CAC-C3C-C4C	3.29	129.07	124.81
23	b	616	CLA	CHD-C4C-NC	3.28	129.38	124.20
23	C	511	CLA	C3C-C4C-NC	3.28	114.25	110.57
23	C	512	CLA	C4-C3-C5	3.28	120.79	115.27
23	B	605	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	c	507	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	c	509	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
25	D	406	BCR	C3-C4-C5	-3.27	108.24	114.08
23	c	513	CLA	CAC-C3C-C4C	3.27	129.05	124.81
29	A	414	PL9	C20-C19-C21	3.27	120.77	115.27
25	c	515	BCR	C38-C26-C25	-3.27	120.86	124.53
23	b	609	CLA	O2A-CGA-CBA	3.26	122.14	111.91
23	A	408	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	B	607	CLA	CMB-C2B-C1B	3.26	130.33	125.37
23	B	609	CLA	C3B-C2B-C1B	-3.26	103.23	107.16
31	A	416	LHG	O8-C23-O10	-3.25	115.38	123.59
25	A	409	BCR	C15-C14-C13	-3.25	122.67	127.31
23	A	406	CLA	C1C-C2C-C3C	-3.25	103.54	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	CMB-C2B-C1B	3.25	130.31	125.37
23	a	405	CLA	C3B-C4B-NB	3.25	113.53	110.52
23	B	607	CLA	O2D-CGD-O1D	-3.24	117.49	123.84
23	b	604	CLA	CMC-C2C-C1C	3.24	129.98	125.04
25	d	405	BCR	C16-C17-C18	-3.24	122.68	127.31
23	A	404	CLA	O2A-CGA-O1A	-3.24	115.41	123.59
23	b	612	CLA	C4-C3-C5	3.24	120.72	115.27
23	c	502	CLA	CHC-C1C-C2C	-3.24	117.73	126.73
23	d	403	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
25	t	101	BCR	C21-C20-C19	-3.24	113.11	123.22
23	c	506	CLA	C1-C2-C3	-3.24	120.45	126.04
40	v	201	HEC	CHA-C1A-NA	3.23	127.94	124.44
23	A	408	CLA	C3B-C4B-NB	3.23	113.52	110.52
23	b	605	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	b	615	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
23	B	608	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	b	608	CLA	CMC-C2C-C1C	3.23	129.96	125.04
25	C	515	BCR	C33-C5-C6	-3.23	120.90	124.53
23	B	603	CLA	CMB-C2B-C1B	3.23	130.28	125.37
25	D	406	BCR	C28-C27-C26	-3.23	108.32	114.08
23	c	513	CLA	C1-C2-C3	-3.22	120.47	126.04
23	c	501	CLA	CMB-C2B-C1B	3.22	130.28	125.37
25	T	101	BCR	C15-C14-C13	3.22	131.91	127.31
23	B	603	CLA	O2A-CGA-CBA	3.22	122.02	111.91
25	b	617	BCR	C16-C17-C18	-3.22	122.71	127.31
23	b	610	CLA	O2A-CGA-CBA	3.22	122.01	111.91
34	c	522	HTG	C1-O5-C5	3.22	118.52	112.58
29	A	414	PL9	C37-C38-C39	-3.21	119.92	127.66
23	b	602	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
25	T	101	BCR	C12-C13-C14	-3.21	114.01	118.94
23	c	510	CLA	CBC-CAC-C3C	-3.21	103.58	112.43
23	B	613	CLA	C4-C3-C5	3.21	120.66	115.27
23	D	404	CLA	O2A-CGA-CBA	3.21	121.97	111.91
23	c	503	CLA	CMB-C2B-C1B	3.20	130.25	125.37
23	B	601	CLA	C3B-C4B-NB	3.20	113.49	110.52
29	a	414	PL9	C42-C43-C44	-3.20	119.95	127.66
25	B	618	BCR	C2-C1-C6	3.20	115.41	110.48
23	B	610	CLA	C1-C2-C3	-3.20	120.51	126.04
23	b	603	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
23	b	616	CLA	CMB-C2B-C1B	3.19	130.24	125.37
23	a	405	CLA	CHD-C4C-NC	3.19	129.24	124.20
23	C	504	CLA	CHC-C1C-C2C	-3.19	117.86	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	CAC-C3C-C4C	3.19	128.95	124.81
23	A	404	CLA	O2D-CGD-CBD	3.19	116.93	111.27
23	A	406	CLA	C1-C2-C3	-3.19	120.53	126.04
23	B	610	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
23	b	612	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	D	405	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	c	509	CLA	CAC-C3C-C4C	3.18	128.94	124.81
29	d	406	PL9	C25-C24-C26	3.18	120.62	115.27
23	C	508	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
23	C	502	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
23	A	406	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	C	509	CLA	CAC-C3C-C4C	3.17	128.92	124.81
29	d	406	PL9	C36-C37-C38	-3.17	101.46	111.88
38	e	103	HEM	C4D-ND-C1D	3.17	108.34	105.07
23	c	512	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	b	610	CLA	C4-C3-C5	3.16	120.59	115.27
23	b	607	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
24	a	407	PHO	C4-C3-C5	3.16	120.59	115.27
31	A	416	LHG	O7-C7-C8	3.16	118.32	111.50
35	M	101	LMT	O1'-C1'-C2'	3.16	113.23	108.30
23	b	606	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
23	b	608	CLA	CHD-C4C-NC	3.16	129.18	124.20
40	V	202	HEC	CHA-C1A-NA	3.16	127.85	124.44
23	c	502	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
23	C	506	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
38	e	103	HEM	CHD-C1D-ND	3.15	127.84	124.42
23	B	616	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
23	a	404	CLA	O2A-CGA-O1A	-3.15	115.64	123.59
26	a	412	SQD	C3-C4-C5	3.15	115.86	110.24
23	C	507	CLA	C4-C3-C5	3.15	120.57	115.27
23	b	613	CLA	O2A-CGA-O1A	-3.15	115.65	123.59
23	B	609	CLA	CHD-C4C-NC	3.14	129.16	124.20
23	B	602	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
23	d	404	CLA	CAC-C3C-C4C	3.14	128.89	124.81
23	c	505	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	c	510	CLA	CHD-C4C-NC	3.14	129.15	124.20
34	B	622	HTG	C1-O5-C5	3.14	118.37	112.58
23	a	404	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	b	614	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	b	614	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
23	C	509	CLA	O2A-CGA-O1A	-3.14	115.68	123.59
23	B	611	CLA	C1-C2-C3	-3.13	120.62	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	620	LMG	O7-C10-C11	3.13	118.25	111.50
23	C	509	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
23	D	405	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
23	c	505	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
23	a	404	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
31	e	101	LHG	O7-C7-C8	3.13	118.25	111.50
25	c	515	BCR	C15-C14-C13	-3.13	122.84	127.31
26	a	410	SQD	O47-C7-O49	-3.13	116.14	123.70
35	D	403	LMT	O1B-C4'-C3'	3.13	115.60	107.28
23	c	508	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	b	603	CLA	O2A-CGA-CBA	3.13	121.72	111.91
23	D	404	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	c	513	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
23	c	506	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
23	b	606	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	a	404	CLA	C1-C2-C3	-3.12	120.65	126.04
23	c	511	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
23	c	502	CLA	CMB-C2B-C1B	3.12	130.12	125.37
23	c	510	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
23	c	512	CLA	C3B-C4B-NB	3.12	113.41	110.52
23	B	608	CLA	O2A-CGA-CBA	3.11	121.68	111.91
23	b	611	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
23	b	616	CLA	O2A-CGA-CBA	3.11	121.68	111.91
23	c	511	CLA	CHD-C4C-NC	3.11	129.11	124.20
23	A	408	CLA	CAA-C2A-C3A	-3.11	104.25	112.78
29	d	406	PL9	C40-C39-C41	3.11	120.50	115.27
33	C	520	LMG	O7-C10-C11	3.11	118.20	111.50
23	b	604	CLA	O2A-CGA-CBA	3.11	121.67	111.91
23	b	608	CLA	C1-C2-C3	-3.11	120.67	126.04
23	c	507	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	B	611	CLA	CMC-C2C-C1C	3.11	129.77	125.04
23	B	601	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
26	B	620	SQD	O48-C23-C24	3.10	121.65	111.91
23	b	611	CLA	CAC-C3C-C4C	3.10	128.84	124.81
23	b	611	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
23	C	512	CLA	C1-C2-C3	-3.10	120.68	126.04
23	B	605	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	a	408	CLA	CAC-C3C-C4C	3.10	128.83	124.81
26	a	410	SQD	C44-O6-C1	-3.10	107.69	113.74
23	D	404	CLA	CHC-C1C-C2C	-3.10	118.13	126.73
23	C	505	CLA	CMC-C2C-C1C	3.10	129.75	125.04
25	B	618	BCR	C3-C4-C5	-3.10	108.55	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
23	B	603	CLA	CHC-C1C-C2C	-3.09	118.14	126.73
25	k	101	BCR	C15-C14-C13	-3.09	122.90	127.31
23	c	503	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	b	607	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	D	404	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
23	B	606	CLA	C4-C3-C5	3.09	120.46	115.27
25	T	101	BCR	C11-C10-C9	-3.09	122.91	127.31
25	A	409	BCR	C37-C22-C21	-3.08	118.60	122.92
23	c	510	CLA	C3C-C4C-NC	3.08	114.03	110.57
23	b	612	CLA	O2A-CGA-CBA	3.08	121.58	111.91
23	B	612	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
23	C	506	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
29	D	407	PL9	C12-C13-C14	-3.08	120.24	127.66
23	C	511	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
23	B	616	CLA	CHD-C4C-NC	3.08	129.05	124.20
23	B	602	CLA	CMB-C2B-C1B	3.08	130.06	125.37
33	b	620	LMG	O8-C28-C29	3.08	121.56	111.91
23	b	606	CLA	C3B-C4B-NB	3.08	113.37	110.52
23	B	611	CLA	CHD-C4C-NC	3.07	129.05	124.20
23	d	401	CLA	C1-C2-C3	-3.07	120.73	126.04
24	A	407	PHO	C4D-CHA-CBD	3.07	109.91	108.52
25	C	516	BCR	C15-C14-C13	-3.07	122.92	127.31
23	B	612	CLA	C3B-C4B-NB	3.07	113.36	110.52
34	B	624	HTG	O5-C1-C2	3.07	114.17	110.31
23	c	507	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	C	505	CLA	CHB-C1B-NB	-3.06	121.02	124.26
23	B	616	CLA	CMB-C2B-C1B	3.06	130.03	125.37
25	C	516	BCR	C33-C5-C6	-3.06	121.09	124.53
23	d	404	CLA	CHD-C4C-NC	3.06	129.02	124.20
23	c	511	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	b	605	CLA	CHD-C4C-NC	3.05	129.02	124.20
23	d	401	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
23	b	616	CLA	C4-C3-C5	3.05	120.41	115.27
23	d	404	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	C	510	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	b	612	CLA	CAC-C3C-C4C	3.05	128.77	124.81
26	a	412	SQD	O7-S-C6	3.05	110.56	106.94
40	v	201	HEC	CHD-C1D-ND	3.04	128.12	124.37
23	B	615	CLA	CHD-C4C-NC	3.04	128.99	124.20
29	D	407	PL9	C22-C23-C24	-3.04	120.35	127.66
23	C	512	CLA	C4C-C3C-C2C	-3.04	102.47	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	C3B-C4B-NB	3.04	113.33	110.52
23	B	604	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
25	b	619	BCR	C15-C14-C13	-3.03	122.98	127.31
26	A	410	SQD	O48-C23-C24	3.03	121.42	111.91
23	B	609	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	C	511	CLA	O2A-CGA-CBA	3.03	121.40	111.91
23	a	408	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	c	511	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
25	a	409	BCR	C11-C10-C9	-3.02	122.99	127.31
26	L	101	SQD	C3-C4-C5	3.02	115.63	110.24
23	b	616	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	b	606	CLA	CHD-C4C-NC	3.02	128.97	124.20
23	B	613	CLA	O2A-CGA-CBA	3.02	121.39	111.91
25	Y	101	BCR	C16-C17-C18	-3.02	123.00	127.31
23	b	604	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	B	614	CLA	CBC-CAC-C3C	-3.02	104.10	112.43
23	c	506	CLA	CAC-C3C-C4C	3.02	128.73	124.81
23	b	605	CLA	O2A-CGA-O1A	-3.02	115.98	123.59
33	b	620	LMG	C7-O1-C1	-3.01	107.85	113.74
23	B	609	CLA	O2A-CGA-CBA	3.01	121.36	111.91
26	D	413	SQD	C44-O6-C1	-3.01	107.85	113.74
26	a	412	SQD	O9-S-C6	3.01	110.52	106.94
40	v	201	HEC	CBC-CAC-C3C	3.01	120.73	112.43
23	a	405	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
23	b	607	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
25	D	406	BCR	C16-C17-C18	-3.01	123.02	127.31
23	c	513	CLA	C4-C3-C5	3.01	120.33	115.27
23	b	607	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
23	B	605	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
23	b	601	CLA	C4-C3-C5	3.01	120.33	115.27
23	a	408	CLA	O2A-CGA-CBA	3.00	121.34	111.91
25	H	101	BCR	C3-C4-C5	-3.00	108.72	114.08
23	b	602	CLA	CMC-C2C-C1C	3.00	129.61	125.04
23	c	505	CLA	CAC-C3C-C4C	3.00	128.70	124.81
33	C	520	LMG	O8-C28-C29	3.00	121.32	111.91
23	b	605	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
23	b	603	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
33	B	621	LMG	O8-C28-C29	2.99	121.29	111.91
23	c	501	CLA	C1-C2-C3	-2.99	120.87	126.04
23	b	602	CLA	C3B-C4B-NB	2.99	113.29	110.52
23	b	607	CLA	C1-O2A-CGA	2.99	124.28	116.44
23	c	501	CLA	C4C-C3C-C2C	-2.99	102.55	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	C3B-C4B-NB	2.99	113.28	110.52
23	C	514	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	b	603	CLA	CHD-C4C-NC	2.98	128.91	124.20
23	a	408	CLA	O2A-CGA-O1A	-2.98	116.06	123.59
23	c	512	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	D	405	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	C	504	CLA	C3B-C4B-NB	2.98	113.28	110.52
23	C	507	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
23	B	601	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
23	b	612	CLA	C3B-C4B-NB	2.98	113.28	110.52
26	a	412	SQD	O48-C23-C24	2.98	121.26	111.91
31	E	101	LHG	O8-C23-C24	2.98	121.25	111.91
31	l	101	LHG	O8-C23-C24	2.98	121.25	111.91
23	c	506	CLA	C4-C3-C5	2.98	120.28	115.27
23	c	503	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
23	c	506	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
23	c	504	CLA	CMB-C2B-C1B	2.97	129.90	125.37
23	b	603	CLA	C3B-C4B-NB	2.97	113.27	110.52
23	A	406	CLA	O2A-CGA-CBA	2.97	121.24	111.91
23	B	614	CLA	O2A-CGA-CBA	2.97	121.23	111.91
26	B	620	SQD	C3-C4-C5	2.97	115.54	110.24
23	b	615	CLA	C4-C3-C5	2.97	120.27	115.27
23	C	511	CLA	CMB-C2B-C1B	2.97	129.89	125.37
23	c	513	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	A	404	CLA	CHC-C1C-C2C	-2.97	118.48	126.73
23	C	514	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
26	A	412	SQD	O47-C7-C8	2.97	117.90	111.50
23	c	501	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
24	a	407	PHO	CMA-C3A-C4A	-2.97	107.88	114.38
23	b	601	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	b	613	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	c	502	CLA	O2A-CGA-CBA	2.96	121.20	111.91
23	b	607	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
29	a	414	PL9	C20-C19-C21	2.96	120.25	115.27
23	C	504	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	a	406	PHO	CMA-C3A-C4A	-2.96	107.90	114.38
23	b	613	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
25	B	619	BCR	C37-C22-C21	-2.96	118.78	122.92
23	b	614	CLA	O2A-CGA-CBA	2.96	121.18	111.91
23	c	512	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
24	D	401	PHO	O1D-CGD-CBD	-2.95	119.82	124.74
33	c	520	LMG	O8-C28-C29	2.95	121.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	CAC-C3C-C4C	2.95	128.64	124.81
26	a	412	SQD	C1-O5-C5	2.95	119.48	113.69
24	a	407	PHO	C1A-C2A-C3A	-2.95	100.03	102.84
23	C	512	CLA	CHD-C4C-NC	2.95	128.85	124.20
29	A	414	PL9	C10-C9-C11	2.95	120.23	115.27
23	a	408	CLA	CMB-C2B-C1B	2.95	129.86	125.37
25	t	101	BCR	C35-C13-C12	2.95	122.72	118.08
23	d	403	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
23	B	601	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
25	A	409	BCR	C38-C26-C25	-2.94	121.22	124.53
23	B	612	CLA	CAC-C3C-C4C	2.94	128.63	124.81
25	A	409	BCR	C11-C10-C9	-2.94	123.11	127.31
23	B	614	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	b	616	CLA	CAC-C3C-C4C	2.94	128.63	124.81
23	d	404	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
23	B	601	CLA	CHD-C4C-NC	2.94	128.83	124.20
23	C	510	CLA	C3B-C4B-NB	2.94	113.24	110.52
34	B	622	HTG	C1'-S1-C1	2.94	105.58	100.09
25	c	514	BCR	C24-C23-C22	-2.94	121.80	126.23
23	C	513	CLA	O2A-CGA-CBA	2.94	121.12	111.91
25	d	405	BCR	C37-C22-C23	2.94	122.70	118.08
26	L	101	SQD	O48-C23-C24	2.94	121.12	111.91
25	B	618	BCR	C38-C26-C25	-2.94	121.23	124.53
31	d	409	LHG	O8-C23-C24	2.93	121.12	111.91
23	b	611	CLA	O2A-CGA-CBA	2.93	121.11	111.91
23	B	616	CLA	C3B-C4B-NB	2.93	113.24	110.52
23	B	615	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	B	606	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	D	404	CLA	O2A-CGA-O1A	-2.93	116.21	123.59
23	B	602	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	b	610	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	C	507	CLA	C3B-C4B-NB	2.92	113.22	110.52
23	c	505	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	B	601	CLA	O2A-CGA-CBA	2.92	121.06	111.91
25	t	101	BCR	C19-C18-C17	-2.92	114.47	118.94
23	C	506	CLA	CMB-C2B-C1B	2.91	129.81	125.37
23	C	511	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
31	D	408	LHG	O7-C7-C8	2.91	117.78	111.50
23	C	513	CLA	CBC-CAC-C3C	-2.91	104.40	112.43
23	B	615	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
23	c	513	CLA	C3B-C4B-NB	2.91	113.21	110.52
23	a	404	CLA	C4-C3-C5	2.91	120.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	CHD-C4C-NC	2.91	128.79	124.20
26	L	101	SQD	C44-O6-C1	-2.91	108.06	113.74
23	c	503	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	d	406	PL9	C35-C34-C36	2.91	120.16	115.27
29	D	407	PL9	C7-C8-C9	-2.91	121.95	126.79
33	z	101	LMG	O8-C28-C29	2.91	121.03	111.91
23	C	514	CLA	CAC-C3C-C4C	2.90	128.58	124.81
23	B	615	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	B	619	BCR	C24-C23-C22	-2.90	121.85	126.23
35	I	101	LMT	O1B-C4'-C3'	2.90	115.00	107.28
25	K	102	BCR	C3-C4-C5	-2.90	108.90	114.08
23	B	609	CLA	C1-C2-C3	-2.90	121.03	126.04
23	a	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	B	604	CLA	CMC-C2C-C1C	2.90	129.45	125.04
36	h	102	DGD	O1G-C1A-C2A	2.90	121.00	111.91
36	C	519	DGD	O1G-C1A-C2A	2.90	121.00	111.91
25	c	514	BCR	C38-C26-C25	-2.90	121.28	124.53
24	D	401	PHO	CMB-C2B-C3B	2.90	130.09	124.68
29	D	407	PL9	C40-C39-C41	2.90	120.14	115.27
23	b	602	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	b	614	CLA	CMC-C2C-C1C	2.89	129.45	125.04
25	c	515	BCR	C2-C1-C6	2.89	114.94	110.48
36	h	102	DGD	O2G-C1B-C2B	2.89	117.73	111.50
23	d	404	CLA	CMB-C2B-C1B	2.89	129.77	125.37
23	A	406	CLA	CHD-C4C-NC	2.89	128.75	124.20
23	C	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	C	513	CLA	CHD-C4C-NC	2.88	128.75	124.20
23	C	511	CLA	C3B-C4B-NB	2.88	113.19	110.52
36	c	516	DGD	C2G-O2G-C1B	-2.88	110.69	117.79
23	b	613	CLA	C4-C3-C5	2.88	120.12	115.27
23	c	505	CLA	C3B-C4B-NB	2.87	113.18	110.52
33	J	101	LMG	O8-C28-C29	2.87	120.93	111.91
23	c	504	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	C	514	CLA	CHD-C4C-NC	2.87	128.73	124.20
25	c	514	BCR	C34-C9-C10	-2.87	118.90	122.92
23	C	506	CLA	CAC-C3C-C4C	2.87	128.54	124.81
31	A	417	LHG	O8-C23-C24	2.87	120.92	111.91
23	b	608	CLA	C3B-C4B-NB	2.87	113.18	110.52
25	t	101	BCR	C7-C6-C5	-2.87	114.52	121.46
23	C	514	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	A	407	PHO	CMB-C2B-C3B	2.86	130.04	124.68
23	b	615	CLA	C4C-C3C-C2C	-2.86	102.72	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	V	202	HEC	CHD-C1D-ND	2.86	127.90	124.37
23	A	406	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
23	d	403	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
31	d	409	LHG	O8-C23-O10	-2.86	116.37	123.59
25	Y	101	BCR	C16-C15-C14	-2.86	117.61	123.47
24	a	406	PHO	O2A-CGA-CBA	2.86	120.88	111.91
23	B	614	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
23	b	603	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
29	D	407	PL9	C10-C9-C11	2.86	120.08	115.27
23	b	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	c	507	CLA	CAC-C3C-C4C	2.86	128.51	124.81
29	d	406	PL9	C22-C23-C24	-2.85	120.79	127.66
23	C	511	CLA	CAC-C3C-C4C	2.85	128.51	124.81
29	A	414	PL9	C42-C43-C44	-2.85	120.79	127.66
25	c	515	BCR	C16-C17-C18	-2.85	123.24	127.31
25	t	101	BCR	C7-C8-C9	-2.85	121.93	126.23
23	A	404	CLA	CAA-CBA-CGA	-2.85	104.93	113.25
23	C	513	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	c	506	CLA	CGD-CBD-CAD	-2.85	101.51	110.73
23	c	501	CLA	C4-C3-C5	2.85	120.06	115.27
23	B	610	CLA	CHC-C1C-C2C	-2.85	118.83	126.73
33	j	101	LMG	C8-O7-C10	-2.84	110.79	117.79
34	b	625	HTG	O5-C5-C4	2.84	114.86	109.69
23	D	405	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
25	y	101	BCR	C21-C20-C19	-2.84	114.35	123.22
23	C	514	CLA	CMC-C2C-C1C	2.84	129.37	125.04
23	C	510	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	C	513	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
23	b	609	CLA	CMC-C2C-C1C	2.84	129.36	125.04
23	B	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
26	A	410	SQD	O9-S-C6	2.84	110.31	106.94
23	B	603	CLA	CAC-C3C-C4C	2.84	128.49	124.81
25	a	409	BCR	C15-C14-C13	-2.84	123.26	127.31
23	B	605	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
23	C	508	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
23	b	601	CLA	CHD-C4C-NC	2.84	128.67	124.20
34	C	521	HTG	O5-C1-C2	2.84	113.88	110.31
25	Y	101	BCR	C38-C26-C25	-2.83	121.34	124.53
23	A	405	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
40	V	202	HEC	CBB-CAB-C3B	2.83	120.24	112.43
23	b	611	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
23	b	614	CLA	O2A-CGA-O1A	-2.83	116.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	405	CLA	C3B-C4B-NB	2.83	113.14	110.52
23	B	613	CLA	O2D-CGD-CBD	2.83	116.29	111.27
31	d	408	LHG	O7-C7-C8	2.83	117.59	111.50
24	a	406	PHO	CMB-C2B-C3B	2.83	129.97	124.68
23	b	614	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
23	b	608	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
23	A	404	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
23	C	504	CLA	CMB-C2B-C1B	2.82	129.67	125.37
25	y	101	BCR	C15-C14-C13	-2.82	123.29	127.31
23	c	503	CLA	O2A-CGA-CBA	2.82	120.75	111.91
23	C	508	CLA	C4-C3-C5	2.82	120.01	115.27
23	b	609	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
26	D	413	SQD	C3-C4-C5	2.81	115.26	110.24
23	b	615	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	b	602	CLA	O2A-CGA-CBA	2.81	120.73	111.91
24	a	406	PHO	C4A-C3A-C2A	-2.81	100.17	102.84
23	b	610	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
33	C	501	LMG	C7-O1-C1	-2.81	108.26	113.74
25	a	409	BCR	C20-C21-C22	-2.80	123.31	127.31
23	c	503	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	C	505	CLA	C1-O2A-CGA	2.80	123.80	116.44
23	B	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	c	502	CLA	C1-C2-C3	-2.80	121.19	126.04
23	B	602	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	c	510	CLA	CMC-C2C-C1C	2.80	129.31	125.04
25	B	617	BCR	C38-C26-C25	-2.80	121.38	124.53
23	B	603	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	b	603	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
24	a	407	PHO	CMB-C2B-C3B	2.80	129.92	124.68
23	B	604	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
23	B	616	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	B	613	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
25	b	618	BCR	C38-C26-C25	-2.80	121.39	124.53
23	a	408	CLA	CMA-C3A-C2A	-2.80	102.55	113.83
29	D	407	PL9	C7-C3-C4	2.79	119.15	116.88
35	D	402	LMT	O1'-C1'-C2'	2.79	112.66	108.30
23	B	610	CLA	C3B-C4B-NB	2.79	113.11	110.52
23	c	509	CLA	C1-O2A-CGA	2.79	123.77	116.44
23	B	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	c	509	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	t	101	BCR	C1-C6-C7	2.79	123.67	115.78
23	b	611	CLA	CBC-CAC-C3C	-2.79	104.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	620	LMG	O6-C5-C4	2.79	114.76	109.69
23	c	511	CLA	CMB-C2B-C1B	2.79	129.62	125.37
23	D	404	CLA	CMC-C2C-C1C	2.79	129.28	125.04
23	c	509	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	b	613	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
23	B	604	CLA	C4-C3-C5	2.78	119.95	115.27
23	c	503	CLA	C4-C3-C5	2.78	119.95	115.27
23	C	503	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
23	C	512	CLA	CMB-C2B-C1B	2.78	129.61	125.37
23	C	507	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	a	405	CLA	CMB-C2B-C1B	2.78	129.60	125.37
23	c	501	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
23	B	607	CLA	C3B-C4B-NB	2.78	113.09	110.52
34	B	622	HTG	O5-C1-C2	2.78	113.81	110.31
25	B	619	BCR	C15-C14-C13	-2.78	123.34	127.31
23	B	612	CLA	C4-C3-C5	2.78	119.95	115.27
26	D	413	SQD	O47-C7-O49	-2.78	116.99	123.70
29	d	406	PL9	C51-C49-C50	2.78	120.74	114.60
25	d	405	BCR	C40-C30-C25	-2.78	105.79	110.30
23	D	404	CLA	CMB-C2B-C1B	2.77	129.59	125.37
23	B	612	CLA	CMC-C2C-C1C	2.77	129.26	125.04
23	b	613	CLA	CHD-C4C-NC	2.77	128.57	124.20
31	D	409	LHG	O8-C23-C24	2.77	120.61	111.91
25	B	619	BCR	C38-C26-C25	-2.77	121.42	124.53
23	b	602	CLA	CAC-C3C-C4C	2.77	128.40	124.81
23	B	605	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
23	C	503	CLA	C3B-C4B-NB	2.77	113.08	110.52
23	B	614	CLA	C4-C3-C5	2.77	119.92	115.27
23	b	606	CLA	CHC-C1C-C2C	-2.77	119.05	126.73
23	c	511	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	C	502	CLA	CHD-C4C-NC	2.76	128.56	124.20
23	b	610	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
25	d	405	BCR	C16-C15-C14	-2.76	117.81	123.47
23	C	505	CLA	CHC-C1C-C2C	-2.76	119.06	126.73
25	b	619	BCR	C24-C23-C22	-2.76	122.06	126.23
23	B	615	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
33	c	519	LMG	O8-C28-C29	2.76	120.56	111.91
25	c	515	BCR	C21-C20-C19	-2.76	114.61	123.22
23	A	405	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
23	c	511	CLA	CAA-CBA-CGA	-2.76	105.20	113.25
23	A	405	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
23	B	607	CLA	C4C-C3C-C2C	-2.75	102.88	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	413	SQD	C1-C2-C3	-2.75	104.26	110.00
25	k	101	BCR	C3-C4-C5	-2.75	109.16	114.08
40	v	201	HEC	C4A-NA-C1A	2.75	108.05	105.35
23	c	507	CLA	CHC-C1C-C2C	-2.75	119.08	126.73
23	A	406	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
23	C	513	CLA	C4-C3-C5	2.75	119.90	115.27
23	c	512	CLA	C4-C3-C5	2.75	119.90	115.27
23	b	614	CLA	CMB-C2B-C1B	2.75	129.56	125.37
23	c	504	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
36	C	518	DGD	O1G-C1A-C2A	2.75	120.54	111.91
23	c	511	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
23	A	408	CLA	CMA-C3A-C2A	-2.75	102.74	113.83
23	c	507	CLA	C1-C2-C3	-2.75	121.29	126.04
34	b	628	HTG	O5-C5-C4	2.75	114.69	109.69
23	c	512	CLA	CBA-CAA-C2A	-2.75	105.76	113.86
25	C	515	BCR	C23-C24-C25	-2.75	119.49	127.20
23	C	511	CLA	CHD-C4C-NC	2.75	128.53	124.20
23	b	615	CLA	C11-C12-C13	-2.75	107.04	115.92
23	c	505	CLA	CHD-C4C-NC	2.75	128.53	124.20
25	B	617	BCR	C11-C10-C9	-2.74	123.39	127.31
23	A	404	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
23	B	613	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
34	c	522	HTG	O5-C1-C2	2.74	113.77	110.31
24	a	406	PHO	C1-C2-C3	-2.74	121.30	126.04
25	b	617	BCR	C15-C14-C13	-2.74	123.40	127.31
23	c	512	CLA	O2A-CGA-CBA	2.74	120.51	111.91
33	Z	102	LMG	O6-C5-C4	2.74	114.67	109.69
23	C	507	CLA	O2A-CGA-CBA	2.74	120.51	111.91
23	C	506	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	b	601	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
23	c	503	CLA	C1-C2-C3	-2.74	121.31	126.04
23	B	611	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
23	a	408	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
23	b	602	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	c	512	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	c	509	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
25	k	101	BCR	C2-C1-C6	2.73	114.69	110.48
23	C	506	CLA	C3B-C4B-NB	2.73	113.05	110.52
25	D	406	BCR	C33-C5-C6	-2.73	121.46	124.53
23	a	404	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
23	B	604	CLA	CMB-C2B-C1B	2.73	129.53	125.37
25	a	409	BCR	C37-C22-C21	-2.73	119.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	CHD-C4C-NC	2.73	128.50	124.20
23	b	612	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
36	c	516	DGD	O3G-C3G-C2G	-2.73	104.32	110.90
23	D	404	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	B	608	CLA	C4-C3-C5	2.72	119.85	115.27
25	A	409	BCR	C20-C21-C22	-2.72	123.42	127.31
23	c	512	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	a	405	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	b	604	CLA	CAC-C3C-C4C	2.72	128.34	124.81
23	D	404	CLA	C4-C3-C5	2.72	119.85	115.27
23	C	503	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	c	502	CLA	CHD-C4C-NC	2.72	128.49	124.20
29	a	414	PL9	C35-C34-C36	2.72	119.84	115.27
23	B	610	CLA	CMB-C2B-C1B	2.72	129.51	125.37
23	A	408	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	B	607	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
23	D	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
23	B	608	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
24	D	401	PHO	CMA-C3A-C4A	-2.71	108.43	114.38
23	C	505	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	d	403	CLA	C4-C3-C5	2.71	119.83	115.27
23	a	405	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
23	C	506	CLA	O2A-CGA-CBA	2.71	120.42	111.91
23	B	609	CLA	C3B-C4B-NB	2.71	113.03	110.52
23	B	613	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
23	c	504	CLA	CHD-C4C-NC	2.71	128.47	124.20
35	B	630	LMT	O5'-C5'-C4'	2.71	115.46	109.75
23	C	514	CLA	C3B-C4B-NB	2.71	113.03	110.52
23	C	508	CLA	CAC-C3C-C4C	2.71	128.32	124.81
23	b	607	CLA	C4-C3-C5	2.71	119.83	115.27
23	B	611	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
36	C	519	DGD	O2G-C1B-C2B	2.71	117.33	111.50
23	c	508	CLA	CHC-C1C-C2C	-2.71	119.22	126.73
23	c	504	CLA	CED-O2D-CGD	2.70	122.06	115.94
23	c	507	CLA	C4-C3-C5	2.70	119.82	115.27
23	A	408	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
29	A	414	PL9	C12-C13-C14	-2.70	121.16	127.66
23	c	506	CLA	CHD-C4C-NC	2.70	128.46	124.20
29	D	407	PL9	C27-C28-C29	-2.70	121.16	127.66
23	c	513	CLA	O2A-CGA-CBA	2.70	120.38	111.91
23	d	404	CLA	O2A-CGA-CBA	2.70	120.37	111.91
23	C	514	CLA	C4-C3-C5	2.70	119.81	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	B	616	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
24	a	406	PHO	O2D-CGD-O1D	-2.70	118.56	123.84
23	C	502	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	b	602	CLA	C11-C10-C8	-2.70	107.21	115.92
23	B	612	CLA	O2A-CGA-CBA	2.70	120.37	111.91
23	c	507	CLA	C6-C7-C8	-2.70	107.21	115.92
23	c	504	CLA	O2A-CGA-CBA	2.69	120.36	111.91
23	b	612	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
25	c	515	BCR	C33-C5-C6	-2.69	121.50	124.53
25	k	101	BCR	C20-C21-C22	-2.69	123.47	127.31
35	D	403	LMT	C4B-C3B-C2B	2.69	115.52	110.82
23	B	608	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
23	b	605	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	c	506	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	B	607	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
23	b	613	CLA	C1-C2-C3	-2.69	121.39	126.04
23	A	406	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	b	602	CLA	CHC-C1C-C2C	-2.68	119.27	126.73
29	a	414	PL9	C25-C24-C26	2.68	119.78	115.27
23	B	604	CLA	O2A-CGA-CBA	2.68	120.31	111.91
23	b	603	CLA	CMC-C2C-C1C	2.68	129.12	125.04
25	C	515	BCR	C7-C8-C9	-2.68	122.19	126.23
23	C	512	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
23	c	510	CLA	CMB-C2B-C1B	2.68	129.44	125.37
29	D	407	PL9	C36-C37-C38	-2.67	103.10	111.88
23	B	606	CLA	CMB-C2B-C1B	2.67	129.44	125.37
23	C	511	CLA	C4-C3-C5	2.67	119.77	115.27
23	c	506	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	c	501	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	C	512	CLA	O2A-CGA-CBA	2.67	120.29	111.91
25	A	409	BCR	C8-C7-C6	-2.67	119.70	127.20
23	c	510	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	a	407	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
31	D	409	LHG	O8-C23-O10	-2.67	116.87	123.59
23	B	603	CLA	CBC-CAC-C3C	-2.66	105.08	112.43
33	b	620	LMG	C1-C2-C3	-2.66	104.45	110.00
23	D	405	CLA	C4-C3-C5	2.66	119.75	115.27
23	c	504	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
23	C	513	CLA	CBA-CAA-C2A	-2.66	106.00	113.86
23	b	604	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
25	b	617	BCR	C20-C21-C22	-2.66	123.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C1-C2-C3	-2.66	121.44	126.04
23	c	508	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	c	508	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	C	504	CLA	O2A-CGA-CBA	2.66	120.25	111.91
34	C	521	HTG	C1-O5-C5	2.66	117.48	112.58
23	b	616	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	b	602	CLA	C11-C12-C13	-2.66	107.33	115.92
23	b	605	CLA	CED-O2D-CGD	2.66	121.94	115.94
23	A	404	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
29	A	414	PL9	C25-C24-C26	2.66	119.74	115.27
29	D	407	PL9	C20-C19-C21	2.66	119.74	115.27
23	B	602	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	d	405	BCR	C39-C30-C25	-2.65	106.00	110.30
23	B	610	CLA	CAC-C3C-C4C	2.65	128.25	124.81
24	D	401	PHO	C4-C3-C5	2.65	119.73	115.27
36	h	102	DGD	C3G-O3G-C1D	-2.65	108.56	113.74
25	a	409	BCR	C32-C1-C6	-2.65	106.00	110.30
23	A	404	CLA	CMC-C2C-C1C	2.65	129.07	125.04
25	K	102	BCR	C15-C14-C13	-2.65	123.53	127.31
23	C	504	CLA	C1-C2-C3	-2.65	121.47	126.04
23	b	610	CLA	CHC-C1C-C2C	-2.65	119.38	126.73
23	b	608	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	c	511	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
29	A	414	PL9	C35-C34-C36	2.64	119.72	115.27
23	b	614	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
23	d	401	CLA	C4-C3-C5	2.64	119.72	115.27
23	B	616	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	e	101	LHG	O8-C23-C24	2.64	120.20	111.91
23	a	405	CLA	C1-C2-C3	-2.64	121.47	126.04
23	B	609	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
35	D	403	LMT	O5'-C5'-C4'	2.64	115.32	109.75
29	d	406	PL9	C31-C32-C33	-2.64	103.21	111.88
31	E	101	LHG	C5-O7-C7	-2.64	111.30	117.79
23	C	513	CLA	CMB-C2B-C1B	2.64	129.39	125.37
23	c	503	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
25	A	409	BCR	C16-C17-C18	-2.64	123.55	127.31
25	a	409	BCR	C37-C22-C23	2.64	122.23	118.08
29	A	414	PL9	C17-C18-C19	-2.63	121.32	127.66
31	D	408	LHG	O8-C23-O10	-2.63	116.95	123.59
23	c	511	CLA	CMC-C2C-C1C	2.63	129.05	125.04
25	B	618	BCR	C37-C22-C23	2.63	122.22	118.08
23	b	603	CLA	C2A-C1A-CHA	-2.63	119.26	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	619	BCR	C10-C11-C12	-2.63	115.01	123.22
23	B	606	CLA	C3B-C4B-NB	2.63	112.95	110.52
23	c	508	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	d	404	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	C	505	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
23	B	605	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	A	408	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
23	C	505	CLA	CHD-C4C-NC	2.63	128.34	124.20
23	c	503	CLA	C3B-C4B-NB	2.63	112.95	110.52
29	D	407	PL9	C51-C49-C50	2.63	120.40	114.60
23	b	604	CLA	C3B-C4B-NB	2.63	112.95	110.52
26	f	101	SQD	O48-C23-C24	2.63	120.15	111.91
23	C	503	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	C	513	CLA	C3B-C4B-NB	2.62	112.95	110.52
33	Z	101	LMG	O8-C28-C29	2.62	120.14	111.91
23	B	607	CLA	CHD-C4C-NC	2.62	128.34	124.20
23	d	403	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	C	509	CLA	O2A-CGA-CBA	2.62	120.14	111.91
25	c	515	BCR	C3-C4-C5	-2.62	109.40	114.08
23	c	507	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	A	412	SQD	O48-C23-O10	-2.62	116.98	123.59
23	b	609	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	B	609	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	b	611	CLA	CHD-C4C-NC	2.62	128.32	124.20
23	b	612	CLA	CHD-C4C-NC	2.62	128.32	124.20
25	K	102	BCR	C2-C1-C6	2.61	114.50	110.48
25	c	514	BCR	C28-C27-C26	-2.61	109.41	114.08
23	b	604	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
25	D	406	BCR	C40-C30-C25	-2.61	106.06	110.30
23	b	612	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	B	604	CLA	CHD-C4C-NC	2.61	128.32	124.20
23	b	603	CLA	C4-C3-C5	2.61	119.67	115.27
25	d	405	BCR	C21-C20-C19	-2.61	115.08	123.22
23	A	408	CLA	CMB-C2B-C1B	2.61	129.34	125.37
23	B	608	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
25	B	619	BCR	C21-C20-C19	-2.61	115.08	123.22
23	B	614	CLA	C1-C2-C3	-2.61	121.53	126.04
23	d	404	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
23	a	404	CLA	CHB-C4A-NA	2.61	128.12	124.51
29	A	414	PL9	C53-C6-C1	2.61	120.32	114.99
25	D	406	BCR	C29-C30-C25	2.60	114.49	110.48
23	C	506	CLA	C1-C2-C3	-2.60	121.54	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	O2A-CGA-CBA	2.60	120.08	111.91
23	b	609	CLA	CHD-C4C-NC	2.60	128.31	124.20
29	a	414	PL9	C53-C6-C1	2.60	120.31	114.99
23	C	507	CLA	CMB-C2B-C1B	2.60	129.33	125.37
25	C	516	BCR	C15-C16-C17	-2.60	118.15	123.47
23	B	611	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	b	606	CLA	C1-C2-C3	-2.60	121.55	126.04
29	A	414	PL9	C40-C39-C41	2.60	119.64	115.27
23	C	503	CLA	C1-C2-C3	-2.60	121.55	126.04
23	B	615	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	C	506	CLA	C4-C3-C5	2.60	119.64	115.27
23	d	401	CLA	CMA-C3A-C2A	-2.60	103.36	113.83
23	B	602	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
35	M	101	LMT	C1-O1'-C1'	-2.59	109.54	113.84
23	d	403	CLA	CMB-C2B-C1B	2.59	129.32	125.37
23	b	614	CLA	CHD-C4C-NC	2.59	128.29	124.20
31	d	407	LHG	O8-C23-O10	-2.59	117.05	123.59
29	d	406	PL9	C15-C14-C16	2.59	119.63	115.27
23	b	601	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	c	511	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	b	608	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	D	405	CLA	CAC-C3C-C4C	2.59	128.17	124.81
25	b	618	BCR	C28-C27-C26	-2.59	109.45	114.08
23	b	601	CLA	C3B-C4B-NB	2.59	112.92	110.52
25	Y	101	BCR	C10-C11-C12	-2.59	115.14	123.22
23	d	401	CLA	CHB-C1B-NB	-2.59	121.52	124.26
23	d	401	CLA	C11-C12-C13	-2.59	107.56	115.92
23	B	604	CLA	C1-O2A-CGA	2.59	123.23	116.44
23	C	502	CLA	O2A-CGA-CBA	2.59	120.02	111.91
29	A	414	PL9	C45-C44-C46	2.58	119.62	115.27
33	b	620	LMG	C8-O7-C10	-2.58	111.43	117.79
23	b	602	CLA	C1-C2-C3	-2.58	121.57	126.04
25	D	406	BCR	C15-C14-C13	-2.58	123.62	127.31
23	b	615	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
25	B	617	BCR	C16-C17-C18	-2.58	123.63	127.31
25	D	406	BCR	C37-C22-C23	2.58	122.14	118.08
34	C	522	HTG	C3-C4-C5	2.58	114.84	110.24
23	C	511	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	C	507	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	A	406	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
25	t	101	BCR	C3-C4-C5	-2.57	109.48	114.08
23	B	607	CLA	C4-C3-C5	2.57	119.60	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
38	E	103	HEM	CHA-C4D-ND	2.57	127.55	124.37
23	C	509	CLA	C4-C3-C5	2.57	119.60	115.27
23	c	502	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	B	604	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
25	B	618	BCR	C28-C27-C26	-2.57	109.49	114.08
23	B	611	CLA	OBD-CAD-C3D	-2.57	122.34	128.52
36	C	519	DGD	O1G-C1A-O1A	-2.57	117.11	123.59
36	c	516	DGD	C6D-O5D-C1E	-2.57	108.72	113.74
23	d	404	CLA	CHC-C1C-C2C	-2.57	119.60	126.73
23	A	405	CLA	CMB-C2B-C1B	2.57	129.28	125.37
38	E	103	HEM	CBD-CAD-C3D	-2.57	105.50	112.63
26	a	412	SQD	O5-C5-C4	2.56	114.35	109.69
25	b	618	BCR	C24-C23-C22	-2.56	122.36	126.23
23	c	507	CLA	C3B-C4B-NB	2.56	112.89	110.52
25	b	619	BCR	C39-C30-C25	-2.56	106.14	110.30
25	h	101	BCR	C37-C22-C21	-2.56	119.33	122.92
23	B	601	CLA	CMB-C2B-C1B	2.56	129.27	125.37
26	A	410	SQD	C45-O47-C7	-2.56	111.49	117.79
25	k	101	BCR	C7-C8-C9	-2.56	122.37	126.23
23	b	601	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	h	101	BCR	C10-C11-C12	-2.56	115.24	123.22
25	b	619	BCR	C2-C1-C6	2.56	114.42	110.48
36	c	517	DGD	O1G-C1A-C2A	2.56	119.93	111.91
23	b	604	CLA	CHD-C4C-NC	2.56	128.23	124.20
23	C	504	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	A	407	PHO	C6-C5-C3	-2.55	106.76	113.45
23	c	506	CLA	CMB-C2B-C1B	2.55	129.25	125.37
23	b	601	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
38	E	103	HEM	C4D-ND-C1D	2.54	107.70	105.07
23	B	606	CLA	O2A-CGA-CBA	2.54	119.89	111.91
26	D	413	SQD	O8-S-C6	2.54	109.79	105.74
38	E	103	HEM	C4B-C3B-C2B	-2.54	105.10	107.11
23	c	506	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
23	C	507	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	b	608	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
23	c	509	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
24	A	407	PHO	O2D-CGD-O1D	-2.54	118.87	123.84
36	C	518	DGD	O1G-C1A-O1A	-2.54	117.18	123.59
25	b	618	BCR	C29-C30-C25	2.54	114.39	110.48
23	A	405	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	a	404	CLA	C2A-C1A-CHA	-2.54	119.42	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	619	BCR	C4-C5-C6	-2.54	119.05	122.73
23	d	403	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
23	A	406	CLA	C3B-C4B-NB	2.53	112.87	110.52
33	a	416	LMG	O6-C5-C4	2.53	114.29	109.69
25	B	617	BCR	C31-C1-C6	-2.53	106.20	110.30
25	B	618	BCR	C36-C18-C19	2.53	122.06	118.08
23	b	606	CLA	CAC-C3C-C4C	2.53	128.09	124.81
23	a	408	CLA	CMC-C2C-C1C	2.53	128.89	125.04
33	C	501	LMG	C9-C8-C7	-2.52	105.82	111.79
26	D	413	SQD	O48-C23-C24	2.52	119.83	111.91
23	b	610	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	B	612	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	b	613	CLA	CMC-C2C-C1C	2.52	128.88	125.04
25	C	516	BCR	C38-C26-C25	-2.52	121.70	124.53
23	C	506	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
23	C	508	CLA	O2A-CGA-CBA	2.52	119.81	111.91
23	c	513	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	C	506	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	b	604	CLA	C4-C3-C5	2.52	119.51	115.27
23	C	507	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
40	V	202	HEC	C3B-C4B-NB	-2.52	107.36	110.17
23	b	611	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
23	c	505	CLA	C1-C2-C3	-2.51	121.70	126.04
25	Y	101	BCR	C37-C22-C23	2.51	122.04	118.08
23	C	510	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	B	601	CLA	CAC-C3C-C4C	2.51	128.07	124.81
23	C	508	CLA	C1-C2-C3	-2.51	121.70	126.04
23	B	611	CLA	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407	PHO	O2A-CGA-CBA	2.51	119.78	111.91
31	d	407	LHG	O8-C23-C24	2.51	119.78	111.91
25	y	101	BCR	C24-C23-C22	-2.51	122.44	126.23
23	c	513	CLA	CHD-C4C-NC	2.51	128.15	124.20
25	T	101	BCR	C7-C6-C5	-2.51	115.39	121.46
23	B	607	CLA	CMC-C2C-C1C	2.51	128.85	125.04
25	y	101	BCR	C37-C22-C23	2.50	122.02	118.08
23	b	602	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	b	615	CLA	CAC-C3C-C4C	2.50	128.05	124.81
25	a	409	BCR	C15-C16-C17	-2.50	118.35	123.47
26	a	410	SQD	O48-C23-C24	2.50	119.75	111.91
25	K	102	BCR	C36-C18-C19	2.50	122.01	118.08
25	c	514	BCR	C33-C5-C6	-2.50	121.72	124.53
23	A	405	CLA	CAA-CBA-CGA	2.50	120.55	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
25	K	102	BCR	C33-C5-C6	-2.50	121.72	124.53
35	D	403	LMT	C1-O1'-C1'	-2.50	109.70	113.84
23	B	613	CLA	CHD-C4C-NC	2.50	128.14	124.20
25	d	405	BCR	C38-C26-C25	-2.49	121.73	124.53
23	B	610	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	B	602	CLA	CED-O2D-CGD	2.49	121.57	115.94
40	v	201	HEC	CBB-CAB-C3B	2.49	119.30	112.43
23	b	611	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	C	510	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	b	603	CLA	CHC-C1C-C2C	-2.49	119.81	126.73
23	C	511	CLA	CMC-C2C-C1C	2.49	128.83	125.04
23	B	610	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
23	B	613	CLA	CED-O2D-CGD	2.49	121.57	115.94
29	D	407	PL9	C37-C38-C39	-2.49	121.67	127.66
23	c	508	CLA	C4-C3-C5	2.49	119.45	115.27
23	B	615	CLA	CAC-C3C-C4C	2.49	128.04	124.81
23	B	603	CLA	CHD-C4C-NC	2.49	128.12	124.20
40	v	201	HEC	C3B-C4B-NB	-2.48	107.40	110.17
23	C	513	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
35	b	627	LMT	C1'-C2'-C3'	2.48	115.17	110.00
24	a	406	PHO	C1A-C2A-C3A	-2.48	100.48	102.84
23	c	505	CLA	CED-O2D-CGD	2.48	121.55	115.94
23	B	612	CLA	CHB-C1B-NB	-2.48	121.63	124.26
29	d	406	PL9	C37-C38-C39	-2.48	121.69	127.66
23	b	602	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
23	C	510	CLA	CHC-C1C-C2C	-2.48	119.85	126.73
26	A	410	SQD	O48-C23-O10	-2.48	117.34	123.59
23	B	608	CLA	CMB-C2B-C1B	2.47	129.14	125.37
25	A	409	BCR	C36-C18-C19	2.47	121.98	118.08
25	C	515	BCR	C11-C10-C9	-2.47	123.78	127.31
33	J	101	LMG	O8-C28-O10	-2.47	117.35	123.59
25	C	515	BCR	C20-C21-C22	-2.47	123.78	127.31
25	h	101	BCR	C16-C15-C14	-2.47	118.41	123.47
23	c	506	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
23	c	509	CLA	CMB-C2B-C1B	2.47	129.13	125.37
23	C	511	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
33	Z	102	LMG	C9-C8-C7	-2.47	105.95	111.79
23	B	608	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	C	514	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
23	b	614	CLA	CHB-C1B-NB	-2.47	121.64	124.26
23	c	508	CLA	C1-C2-C3	-2.47	121.77	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	501	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
29	d	406	PL9	C17-C18-C19	-2.47	121.72	127.66
23	B	607	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	b	616	CLA	C1-C2-C3	-2.47	121.78	126.04
23	a	404	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
25	y	101	BCR	C10-C11-C12	-2.46	115.53	123.22
23	C	505	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
23	c	503	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
36	C	518	DGD	C2G-O2G-C1B	-2.46	111.73	117.79
29	D	407	PL9	C15-C14-C16	2.46	119.41	115.27
23	D	405	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
23	C	513	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
23	B	606	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	H	101	BCR	C29-C30-C25	2.46	114.27	110.48
33	c	520	LMG	O8-C28-O10	-2.46	117.39	123.59
33	Z	102	LMG	C1-O6-C5	2.46	118.51	113.69
23	b	616	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
29	d	406	PL9	C12-C13-C14	-2.46	121.75	127.66
23	b	608	CLA	CBC-CAC-C3C	-2.45	105.66	112.43
23	b	604	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
23	C	506	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
23	B	606	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
29	d	406	PL9	C53-C6-C1	2.45	120.00	114.99
23	d	401	CLA	C1-O2A-CGA	2.45	122.87	116.44
23	B	601	CLA	C4-C3-C5	2.45	119.39	115.27
23	C	502	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
23	c	503	CLA	CAC-C3C-C4C	2.45	127.99	124.81
23	C	502	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
36	H	102	DGD	O1G-C1A-C2A	2.44	119.58	111.91
23	c	510	CLA	C4-C3-C2	-2.44	117.41	123.68
25	B	618	BCR	C36-C18-C17	-2.44	119.50	122.92
23	b	610	CLA	CHD-C4C-NC	2.44	128.05	124.20
23	a	408	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	C	516	BCR	C3-C4-C5	-2.44	109.72	114.08
23	c	505	CLA	C4-C3-C5	2.44	119.37	115.27
23	B	608	CLA	CMC-C2C-C1C	2.43	128.75	125.04
23	b	601	CLA	CMB-C2B-C1B	2.43	129.08	125.37
23	c	501	CLA	CHD-C4C-NC	2.43	128.04	124.20
25	B	619	BCR	C7-C8-C9	-2.43	122.56	126.23
23	A	405	CLA	CMA-C3A-C2A	-2.43	104.01	113.83
23	a	408	CLA	C4-C3-C5	2.43	119.36	115.27
24	D	401	PHO	O2D-CGD-O1D	-2.43	119.08	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	O2A-CGA-CBA	2.43	119.54	111.91
31	d	408	LHG	O8-C23-C24	2.43	119.54	111.91
23	b	606	CLA	CMB-C2B-C1B	2.43	129.07	125.37
23	b	613	CLA	CMB-C2B-C1B	2.43	129.07	125.37
23	A	405	CLA	CHC-C1C-C2C	-2.43	119.97	126.73
23	d	401	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
23	b	611	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	b	612	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
25	b	618	BCR	C37-C22-C21	-2.43	119.52	122.92
23	C	509	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	c	508	CLA	CHD-C4C-NC	2.43	128.03	124.20
25	b	617	BCR	C37-C22-C21	-2.43	119.52	122.92
23	B	614	CLA	CHB-C1B-NB	-2.43	121.69	124.26
23	b	606	CLA	CMC-C2C-C1C	2.43	128.73	125.04
25	b	617	BCR	C32-C1-C6	-2.43	106.36	110.30
23	C	509	CLA	CHB-C1B-NB	-2.43	121.69	124.26
23	C	502	CLA	C4-C3-C5	2.42	119.35	115.27
36	c	516	DGD	C3G-C2G-C1G	-2.42	106.06	111.79
23	a	405	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
40	V	202	HEC	CBA-CAA-C2A	-2.42	105.90	112.63
23	A	404	CLA	CED-O2D-CGD	2.42	121.42	115.94
23	B	615	CLA	C4-C3-C5	2.42	119.34	115.27
25	t	101	BCR	C37-C22-C21	-2.42	119.53	122.92
23	A	408	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	B	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
33	Z	102	LMG	O6-C1-C2	2.42	115.47	110.35
26	L	101	SQD	O8-S-C6	2.42	109.59	105.74
29	D	407	PL9	C42-C41-C39	-2.42	105.02	112.98
23	C	504	CLA	CHD-C4C-NC	2.42	128.01	124.20
23	b	616	CLA	CHC-C1C-C2C	-2.42	120.02	126.73
23	a	404	CLA	CHD-C4C-NC	2.42	128.01	124.20
23	b	606	CLA	O2A-CGA-CBA	2.42	119.49	111.91
23	c	504	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
25	d	405	BCR	C38-C26-C27	2.41	118.25	113.62
23	c	502	CLA	CAC-C3C-C4C	2.41	127.94	124.81
23	c	509	CLA	CMC-C2C-C1C	2.41	128.72	125.04
23	b	609	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
25	c	515	BCR	C37-C22-C23	2.41	121.88	118.08
29	a	414	PL9	C7-C8-C9	-2.41	122.78	126.79
40	V	202	HEC	C2A-C1A-NA	-2.41	107.98	110.32
26	f	101	SQD	O5-C5-C4	2.41	114.07	109.69
23	B	602	CLA	CBC-CAC-C3C	-2.41	105.78	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
23	B	616	CLA	CAC-C3C-C4C	2.41	127.94	124.81
23	A	405	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
23	C	508	CLA	CHD-C4C-NC	2.41	128.00	124.20
23	B	605	CLA	CHC-C1C-C2C	-2.41	120.05	126.73
23	b	601	CLA	CAC-C3C-C4C	2.41	127.93	124.81
23	C	503	CLA	CMC-C2C-C1C	2.41	128.70	125.04
23	B	602	CLA	CHD-C4C-NC	2.40	127.99	124.20
24	a	407	PHO	O1D-CGD-CBD	-2.40	120.73	124.74
29	a	414	PL9	C51-C49-C50	2.40	119.91	114.60
23	B	612	CLA	C11-C12-C13	-2.40	108.15	115.92
33	j	101	LMG	O8-C28-C29	2.40	119.45	111.91
23	B	616	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	B	610	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
38	E	103	HEM	CHD-C1D-ND	2.40	127.03	124.42
23	b	612	CLA	CMC-C2C-C1C	2.40	128.69	125.04
33	C	520	LMG	O8-C28-O10	-2.40	117.54	123.59
23	b	616	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
33	b	620	LMG	O8-C28-O10	-2.40	117.54	123.59
23	B	610	CLA	C4-C3-C5	2.40	119.30	115.27
23	d	403	CLA	CAC-C3C-C4C	2.39	127.92	124.81
23	B	601	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
35	D	403	LMT	O1B-C4'-C5'	-2.39	102.90	109.45
23	C	508	CLA	C3B-C4B-NB	2.39	112.73	110.52
23	d	403	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
25	C	516	BCR	C16-C17-C18	-2.39	123.90	127.31
26	a	410	SQD	O48-C23-O10	-2.39	117.56	123.59
23	c	501	CLA	C3B-C4B-NB	2.39	112.73	110.52
23	C	514	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
25	y	101	BCR	C28-C27-C26	-2.39	109.81	114.08
23	B	612	CLA	CMB-C2B-C1B	2.39	129.00	125.37
25	a	409	BCR	C8-C7-C6	-2.39	120.50	127.20
26	L	101	SQD	C1-C2-C3	-2.38	105.03	110.00
23	b	610	CLA	C3B-C4B-NB	2.38	112.73	110.52
23	B	605	CLA	C4-C3-C5	2.38	119.28	115.27
23	c	502	CLA	CMC-C2C-C1C	2.38	128.66	125.04
23	B	616	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
23	B	613	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
33	B	621	LMG	C7-O1-C1	-2.38	109.10	113.74
23	B	610	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	d	404	CLA	C3B-C4B-NB	2.38	112.72	110.52
23	c	510	CLA	CAC-C3C-C4C	2.38	127.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CGD-CBD-CAD	-2.37	103.04	110.73
24	a	406	PHO	O1D-CGD-CBD	-2.37	120.79	124.74
23	c	505	CLA	CHC-C1C-C2C	-2.37	120.14	126.73
23	B	611	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	B	616	CLA	C4-C3-C5	2.37	119.26	115.27
34	V	203	HTG	C1-C2-C3	2.37	112.58	109.67
29	A	414	PL9	C51-C49-C50	2.37	119.83	114.60
25	C	515	BCR	C38-C26-C25	-2.37	121.87	124.53
23	c	508	CLA	CMC-C2C-C1C	2.37	128.64	125.04
23	C	502	CLA	CMB-C2B-C1B	2.36	128.97	125.37
36	c	518	DGD	O3G-C3G-C2G	-2.36	105.20	110.90
23	b	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
36	C	517	DGD	C4E-C3E-C2E	-2.36	106.70	110.82
23	b	605	CLA	CAC-C3C-C4C	2.36	127.88	124.81
23	c	507	CLA	CMC-C2C-C1C	2.36	128.64	125.04
23	c	513	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
23	b	601	CLA	CMC-C2C-C1C	2.36	128.63	125.04
25	T	101	BCR	C35-C13-C12	2.36	121.80	118.08
23	c	504	CLA	C4-C3-C5	2.36	119.24	115.27
26	f	101	SQD	C4-C3-C2	-2.36	106.71	110.82
35	b	627	LMT	O5'-C1'-C2'	2.36	115.34	110.35
40	v	201	HEC	C2A-C1A-NA	-2.36	108.03	110.32
23	C	507	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
25	T	101	BCR	C1-C6-C7	2.35	122.44	115.78
24	D	401	PHO	C4A-C3A-C2A	-2.35	100.60	102.84
23	B	606	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
40	v	201	HEC	O2D-CGD-CBD	2.35	121.59	114.03
25	a	409	BCR	C33-C5-C6	-2.35	121.89	124.53
23	c	510	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
23	d	403	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
23	c	505	CLA	O2A-CGA-CBA	2.35	119.27	111.91
23	B	610	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
25	c	515	BCR	C32-C1-C6	-2.34	106.50	110.30
23	C	508	CLA	C6-C7-C8	-2.34	108.35	115.92
23	a	408	CLA	CMA-C3A-C4A	-2.34	105.48	111.77
24	A	407	PHO	C4-C3-C5	2.34	119.21	115.27
23	B	614	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
23	d	403	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
23	C	505	CLA	C4-C3-C5	2.34	119.21	115.27
25	H	101	BCR	C2-C1-C6	2.34	114.08	110.48
23	C	511	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
23	b	602	CLA	CMB-C2B-C1B	2.34	128.93	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C4C-C3C-C2C	-2.33	103.49	106.90
23	b	601	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	C	514	CLA	O2A-CGA-CBA	2.33	119.23	111.91
23	B	605	CLA	C3B-C4B-NB	2.33	112.68	110.52
23	C	505	CLA	C1-C2-C3	-2.33	122.01	126.04
23	A	406	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
23	b	614	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
23	C	512	CLA	C11-C10-C8	-2.33	108.39	115.92
23	d	404	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
23	b	602	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	c	513	CLA	CHC-C1C-C2C	-2.33	120.26	126.73
23	a	408	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
23	B	608	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	k	101	BCR	C10-C11-C12	-2.33	115.96	123.22
25	t	101	BCR	C20-C21-C22	-2.32	123.99	127.31
23	a	404	CLA	CMC-C2C-C1C	2.32	128.58	125.04
23	A	404	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	c	505	CLA	CHB-C1B-NB	-2.32	121.80	124.26
26	f	101	SQD	O47-C7-O49	-2.32	118.09	123.70
23	c	506	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
23	C	507	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
23	B	611	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
23	c	509	CLA	CHB-C1B-NB	-2.32	121.81	124.26
23	a	404	CLA	CAC-C3C-C4C	2.32	127.81	124.81
23	C	512	CLA	CHB-C1B-NB	-2.31	121.81	124.26
23	d	404	CLA	C4-C3-C5	2.31	119.16	115.27
25	B	618	BCR	C10-C11-C12	-2.31	116.00	123.22
33	j	101	LMG	O7-C10-O9	-2.31	118.11	123.70
23	C	511	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
23	C	513	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
23	C	502	CLA	CHB-C1B-NB	-2.31	121.81	124.26
23	b	616	CLA	CMC-C2C-C1C	2.31	128.56	125.04
26	D	413	SQD	C46-C45-C44	-2.31	106.33	111.79
38	E	103	HEM	CMD-C2D-C1D	2.31	128.56	125.04
23	A	405	CLA	C4-C3-C5	2.31	119.15	115.27
23	D	405	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
29	D	407	PL9	C7-C3-C2	-2.31	120.27	123.30
23	C	505	CLA	CAC-C3C-C4C	2.31	127.80	124.81
36	H	102	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
23	B	609	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	b	602	CLA	C4-C3-C5	2.30	119.15	115.27
23	b	601	CLA	CBC-CAC-C3C	-2.30	106.08	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	101	BCR	C40-C30-C25	-2.30	106.56	110.30
36	c	518	DGD	O2G-C1B-C2B	2.30	116.46	111.50
36	h	102	DGD	O1G-C1A-O1A	-2.30	117.78	123.59
25	c	515	BCR	C11-C10-C9	-2.30	124.03	127.31
25	T	101	BCR	C2-C1-C6	2.30	114.02	110.48
36	c	518	DGD	O5D-C6D-C5D	-2.30	104.80	109.05
25	c	514	BCR	C2-C1-C6	2.30	114.02	110.48
23	A	406	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	b	606	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	d	404	CLA	C1-C2-C3	-2.30	122.07	126.04
23	C	503	CLA	C4-C3-C5	2.30	119.13	115.27
23	c	510	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
33	z	101	LMG	C8-O7-C10	-2.30	112.14	117.79
23	a	405	CLA	C4-C3-C5	2.30	119.13	115.27
34	C	522	HTG	O5-C1-C2	2.29	113.20	110.31
23	c	505	CLA	C1-O2A-CGA	2.29	122.46	116.44
25	a	409	BCR	C38-C26-C25	-2.29	121.96	124.53
23	C	513	CLA	C1-C2-C3	-2.29	122.08	126.04
33	a	416	LMG	O8-C28-C29	2.29	119.09	111.91
23	a	405	CLA	C1-O2A-CGA	2.29	122.45	116.44
23	b	602	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
25	B	619	BCR	C2-C3-C4	-2.29	106.27	111.38
23	C	513	CLA	CHB-C4A-NA	2.29	127.67	124.51
40	V	202	HEC	CMD-C2D-C1D	2.29	128.52	125.04
23	C	503	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
26	a	410	SQD	C3-C4-C5	2.29	114.32	110.24
25	b	617	BCR	C24-C23-C22	-2.28	122.78	126.23
33	b	620	LMG	C4-C3-C2	-2.28	106.84	110.82
23	B	607	CLA	CAA-CBA-CGA	2.28	119.92	113.25
23	D	404	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
23	B	614	CLA	CMC-C2C-C1C	2.28	128.51	125.04
25	c	515	BCR	C35-C13-C14	-2.28	119.73	122.92
25	H	101	BCR	C2-C3-C4	-2.28	106.28	111.38
23	A	406	CLA	CHB-C1B-NB	-2.28	121.84	124.26
31	A	416	LHG	C5-O7-C7	-2.28	112.17	117.79
23	c	512	CLA	C1-O2A-CGA	2.28	122.43	116.44
31	d	408	LHG	O8-C23-O10	-2.28	117.84	123.59
23	A	404	CLA	C4-C3-C5	2.28	119.11	115.27
25	k	101	BCR	C39-C30-C25	-2.28	106.60	110.30
23	d	404	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
33	j	101	LMG	O8-C28-O10	-2.28	117.84	123.59
23	B	605	CLA	CAC-C3C-C4C	2.28	127.76	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	101	BCR	C40-C30-C25	-2.28	106.61	110.30
23	b	608	CLA	C4-C3-C5	2.28	119.10	115.27
23	c	508	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
23	b	606	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
34	b	628	HTG	O5-C1-C2	2.27	113.17	110.31
23	c	507	CLA	O2A-CGA-CBA	2.27	119.04	111.91
29	d	406	PL9	C30-C29-C31	2.27	119.09	115.27
23	c	509	CLA	C4-C3-C5	2.27	119.09	115.27
38	E	103	HEM	O2A-CGA-CBA	2.27	121.32	114.03
26	L	101	SQD	O47-C7-O49	-2.27	118.22	123.70
23	c	503	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
36	C	517	DGD	O1G-C1A-O1A	-2.27	117.86	123.59
23	C	506	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
25	T	101	BCR	C16-C15-C14	2.27	128.12	123.47
33	Z	101	LMG	C4-C3-C2	2.27	114.78	110.82
36	c	518	DGD	O1G-C1A-C2A	2.27	119.02	111.91
23	C	512	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
23	b	613	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	C	513	CLA	CMC-C2C-C1C	2.26	128.48	125.04
23	c	510	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
24	D	401	PHO	CMC-C2C-C1C	2.26	128.99	124.73
23	c	504	CLA	CHB-C1B-NB	-2.26	121.87	124.26
23	B	611	CLA	CMB-C2B-C1B	2.25	128.80	125.37
23	a	405	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	C	508	CLA	CMC-C2C-C1C	2.25	128.47	125.04
25	t	101	BCR	C16-C15-C14	-2.25	118.86	123.47
25	B	617	BCR	C28-C27-C26	-2.25	110.05	114.08
23	B	613	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
23	C	514	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
23	a	404	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
40	v	201	HEC	CHD-C4C-NC	2.25	127.99	123.85
23	A	404	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
23	D	405	CLA	CHB-C4A-NA	2.25	127.62	124.51
40	V	202	HEC	CHB-C1B-C2B	-2.25	121.46	124.98
23	B	612	CLA	CHD-C4C-NC	2.25	127.75	124.20
23	B	612	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	b	615	CLA	O2A-CGA-CBA	2.25	118.96	111.91
23	A	405	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	B	609	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	b	610	CLA	C4-C3-C2	-2.25	117.91	123.68
25	c	515	BCR	C20-C21-C22	-2.25	124.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	101	BCR	C11-C10-C9	-2.25	124.10	127.31
29	D	407	PL9	C25-C24-C26	2.25	119.05	115.27
23	d	404	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
23	c	501	CLA	CMC-C2C-C1C	2.24	128.46	125.04
29	a	414	PL9	C40-C39-C41	2.24	119.04	115.27
23	A	408	CLA	O2A-CGA-CBA	2.24	118.95	111.91
23	D	405	CLA	O2A-CGA-CBA	2.24	118.94	111.91
25	t	101	BCR	C29-C28-C27	-2.24	106.37	111.38
23	c	512	CLA	CHB-C1B-NB	-2.24	121.89	124.26
25	D	406	BCR	C21-C20-C19	-2.24	116.23	123.22
23	C	511	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	B	611	CLA	CAC-C3C-C4C	2.24	127.71	124.81
25	C	516	BCR	C21-C20-C19	-2.24	116.24	123.22
24	a	406	PHO	CBA-CAA-C2A	-2.23	107.28	113.81
23	C	503	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
23	B	616	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
36	C	517	DGD	O3G-C3G-C2G	-2.23	105.51	110.90
34	B	622	HTG	O2-C2-C3	-2.23	105.19	110.35
23	C	513	CLA	CAC-C3C-C4C	2.23	127.70	124.81
23	b	616	CLA	C11-C12-C13	-2.23	108.71	115.92
23	C	502	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
35	D	403	LMT	C1B-O5B-C5B	-2.23	109.31	113.69
25	c	515	BCR	C37-C22-C21	-2.23	119.80	122.92
23	b	608	CLA	CAC-C3C-C4C	2.23	127.70	124.81
23	C	506	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	C	502	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
25	H	101	BCR	C7-C6-C5	2.23	126.86	121.46
23	B	609	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
24	D	401	PHO	CBA-CAA-C2A	-2.23	107.30	113.81
23	c	504	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	B	609	CLA	CED-O2D-CGD	2.23	120.97	115.94
25	c	515	BCR	C15-C16-C17	-2.23	118.91	123.47
23	b	614	CLA	C4-C3-C5	2.23	119.01	115.27
23	A	408	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
23	b	609	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
23	C	512	CLA	CHB-C4A-NA	2.22	127.59	124.51
26	A	410	SQD	O47-C7-O49	-2.22	118.34	123.70
23	B	615	CLA	O2A-CGA-CBA	2.22	118.87	111.91
29	a	414	PL9	C45-C44-C46	2.22	119.00	115.27
23	B	602	CLA	C1-C2-C3	-2.22	122.21	126.04
23	B	605	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	c	501	CLA	CBC-CAC-C3C	-2.22	106.32	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405	CLA	O2A-CGA-CBA	2.21	118.86	111.91
25	B	619	BCR	C10-C11-C12	-2.21	116.31	123.22
23	C	509	CLA	CMB-C2B-C1B	2.21	128.74	125.37
23	b	607	CLA	CHD-C4C-NC	2.21	127.69	124.20
31	D	408	LHG	O8-C23-C24	2.21	118.85	111.91
25	c	515	BCR	C40-C30-C25	-2.21	106.71	110.30
25	y	101	BCR	C16-C15-C14	-2.21	118.95	123.47
23	d	401	CLA	CAA-CBA-CGA	2.21	119.71	113.25
25	c	514	BCR	C37-C22-C21	-2.21	119.83	122.92
25	b	619	BCR	C37-C22-C23	2.21	121.56	118.08
23	b	601	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
36	C	519	DGD	O6D-C1D-O3G	-2.21	104.75	109.97
23	B	611	CLA	CED-O2D-CGD	2.20	120.92	115.94
33	C	501	LMG	O8-C28-C29	2.20	118.82	111.91
31	d	407	LHG	O7-C7-O9	-2.20	118.38	123.70
23	B	602	CLA	C1-O2A-CGA	2.20	122.22	116.44
23	b	606	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
24	a	407	PHO	CBA-CAA-C2A	-2.20	107.38	113.81
23	b	616	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
23	b	616	CLA	C3B-C4B-NB	2.20	112.56	110.52
23	c	510	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	C	508	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	a	405	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	b	606	CLA	C1-O2A-CGA	2.20	122.21	116.44
25	b	618	BCR	C20-C21-C22	-2.20	124.17	127.31
35	B	631	LMT	O1'-C1'-C2'	2.20	111.73	108.30
25	H	101	BCR	C31-C1-C6	-2.19	106.74	110.30
23	b	609	CLA	C7-C6-C5	-2.19	107.40	113.36
23	B	604	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
23	C	504	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	c	513	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	B	610	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
25	H	101	BCR	C36-C18-C17	-2.19	119.86	122.92
23	B	604	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
31	E	101	LHG	O8-C23-O10	-2.19	118.07	123.59
24	A	407	PHO	CMA-C3A-C4A	-2.19	109.59	114.38
23	c	505	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
25	A	409	BCR	C31-C1-C6	-2.18	106.75	110.30
23	B	606	CLA	CMC-C2C-C1C	2.18	128.37	125.04
29	d	406	PL9	C45-C44-C46	2.18	118.94	115.27
23	c	507	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	c	506	CLA	CHB-C4A-NA	2.18	127.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	PHO	CED-O2D-CGD	2.18	120.86	115.94
23	c	510	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
29	D	407	PL9	C45-C44-C46	2.18	118.93	115.27
23	b	607	CLA	CMC-C2C-C1C	2.18	128.35	125.04
23	c	512	CLA	CMA-C3A-C4A	-2.18	105.92	111.77
25	H	101	BCR	C16-C15-C14	-2.18	119.02	123.47
23	B	613	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
23	A	406	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
23	B	605	CLA	O2A-CGA-CBA	2.18	118.73	111.91
23	d	404	CLA	C1-O2A-CGA	2.18	122.15	116.44
36	H	102	DGD	C3G-O3G-C1D	-2.17	109.49	113.74
38	e	103	HEM	CHA-C1A-NA	2.17	127.85	123.85
23	c	512	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
23	C	503	CLA	O2A-CGA-CBA	2.17	118.73	111.91
23	b	605	CLA	C1-C2-C3	-2.17	122.29	126.04
25	k	101	BCR	C36-C18-C19	2.17	121.49	118.08
25	C	516	BCR	C34-C9-C10	-2.17	119.89	122.92
23	d	401	CLA	CHB-C4A-NA	2.17	127.51	124.51
29	A	414	PL9	C47-C48-C49	-2.17	120.34	127.75
33	z	101	LMG	C7-O1-C1	-2.17	109.51	113.74
40	V	202	HEC	C4A-NA-C1A	2.17	107.47	105.35
23	a	405	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
31	D	409	LHG	O7-C7-O9	-2.17	118.47	123.70
25	b	619	BCR	C21-C20-C19	-2.17	116.46	123.22
23	B	603	CLA	C2A-C1A-CHA	-2.16	120.07	123.86
23	C	509	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
23	a	404	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
23	C	510	CLA	C11-C12-C13	-2.16	108.93	115.92
24	a	406	PHO	CBC-CAC-C3C	-2.16	109.72	112.88
25	T	101	BCR	C37-C22-C23	2.16	121.48	118.08
29	D	407	PL9	C17-C18-C19	-2.16	122.46	127.66
25	c	514	BCR	C3-C4-C5	-2.16	110.22	114.08
24	A	407	PHO	O2A-CGA-O1A	-2.16	118.14	123.59
23	c	504	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
23	c	511	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
23	B	607	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	A	404	CLA	CHB-C1B-NB	-2.16	121.97	124.26
25	Y	101	BCR	C36-C18-C19	2.15	121.47	118.08
23	a	405	CLA	CHB-C4A-NA	2.15	127.49	124.51
35	b	627	LMT	C3'-C4'-C5'	-2.15	105.99	110.93
23	C	505	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
23	A	406	CLA	C4-C3-C5	2.15	118.89	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	618	BCR	C16-C17-C18	-2.15	124.24	127.31
23	B	602	CLA	C11-C12-C13	-2.15	108.98	115.92
23	C	513	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	c	513	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
34	B	624	HTG	C1-C2-C3	2.14	114.82	110.59
23	c	509	CLA	CHD-C4C-NC	2.14	127.58	124.20
26	A	412	SQD	O9-S-C6	2.14	109.48	106.94
35	m	102	LMT	C1B-O5B-C5B	2.14	117.89	113.69
23	B	601	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	B	602	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
40	v	201	HEC	O2A-CGA-CBA	2.14	120.90	114.03
23	b	613	CLA	CHB-C1B-NB	-2.14	121.99	124.26
23	C	510	CLA	CMB-C2B-C1B	2.14	128.62	125.37
25	h	101	BCR	C20-C21-C22	-2.14	124.26	127.31
23	C	510	CLA	C4-C3-C5	2.14	118.86	115.27
23	b	610	CLA	C11-C12-C13	-2.14	109.02	115.92
23	C	510	CLA	C1-O2A-CGA	2.13	122.05	116.44
23	B	615	CLA	C1-O2A-CGA	2.13	122.04	116.44
23	d	401	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
23	C	513	CLA	CHB-C1B-C2B	-2.13	121.21	127.24
35	D	403	LMT	C3B-C4B-C5B	2.13	114.05	110.24
25	C	515	BCR	C11-C12-C13	-2.13	120.42	126.42
29	d	406	PL9	C27-C28-C29	-2.13	122.53	127.66
23	c	502	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	B	603	CLA	C5-C3-C2	-2.13	116.81	121.12
25	a	409	BCR	C28-C27-C26	-2.13	110.28	114.08
23	a	408	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
23	D	404	CLA	C4-C3-C2	-2.12	118.23	123.68
29	D	407	PL9	C30-C29-C31	2.12	118.84	115.27
23	B	608	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
40	v	201	HEC	CBA-CAA-C2A	-2.12	106.74	112.63
25	c	515	BCR	C35-C13-C12	2.12	121.42	118.08
38	E	103	HEM	CBA-CAA-C2A	-2.12	106.74	112.63
23	b	603	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
25	t	101	BCR	C33-C5-C4	2.12	117.69	113.62
35	I	101	LMT	O1'-C1'-C2'	2.12	111.61	108.30
23	c	502	CLA	CHB-C4A-NA	2.12	127.44	124.51
23	C	504	CLA	CHB-C1B-C2B	-2.12	121.26	127.24
26	A	410	SQD	O8-S-C6	2.12	109.11	105.74
23	A	406	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
38	E	103	HEM	CHA-C1A-NA	2.11	127.73	123.85
35	M	103	LMT	O5'-C5'-C4'	2.11	114.21	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	c	506	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
23	c	502	CLA	CHB-C1B-NB	-2.11	122.02	124.26
24	D	401	PHO	C1-O2A-CGA	2.11	121.98	116.44
23	a	405	CLA	CMC-C2C-C1C	2.11	128.25	125.04
36	c	517	DGD	O5D-C1E-C2E	2.11	111.60	108.30
25	b	618	BCR	C15-C16-C17	-2.11	119.15	123.47
26	D	413	SQD	O5-C1-C2	-2.11	105.88	110.35
23	A	404	CLA	CMA-C3A-C2A	-2.11	105.32	113.83
24	a	406	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
26	B	620	SQD	O48-C46-C45	2.11	114.57	108.43
23	B	611	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
34	b	622	HTG	C1-O5-C5	2.11	116.47	112.58
23	C	512	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
25	h	101	BCR	C37-C22-C23	2.11	121.39	118.08
33	c	520	LMG	C9-C8-C7	-2.11	106.81	111.79
31	l	101	LHG	O8-C23-O10	-2.10	118.28	123.59
26	A	412	SQD	C46-C45-C44	-2.10	106.81	111.79
31	d	407	LHG	C5-O7-C7	-2.10	112.61	117.79
35	D	402	LMT	O5B-C5B-C4B	2.10	113.51	109.69
23	B	614	CLA	CHC-C1C-NC	2.10	127.39	124.20
25	K	102	BCR	C11-C10-C9	-2.10	124.31	127.31
23	d	403	CLA	CHD-C4C-NC	2.10	127.52	124.20
33	J	101	LMG	O7-C10-O9	-2.10	118.63	123.70
25	B	617	BCR	C36-C18-C17	-2.10	119.98	122.92
23	b	616	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
23	b	613	CLA	CAC-C3C-C4C	2.10	127.53	124.81
25	B	617	BCR	C33-C5-C4	2.10	117.64	113.62
23	A	405	CLA	C1-C2-C3	-2.10	122.42	126.04
23	b	607	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
25	k	101	BCR	C34-C9-C8	2.10	121.38	118.08
23	A	406	CLA	CHC-C4B-NB	-2.10	122.04	124.26
25	t	101	BCR	C28-C27-C26	-2.09	110.34	114.08
23	B	613	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
23	A	404	CLA	CMB-C2B-C1B	2.09	128.56	125.37
33	c	519	LMG	O8-C28-O10	-2.09	118.31	123.59
23	B	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	606	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
23	C	510	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
23	A	405	CLA	C11-C10-C8	-2.09	109.17	115.92
34	V	203	HTG	C1-O5-C5	2.09	115.02	112.19
23	b	613	CLA	C2A-C1A-CHA	-2.09	120.21	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B	630	LMT	C1'-O5'-C5'	2.09	117.79	113.69
26	D	413	SQD	O48-C23-O10	-2.09	118.32	123.59
23	A	405	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
23	B	615	CLA	CHA-C1A-NA	-2.09	121.62	126.40
23	C	510	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	c	502	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
36	C	519	DGD	O6E-C1E-O5D	-2.08	105.04	109.97
38	e	103	HEM	CBD-CAD-C3D	-2.08	106.84	112.63
23	c	508	CLA	CMB-C2B-C1B	2.08	128.54	125.37
23	b	603	CLA	CHB-C1B-C2B	-2.08	121.35	127.24
25	b	617	BCR	C11-C10-C9	-2.08	124.34	127.31
23	C	506	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
36	H	102	DGD	O1G-C1A-O1A	-2.08	118.34	123.59
23	B	614	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
25	B	618	BCR	C35-C13-C14	-2.08	120.01	122.92
25	B	619	BCR	C37-C22-C23	2.08	121.35	118.08
36	c	517	DGD	C1D-O6D-C5D	2.08	117.77	113.69
40	V	202	HEC	CAD-CBD-CGD	2.08	118.08	113.60
35	m	102	LMT	O1B-C1B-C2B	2.08	113.48	108.10
33	Z	102	LMG	C7-O1-C1	-2.08	109.69	113.74
23	b	614	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
23	d	403	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	B	617	BCR	C29-C30-C25	2.07	113.67	110.48
36	h	102	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
23	c	506	CLA	CMC-C2C-C1C	2.07	128.19	125.04
35	a	417	LMT	C1B-O1B-C4'	-2.07	112.84	117.96
25	h	101	BCR	C15-C14-C13	-2.07	124.35	127.31
25	k	101	BCR	C34-C9-C10	-2.07	120.02	122.92
23	B	601	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
25	Y	101	BCR	C28-C27-C26	-2.07	110.38	114.08
23	B	604	CLA	C6-C7-C8	-2.07	109.23	115.92
34	b	623	HTG	C1-O5-C5	2.07	116.39	112.58
23	d	401	CLA	CMB-C2B-C1B	2.07	128.52	125.37
23	D	405	CLA	CHC-C4B-NB	-2.07	122.07	124.26
23	C	507	CLA	CED-O2D-CGD	2.07	120.61	115.94
23	c	507	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
25	Y	101	BCR	C29-C28-C27	-2.06	106.76	111.38
23	c	504	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	B	602	CLA	CHB-C4A-NA	2.06	127.37	124.51
23	c	510	CLA	CHB-C4A-NA	2.06	127.37	124.51
23	B	609	CLA	C7-C6-C5	-2.06	107.76	113.36
35	e	102	LMT	C1B-C2B-C3B	2.06	114.29	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405	CLA	O2A-CGA-CBA	2.06	118.38	111.91
23	a	404	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
25	b	617	BCR	C38-C26-C25	-2.06	122.21	124.53
36	c	516	DGD	O2G-C1B-O1B	-2.06	118.72	123.70
23	C	504	CLA	CHC-C1C-NC	2.06	127.33	124.20
25	b	619	BCR	C20-C21-C22	-2.06	124.37	127.31
26	B	620	SQD	O9-S-C6	2.06	109.38	106.94
23	b	613	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
23	d	401	CLA	CMC-C2C-C1C	2.05	128.17	125.04
29	a	414	PL9	C17-C18-C19	-2.05	122.72	127.66
38	E	103	HEM	O2D-CGD-CBD	2.05	120.62	114.03
36	C	517	DGD	O1G-C1A-C2A	2.05	118.35	111.91
33	B	621	LMG	O8-C28-O10	-2.05	118.42	123.59
23	B	607	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	C	505	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
25	D	406	BCR	C10-C11-C12	-2.05	116.83	123.22
23	D	404	CLA	OBD-CAD-C3D	-2.05	123.60	128.52
26	B	620	SQD	O5-C1-C2	-2.05	106.02	110.35
23	B	603	CLA	CHB-C1B-C2B	-2.05	121.46	127.24
23	C	513	CLA	C11-C12-C13	-2.05	109.31	115.92
40	v	201	HEC	CHB-C1B-C2B	-2.05	121.78	124.98
23	b	605	CLA	CHB-C1B-NB	-2.05	122.09	124.26
26	B	620	SQD	O48-C23-O10	-2.04	118.43	123.59
23	c	503	CLA	C2A-C1A-CHA	-2.04	120.28	123.86
23	B	614	CLA	CHB-C4A-NA	2.04	127.34	124.51
38	E	103	HEM	C4A-NA-C1A	2.04	107.35	105.35
25	A	409	BCR	C7-C8-C9	-2.04	123.15	126.23
36	c	518	DGD	O6D-C1D-O3G	-2.04	105.14	109.97
31	E	101	LHG	O7-C7-O9	-2.04	118.77	123.70
23	C	512	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
25	b	619	BCR	C28-C27-C26	-2.04	110.43	114.08
36	c	517	DGD	O2G-C1B-O1B	-2.04	118.77	123.70
25	b	617	BCR	C15-C16-C17	-2.04	119.30	123.47
23	b	615	CLA	C6-C7-C8	-2.04	109.34	115.92
23	b	611	CLA	CMB-C2B-C1B	2.04	128.47	125.37
29	D	407	PL9	C45-C44-C43	-2.04	118.46	123.68
25	T	101	BCR	C3-C4-C5	-2.04	110.44	114.08
23	B	602	CLA	C11-C10-C8	-2.04	109.34	115.92
23	a	408	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	b	610	CLA	CMC-C2C-C1C	2.03	128.14	125.04
23	d	404	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	c	510	CLA	C11-C10-C8	-2.03	109.35	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	H	102	DGD	O6E-C5E-C6E	2.03	111.49	106.44
25	B	619	BCR	C29-C30-C25	2.03	113.61	110.48
25	D	406	BCR	C30-C25-C24	2.03	121.52	115.78
23	b	604	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
25	K	102	BCR	C38-C26-C25	-2.03	122.25	124.53
23	C	508	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	A	408	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
23	a	408	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
23	A	406	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	C	511	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
23	d	403	CLA	CHB-C4A-NA	2.03	127.31	124.51
23	B	607	CLA	C1-O2A-CGA	2.02	121.76	116.44
24	A	407	PHO	C6-C7-C8	-2.02	109.38	115.92
23	B	601	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
23	b	602	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
23	B	606	CLA	C1-O2A-CGA	2.02	121.75	116.44
25	a	409	BCR	C2-C1-C6	2.02	113.59	110.48
33	J	101	LMG	C8-O7-C10	-2.02	112.82	117.79
25	c	514	BCR	C21-C20-C19	-2.02	116.91	123.22
23	c	507	CLA	C11-C10-C8	-2.02	109.39	115.92
36	c	518	DGD	C3G-C2G-C1G	-2.02	107.01	111.79
36	C	518	DGD	O6E-C5E-C6E	2.02	111.45	106.44
23	d	404	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
34	B	627	HTG	C1-O5-C5	2.02	116.30	112.58
23	D	405	CLA	CHB-C1B-NB	-2.02	122.12	124.26
23	B	613	CLA	C7-C6-C5	-2.01	107.89	113.36
26	B	620	SQD	O5-C5-C4	2.01	113.35	109.69
29	d	406	PL9	C36-C34-C33	-2.01	117.05	121.12
40	v	201	HEC	CHB-C4A-NA	2.01	126.61	124.44
36	c	517	DGD	O1G-C1A-O1A	-2.01	118.52	123.59
23	C	505	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	b	615	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
23	C	505	CLA	CMB-C2B-C1B	2.01	128.43	125.37
23	C	505	CLA	O2A-CGA-CBA	2.01	118.20	111.91
23	b	602	CLA	C7-C6-C5	-2.01	107.91	113.36
36	C	519	DGD	C3G-C2G-C1G	-2.01	107.04	111.79
36	C	518	DGD	C3G-O3G-C1D	-2.01	109.82	113.74
23	d	401	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
25	d	405	BCR	C35-C13-C14	-2.00	120.12	122.92
23	b	607	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	a	414	PL9	C12-C13-C14	-2.00	122.84	127.66
35	e	102	LMT	O1B-C1B-C2B	2.00	113.29	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	201	HEC	NA

All (1400) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	B	616	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	C2B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	514	CLA	C2B-C3B-CAB-CBB
23	C	514	CLA	C4B-C3B-CAB-CBB
23	D	405	CLA	C2-C3-C5-C6
23	D	405	CLA	C4-C3-C5-C6
23	a	405	CLA	C4B-C3B-CAB-CBB
23	a	408	CLA	C2B-C3B-CAB-CBB
23	a	408	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	C2-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	d	404	CLA	C2B-C3B-CAB-CBB
23	d	404	CLA	C4B-C3B-CAB-CBB
25	D	406	BCR	C7-C8-C9-C10
25	D	406	BCR	C7-C8-C9-C34
25	D	406	BCR	C21-C22-C23-C24
25	D	406	BCR	C37-C22-C23-C24
25	D	406	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	d	405	BCR	C7-C8-C9-C10
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C21-C22-C23-C24
25	d	405	BCR	C37-C22-C23-C24
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
26	D	413	SQD	O49-C7-O47-C45
26	D	413	SQD	C8-C7-O47-C45
26	D	413	SQD	C5-C6-S-O7
26	D	413	SQD	C5-C6-S-O8
26	D	413	SQD	C5-C6-S-O9
26	L	101	SQD	O49-C7-O47-C45
26	L	101	SQD	C5-C6-S-O7
26	L	101	SQD	C5-C6-S-O8
26	L	101	SQD	C5-C6-S-O9
26	a	412	SQD	O6-C44-C45-O47
26	f	101	SQD	O49-C7-O47-C45
26	f	101	SQD	C8-C7-O47-C45
26	f	101	SQD	C5-C6-S-O7
26	f	101	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
26	f	101	SQD	C5-C6-S-O9
27	A	411	GOL	O1-C1-C2-C3
27	B	625	GOL	O1-C1-C2-C3
27	B	626	GOL	C1-C2-C3-O3
27	C	523	GOL	O1-C1-C2-O2
27	C	523	GOL	O1-C1-C2-C3
27	a	411	GOL	C1-C2-C3-O3
27	d	402	GOL	O1-C1-C2-C3
29	A	414	PL9	C13-C14-C16-C17
29	A	414	PL9	C15-C14-C16-C17
29	A	414	PL9	C23-C24-C26-C27
29	A	414	PL9	C25-C24-C26-C27
29	d	406	PL9	C39-C41-C42-C43
31	A	416	LHG	C4-O6-P-O5
31	A	417	LHG	O1-C1-C2-C3
31	A	417	LHG	C3-O3-P-O4
31	A	417	LHG	C4-O6-P-O4
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O4
31	D	409	LHG	C4-O6-P-O4
31	E	101	LHG	O1-C1-C2-C3
31	E	101	LHG	C1-C2-C3-O3
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
31	d	407	LHG	O1-C1-C2-C3
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O5
31	d	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O4
31	d	409	LHG	C4-O6-P-O4
31	e	101	LHG	C3-O3-P-O5
31	e	101	LHG	C3-O3-P-O6
31	e	101	LHG	O10-C23-O8-C6
31	e	101	LHG	C24-C23-O8-C6
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
33	C	501	LMG	C11-C10-O7-C8
33	Z	102	LMG	C2-C1-O1-C7
33	Z	102	LMG	O9-C10-O7-C8
33	Z	102	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	a	416	LMG	O9-C10-O7-C8
33	c	520	LMG	C11-C10-O7-C8
33	z	101	LMG	C11-C10-O7-C8
34	B	622	HTG	C2'-C1'-S1-C1
34	B	623	HTG	C2'-C1'-S1-C1
34	B	624	HTG	O5-C1-S1-C1'
35	B	629	LMT	C2'-C1'-O1'-C1
35	B	629	LMT	O5'-C1'-O1'-C1
35	B	630	LMT	C2'-C1'-O1'-C1
35	B	630	LMT	O5'-C1'-O1'-C1
35	B	631	LMT	C2'-C1'-O1'-C1
35	B	631	LMT	O5'-C1'-O1'-C1
35	B	631	LMT	C2-C1-O1'-C1'
35	D	402	LMT	C2'-C1'-O1'-C1
35	D	402	LMT	O5'-C1'-O1'-C1
35	E	102	LMT	C2'-C1'-O1'-C1
35	E	102	LMT	O5'-C1'-O1'-C1
35	I	101	LMT	C2'-C1'-O1'-C1
35	I	101	LMT	O5'-C1'-O1'-C1
35	M	103	LMT	C2'-C1'-O1'-C1
35	M	103	LMT	O5'-C1'-O1'-C1
35	a	417	LMT	C2'-C1'-O1'-C1
35	a	417	LMT	O5'-C1'-O1'-C1
35	b	621	LMT	O5'-C1'-O1'-C1
35	b	627	LMT	O5'-C1'-O1'-C1
35	b	627	LMT	C2-C1-O1'-C1'
35	e	102	LMT	C2'-C1'-O1'-C1
35	e	102	LMT	O5'-C1'-O1'-C1
38	E	103	HEM	C2C-C3C-CAC-CBC
38	E	103	HEM	C4C-C3C-CAC-CBC
38	e	103	HEM	C2C-C3C-CAC-CBC
38	e	103	HEM	C4C-C3C-CAC-CBC
35	D	403	LMT	C3'-C4'-O1B-C1B
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
33	c	520	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
35	I	101	LMT	C3'-C4'-O1B-C1B
23	A	408	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	L	101	SQD	C8-C7-O47-C45
33	a	416	LMG	C11-C10-O7-C8
23	d	401	CLA	CBD-CGD-O2D-CED
33	c	520	LMG	O6-C5-C6-O5
23	c	504	CLA	C4-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	c	504	CLA	C2-C3-C5-C6
23	a	405	CLA	CBD-CGD-O2D-CED
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C3-C5-C6-C7
34	c	521	HTG	S1-C1'-C2'-C3'
33	C	501	LMG	O9-C10-O7-C8
35	D	403	LMT	C4'-C5'-C6'-O6'
34	B	624	HTG	O5-C5-C6-O6
23	C	502	CLA	CBD-CGD-O2D-CED
31	D	408	LHG	O2-C2-C3-O3
31	E	101	LHG	O2-C2-C3-O3
31	d	408	LHG	O2-C2-C3-O3
23	b	616	CLA	C3-C5-C6-C7
23	c	506	CLA	C3-C5-C6-C7
33	Z	101	LMG	O6-C5-C6-O5
35	I	101	LMT	O5B-C5B-C6B-O6B
34	b	625	HTG	O5-C5-C6-O6
34	b	628	HTG	S1-C1'-C2'-C3'
35	M	103	LMT	O5'-C5'-C6'-O6'
35	D	403	LMT	O5'-C5'-C6'-O6'
23	C	508	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	d	404	CLA	C2-C3-C5-C6
33	j	101	LMG	C10-C11-C12-C13
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
35	D	403	LMT	O5B-C5B-C6B-O6B
29	A	414	PL9	C14-C16-C17-C18
29	D	407	PL9	C39-C41-C42-C43
34	d	411	HTG	C4-C5-C6-O6
35	E	102	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C1-C2-C3-O3
35	D	403	LMT	C4B-C5B-C6B-O6B
23	c	512	CLA	C3-C5-C6-C7
23	A	408	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
31	D	409	LHG	C24-C23-O8-C6
34	B	623	HTG	C4-C5-C6-O6
26	A	412	SQD	C26-C27-C28-C29
33	c	520	LMG	C4-C5-C6-O5
23	A	405	CLA	C15-C16-C17-C18
23	C	508	CLA	C5-C6-C7-C8
35	b	621	LMT	C2'-C1'-O1'-C1
35	b	627	LMT	C2'-C1'-O1'-C1
31	D	408	LHG	C32-C33-C34-C35
23	B	601	CLA	C11-C10-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	c	502	CLA	C14-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C9
23	C	502	CLA	C15-C16-C17-C18
25	H	101	BCR	C7-C8-C9-C34
25	K	102	BCR	C7-C8-C9-C34
25	Y	101	BCR	C37-C22-C23-C24
25	y	101	BCR	C37-C22-C23-C24
25	H	101	BCR	C7-C8-C9-C10
33	J	101	LMG	O6-C5-C6-O5
26	A	410	SQD	C8-C7-O47-C45
23	C	511	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	O1A-CGA-O2A-C1
23	b	606	CLA	C10-C11-C12-C13
34	b	623	HTG	O5-C5-C6-O6
23	B	601	CLA	C5-C6-C7-C8
33	Z	102	LMG	C10-C11-C12-C13
23	C	514	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	C15-C16-C17-C18
23	B	605	CLA	C5-C6-C7-C8
23	B	614	CLA	C5-C6-C7-C8
23	B	614	CLA	C8-C10-C11-C12
23	B	614	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C8-C10-C11-C12
23	a	408	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
23	c	502	CLA	C15-C16-C17-C18
33	c	520	LMG	C10-C11-C12-C13
36	C	518	DGD	C1A-C2A-C3A-C4A
23	B	606	CLA	C13-C15-C16-C17
23	a	404	CLA	C15-C16-C17-C18
35	B	631	LMT	O1'-C1-C2-C3
23	b	614	CLA	C13-C15-C16-C17
35	I	101	LMT	O1'-C1-C2-C3
23	c	510	CLA	C10-C11-C12-C13
34	b	628	HTG	O5-C5-C6-O6
23	A	408	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	A	408	CLA	O1A-CGA-O2A-C1
25	T	101	BCR	C13-C14-C15-C16
23	a	408	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	601	CLA	C8-C10-C11-C12
23	b	605	CLA	C8-C10-C11-C12
31	D	409	LHG	O10-C23-O8-C6
23	b	604	CLA	CBD-CGD-O2D-CED
35	B	631	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
23	B	616	CLA	C10-C11-C12-C13
26	D	413	SQD	C7-C8-C9-C10
36	c	516	DGD	O6D-C5D-C6D-O5D
35	B	631	LMT	O5'-C5'-C6'-O6'
26	A	410	SQD	O49-C7-O47-C45
34	B	624	HTG	C4-C5-C6-O6
23	B	602	CLA	C15-C16-C17-C18
23	d	404	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	C11-C10-C9-C8
35	I	101	LMT	C4B-C5B-C6B-O6B
23	C	511	CLA	C5-C6-C7-C8
23	c	507	CLA	C8-C10-C11-C12
31	D	408	LHG	C4-O6-P-O3
31	E	101	LHG	C3-O3-P-O6
31	l	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
23	D	405	CLA	C3-C5-C6-C7
35	D	402	LMT	C1-C2-C3-C4
23	c	501	CLA	O1D-CGD-O2D-CED
31	d	408	LHG	C1-C2-C3-O3
23	B	604	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	b	614	CLA	C3-C5-C6-C7
23	c	512	CLA	C13-C15-C16-C17
26	A	410	SQD	C11-C10-C9-C8
36	C	517	DGD	O6D-C5D-C6D-O5D
23	b	614	CLA	C15-C16-C17-C18
23	b	615	CLA	C13-C15-C16-C17
33	b	620	LMG	C38-C39-C40-C41
35	b	627	LMT	C2-C3-C4-C5
35	m	102	LMT	C11-C10-C9-C8
36	C	517	DGD	CAA-CBA-CCA-CDA
23	a	404	CLA	CBD-CGD-O2D-CED
33	b	620	LMG	C11-C10-O7-C8
26	A	412	SQD	C18-C19-C20-C21
26	a	410	SQD	C9-C10-C11-C12
26	a	410	SQD	C11-C12-C13-C14
31	d	409	LHG	C32-C33-C34-C35
33	B	621	LMG	C17-C18-C19-C20
33	Z	101	LMG	C16-C17-C18-C19
33	a	416	LMG	C31-C32-C33-C34
35	e	102	LMT	C3-C4-C5-C6
36	C	517	DGD	C4D-C5D-C6D-O5D
26	A	410	SQD	C9-C10-C11-C12
26	L	101	SQD	C14-C15-C16-C17
26	L	101	SQD	C24-C25-C26-C27
26	a	410	SQD	C13-C14-C15-C16
31	d	409	LHG	C34-C35-C36-C37
33	Z	101	LMG	C17-C18-C19-C20
36	C	518	DGD	C7B-C8B-C9B-CAB
36	H	102	DGD	CAB-CBB-CCB-CDB
33	b	620	LMG	O9-C10-O7-C8
31	d	408	LHG	C13-C14-C15-C16
33	c	519	LMG	C33-C34-C35-C36
36	C	518	DGD	C9A-CAA-CBA-CCA
26	f	101	SQD	C28-C29-C30-C31
31	A	417	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	D	409	LHG	C29-C30-C31-C32
36	c	517	DGD	C7A-C8A-C9A-CAA
33	a	416	LMG	C30-C31-C32-C33
35	B	630	LMT	C2-C3-C4-C5
35	E	102	LMT	O5'-C5'-C6'-O6'
35	m	102	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C2E-C1E-O5D-C6D
36	C	518	DGD	C2E-C1E-O5D-C6D
26	D	413	SQD	C30-C31-C32-C33
33	B	621	LMG	C36-C37-C38-C39
33	C	520	LMG	C11-C12-C13-C14
33	Z	101	LMG	C15-C16-C17-C18
23	B	615	CLA	C8-C10-C11-C12
23	b	610	CLA	C15-C16-C17-C18
23	C	507	CLA	C16-C17-C18-C20
23	d	401	CLA	O1D-CGD-O2D-CED
34	B	623	HTG	O5-C5-C6-O6
34	d	411	HTG	O5-C5-C6-O6
23	c	505	CLA	C4-C3-C5-C6
24	D	401	PHO	C4-C3-C5-C6
29	D	407	PL9	C15-C14-C16-C17
26	a	412	SQD	C25-C26-C27-C28
31	E	101	LHG	C24-C25-C26-C27
33	c	519	LMG	C4-C5-C6-O5
23	B	615	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
23	C	511	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	d	401	CLA	C11-C12-C13-C14
31	A	417	LHG	C23-C24-C25-C26
26	A	412	SQD	C16-C17-C18-C19
26	D	413	SQD	C24-C25-C26-C27
33	J	101	LMG	C30-C31-C32-C33
35	b	621	LMT	C3-C4-C5-C6
35	b	627	LMT	C3-C4-C5-C6
36	c	516	DGD	C5A-C6A-C7A-C8A
23	c	507	CLA	C2A-CAA-CBA-CGA
23	a	408	CLA	O1A-CGA-O2A-C1
36	c	516	DGD	C4D-C5D-C6D-O5D
26	A	410	SQD	C15-C16-C17-C18
26	A	412	SQD	C25-C26-C27-C28
33	b	620	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	b	625	HTG	C3'-C4'-C5'-C6'
27	B	625	GOL	C1-C2-C3-O3
27	b	624	GOL	O1-C1-C2-C3
31	A	416	LHG	O1-C1-C2-C3
23	d	404	CLA	C3-C5-C6-C7
34	C	522	HTG	O5-C5-C6-O6
23	B	605	CLA	C8-C10-C11-C12
26	D	413	SQD	C32-C33-C34-C35
26	a	412	SQD	C27-C28-C29-C30
26	f	101	SQD	C25-C26-C27-C28
31	A	417	LHG	C13-C14-C15-C16
31	D	408	LHG	C13-C14-C15-C16
31	d	408	LHG	C14-C15-C16-C17
33	C	501	LMG	C37-C38-C39-C40
33	j	101	LMG	C29-C30-C31-C32
36	H	102	DGD	C6A-C7A-C8A-C9A
23	B	602	CLA	C4B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
23	B	608	CLA	C16-C17-C18-C19
33	Z	102	LMG	O6-C1-O1-C7
35	m	102	LMT	O5'-C1'-O1'-C1
36	C	517	DGD	O6E-C1E-O5D-C6D
26	B	620	SQD	C33-C34-C35-C36
26	a	412	SQD	C10-C11-C12-C13
31	A	417	LHG	C25-C26-C27-C28
31	l	101	LHG	C27-C28-C29-C30
33	C	520	LMG	C12-C13-C14-C15
33	a	416	LMG	C35-C36-C37-C38
26	a	410	SQD	C30-C31-C32-C33
33	B	621	LMG	C28-C29-C30-C31
23	d	404	CLA	O1A-CGA-O2A-C1
33	b	620	LMG	C39-C40-C41-C42
23	a	405	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBA-CGA-O2A-C1
33	J	101	LMG	C34-C35-C36-C37
23	c	509	CLA	C5-C6-C7-C8
26	B	620	SQD	C18-C19-C20-C21
35	B	629	LMT	C5-C6-C7-C8
36	H	102	DGD	CCA-CDA-CEA-CFA
23	C	502	CLA	O1D-CGD-O2D-CED
23	B	608	CLA	C16-C17-C18-C20
26	a	410	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	CBA-CCA-CDA-CEA
36	H	102	DGD	CBB-CCB-CDB-CEB
34	B	622	HTG	C1'-C2'-C3'-C4'
35	B	629	LMT	C11-C10-C9-C8
33	C	520	LMG	C28-C29-C30-C31
23	C	506	CLA	C4-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
24	D	401	PHO	C2-C3-C5-C6
29	D	407	PL9	C13-C14-C16-C17
26	L	101	SQD	C26-C27-C28-C29
31	d	407	LHG	C25-C26-C27-C28
36	C	519	DGD	CAA-CBA-CCA-CDA
27	A	411	GOL	O1-C1-C2-O2
27	B	625	GOL	O1-C1-C2-O2
27	B	626	GOL	O2-C2-C3-O3
27	d	402	GOL	O1-C1-C2-O2
31	d	407	LHG	O1-C1-C2-O2
33	z	101	LMG	C18-C19-C20-C21
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB
23	a	405	CLA	C2B-C3B-CAB-CBB
23	b	616	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
33	c	520	LMG	C37-C38-C39-C40
23	c	509	CLA	C3-C5-C6-C7
26	L	101	SQD	C27-C28-C29-C30
33	Z	102	LMG	C19-C20-C21-C22
36	C	518	DGD	CCB-CDB-CEB-CFB
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
26	L	101	SQD	C13-C14-C15-C16
26	a	412	SQD	C24-C25-C26-C27
31	A	417	LHG	C24-C25-C26-C27
31	e	101	LHG	C26-C27-C28-C29
33	j	101	LMG	C38-C39-C40-C41
31	D	409	LHG	C13-C14-C15-C16
25	D	406	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
31	d	408	LHG	C16-C17-C18-C19
31	d	408	LHG	C30-C31-C32-C33
36	C	517	DGD	C3B-C4B-C5B-C6B
31	d	409	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C8-C10-C11-C12
33	B	621	LMG	C11-C10-O7-C8
31	A	416	LHG	C25-C26-C27-C28
31	A	416	LHG	C32-C33-C34-C35
31	d	407	LHG	C34-C35-C36-C37
33	J	101	LMG	C36-C37-C38-C39
23	B	601	CLA	O1A-CGA-O2A-C1
23	A	408	CLA	C4-C3-C5-C6
23	A	408	CLA	C6-C7-C8-C10
23	C	511	CLA	C2-C3-C5-C6
23	C	511	CLA	C6-C7-C8-C10
23	b	603	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	614	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	d	401	CLA	C11-C12-C13-C15
34	C	522	HTG	S1-C1'-C2'-C3'
23	b	605	CLA	C3-C5-C6-C7
31	d	409	LHG	O10-C23-O8-C6
33	J	101	LMG	C20-C21-C22-C23
34	B	624	HTG	C3'-C4'-C5'-C6'
23	c	513	CLA	C10-C11-C12-C13
23	B	610	CLA	C16-C17-C18-C19
23	b	601	CLA	CBA-CGA-O2A-C1
31	D	409	LHG	C15-C16-C17-C18
31	l	101	LHG	C12-C13-C14-C15
31	l	101	LHG	C14-C15-C16-C17
23	A	404	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	601	CLA	C10-C11-C12-C13
33	B	621	LMG	C18-C19-C20-C21
35	b	621	LMT	C4-C5-C6-C7
34	b	628	HTG	C1'-C2'-C3'-C4'
26	D	413	SQD	C11-C10-C9-C8
35	e	102	LMT	C5-C6-C7-C8
36	c	517	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	CBB-CCB-CDB-CEB
23	c	502	CLA	C16-C17-C18-C20
36	C	518	DGD	O6E-C1E-O5D-C6D
36	c	516	DGD	O6E-C1E-O5D-C6D
23	b	611	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	B	621	LMG	C32-C33-C34-C35
33	C	520	LMG	C17-C18-C19-C20
33	j	101	LMG	C21-C22-C23-C24
33	a	416	LMG	C39-C40-C41-C42
23	c	512	CLA	C10-C11-C12-C13
26	a	410	SQD	C27-C28-C29-C30
31	d	408	LHG	C9-C10-C11-C12
33	B	621	LMG	O9-C10-O7-C8
23	b	608	CLA	C3-C5-C6-C7
31	l	101	LHG	C34-C35-C36-C37
23	C	509	CLA	C10-C11-C12-C13
26	a	410	SQD	C34-C35-C36-C37
35	E	102	LMT	C5-C6-C7-C8
35	b	627	LMT	C11-C10-C9-C8
36	C	518	DGD	CCA-CDA-CEA-CFA
33	Z	101	LMG	C4-C5-C6-O5
33	c	519	LMG	C34-C35-C36-C37
23	C	511	CLA	C4-C3-C5-C6
36	c	517	DGD	C1B-C2B-C3B-C4B
29	A	414	PL9	C4-C3-C7-C8
29	a	414	PL9	C4-C3-C7-C8
31	d	407	LHG	C33-C34-C35-C36
33	J	101	LMG	C14-C15-C16-C17
36	h	102	DGD	C5B-C6B-C7B-C8B
23	A	408	CLA	C6-C7-C8-C9
23	B	602	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	509	CLA	C14-C13-C15-C16
36	c	516	DGD	O6E-C5E-C6E-O5E
33	C	520	LMG	C37-C38-C39-C40
36	C	518	DGD	C8A-C9A-CAA-CBA
23	b	601	CLA	C3-C5-C6-C7
31	d	407	LHG	C32-C33-C34-C35
33	Z	102	LMG	O6-C5-C6-O5
34	B	627	HTG	O5-C5-C6-O6
36	C	517	DGD	O6E-C5E-C6E-O5E
25	b	619	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	a	404	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
31	D	409	LHG	C28-C29-C30-C31
25	y	101	BCR	C21-C22-C23-C24
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C16-C17-C18-C20
31	A	416	LHG	C18-C19-C20-C21
33	c	519	LMG	C31-C32-C33-C34
23	b	608	CLA	C13-C15-C16-C17
23	c	506	CLA	C13-C15-C16-C17
31	A	417	LHG	C3-O3-P-O6
31	A	417	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O3
31	d	409	LHG	C4-O6-P-O3
34	B	623	HTG	C2'-C3'-C4'-C5'
23	C	503	CLA	C3-C5-C6-C7
31	l	101	LHG	C16-C17-C18-C19
35	B	629	LMT	C7-C8-C9-C10
35	m	102	LMT	C7-C8-C9-C10
35	B	631	LMT	C7-C8-C9-C10
34	b	625	HTG	C4-C5-C6-O6
23	B	615	CLA	C16-C17-C18-C20
23	C	507	CLA	C16-C17-C18-C19
26	f	101	SQD	C31-C32-C33-C34
31	d	409	LHG	C33-C34-C35-C36
23	c	508	CLA	C5-C6-C7-C8
35	D	402	LMT	C3-C4-C5-C6
23	B	605	CLA	C4-C3-C5-C6
36	c	518	DGD	CAB-CBB-CCB-CDB
23	b	613	CLA	CBD-CGD-O2D-CED
31	A	417	LHG	C12-C13-C14-C15
23	b	601	CLA	O1A-CGA-O2A-C1
33	Z	101	LMG	C18-C19-C20-C21
33	j	101	LMG	O6-C5-C6-O5
35	I	101	LMT	O5'-C5'-C6'-O6'
26	A	410	SQD	O6-C44-C45-C46
26	L	101	SQD	C44-C45-C46-O48
26	a	412	SQD	O6-C44-C45-C46
31	D	409	LHG	C4-C5-C6-O8
33	Z	101	LMG	C8-C7-O1-C1
36	C	518	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	517	DGD	C5D-C6D-O5D-C1E
31	D	408	LHG	C17-C18-C19-C20
36	C	519	DGD	CBA-CCA-CDA-CEA
34	c	522	HTG	O5-C5-C6-O6
23	B	602	CLA	C13-C15-C16-C17
23	b	613	CLA	C5-C6-C7-C8
23	d	404	CLA	C5-C6-C7-C8
35	D	402	LMT	C5-C6-C7-C8
23	a	404	CLA	O1D-CGD-O2D-CED
29	a	414	PL9	C14-C16-C17-C18
31	D	408	LHG	C28-C29-C30-C31
33	C	520	LMG	C15-C16-C17-C18
26	B	620	SQD	C24-C23-O48-C46
27	a	411	GOL	O2-C2-C3-O3
31	A	416	LHG	O1-C1-C2-O2
31	E	101	LHG	O1-C1-C2-O2
31	l	101	LHG	C26-C27-C28-C29
36	c	517	DGD	CBA-CCA-CDA-CEA
23	B	601	CLA	CAA-CBA-CGA-O2A
35	B	629	LMT	C4'-C5'-C6'-O6'
23	A	406	CLA	C2C-C3C-CAC-CBC
35	a	417	LMT	C11-C10-C9-C8
23	B	615	CLA	C13-C15-C16-C17
23	C	514	CLA	C4-C3-C5-C6
33	c	519	LMG	C21-C22-C23-C24
23	c	502	CLA	C16-C17-C18-C19
26	a	410	SQD	C10-C11-C12-C13
35	a	417	LMT	C4-C5-C6-C7
23	c	506	CLA	C10-C11-C12-C13
31	A	416	LHG	C29-C30-C31-C32
23	a	404	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C2-C1-O2A-CGA
33	C	520	LMG	C36-C37-C38-C39
35	M	103	LMT	C6-C7-C8-C9
31	E	101	LHG	C25-C26-C27-C28
35	B	630	LMT	C6-C7-C8-C9
23	b	612	CLA	C10-C11-C12-C13
34	b	628	HTG	C3'-C4'-C5'-C6'
36	c	517	DGD	C2E-C1E-O5D-C6D
40	V	202	HEC	C2B-C3B-CAB-CBB
26	f	101	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
33	a	416	LMG	O7-C8-C9-O8
31	e	101	LHG	C11-C12-C13-C14
23	D	405	CLA	C8-C10-C11-C12
23	B	615	CLA	C16-C17-C18-C19
34	B	623	HTG	C3'-C4'-C5'-C6'
29	d	406	PL9	C15-C14-C16-C17
35	M	103	LMT	C4'-C5'-C6'-O6'
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	509	CLA	C12-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C15
36	h	102	DGD	O2G-C1B-C2B-C3B
23	b	607	CLA	C3-C5-C6-C7
23	B	604	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C12-C13-C14
23	d	404	CLA	C11-C10-C8-C9
36	H	102	DGD	C7B-C8B-C9B-CAB
23	B	611	CLA	C13-C15-C16-C17
26	A	410	SQD	C12-C13-C14-C15
26	B	620	SQD	O10-C23-O48-C46
33	B	621	LMG	C14-C15-C16-C17
25	K	102	BCR	C7-C8-C9-C10
34	B	622	HTG	C2'-C3'-C4'-C5'
36	c	517	DGD	C9B-CAB-CBB-CCB
35	e	102	LMT	C4'-C5'-C6'-O6'
23	c	511	CLA	CBA-CGA-O2A-C1
33	B	621	LMG	C37-C38-C39-C40
34	c	521	HTG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
23	A	406	CLA	C4B-C3B-CAB-CBB
23	A	408	CLA	C4B-C3B-CAB-CBB
23	B	607	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C4B-C3B-CAB-CBB
29	a	414	PL9	C9-C11-C12-C13
33	Z	102	LMG	C17-C18-C19-C20
33	j	101	LMG	C35-C36-C37-C38
36	c	517	DGD	CAA-CBA-CCA-CDA
36	c	518	DGD	CBA-CCA-CDA-CEA
29	a	414	PL9	C20-C19-C21-C22
23	C	507	CLA	C2-C3-C5-C6
29	d	406	PL9	C13-C14-C16-C17
23	B	613	CLA	C15-C16-C17-C18
35	E	102	LMT	C9-C10-C11-C12
36	c	517	DGD	C7B-C8B-C9B-CAB
23	b	602	CLA	C16-C17-C18-C19
23	C	512	CLA	CBA-CGA-O2A-C1
23	b	611	CLA	CBA-CGA-O2A-C1
26	a	412	SQD	C24-C23-O48-C46
33	C	520	LMG	C10-C11-C12-C13
23	C	507	CLA	C3A-C2A-CAA-CBA
26	f	101	SQD	C34-C35-C36-C37
33	B	621	LMG	C33-C34-C35-C36
36	c	517	DGD	C2B-C3B-C4B-C5B
36	C	519	DGD	CDA-CEA-CFA-CGA
24	A	407	PHO	C2C-C3C-CAC-CBC
33	Z	101	LMG	C33-C34-C35-C36
35	e	102	LMT	C2B-C1B-O1B-C4'
23	b	602	CLA	C16-C17-C18-C20
36	c	516	DGD	C2A-C1A-O1G-C1G
31	e	101	LHG	C14-C15-C16-C17
31	E	101	LHG	C4-C5-C6-O8
31	e	101	LHG	C4-C5-C6-O8
33	b	620	LMG	O1-C7-C8-C9
36	C	517	DGD	C9A-CAA-CBA-CCA
36	C	517	DGD	C8A-C9A-CAA-CBA
29	a	414	PL9	C45-C44-C46-C47
36	C	519	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C2-C3-C5-C6
31	d	409	LHG	C30-C31-C32-C33
36	h	102	DGD	CDA-CEA-CFA-CGA
23	c	511	CLA	O1A-CGA-O2A-C1
35	B	629	LMT	O5'-C5'-C6'-O6'
36	H	102	DGD	C9B-CAB-CBB-CCB
23	B	601	CLA	C2A-CAA-CBA-CGA
31	A	417	LHG	O1-C1-C2-O2
23	b	603	CLA	C13-C15-C16-C17
36	c	516	DGD	CDB-CEB-CFB-CGB
23	D	405	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
23	C	507	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
33	a	416	LMG	C20-C21-C22-C23
34	b	628	HTG	C2'-C3'-C4'-C5'
26	A	410	SQD	O6-C44-C45-O47
26	B	620	SQD	O47-C45-C46-O48
26	L	101	SQD	O47-C45-C46-O48
31	D	409	LHG	O7-C5-C6-O8
33	b	620	LMG	O1-C7-C8-O7
24	a	407	PHO	C2C-C3C-CAC-CBC
36	c	517	DGD	O6E-C1E-O5D-C6D
23	b	615	CLA	C5-C6-C7-C8
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
29	a	414	PL9	C18-C19-C21-C22
29	a	414	PL9	C43-C44-C46-C47
33	C	520	LMG	C16-C17-C18-C19
36	h	102	DGD	C9A-CAA-CBA-CCA
23	B	604	CLA	C13-C15-C16-C17
23	A	408	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	C	503	CLA	C14-C13-C15-C16
23	D	405	CLA	C11-C10-C8-C9
23	b	609	CLA	C6-C7-C8-C9
26	A	412	SQD	C15-C16-C17-C18
33	C	520	LMG	C13-C14-C15-C16
23	C	510	CLA	CBD-CGD-O2D-CED
33	Z	102	LMG	C11-C12-C13-C14
23	B	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	D	409	LHG	C2-C3-O3-P
23	C	512	CLA	O1A-CGA-O2A-C1
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
25	Y	101	BCR	C21-C22-C23-C24
23	b	603	CLA	C10-C11-C12-C13
31	d	408	LHG	C28-C29-C30-C31
33	a	416	LMG	C36-C37-C38-C39
23	A	404	CLA	C13-C15-C16-C17
23	C	507	CLA	C13-C15-C16-C17
31	l	101	LHG	O6-C4-C5-C6
36	h	102	DGD	C9B-CAB-CBB-CCB
23	B	604	CLA	C6-C7-C8-C10
23	B	614	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	C	502	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	b	603	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C12-C13-C15
23	c	502	CLA	C12-C13-C15-C16
23	d	404	CLA	C11-C10-C8-C7
26	L	101	SQD	C12-C13-C14-C15
23	C	508	CLA	C13-C15-C16-C17
31	e	101	LHG	C9-C10-C11-C12
23	C	507	CLA	C8-C10-C11-C12
24	a	407	PHO	C8-C10-C11-C12
23	B	604	CLA	C2C-C3C-CAC-CBC
31	A	416	LHG	C24-C25-C26-C27
23	b	602	CLA	C10-C11-C12-C13
33	b	620	LMG	C35-C36-C37-C38
34	b	625	HTG	C2'-C1'-S1-C1
34	c	521	HTG	C2'-C1'-S1-C1
23	b	611	CLA	C3-C5-C6-C7
26	L	101	SQD	C24-C23-O48-C46
33	a	416	LMG	C29-C28-O8-C9
31	D	409	LHG	C17-C18-C19-C20
23	B	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	D	401	PHO	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
26	B	620	SQD	C46-C45-O47-C7
26	L	101	SQD	C46-C45-O47-C7
38	e	103	HEM	C2B-C3B-CAB-CBB
23	C	512	CLA	C3-C5-C6-C7
23	B	611	CLA	C8-C10-C11-C12
23	c	506	CLA	C15-C16-C17-C18
23	d	401	CLA	C15-C16-C17-C18
31	d	407	LHG	C24-C23-O8-C6
31	A	417	LHG	C14-C15-C16-C17
31	d	408	LHG	C26-C27-C28-C29
36	C	519	DGD	O6D-C1D-O3G-C3G
23	c	512	CLA	C15-C16-C17-C18
31	E	101	LHG	C23-C24-C25-C26
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	f	101	SQD	C44-C45-C46-O48
23	c	509	CLA	CBD-CGD-O2D-CED
23	b	611	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C3-C5-C6-C7
23	A	405	CLA	C2C-C3C-CAC-CBC
36	C	519	DGD	O6E-C5E-C6E-O5E
23	b	602	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C8-C10-C11-C12
26	A	412	SQD	O49-C7-O47-C45
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	D	405	CLA	O1A-CGA-O2A-C1
26	a	412	SQD	O10-C23-O48-C46
31	D	408	LHG	O10-C23-O8-C6
36	C	519	DGD	O1A-C1A-O1G-C1G
36	c	516	DGD	O1A-C1A-O1G-C1G
36	h	102	DGD	CBA-CCA-CDA-CEA
36	c	516	DGD	C2E-C1E-O5D-C6D
23	b	604	CLA	C13-C15-C16-C17
29	A	414	PL9	C2-C3-C7-C8
31	A	416	LHG	C11-C12-C13-C14
26	a	410	SQD	O6-C44-C45-O47
26	f	101	SQD	O47-C45-C46-O48
23	B	608	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	d	401	CLA	C13-C15-C16-C17
31	d	409	LHG	C9-C10-C11-C12
23	C	510	CLA	C3-C5-C6-C7
26	A	412	SQD	C8-C7-O47-C45
23	b	601	CLA	C4-C3-C5-C6
29	A	414	PL9	C30-C29-C31-C32
26	A	410	SQD	C18-C19-C20-C21
31	A	416	LHG	C33-C34-C35-C36
36	H	102	DGD	CCB-CDB-CEB-CFB
31	d	407	LHG	O10-C23-O8-C6
36	c	516	DGD	CDA-CEA-CFA-CGA
23	C	502	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
35	e	102	LMT	C4-C5-C6-C7
23	a	408	CLA	C16-C17-C18-C20
34	b	623	HTG	C4-C5-C6-O6
26	D	413	SQD	C27-C28-C29-C30
23	B	604	CLA	C3-C5-C6-C7
33	B	621	LMG	O6-C5-C6-O5
23	A	408	CLA	C16-C17-C18-C19
31	E	101	LHG	C15-C16-C17-C18
36	h	102	DGD	C4B-C5B-C6B-C7B
25	k	101	BCR	C9-C10-C11-C12
31	d	408	LHG	O10-C23-O8-C6
33	a	416	LMG	O10-C28-O8-C9
23	A	405	CLA	C13-C15-C16-C17
31	d	409	LHG	C29-C30-C31-C32
29	A	414	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C10-C11-C12-C13
33	j	101	LMG	C19-C20-C21-C22
26	L	101	SQD	O10-C23-O48-C46
23	C	513	CLA	C4B-C3B-CAB-CBB
23	b	601	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
31	A	417	LHG	C4-O6-P-O5
31	D	408	LHG	C3-O3-P-O4
31	D	408	LHG	C4-O6-P-O5
31	d	408	LHG	C4-O6-P-O5
31	d	409	LHG	C4-O6-P-O5
23	A	406	CLA	C16-C17-C18-C19
35	E	102	LMT	O1'-C1-C2-C3
35	m	102	LMT	C9-C10-C11-C12
26	L	101	SQD	O5-C1-O6-C44
23	c	512	CLA	CBA-CGA-O2A-C1
31	d	408	LHG	C24-C23-O8-C6
29	d	406	PL9	C9-C11-C12-C13
23	C	513	CLA	C3-C5-C6-C7
31	D	408	LHG	C33-C34-C35-C36
31	d	409	LHG	C26-C27-C28-C29
33	j	101	LMG	C16-C17-C18-C19
35	e	102	LMT	O5B-C1B-O1B-C4'
34	B	622	HTG	C3'-C4'-C5'-C6'
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
34	c	521	HTG	C3'-C4'-C5'-C6'
34	B	623	HTG	C4'-C5'-C6'-C7'
23	b	613	CLA	O1D-CGD-O2D-CED
23	A	406	CLA	C12-C13-C15-C16
23	B	604	CLA	C11-C12-C13-C15
23	B	605	CLA	C6-C7-C8-C10
23	C	514	CLA	C6-C7-C8-C10
23	b	601	CLA	C2-C3-C5-C6
23	c	512	CLA	C6-C7-C8-C10
33	z	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
34	c	521	HTG	C2-C1-S1-C1'
23	B	606	CLA	C10-C11-C12-C13
23	c	509	CLA	C13-C15-C16-C17
33	Z	101	LMG	C37-C38-C39-C40
23	b	605	CLA	O1A-CGA-O2A-C1
36	h	102	DGD	CAB-CBB-CCB-CDB
26	f	101	SQD	O6-C44-C45-C46
33	a	416	LMG	C7-C8-C9-O8
31	E	101	LHG	O7-C5-C6-O8
31	e	101	LHG	O7-C5-C6-O8
33	Z	102	LMG	C15-C16-C17-C18
33	j	101	LMG	C14-C15-C16-C17
35	B	629	LMT	C3-C4-C5-C6
23	b	609	CLA	O1A-CGA-O2A-C1
31	d	407	LHG	C11-C12-C13-C14
31	l	101	LHG	C9-C10-C11-C12
35	D	403	LMT	C5-C6-C7-C8
35	M	103	LMT	O5B-C5B-C6B-O6B
36	c	517	DGD	C2G-C3G-O3G-C1D
23	c	508	CLA	C16-C17-C18-C19
35	M	103	LMT	O1'-C1-C2-C3
29	D	407	PL9	C30-C29-C31-C32
29	D	407	PL9	C45-C44-C46-C47
23	A	408	CLA	C2-C3-C5-C6
29	A	414	PL9	C28-C29-C31-C32
29	D	407	PL9	C28-C29-C31-C32
23	b	604	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	C11-C12-C13-C14
23	C	513	CLA	C11-C10-C8-C9
23	a	408	CLA	C11-C10-C8-C9
23	b	601	CLA	C11-C10-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C12-C13-C14
23	c	512	CLA	O1A-CGA-O2A-C1
33	c	519	LMG	C29-C30-C31-C32
23	B	604	CLA	C4C-C3C-CAC-CBC
40	v	201	HEC	C2B-C3B-CAB-CBB
29	a	414	PL9	C39-C41-C42-C43
36	c	518	DGD	O1A-C1A-O1G-C1G
36	H	102	DGD	O2G-C1B-C2B-C3B
31	D	409	LHG	C30-C31-C32-C33
33	c	519	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
23	A	406	CLA	C4C-C3C-CAC-CBC
23	b	601	CLA	CAA-CBA-CGA-O2A
31	D	409	LHG	C10-C11-C12-C13
23	A	406	CLA	C2B-C3B-CAB-CBB
23	A	408	CLA	C2B-C3B-CAB-CBB
23	B	603	CLA	C2B-C3B-CAB-CBB
23	B	607	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	b	601	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C2B-C3B-CAB-CBB
35	D	402	LMT	O1'-C1-C2-C3
31	d	407	LHG	C24-C25-C26-C27
35	D	403	LMT	C6-C7-C8-C9
35	b	621	LMT	C11-C10-C9-C8
23	C	514	CLA	C2-C3-C5-C6
26	D	413	SQD	C23-C24-C25-C26
33	C	501	LMG	C12-C13-C14-C15
36	H	102	DGD	C4A-C5A-C6A-C7A
31	e	101	LHG	C24-C25-C26-C27
33	b	620	LMG	C22-C23-C24-C25
23	B	602	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
33	a	416	LMG	C10-C11-C12-C13
23	c	510	CLA	O1A-CGA-O2A-C1
35	M	103	LMT	O5B-C1B-O1B-C4'
31	d	409	LHG	C2-C3-O3-P
34	b	623	HTG	S1-C1'-C2'-C3'
23	b	616	CLA	O1A-CGA-O2A-C1
23	A	405	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	C	507	CLA	C5-C6-C7-C8
31	d	407	LHG	C7-C8-C9-C10
25	C	516	BCR	C1-C6-C7-C8
25	C	516	BCR	C5-C6-C7-C8
23	B	605	CLA	C2-C3-C5-C6
29	A	414	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
33	b	620	LMG	C37-C38-C39-C40
35	D	403	LMT	C2-C3-C4-C5
23	b	609	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
33	z	101	LMG	O6-C1-O1-C7
23	C	503	CLA	C10-C11-C12-C13
36	C	519	DGD	C2D-C1D-O3G-C3G
40	V	202	HEC	C4B-C3B-CAB-CBB
31	E	101	LHG	C4-O6-P-O3
36	c	518	DGD	CCB-CDB-CEB-CFB
23	a	404	CLA	C16-C17-C18-C19
31	A	417	LHG	C30-C31-C32-C33
35	B	629	LMT	C4-C5-C6-C7
23	b	612	CLA	C13-C15-C16-C17
23	C	513	CLA	C11-C10-C8-C7
23	D	405	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
26	A	410	SQD	C16-C17-C18-C19
23	C	506	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C9
23	C	506	CLA	C5-C6-C7-C8
33	c	519	LMG	C35-C36-C37-C38
33	c	520	LMG	C36-C37-C38-C39
26	f	101	SQD	C29-C30-C31-C32
31	A	417	LHG	C16-C17-C18-C19
23	b	613	CLA	O1A-CGA-O2A-C1
23	d	404	CLA	C16-C17-C18-C20
23	c	510	CLA	CBA-CGA-O2A-C1
35	E	102	LMT	C2B-C1B-O1B-C4'
35	e	102	LMT	C1-C2-C3-C4
29	a	414	PL9	C25-C24-C26-C27
23	C	514	CLA	O1A-CGA-O2A-C1
23	a	408	CLA	C16-C17-C18-C19
23	C	514	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C2A-C1A-O1G-C1G
29	a	414	PL9	C2-C3-C7-C8
23	a	408	CLA	C15-C16-C17-C18
34	b	625	HTG	C1'-C2'-C3'-C4'
23	C	513	CLA	CBA-CGA-O2A-C1
36	C	518	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
25	t	101	BCR	C15-C16-C17-C18
35	M	103	LMT	C2B-C1B-O1B-C4'
23	b	609	CLA	C13-C15-C16-C17
23	D	404	CLA	C2C-C3C-CAC-CBC
35	m	102	LMT	C6-C7-C8-C9
31	A	417	LHG	C11-C12-C13-C14
23	C	507	CLA	C3-C5-C6-C7
26	a	412	SQD	C12-C13-C14-C15
33	c	519	LMG	O6-C5-C6-O5
23	C	513	CLA	O1A-CGA-O2A-C1
23	B	608	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
35	M	103	LMT	C4B-C5B-C6B-O6B
26	L	101	SQD	C10-C11-C12-C13
35	E	102	LMT	C3-C4-C5-C6
33	C	501	LMG	O8-C28-C29-C30
33	J	101	LMG	C19-C20-C21-C22
33	z	101	LMG	C12-C13-C14-C15
36	H	102	DGD	C6B-C7B-C8B-C9B
23	A	406	CLA	C3A-C2A-CAA-CBA
23	b	608	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	A	406	CLA	C16-C17-C18-C20
23	B	612	CLA	CBA-CGA-O2A-C1
33	j	101	LMG	C28-C29-C30-C31
29	D	407	PL9	C43-C44-C46-C47
23	A	404	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C14
23	C	510	CLA	C6-C7-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	c	508	CLA	C16-C17-C18-C20
26	B	620	SQD	C11-C10-C9-C8
31	l	101	LHG	C24-C25-C26-C27
36	C	517	DGD	CCA-CDA-CEA-CFA
26	a	410	SQD	O6-C44-C45-C46
33	C	501	LMG	C14-C15-C16-C17
24	D	401	PHO	CBA-CGA-O2A-C1
36	C	519	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C10-C11-C12-C13
33	b	620	LMG	C19-C20-C21-C22
38	E	103	HEM	CAD-CBD-CGD-O1D
36	h	102	DGD	O1B-C1B-C2B-C3B
23	a	405	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	C11-C12-C13-C15
23	B	615	CLA	C11-C12-C13-C15
23	d	404	CLA	C12-C13-C15-C16
31	d	407	LHG	C17-C18-C19-C20
23	B	601	CLA	CAA-CBA-CGA-O1A
26	D	413	SQD	C29-C30-C31-C32
23	C	510	CLA	O1D-CGD-O2D-CED
35	E	102	LMT	O5B-C1B-O1B-C4'
31	l	101	LHG	C13-C14-C15-C16
23	B	613	CLA	C13-C15-C16-C17
31	A	416	LHG	C28-C29-C30-C31
23	b	616	CLA	C4-C3-C5-C6
31	D	408	LHG	C9-C10-C11-C12
33	j	101	LMG	C15-C16-C17-C18
23	b	603	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
35	M	101	LMT	C2-C3-C4-C5
40	v	201	HEC	CAD-CBD-CGD-O2D
23	C	508	CLA	C2A-CAA-CBA-CGA
25	a	409	BCR	C19-C20-C21-C22
23	a	405	CLA	C13-C15-C16-C17
31	A	417	LHG	C32-C33-C34-C35
26	A	412	SQD	O5-C1-O6-C44
34	b	622	HTG	C2'-C3'-C4'-C5'
23	c	509	CLA	O1D-CGD-O2D-CED
29	d	406	PL9	C34-C36-C37-C38
38	e	103	HEM	CAD-CBD-CGD-O1D
23	b	614	CLA	C2-C1-O2A-CGA
23	B	603	CLA	CBD-CGD-O2D-CED
36	C	518	DGD	C4A-C5A-C6A-C7A
31	d	409	LHG	C31-C32-C33-C34
23	c	504	CLA	C11-C12-C13-C14
33	c	519	LMG	C30-C31-C32-C33
23	b	606	CLA	CBD-CGD-O2D-CED
26	B	620	SQD	C34-C35-C36-C37
31	l	101	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
26	D	413	SQD	C28-C29-C30-C31
35	M	101	LMT	O5'-C5'-C6'-O6'
35	m	102	LMT	O5'-C5'-C6'-O6'
40	v	201	HEC	C4B-C3B-CAB-CBB
23	B	615	CLA	C3-C5-C6-C7
25	A	409	BCR	C1-C6-C7-C8
25	D	406	BCR	C1-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C30
25	d	405	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
34	b	628	HTG	C4-C5-C6-O6
27	B	626	GOL	O1-C1-C2-C3
23	b	613	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	C4-C3-C5-C6
29	D	407	PL9	C35-C34-C36-C37
29	a	414	PL9	C15-C14-C16-C17
23	D	405	CLA	C10-C11-C12-C13
23	b	607	CLA	C13-C15-C16-C17
40	v	201	HEC	CAD-CBD-CGD-O1D
35	I	101	LMT	C1-C2-C3-C4
38	E	103	HEM	CAD-CBD-CGD-O2D
38	e	103	HEM	CAA-CBA-CGA-O2A
31	D	409	LHG	O6-C4-C5-O7
26	a	410	SQD	C31-C32-C33-C34
38	e	103	HEM	CAA-CBA-CGA-O1A
23	c	503	CLA	C2A-CAA-CBA-CGA
23	A	405	CLA	C4C-C3C-CAC-CBC
33	b	620	LMG	C33-C34-C35-C36
36	C	519	DGD	C8B-C9B-CAB-CBB
23	B	608	CLA	C4B-C3B-CAB-CBB
24	D	401	PHO	O1A-CGA-O2A-C1
26	L	101	SQD	C11-C10-C9-C8
23	B	616	CLA	C11-C12-C13-C15
23	C	503	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C7
23	c	510	CLA	C2-C3-C5-C6
23	c	510	CLA	C6-C7-C8-C10
23	b	603	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C2-C1-O6-C44
33	C	501	LMG	C29-C30-C31-C32
36	C	517	DGD	C7A-C8A-C9A-CAA
34	b	625	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
23	B	609	CLA	O1A-CGA-O2A-C1
23	b	606	CLA	C16-C17-C18-C19
33	Z	102	LMG	C18-C19-C20-C21
35	M	103	LMT	C1-C2-C3-C4
23	b	611	CLA	C13-C15-C16-C17
33	a	416	LMG	C29-C30-C31-C32
34	c	521	HTG	O5-C1-S1-C1'
31	l	101	LHG	O7-C7-C8-C9
29	d	406	PL9	C45-C44-C46-C47
23	d	404	CLA	C10-C11-C12-C13
33	a	416	LMG	C21-C22-C23-C24
33	c	519	LMG	C32-C33-C34-C35
23	B	612	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	C2-C3-C5-C6
35	I	101	LMT	C5'-C4'-O1B-C1B
36	c	516	DGD	C6B-C7B-C8B-C9B
23	b	615	CLA	C16-C17-C18-C19
23	A	406	CLA	C14-C13-C15-C16
23	B	604	CLA	C11-C12-C13-C14
23	B	605	CLA	C14-C13-C15-C16
23	B	611	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
38	E	103	HEM	CAA-CBA-CGA-O1A
31	d	408	LHG	C35-C36-C37-C38
23	B	612	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
33	j	101	LMG	C36-C37-C38-C39
23	B	613	CLA	CAA-CBA-CGA-O2A
31	e	101	LHG	O8-C23-C24-C25
40	V	202	HEC	CAD-CBD-CGD-O1D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	609	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
24	a	406	PHO	CAD-CBD-CGD-O2D
23	b	607	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C19
23	B	609	CLA	C13-C15-C16-C17
36	c	517	DGD	O1B-C1B-O2G-C2G
38	e	103	HEM	CAD-CBD-CGD-O2D
23	B	612	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	CAA-CBA-CGA-O2A
23	b	613	CLA	CAA-CBA-CGA-O2A
26	a	412	SQD	O48-C23-C24-C25
33	C	520	LMG	O8-C28-C29-C30
33	Z	102	LMG	O7-C10-C11-C12
33	C	501	LMG	C16-C17-C18-C19
36	C	519	DGD	C6B-C7B-C8B-C9B
23	B	607	CLA	C4-C3-C5-C6
29	D	407	PL9	C33-C34-C36-C37
26	f	101	SQD	O47-C7-C8-C9
33	C	520	LMG	O7-C10-C11-C12
25	b	619	BCR	C21-C22-C23-C24
26	B	620	SQD	C16-C17-C18-C19
23	b	603	CLA	O1A-CGA-O2A-C1
31	d	408	LHG	C25-C26-C27-C28
23	b	612	CLA	CAA-CBA-CGA-O2A
33	J	101	LMG	O7-C10-C11-C12
34	b	622	HTG	C4'-C5'-C6'-C7'
40	V	202	HEC	CAD-CBD-CGD-O2D
31	l	101	LHG	C35-C36-C37-C38
23	B	602	CLA	O2A-C1-C2-C3
23	b	602	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
24	D	401	PHO	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
26	A	412	SQD	C30-C31-C32-C33
36	C	519	DGD	C3A-C4A-C5A-C6A
36	H	102	DGD	CDB-CEB-CFB-CGB
38	e	103	HEM	C4B-C3B-CAB-CBB
23	a	405	CLA	C16-C17-C18-C20
36	C	517	DGD	CDB-CEB-CFB-CGB
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
25	y	101	BCR	C9-C10-C11-C12
31	A	417	LHG	O7-C7-C8-C9
26	L	101	SQD	C29-C30-C31-C32
34	d	411	HTG	C1'-C2'-C3'-C4'
23	c	507	CLA	C5-C6-C7-C8
33	c	519	LMG	O7-C10-C11-C12
36	C	519	DGD	CCB-CDB-CEB-CFB
33	Z	102	LMG	O1-C7-C8-O7
35	b	621	LMT	C6-C7-C8-C9
35	B	630	LMT	C4-C5-C6-C7
23	c	510	CLA	CAA-CBA-CGA-O2A
26	L	101	SQD	C18-C19-C20-C21
23	D	404	CLA	C16-C17-C18-C20
24	D	401	PHO	CHA-CBD-CGD-O1D
26	A	410	SQD	C13-C14-C15-C16
23	A	406	CLA	CBA-CGA-O2A-C1
35	I	101	LMT	C4-C5-C6-C7
23	A	406	CLA	O1A-CGA-O2A-C1
23	A	404	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	D	405	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	c	505	CLA	C6-C7-C8-C10
36	c	517	DGD	CBB-CCB-CDB-CEB
35	B	630	LMT	C3-C4-C5-C6
23	A	404	CLA	C11-C12-C13-C14
23	C	505	CLA	C6-C7-C8-C9
23	c	504	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C17-C18-C19-C20
23	c	508	CLA	C2B-C3B-CAB-CBB
38	E	103	HEM	CAA-CBA-CGA-O2A
34	c	521	HTG	C2'-C3'-C4'-C5'
26	L	101	SQD	O48-C23-C24-C25
31	d	409	LHG	O8-C23-C24-C25
26	A	412	SQD	C5-C6-S-O8
23	C	511	CLA	C16-C17-C18-C20
23	a	404	CLA	C16-C17-C18-C20
29	a	414	PL9	C31-C32-C33-C34
36	h	102	DGD	CAA-CBA-CCA-CDA
33	C	520	LMG	O9-C10-C11-C12
33	C	520	LMG	O10-C28-C29-C30
31	d	408	LHG	C17-C18-C19-C20
23	b	612	CLA	CAA-CBA-CGA-O1A
26	a	412	SQD	O10-C23-C24-C25
31	l	101	LHG	O9-C7-C8-C9
33	C	520	LMG	C32-C33-C34-C35
23	b	604	CLA	C8-C10-C11-C12
31	E	101	LHG	C12-C13-C14-C15
31	l	101	LHG	C28-C29-C30-C31
23	C	507	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C1A-C2A-CAA-CBA
36	C	519	DGD	C1B-C2B-C3B-C4B
31	e	101	LHG	O10-C23-C24-C25
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	CAA-CBA-CGA-O1A
26	f	101	SQD	O49-C7-C8-C9
33	J	101	LMG	O9-C10-C11-C12
33	B	621	LMG	O1-C7-C8-C9
23	B	603	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
34	B	627	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	CDB-CEB-CFB-CGB
35	E	102	LMT	C6-C7-C8-C9
23	B	610	CLA	C13-C15-C16-C17
23	c	513	CLA	C4B-C3B-CAB-CBB
31	A	417	LHG	C3-O3-P-O5
31	D	409	LHG	C4-O6-P-O5
31	E	101	LHG	C4-O6-P-O5
23	B	616	CLA	C16-C17-C18-C20
36	C	519	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	CAA-CBA-CGA-O1A
31	A	417	LHG	O9-C7-C8-C9
33	Z	102	LMG	O9-C10-C11-C12
36	h	102	DGD	C6A-C7A-C8A-C9A
25	A	409	BCR	C5-C6-C7-C8
25	d	405	BCR	C23-C24-C25-C26
23	B	612	CLA	CAA-CBA-CGA-O1A
26	a	410	SQD	C26-C27-C28-C29
35	B	629	LMT	C3'-C4'-O1B-C1B
23	C	506	CLA	CAA-CBA-CGA-O2A
29	D	407	PL9	C11-C12-C13-C14
29	D	407	PL9	C36-C37-C38-C39
23	A	406	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
33	c	519	LMG	O9-C10-C11-C12
36	H	102	DGD	C2B-C3B-C4B-C5B
23	B	606	CLA	C11-C10-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	a	404	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C9
31	e	101	LHG	C23-C24-C25-C26
26	A	412	SQD	C28-C29-C30-C31
35	B	630	LMT	C4'-C5'-C6'-O6'
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
31	d	407	LHG	C1-C2-C3-O3
36	H	102	DGD	C5B-C6B-C7B-C8B
36	c	516	DGD	CCB-CDB-CEB-CFB
31	d	407	LHG	C18-C19-C20-C21
23	B	601	CLA	C11-C10-C8-C7
23	B	615	CLA	C6-C7-C8-C10
23	a	404	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C15
29	a	414	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	O6-C4-C5-O7
23	c	512	CLA	CAA-CBA-CGA-O2A
26	A	410	SQD	O47-C7-C8-C9
33	b	620	LMG	O7-C10-C11-C12
36	C	517	DGD	O2G-C1B-C2B-C3B
23	c	512	CLA	CAA-CBA-CGA-O1A
26	A	410	SQD	O49-C7-C8-C9
31	d	409	LHG	O10-C23-C24-C25
35	D	403	LMT	C3-C4-C5-C6
23	C	509	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
23	c	510	CLA	C13-C15-C16-C17
36	C	518	DGD	CBA-CCA-CDA-CEA
26	L	101	SQD	O10-C23-C24-C25
33	b	620	LMG	O9-C10-C11-C12
33	B	621	LMG	C19-C20-C21-C22
23	b	616	CLA	C10-C11-C12-C13
36	c	516	DGD	O2G-C1B-C2B-C3B
23	B	612	CLA	C13-C15-C16-C17
23	c	510	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	C13-C15-C16-C17
23	b	602	CLA	CAA-CBA-CGA-O2A
23	c	505	CLA	CAA-CBA-CGA-O2A
36	C	517	DGD	O1G-C1A-C2A-C3A
35	b	621	LMT	C3'-C4'-O1B-C1B

There are no ring outliers.

151 monomers are involved in 343 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	518	DGD	2	0
23	B	613	CLA	2	0
23	a	405	CLA	2	0
34	b	622	HTG	2	0
23	c	513	CLA	7	0
23	b	604	CLA	5	0
23	b	601	CLA	2	0
25	C	515	BCR	2	0
35	M	103	LMT	1	0
23	B	614	CLA	4	0
31	e	101	LHG	2	0
24	A	407	PHO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	408	CLA	3	0
23	C	504	CLA	5	0
31	D	408	LHG	2	0
23	B	616	CLA	6	0
23	b	605	CLA	7	0
23	c	509	CLA	5	0
36	c	517	DGD	3	0
25	a	409	BCR	1	0
25	B	619	BCR	3	0
26	A	410	SQD	3	0
26	A	412	SQD	3	0
38	e	103	HEM	3	0
34	c	521	HTG	1	0
23	C	503	CLA	2	0
36	H	102	DGD	1	0
23	C	505	CLA	1	0
29	A	414	PL9	6	0
35	D	403	LMT	2	0
23	c	511	CLA	3	0
34	B	623	HTG	2	0
36	c	516	DGD	3	0
35	I	101	LMT	1	0
23	c	506	CLA	5	0
23	b	616	CLA	3	0
23	D	404	CLA	3	0
23	C	514	CLA	7	0
23	C	509	CLA	3	0
23	b	613	CLA	3	0
25	c	514	BCR	6	0
25	T	101	BCR	5	0
33	b	620	LMG	1	0
26	L	101	SQD	5	0
23	B	605	CLA	6	0
25	b	617	BCR	2	0
33	c	519	LMG	1	0
23	c	510	CLA	3	0
31	A	416	LHG	3	0
35	b	621	LMT	1	0
36	C	519	DGD	1	0
23	b	609	CLA	5	0
23	b	603	CLA	3	0
23	c	508	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	512	CLA	6	0
23	B	607	CLA	1	0
25	d	405	BCR	5	0
34	B	622	HTG	4	0
23	B	603	CLA	1	0
25	b	619	BCR	2	0
23	C	508	CLA	5	0
31	d	408	LHG	3	0
25	c	515	BCR	4	0
23	b	611	CLA	1	0
23	C	510	CLA	1	0
23	b	610	CLA	1	0
23	C	502	CLA	3	0
33	Z	101	LMG	2	0
36	c	518	DGD	3	0
35	D	402	LMT	2	0
23	B	601	CLA	2	0
25	y	101	BCR	1	0
31	d	409	LHG	7	0
33	z	101	LMG	1	0
26	D	413	SQD	1	0
23	a	404	CLA	4	0
25	H	101	BCR	3	0
27	C	523	GOL	1	0
35	M	101	LMT	2	0
23	B	610	CLA	1	0
25	Y	101	BCR	2	0
23	c	507	CLA	4	0
34	b	625	HTG	1	0
26	a	410	SQD	4	0
23	d	403	CLA	4	0
23	C	506	CLA	8	0
33	j	101	LMG	2	0
23	c	501	CLA	3	0
25	A	409	BCR	1	0
24	a	406	PHO	1	0
23	B	604	CLA	4	0
27	a	411	GOL	1	0
25	t	101	BCR	3	0
35	B	630	LMT	3	0
31	A	417	LHG	2	0
33	B	621	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	618	BCR	4	0
23	b	608	CLA	2	0
25	b	618	BCR	3	0
23	B	611	CLA	2	0
24	a	407	PHO	3	0
25	h	101	BCR	5	0
33	Z	102	LMG	1	0
23	b	602	CLA	1	0
23	C	513	CLA	5	0
23	A	405	CLA	2	0
23	B	606	CLA	3	0
33	J	101	LMG	3	0
25	B	617	BCR	1	0
25	D	406	BCR	2	0
23	b	615	CLA	3	0
23	c	502	CLA	3	0
23	B	602	CLA	5	0
23	c	503	CLA	3	0
35	E	102	LMT	1	0
31	D	409	LHG	4	0
23	c	504	CLA	2	0
27	B	625	GOL	1	0
33	a	416	LMG	4	0
34	c	522	HTG	1	0
23	A	406	CLA	2	0
26	B	620	SQD	2	0
27	B	626	GOL	1	0
33	C	501	LMG	7	0
23	C	512	CLA	2	0
25	K	102	BCR	1	0
23	c	505	CLA	5	0
24	D	401	PHO	1	0
23	A	408	CLA	6	0
23	C	507	CLA	9	0
34	C	521	HTG	1	0
36	C	517	DGD	5	0
29	a	414	PL9	4	0
25	C	516	BCR	3	0
23	B	615	CLA	3	0
23	b	612	CLA	4	0
29	D	407	PL9	3	0
38	E	103	HEM	3	0

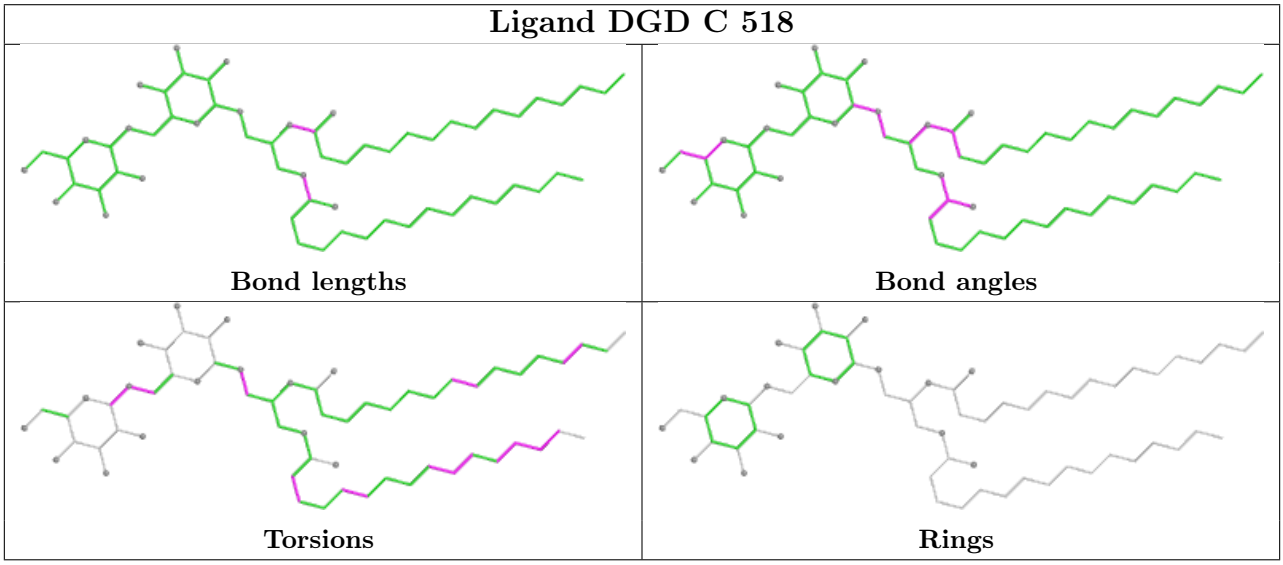
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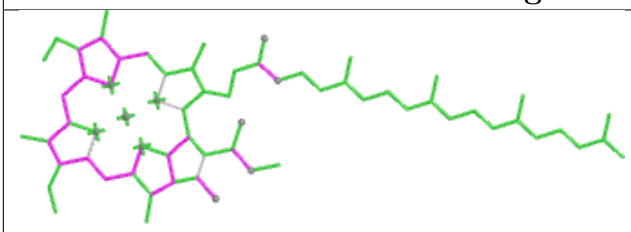
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	629	LMT	1	0
23	A	404	CLA	2	0
31	E	101	LHG	1	0
34	b	628	HTG	1	0
23	B	608	CLA	1	0
23	b	614	CLA	3	0
33	c	520	LMG	1	0
25	k	101	BCR	2	0
23	B	612	CLA	1	0
34	d	411	HTG	1	0
23	d	401	CLA	4	0
23	d	404	CLA	4	0
23	B	609	CLA	4	0

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.

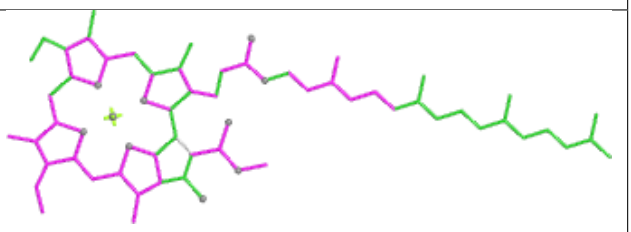
Ligand DGD C 518



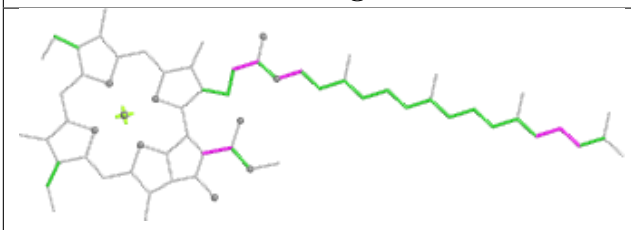
Ligand CLA B 613



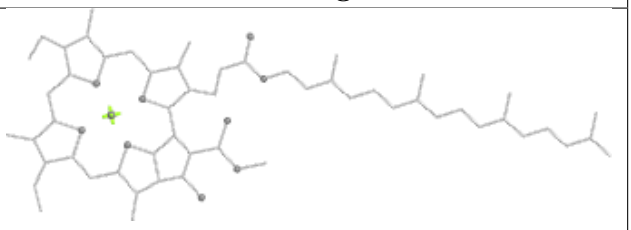
Bond lengths



Bond angles

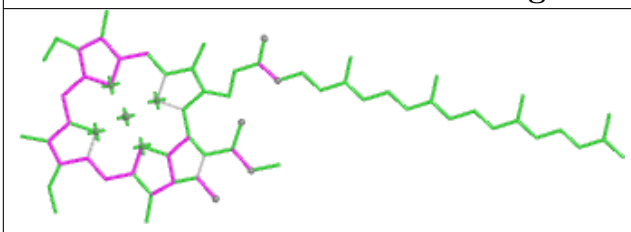


Torsions

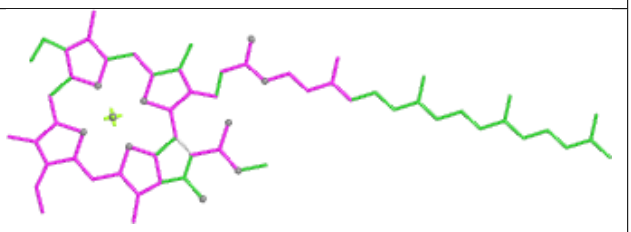


Rings

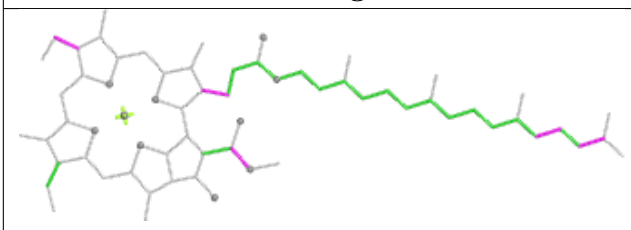
Ligand CLA a 405



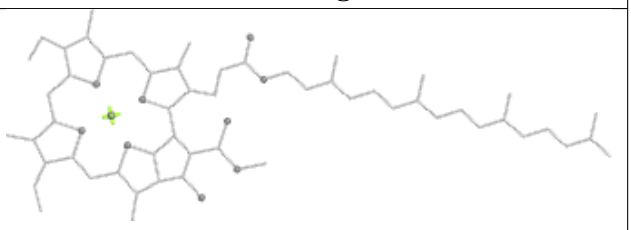
Bond lengths



Bond angles

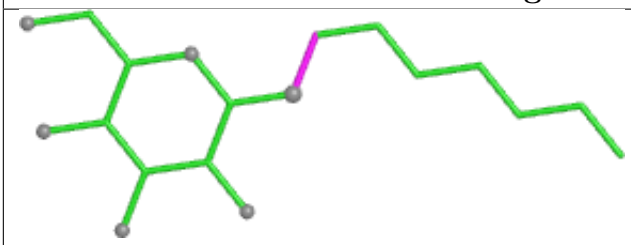


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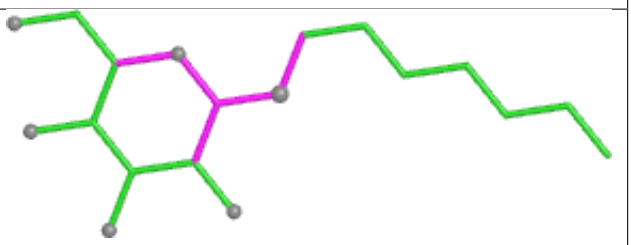


Rings

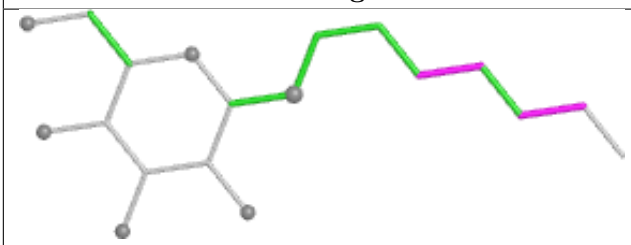
Ligand HTG b 622



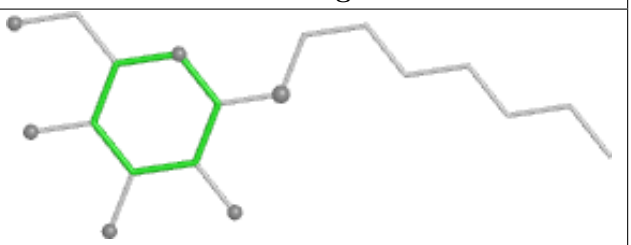
Bond lengths



Bond angles

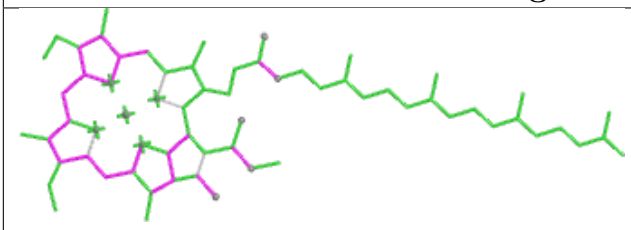


Torsions

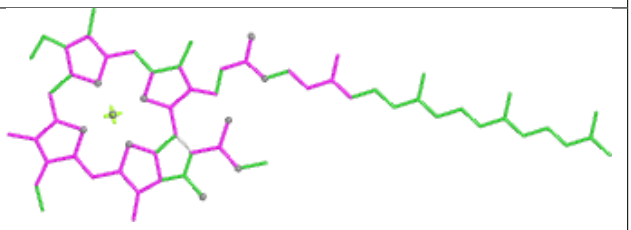


Rings

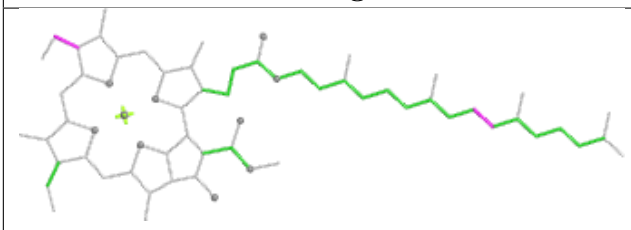
Ligand CLA c 513



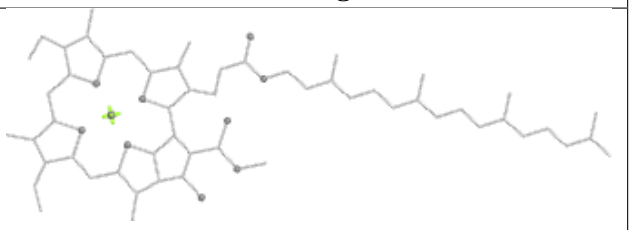
Bond lengths



Bond angles

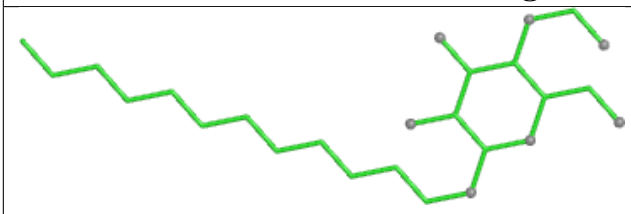


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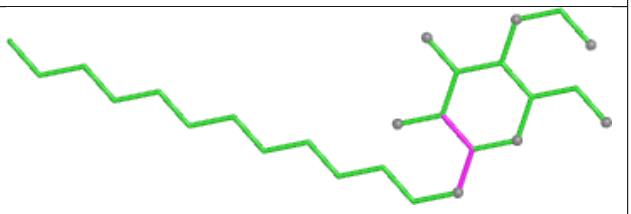


Rings

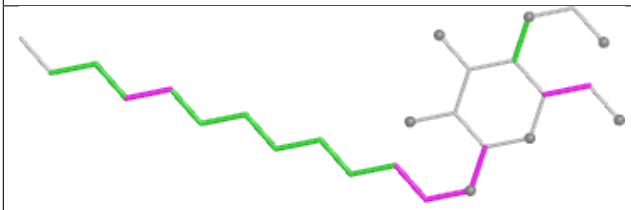
Ligand LMT B 631



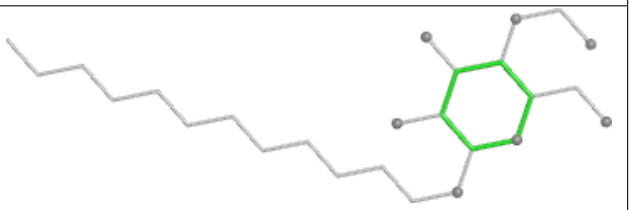
Bond lengths



Bond angles

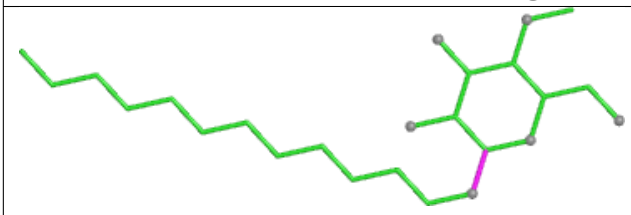


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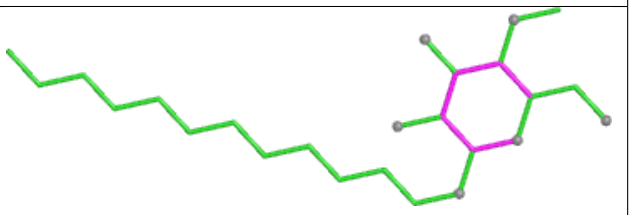


Rings

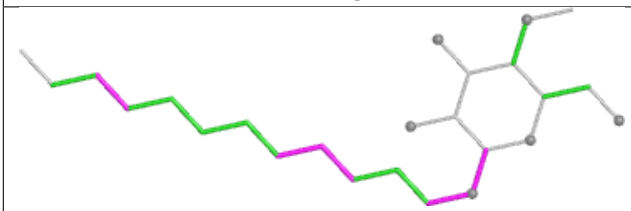
Ligand LMT b 627



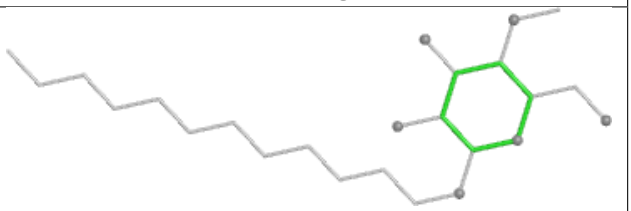
Bond lengths



Bond angles

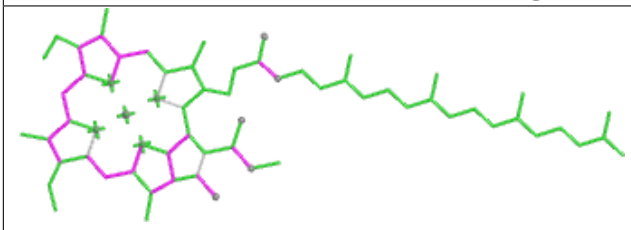


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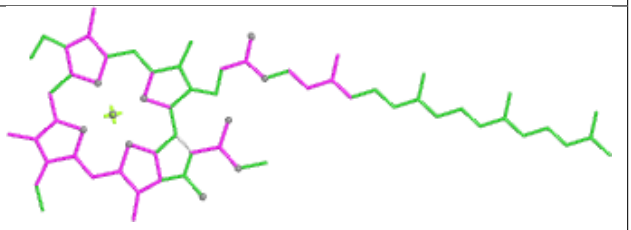


Rings

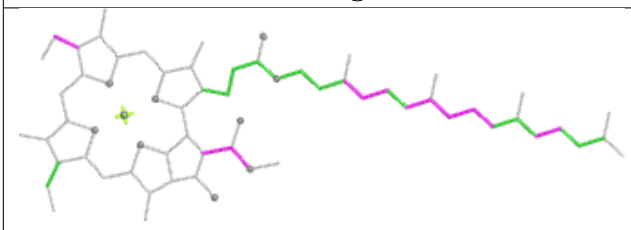
Ligand CLA b 604



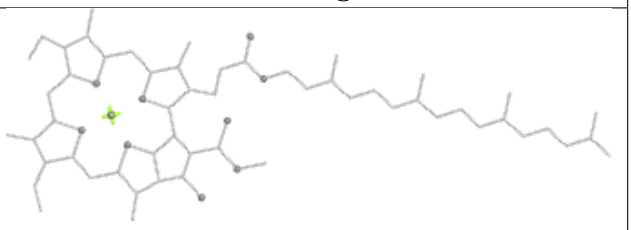
Bond lengths



Bond angles

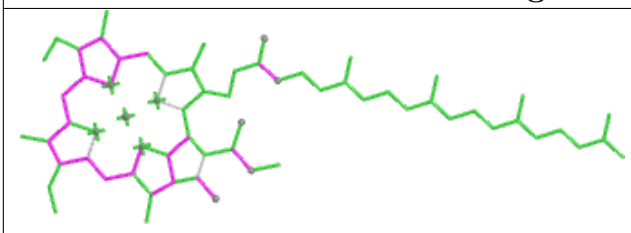


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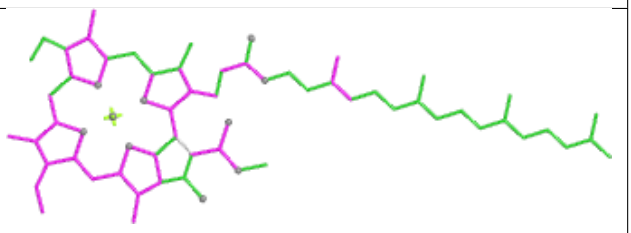


Rings

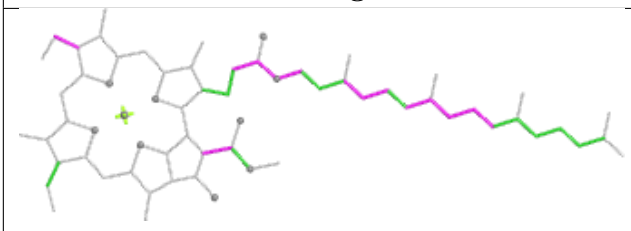
Ligand CLA b 601



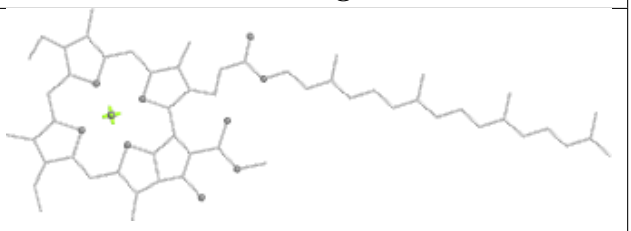
Bond lengths



Bond angles

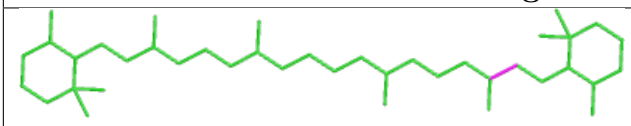


Torsions

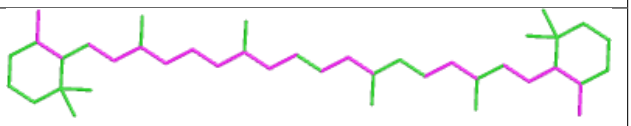


Rings

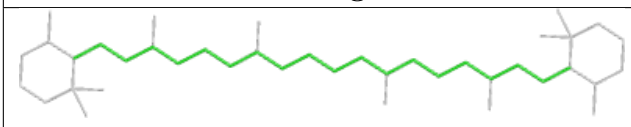
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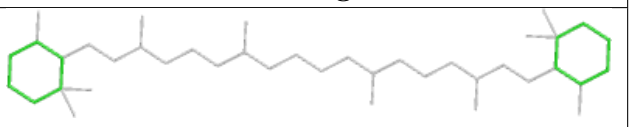
Bond lengths



Bond angles

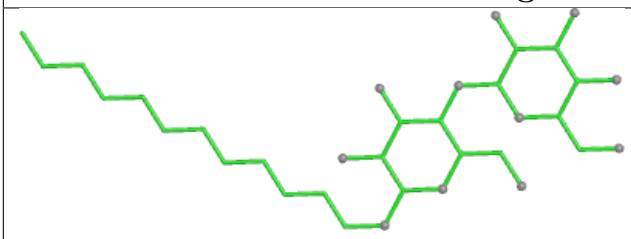


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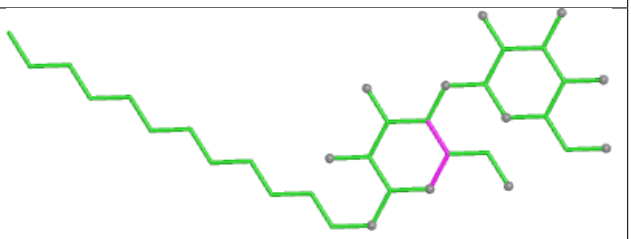


Rings

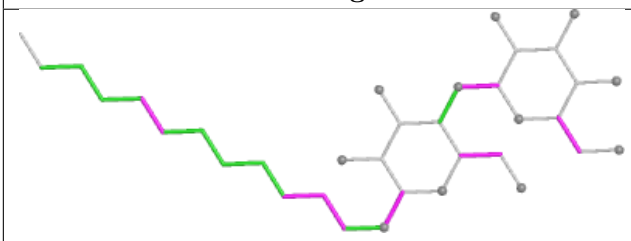
Ligand LMT M 103



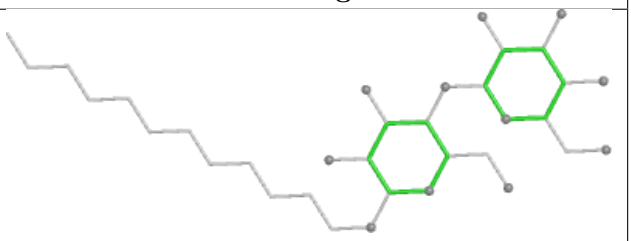
Bond lengths



Bond angles

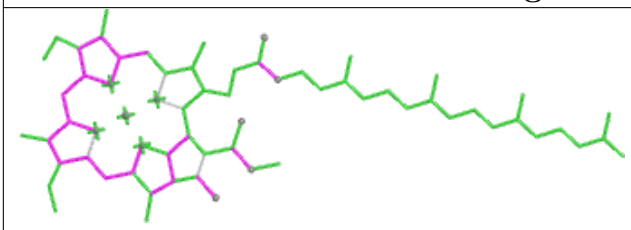


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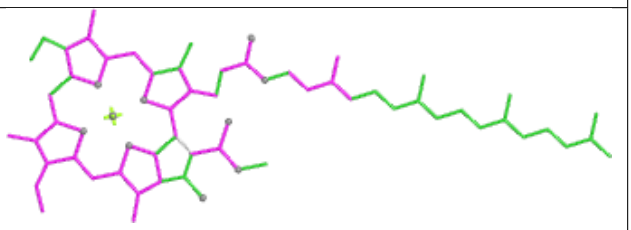


Rings

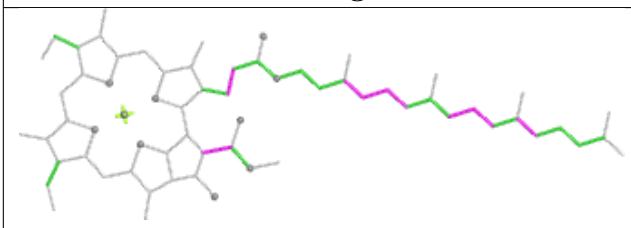
Ligand CLA B 614



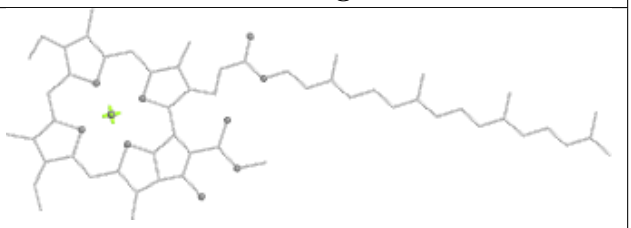
Bond lengths



Bond angles

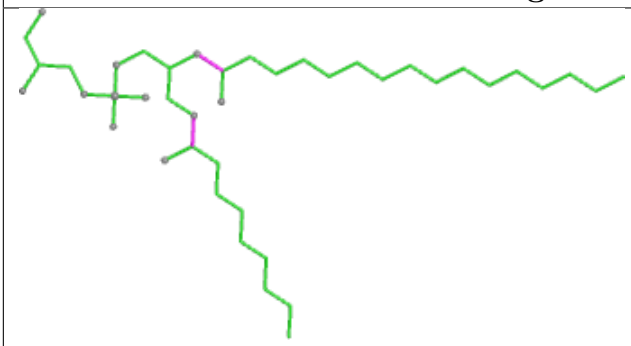


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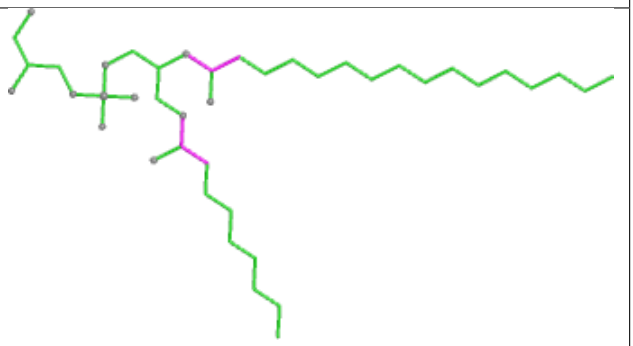


Rings

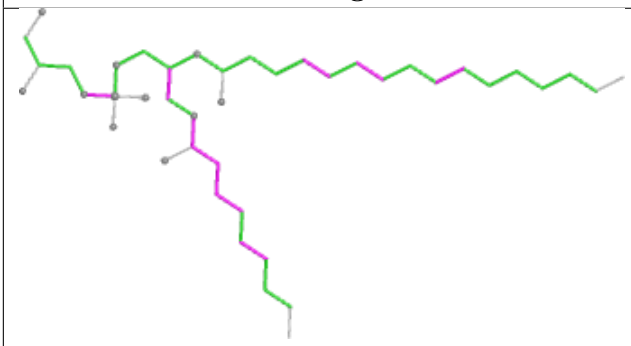
Ligand LHG e 101



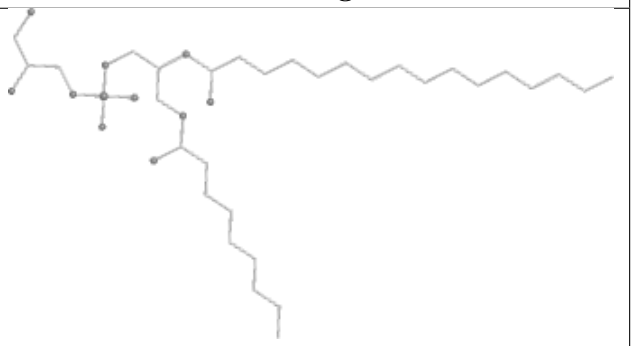
Bond lengths



Bond angles

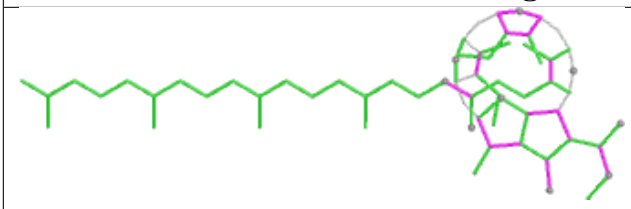


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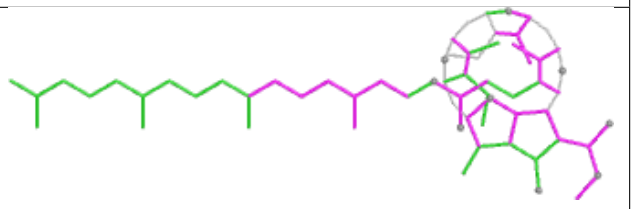


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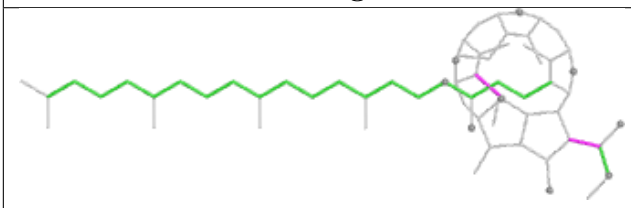
Ligand PHO A 407



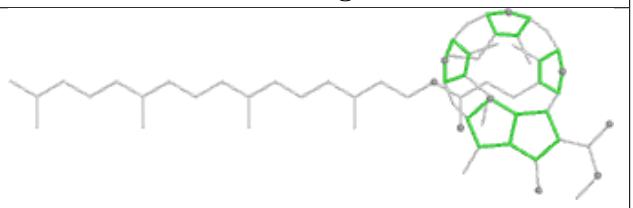
Bond lengths



Bond angles

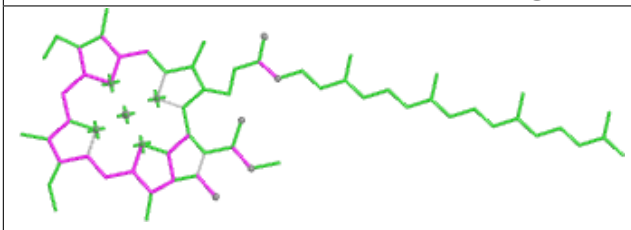


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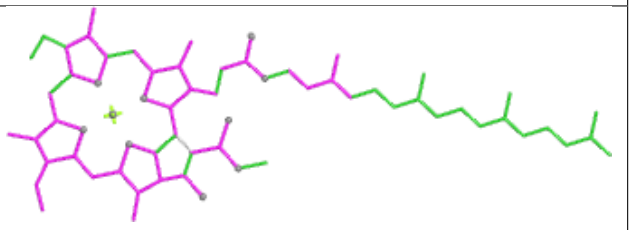


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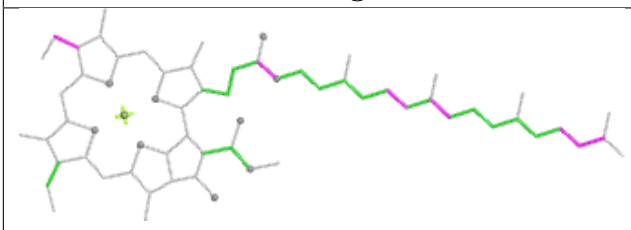
Ligand CLA a 408



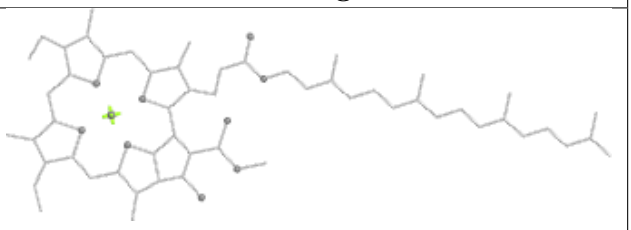
Bond lengths



Bond angles

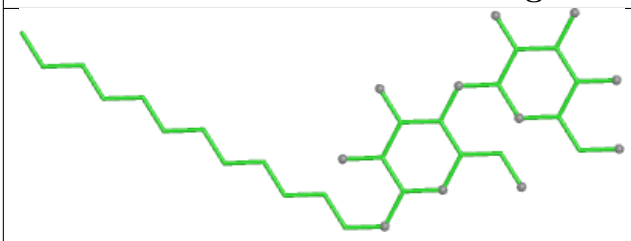


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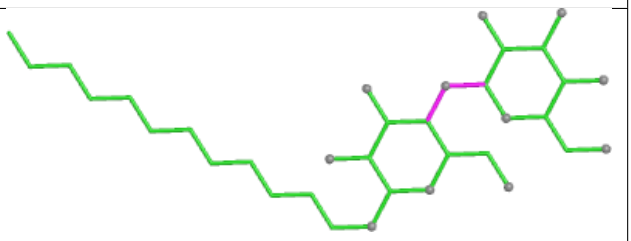


Rings

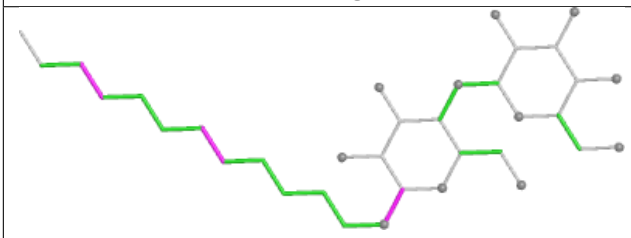
Ligand LMT a 417



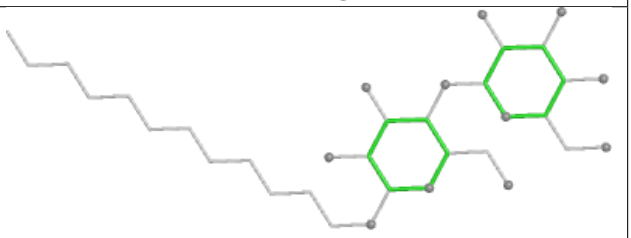
Bond lengths



Bond angles

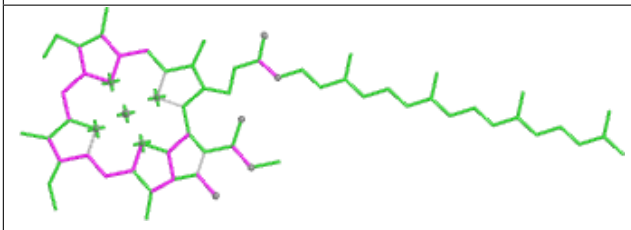


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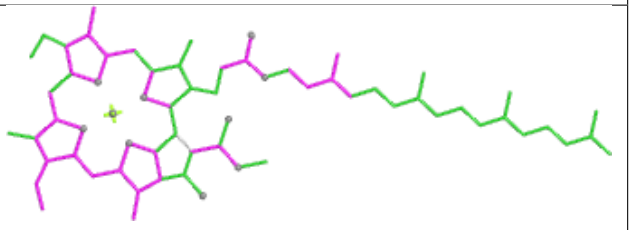


Rings

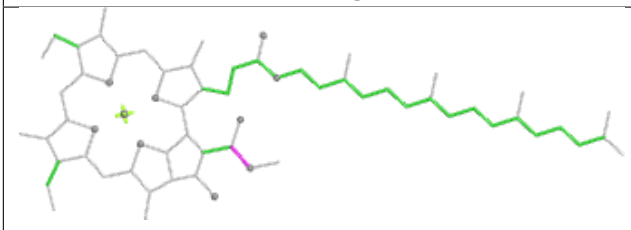
Ligand CLA C 504



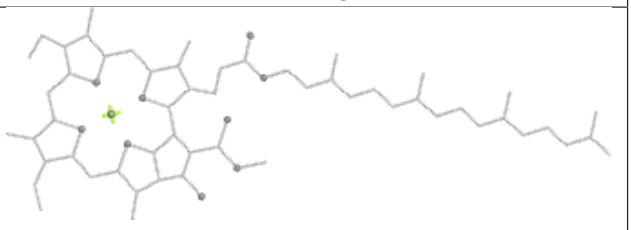
Bond lengths



Bond angles

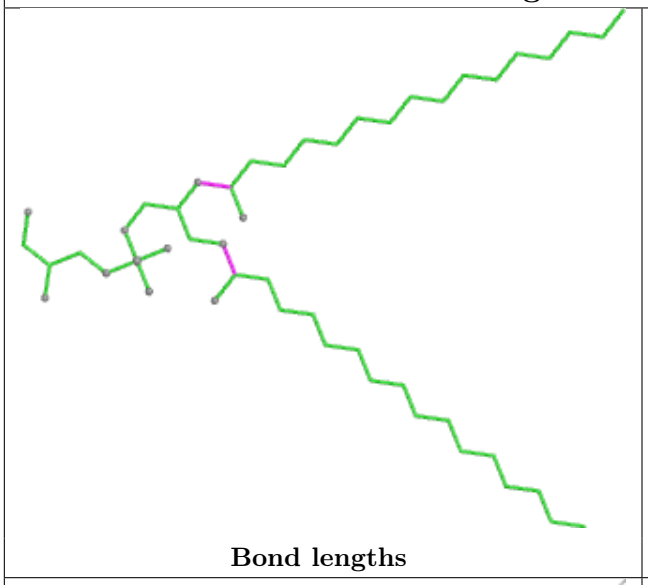


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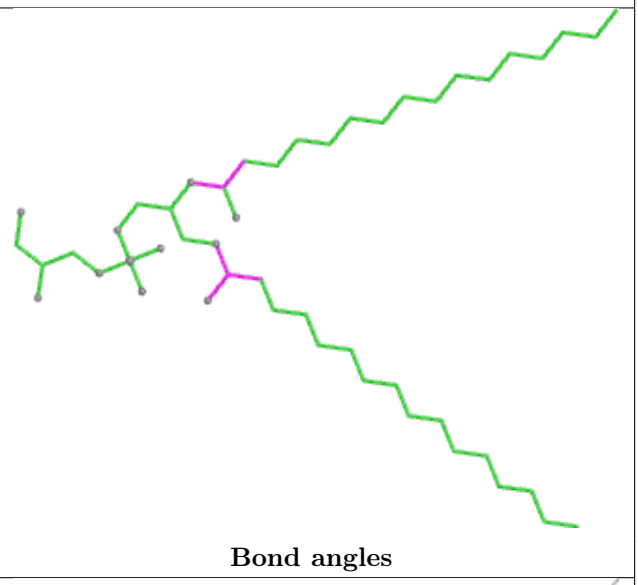


Rings

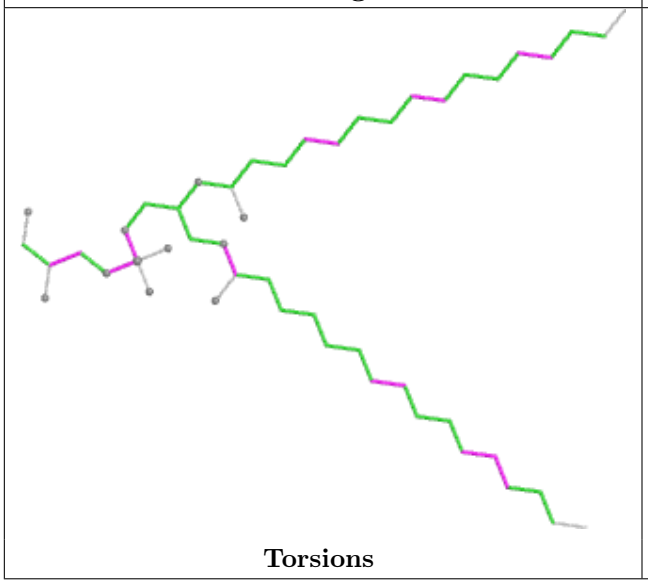
Ligand LHG D 408



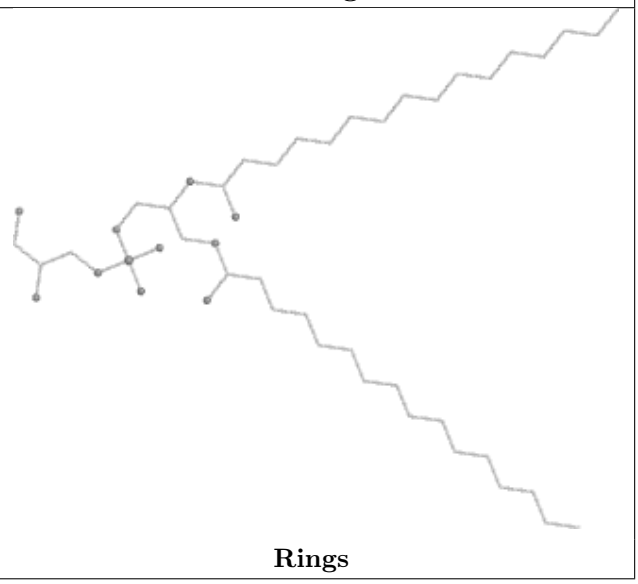
Bond lengths



Bond angles

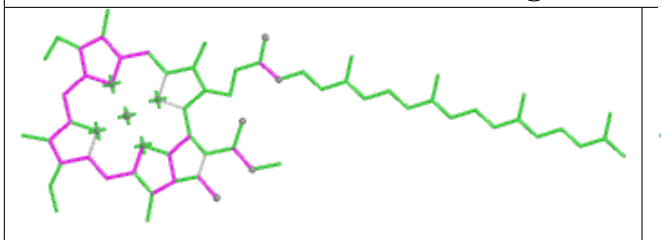


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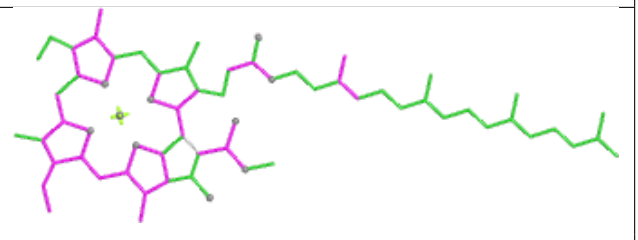


Rings

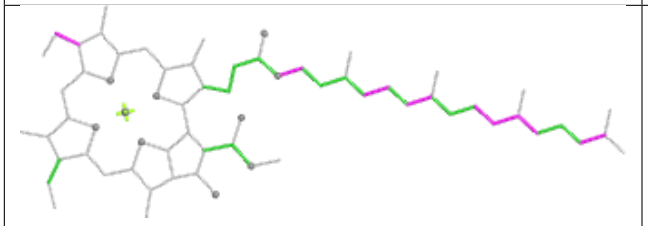
Ligand CLA B 616



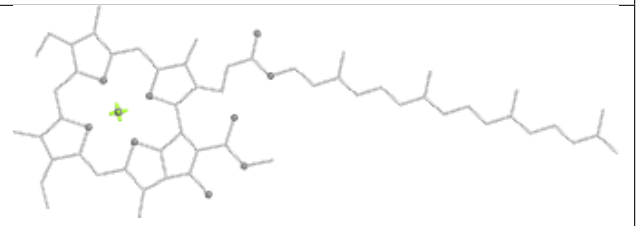
Bond lengths



Bond angles

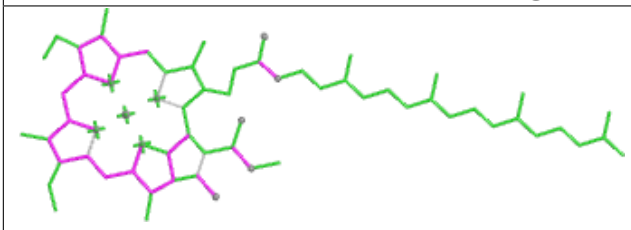


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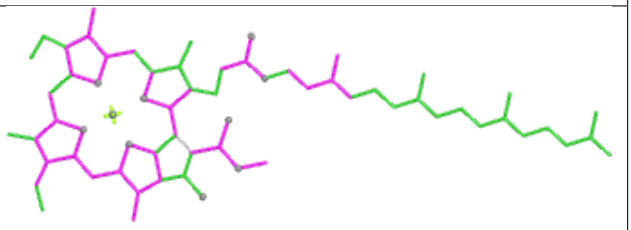


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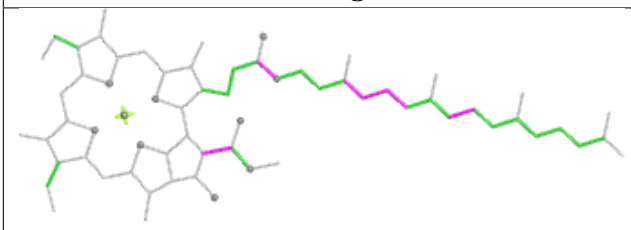
Ligand CLA b 605



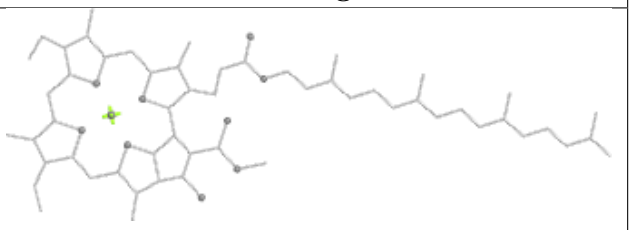
Bond lengths



Bond angles

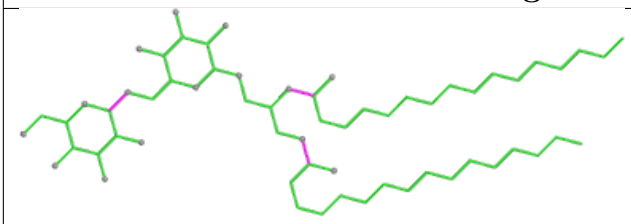


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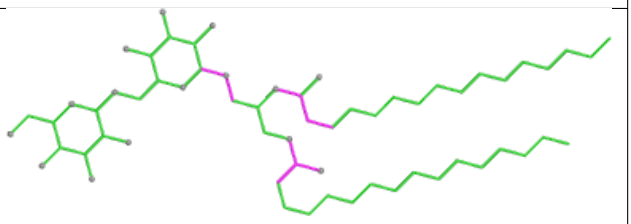


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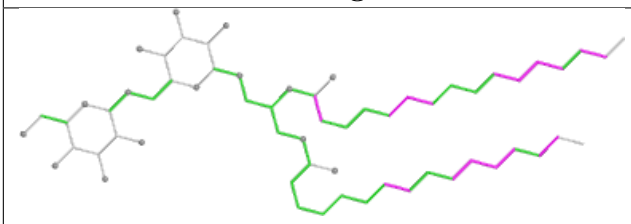
Ligand DGD h 102



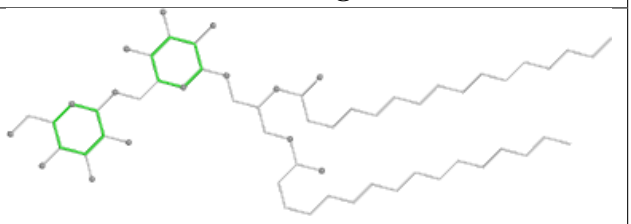
Bond lengths



Bond angles

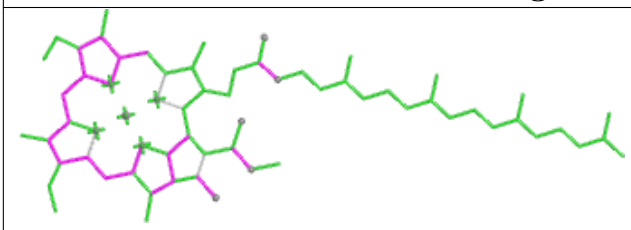


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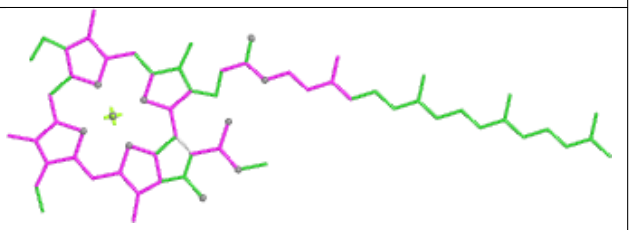


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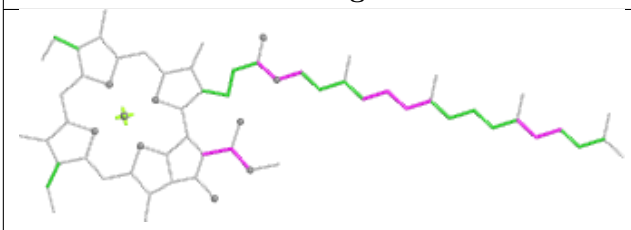
Ligand CLA c 509



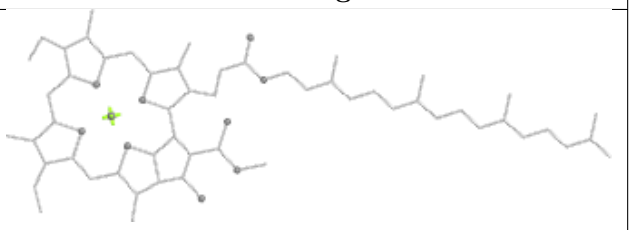
Bond lengths



Bond angles

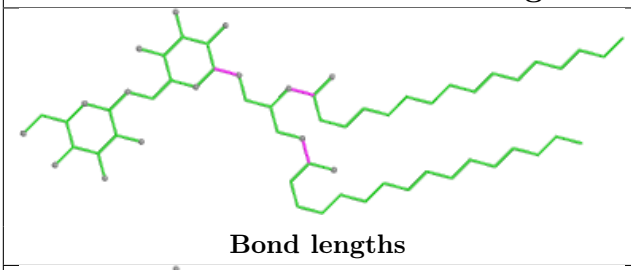


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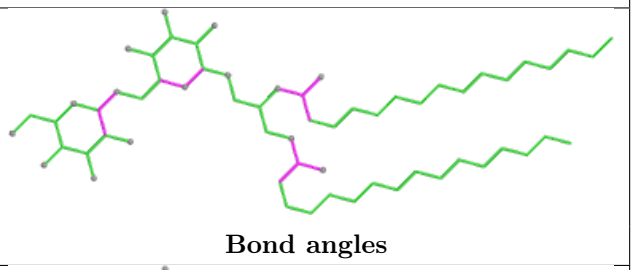


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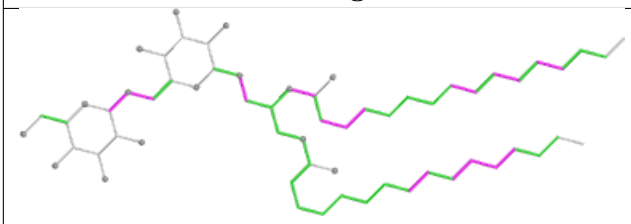
Ligand DGD c 517



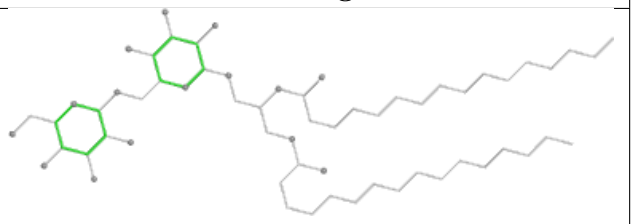
Bond lengths



Bond angles

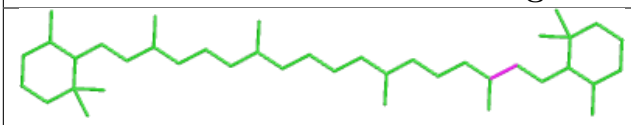


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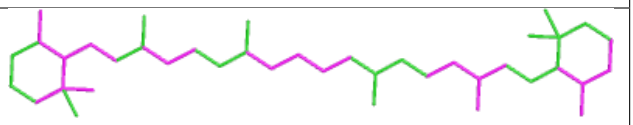


Rings

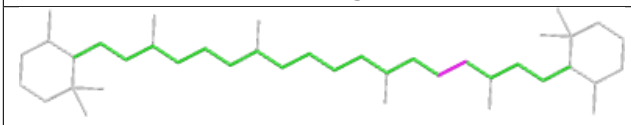
Ligand BCR a 409



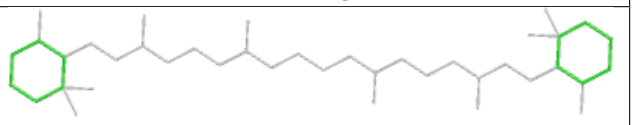
Bond lengths



Bond angles

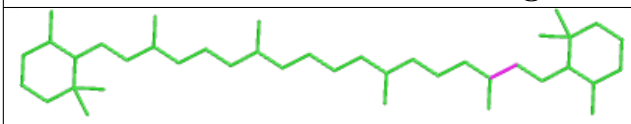


Torsions

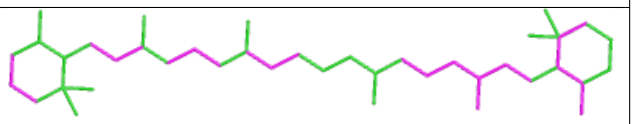


Rings

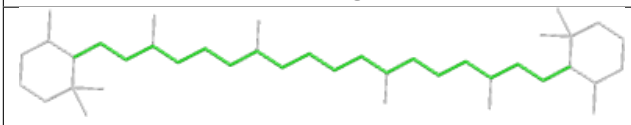
Ligand BCR B 619



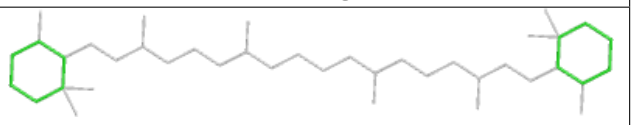
Bond lengths



Bond angles

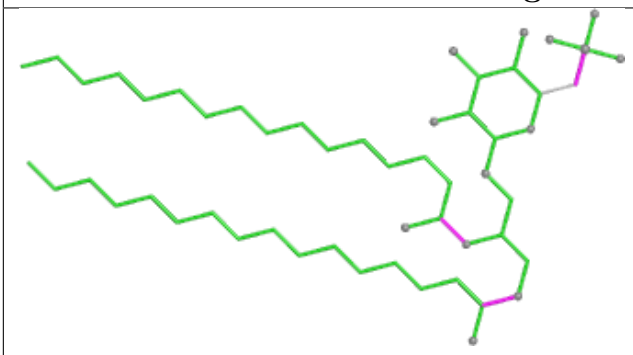


Torsions

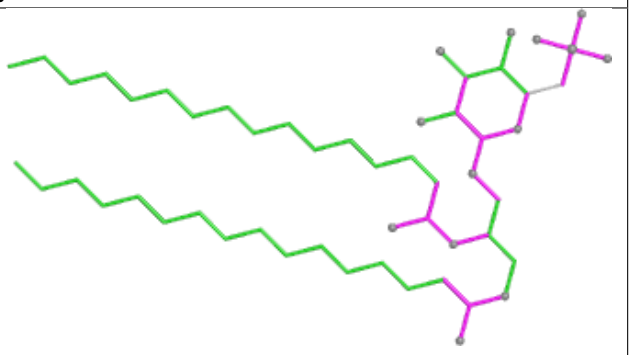


Rings

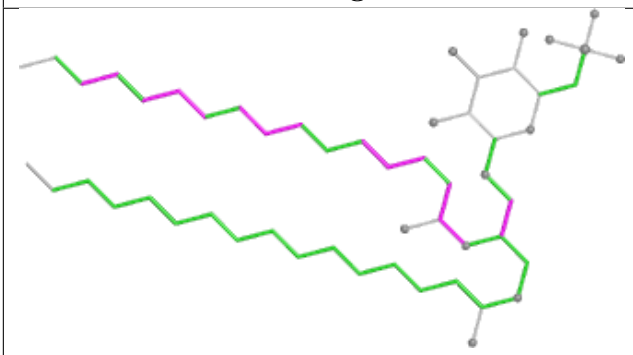
Ligand SQD A 410



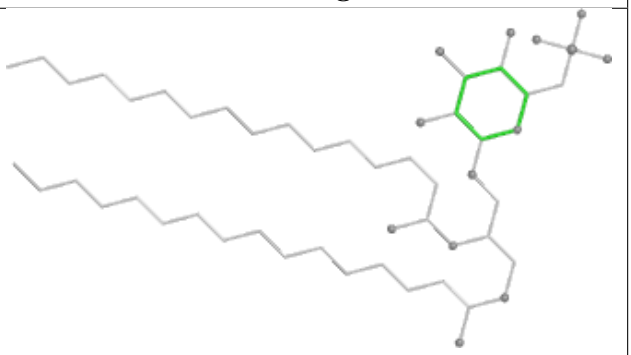
Bond lengths



Bond angles

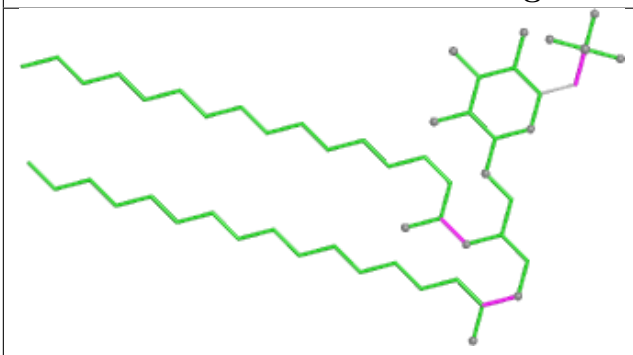


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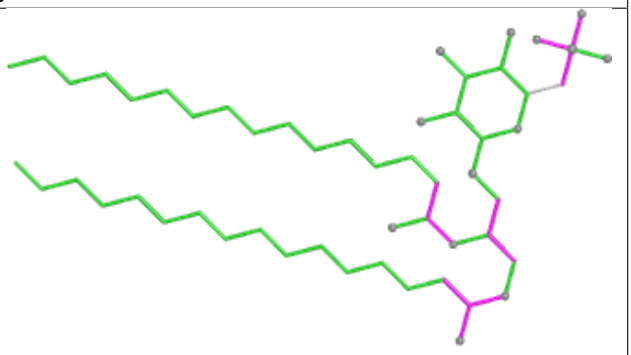


Rings

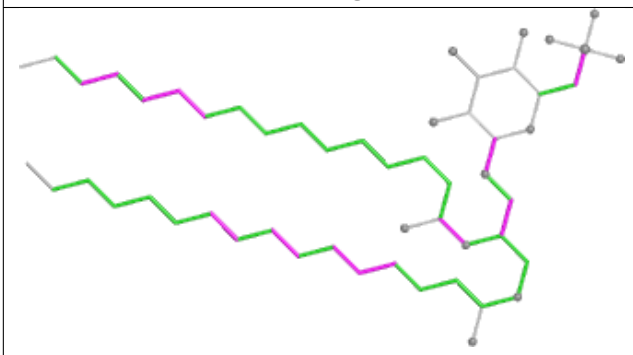
Ligand SQD A 412



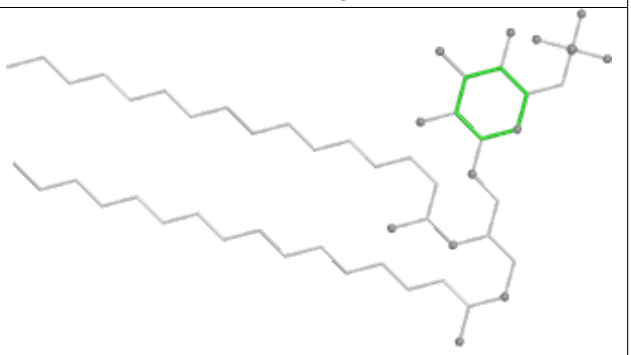
Bond lengths



Bond angles

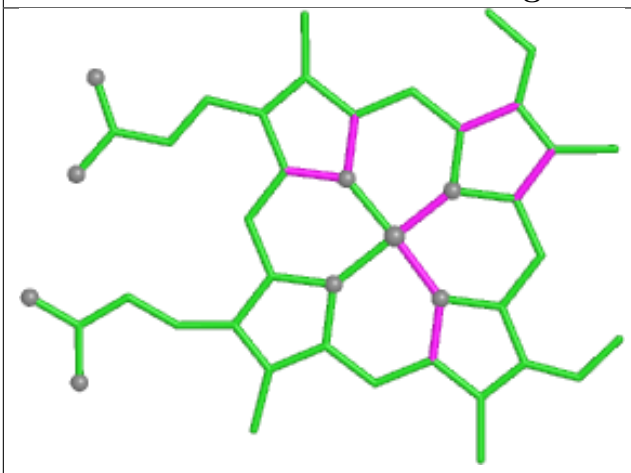


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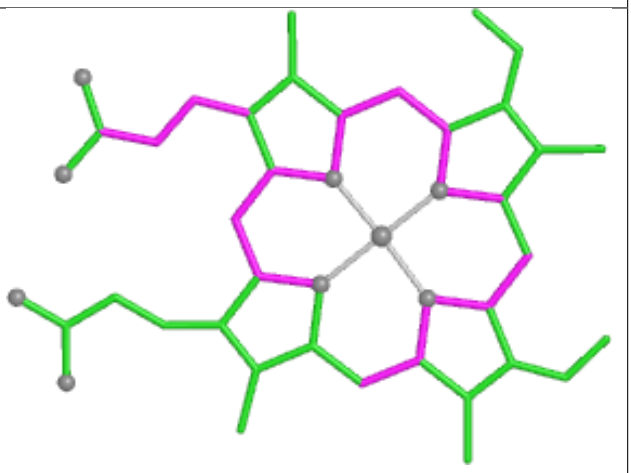


Rings

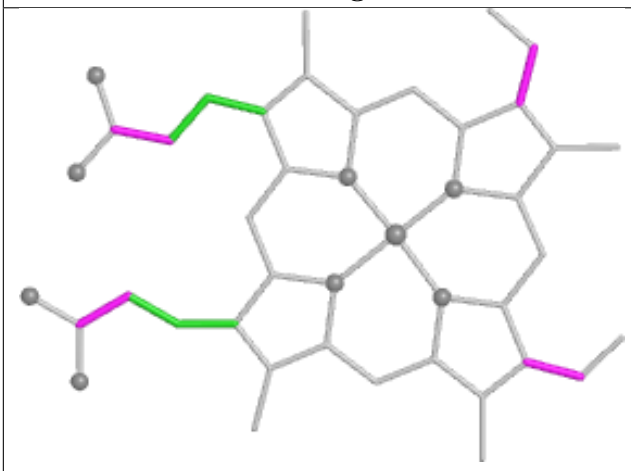
Ligand HEM e 103



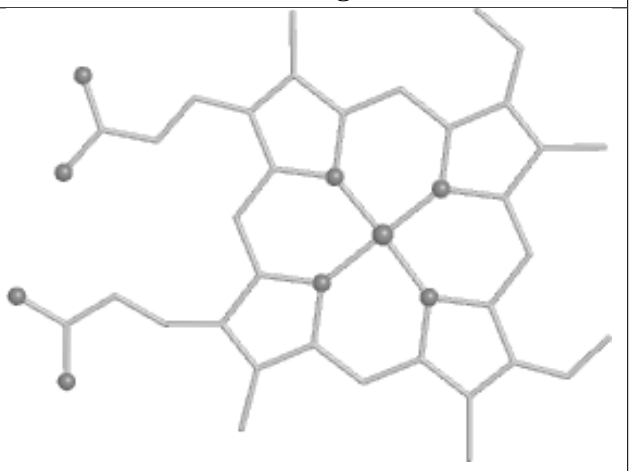
Bond lengths



Bond angles

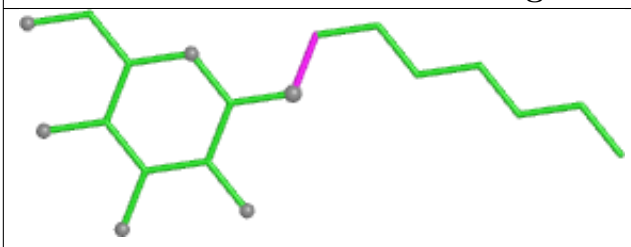


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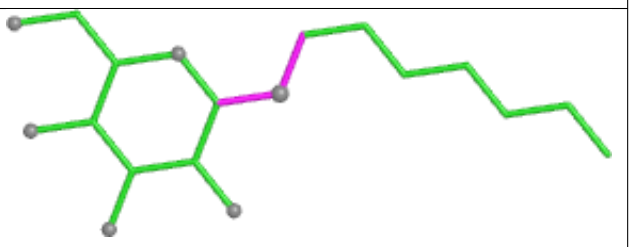


Rings

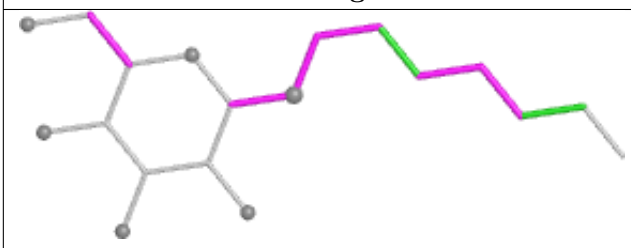
Ligand HTG c 521



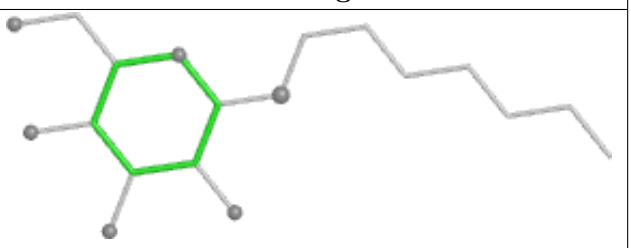
Bond lengths



Bond angles

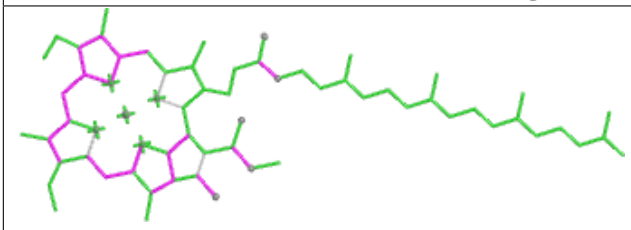


Torsions

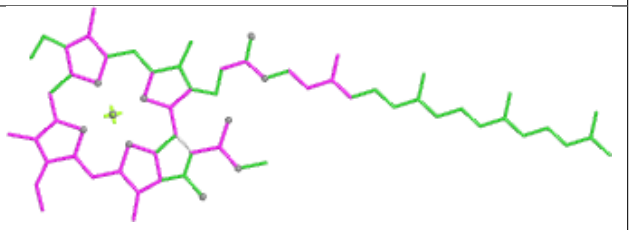


Rings

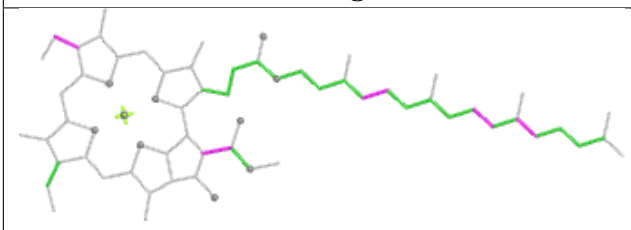
Ligand CLA C 503



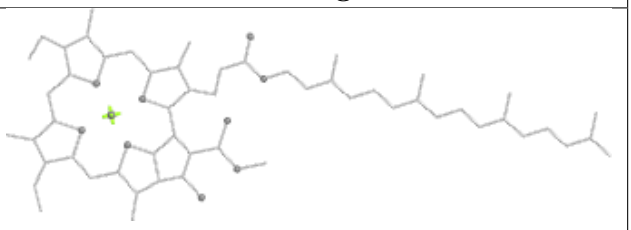
Bond lengths



Bond angles

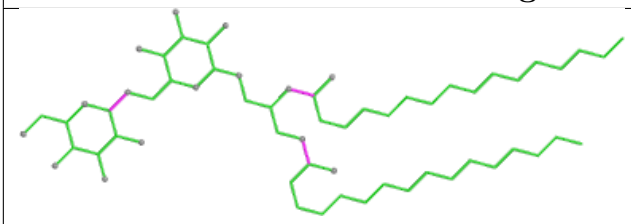


Torsions

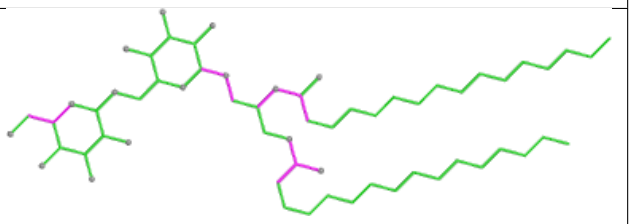


Rings

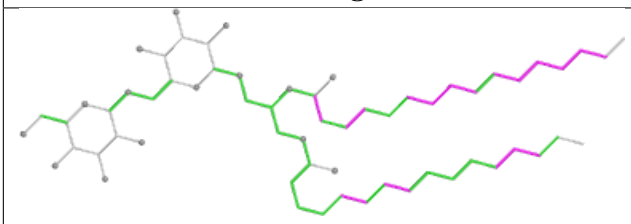
Ligand DGD H 102



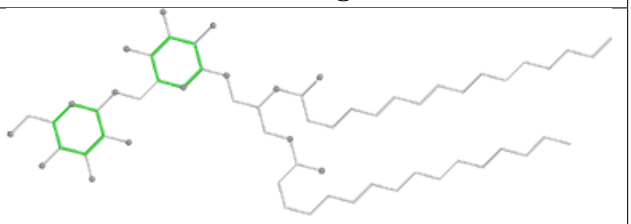
Bond lengths



Bond angles

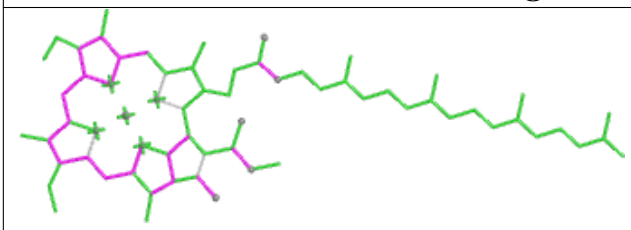


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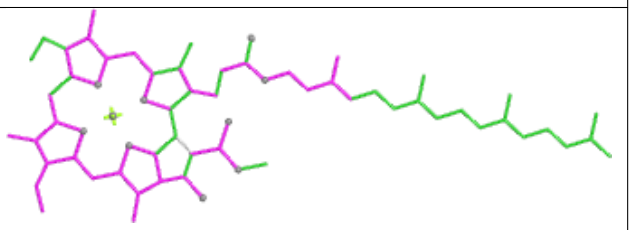


Rings

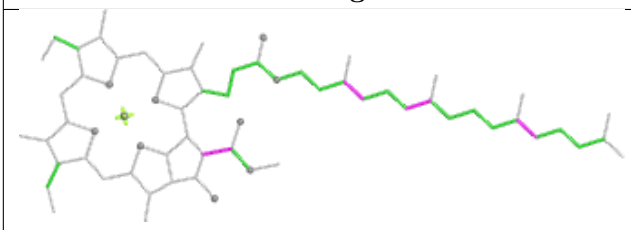
Ligand CLA C 505



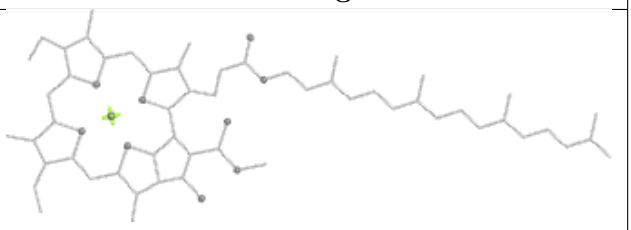
Bond lengths



Bond angles

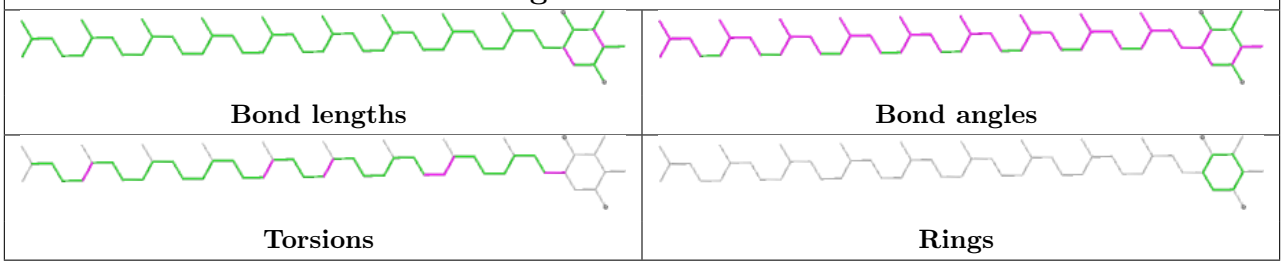


Torsions

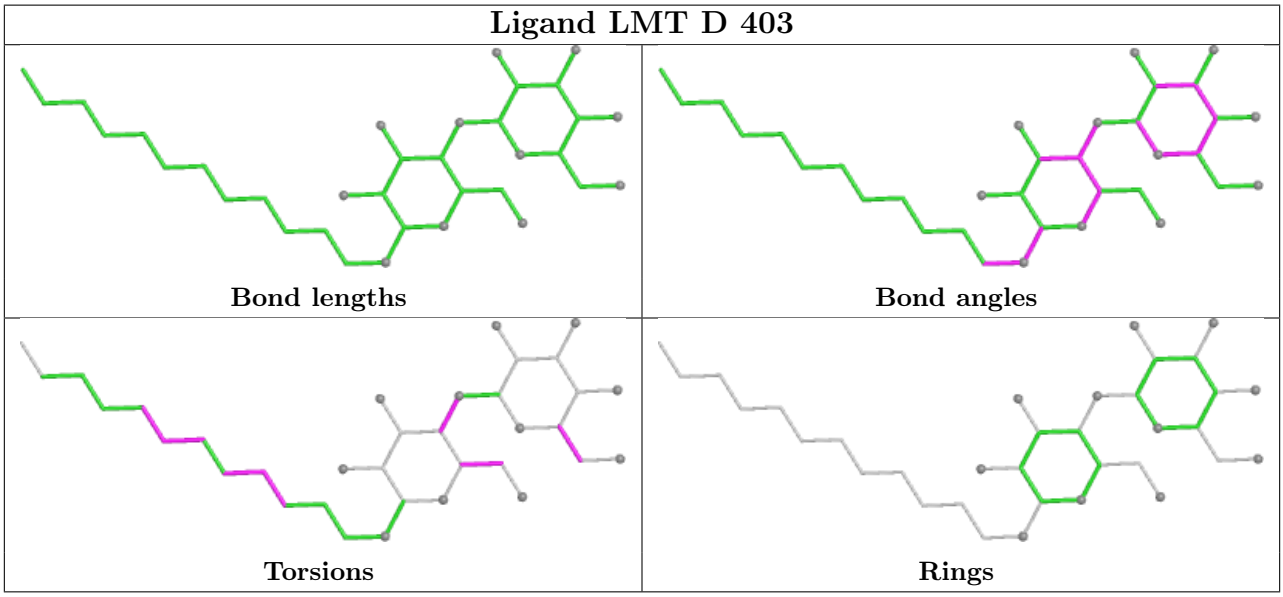


Rings

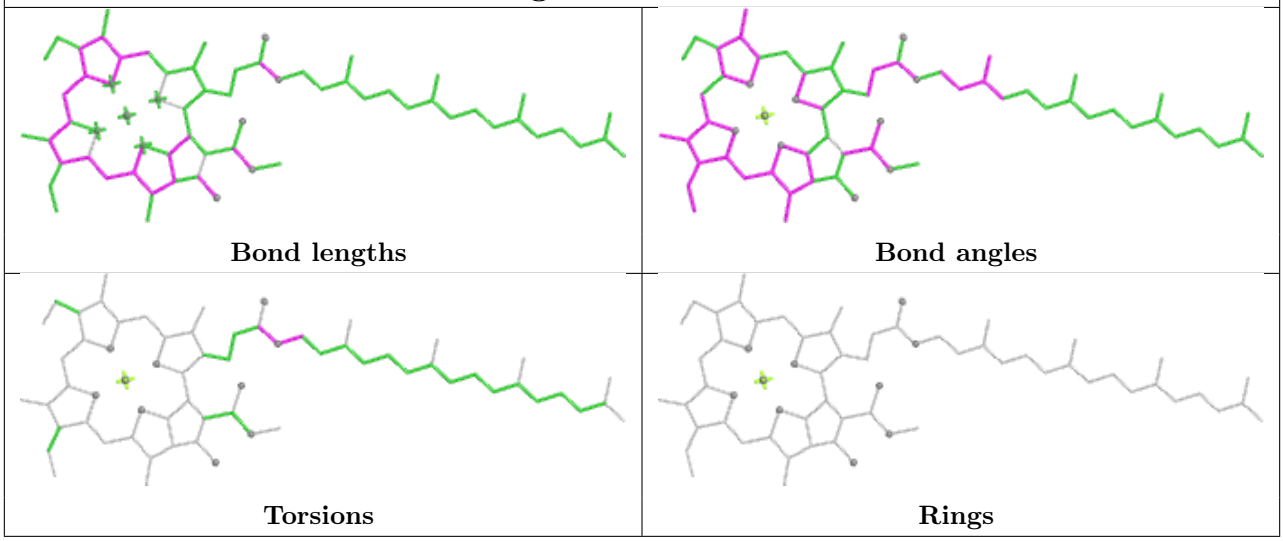
Ligand PL9 A 414



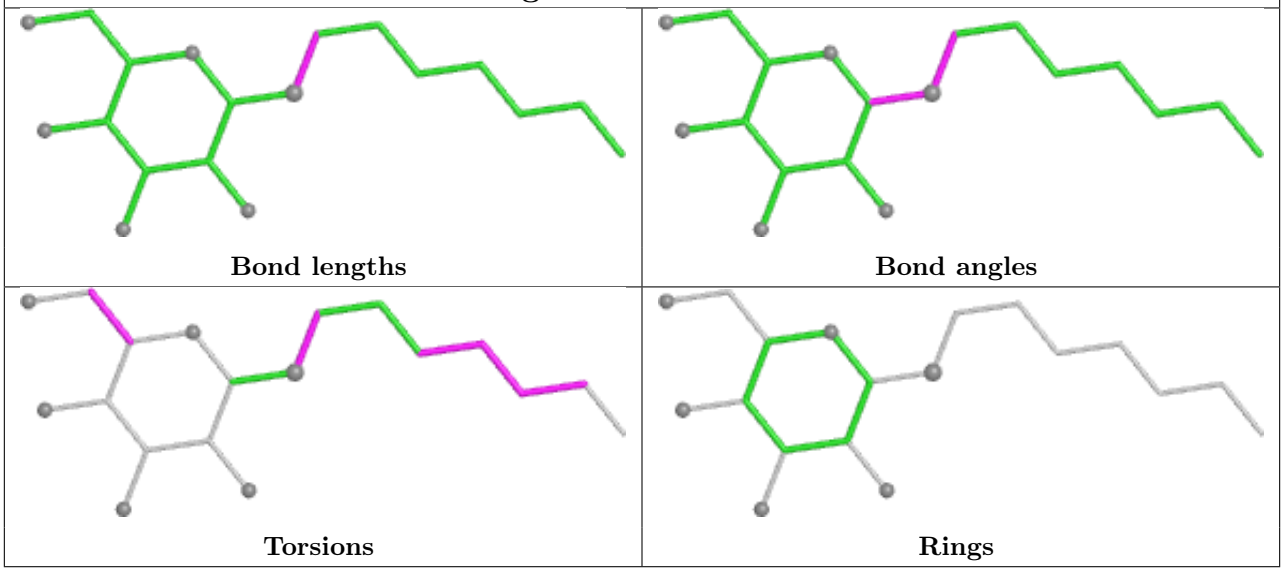
Ligand LMT D 403



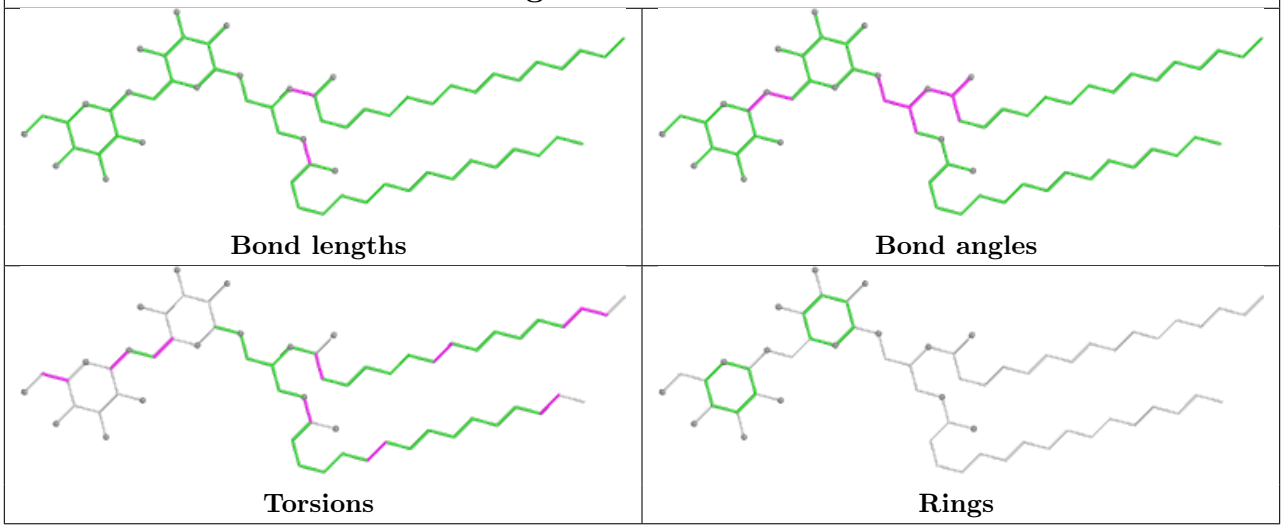
Ligand CLA c 511



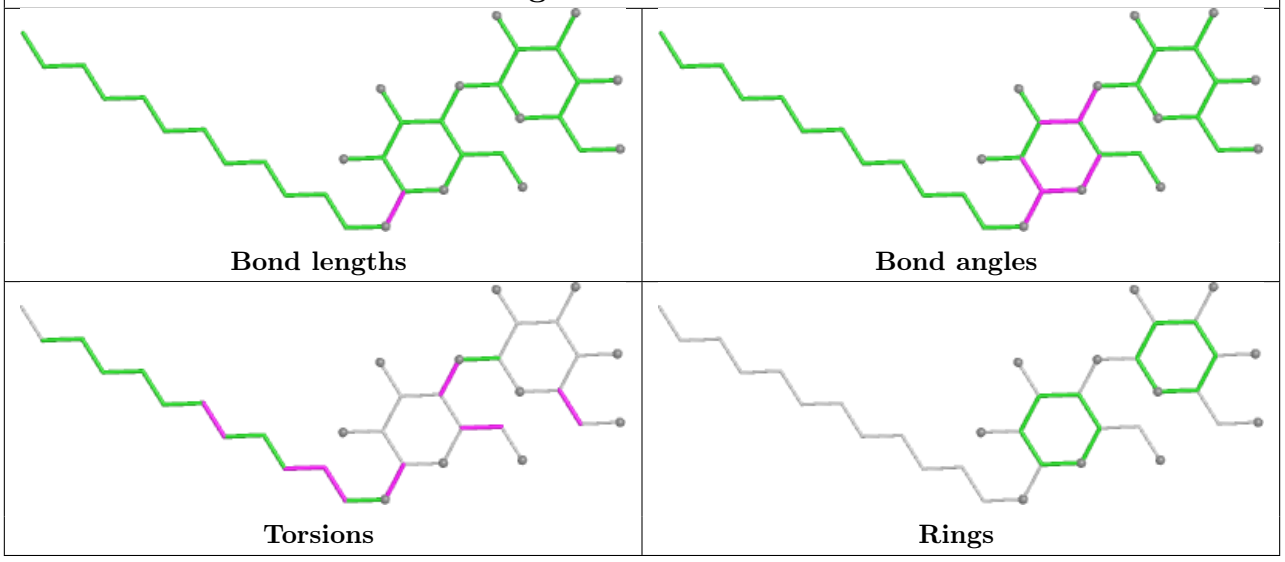
Ligand HTG B 623



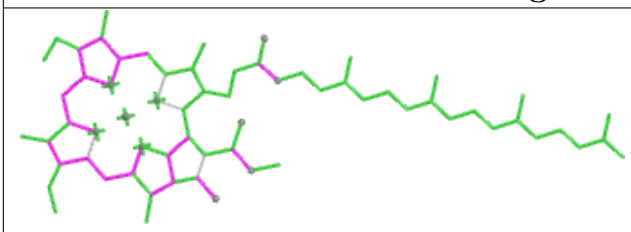
Ligand DGD c 516



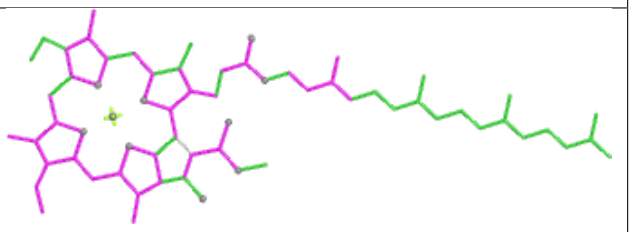
Ligand LMT I 101



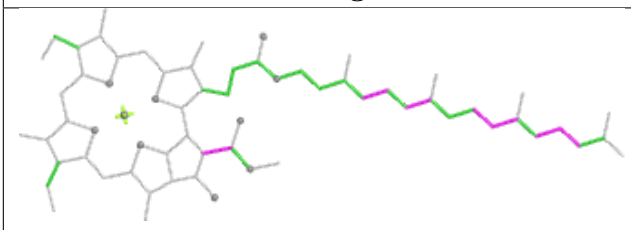
Ligand CLA c 506



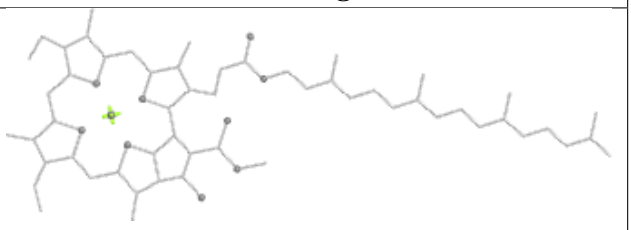
Bond lengths



Bond angles

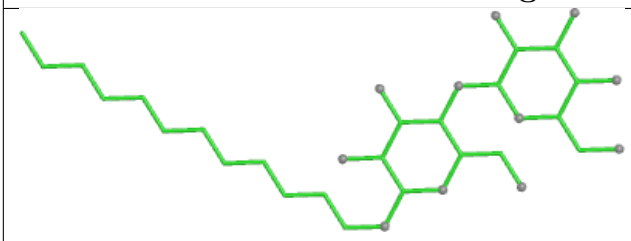


Torsions

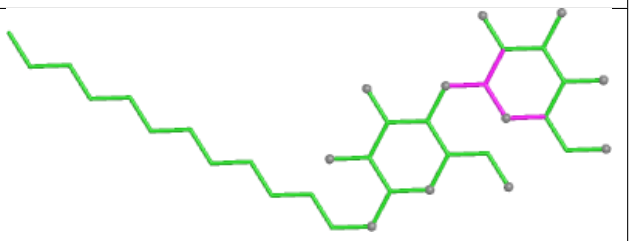


Rings

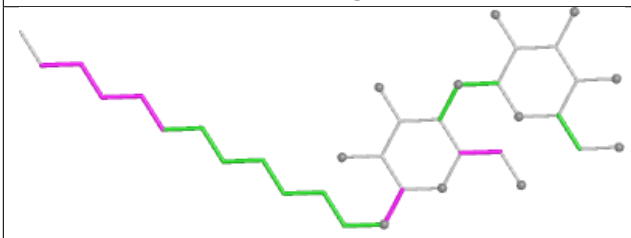
Ligand LMT m 102



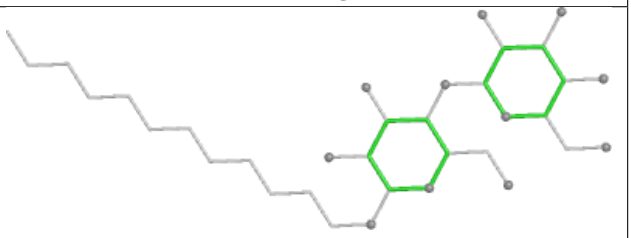
Bond lengths



Bond angles

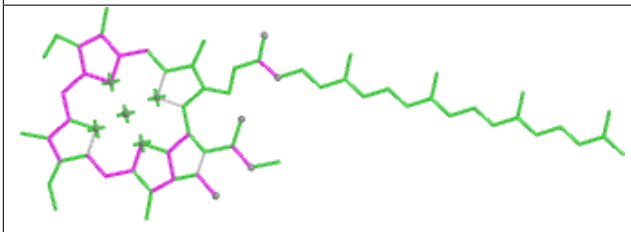


Torsions

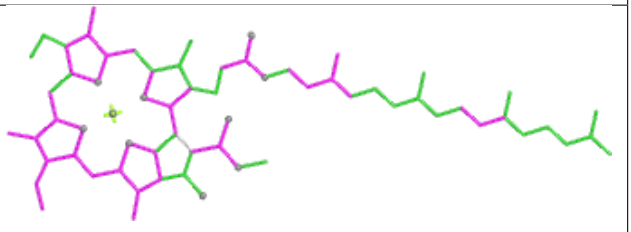


Rings

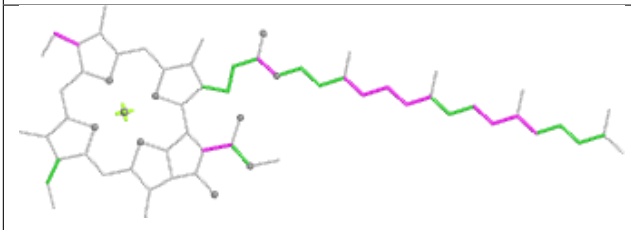
Ligand CLA b 616



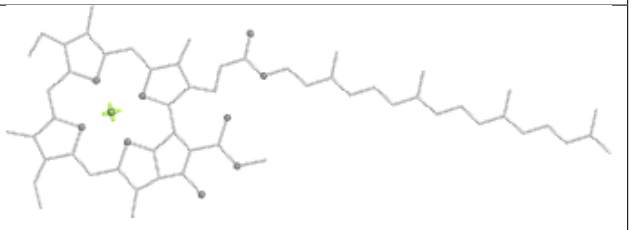
Bond lengths



Bond angles

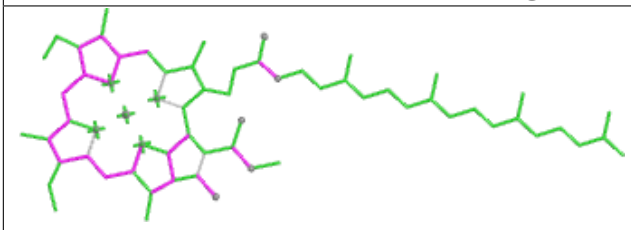


Torsions

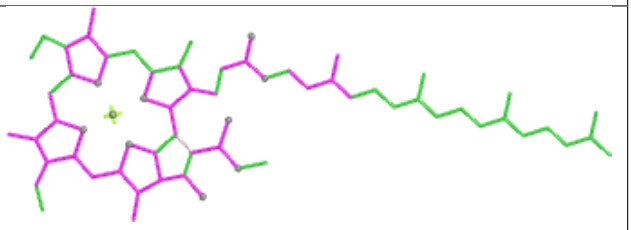


Rings

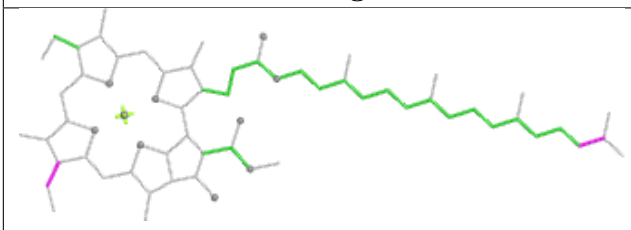
Ligand CLA D 404



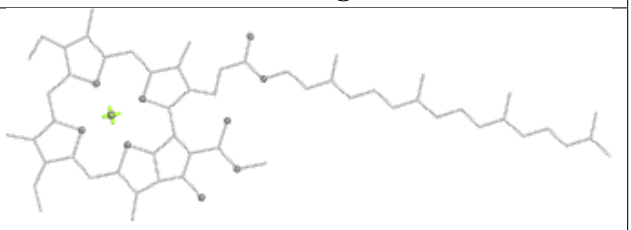
Bond lengths



Bond angles

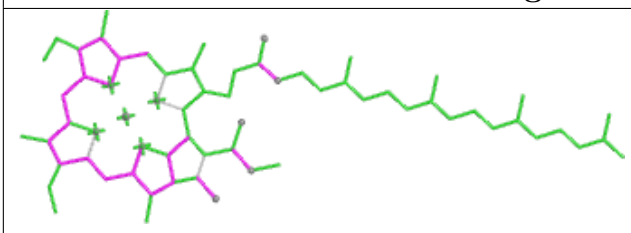


Torsions

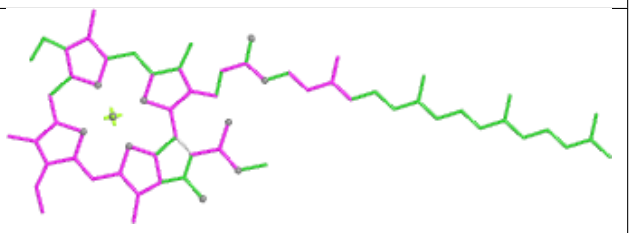


Rings

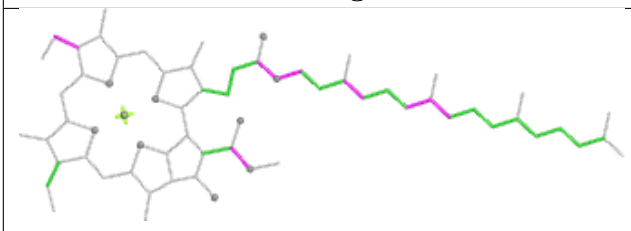
Ligand CLA C 514



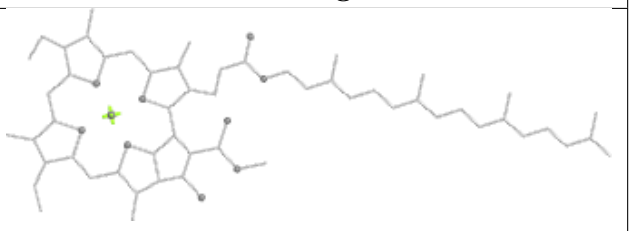
Bond lengths



Bond angles

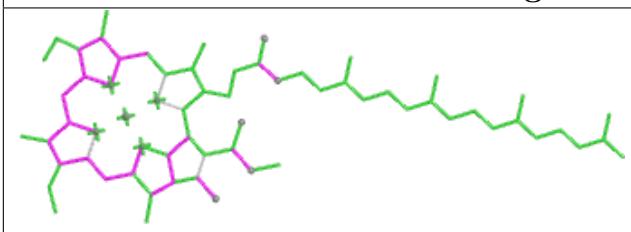


Torsions

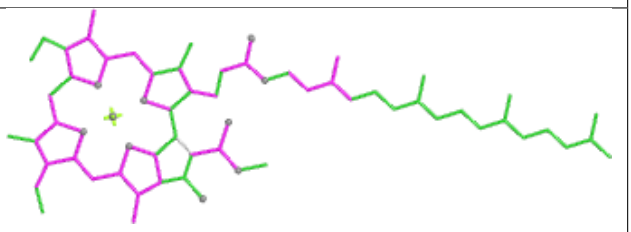


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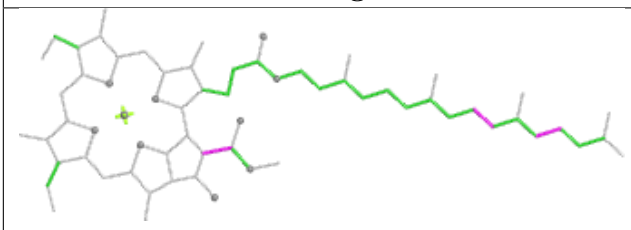
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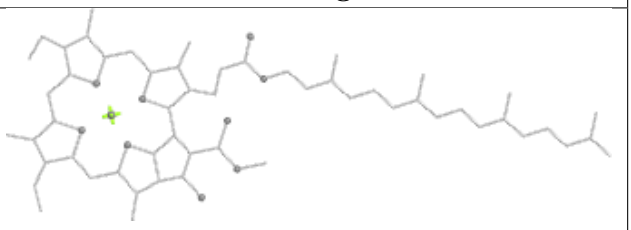
Bond lengths



Bond angles

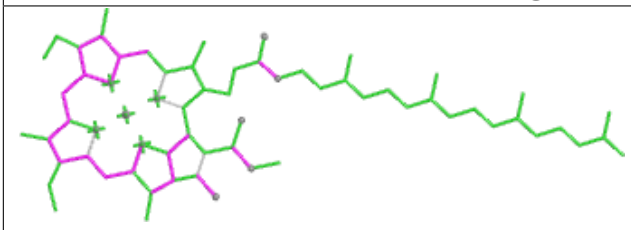


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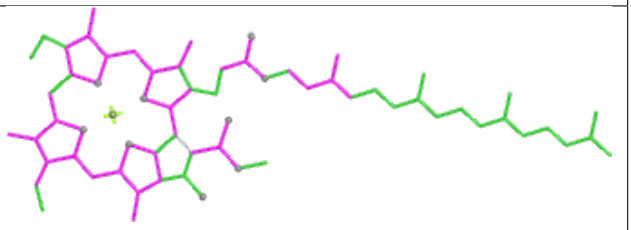


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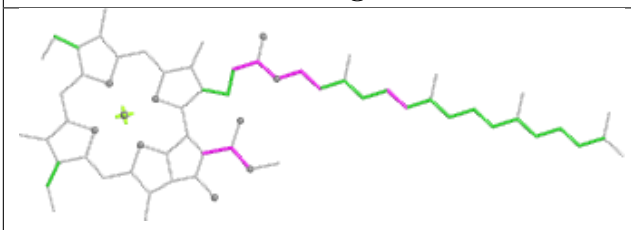
Ligand CLA b 613



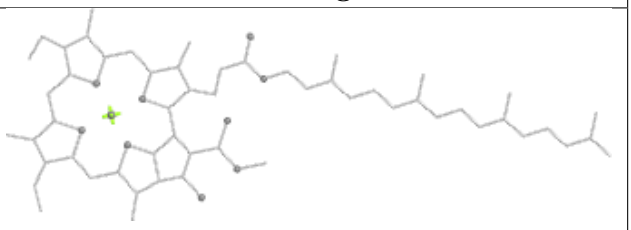
Bond lengths



Bond angles



Torsions

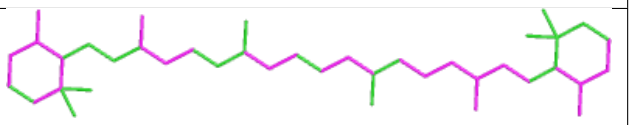


Rings

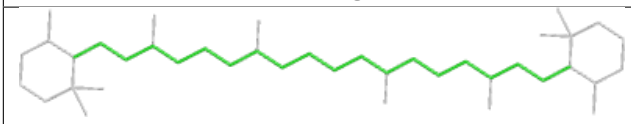
Ligand BCR c 514



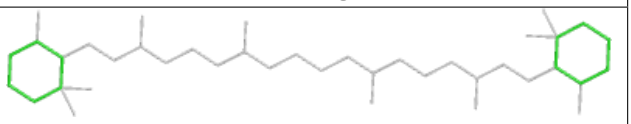
Bond lengths



Bond angles

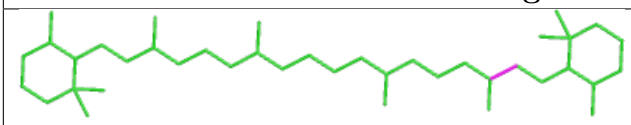


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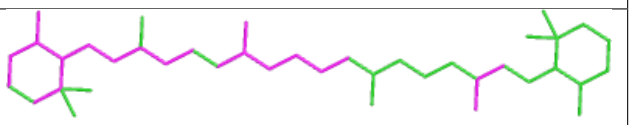


Rings

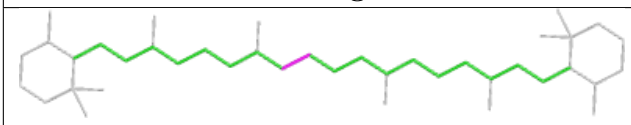
Ligand BCR T 101



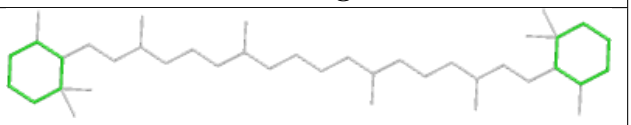
Bond lengths



Bond angles

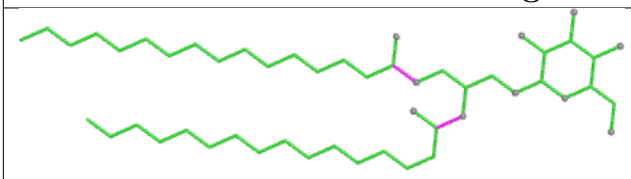


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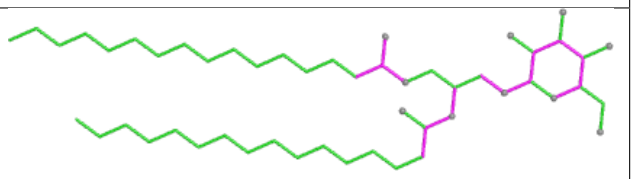


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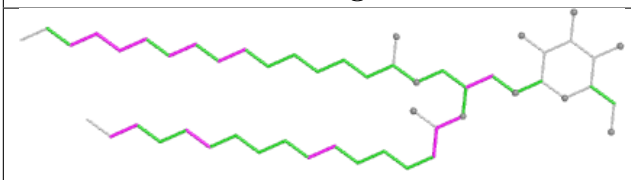
Ligand LMG b 620



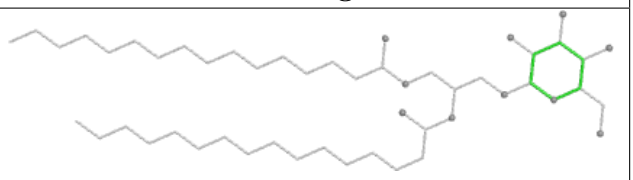
Bond lengths



Bond angles

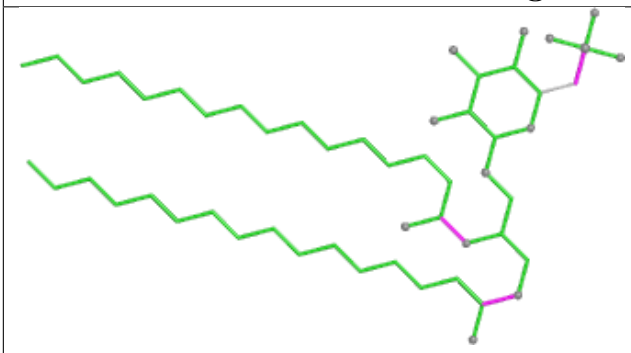


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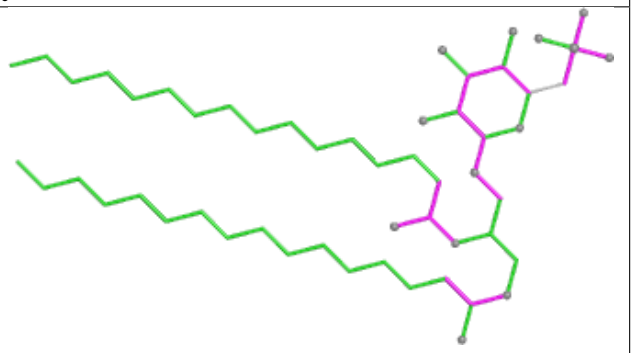


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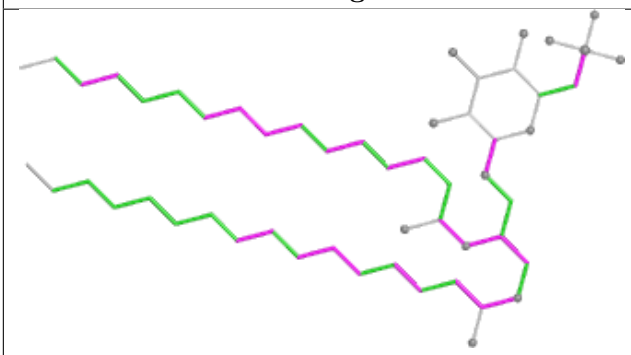
Ligand SQD L 101



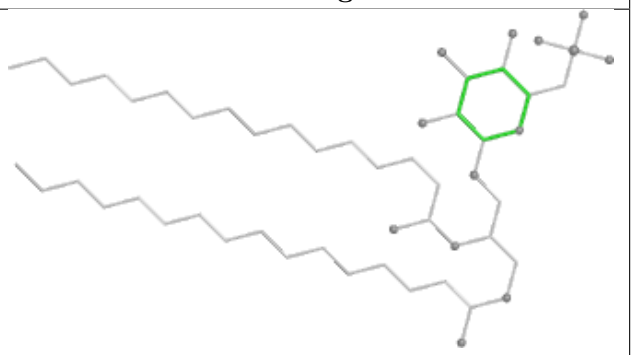
Bond lengths



Bond angles

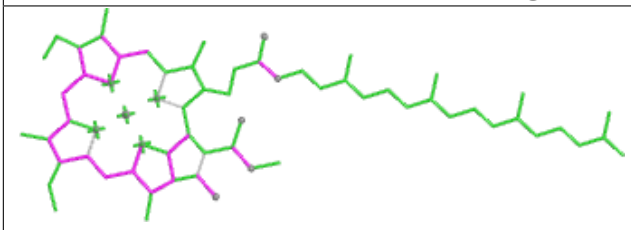


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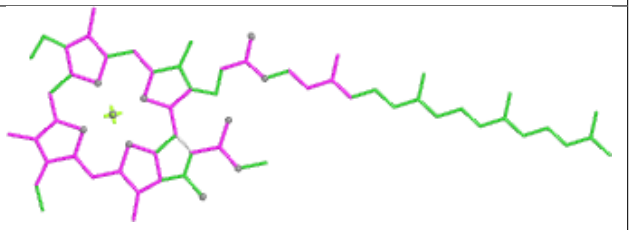


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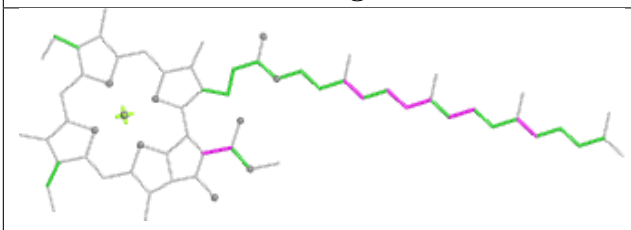
Ligand CLA B 605



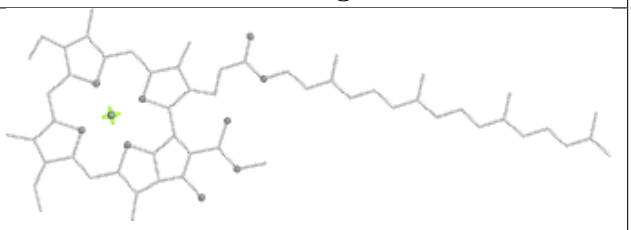
Bond lengths



Bond angles



Torsions

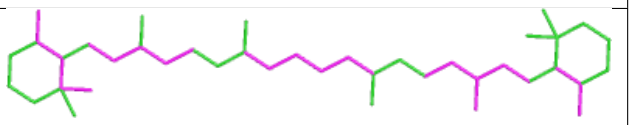


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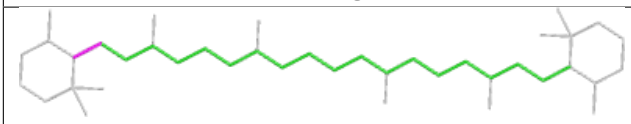
Ligand BCR b 617



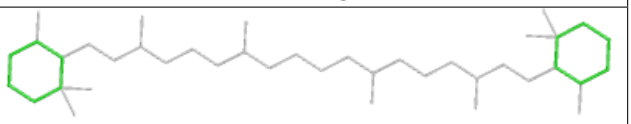
Bond lengths



Bond angles

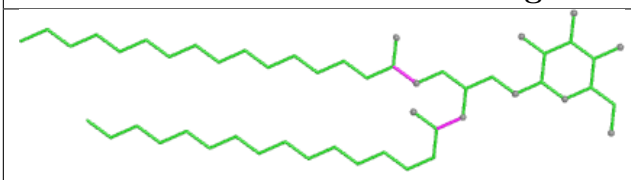


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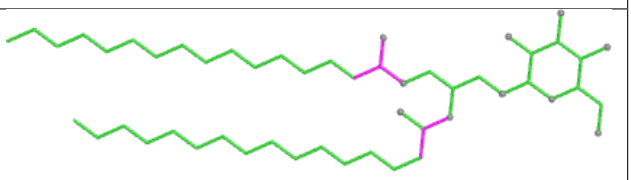


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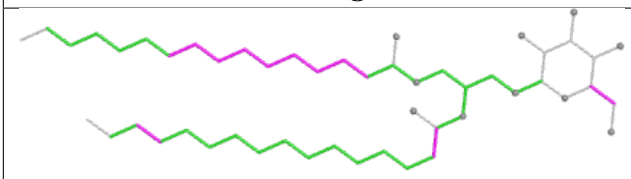
Ligand LMG c 519



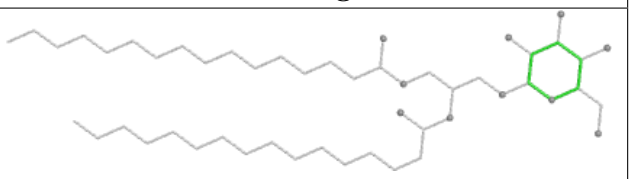
Bond lengths



Bond angles

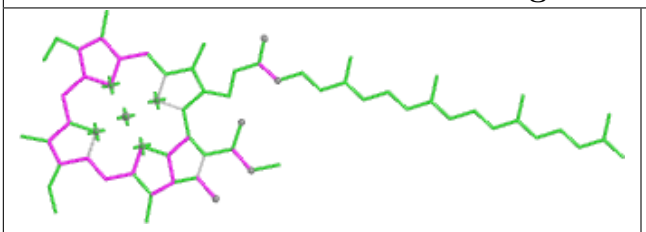


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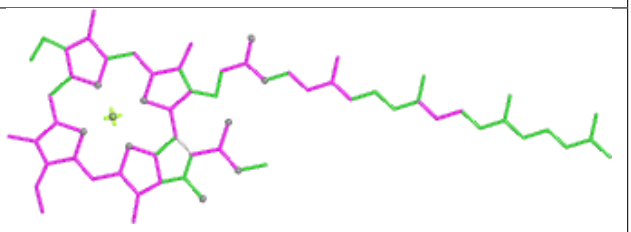


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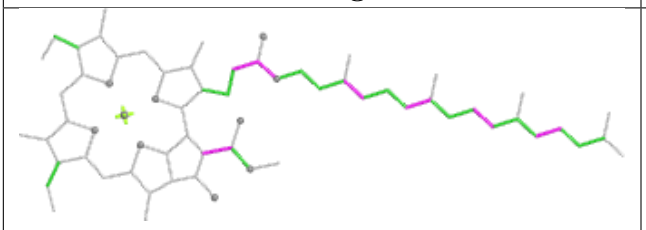
Ligand CLA c 510



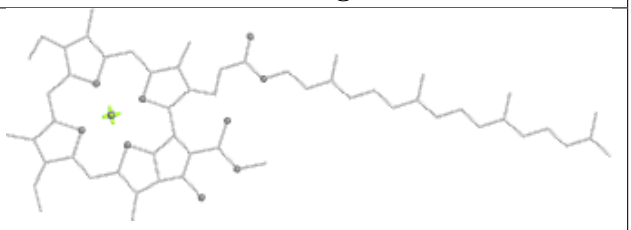
Bond lengths



Bond angles

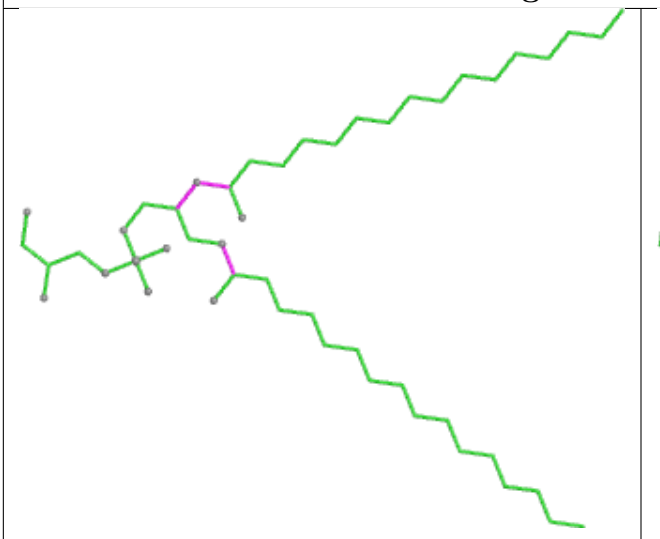


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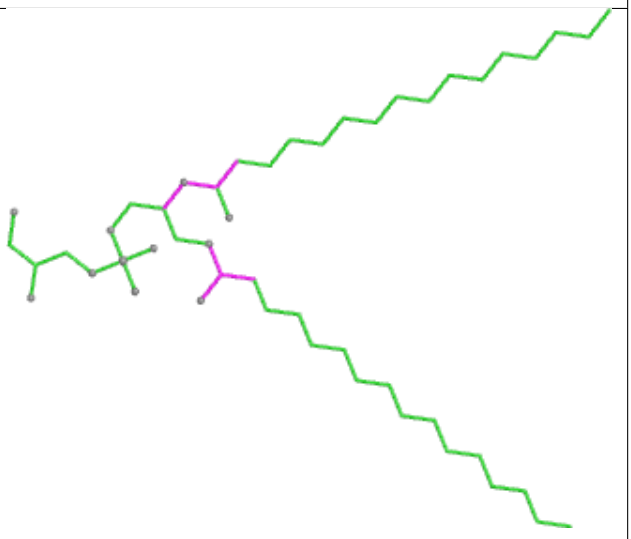


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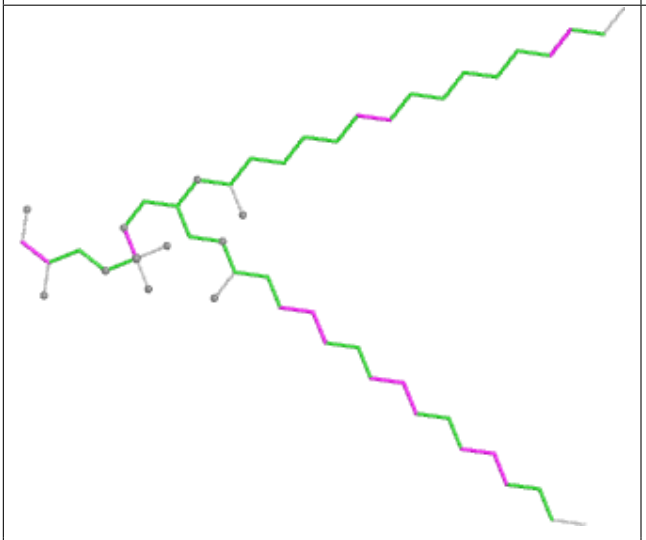
Ligand LHG A 416



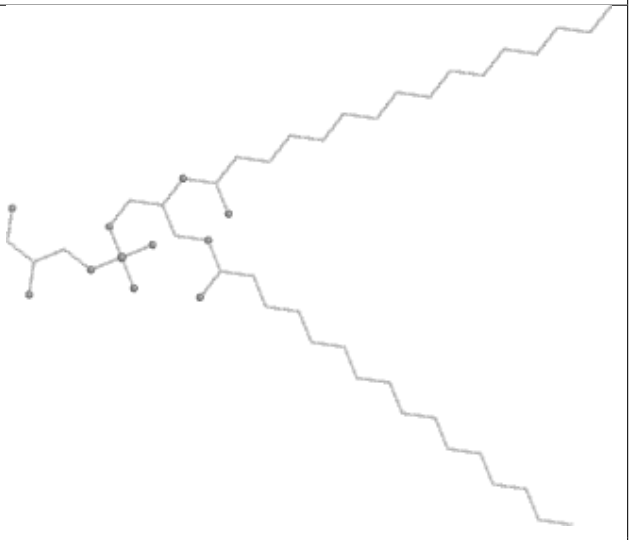
Bond lengths



Bond angles

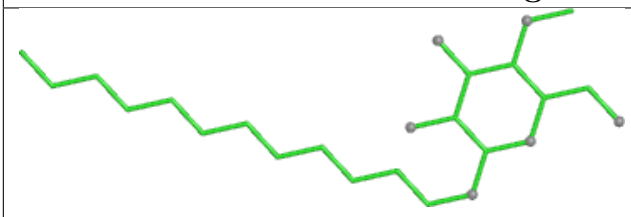


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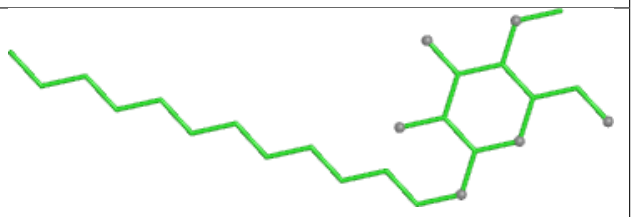


Rings

Ligand LMT b 621



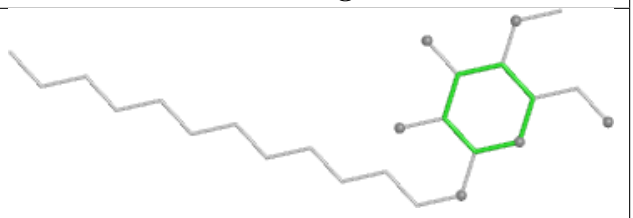
Bond lengths



Bond angles

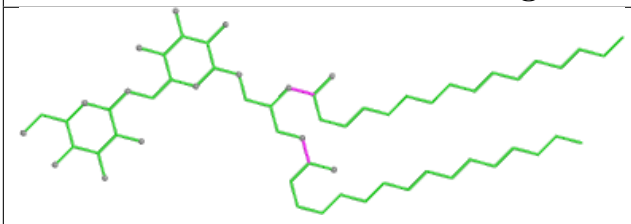


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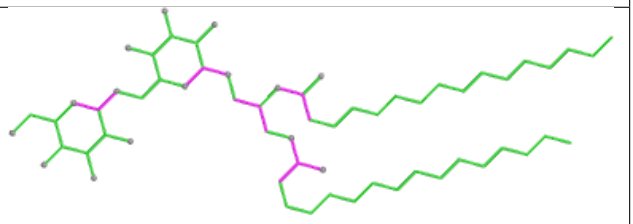


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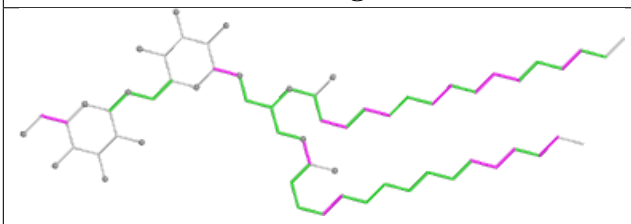
Ligand DGD C 519



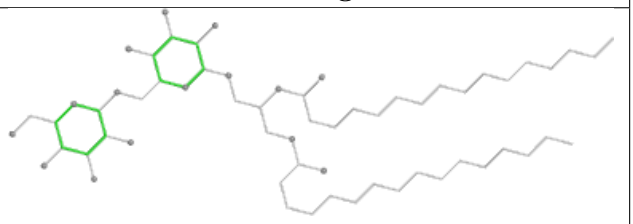
Bond lengths



Bond angles

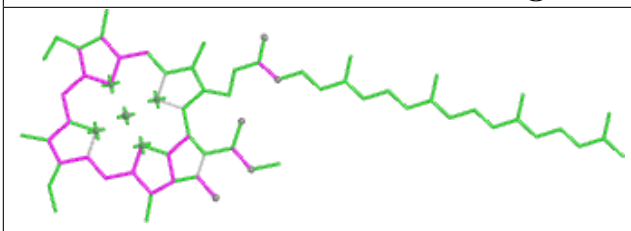


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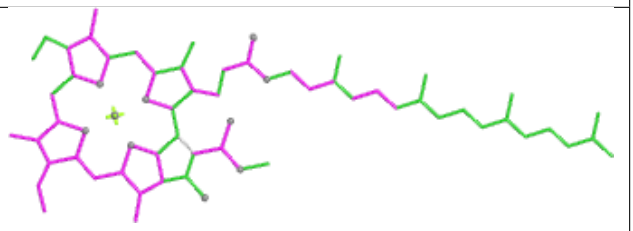


Rings

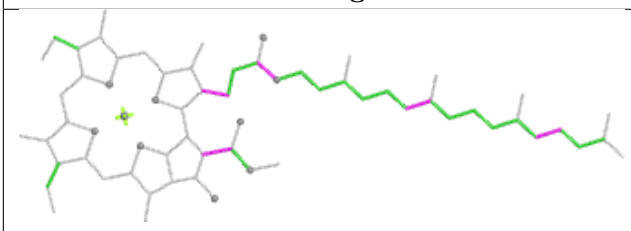
Ligand CLA b 609



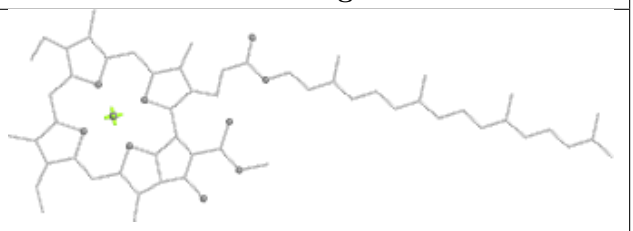
Bond lengths



Bond angles

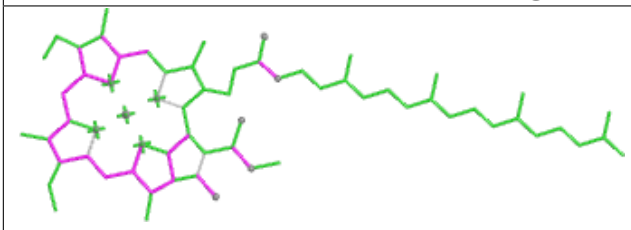


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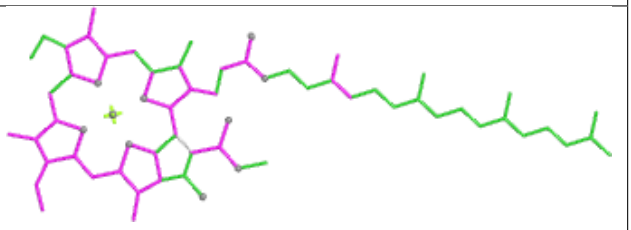


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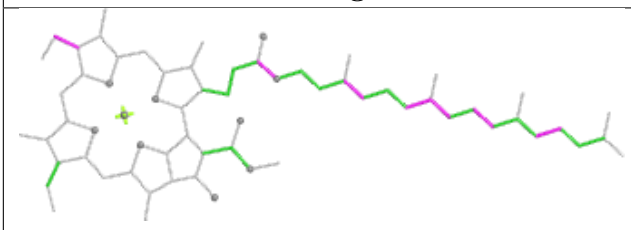
Ligand CLA b 603



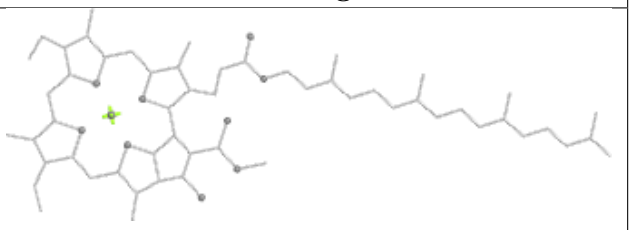
Bond lengths



Bond angles

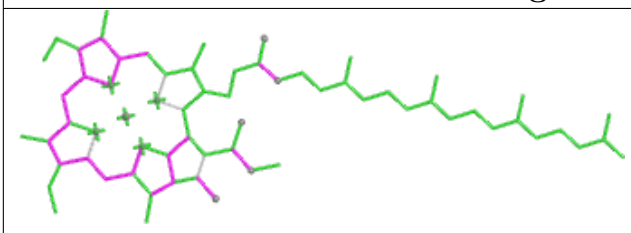


Torsions

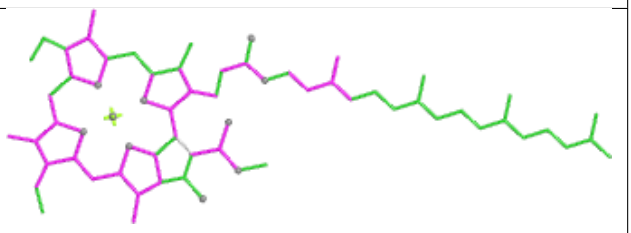


Rings

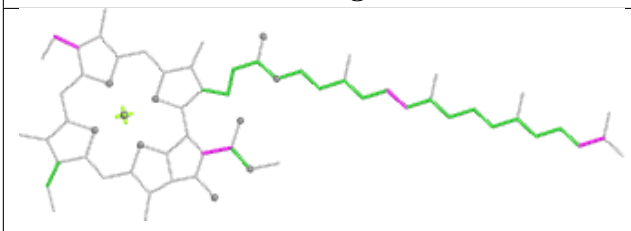
Ligand CLA c 508



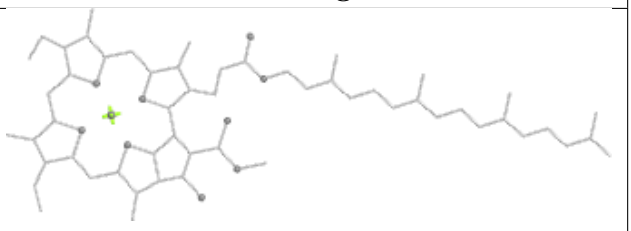
Bond lengths



Bond angles

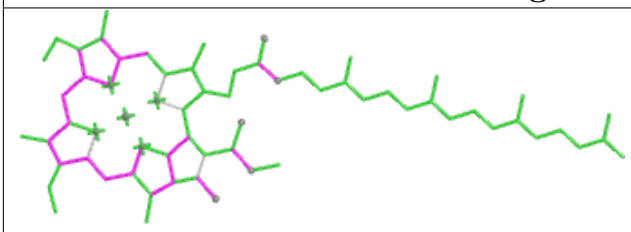


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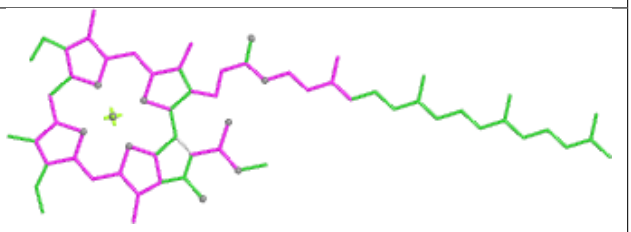


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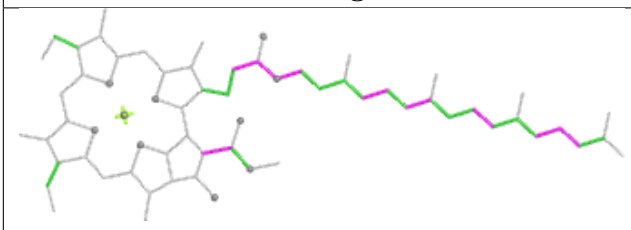
Ligand CLA c 512



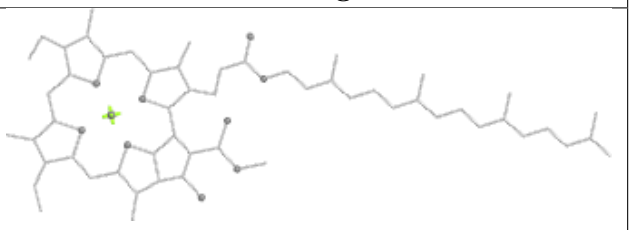
Bond lengths



Bond angles

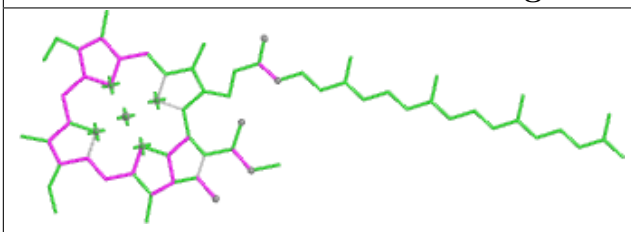


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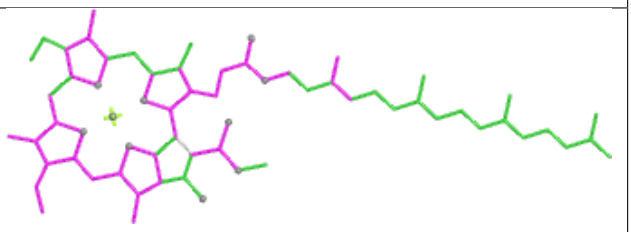


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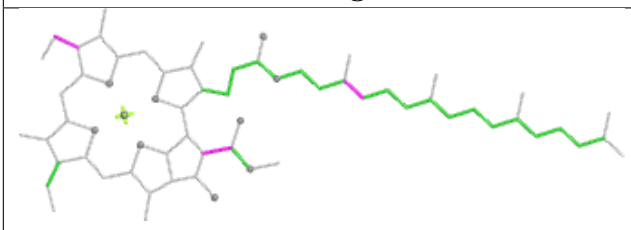
Ligand CLA B 607



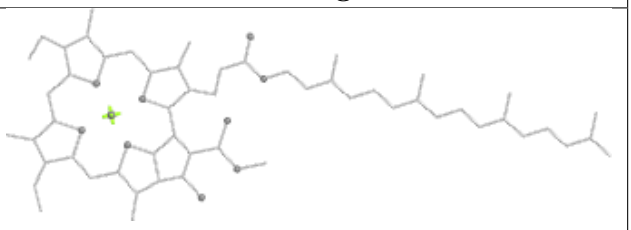
Bond lengths



Bond angles



Torsions

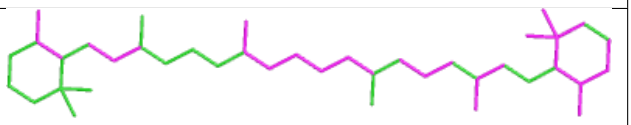


Rings

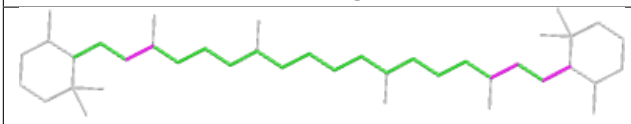
Ligand BCR d 405



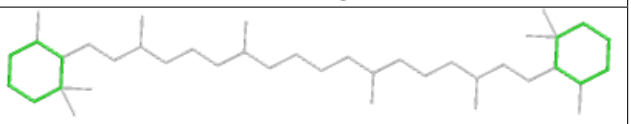
Bond lengths



Bond angles

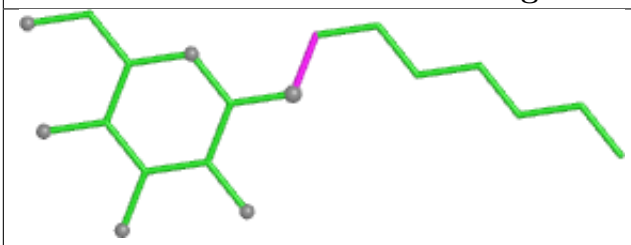


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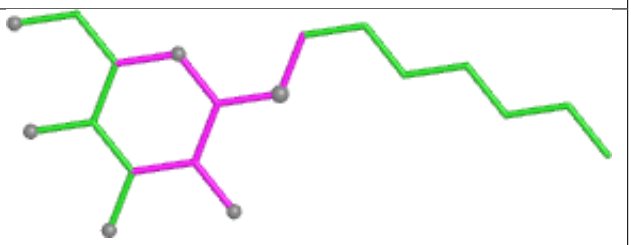


Rings

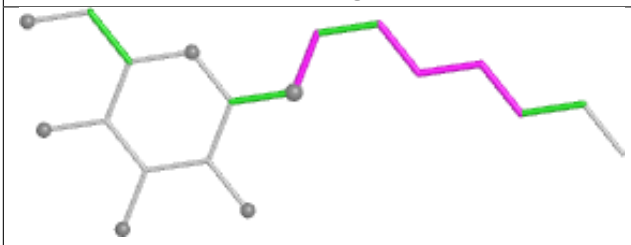
Ligand HTG B 622



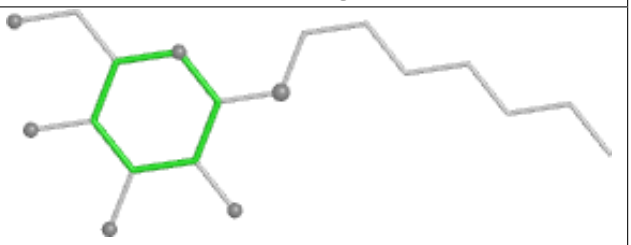
Bond lengths



Bond angles

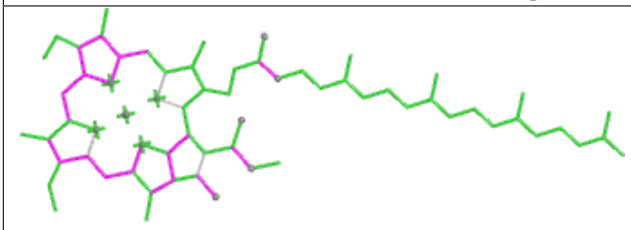


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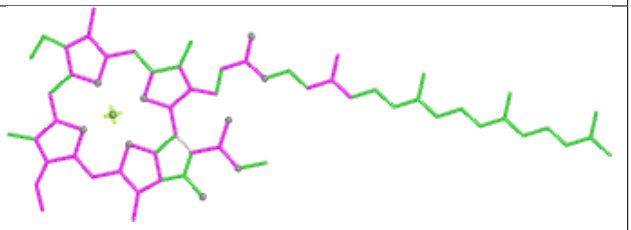


Rings

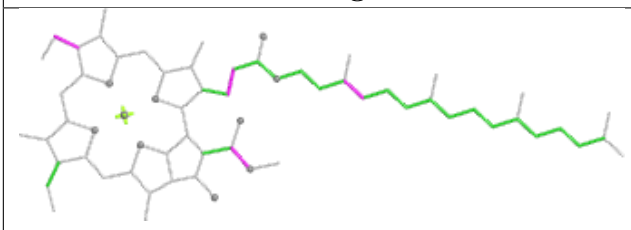
Ligand CLA B 603



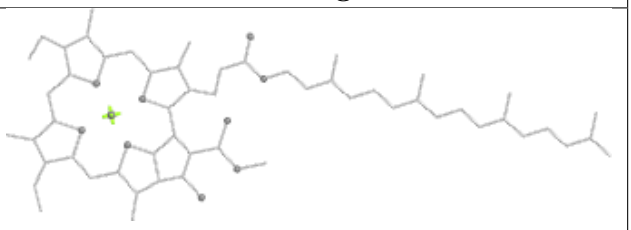
Bond lengths



Bond angles

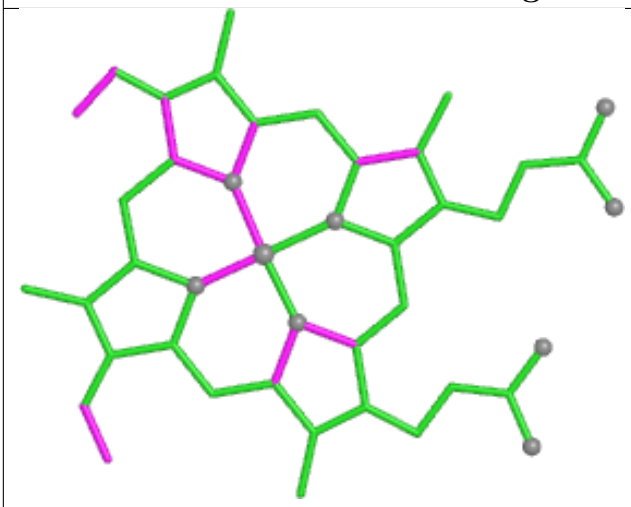


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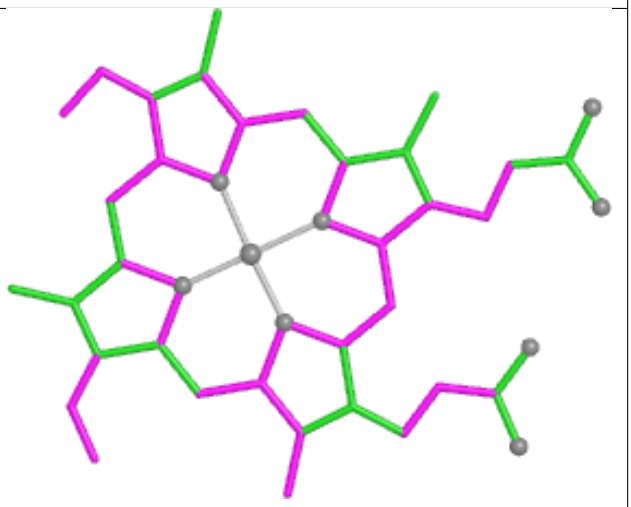


Rings

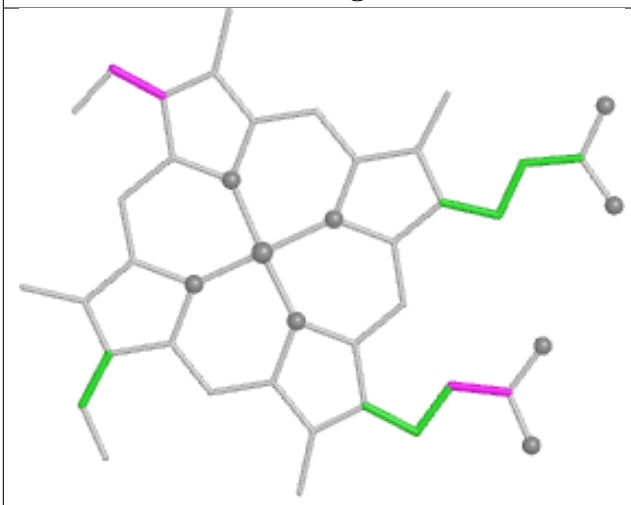
Ligand HEC V 202



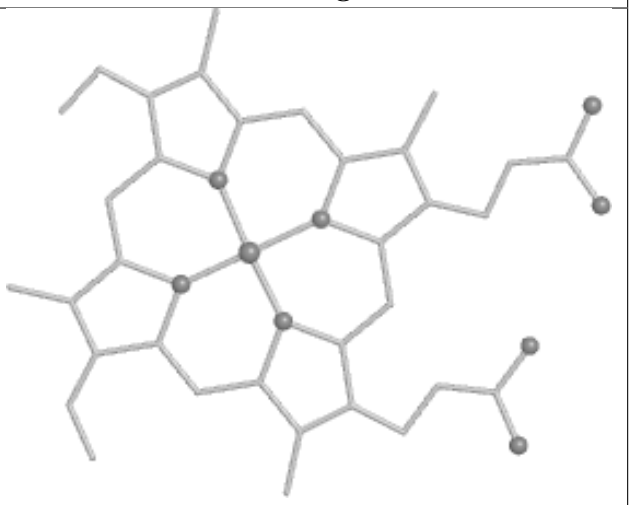
Bond lengths



Bond angles

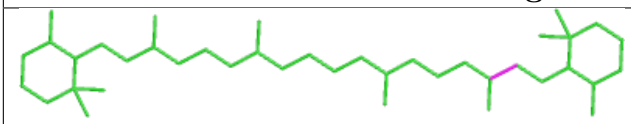


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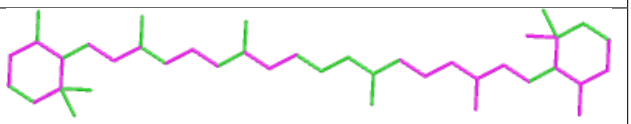


Rings

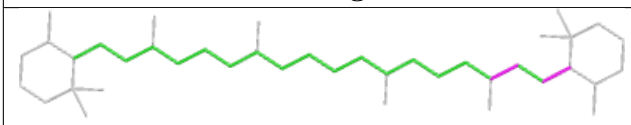
Ligand BCR b 619



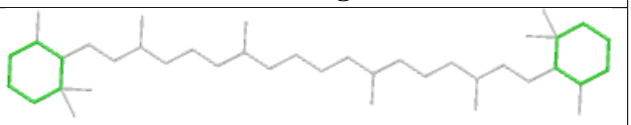
Bond lengths



Bond angles

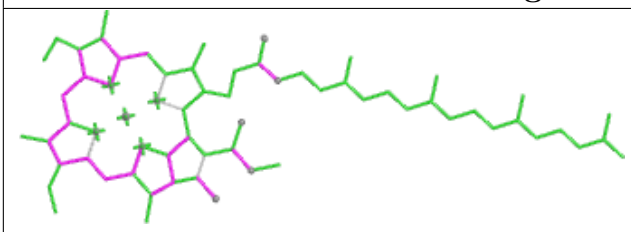


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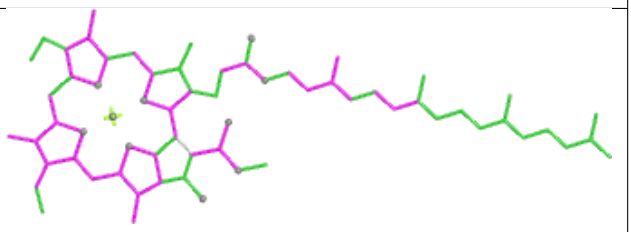


Rings

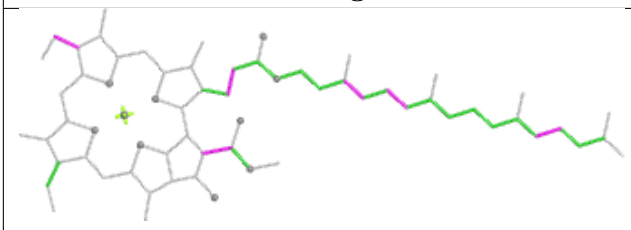
Ligand CLA C 508



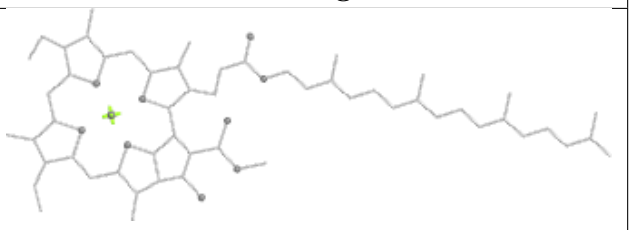
Bond lengths



Bond angles

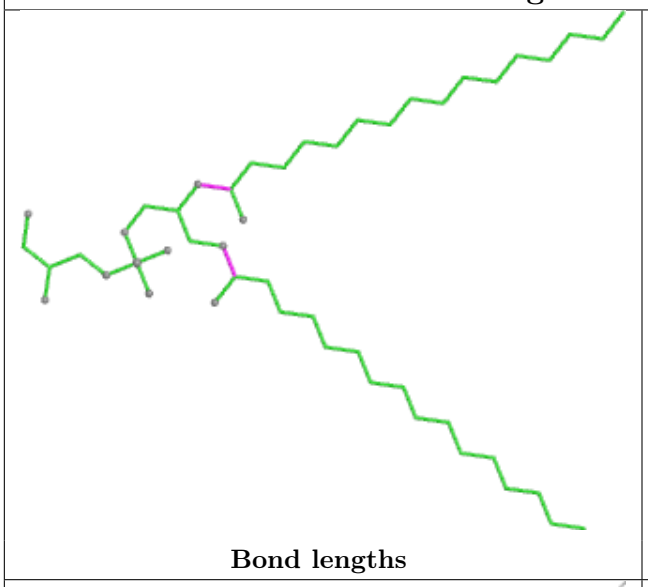


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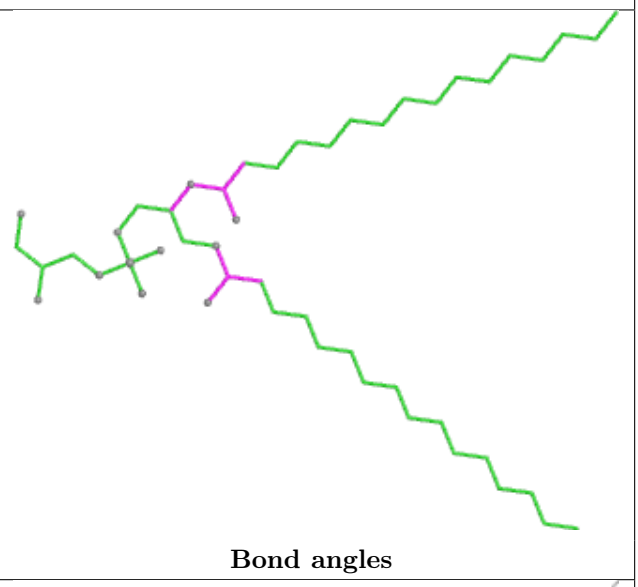


Rings

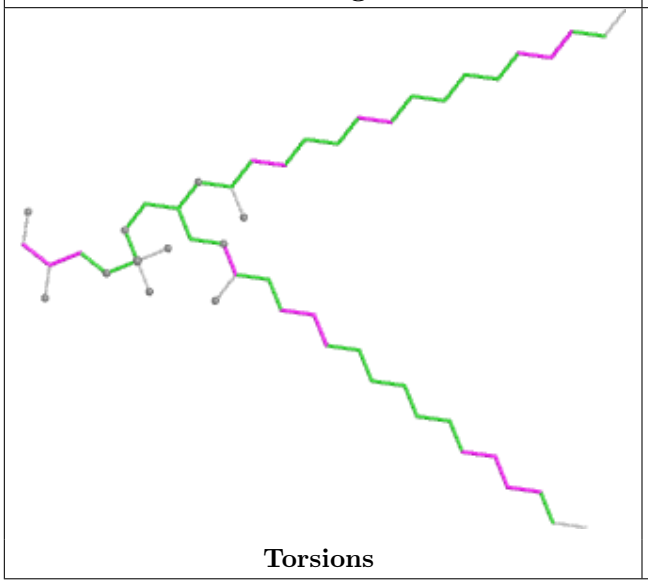
Ligand LHG d 407



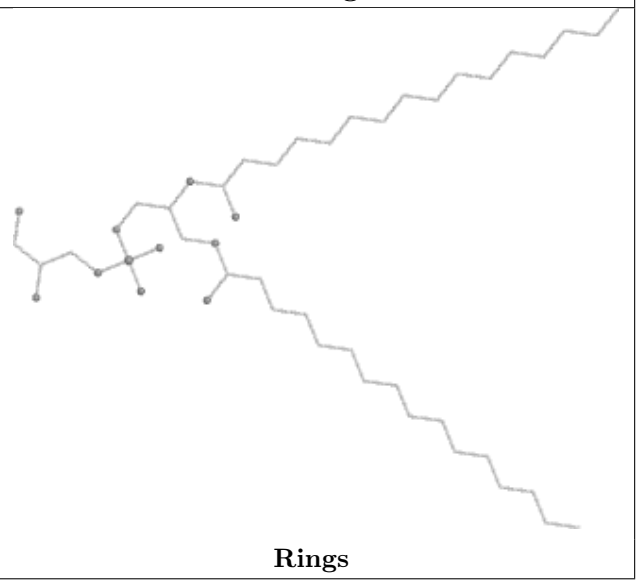
Bond lengths



Bond angles

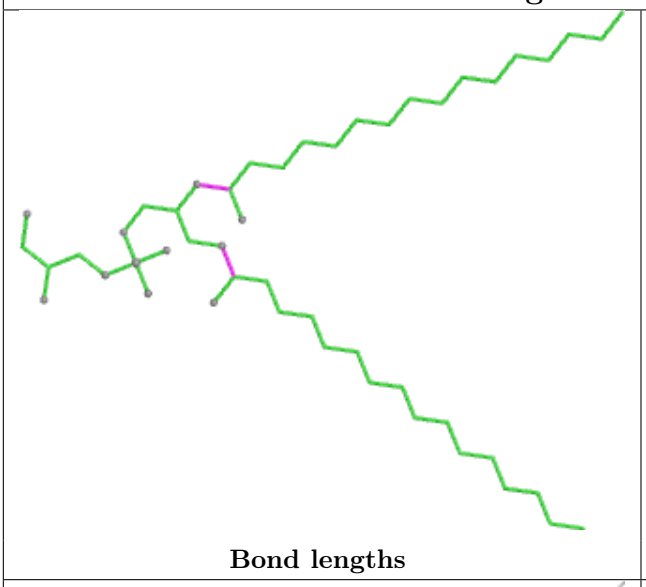


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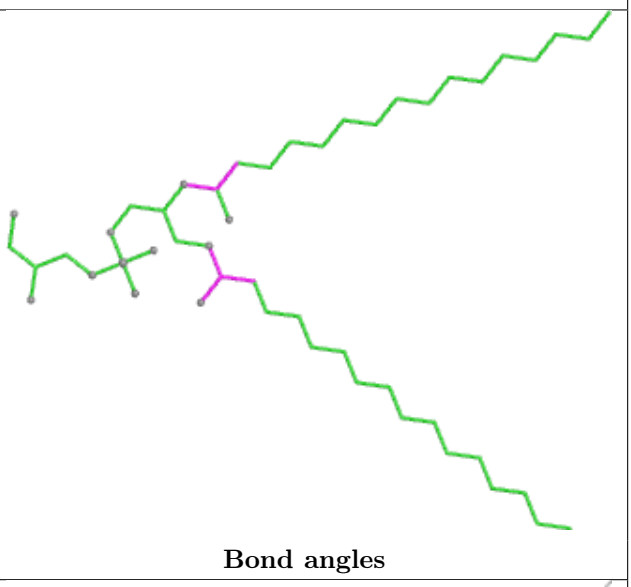


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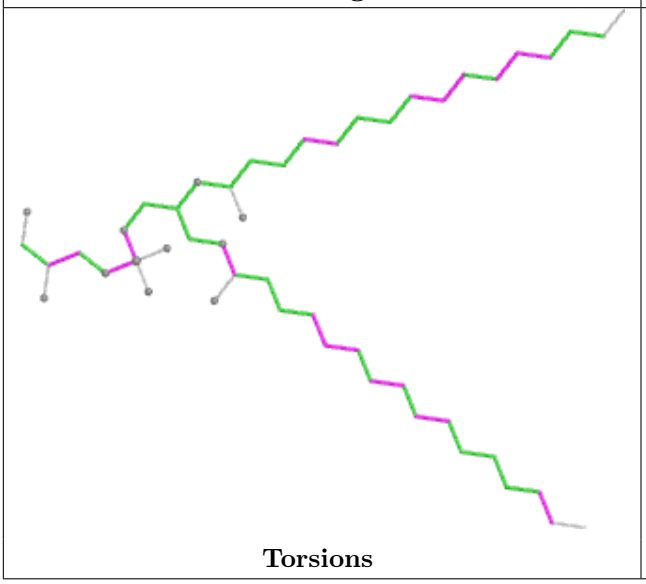
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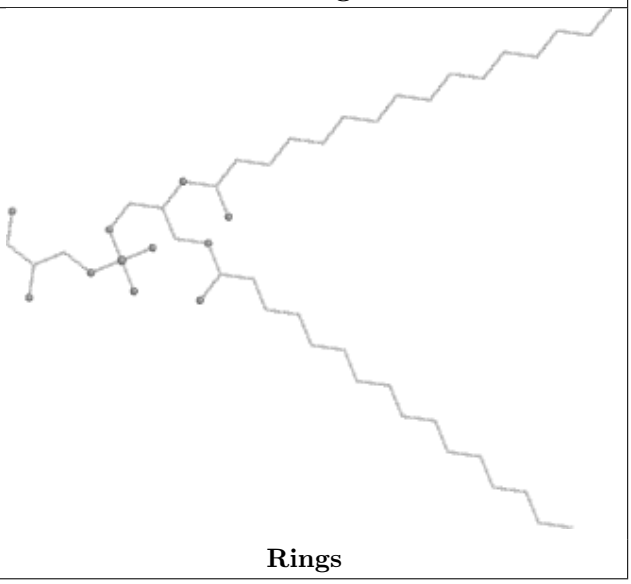
Bond lengths



Bond angles



Torsions

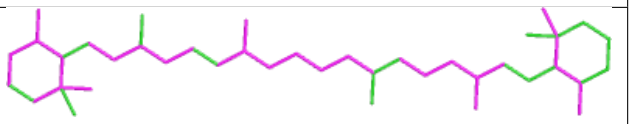


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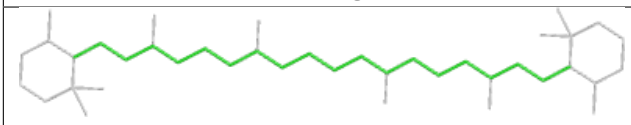
Ligand BCR c 515



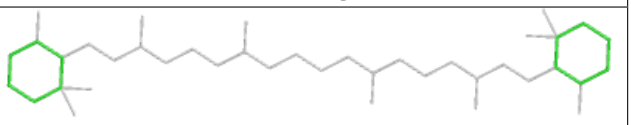
Bond lengths



Bond angles

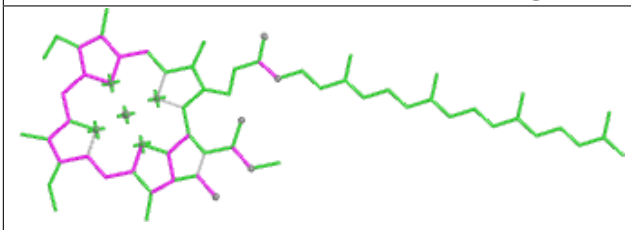


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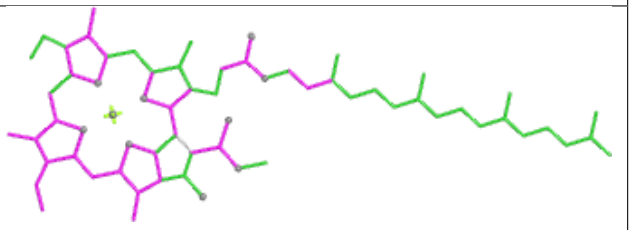


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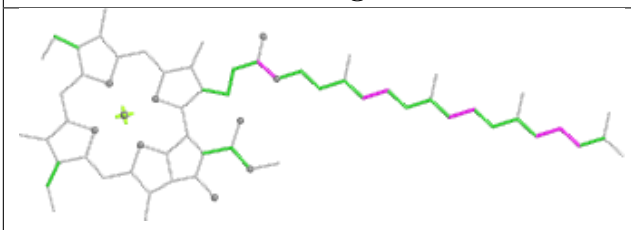
Ligand CLA b 611



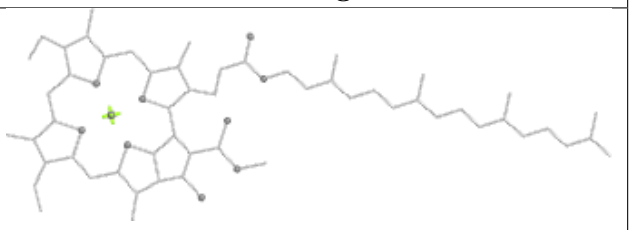
Bond lengths



Bond angles

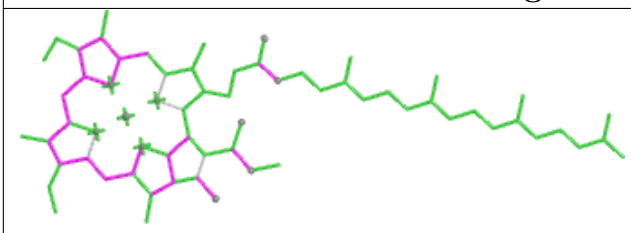


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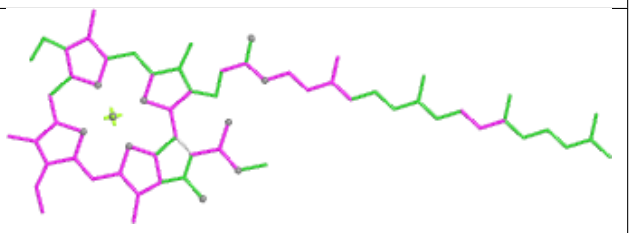


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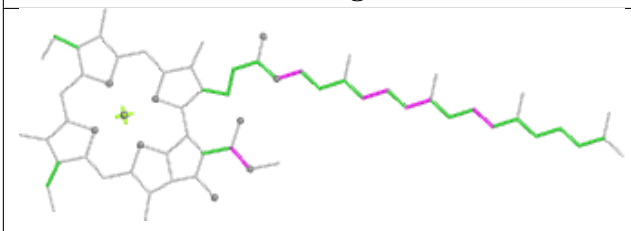
Ligand CLA C 510



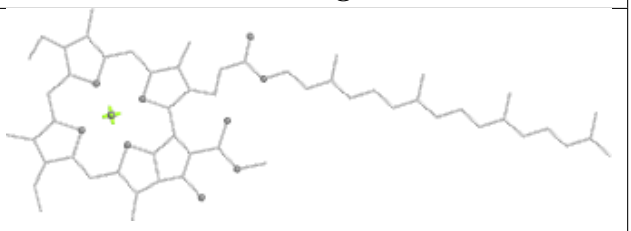
Bond lengths



Bond angles

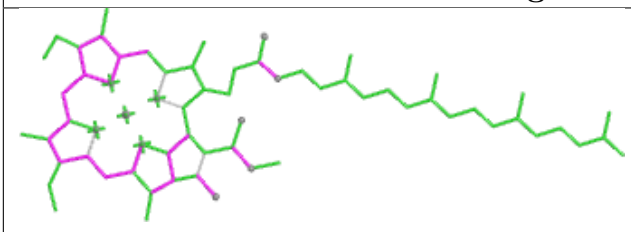


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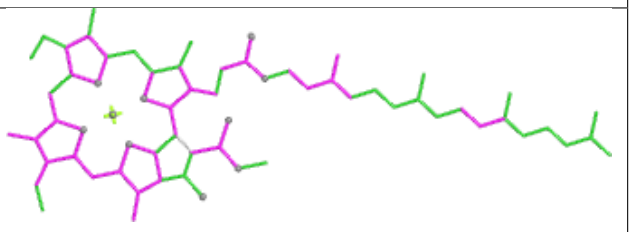


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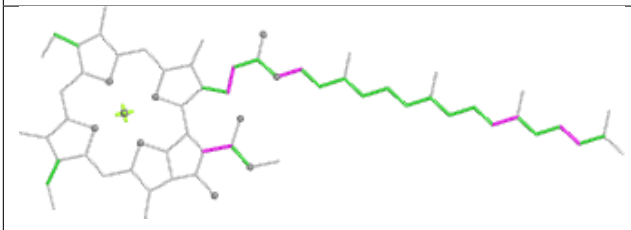
Ligand CLA b 610



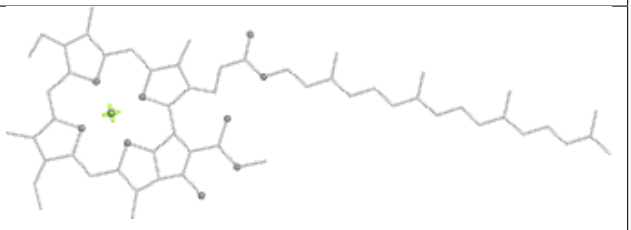
Bond lengths



Bond angles

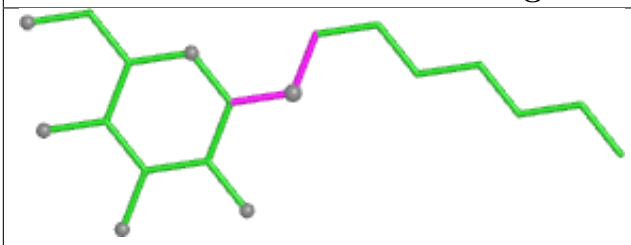


Torsions

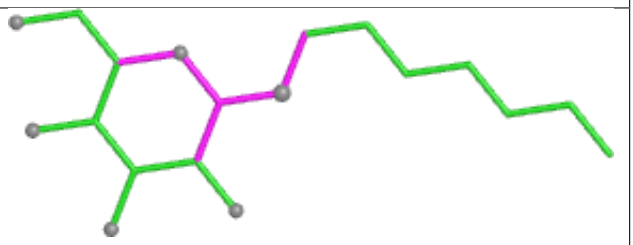


Rings

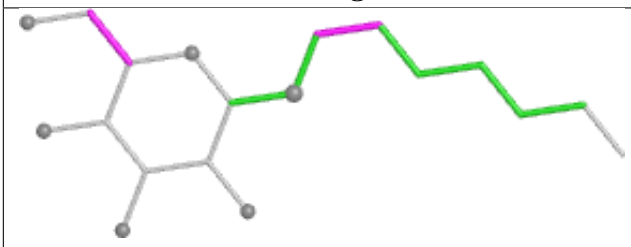
Ligand HTG b 623



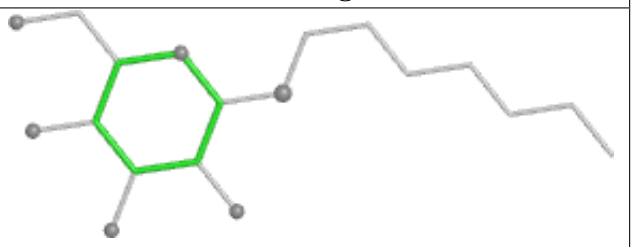
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 d 406



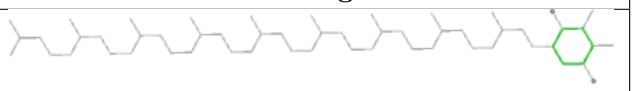
Bond lengths



Bond angles

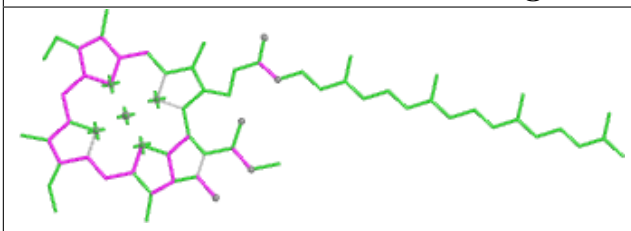


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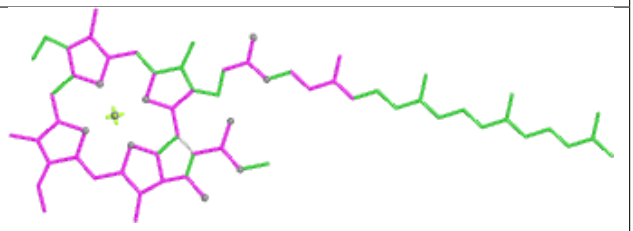


Rings

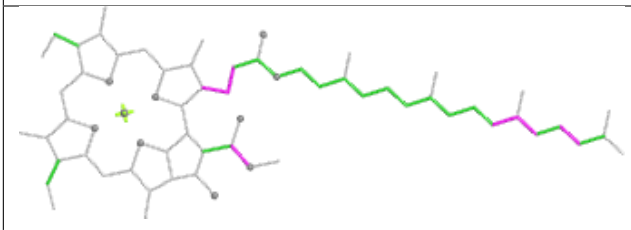
Ligand CLA C 502



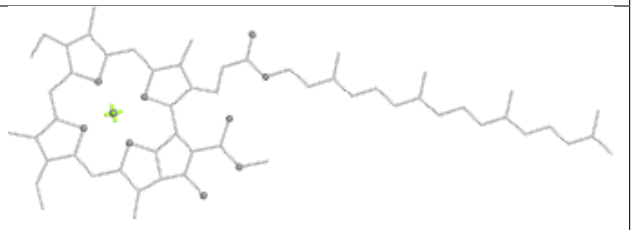
Bond lengths



Bond angles

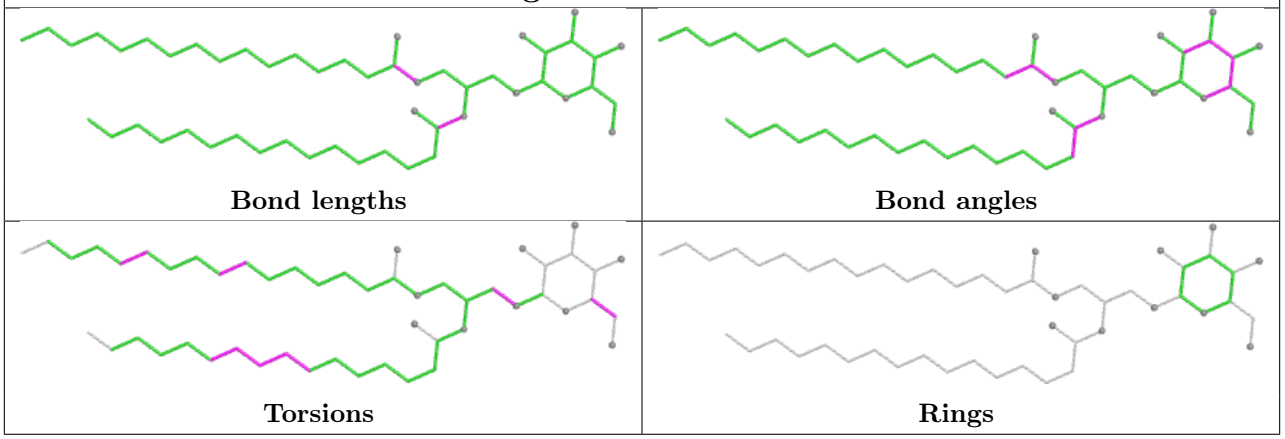


Torsions

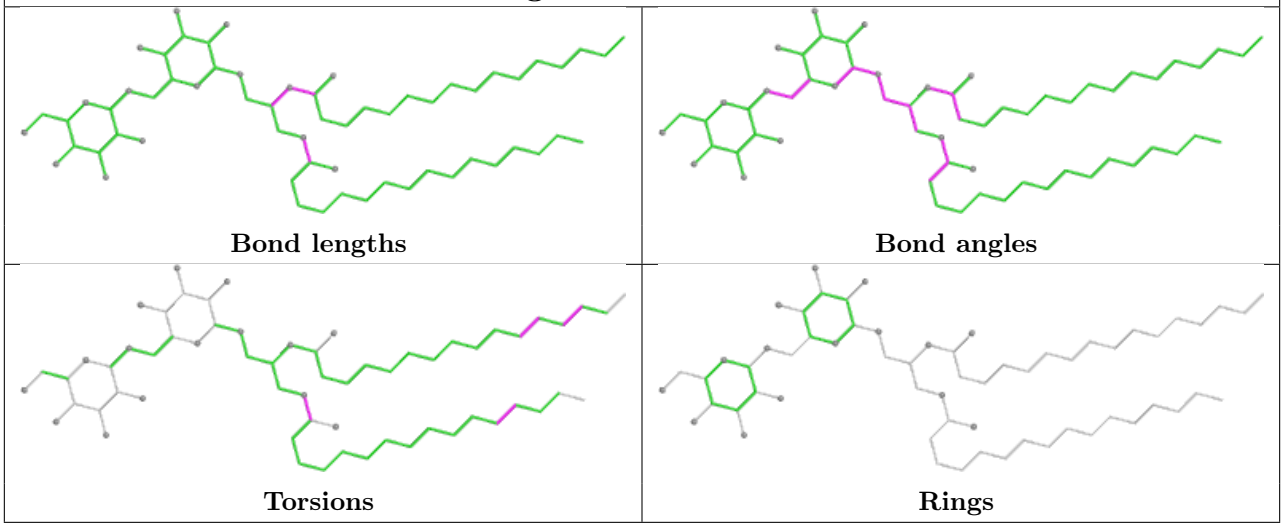


Rings

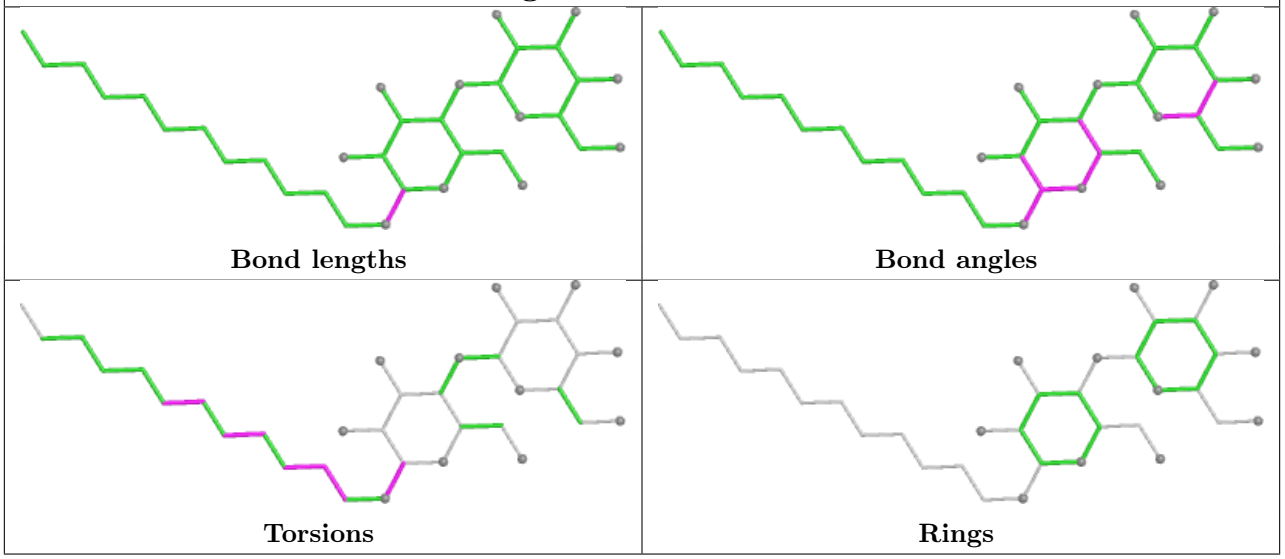
Ligand LMG Z 101

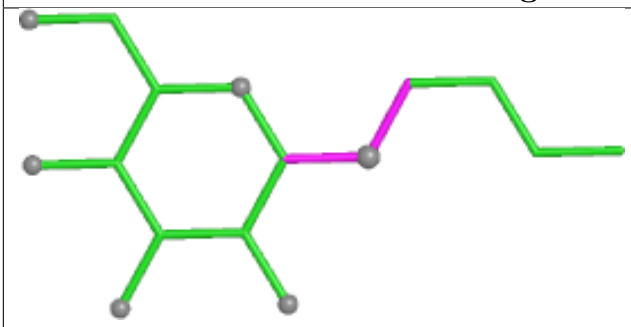
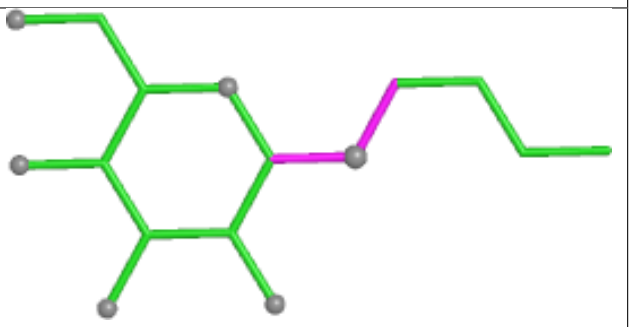
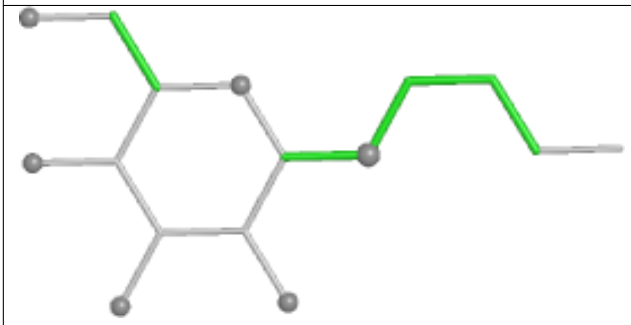
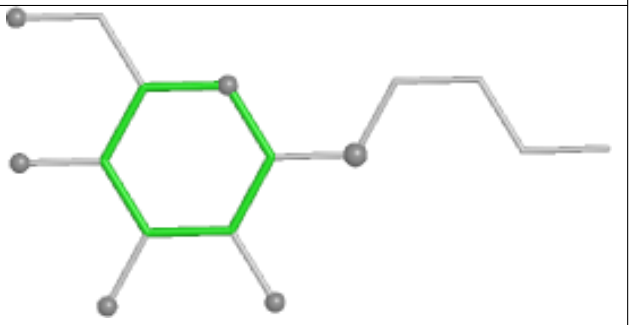


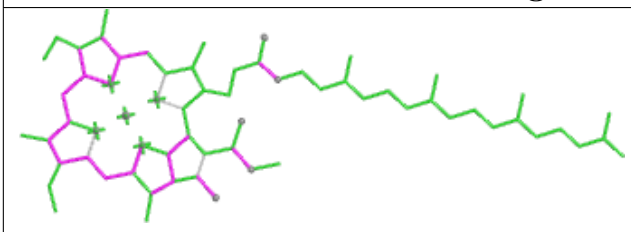
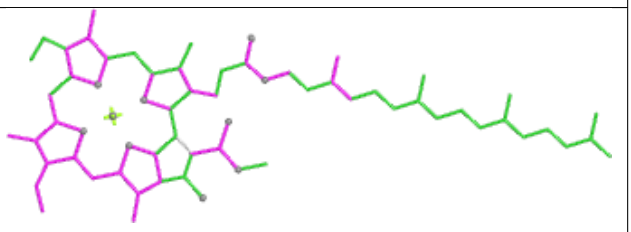
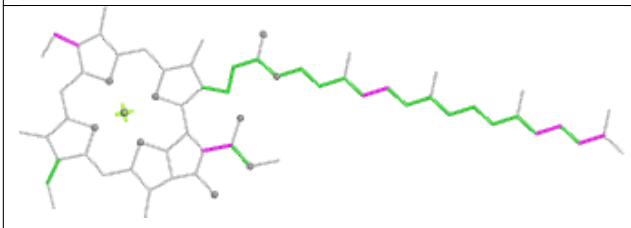
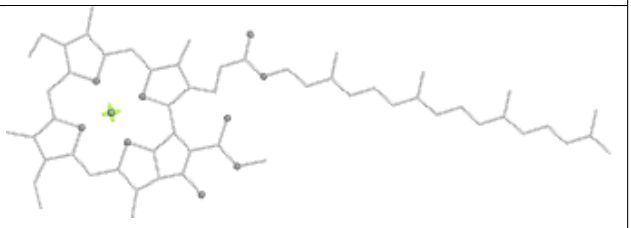
Ligand DGD c 518



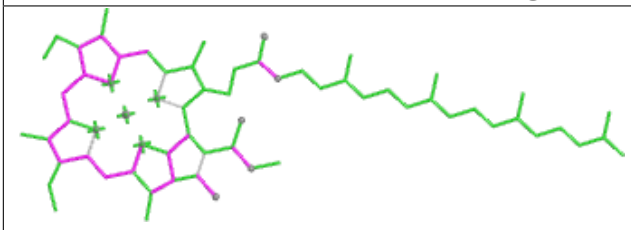
Ligand LMT D 402



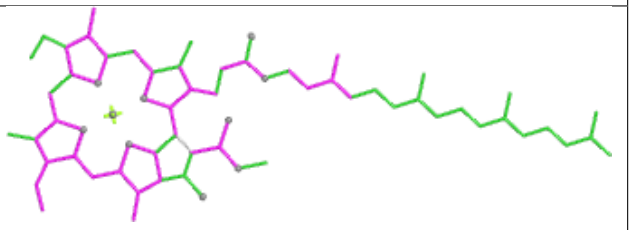
Ligand HTG D 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

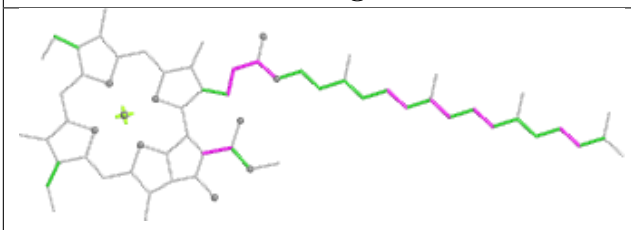
Ligand CLA B 601



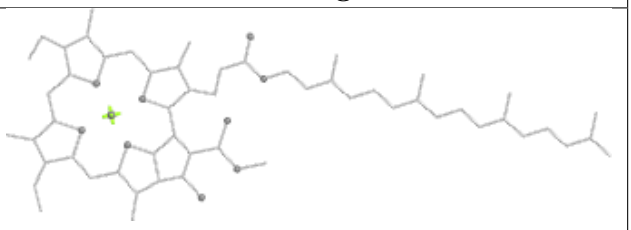
Bond lengths



Bond angles

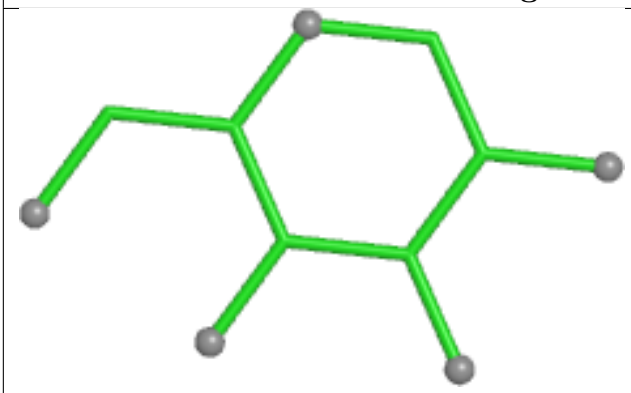


Torsions

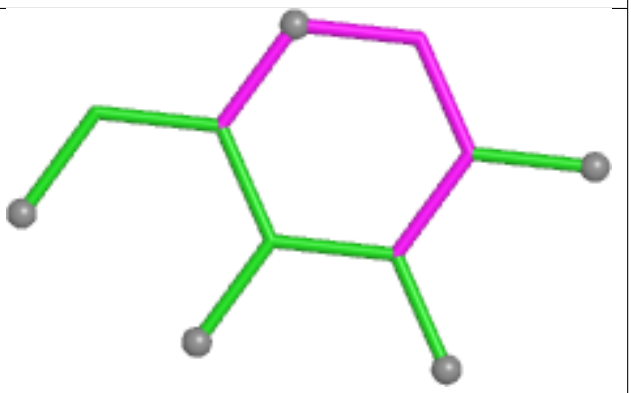


Rings

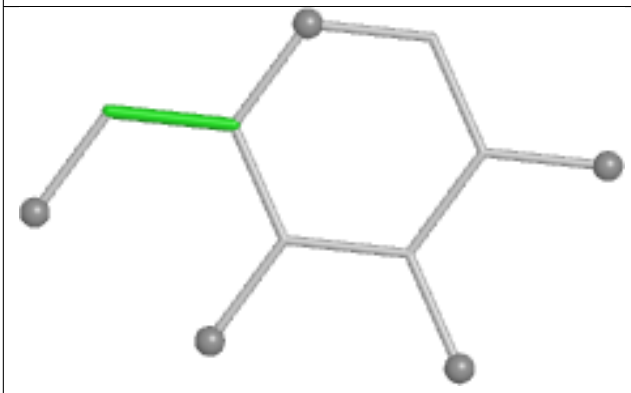
Ligand HTG V 203



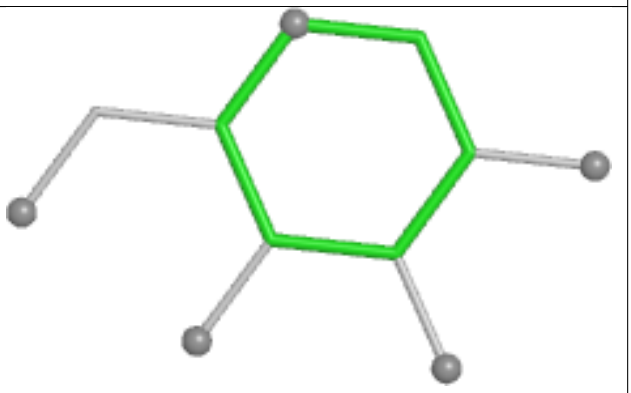
Bond lengths



Bond angles

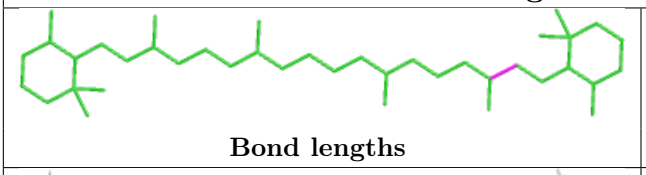


Torsions

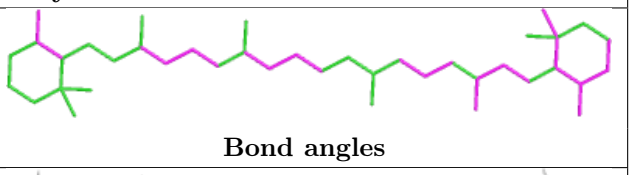


Rings

Ligand BCR y 101



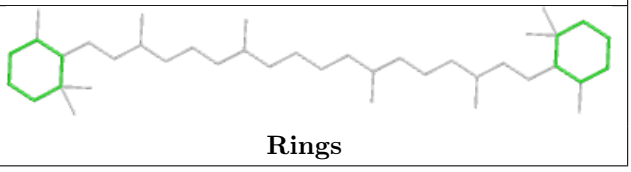
Bond lengths



Bond angles

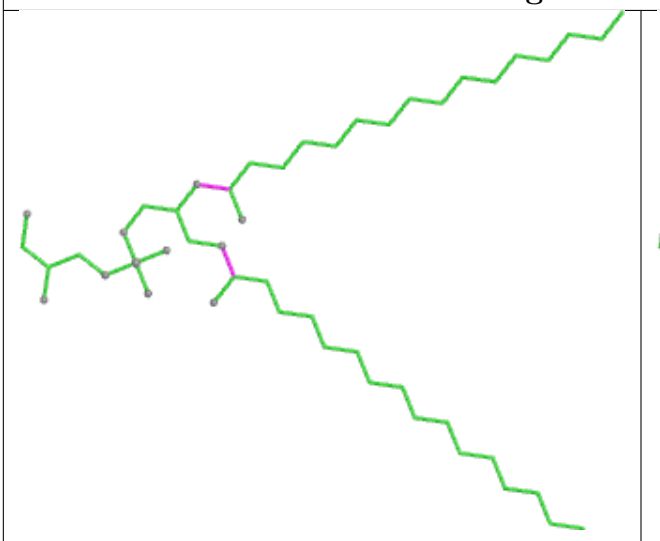


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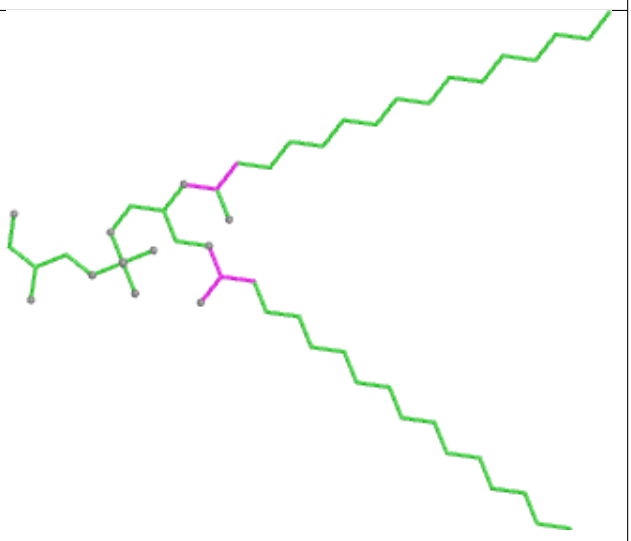


Rings

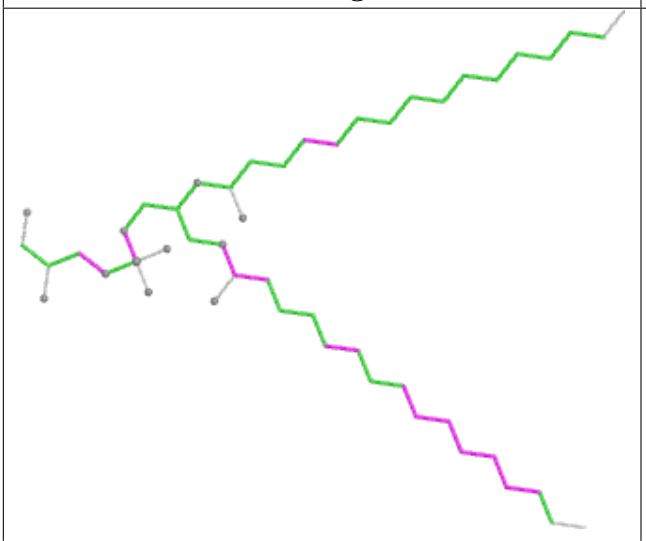
Ligand LHG d 409



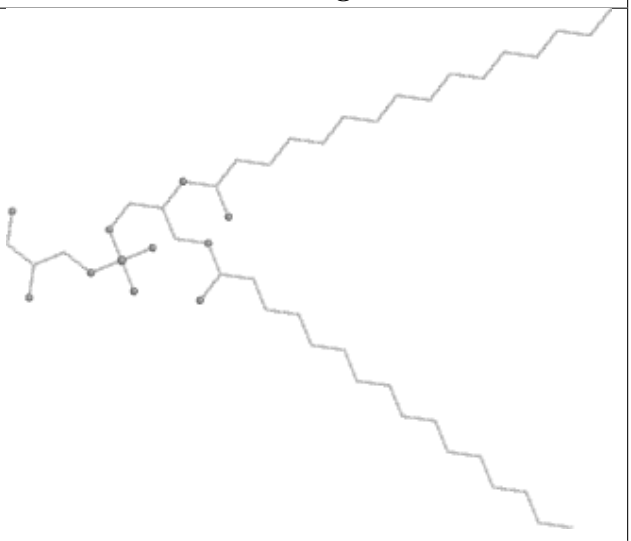
Bond lengths



Bond angles

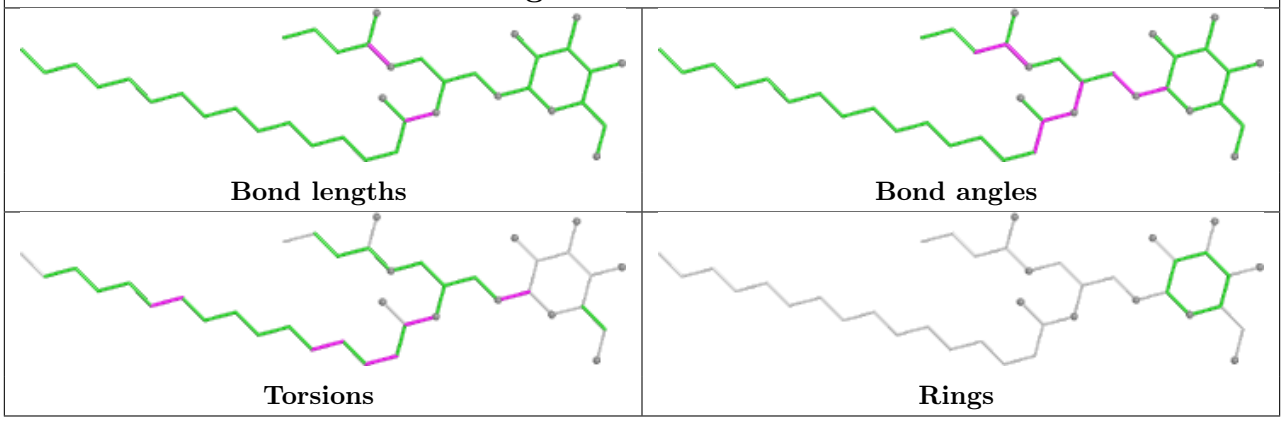


Torsions

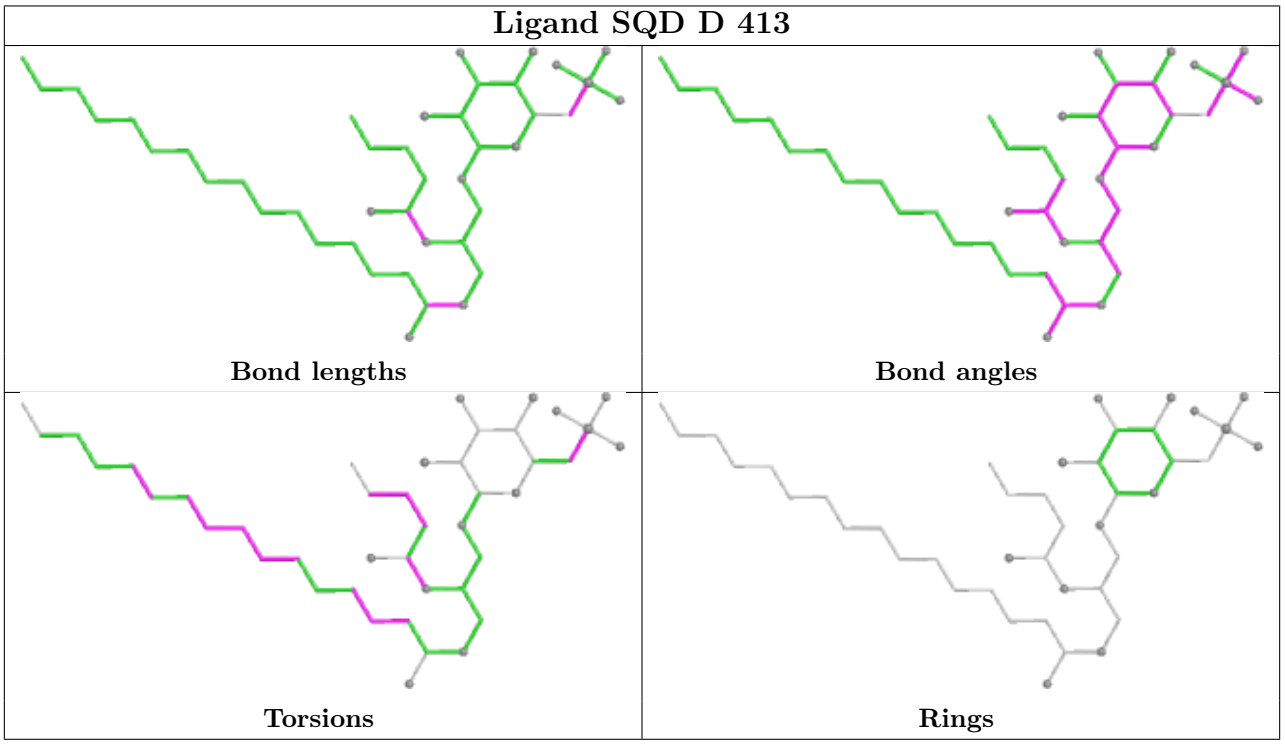


Rings

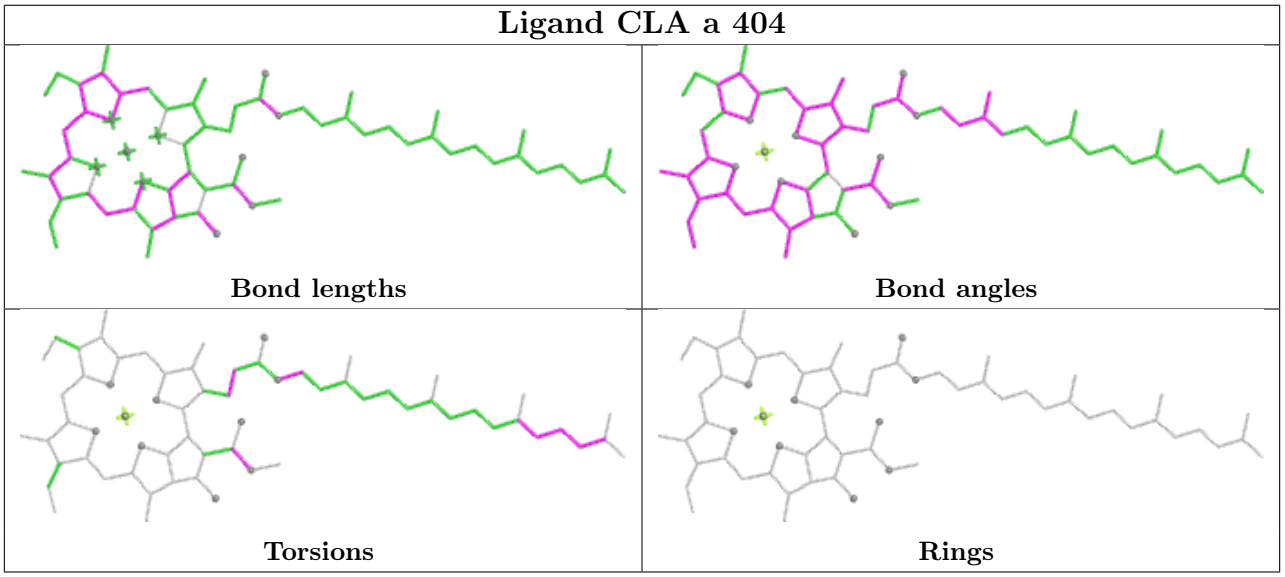
Ligand LMG z 101



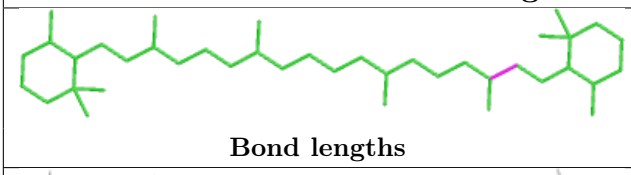
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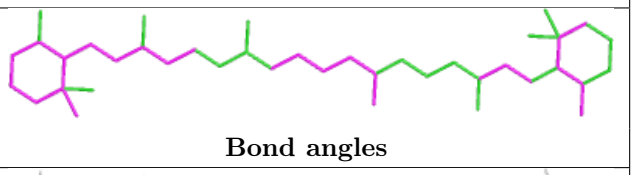
Ligand CLA a 404



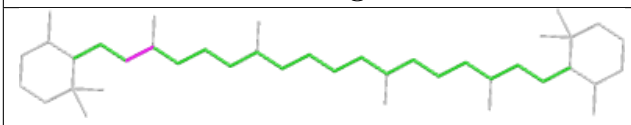
Ligand BCR H 101



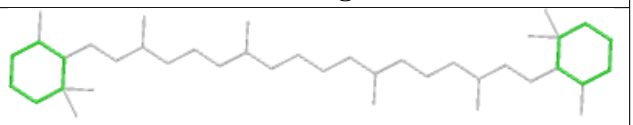
Bond lengths



Bond angles

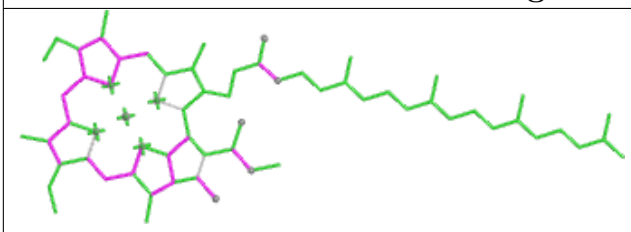


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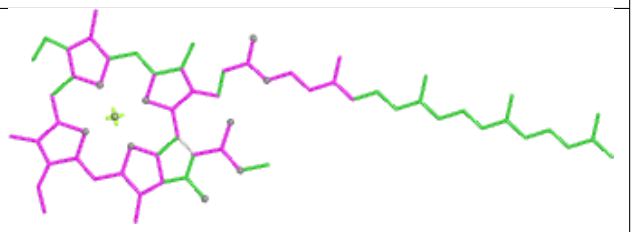


Rings

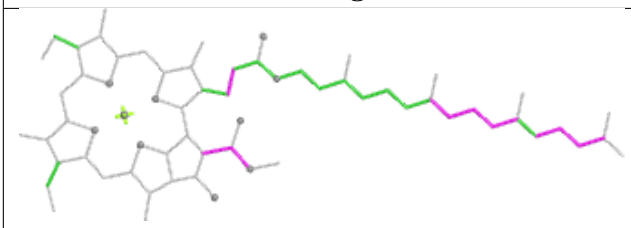
Ligand CLA b 606



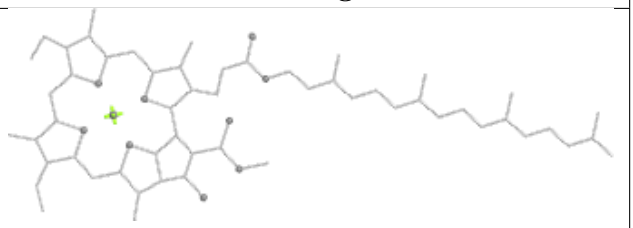
Bond lengths



Bond angles

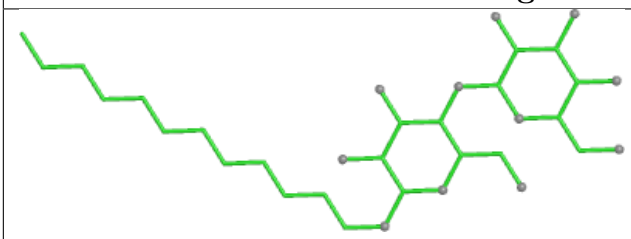


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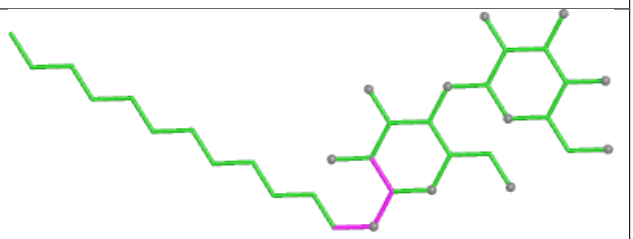


Rings

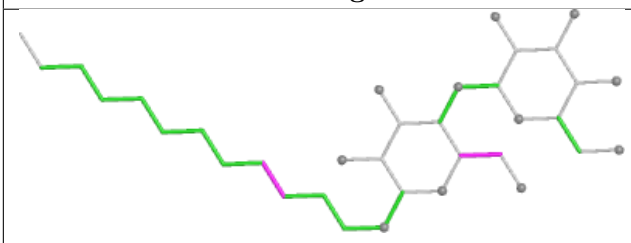
Ligand LMT M 101



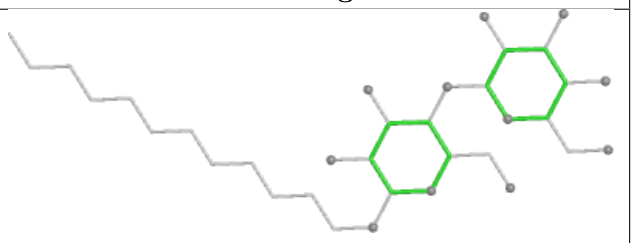
Bond lengths



Bond angles

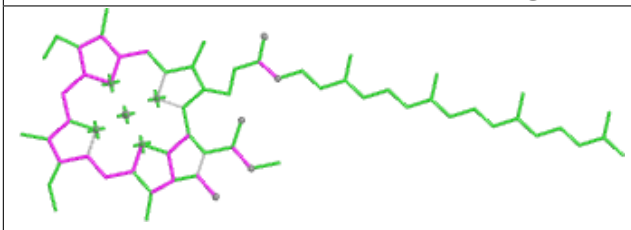


Torsions

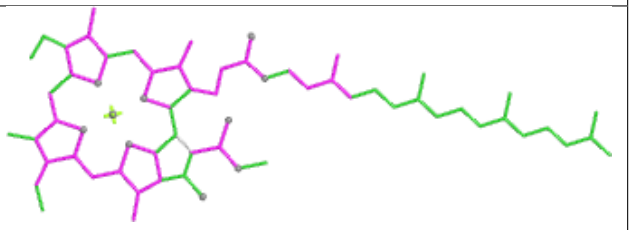


Rings

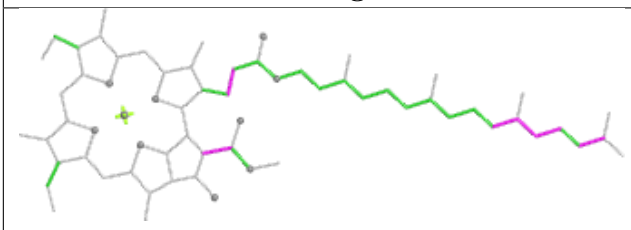
Ligand CLA B 610



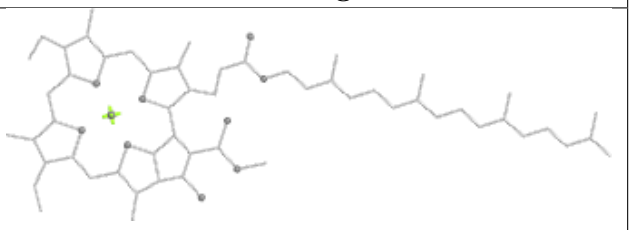
Bond lengths



Bond angles



Torsions



Rings

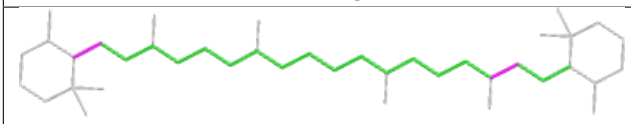
Ligand BCR Y 101



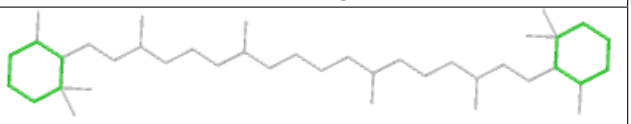
Bond lengths



Bond angles

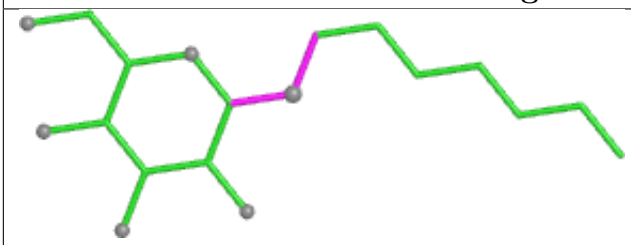


Torsions

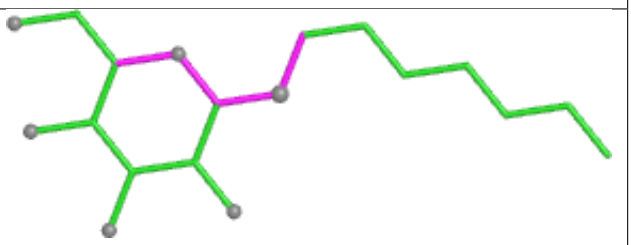


Rings

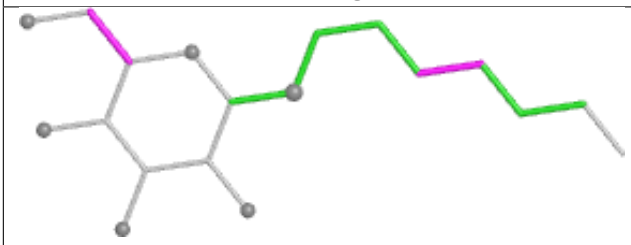
Ligand HTG B 627



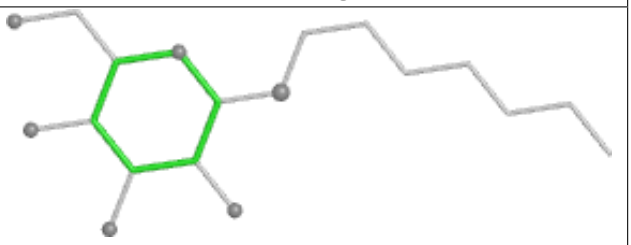
Bond lengths



Bond angles

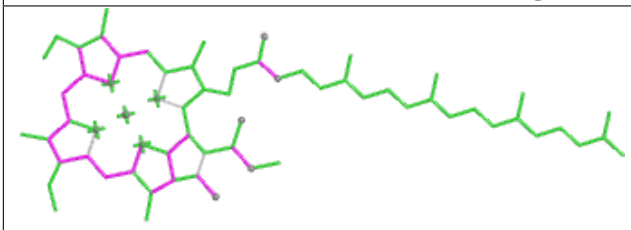


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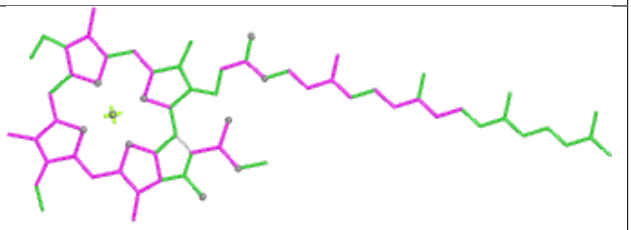


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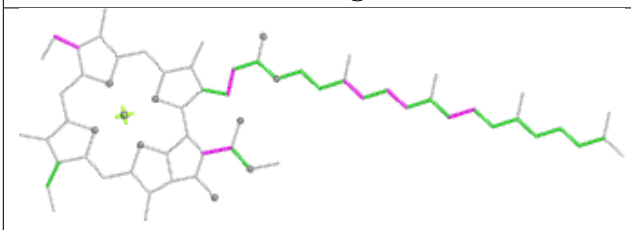
Ligand CLA c 507



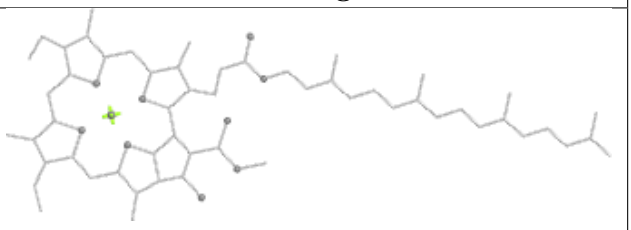
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Bond angles

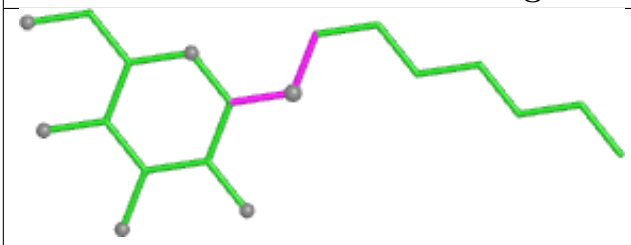


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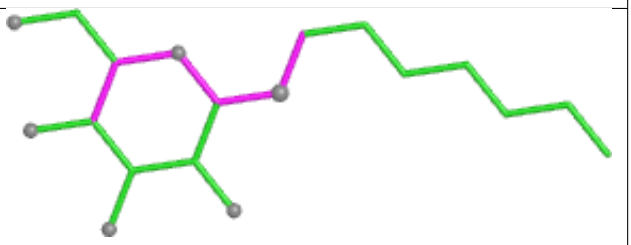


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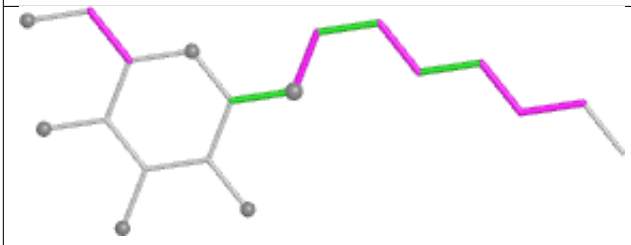
Ligand HTG b 625



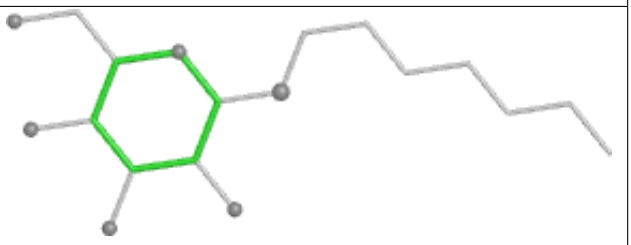
Bond lengths



Bond angles

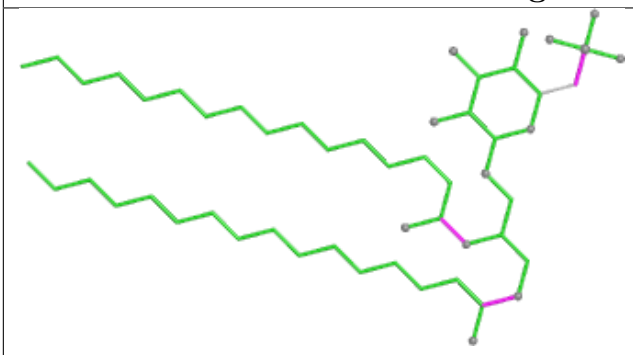


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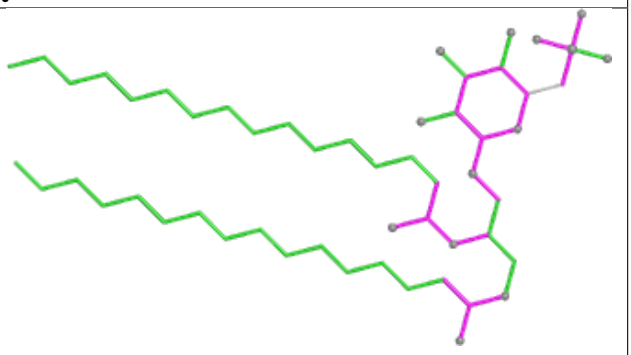


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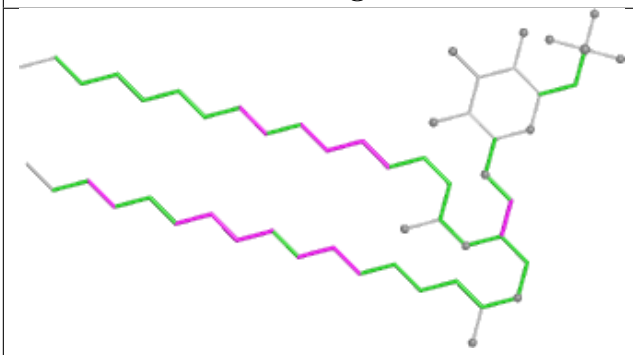
Ligand SQD a 410



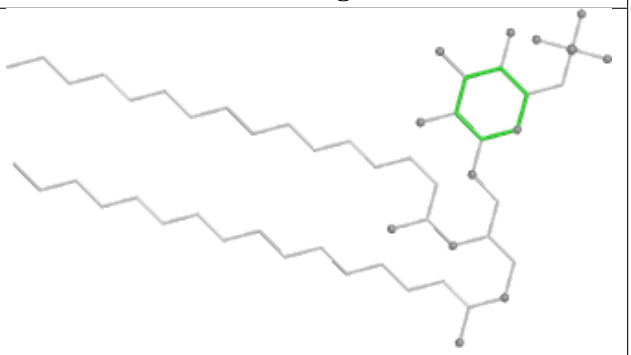
Bond lengths



Bond angles

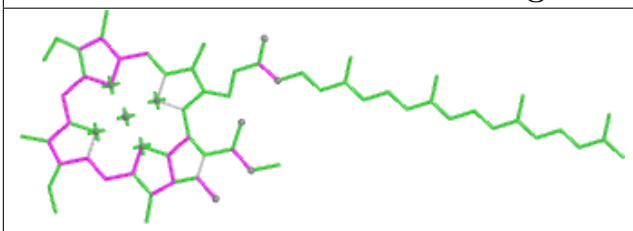


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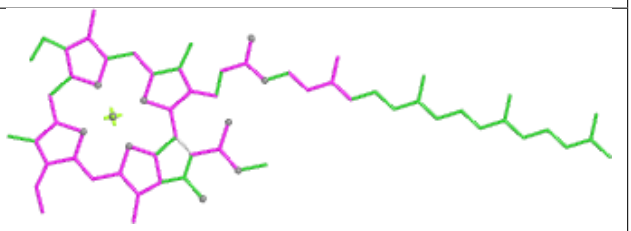


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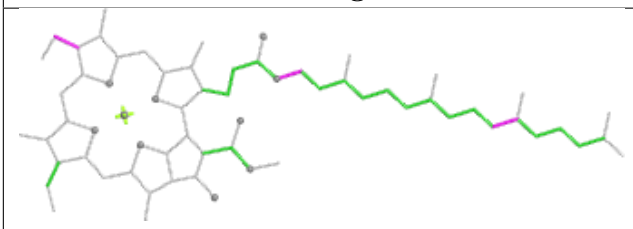
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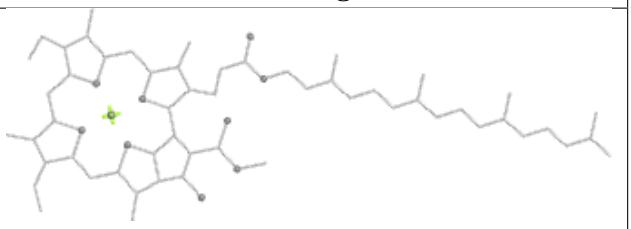
Bond lengths



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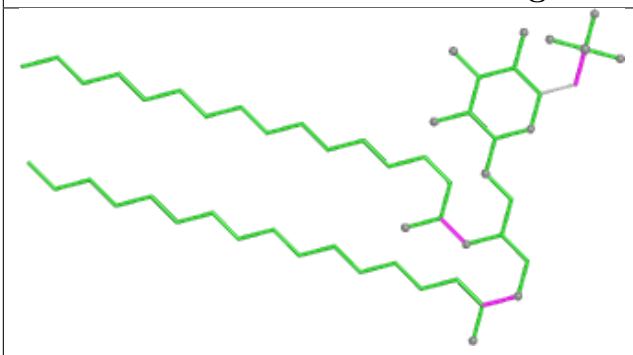


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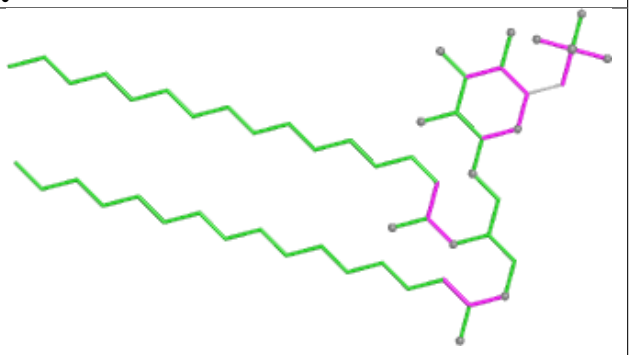


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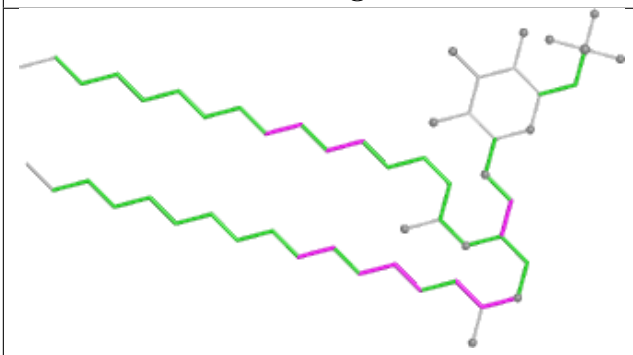
Ligand SQD a 412



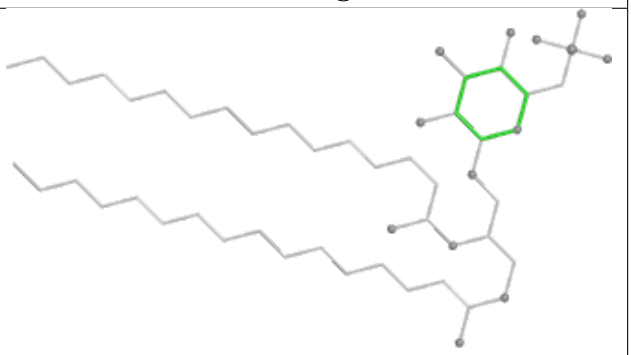
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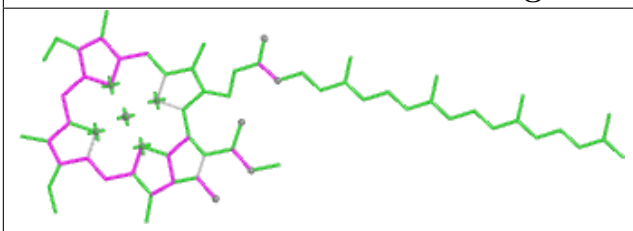


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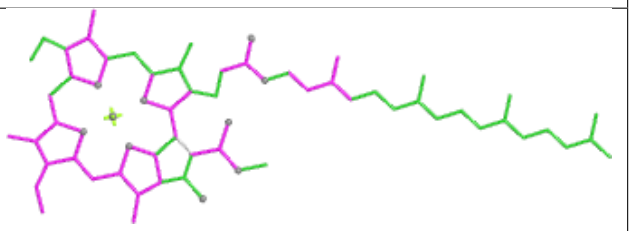


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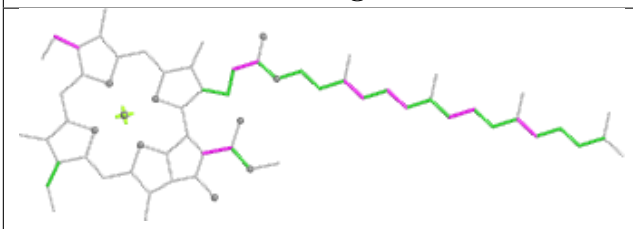
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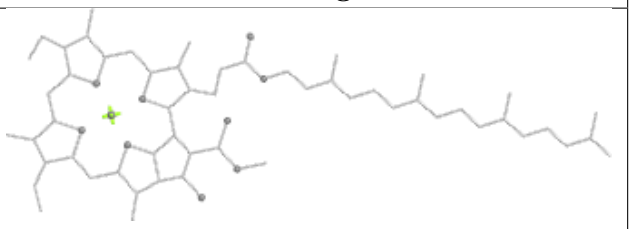
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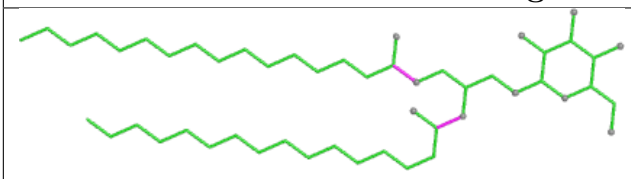


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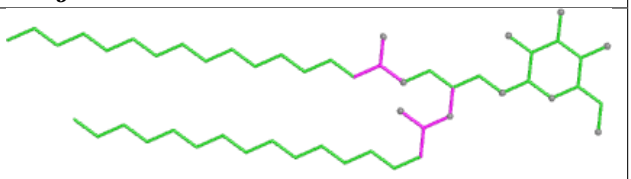


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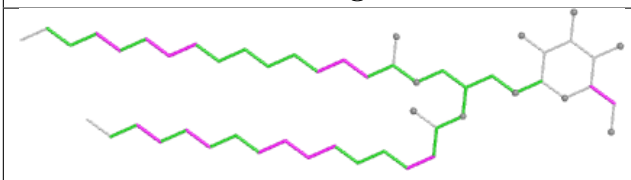
Ligand LMG j 101



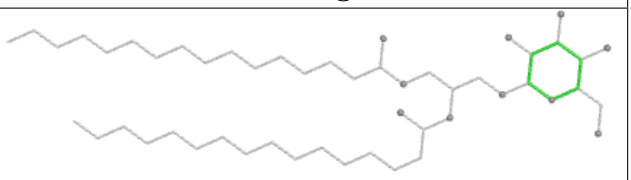
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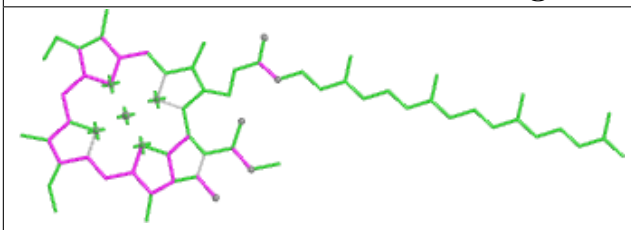


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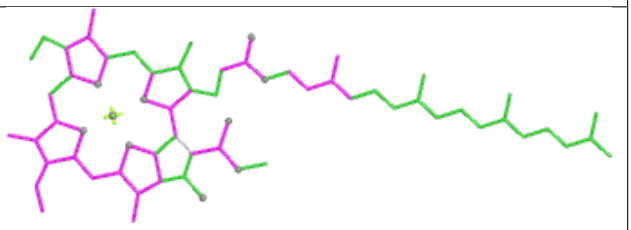


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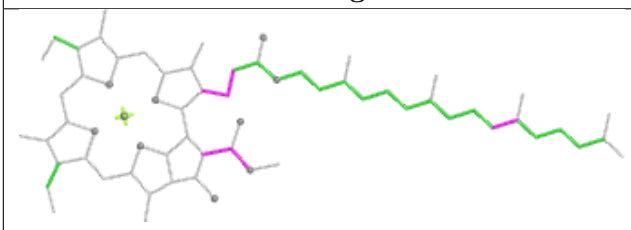
Ligand CLA c 501



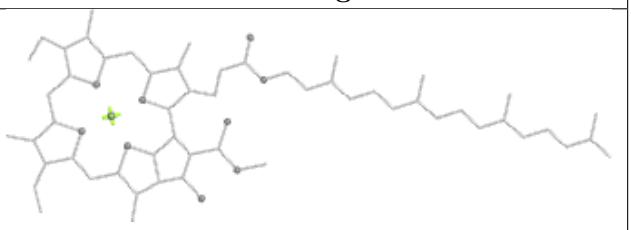
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Bond angles

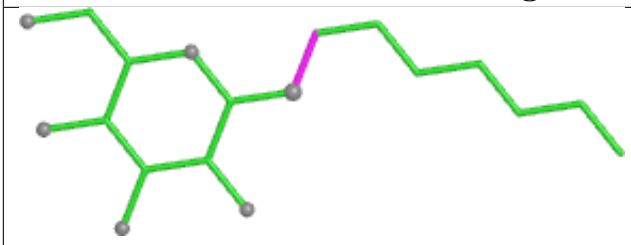


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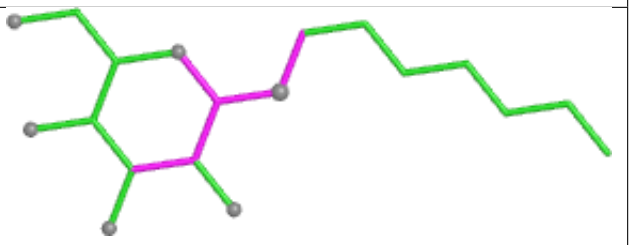


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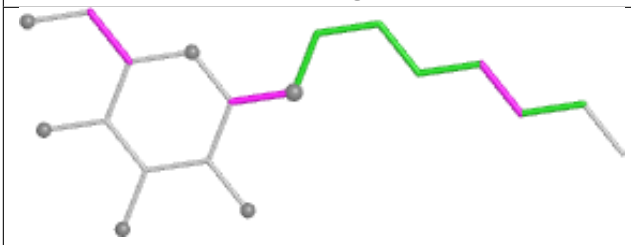
Ligand HTG B 624



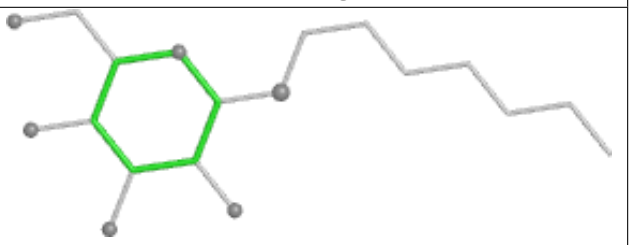
Bond lengths



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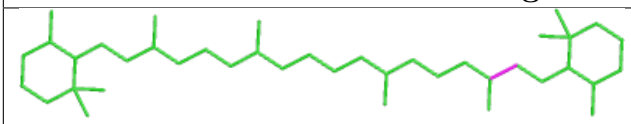


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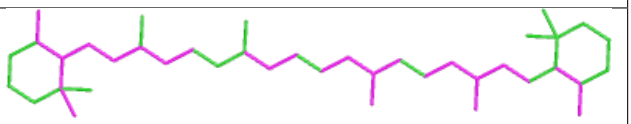


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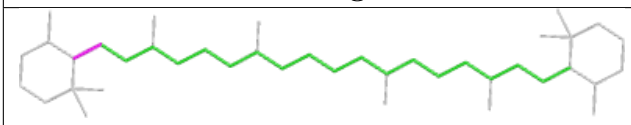
Ligand BCR A 409



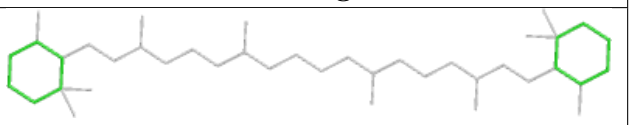
Bond lengths



Bond angles

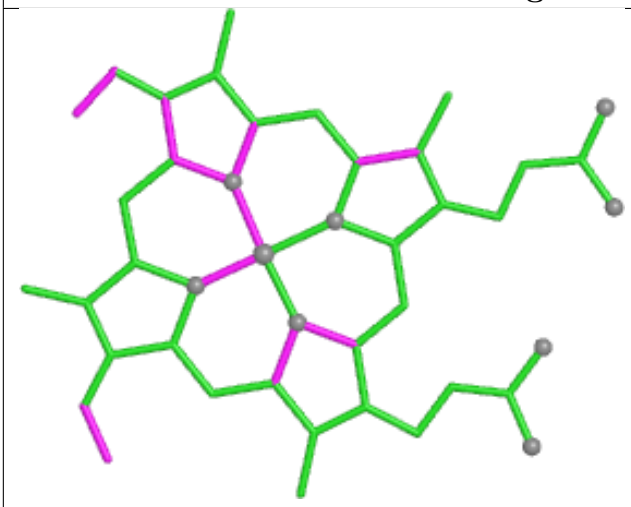


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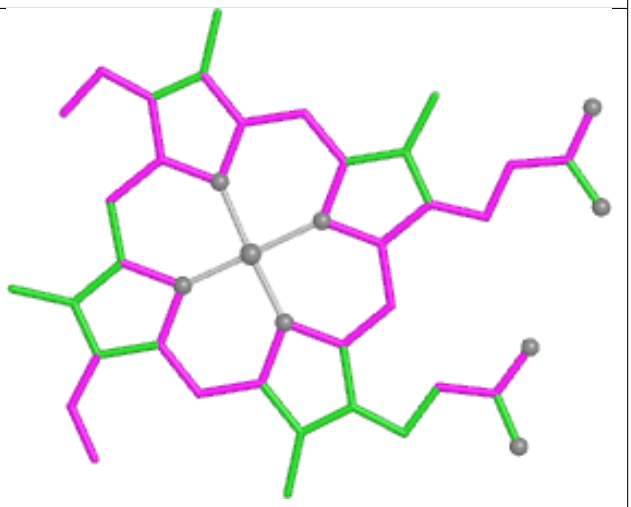


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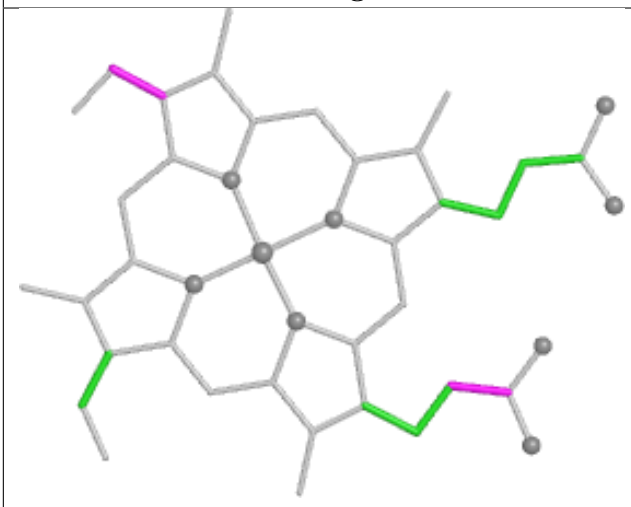
Ligand HEC v 201



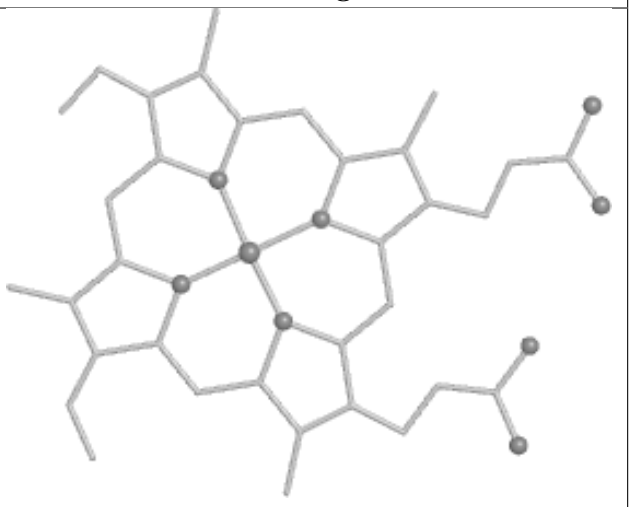
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Bond angles

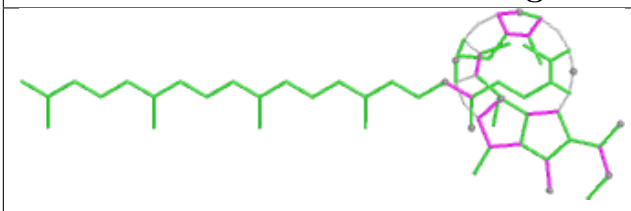


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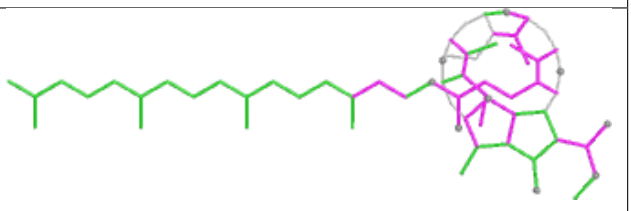


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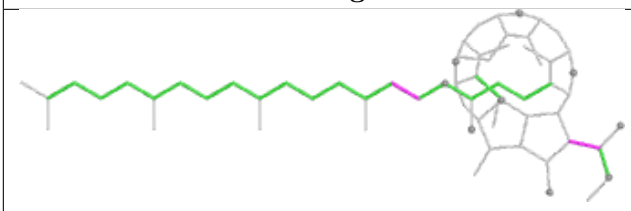
Ligand PHO a 406



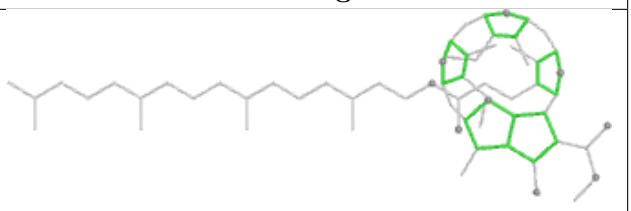
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Bond angles

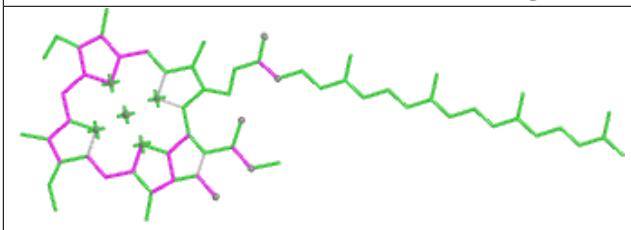


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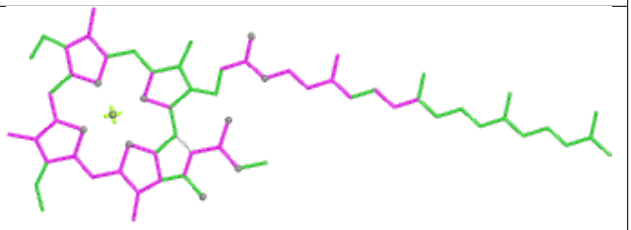


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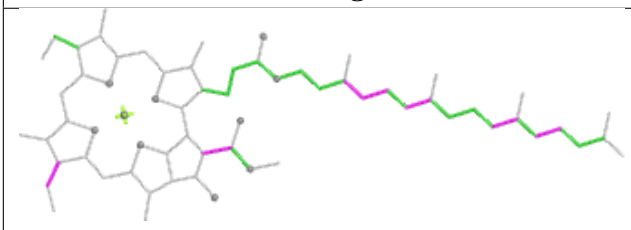
Ligand CLA B 604



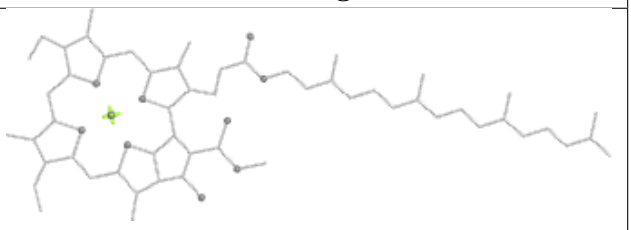
Bond lengths



Bond angles

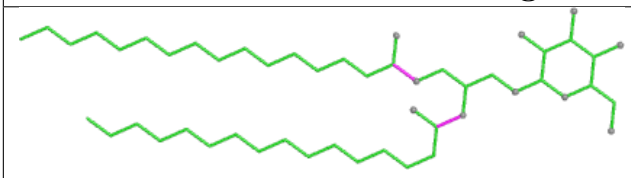


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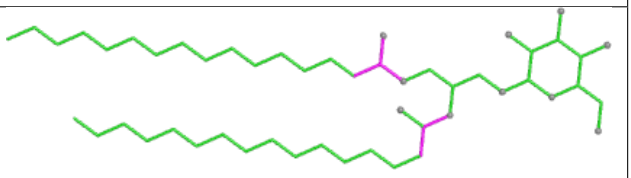


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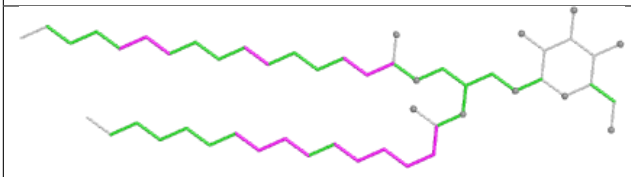
Ligand LMG C 520



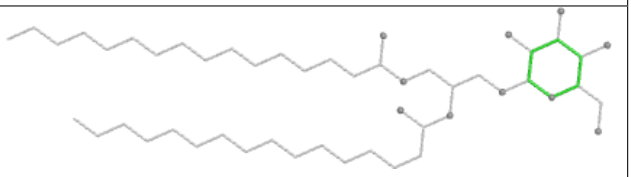
Bond lengths



Bond angles

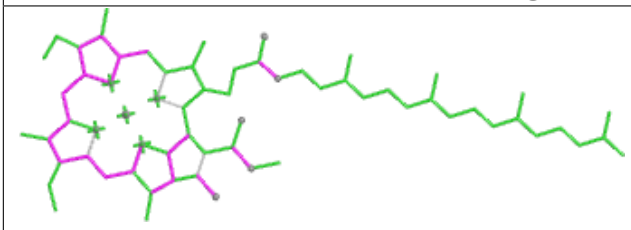


Torsions

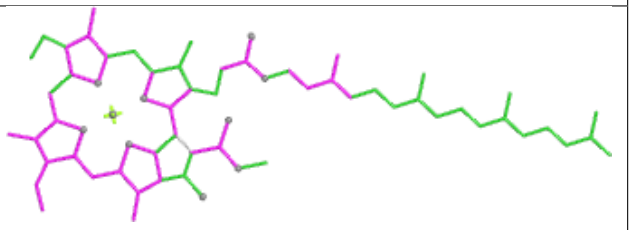


Rings

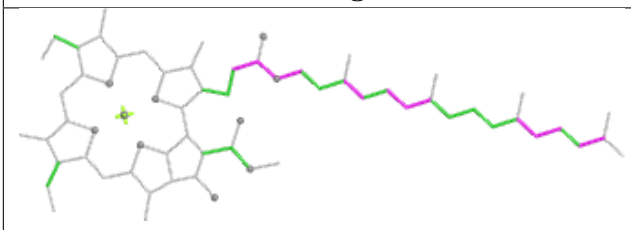
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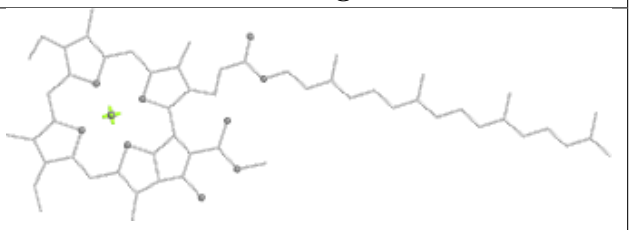
Bond lengths



Bond angles



Torsions

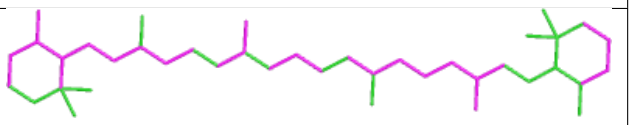


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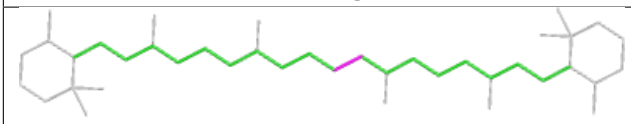
Ligand BCR t 101



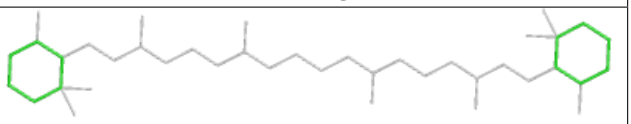
Bond lengths



Bond angles

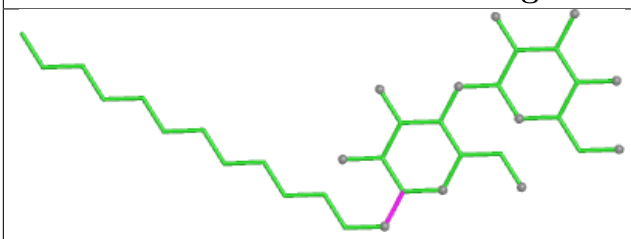


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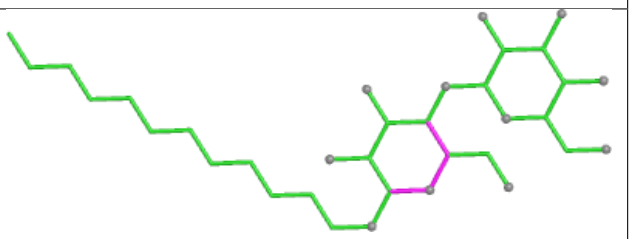


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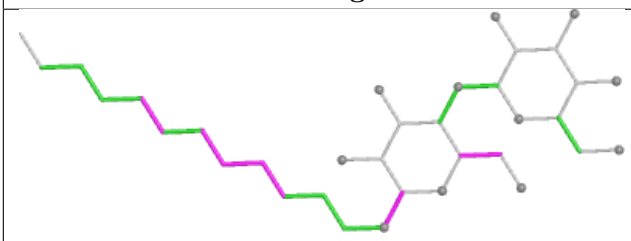
Ligand LMT B 630



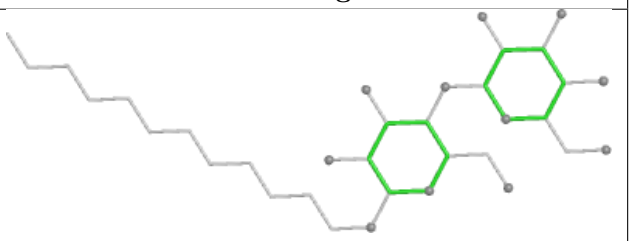
Bond lengths



Bond angles

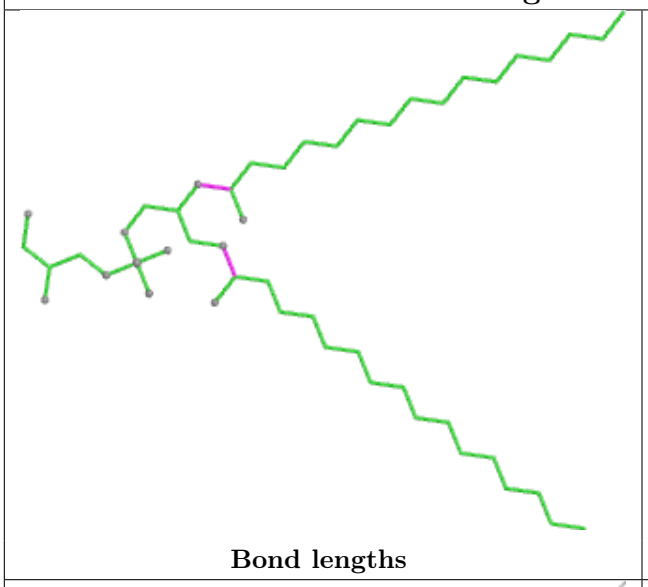


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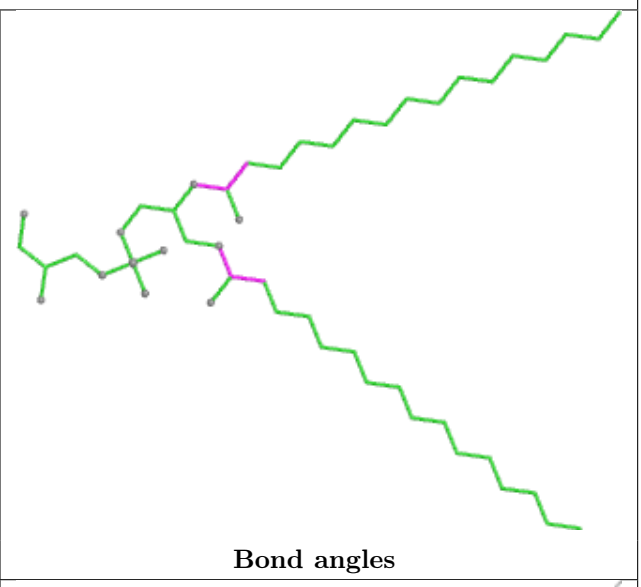


Rings

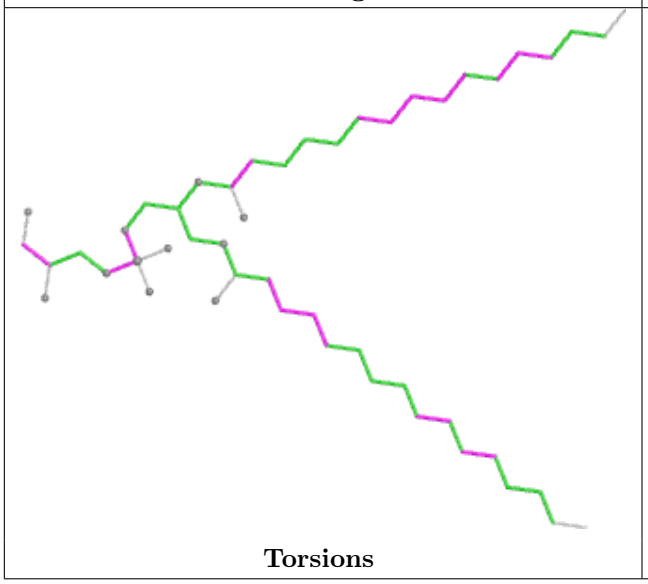
Ligand LHG A 417



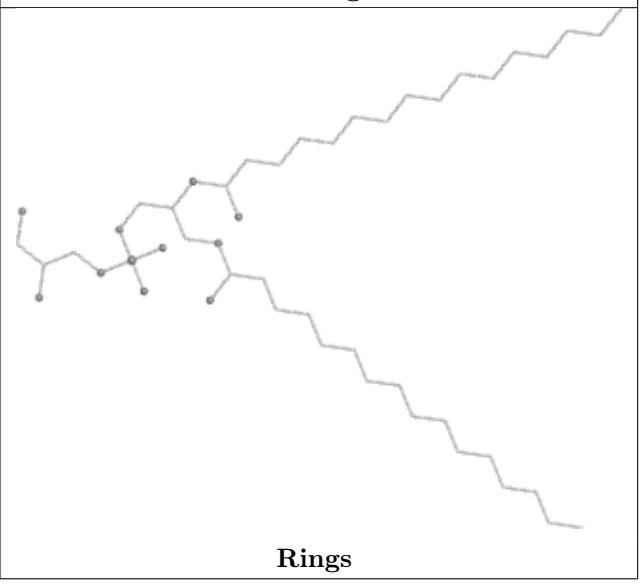
Bond lengths



Bond angles

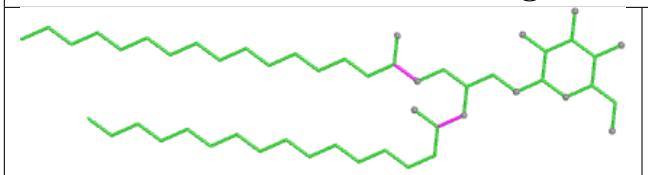


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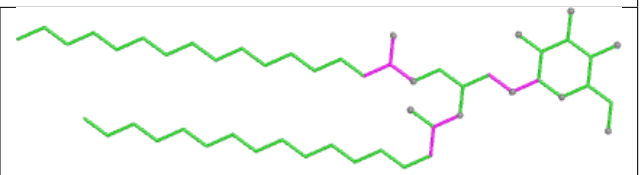


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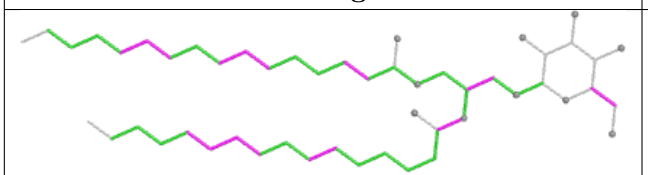
Ligand LMG B 621



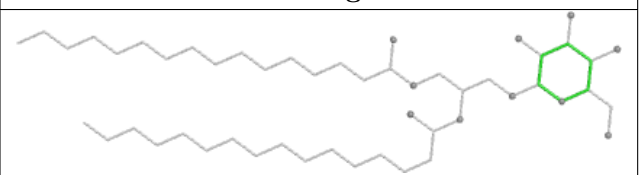
Bond lengths



Bond angles

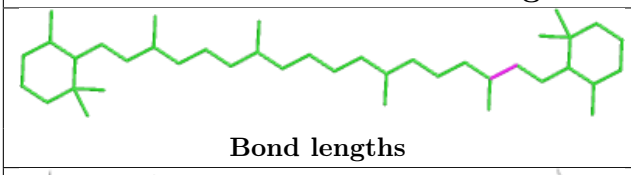


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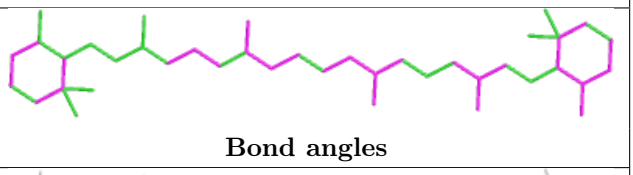


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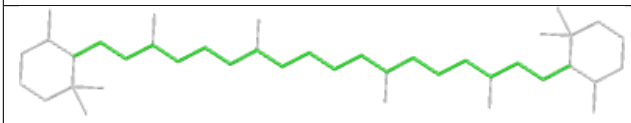
Ligand BCR B 618



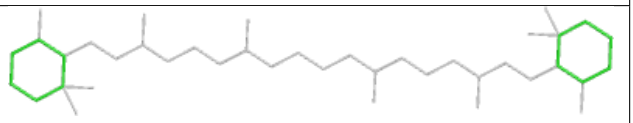
Bond lengths



Bond angles

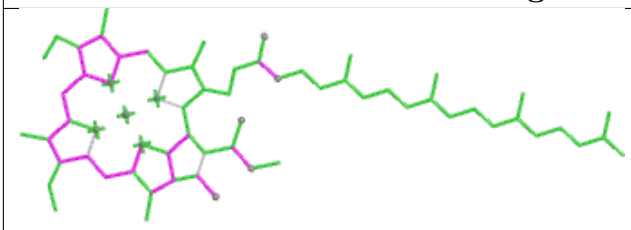


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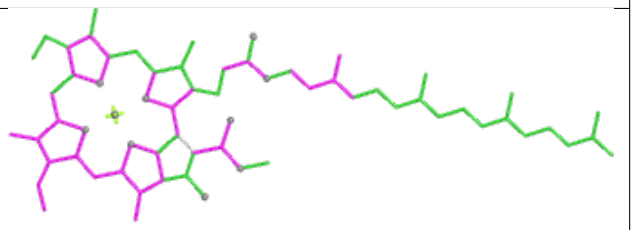


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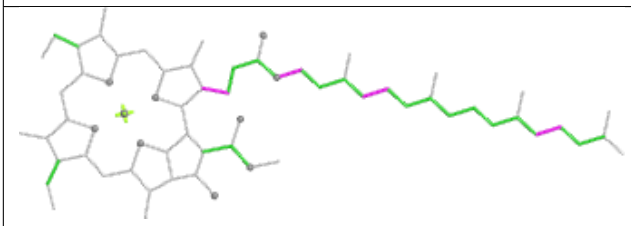
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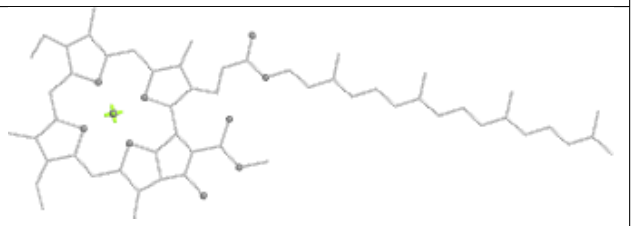
Bond lengths



Bond angles



Torsions

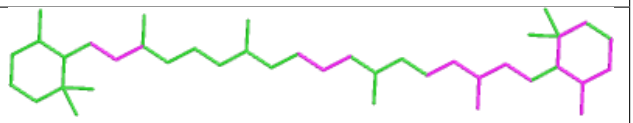


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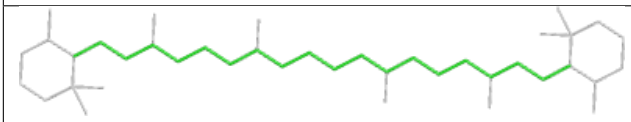
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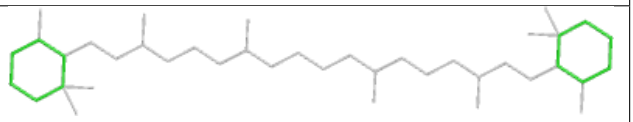
Bond lengths



Bond angles

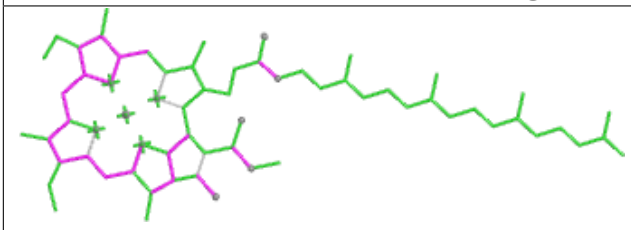


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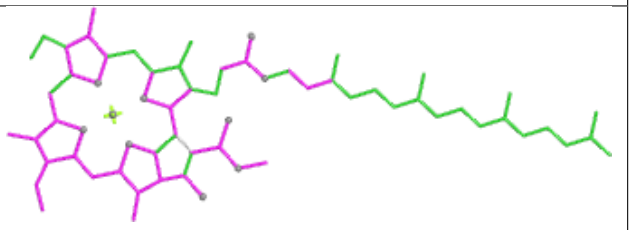


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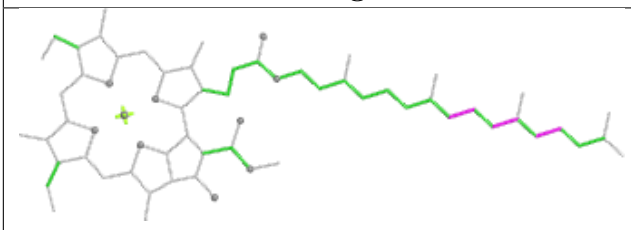
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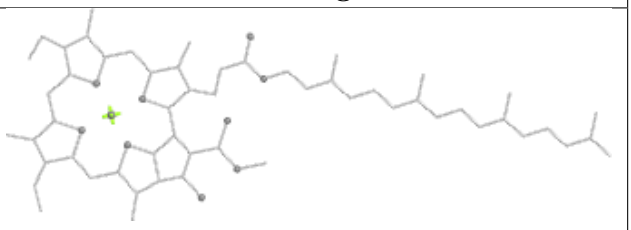
Bond lengths



Bond angles



Torsions

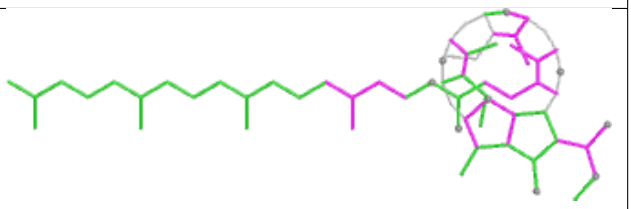


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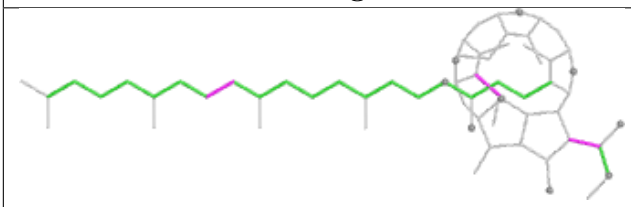
Ligand PHO a 407



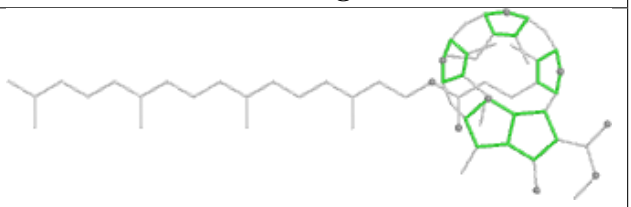
Bond lengths



Bond angles

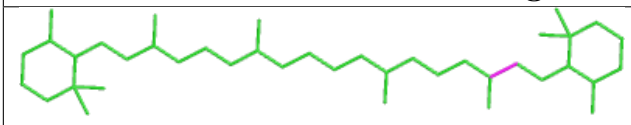


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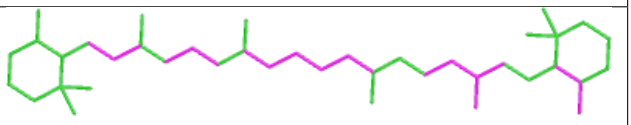


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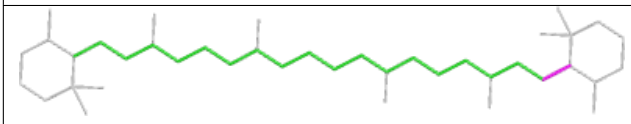
Ligand BCR h 101



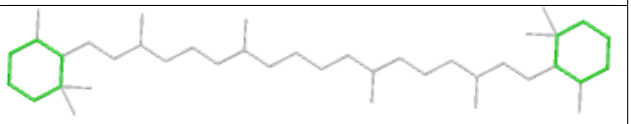
Bond lengths



Bond angles

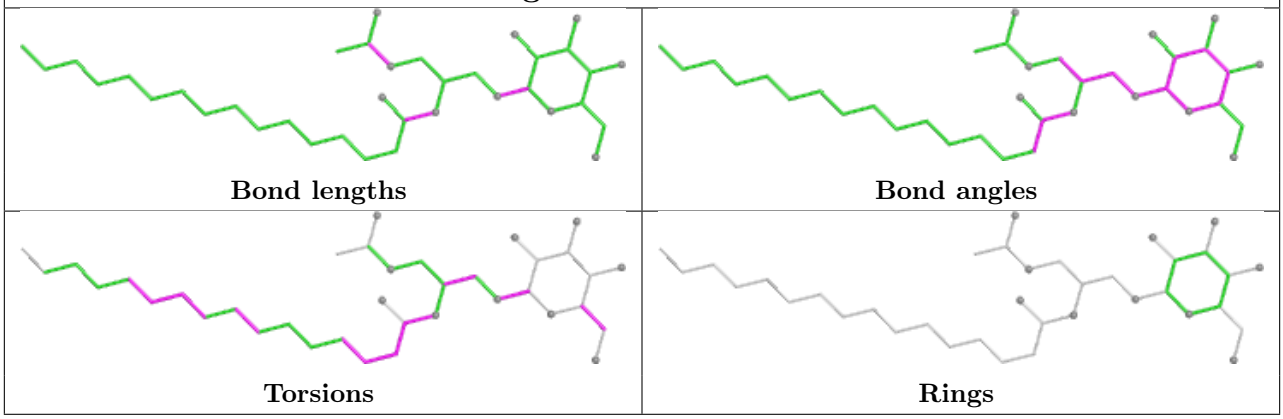


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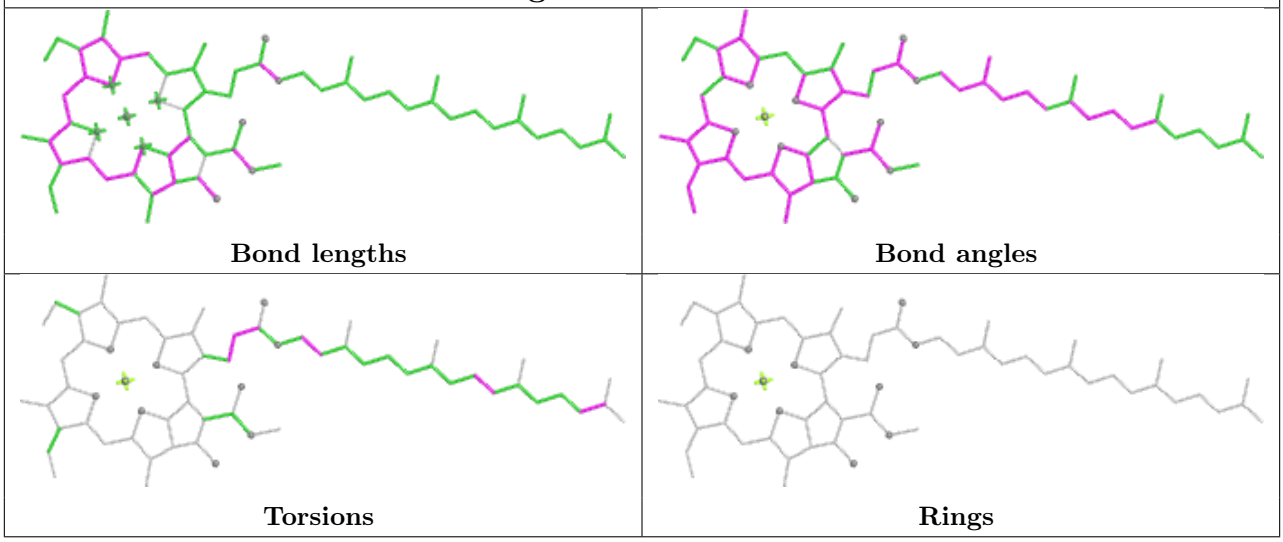


Rings

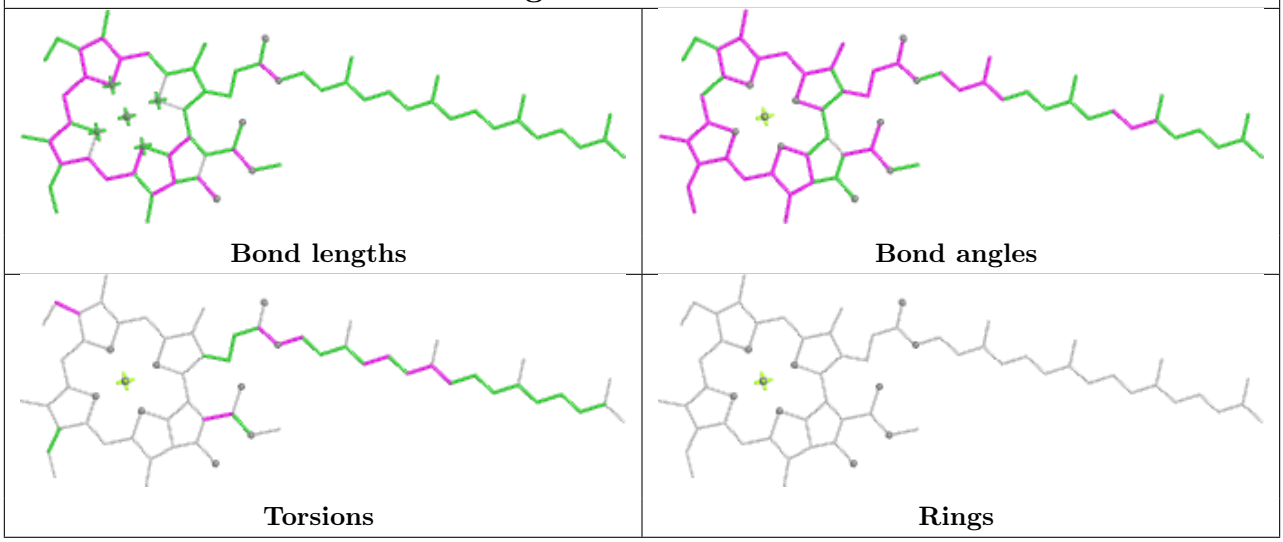
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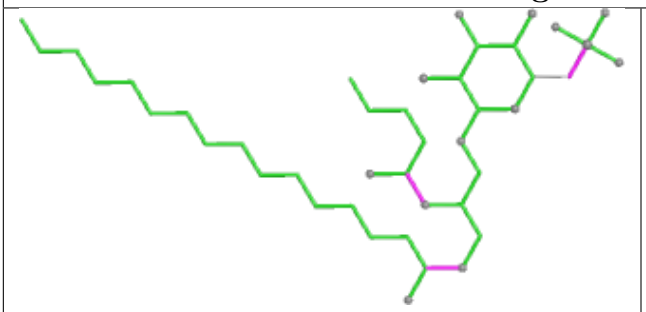
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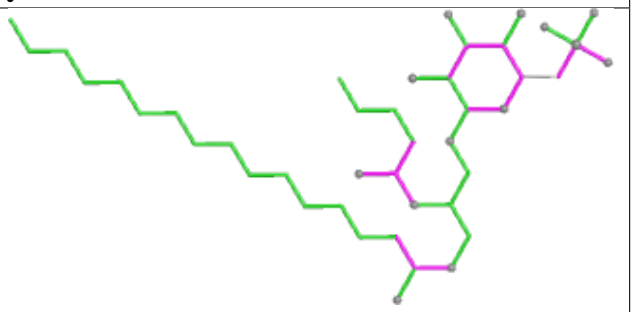
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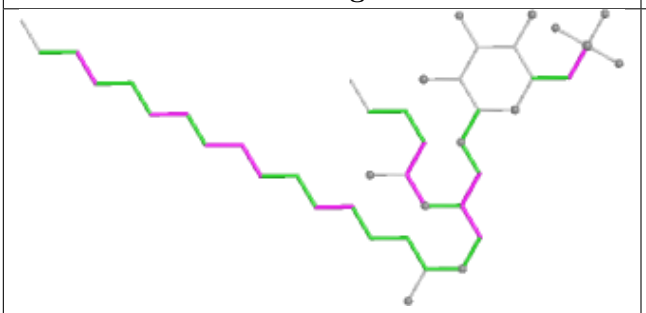
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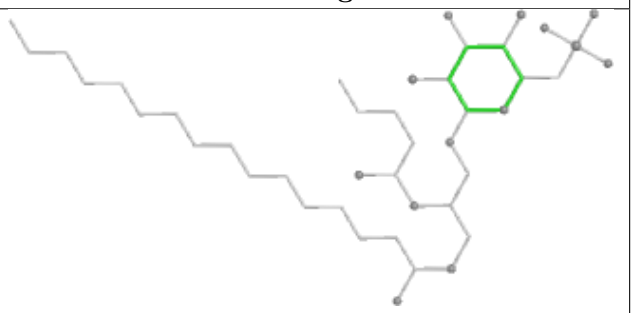
Bond lengths



Bond angles

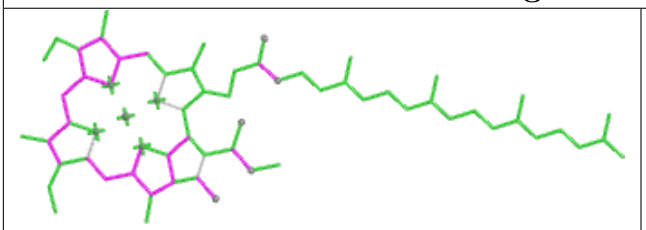


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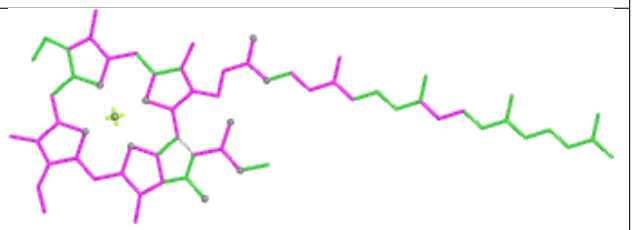


Rings

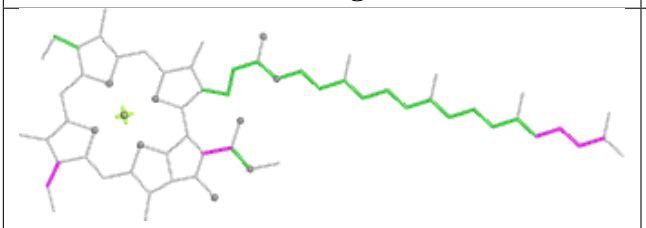
Ligand CLA A 405



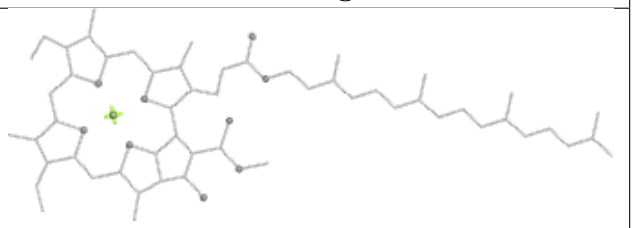
Bond lengths



Bond angles

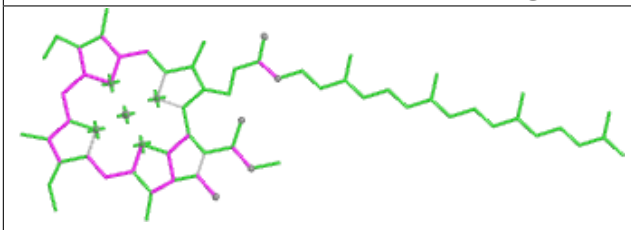


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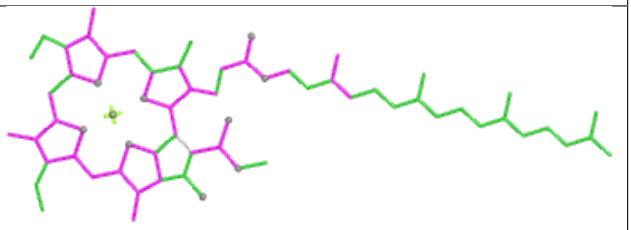


Rings

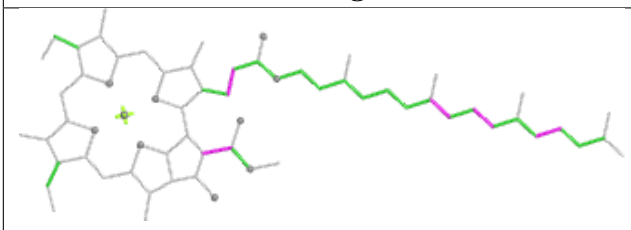
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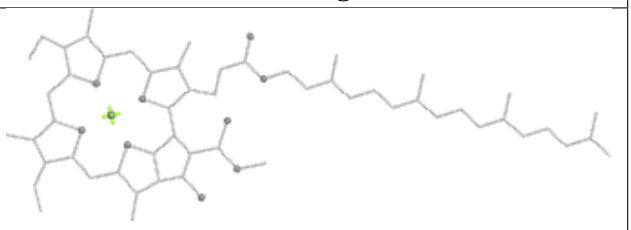
Bond lengths



Bond angles

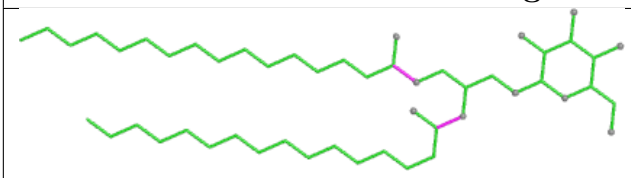


Torsions

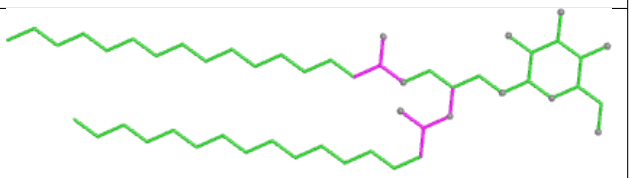


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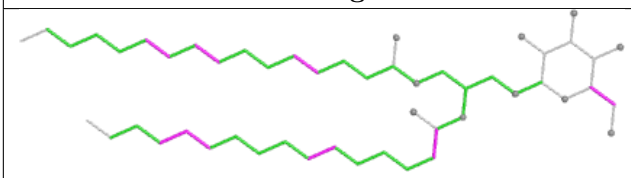
Ligand LMG J 101



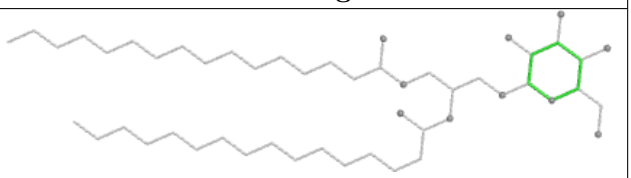
Bond lengths



Bond angles



Torsions



Rings

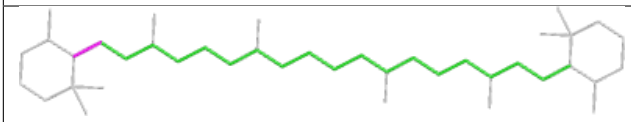
Ligand BCR B 617



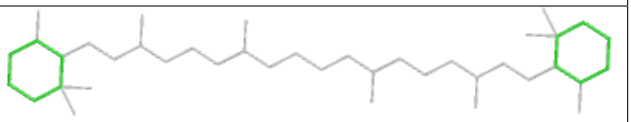
Bond lengths



Bond angles

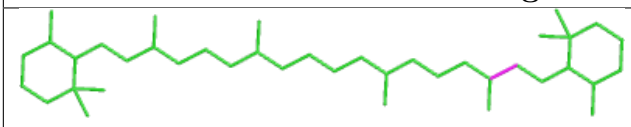


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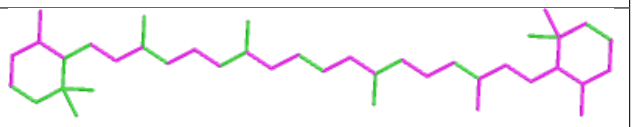


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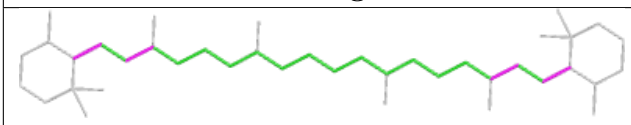
Ligand BCR D 406



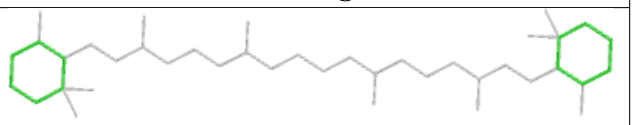
Bond lengths



Bond angles

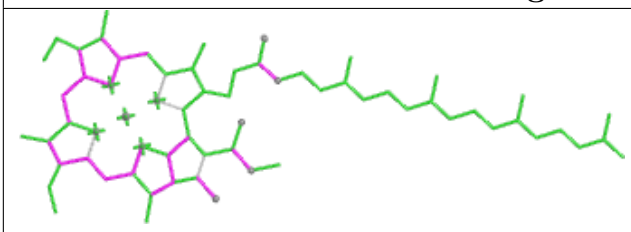


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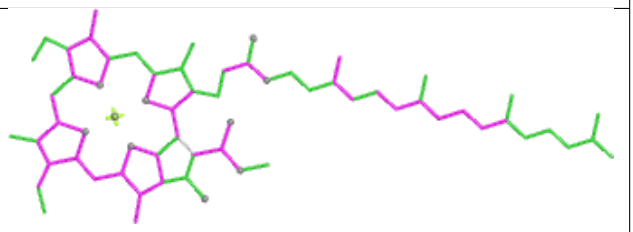


Rings

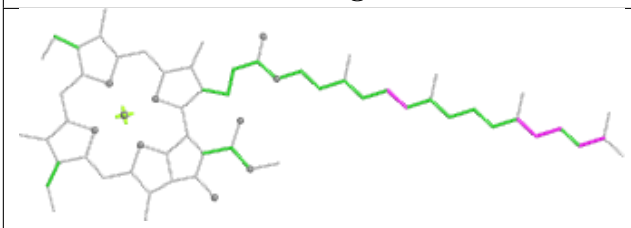
Ligand CLA b 615



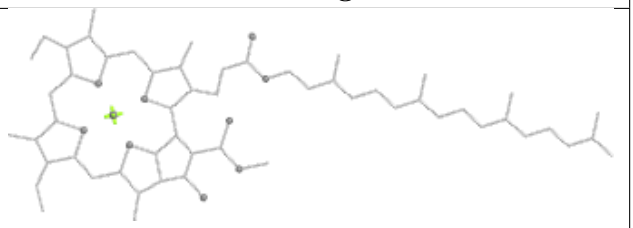
Bond lengths



Bond angles

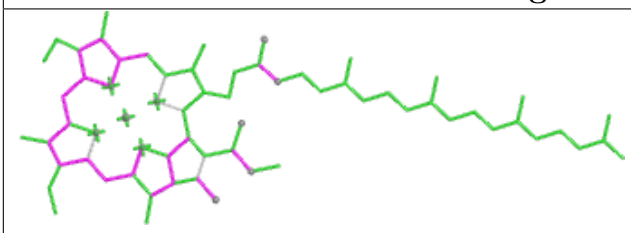


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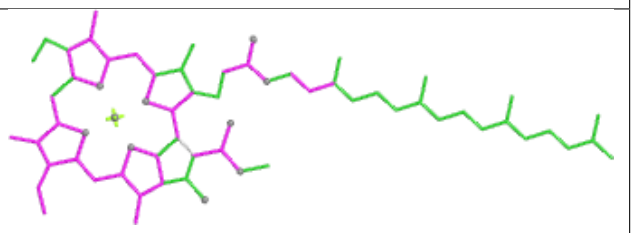


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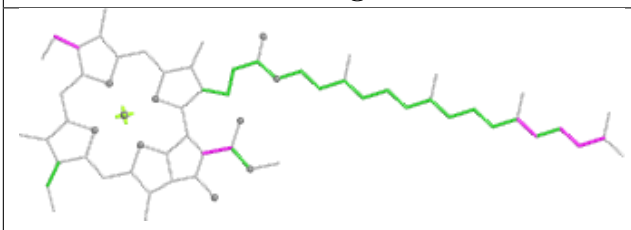
Ligand CLA c 502



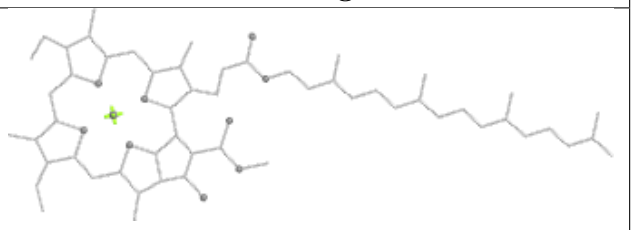
Bond lengths



Bond angles

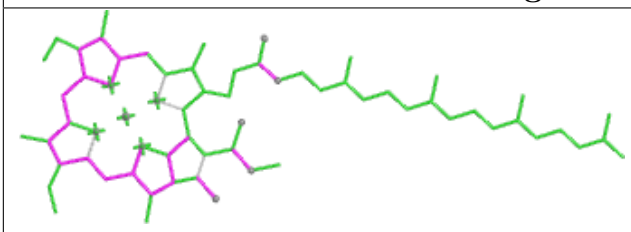


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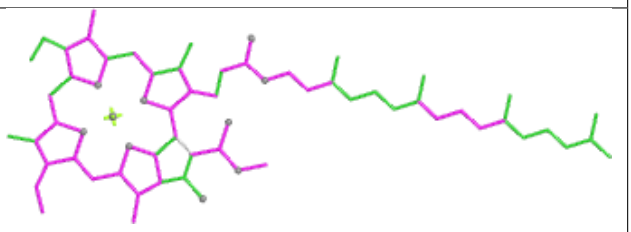


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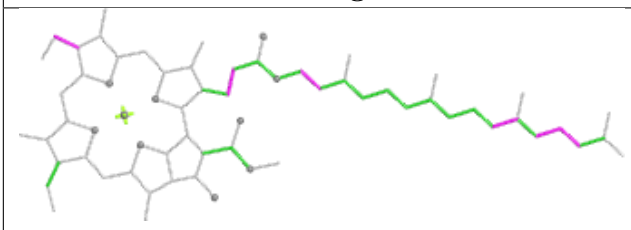
Ligand CLA B 602



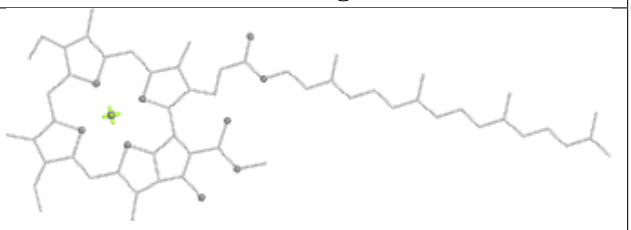
Bond lengths



Bond angles

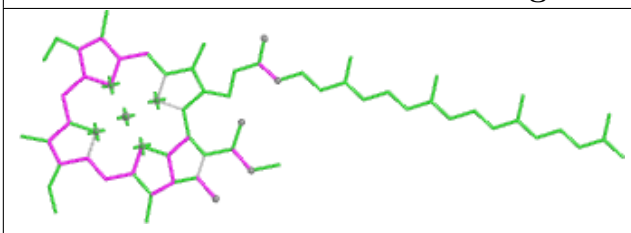


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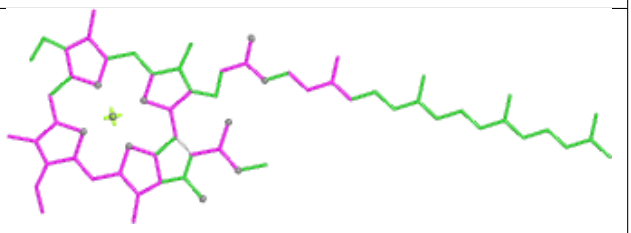


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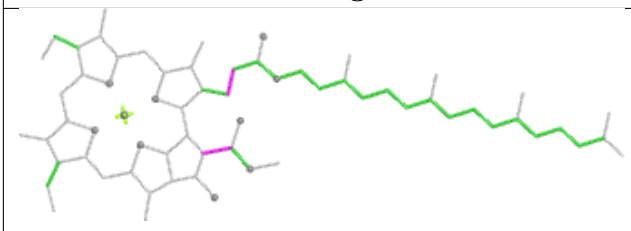
Ligand CLA c 503



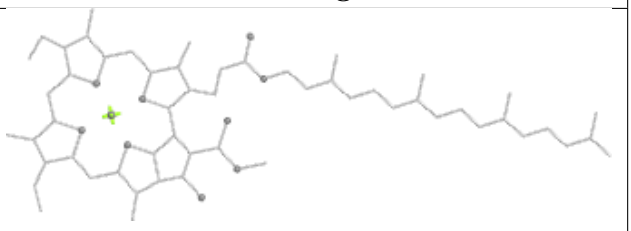
Bond lengths



Bond angles

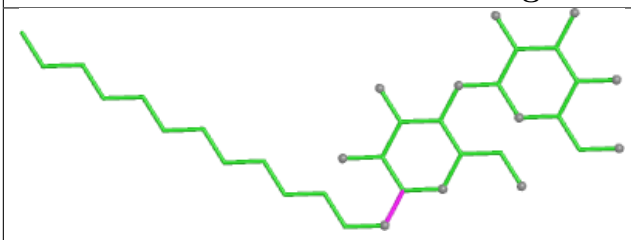


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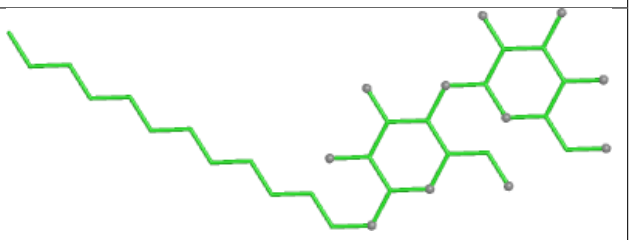


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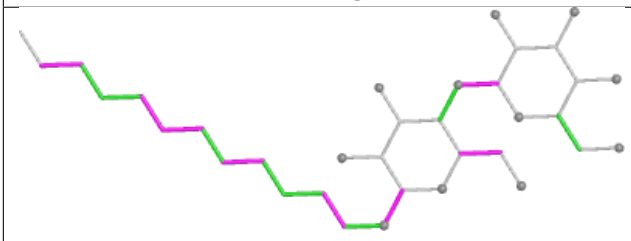
Ligand LMT E 102



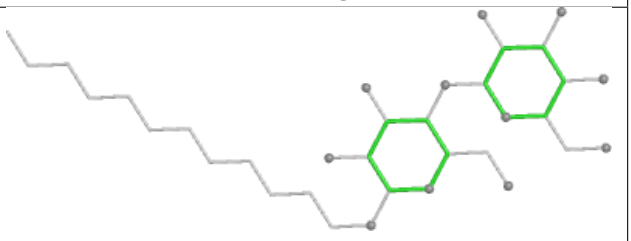
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Bond angles

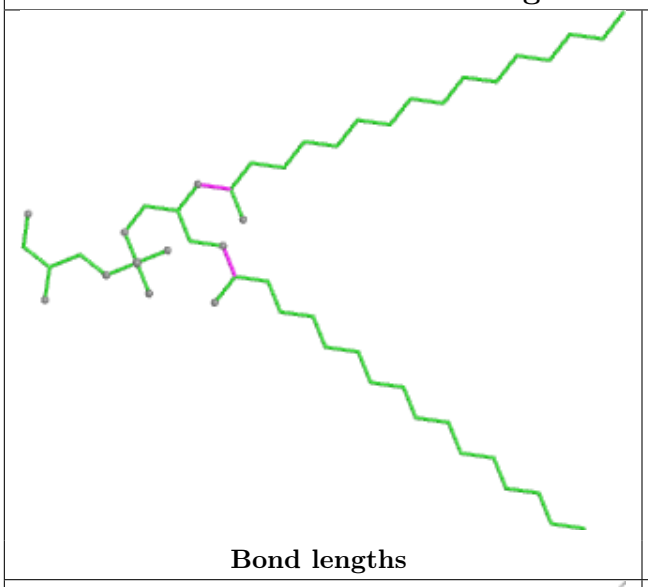


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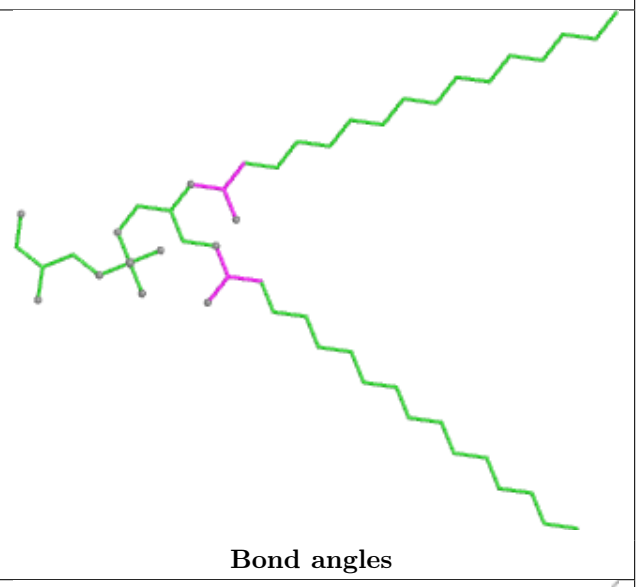


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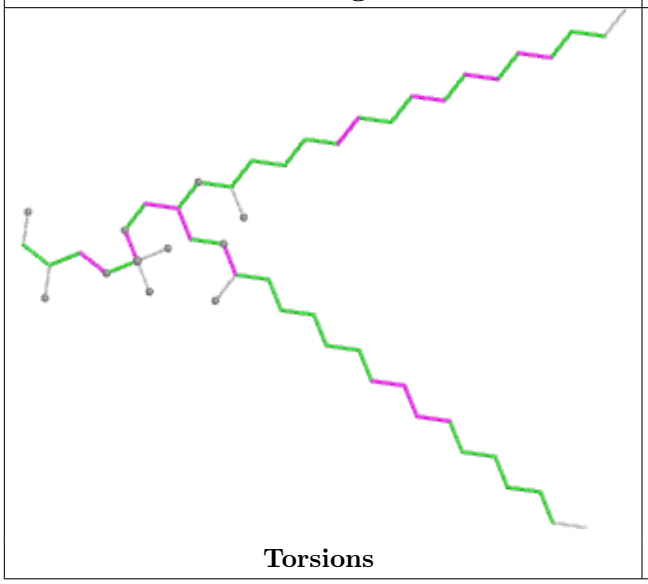
Ligand LHG D 409



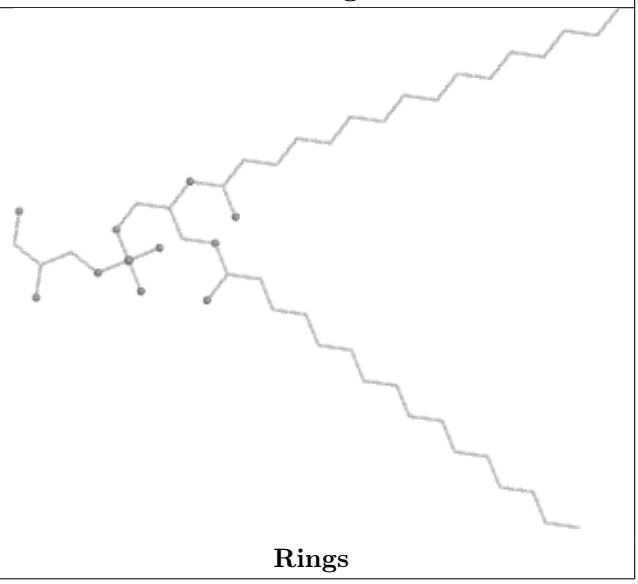
Bond lengths



Bond angles

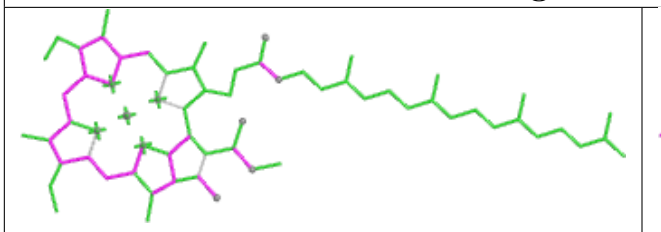


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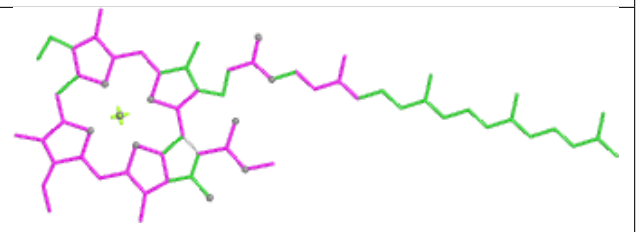


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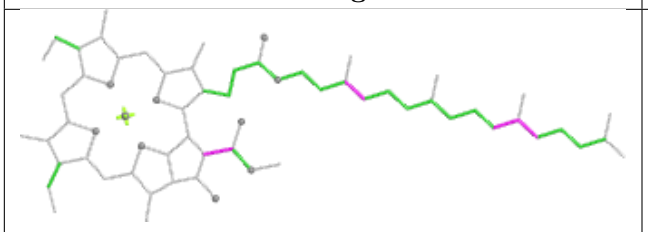
Ligand CLA c 504



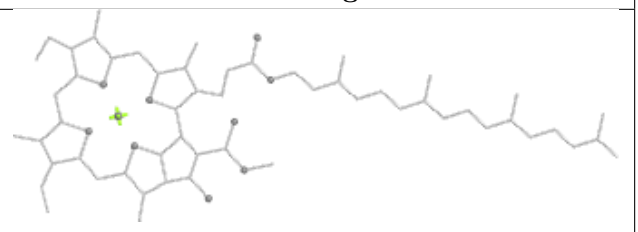
Bond lengths



Bond angles

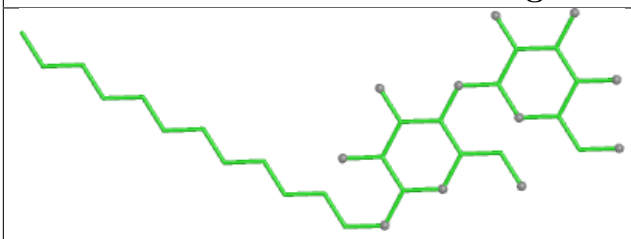


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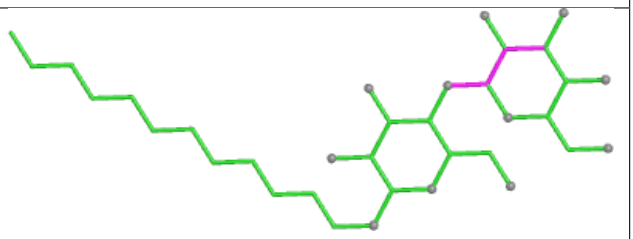


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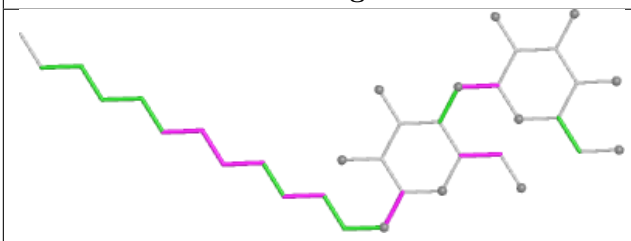
Ligand LMT e 102



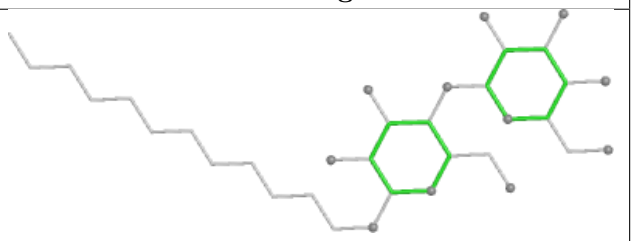
Bond lengths



Bond angles

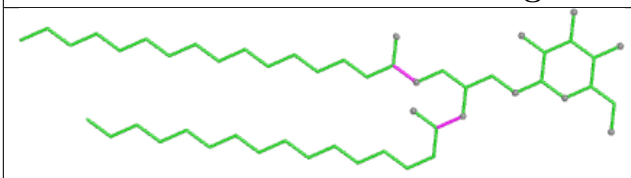


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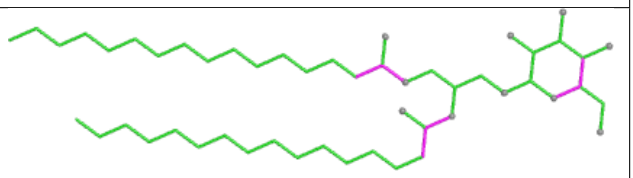


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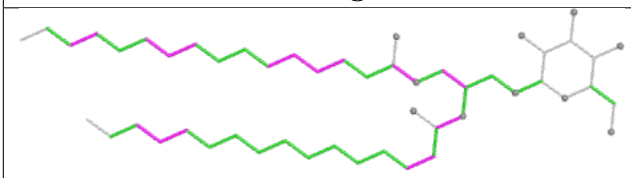
Ligand LMG a 416



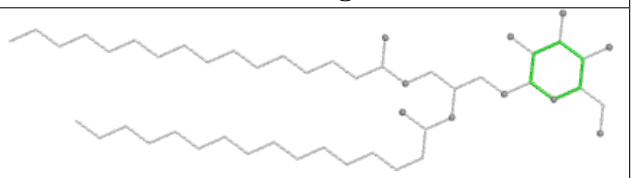
Bond lengths



Bond angles

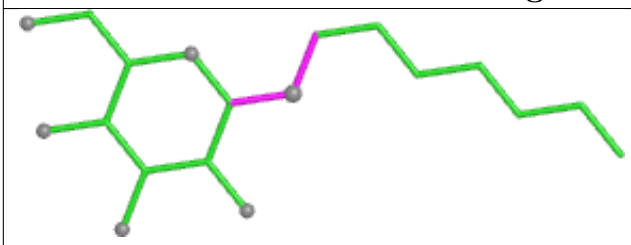


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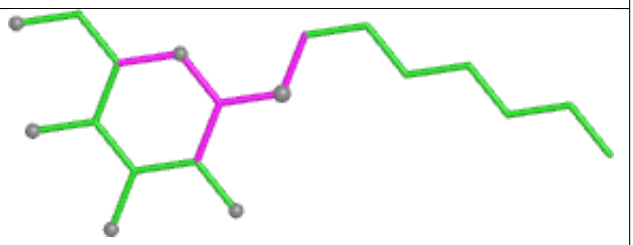


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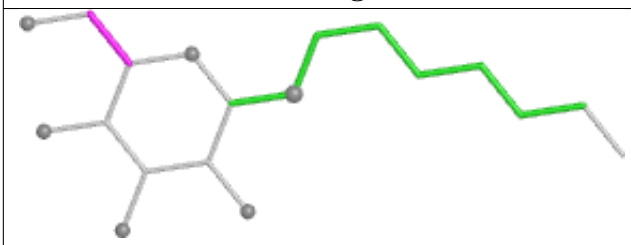
Ligand HTG c 522



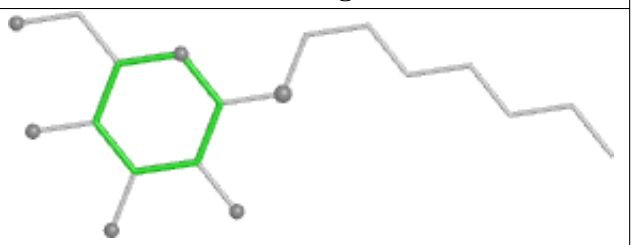
Bond lengths



Bond angles

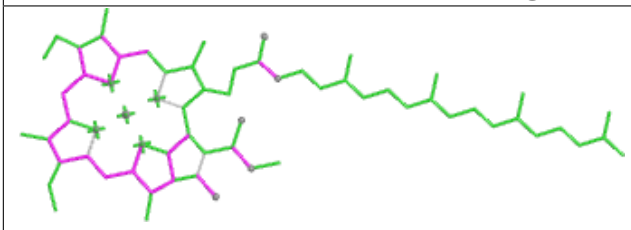


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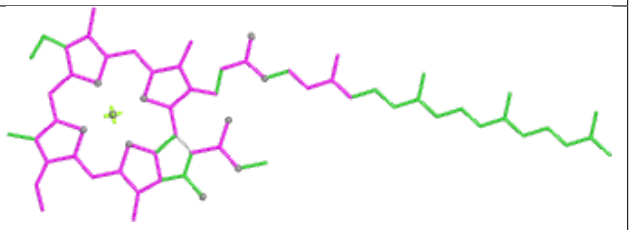


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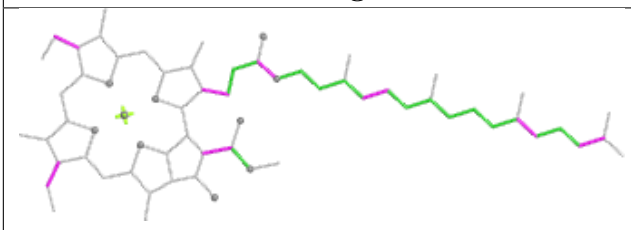
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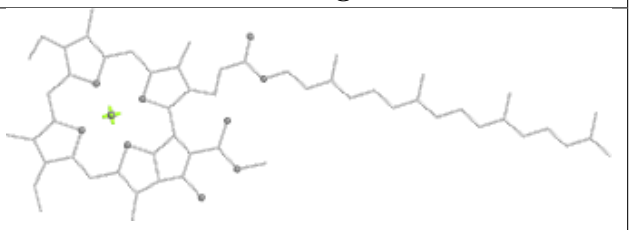
Bond lengths



Bond angles

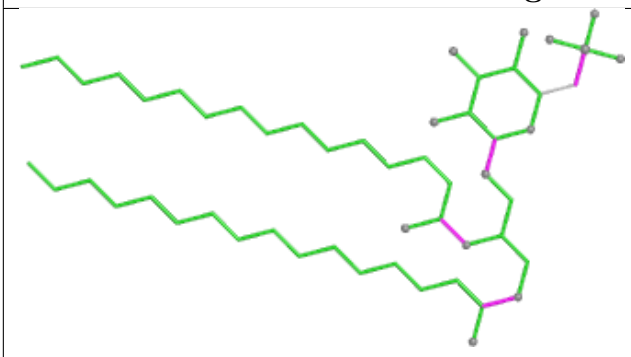


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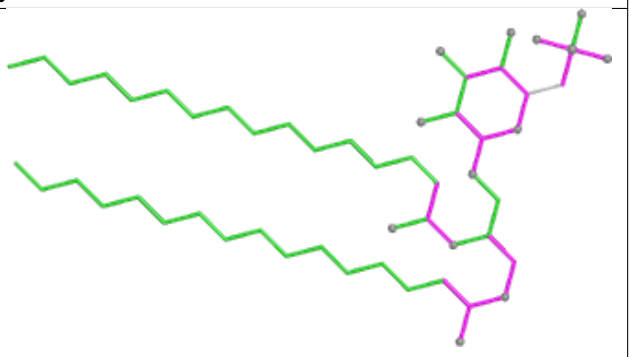


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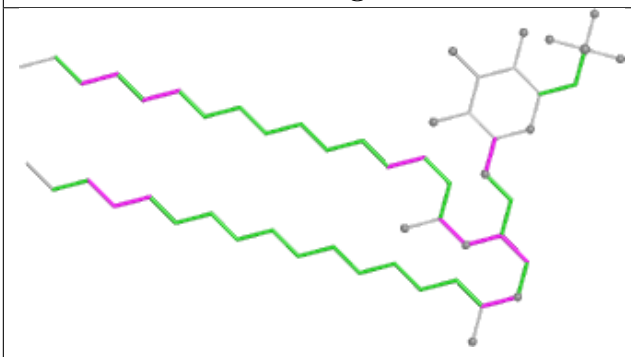
Ligand SQD B 620



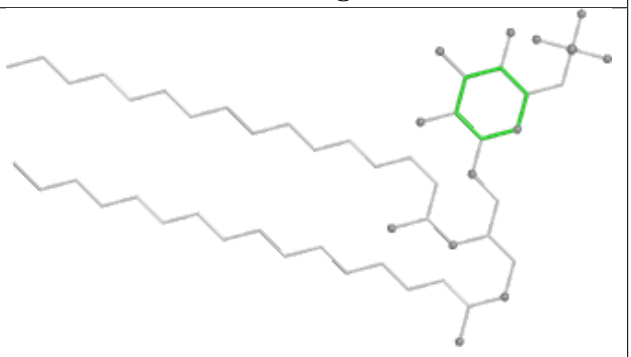
Bond lengths



Bond angles

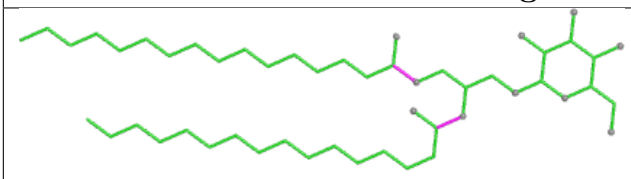


Torsions

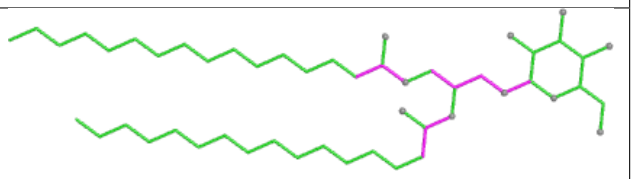


Rings

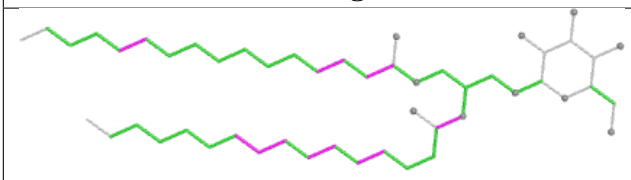
Ligand LMG C 501



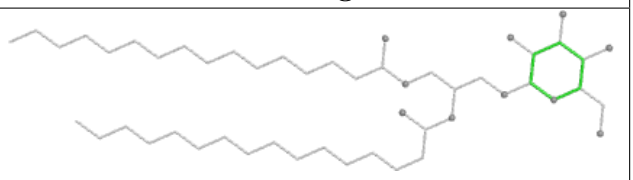
Bond lengths



Bond angles

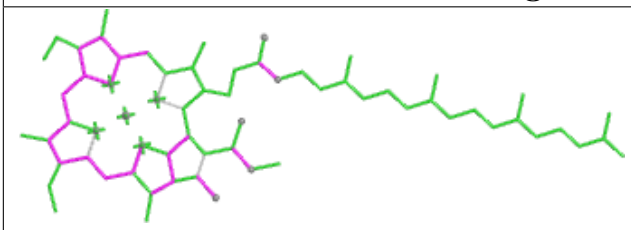


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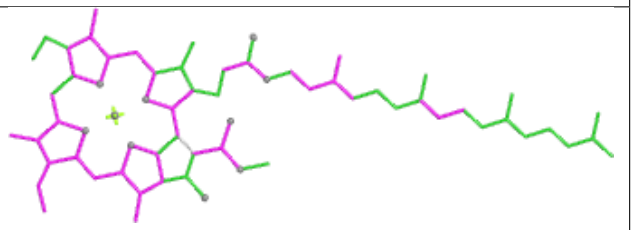


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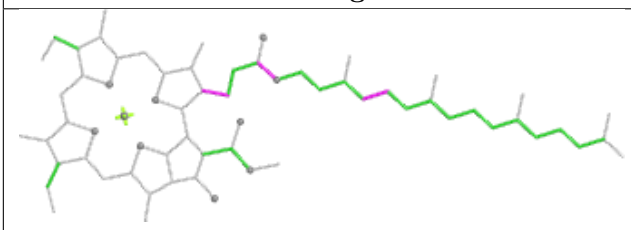
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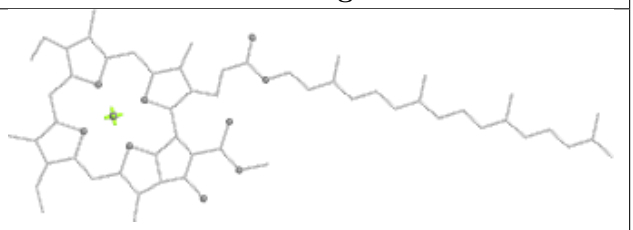
Bond lengths



Bond angles



Torsions



Rings

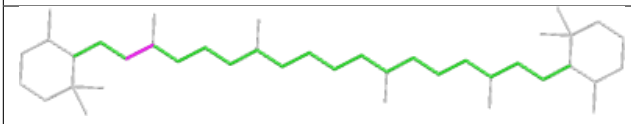
Ligand BCR K 102



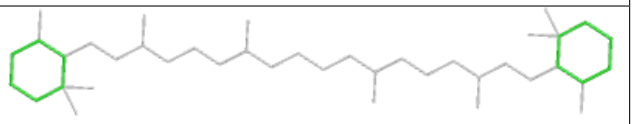
Bond lengths



Bond angles

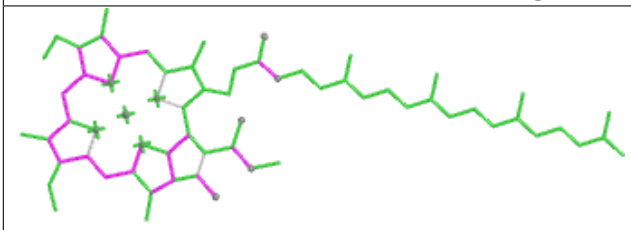


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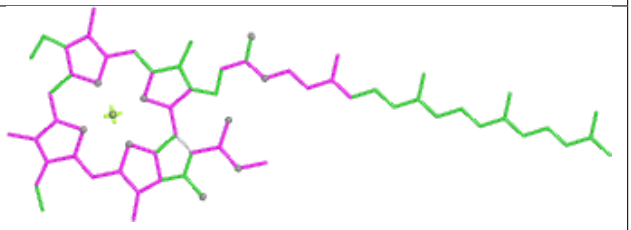


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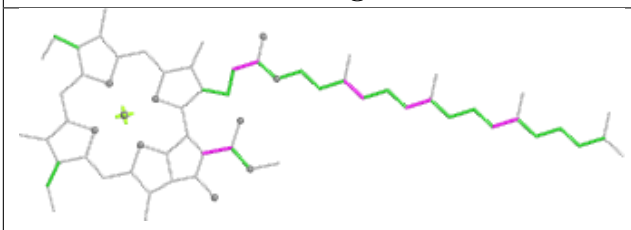
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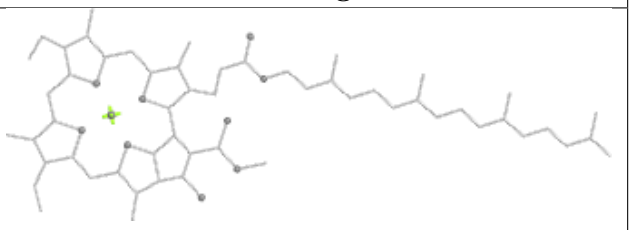
Bond lengths



Bond angles



Torsions

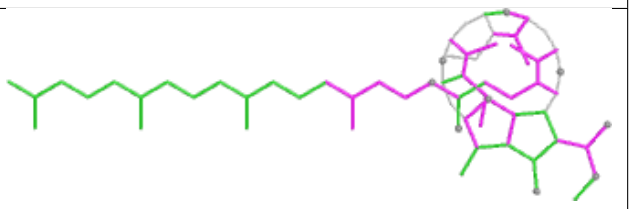


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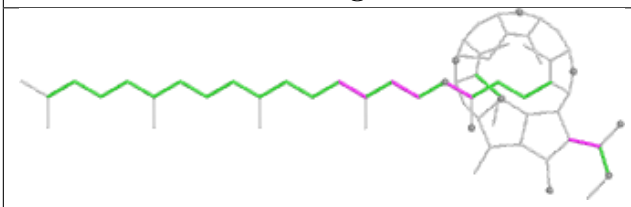
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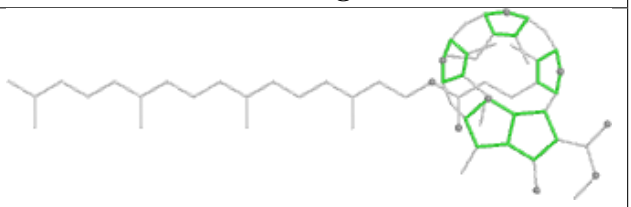
Bond lengths



Bond angles

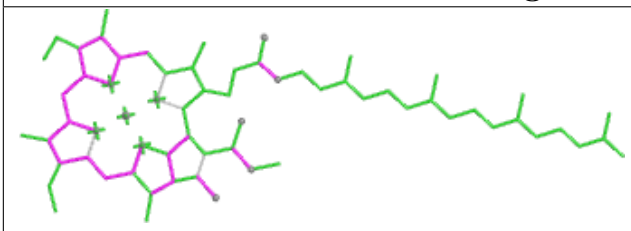


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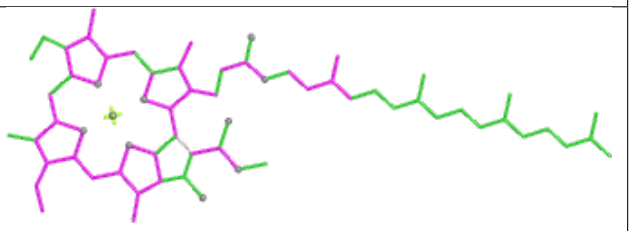


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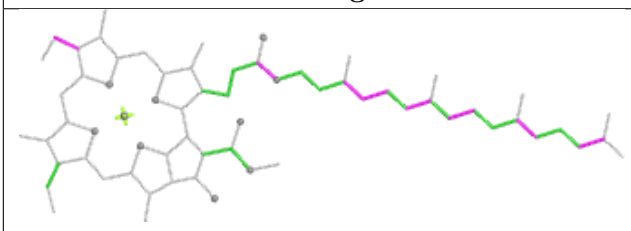
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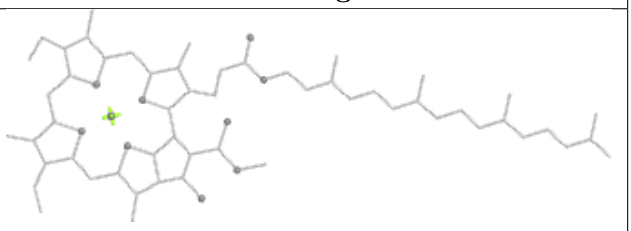
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Bond angles

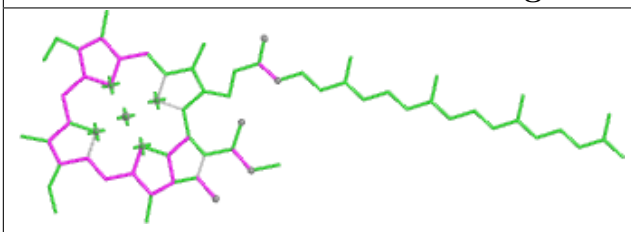


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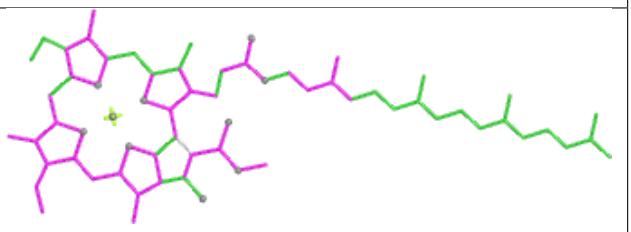


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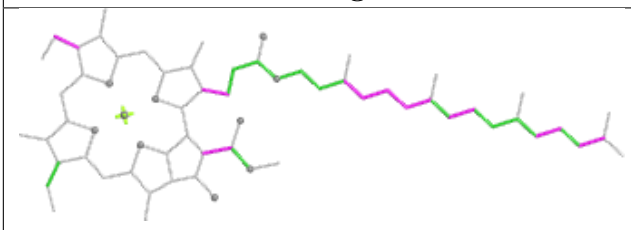
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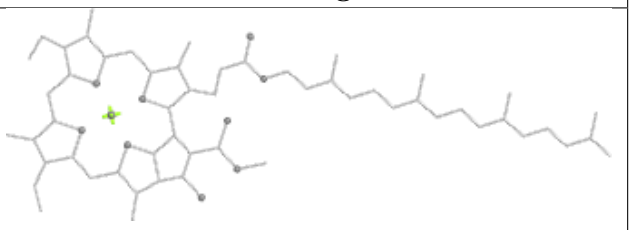
Bond lengths



Bond angles

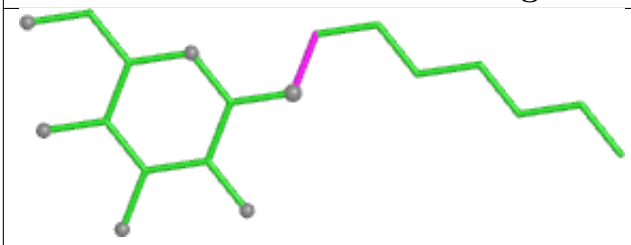


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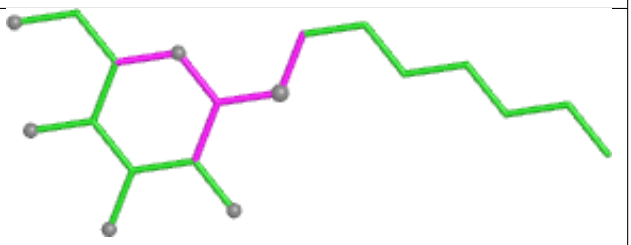


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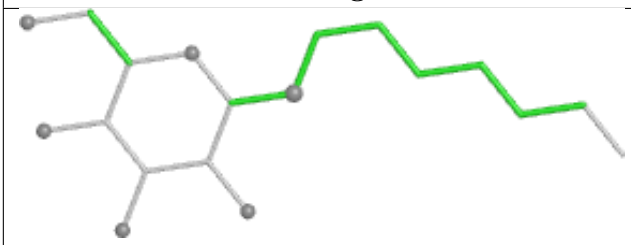
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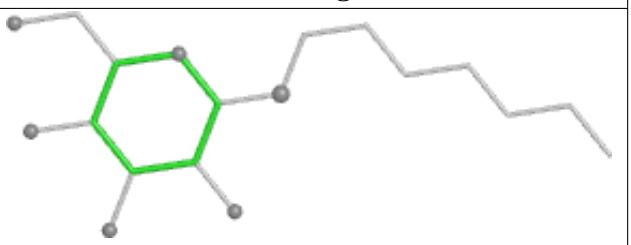
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Bond angles

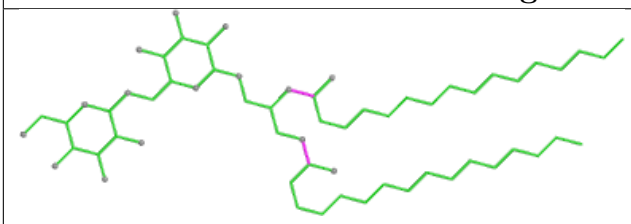


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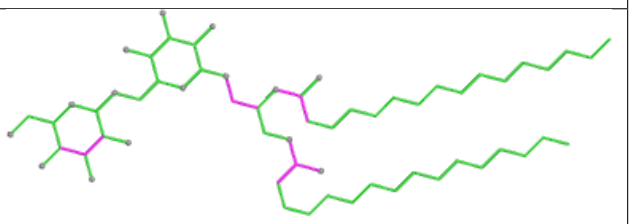


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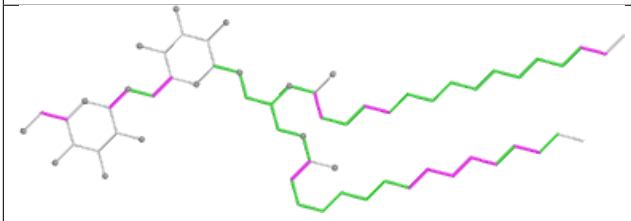
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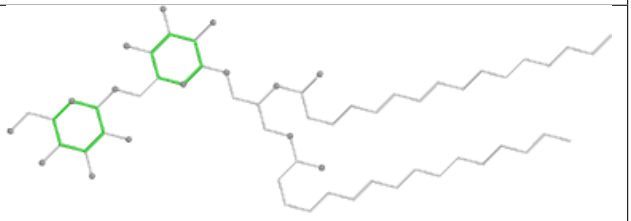
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Bond angles

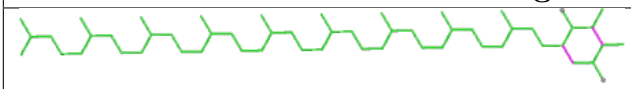


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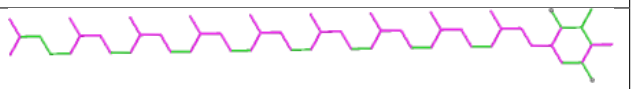


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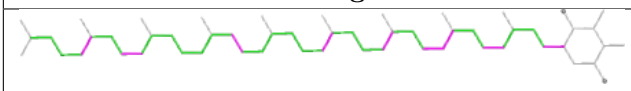
Ligand PL9 a 414



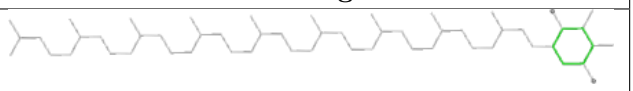
Bond lengths



Bond angles

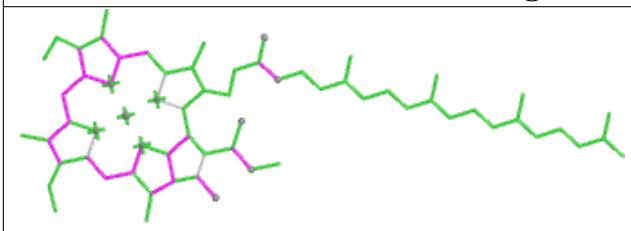


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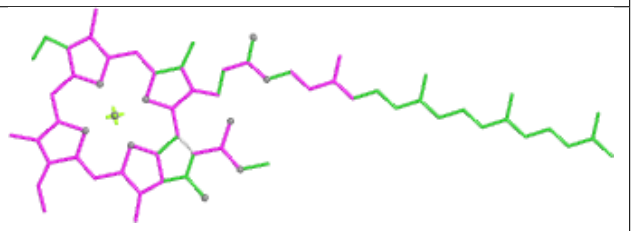


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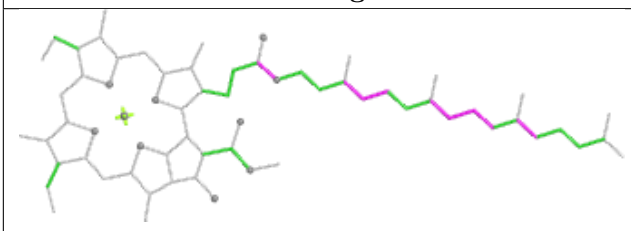
Ligand CLA D 405



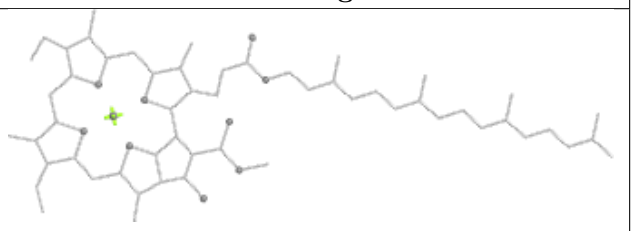
Bond lengths



Bond angles



Torsions

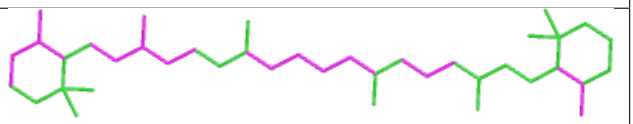


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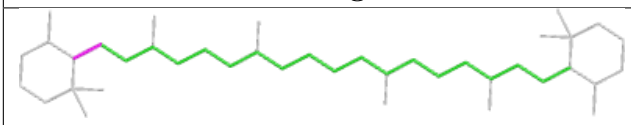
Ligand BCR C 516



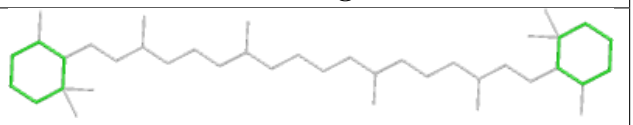
Bond lengths



Bond angles

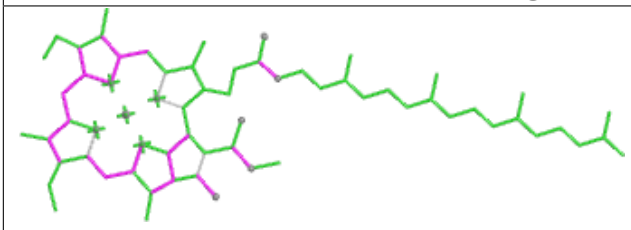


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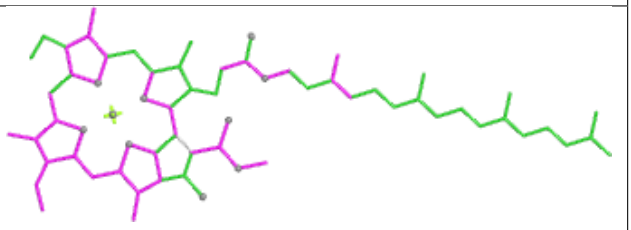


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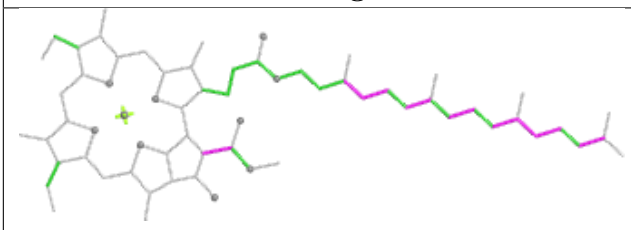
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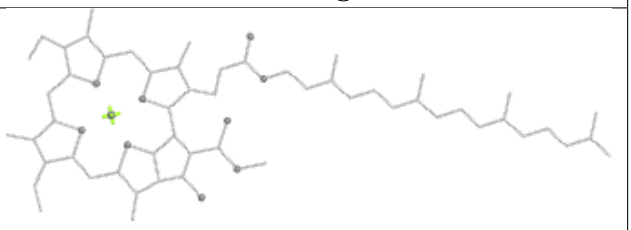
Bond lengths



Bond angles

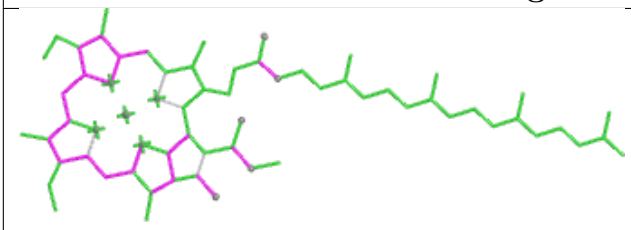


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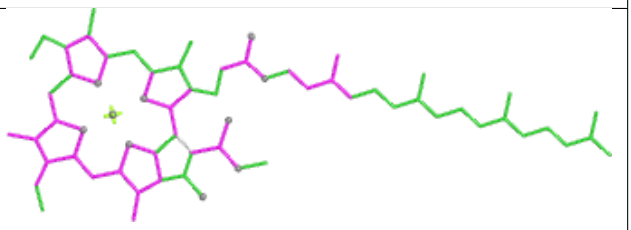


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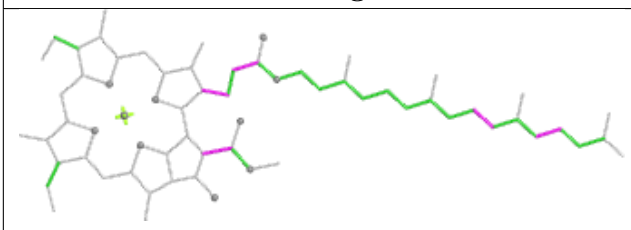
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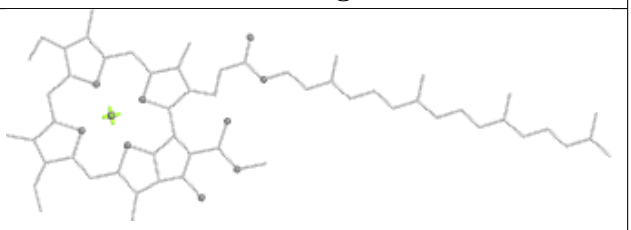
Bond lengths



Bond angles

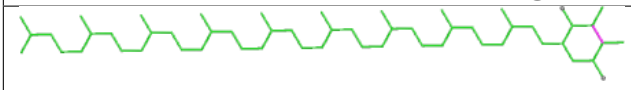


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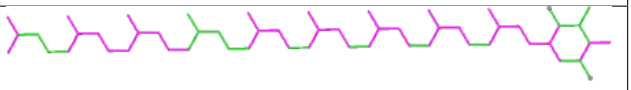


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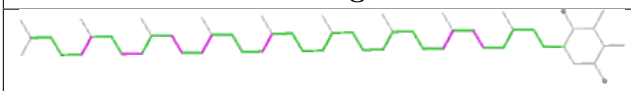
Ligand PL9 D 407



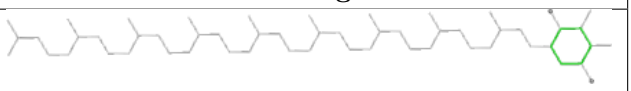
Bond lengths



Bond angles

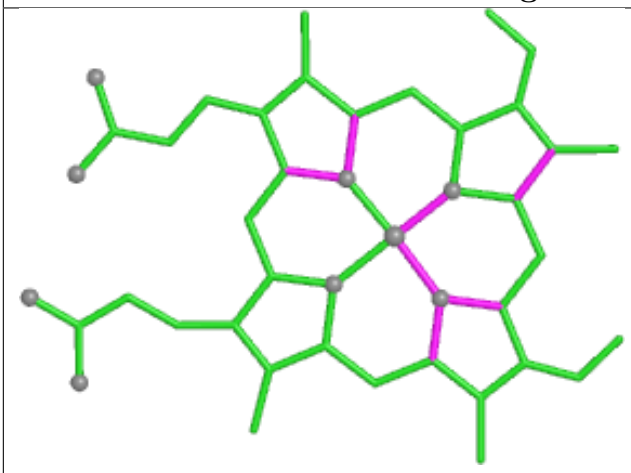


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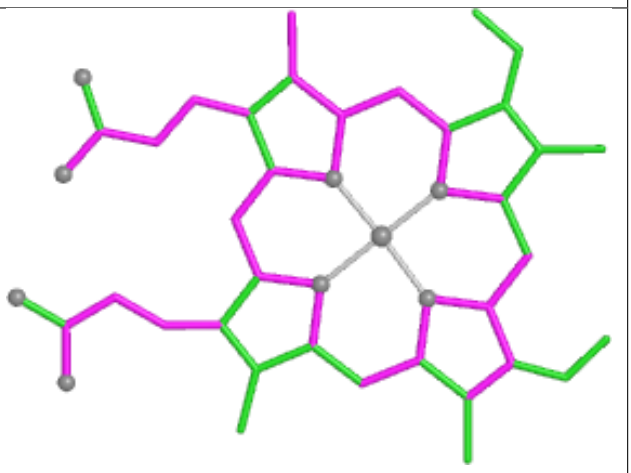


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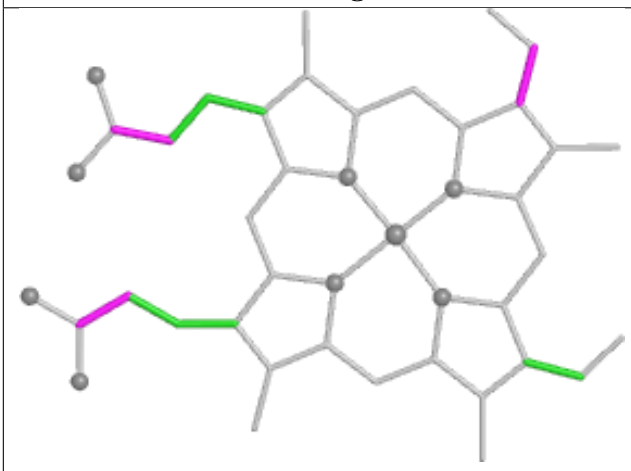
Ligand HEM E 103



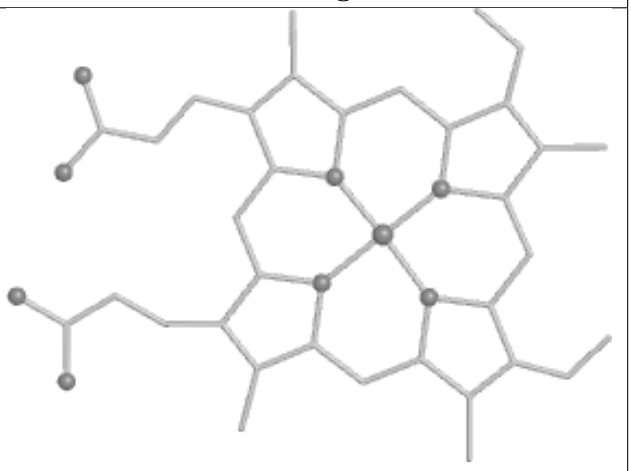
Bond lengths



Bond angles

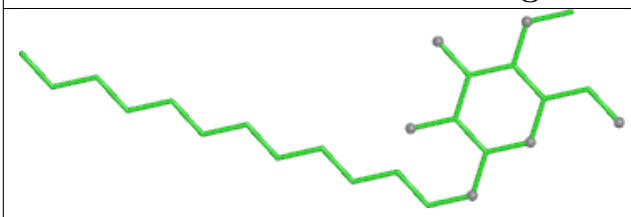


Torsions

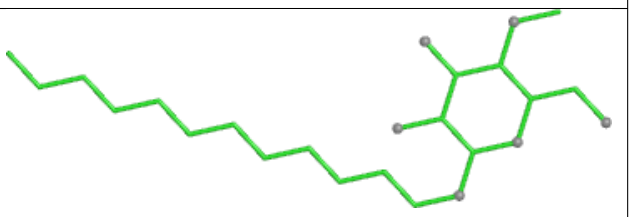


Rings

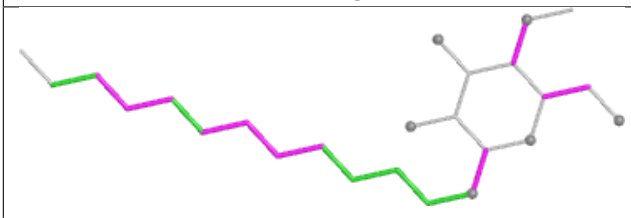
Ligand LMT B 629



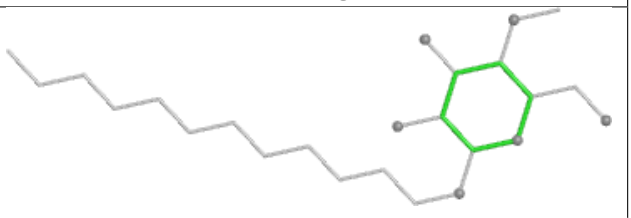
Bond lengths



Bond angles

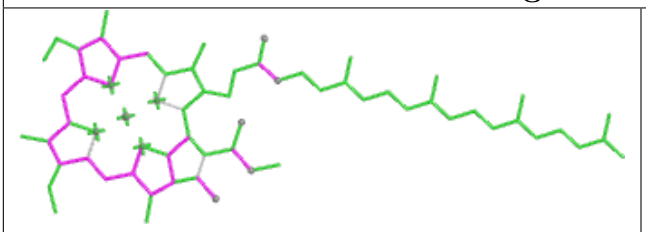


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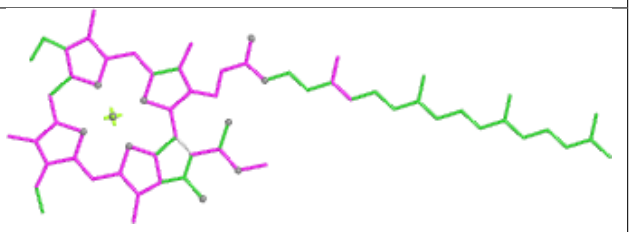


Rings

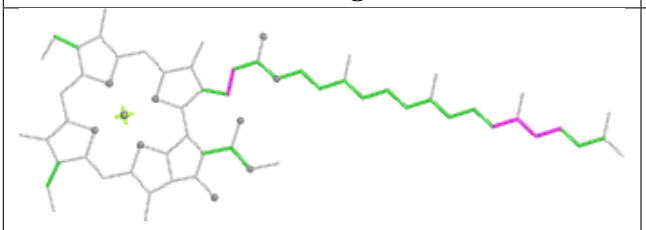
Ligand CLA A 404



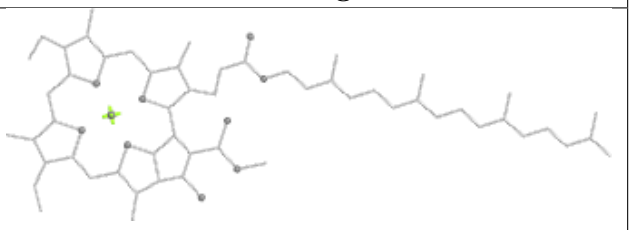
Bond lengths



Bond angles

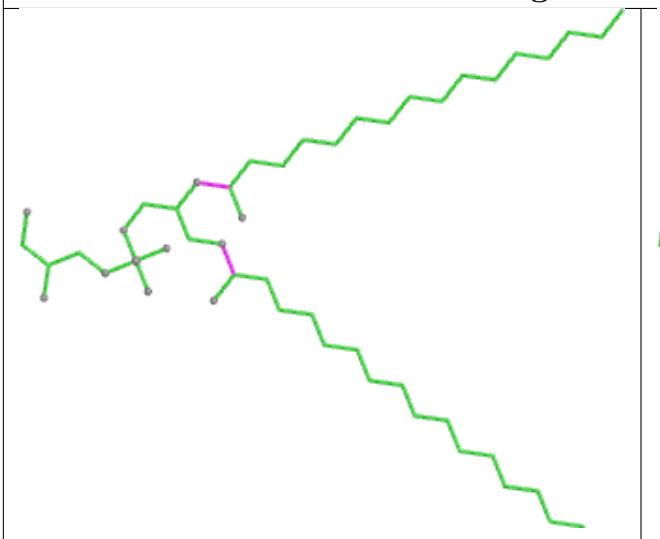


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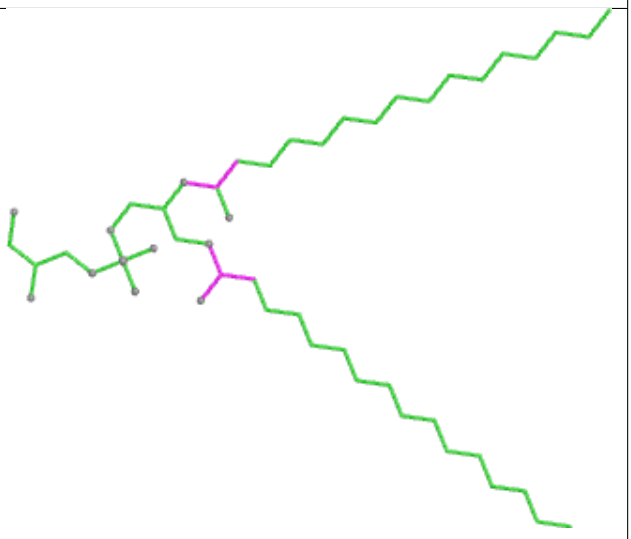


Rings

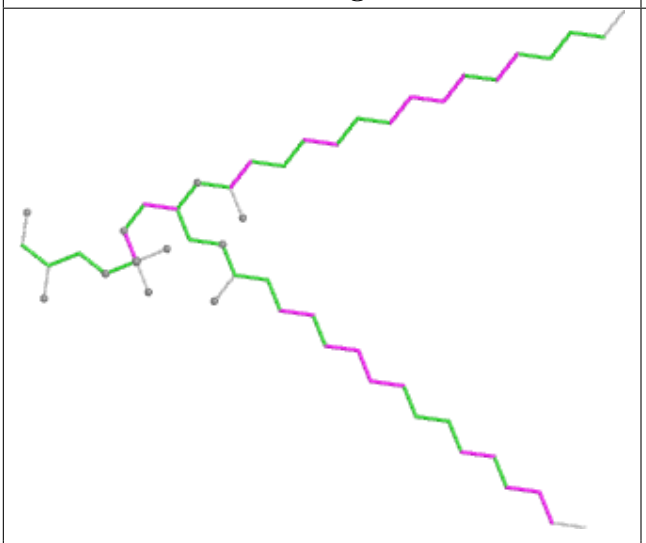
Ligand LHG l 101



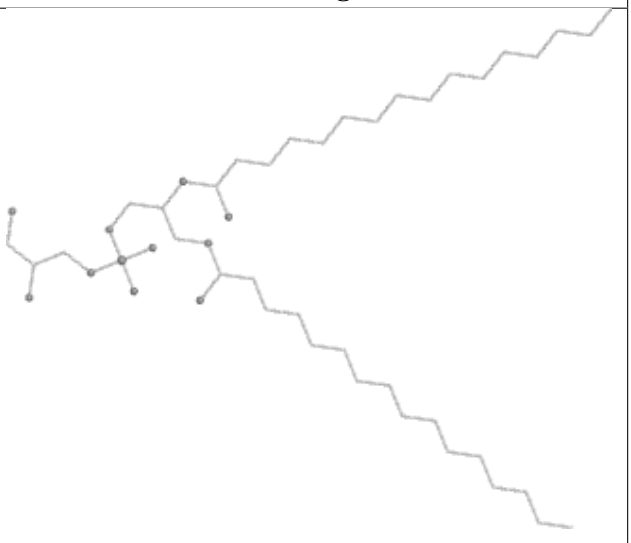
Bond lengths



Bond angles

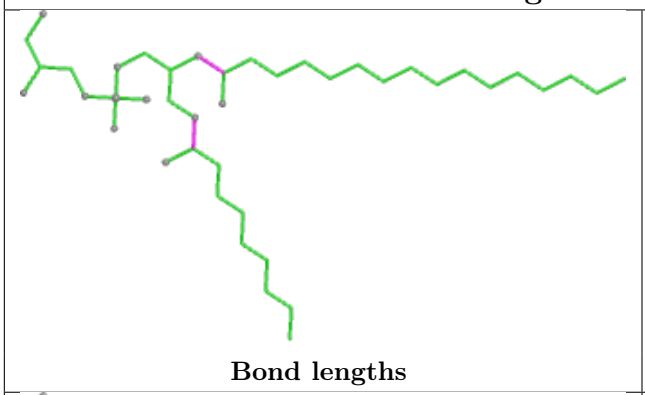


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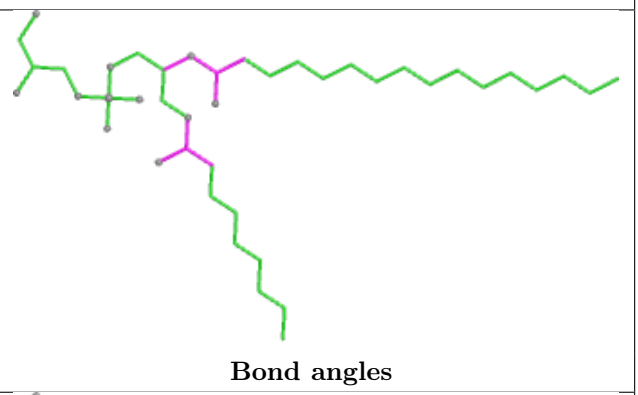


Rings

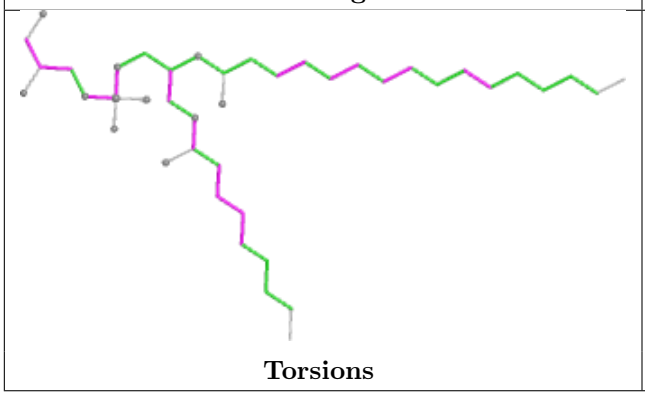
Ligand LHG E 101



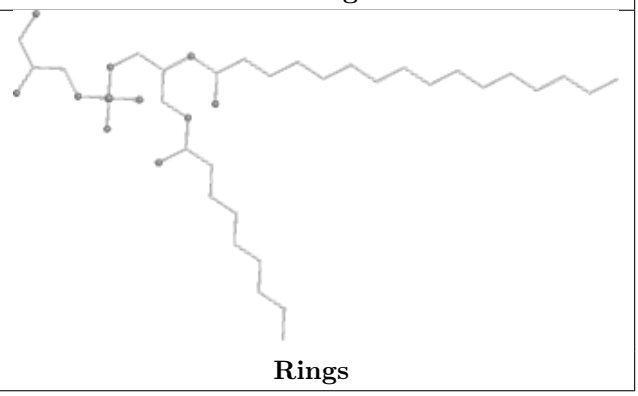
Bond lengths



Bond angles

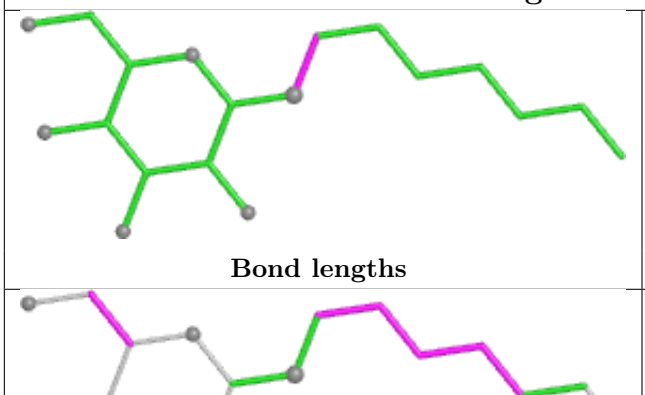


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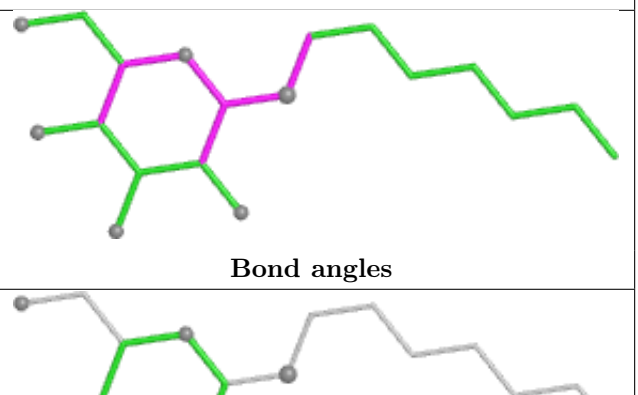


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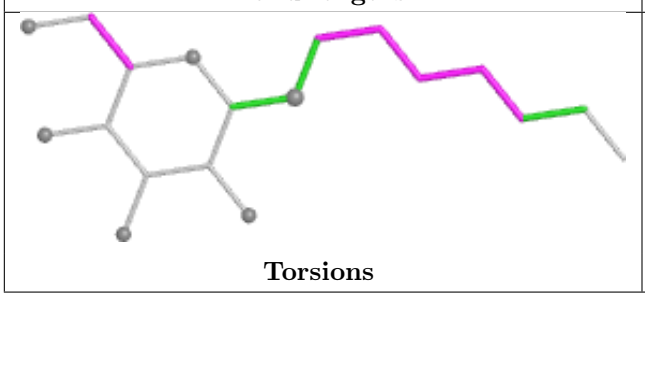
Ligand HTG b 628



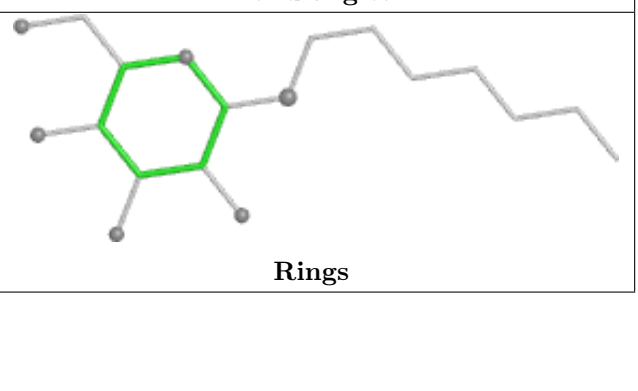
Bond lengths



Bond angles

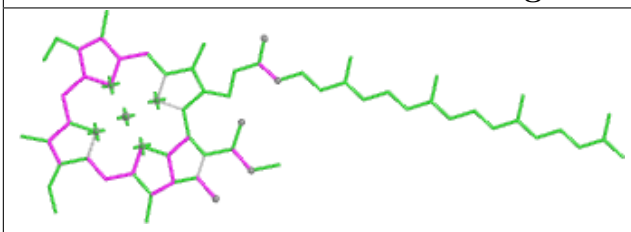


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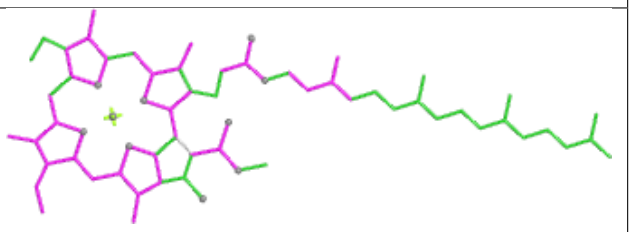


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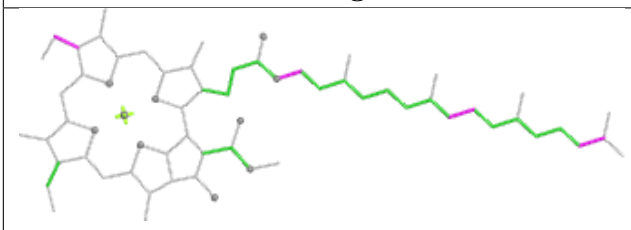
Ligand CLA B 608



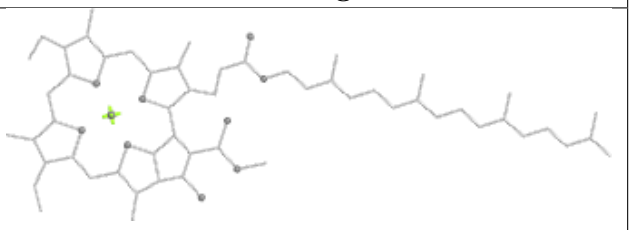
Bond lengths



Bond angles

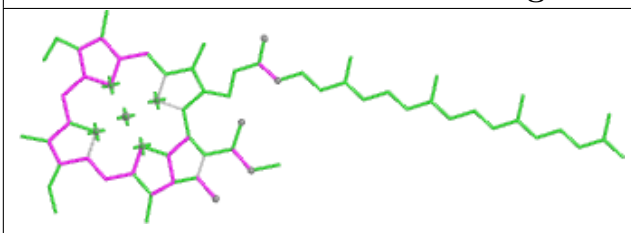


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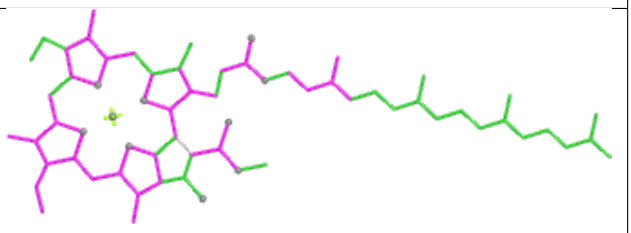


Rings

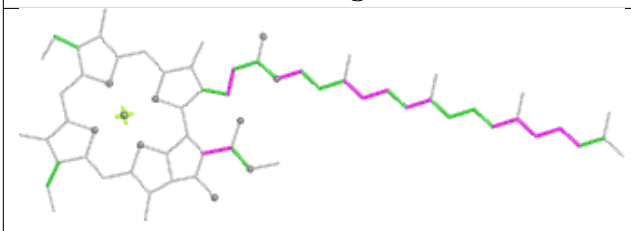
Ligand CLA b 614



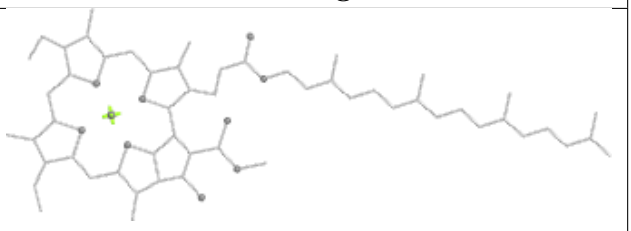
Bond lengths



Bond angles

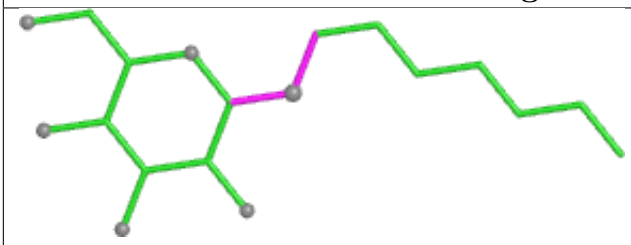


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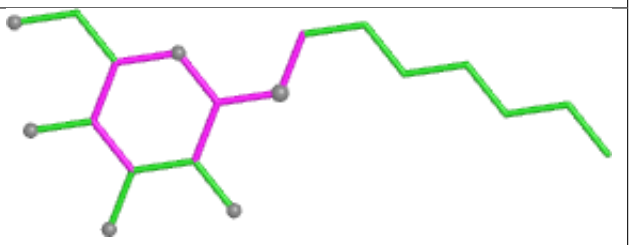


Rings

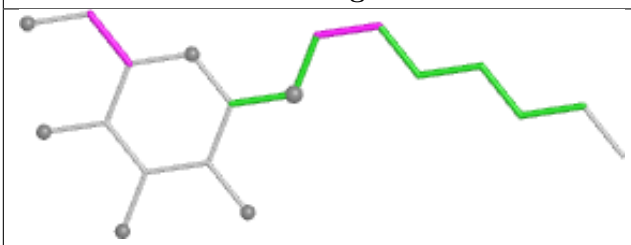
Ligand HTG C 522



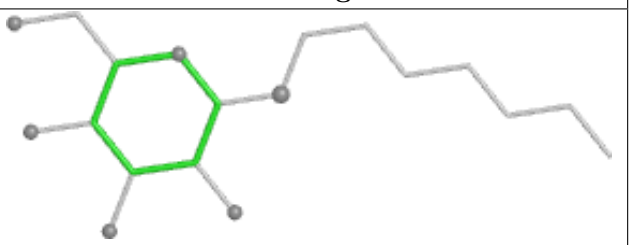
Bond lengths



Bond angles

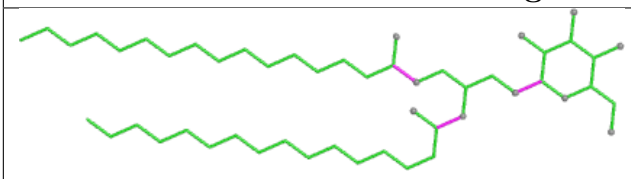


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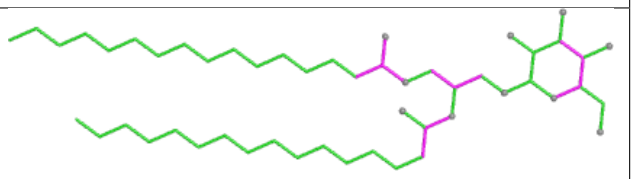


Rings

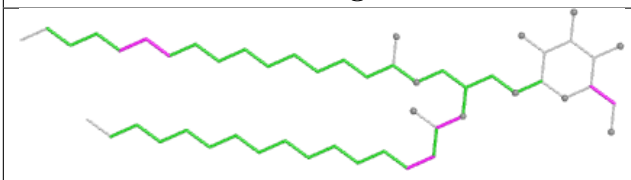
Ligand LMG c 520



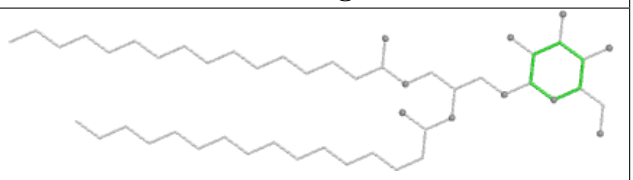
Bond lengths



Bond angles

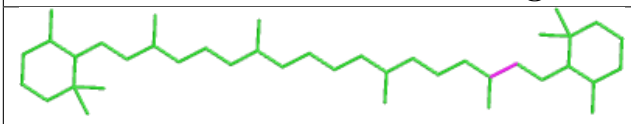


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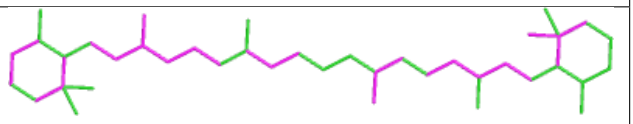


Rings

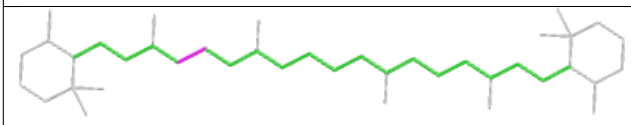
Ligand BCR k 101



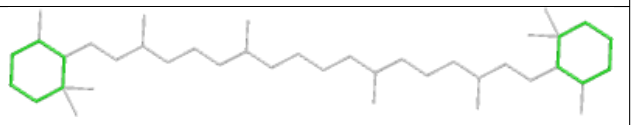
Bond lengths



Bond angles

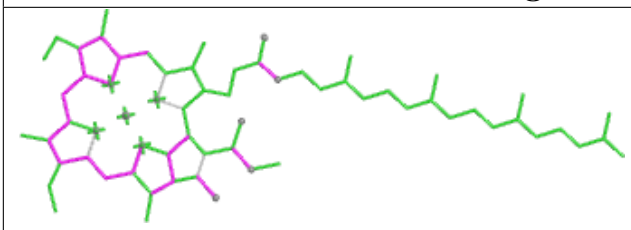


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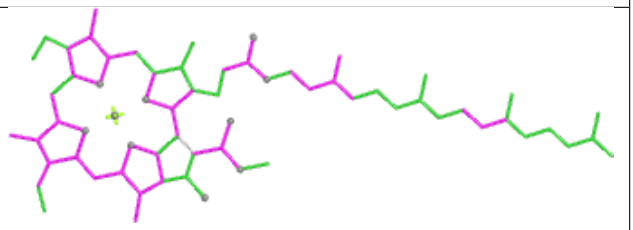


Rings

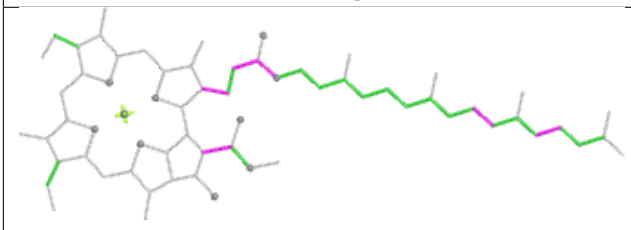
Ligand CLA B 612



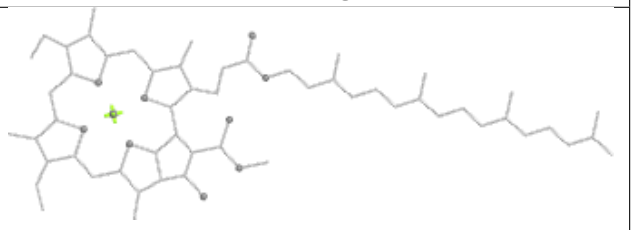
Bond lengths



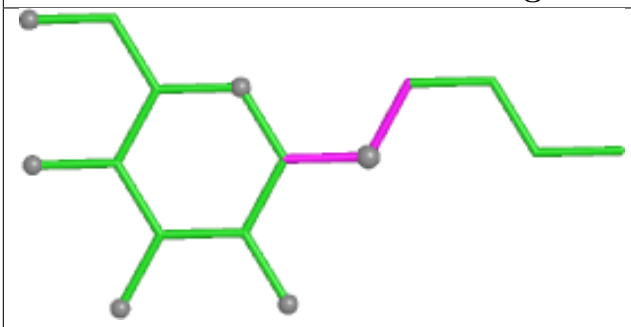
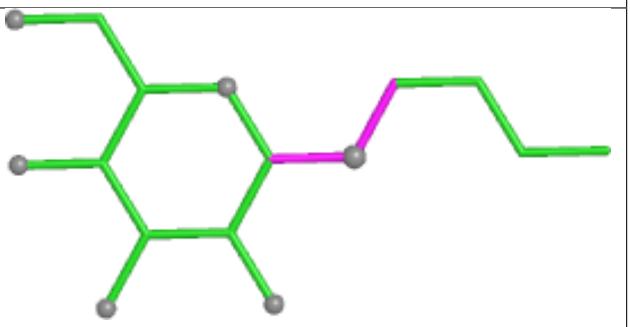
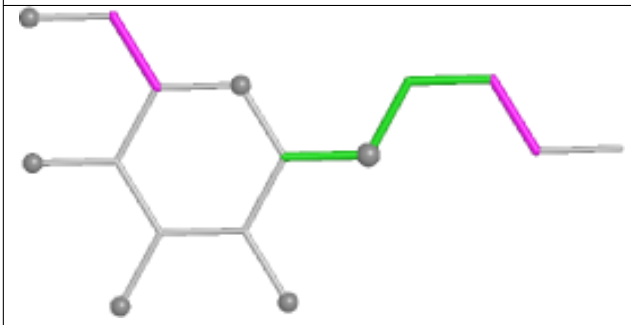
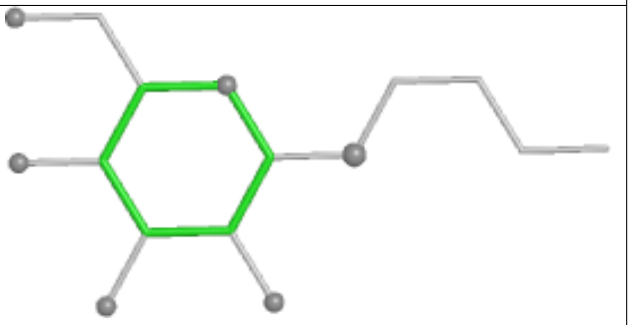
Bond angles

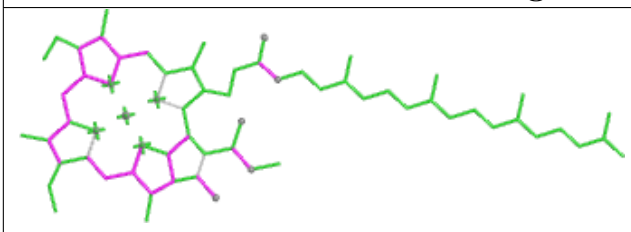
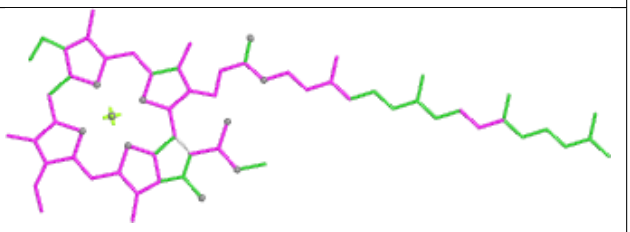
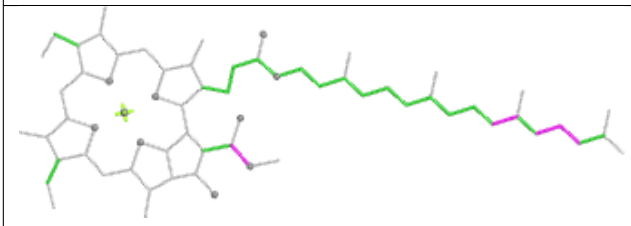
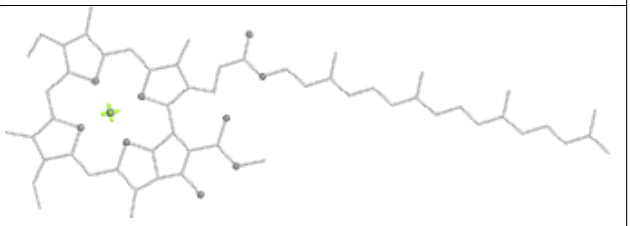


Torsions

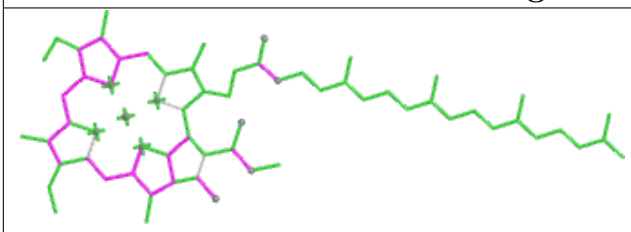


Rings

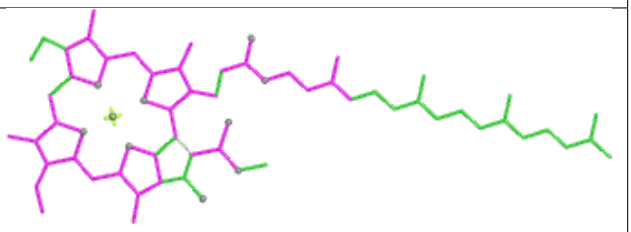
Ligand HTG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

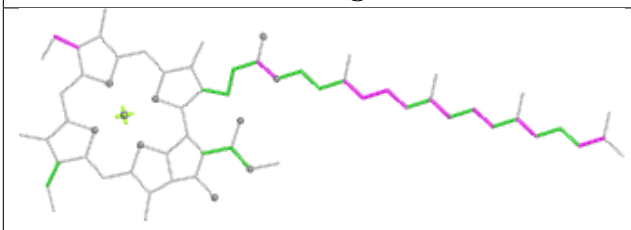
Ligand CLA d 404



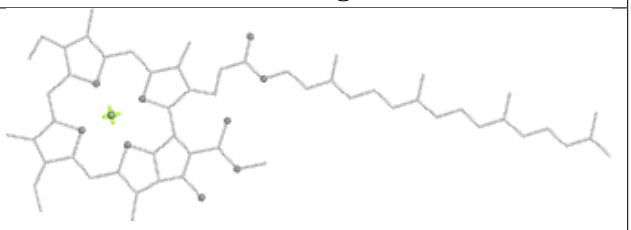
Bond lengths



Bond angles

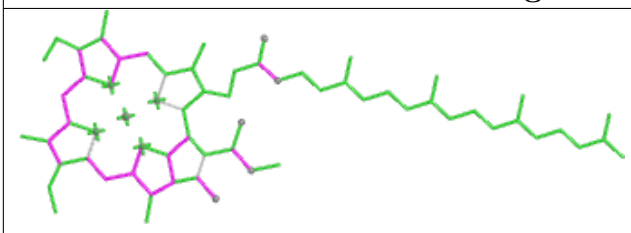


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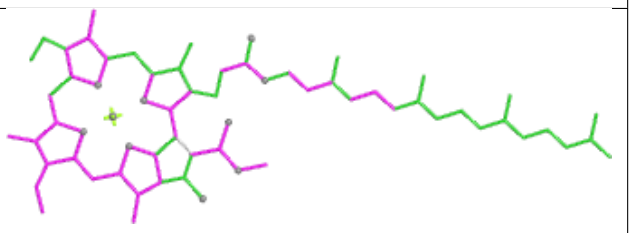


Rings

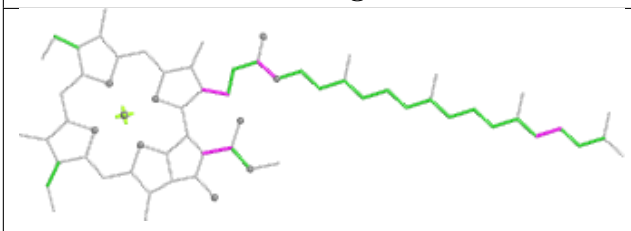
Ligand CLA B 609



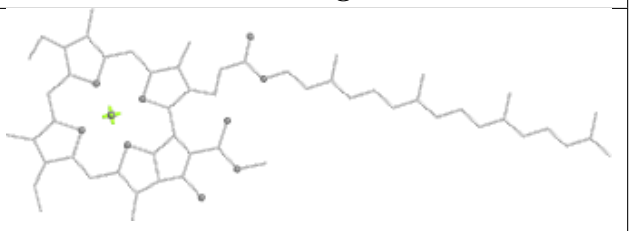
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-1.12	0	100	100	20, 31, 53, 100	3 (0%)
1	a	334/344 (97%)	-1.11	0	100	100	22, 33, 62, 108	5 (1%)
2	B	504/505 (99%)	-1.08	0	100	100	17, 36, 65, 109	8 (1%)
2	b	504/505 (99%)	-1.03	0	100	100	20, 37, 74, 118	4 (0%)
3	C	451/455 (99%)	-1.01	0	100	100	24, 45, 67, 117	4 (0%)
3	c	455/455 (100%)	-0.99	0	100	100	27, 48, 69, 109	5 (1%)
4	D	342/342 (100%)	-1.12	0	100	100	18, 32, 53, 108	1 (0%)
4	d	341/342 (99%)	-1.14	0	100	100	20, 36, 54, 123	1 (0%)
5	E	81/84 (96%)	-0.87	0	100	100	35, 54, 82, 120	1 (1%)
5	e	79/84 (94%)	-0.85	0	100	100	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.97	0	100	100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.87	0	100	100	44, 50, 86, 122	0
7	H	64/65 (98%)	-0.85	1 (1%)	70	67	26, 47, 68, 101	1 (1%)
7	h	65/65 (100%)	-0.97	0	100	100	37, 51, 74, 141	0
8	I	37/38 (97%)	-0.88	0	100	100	37, 46, 88, 130	0
8	i	37/38 (97%)	-0.78	0	100	100	38, 46, 93, 135	0
9	J	38/39 (97%)	-0.98	0	100	100	32, 52, 106, 147	0
9	j	39/39 (100%)	-0.81	0	100	100	40, 51, 107, 129	0
10	K	37/37 (100%)	-1.05	0	100	100	44, 53, 76, 91	0
10	k	37/37 (100%)	-1.06	0	100	100	47, 54, 78, 93	0
11	L	36/37 (97%)	-1.16	0	100	100	15, 26, 89, 129	1 (2%)
11	l	36/37 (97%)	-1.12	0	100	100	17, 28, 87, 128	1 (2%)
12	M	32/36 (88%)	-1.12	0	100	100	16, 29, 49, 117	1 (3%)
12	m	33/36 (91%)	-1.09	0	100	100	24, 29, 72, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.99	0	100	100	22, 45, 100, 157	5 (2%)
13	o	243/244 (99%)	-1.00	0	100	100	24, 46, 99, 144	2 (0%)
14	T	29/32 (90%)	-1.11	0	100	100	23, 28, 60, 96	0
14	t	29/32 (90%)	-1.12	0	100	100	23, 29, 61, 97	0
15	U	96/104 (92%)	-1.08	0	100	100	31, 40, 66, 84	0
15	u	97/104 (93%)	-1.14	0	100	100	32, 43, 68, 101	0
16	V	137/137 (100%)	-1.02	0	100	100	29, 43, 70, 100	0
16	v	137/137 (100%)	-1.02	0	100	100	34, 50, 74, 101	0
17	X	38/40 (95%)	-0.77	0	100	100	44, 56, 82, 110	0
17	x	38/40 (95%)	-0.55	0	100	100	47, 58, 83, 112	0
18	Y	29/30 (96%)	-0.50	0	100	100	56, 71, 112, 114	0
18	y	29/30 (96%)	-0.77	0	100	100	58, 70, 110, 114	0
19	Z	62/62 (100%)	-0.80	0	100	100	57, 72, 117, 152	0
19	z	62/62 (100%)	-0.55	0	100	100	60, 74, 117, 153	0
20	R	34/34 (100%)	0.41	0	100	100	89, 108, 128, 135	0
All	All	5284/5384 (98%)	-1.01	1 (0%)	100	100	15, 41, 82, 157	43 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.97	0.04	31,47,56,62	0
14	FME	T	1	10/11	0.97	0.05	18,32,46,47	0
14	FME	t	1	10/11	0.97	0.04	21,32,41,71	0
8	FME	i	1	10/11	0.98	0.03	37,49,57,62	0
12	FME	m	1	10/11	0.98	0.04	30,42,63,78	0
12	FME	M	1	10/11	0.98	0.06	18,38,70,79	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	A	415	28/-	0.65	0.14	67,87,108,112	0
30	UNL	i	101	40/-	0.67	0.13	48,88,140,147	0
35	LMT	E	102	35/35	0.68	0.14	78,120,147,150	0
30	UNL	m	101	10/-	0.69	0.12	40,50,55,56	0
34	HTG	B	624	19/19	0.71	0.10	57,104,140,144	0
30	UNL	J	102	10/-	0.72	0.15	55,64,89,90	0
34	HTG	D	412	16/19	0.73	0.10	48,115,128,130	0
35	LMT	B	630	35/35	0.73	0.12	33,105,126,134	0
35	LMT	D	402	35/35	0.73	0.11	31,97,113,115	0
33	LMG	Z	101	51/55	0.73	0.11	46,105,140,150	0
34	HTG	B	623	19/19	0.75	0.14	60,84,110,115	0
34	HTG	b	622	19/19	0.75	0.14	74,95,125,130	0
34	HTG	c	521	19/19	0.75	0.10	68,112,134,140	0
30	UNL	a	415	30/-	0.76	0.11	72,90,111,118	0
30	UNL	K	101	34/-	0.77	0.10	55,96,114,125	0
35	LMT	a	417	35/35	0.77	0.11	78,114,130,131	0
35	LMT	e	102	35/35	0.77	0.12	76,134,147,156	0
26	SQD	f	101	43/54	0.78	0.11	85,111,157,164	0
30	UNL	D	411	40/-	0.78	0.11	40,77,117,122	0
35	LMT	I	101	35/35	0.79	0.10	74,108,131,141	0
35	LMT	D	403	35/35	0.79	0.09	48,91,116,117	0
35	LMT	b	621	25/35	0.79	0.10	60,99,144,148	0
34	HTG	C	521	19/19	0.79	0.10	66,101,116,120	0
35	LMT	M	103	35/35	0.80	0.10	40,120,148,154	0
34	HTG	c	522	19/19	0.80	0.11	79,124,142,146	0
30	UNL	M	102	10/-	0.80	0.10	33,52,59,69	0
34	HTG	V	203	11/19	0.80	0.09	71,92,107,108	0
33	LMG	c	520	51/55	0.81	0.09	51,102,132,138	0
34	HTG	b	623	19/19	0.81	0.10	71,109,141,169	0
34	HTG	d	411	16/19	0.81	0.11	81,112,121,122	0
30	UNL	I	102	40/-	0.82	0.11	40,85,135,142	0
30	UNL	b	629	36/-	0.83	0.09	49,80,131,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	b	626	33/-	0.83	0.10	44,78,131,135	0
30	UNL	c	525	32/-	0.84	0.10	71,97,113,119	0
30	UNL	B	628	33/-	0.84	0.10	29,76,136,139	0
30	UNL	j	102	10/-	0.84	0.11	60,75,88,89	0
34	HTG	C	522	19/19	0.84	0.09	58,139,157,179	0
29	PL9	A	414	55/55	0.85	0.13	41,88,105,119	0
35	LMT	M	101	35/35	0.85	0.08	39,80,103,109	0
33	LMG	Z	102	37/55	0.85	0.10	47,97,129,137	0
26	SQD	a	412	54/54	0.86	0.08	44,73,125,133	0
31	LHG	E	101	42/49	0.86	0.09	41,93,108,124	0
31	LHG	e	101	42/49	0.86	0.09	81,118,142,148	0
35	LMT	m	102	35/35	0.86	0.09	34,78,102,109	0
35	LMT	B	629	25/35	0.87	0.10	34,68,124,125	0
27	GOL	a	411	6/6	0.87	0.11	52,60,62,66	0
26	SQD	A	412	54/54	0.87	0.07	39,65,102,118	0
29	PL9	a	414	55/55	0.87	0.12	57,93,112,120	0
34	HTG	b	628	19/19	0.88	0.10	34,65,115,119	0
26	SQD	B	620	54/54	0.89	0.08	41,73,108,113	0
27	GOL	b	624	6/6	0.89	0.08	58,76,78,86	0
34	HTG	B	627	19/19	0.89	0.07	45,63,74,75	0
27	GOL	d	402	6/6	0.89	0.21	33,50,65,68	0
33	LMG	z	101	39/55	0.89	0.10	63,112,140,147	0
33	LMG	C	501	51/55	0.90	0.08	35,74,98,102	0
26	SQD	D	413	43/54	0.90	0.09	64,97,112,116	0
30	UNL	D	410	17/-	0.90	0.08	44,56,91,100	0
30	UNL	x	101	18/-	0.90	0.09	44,63,91,92	0
26	SQD	L	101	54/54	0.90	0.07	47,71,116,121	0
27	GOL	B	626	6/6	0.90	0.12	38,51,55,62	0
25	BCR	D	406	40/40	0.91	0.07	32,42,87,90	0
33	LMG	a	416	51/55	0.91	0.07	41,77,102,118	0
33	LMG	c	519	51/55	0.91	0.08	43,77,114,124	0
35	LMT	b	627	25/35	0.91	0.08	29,61,134,139	0
27	GOL	C	523	6/6	0.91	0.10	44,54,59,60	0
25	BCR	y	101	40/40	0.91	0.07	44,54,70,72	0
35	LMT	B	631	26/35	0.92	0.08	52,80,105,109	0
23	CLA	b	601	65/65	0.92	0.07	43,69,99,126	0
27	GOL	A	411	6/6	0.92	0.07	50,58,65,79	0
33	LMG	C	520	51/55	0.92	0.08	37,69,104,121	0
34	HTG	B	622	19/19	0.93	0.07	34,61,127,132	0
25	BCR	d	405	40/40	0.93	0.07	40,50,74,81	0
23	CLA	c	513	65/65	0.93	0.07	52,73,115,119	0
23	CLA	B	601	65/65	0.93	0.07	39,57,88,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMG	J	101	51/55	0.93	0.07	30,51,88,99	0
33	LMG	j	101	51/55	0.93	0.07	37,53,102,123	0
27	GOL	B	625	6/6	0.93	0.09	48,76,85,89	0
36	DGD	c	517	62/66	0.93	0.06	38,53,112,129	0
37	CA	V	201	1/1	0.93	0.05	93,93,93,93	0
26	SQD	a	410	54/54	0.94	0.07	41,64,98,105	0
25	BCR	K	102	40/40	0.94	0.07	39,47,62,65	0
25	BCR	Y	101	40/40	0.94	0.07	37,49,59,62	0
23	CLA	c	504	65/65	0.94	0.07	37,50,89,111	0
30	UNL	d	410	17/-	0.94	0.06	42,57,85,90	0
33	LMG	b	620	51/55	0.94	0.06	29,50,88,106	0
23	CLA	C	514	65/65	0.94	0.07	46,64,87,95	0
34	HTG	b	625	19/19	0.94	0.06	43,56,83,93	0
26	SQD	A	410	54/54	0.94	0.07	38,62,99,105	0
25	BCR	B	619	40/40	0.94	0.06	28,42,63,67	0
25	BCR	C	515	40/40	0.94	0.07	46,61,72,73	0
23	CLA	C	507	65/65	0.94	0.07	39,55,102,106	0
36	DGD	c	516	62/66	0.94	0.06	33,43,73,95	0
25	BCR	H	101	40/40	0.94	0.06	33,42,63,67	0
30	UNL	X	101	18/-	0.94	0.08	40,53,83,90	0
29	PL9	d	406	55/55	0.95	0.06	23,30,41,58	0
25	BCR	k	101	40/40	0.95	0.07	47,55,79,81	0
25	BCR	t	101	40/40	0.95	0.05	19,42,59,62	0
23	CLA	b	616	65/65	0.95	0.07	31,46,98,105	0
23	CLA	C	513	65/65	0.95	0.07	43,59,94,101	0
23	CLA	c	506	65/65	0.95	0.06	44,58,90,111	0
23	CLA	c	507	65/65	0.95	0.07	41,53,65,68	0
25	BCR	T	101	40/40	0.95	0.05	20,36,45,53	0
31	LHG	A	416	49/49	0.95	0.06	26,44,61,77	0
31	LHG	D	409	49/49	0.95	0.07	29,47,107,124	0
23	CLA	C	505	65/65	0.95	0.06	30,41,79,104	0
36	DGD	C	518	62/66	0.95	0.06	29,46,103,110	0
25	BCR	c	514	40/40	0.95	0.06	52,65,76,79	0
33	LMG	B	621	51/55	0.95	0.06	32,49,79,105	0
36	DGD	c	518	62/66	0.95	0.05	36,46,77,96	0
23	CLA	B	606	65/65	0.95	0.06	26,35,76,99	0
37	CA	c	523	1/1	0.95	0.07	68,68,68,68	0
25	BCR	b	617	40/40	0.96	0.04	20,34,41,44	0
25	BCR	b	618	40/40	0.96	0.04	21,34,49,55	0
25	BCR	b	619	40/40	0.96	0.05	32,45,61,69	0
31	LHG	d	407	49/49	0.96	0.06	25,44,72,87	0
31	LHG	d	409	49/49	0.96	0.07	33,50,98,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	PL9	D	407	55/55	0.96	0.05	20,31,45,54	0
31	LHG	l	101	49/49	0.96	0.05	25,38,55,60	0
23	CLA	B	614	65/65	0.96	0.06	21,31,82,100	0
25	BCR	c	515	40/40	0.96	0.05	37,52,65,75	0
23	CLA	B	616	65/65	0.96	0.07	30,45,113,124	0
25	BCR	h	101	40/40	0.96	0.06	39,50,64,77	0
23	CLA	c	508	65/65	0.96	0.06	35,48,107,118	0
23	CLA	c	511	65/65	0.96	0.07	43,56,74,82	0
23	CLA	c	512	65/65	0.96	0.06	48,64,90,96	0
23	CLA	D	405	65/65	0.96	0.07	31,46,99,111	0
23	CLA	d	404	65/65	0.96	0.07	38,48,98,109	0
24	PHO	a	407	64/64	0.96	0.05	28,35,50,52	0
25	BCR	A	409	40/40	0.96	0.05	22,34,46,49	0
25	BCR	B	618	40/40	0.96	0.04	21,36,54,69	0
23	CLA	a	405	65/65	0.96	0.06	27,36,105,111	0
23	CLA	a	408	65/65	0.96	0.08	28,40,107,115	0
36	DGD	C	517	62/66	0.96	0.05	27,36,81,92	0
25	BCR	C	516	40/40	0.96	0.05	36,48,66,73	0
36	DGD	C	519	62/66	0.96	0.05	28,44,71,95	0
23	CLA	B	602	65/65	0.96	0.05	29,37,55,67	0
23	CLA	b	606	65/65	0.96	0.05	27,42,77,106	0
23	CLA	A	408	65/65	0.96	0.06	26,36,101,109	0
23	CLA	c	501	65/65	0.96	0.05	38,49,64,71	0
23	CLA	C	509	65/65	0.96	0.06	30,43,102,115	0
23	CLA	b	608	65/65	0.97	0.04	32,41,60,68	0
25	BCR	a	409	40/40	0.97	0.04	24,35,45,49	0
23	CLA	b	609	65/65	0.97	0.05	36,44,63,82	0
23	CLA	b	611	65/65	0.97	0.04	25,34,49,61	0
23	CLA	b	612	65/65	0.97	0.05	25,35,48,59	0
23	CLA	b	614	65/65	0.97	0.05	23,34,76,89	0
23	CLA	b	615	65/65	0.97	0.05	29,40,66,81	0
23	CLA	B	609	65/65	0.97	0.05	29,39,53,63	0
23	CLA	C	506	65/65	0.97	0.05	31,40,71,78	0
23	CLA	c	502	65/65	0.97	0.05	37,48,68,73	0
23	CLA	c	503	65/65	0.97	0.05	40,51,63,78	0
23	CLA	B	610	65/65	0.97	0.06	27,36,52,69	0
23	CLA	c	505	65/65	0.97	0.05	32,45,68,86	0
23	CLA	C	508	65/65	0.97	0.05	36,47,60,70	0
23	CLA	B	611	65/65	0.97	0.04	23,30,41,45	0
23	CLA	C	510	65/65	0.97	0.06	36,47,67,69	0
31	LHG	A	417	49/49	0.97	0.05	23,37,55,66	0
31	LHG	D	408	49/49	0.97	0.06	22,34,51,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	509	65/65	0.97	0.06	43,52,66,73	0
23	CLA	c	510	65/65	0.97	0.05	39,47,62,66	0
23	CLA	C	511	65/65	0.97	0.04	33,44,57,61	0
31	LHG	d	408	49/49	0.97	0.05	24,35,53,70	0
23	CLA	C	512	65/65	0.97	0.06	36,52,73,84	0
23	CLA	B	613	65/65	0.97	0.04	21,29,68,78	0
23	CLA	B	603	65/65	0.97	0.05	26,39,52,57	0
24	PHO	A	407	64/64	0.97	0.05	23,31,46,51	0
23	CLA	D	404	65/65	0.97	0.05	20,26,46,52	0
23	CLA	B	615	65/65	0.97	0.04	27,34,61,68	0
25	BCR	B	617	40/40	0.97	0.04	22,31,46,49	0
23	CLA	A	406	65/65	0.97	0.05	22,29,80,89	0
23	CLA	C	502	65/65	0.97	0.05	34,41,60,77	0
23	CLA	C	503	65/65	0.97	0.06	31,42,55,73	0
36	DGD	H	102	62/66	0.97	0.05	26,40,58,66	0
23	CLA	b	602	65/65	0.97	0.05	32,44,60,68	0
23	CLA	b	603	65/65	0.97	0.05	30,40,53,74	0
23	CLA	b	604	65/65	0.97	0.05	23,31,85,96	0
36	DGD	h	102	62/66	0.97	0.05	31,46,62,73	0
23	CLA	C	504	65/65	0.97	0.05	36,44,65,75	0
23	CLA	b	607	65/65	0.97	0.05	20,31,53,63	0
23	CLA	B	604	65/65	0.98	0.05	21,29,92,104	0
23	CLA	B	612	65/65	0.98	0.05	24,29,42,51	0
23	CLA	B	605	65/65	0.98	0.04	22,30,44,48	0
23	CLA	b	605	65/65	0.98	0.05	24,34,52,97	0
23	CLA	d	401	65/65	0.98	0.04	23,26,48,75	0
23	CLA	d	403	65/65	0.98	0.05	25,29,49,62	0
23	CLA	A	405	65/65	0.98	0.04	19,23,41,47	0
23	CLA	B	607	65/65	0.98	0.04	18,27,54,66	0
24	PHO	D	401	64/64	0.98	0.04	21,27,35,45	0
24	PHO	a	406	64/64	0.98	0.04	22,31,40,51	0
23	CLA	a	404	65/65	0.98	0.05	25,30,50,60	0
23	CLA	B	608	65/65	0.98	0.03	27,37,51,55	0
23	CLA	b	610	65/65	0.98	0.04	30,42,51,60	0
22	CL	a	403	1/1	0.98	0.04	34,34,34,34	0
23	CLA	A	404	65/65	0.98	0.04	20,23,41,58	0
37	CA	O	301	1/1	0.98	0.05	87,87,87,87	0
23	CLA	b	613	65/65	0.98	0.04	22,33,67,78	0
32	BCT	a	418	4/4	0.98	0.04	45,52,54,59	0
37	CA	o	301	1/1	0.98	0.02	85,85,85,85	0
38	HEM	E	103	43/43	0.98	0.06	40,54,66,73	0
38	HEM	e	103	43/43	0.98	0.07	48,73,98,105	0

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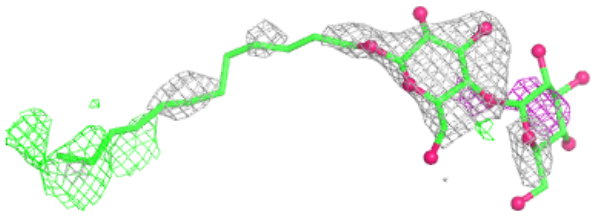
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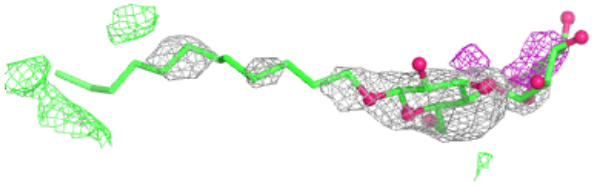
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
39	MG	j	103	1/1	0.98	0.07	51,51,51,51	0
40	HEC	v	201	43/43	0.98	0.05	40,50,59,66	0
22	CL	A	402	1/1	0.99	0.06	24,24,24,24	0
22	CL	A	403	1/1	0.99	0.01	27,27,27,27	0
37	CA	c	524	1/1	0.99	0.05	66,66,66,66	0
32	BCT	A	418	4/4	0.99	0.04	34,39,47,65	0
22	CL	a	402	1/1	0.99	0.04	31,31,31,31	0
21	FE2	A	401	1/1	0.99	0.03	42,42,42,42	0
39	MG	J	103	1/1	0.99	0.08	39,39,39,39	0
37	CA	C	524	1/1	0.99	0.08	62,62,62,62	0
40	HEC	V	202	43/43	0.99	0.04	30,33,44,53	0
21	FE2	a	401	1/1	0.99	0.05	45,45,45,45	0
28	OEX	a	413	10/10	1.00	0.02	27,34,45,53	0
28	OEX	A	413	10/10	1.00	0.02	22,30,43,45	0

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

Electron density around LMT E 102:

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

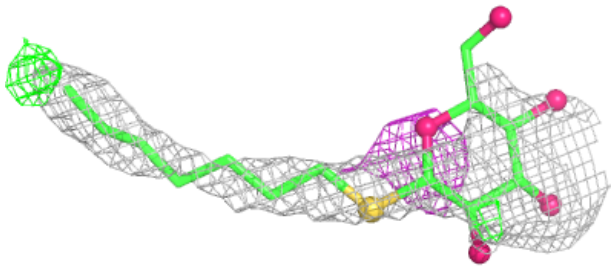


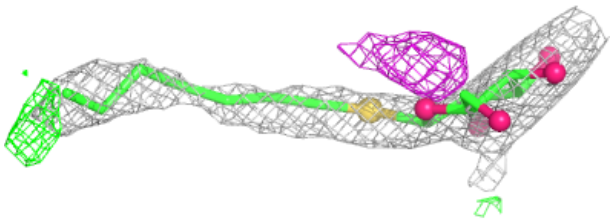


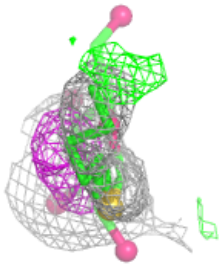


Electron density around HTG B 624:

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

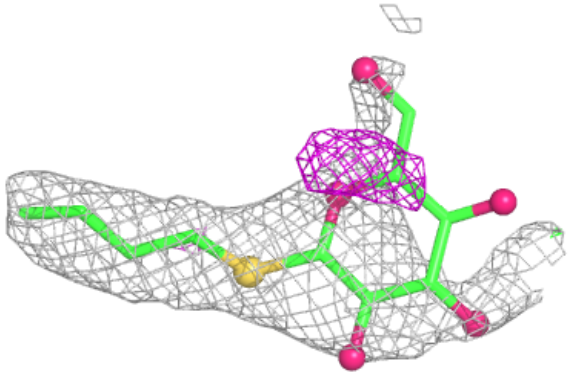


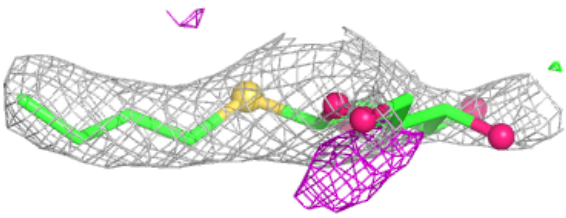


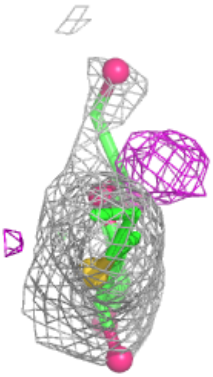


Electron density around HTG D 412:

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

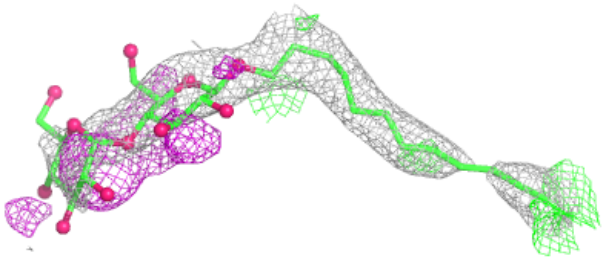


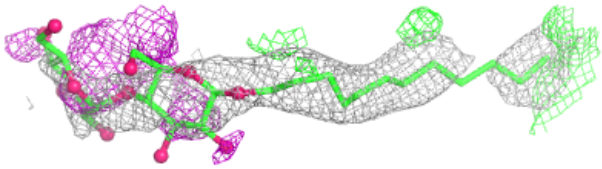


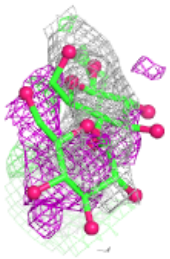


Electron density around LMT B 630:

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

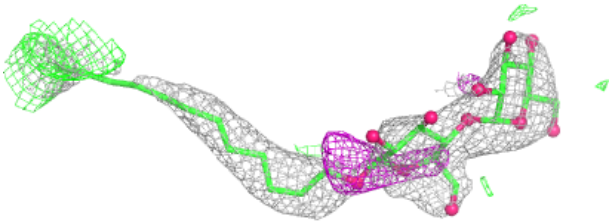


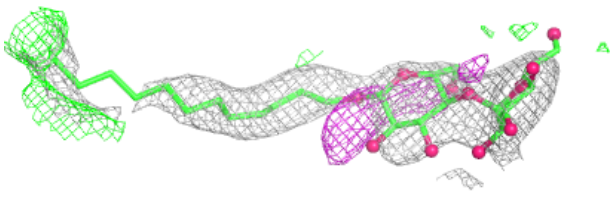


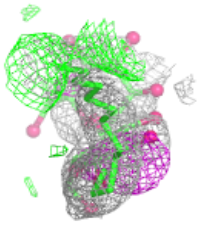


Electron density around LMT D 402:

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

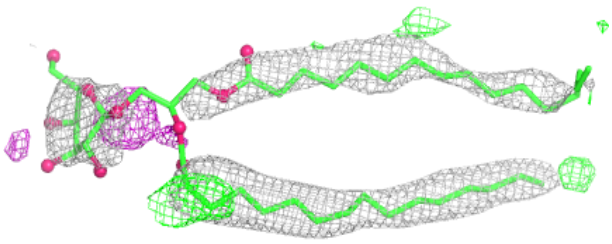


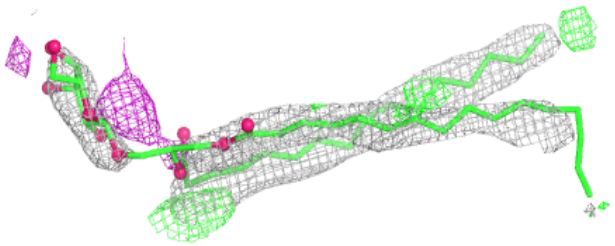


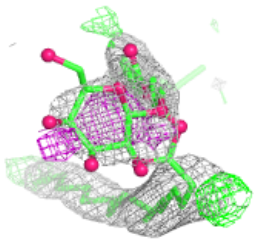


Electron density around LMG Z 101:

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

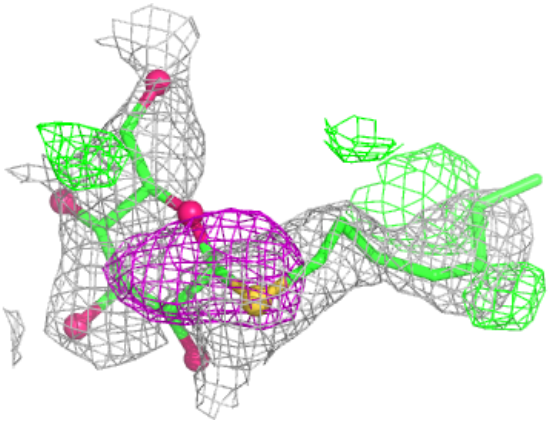


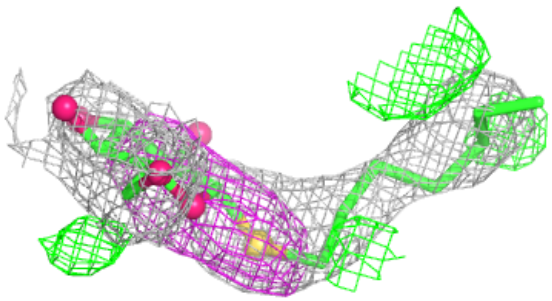


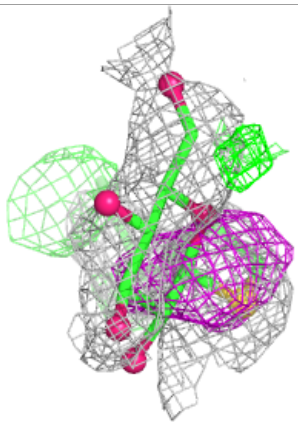


Electron density around HTG B 623:

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

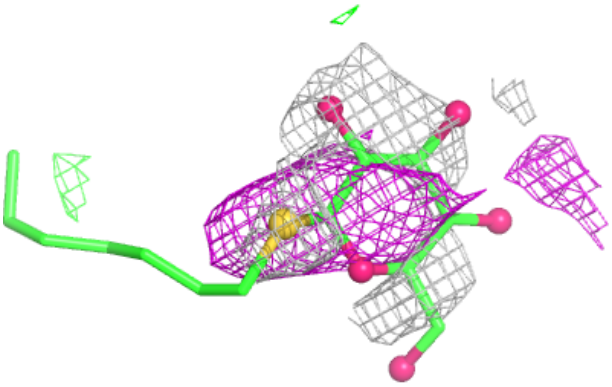


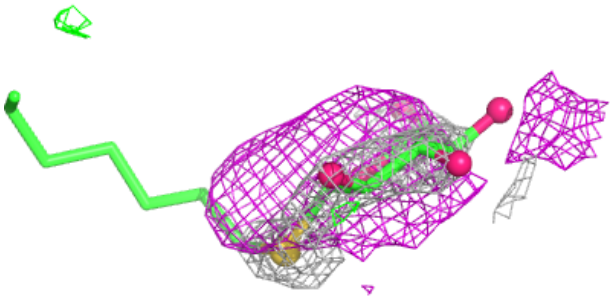


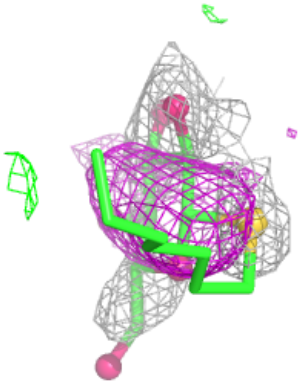


Electron density around HTG b 622:

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

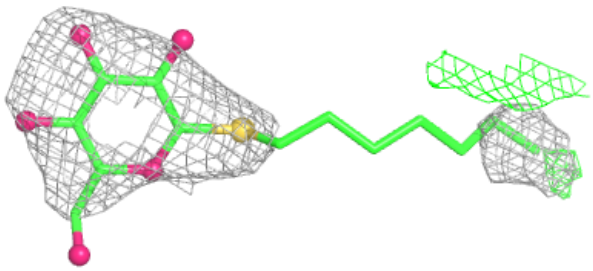


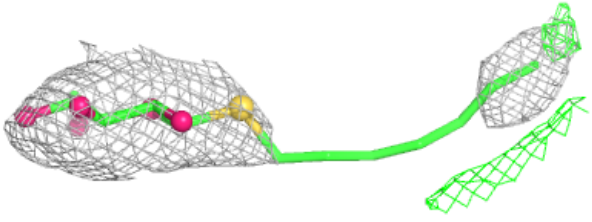


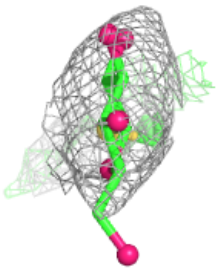


Electron density around HTG c 521:

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

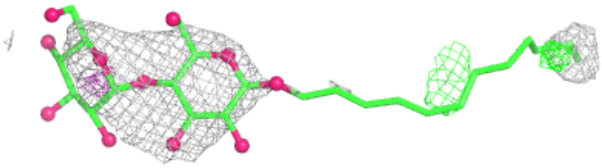


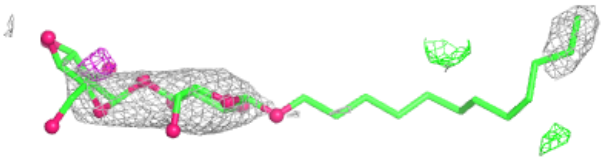


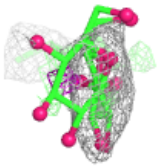


Electron density around LMT a 417:

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

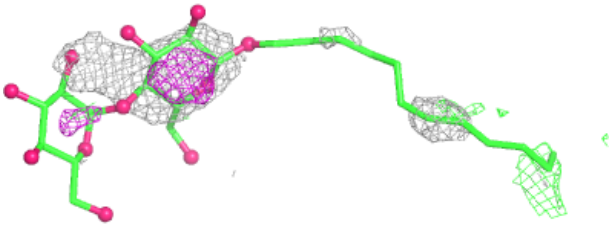


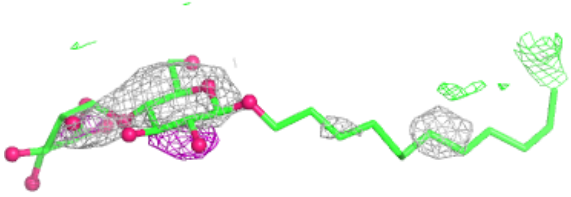


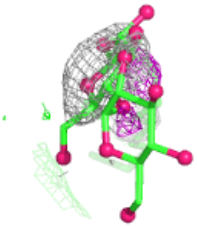


Electron density around LMT e 102:

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



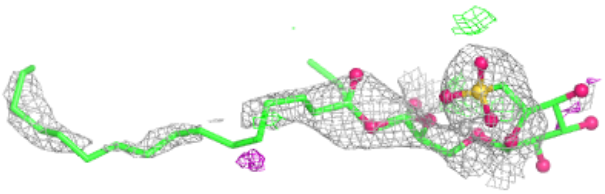




Electron density around SQD f 101:

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

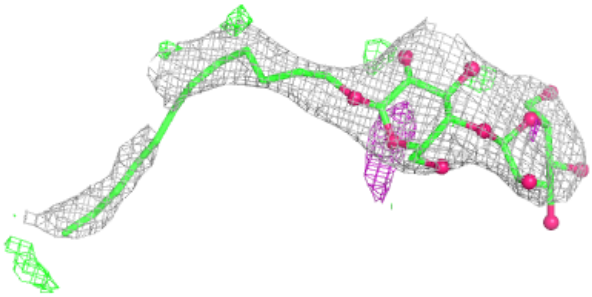


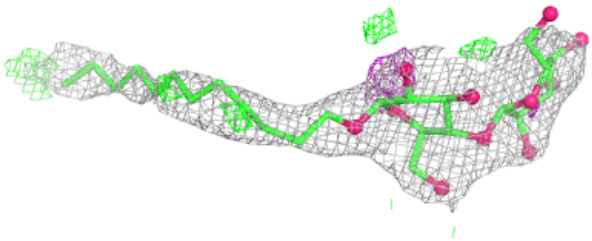


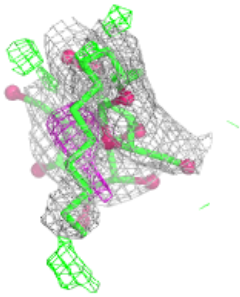


Electron density around LMT I 101:

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

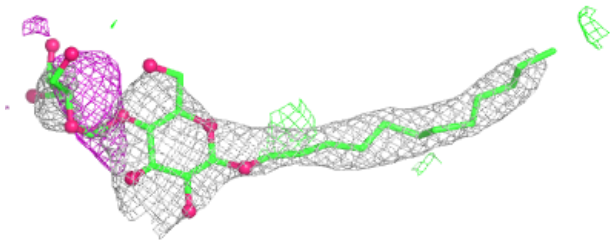


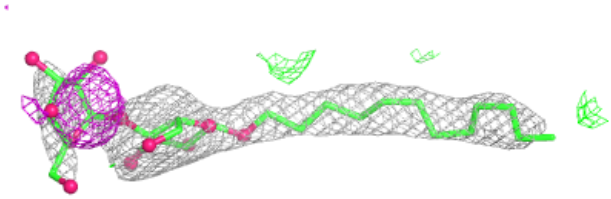


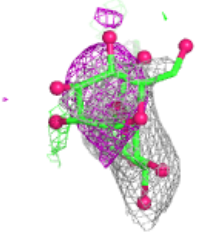


Electron density around LMT D 403:

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

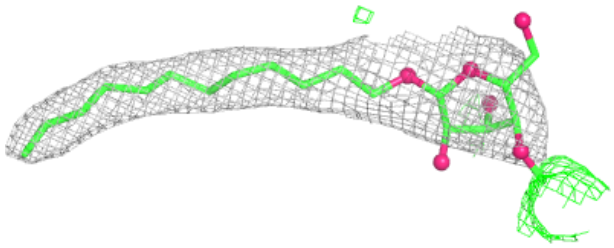


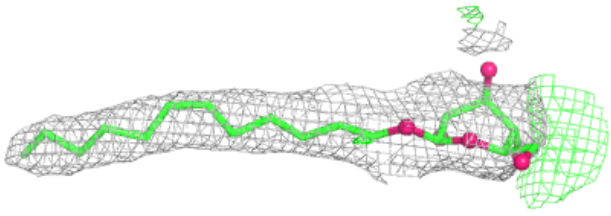


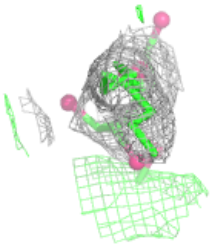


Electron density around LMT b 621:

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

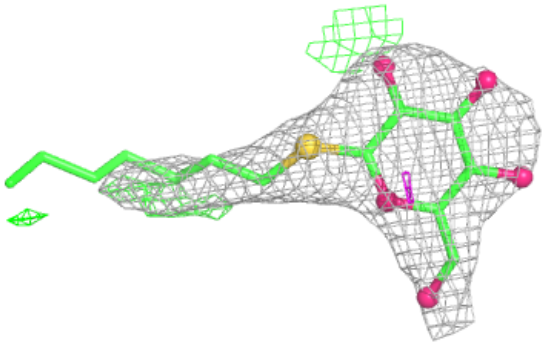


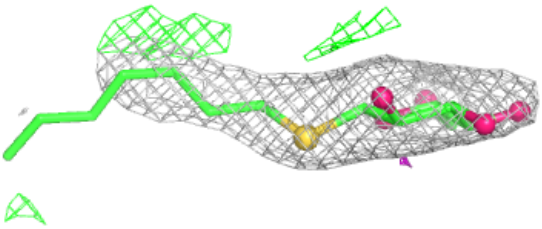


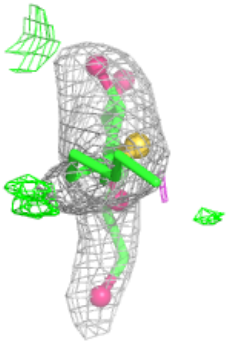


Electron density around HTG C 521:

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

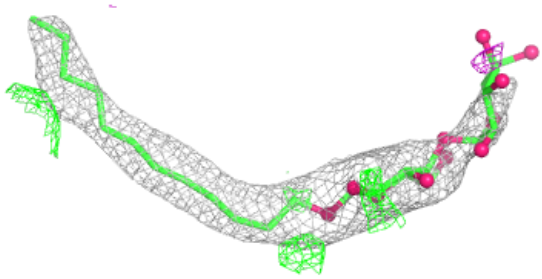


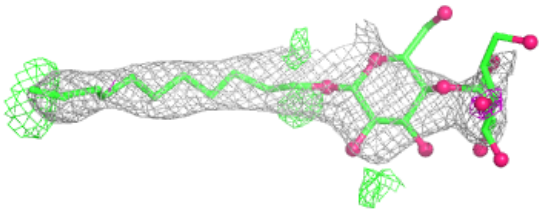


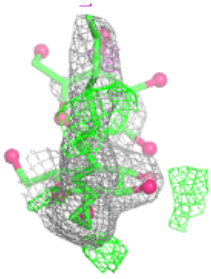


Electron density around LMT M 103:

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

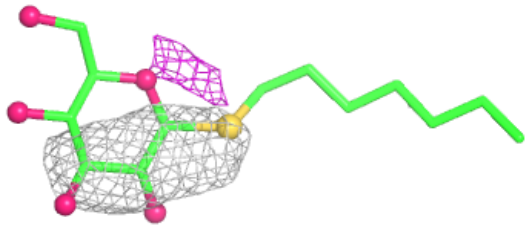


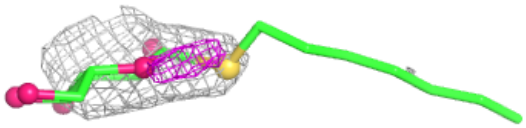


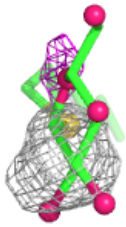


Electron density around HTG c 522:

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

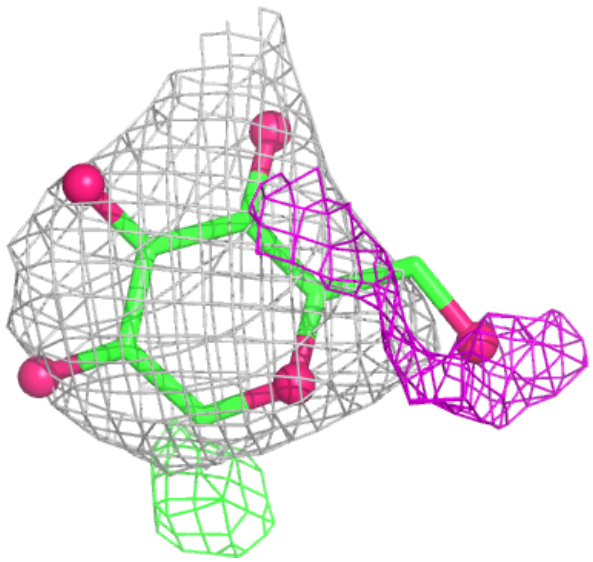


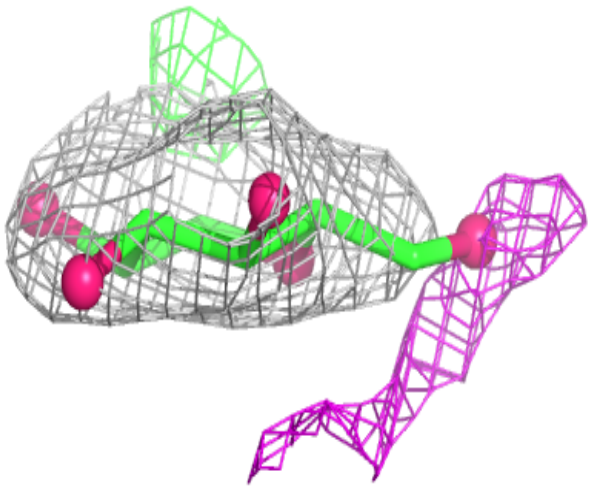


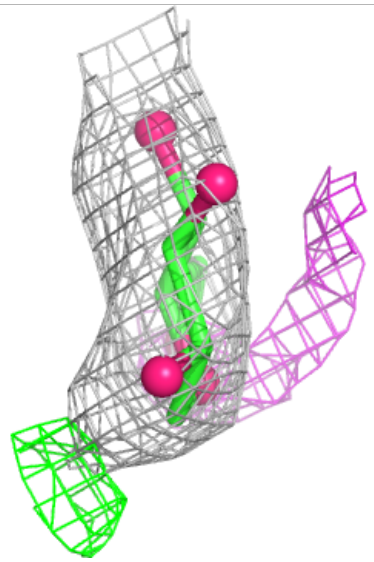


Electron density around HTG V 203:

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

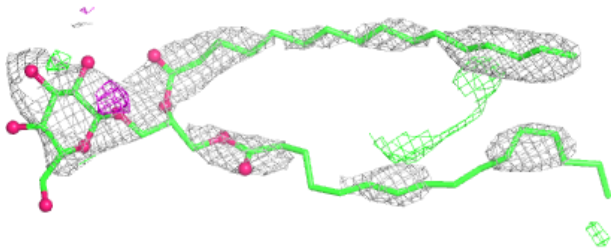


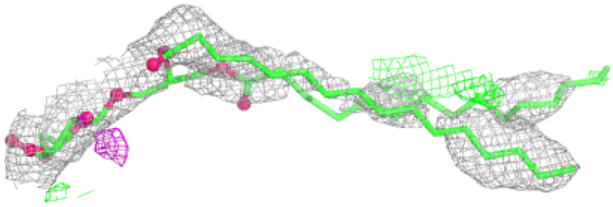


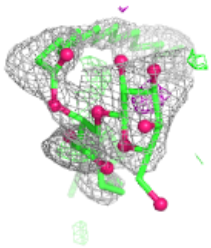


Electron density around LMG c 520:

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

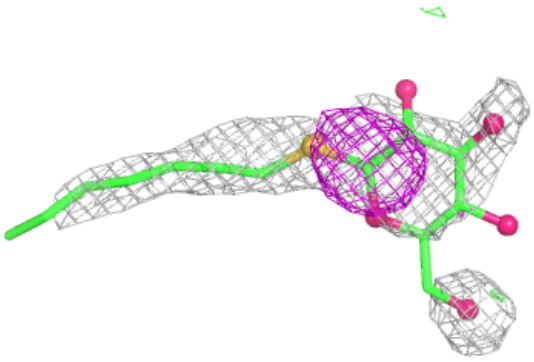


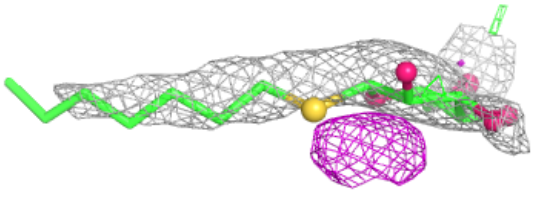


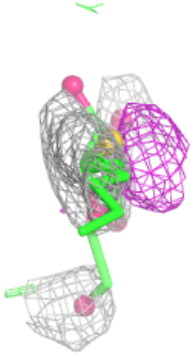


Electron density around HTG b 623:

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

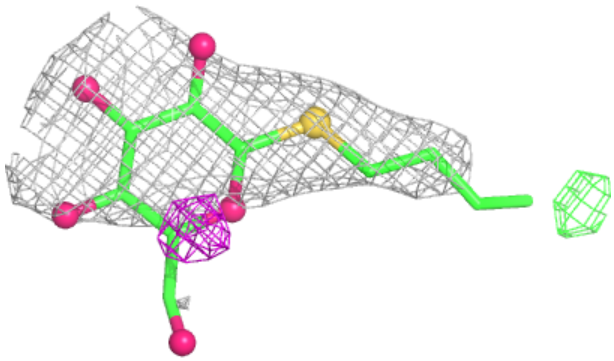


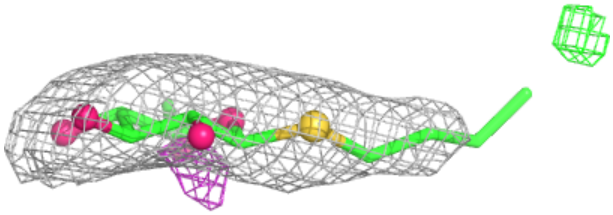


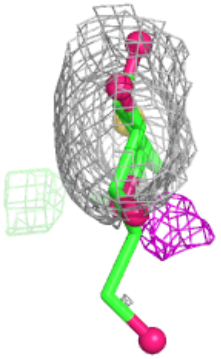


Electron density around HTG d 411:

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

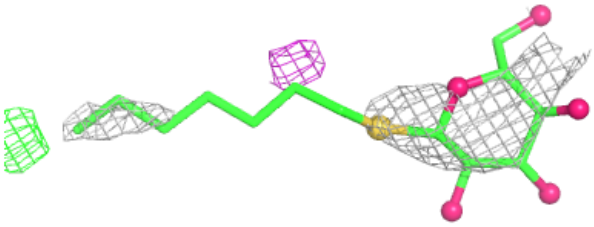


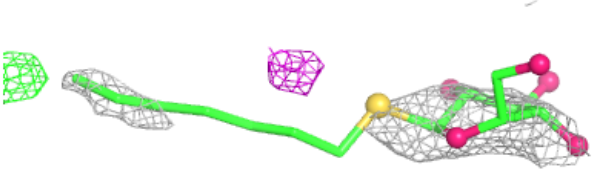


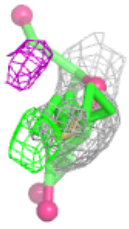


Electron density around HTG C 522:

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

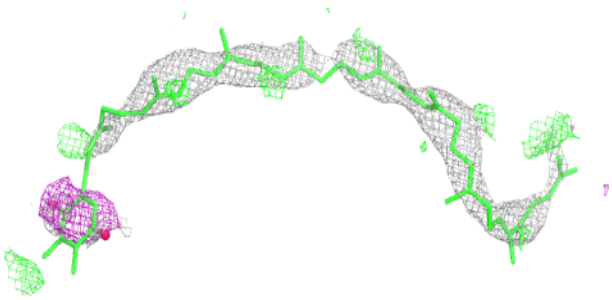


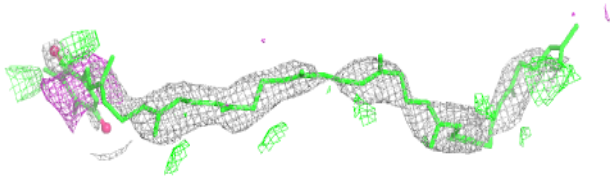


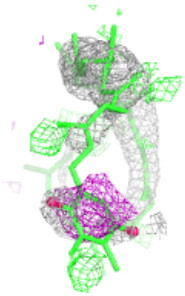


Electron density around PL9 A 414:

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

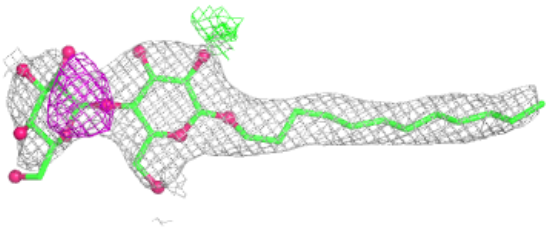


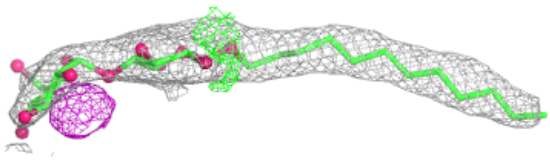


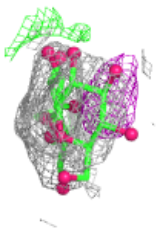


Electron density around LMT M 101:

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

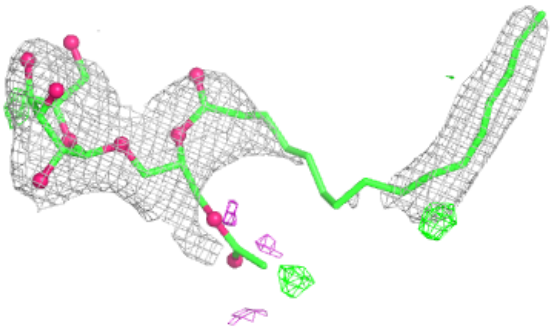


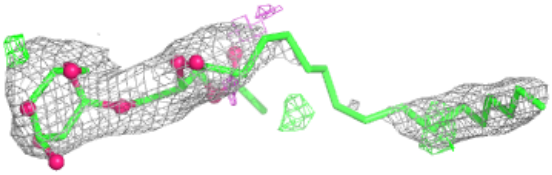


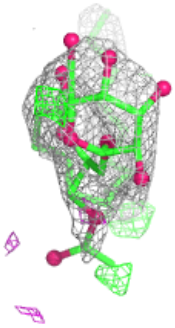


Electron density around LMG Z 102:

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

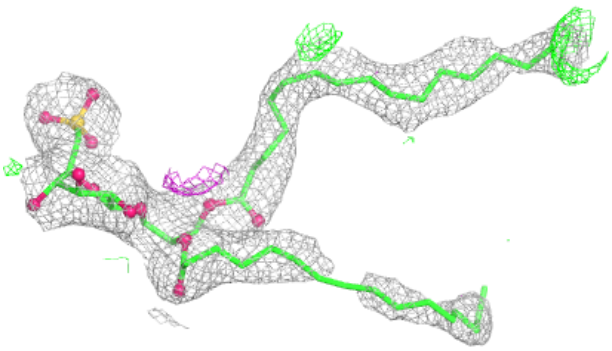


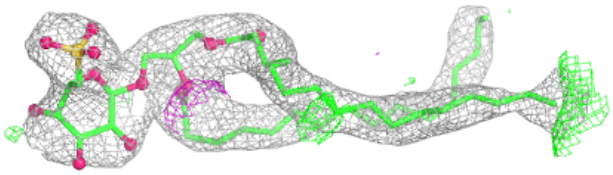


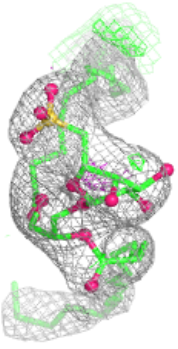


Electron density around SQD a 412:

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

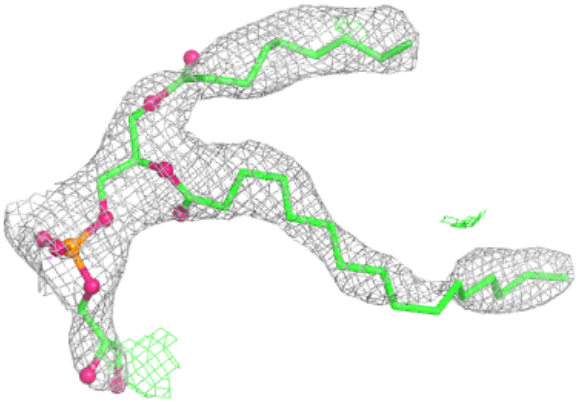


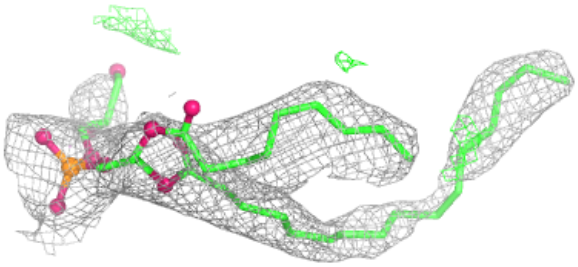


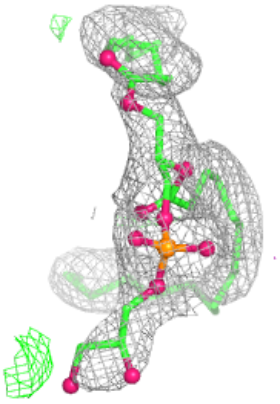


Electron density around LHG E 101:

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

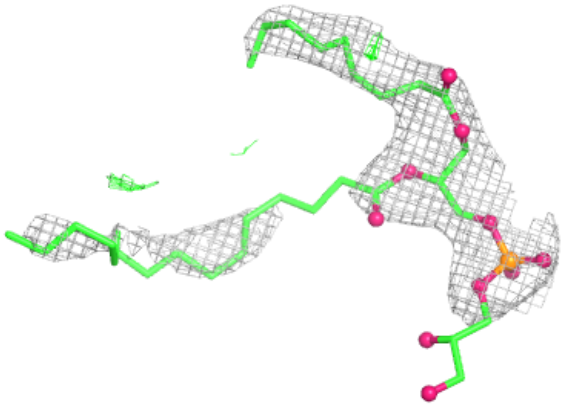


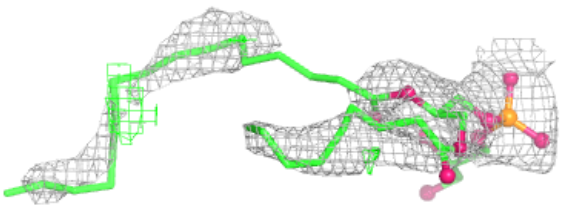


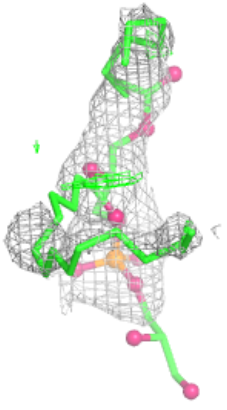


Electron density around LHG e 101:

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

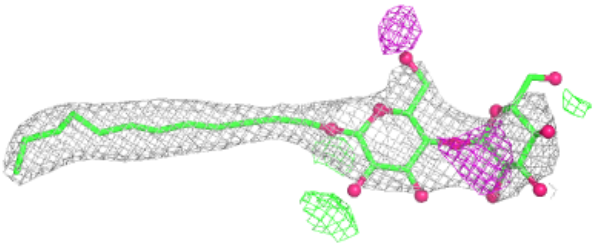


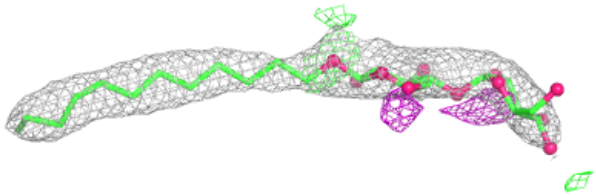


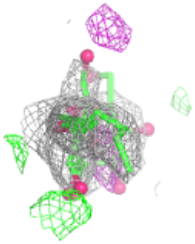


Electron density around LMT m 102:

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

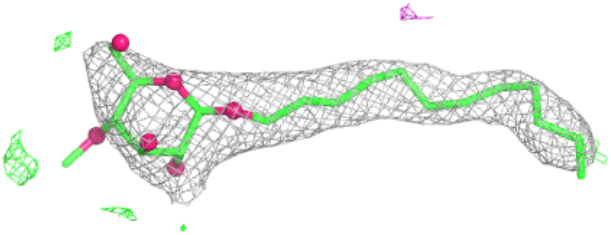


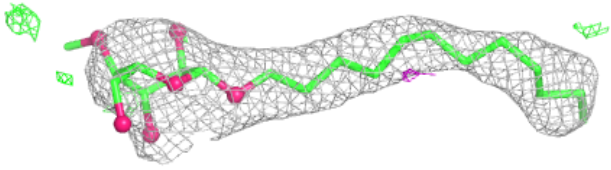


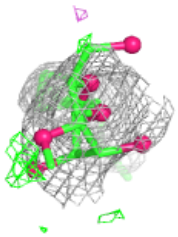


Electron density around LMT B 629:

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

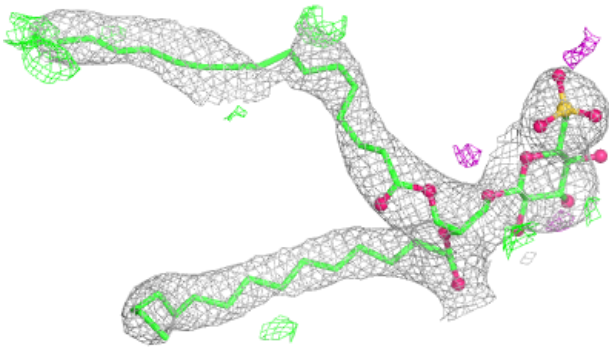


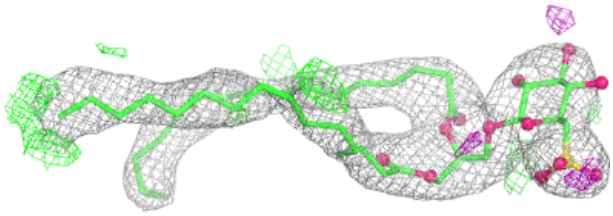


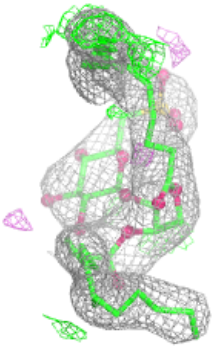


Electron density around SQD A 412:

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

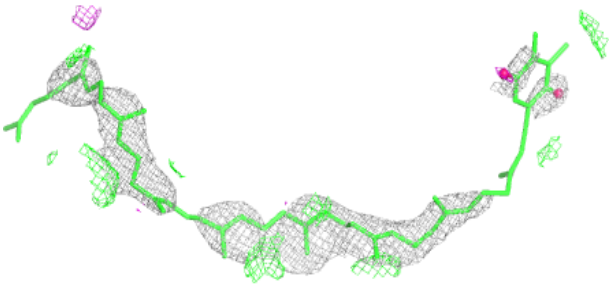


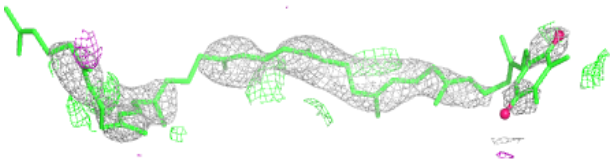


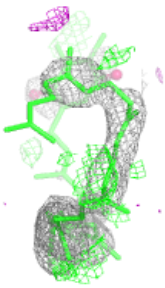


Electron density around PL9 a 414:

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

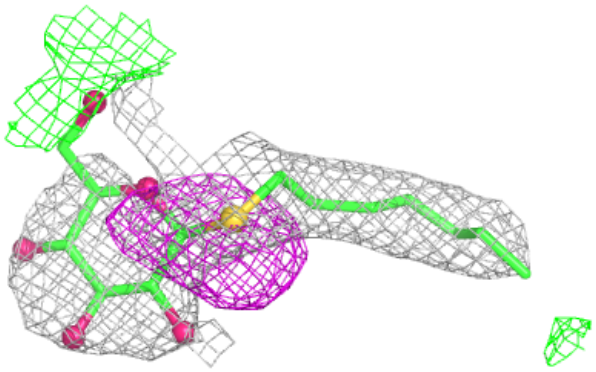


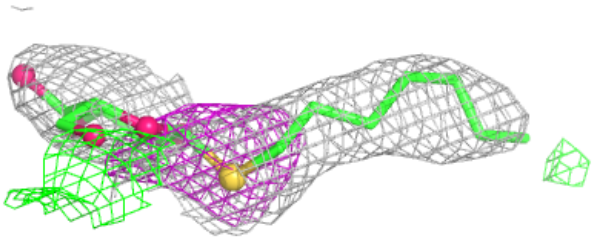


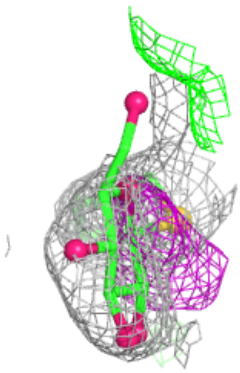


Electron density around HTG b 628:

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

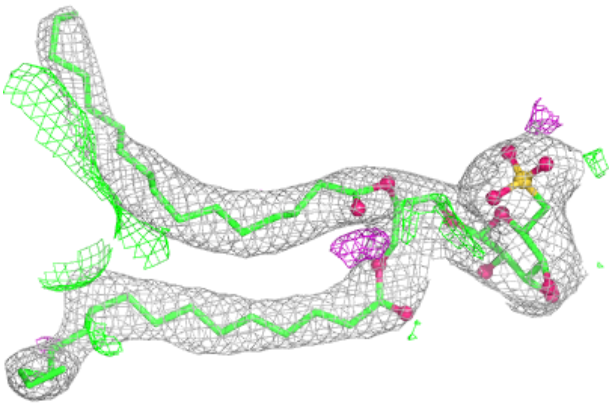


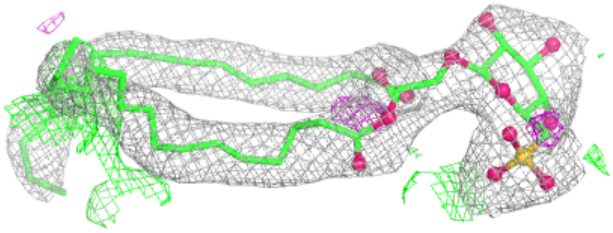


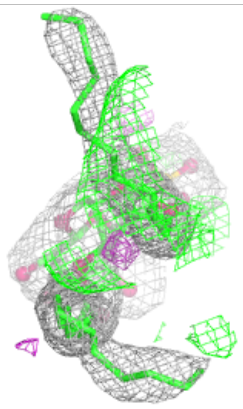


Electron density around SQD B 620:

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

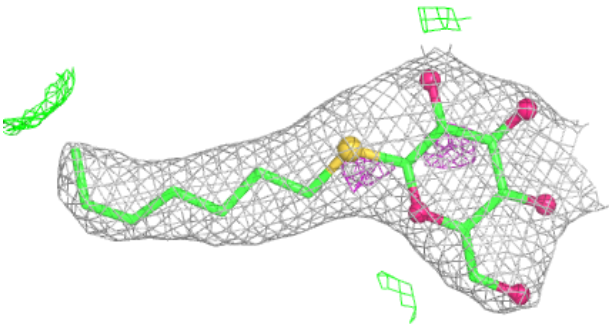


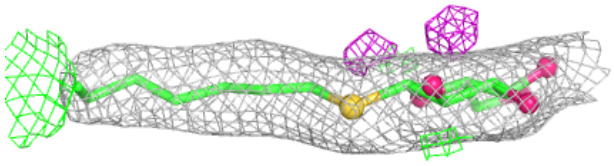


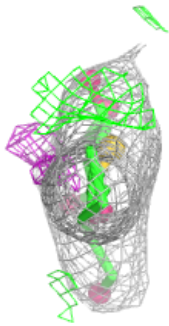


Electron density around HTG B 627:

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

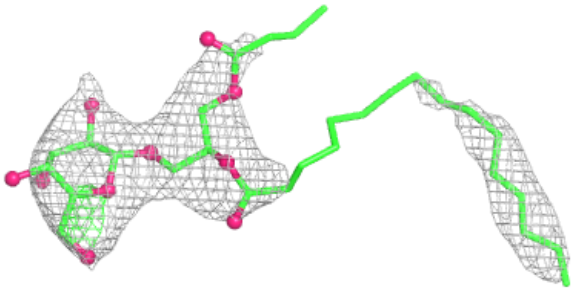


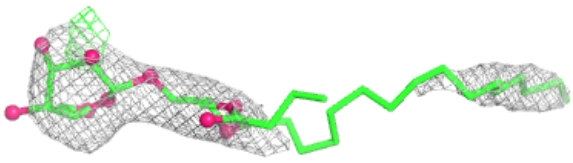


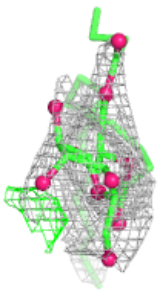


Electron density around LMG z 101:

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

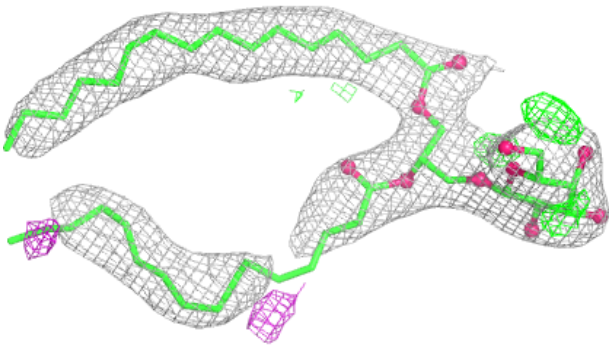


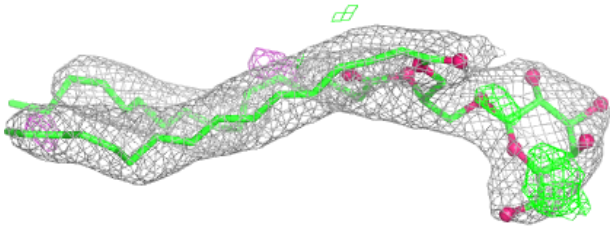


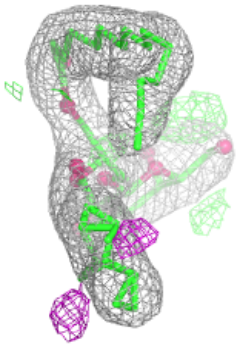


Electron density around LMG C 501:

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

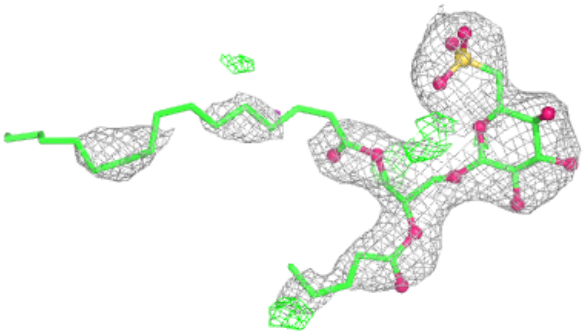


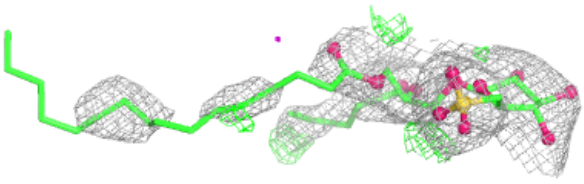


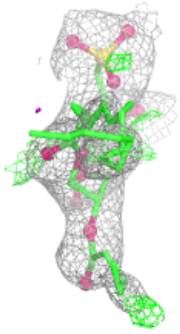


Electron density around SQD D 413:

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

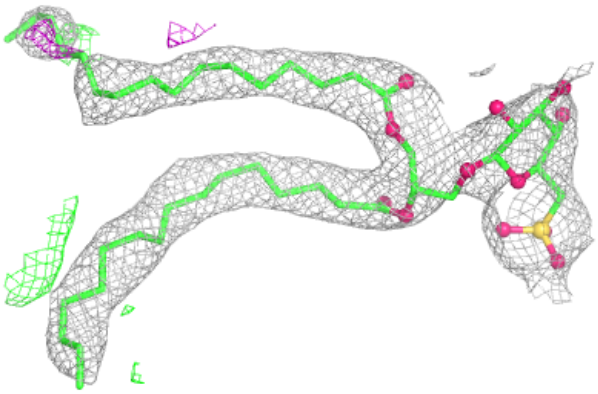


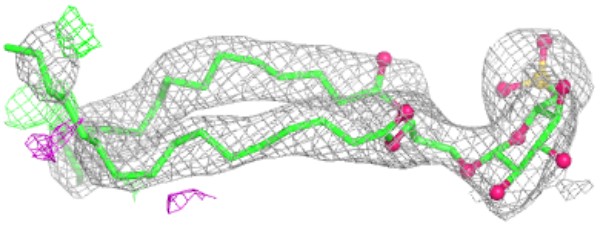


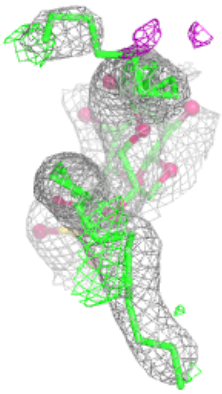


Electron density around SQD L 101:

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

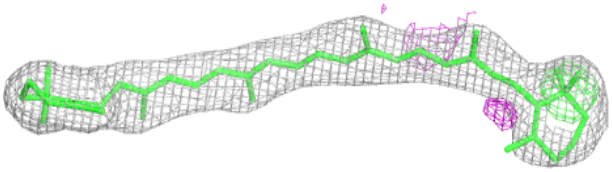


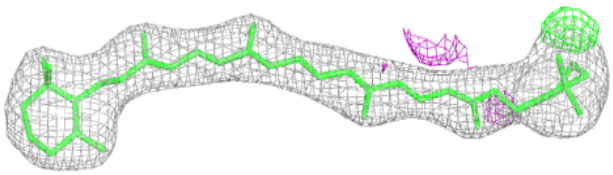


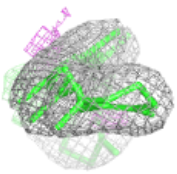


Electron density around BCR D 406:

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

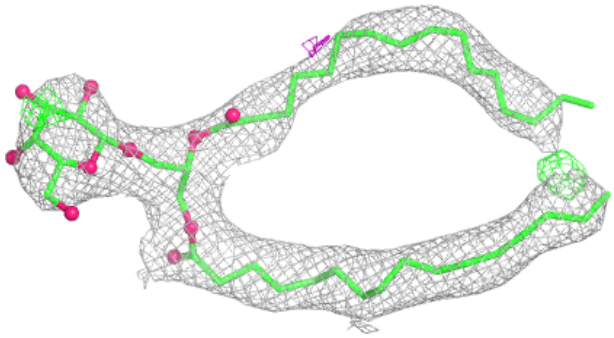


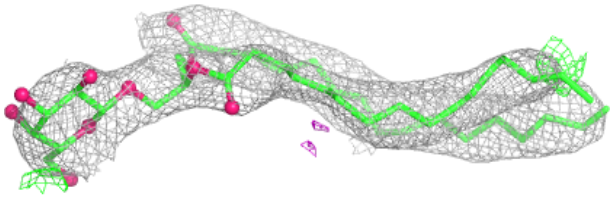


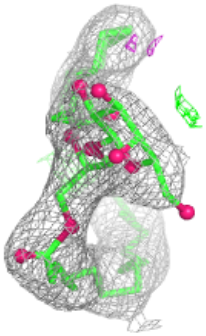


Electron density around LMG a 416:

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

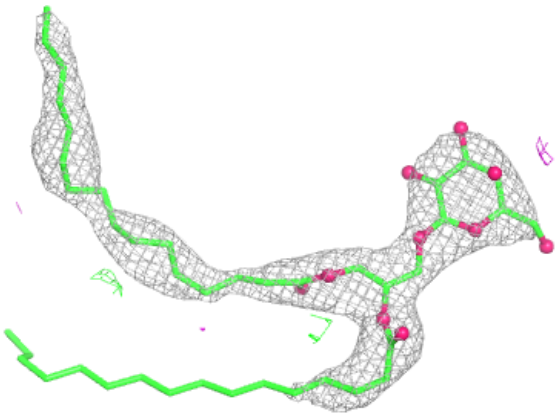


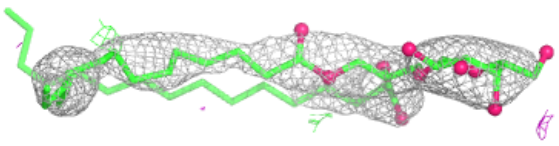


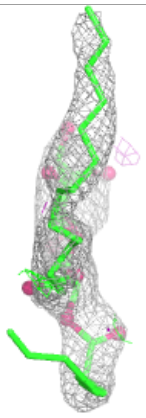


Electron density around LMG c 519:

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

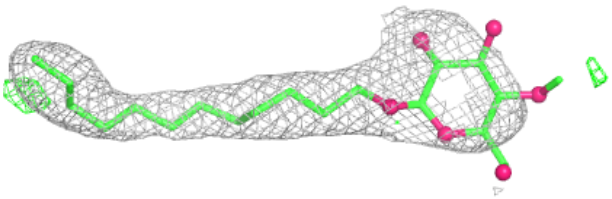


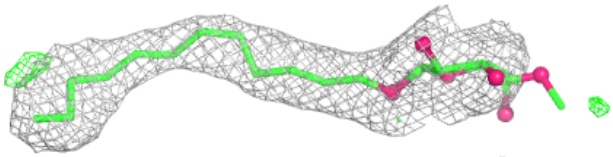


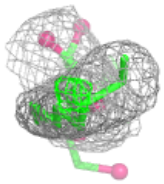


Electron density around LMT b 627:

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

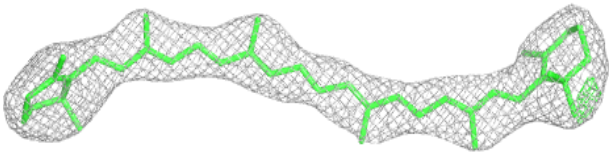


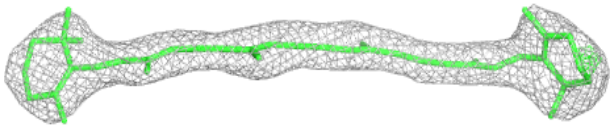


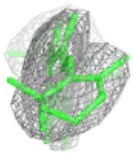


Electron density around BCR y 101:

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

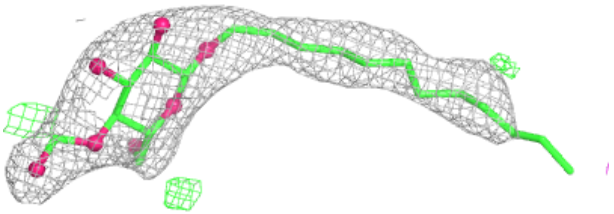


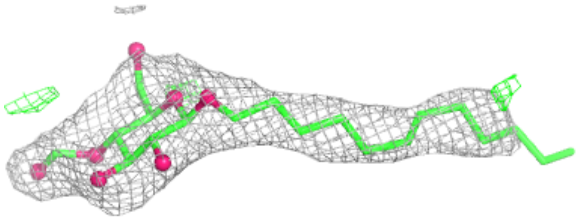


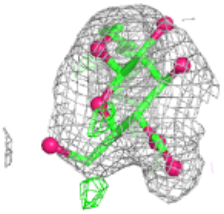


Electron density around LMT B 631:

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

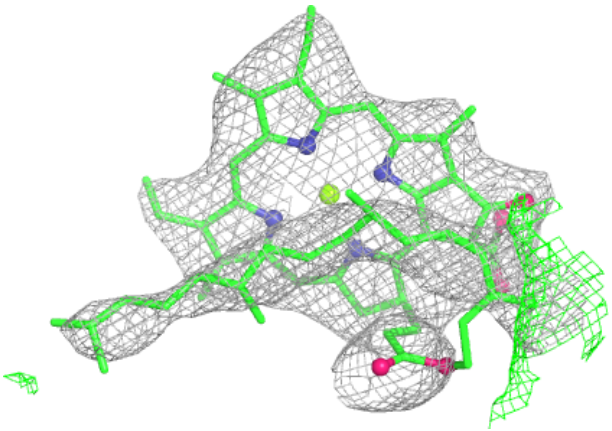


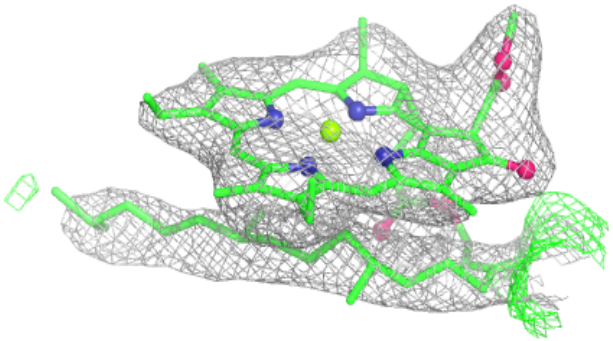


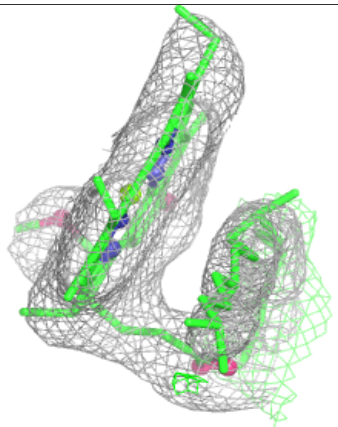


Electron density around CLA b 601:

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

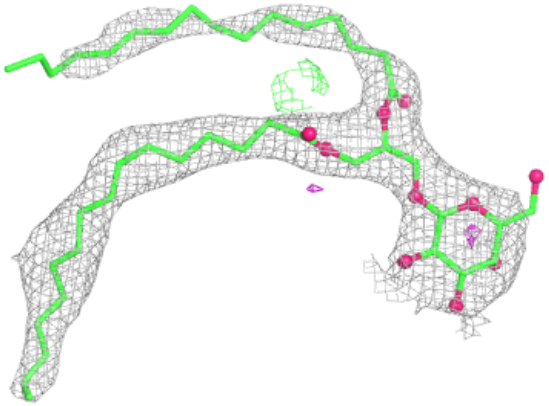


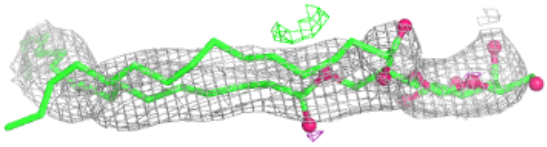




Electron density around LMG C 520:

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

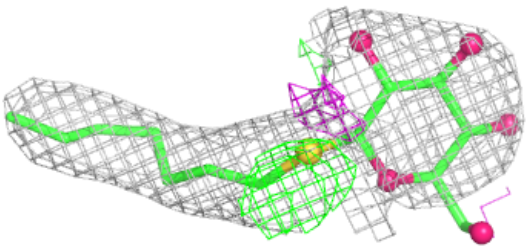


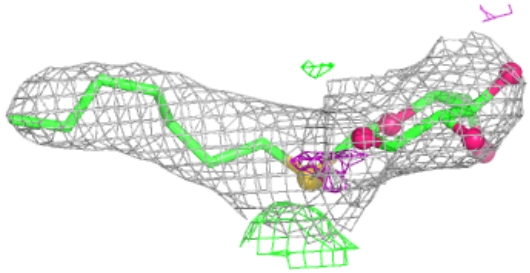


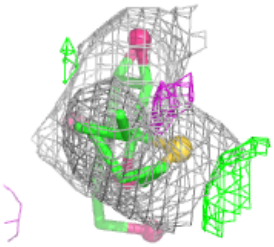


Electron density around HTG B 622:

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

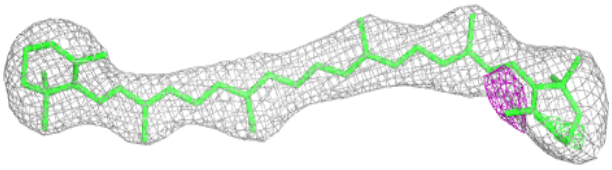


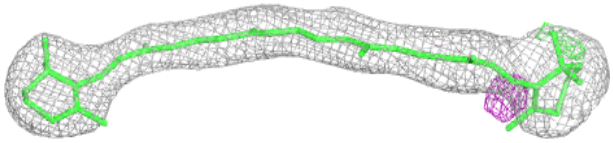


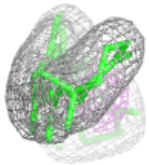


Electron density around BCR d 405:

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

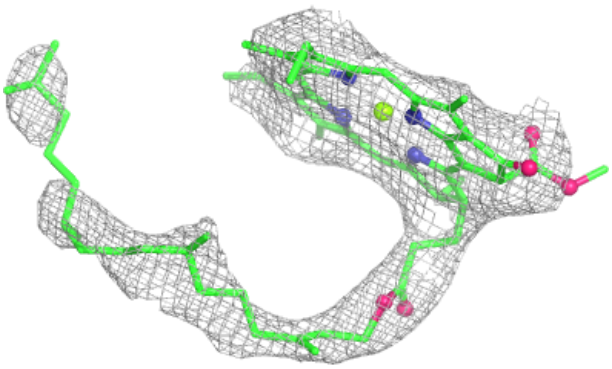


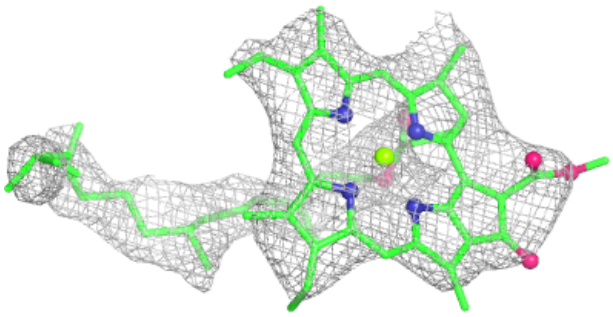




Electron density around CLA c 513:

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

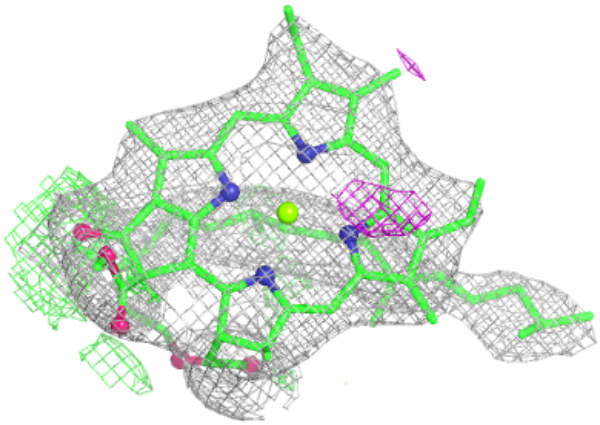


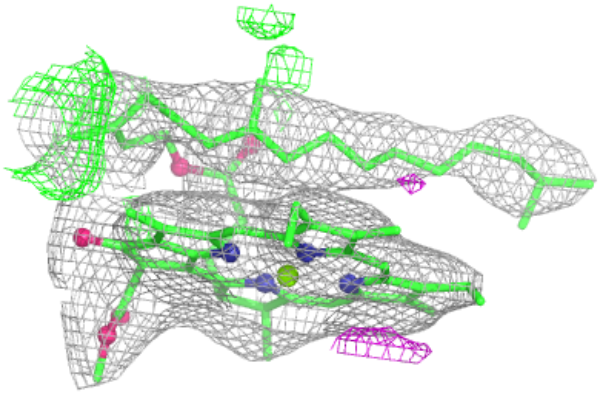


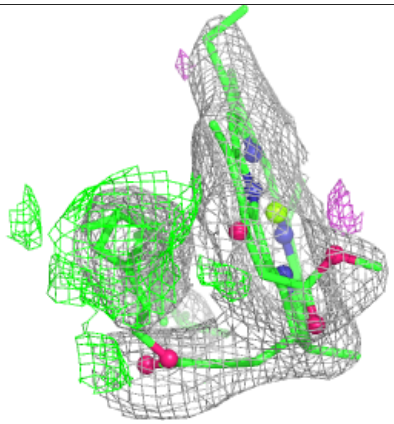


Electron density around CLA B 601:

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

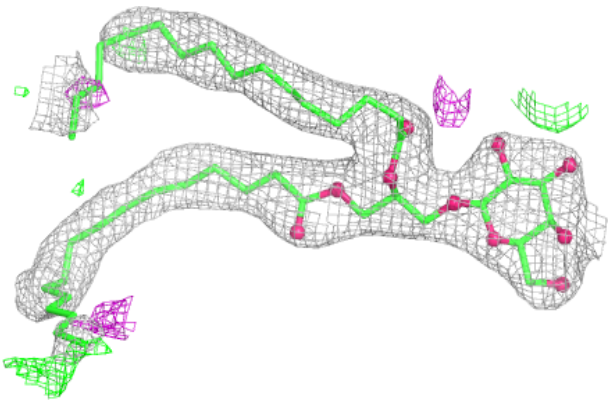


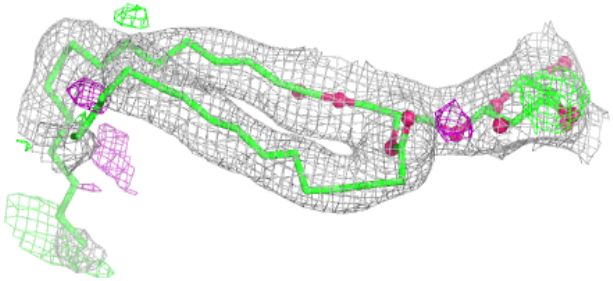




Electron density around LMG J 101:

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

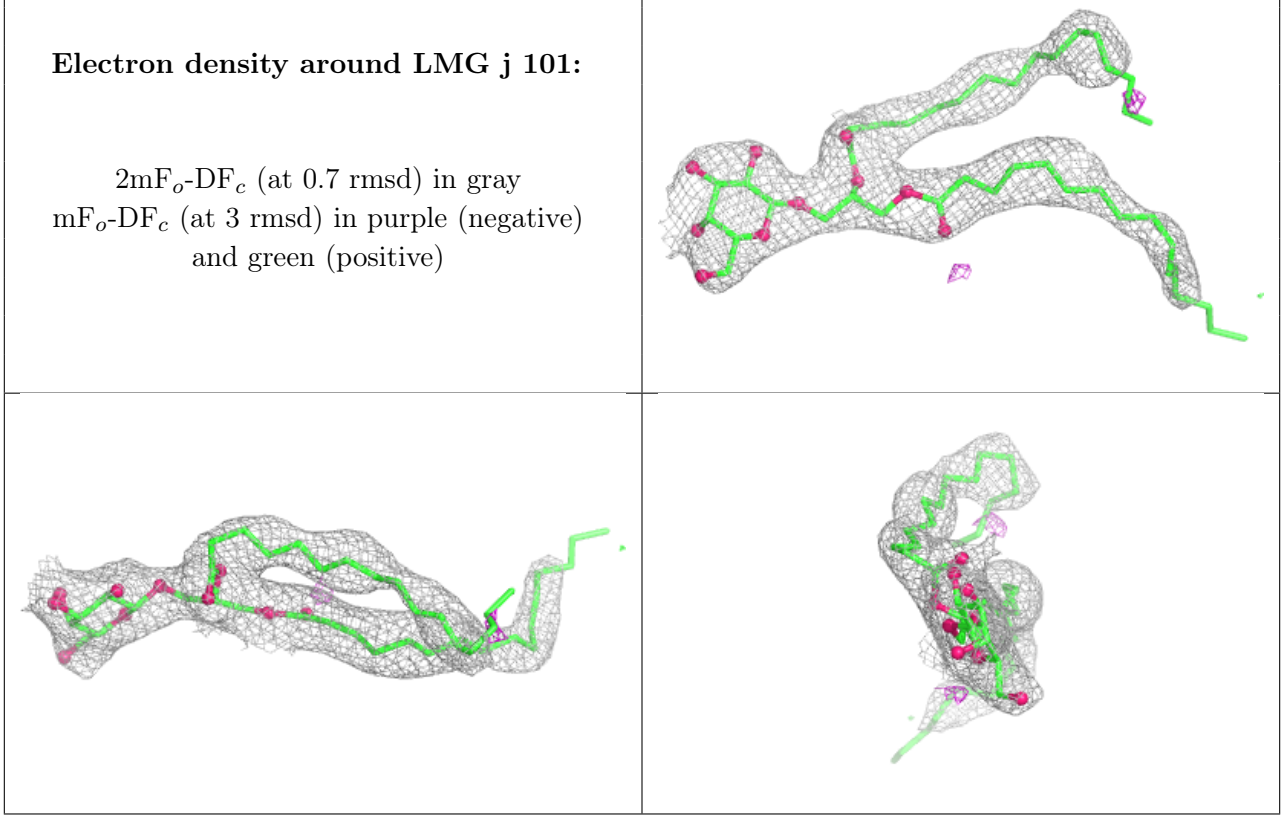






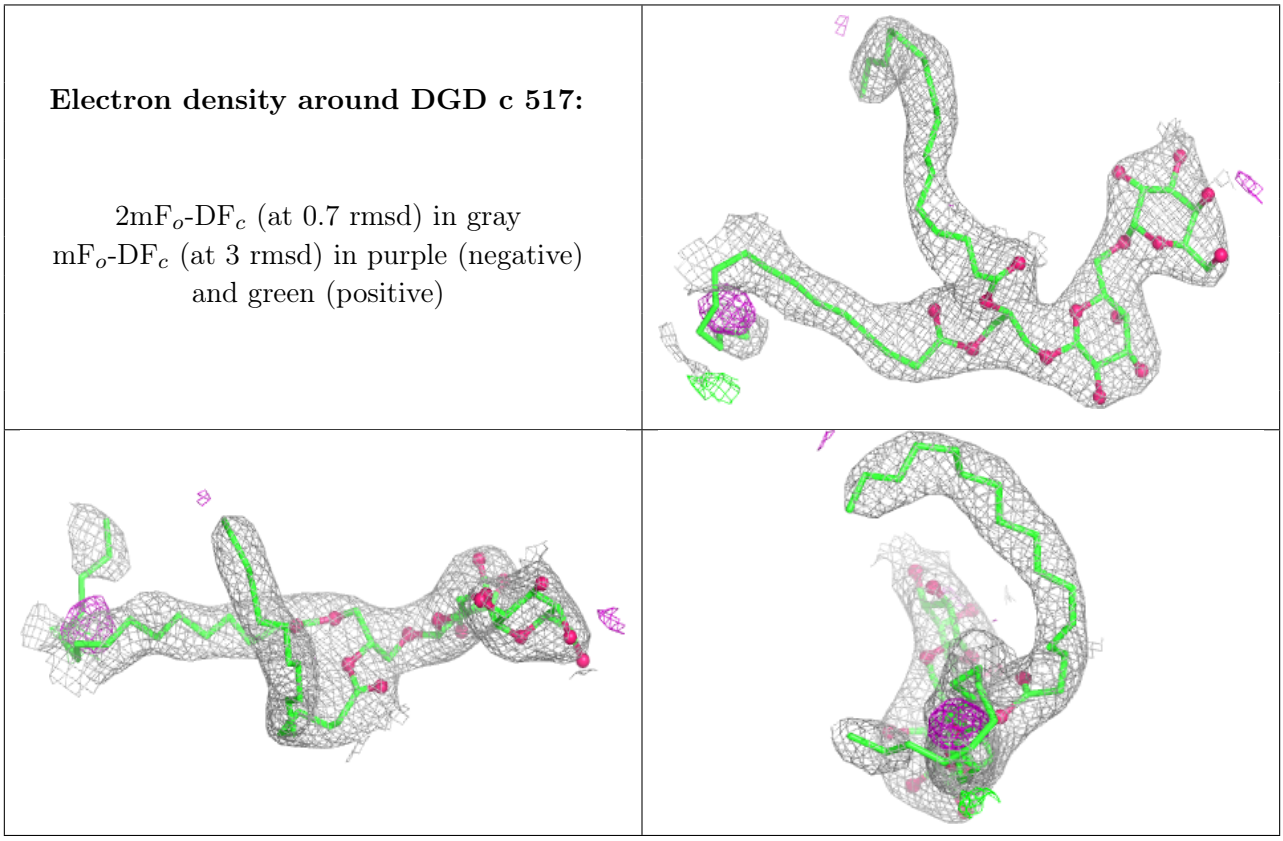
Electron density around LMG j 101:

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



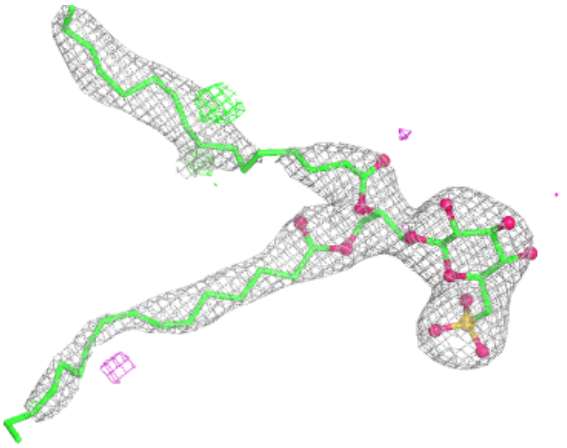
Electron density around DGD c 517:

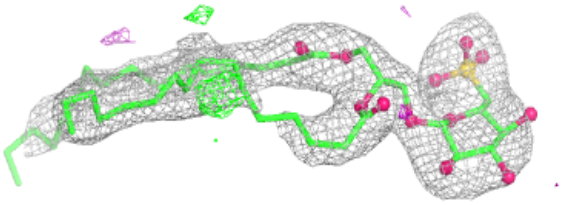
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

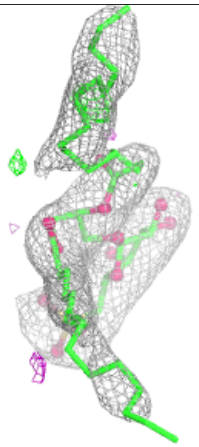


Electron density around SQD a 410:

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

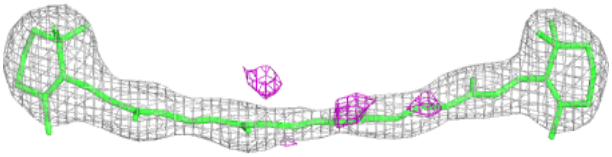


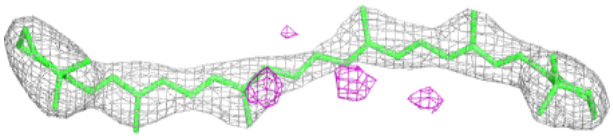


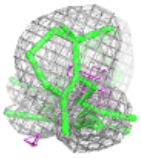


Electron density around BCR K 102:

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

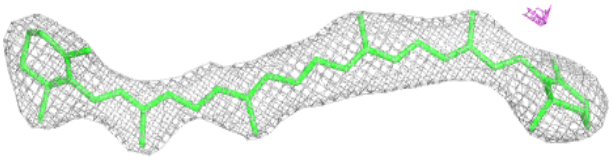


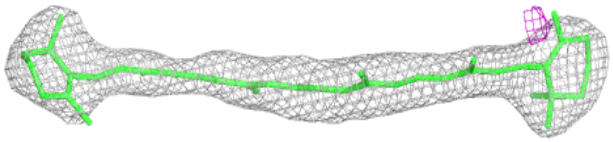


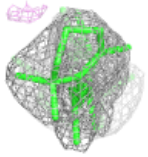


Electron density around BCR Y 101:

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

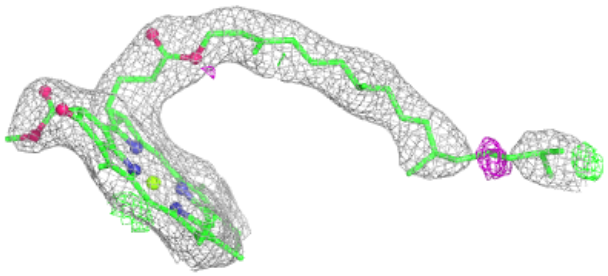


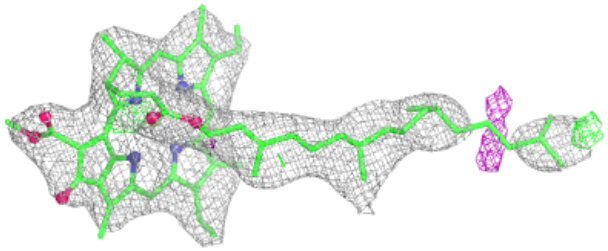


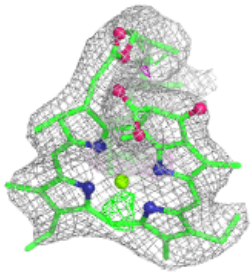


Electron density around CLA c 504:

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

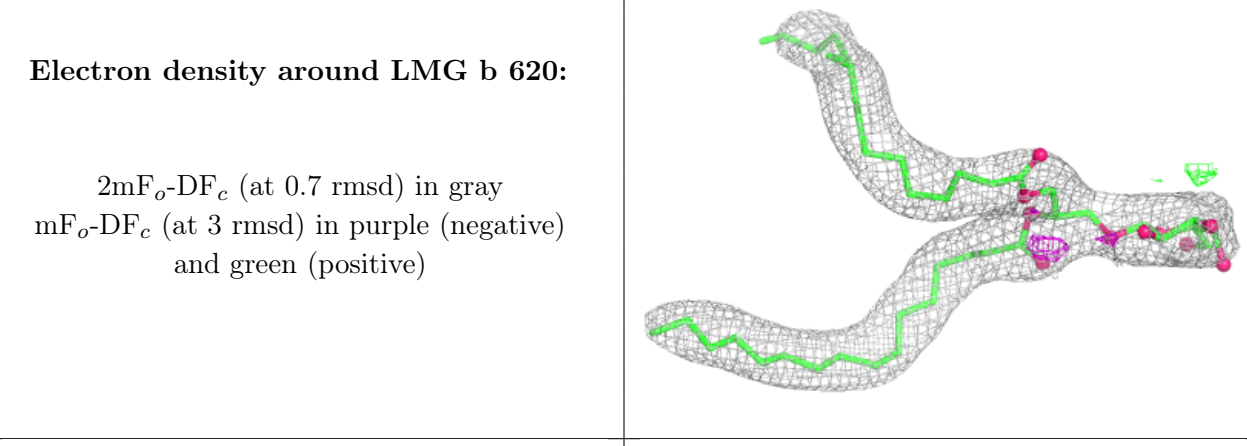






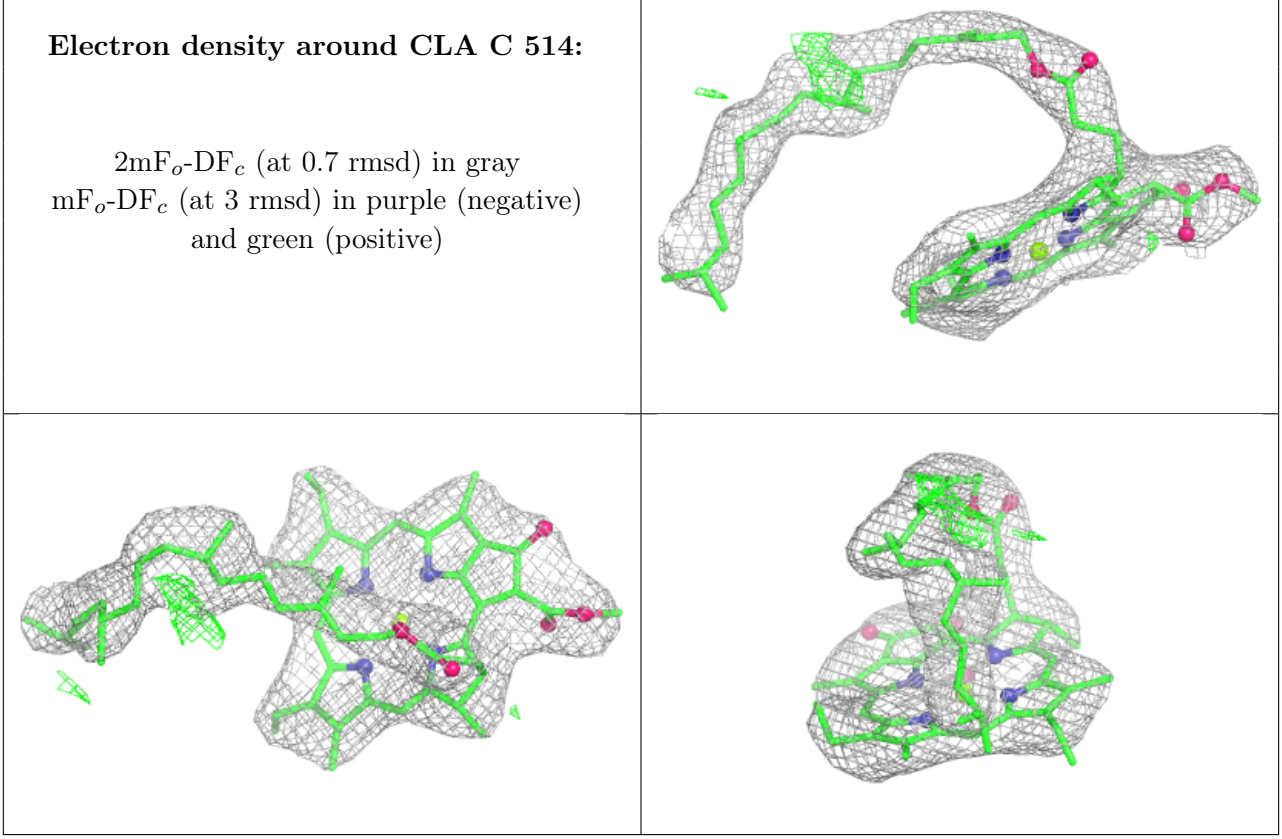
Electron density around LMG b 620:

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



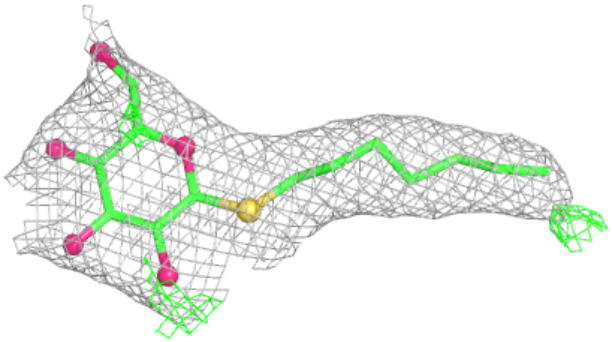
Electron density around CLA C 514:

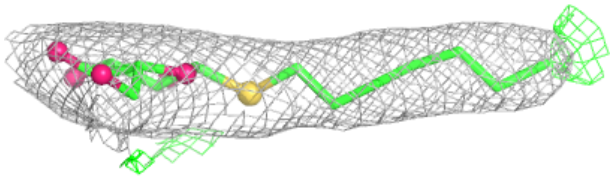
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

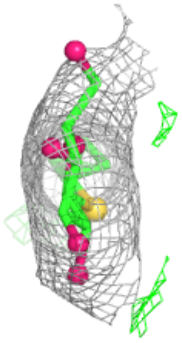


Electron density around HTG b 625:

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

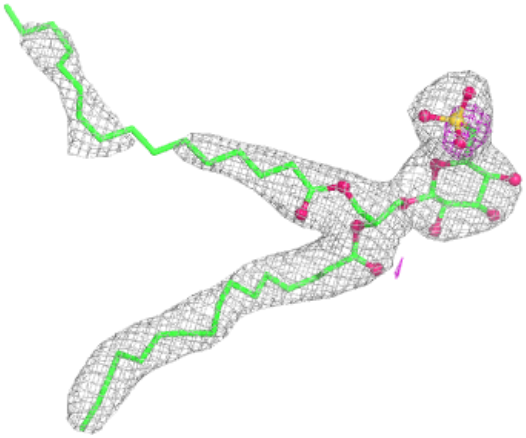


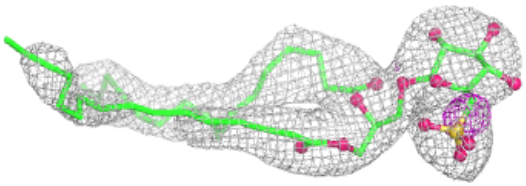


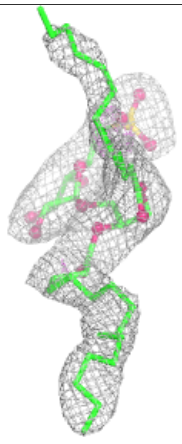


Electron density around SQD A 410:

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

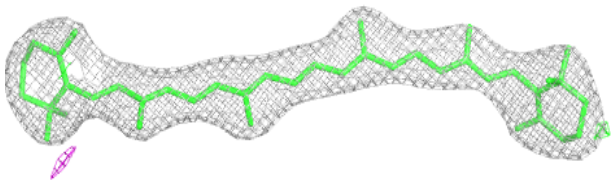


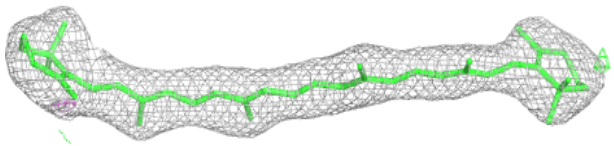


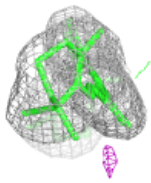


Electron density around BCR B 619:

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

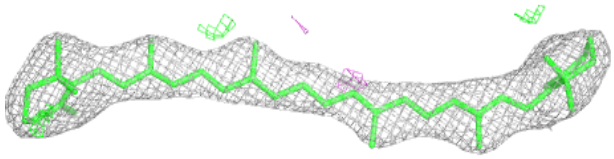


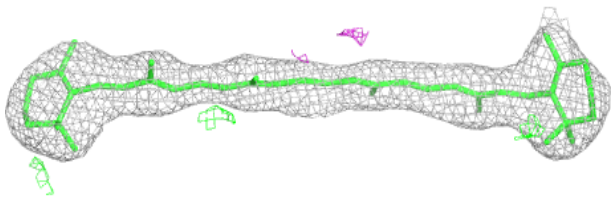


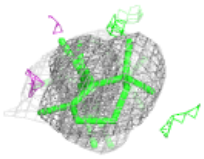


Electron density around BCR C 515:

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

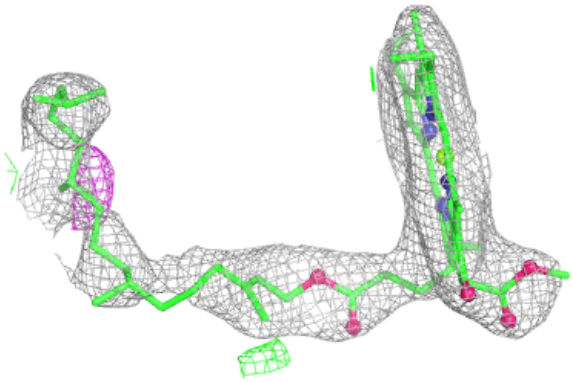


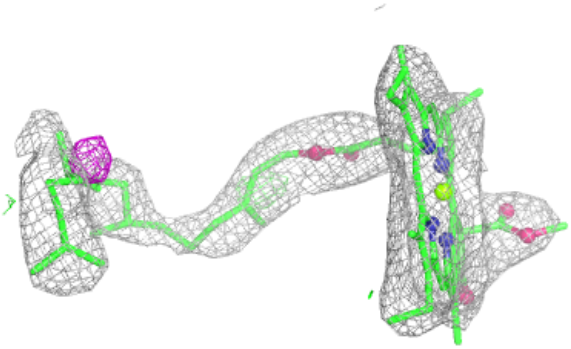


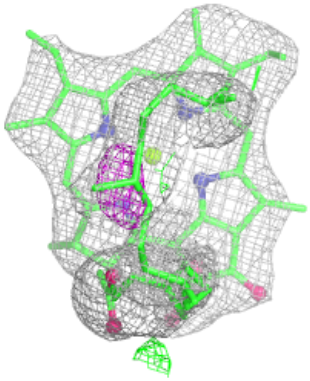


Electron density around CLA C 507:

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

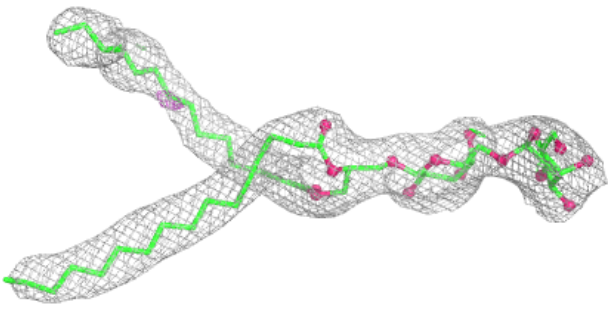


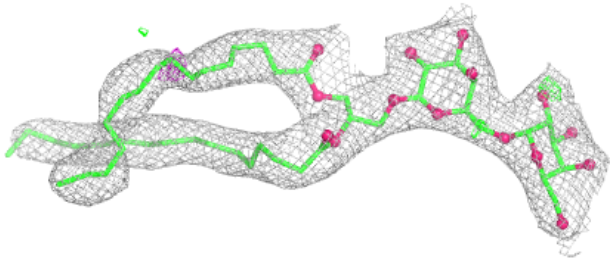


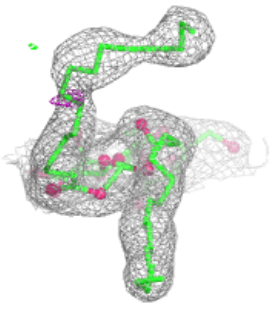


Electron density around DGD c 516:

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

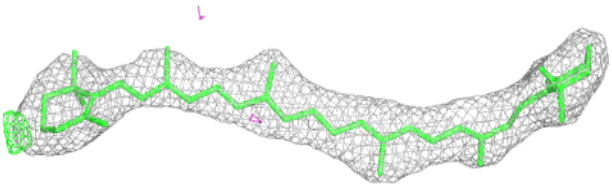


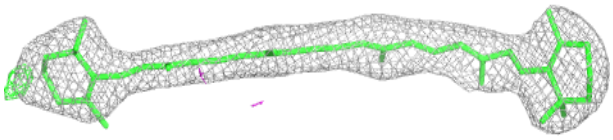


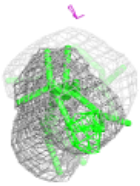


Electron density around BCR H 101:

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

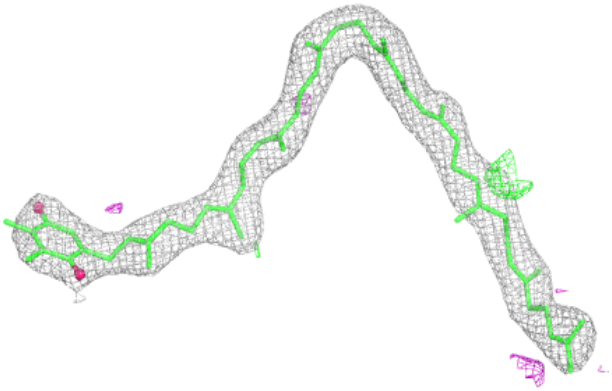


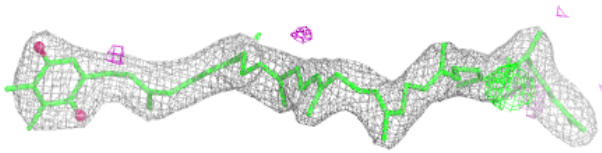




Electron density around PL9 d 406:

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

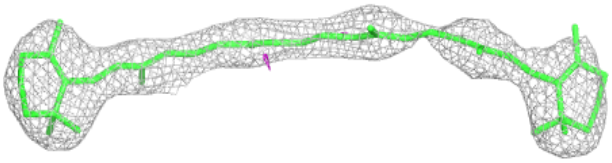


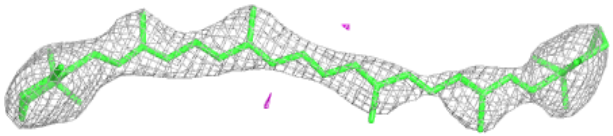


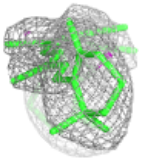


Electron density around BCR k 101:

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

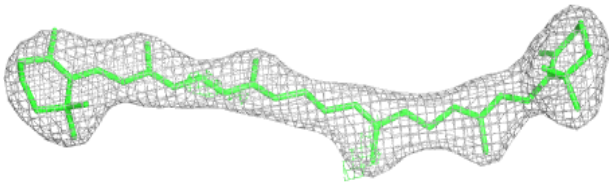


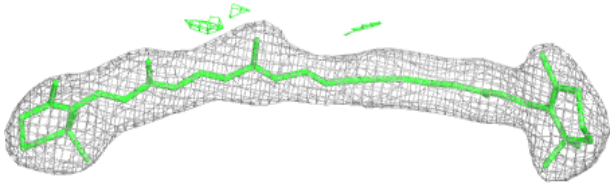


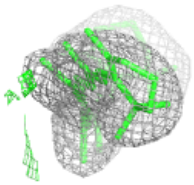


Electron density around BCR t 101:

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

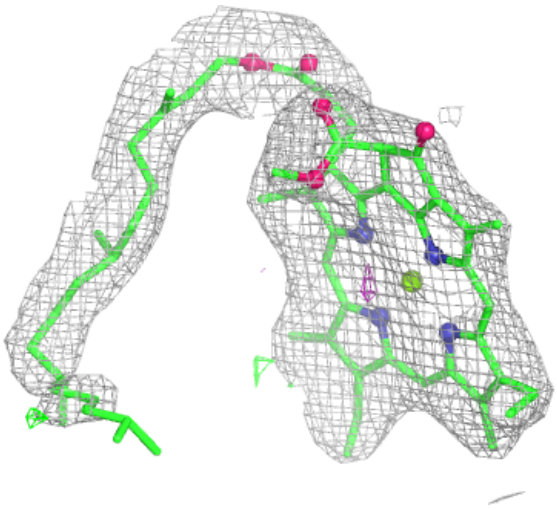


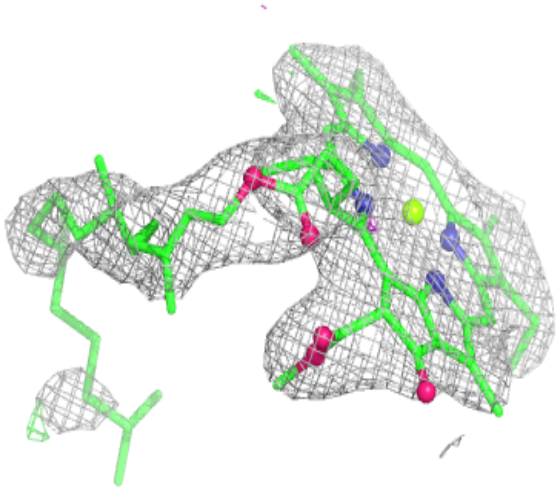


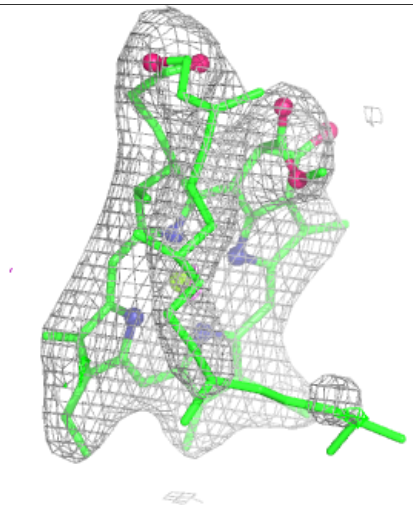


Electron density around CLA b 616:

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

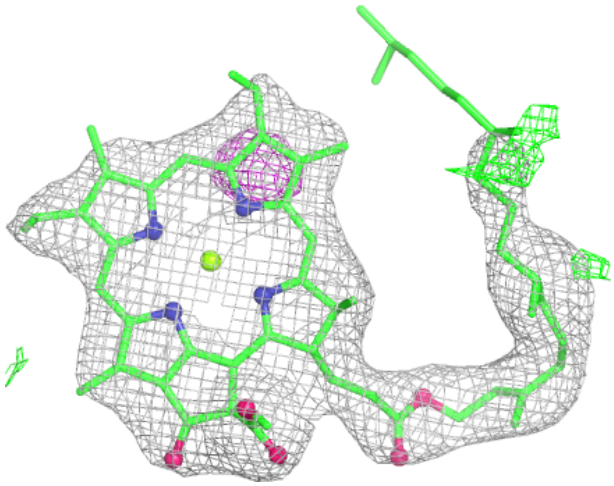


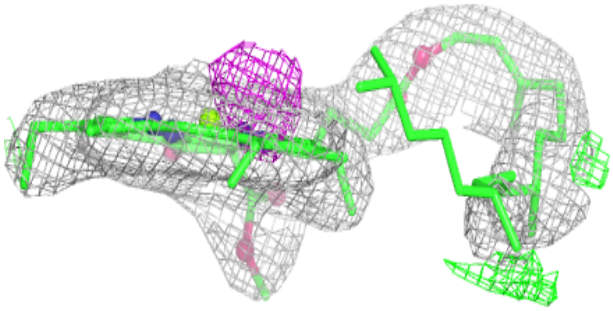


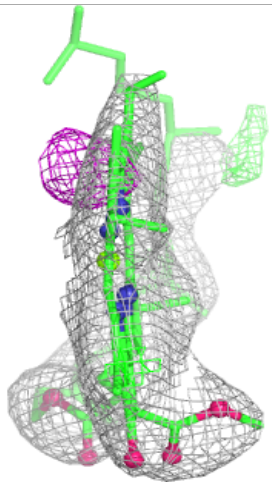


Electron density around CLA C 513:

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

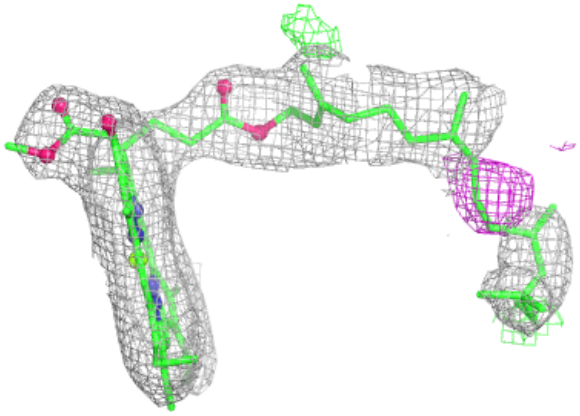


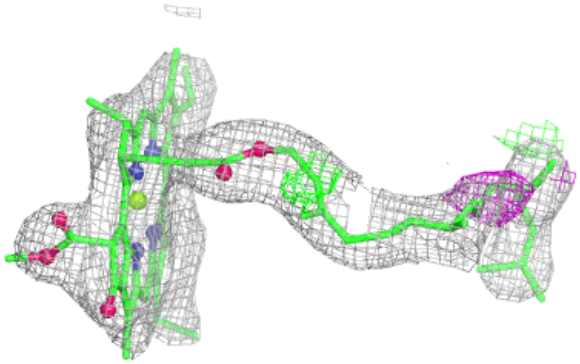


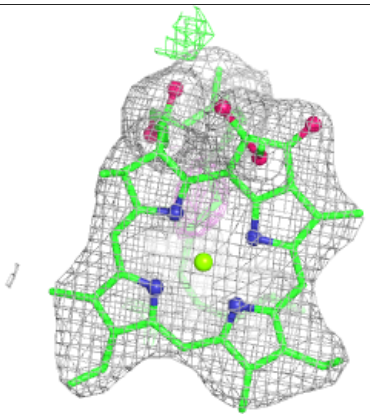


Electron density around CLA c 506:

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

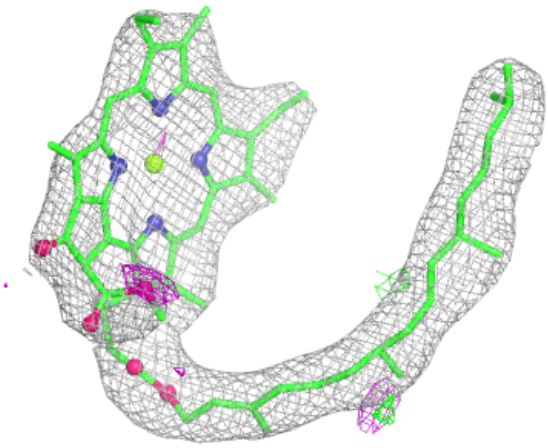


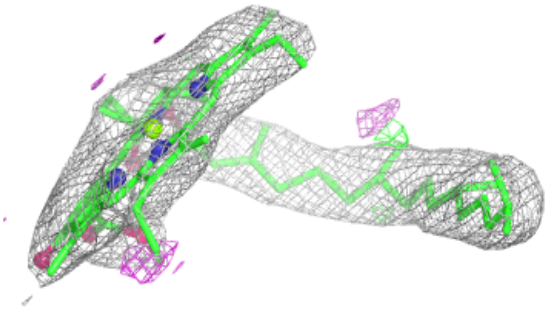


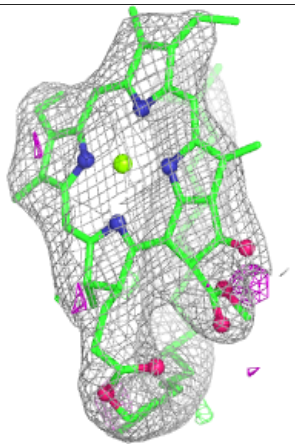


Electron density around CLA c 507:

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

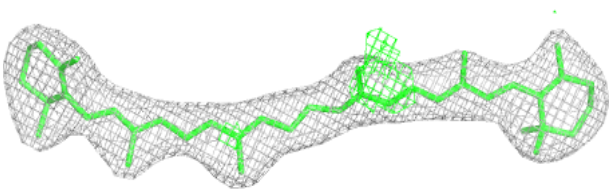


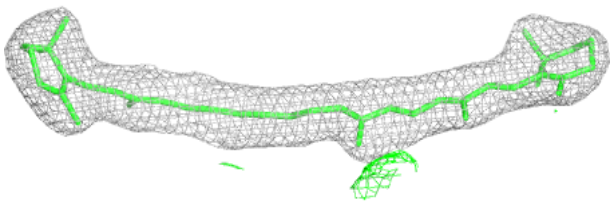


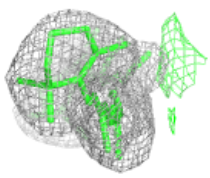


Electron density around BCR T 101:

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

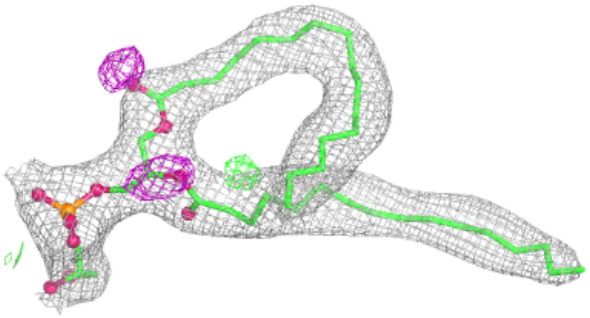


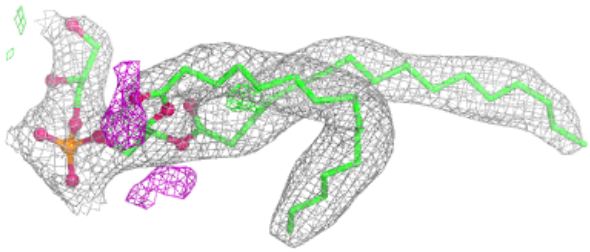


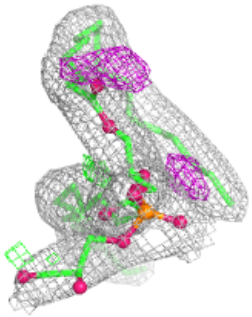


Electron density around LHG A 416:

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

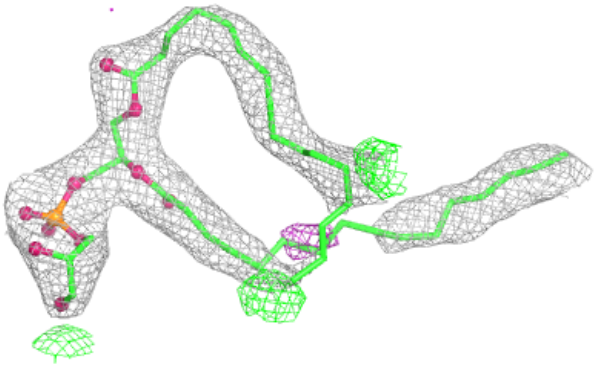


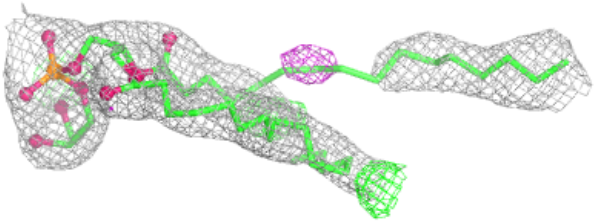


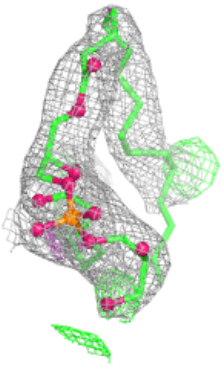


Electron density around LHG D 409:

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

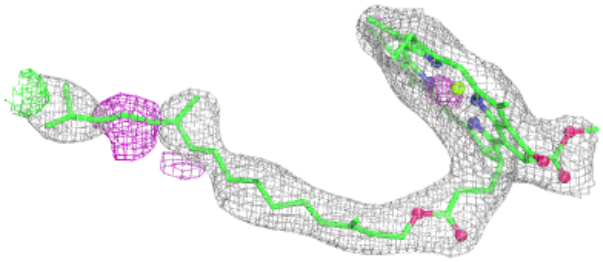


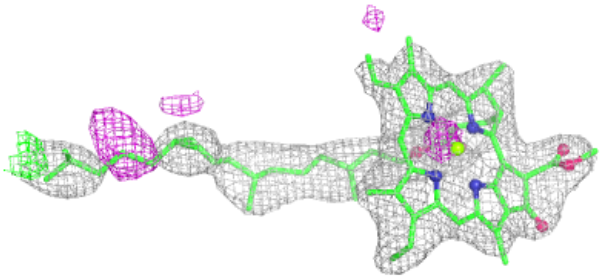


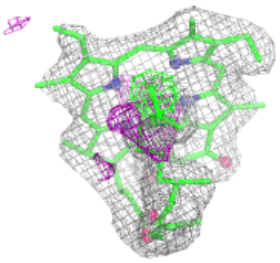


Electron density around CLA C 505:

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

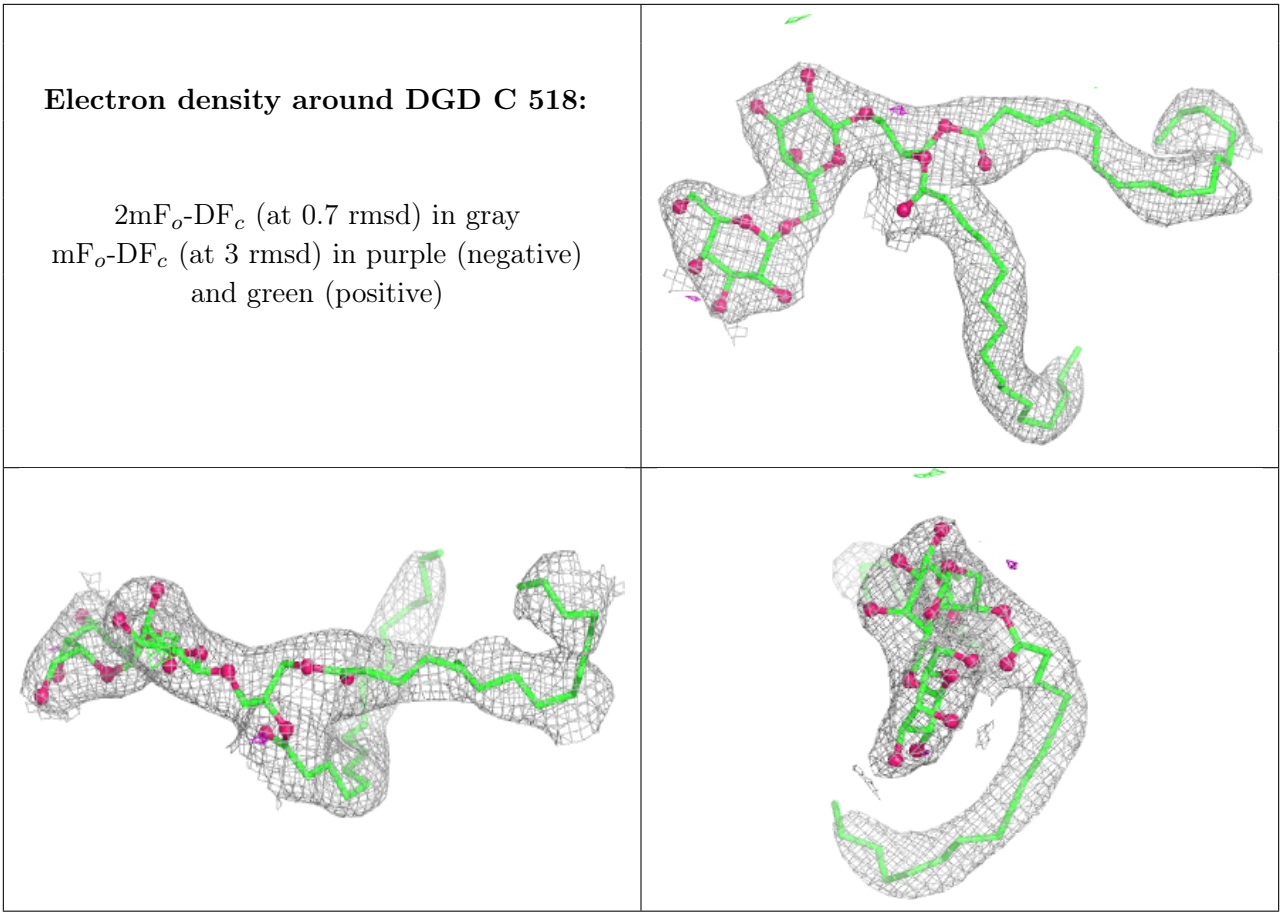






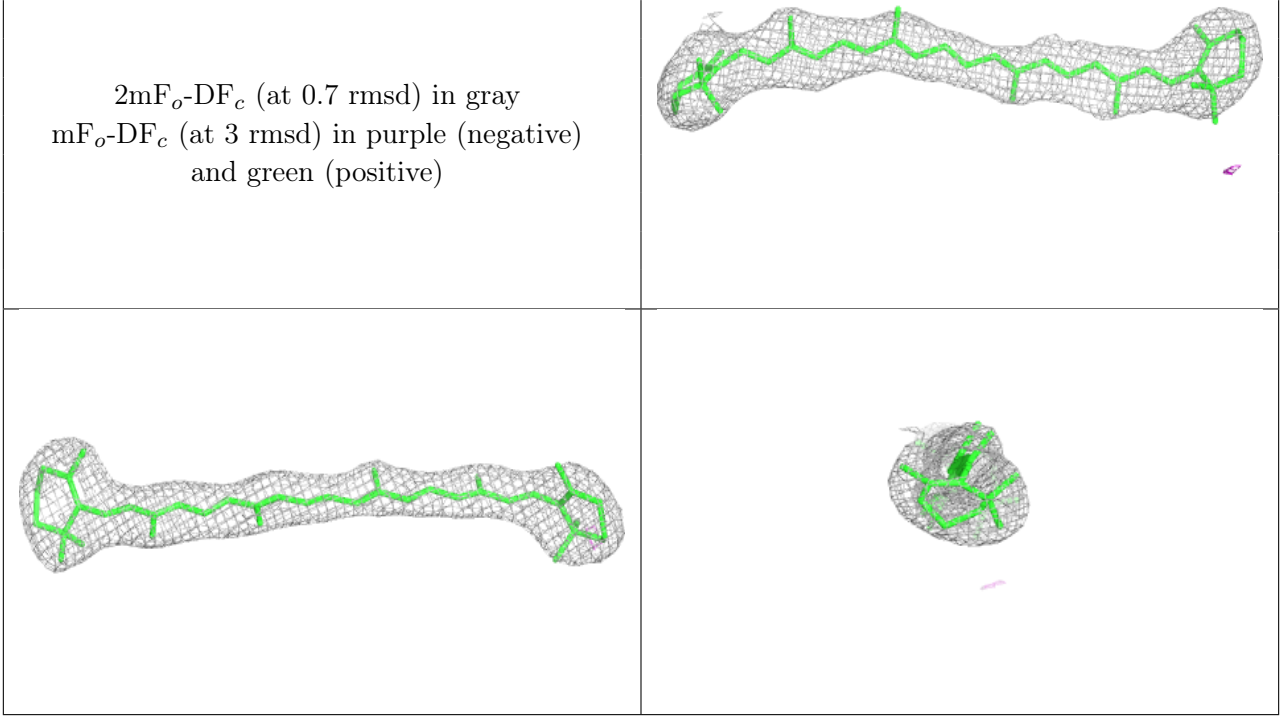
Electron density around DGD C 518:

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



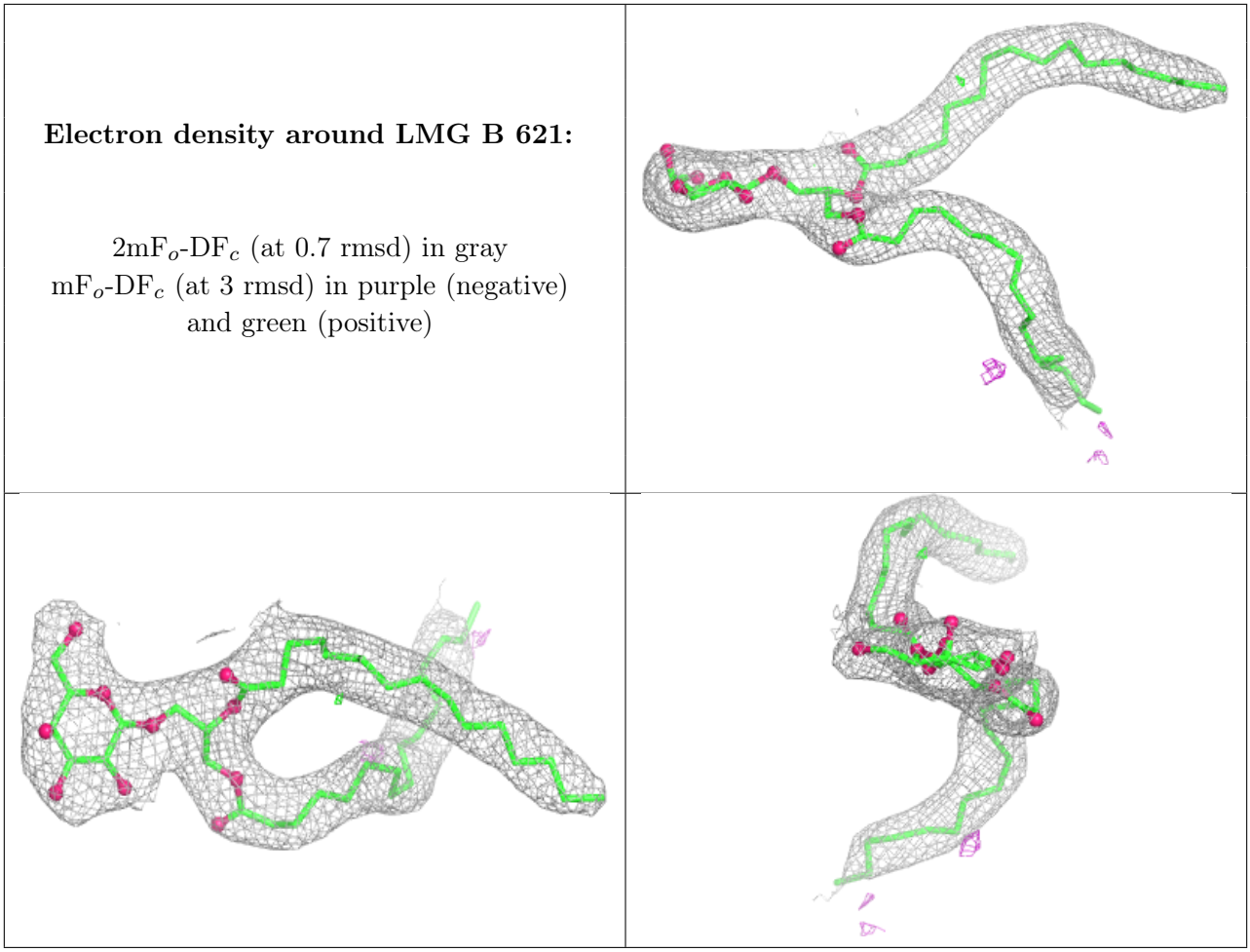
Electron density around BCR c 514:

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



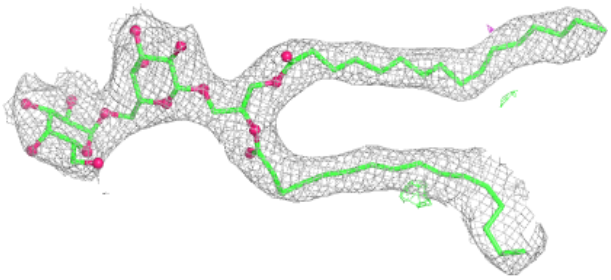
Electron density around LMG B 621:

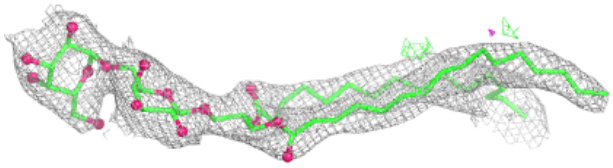
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

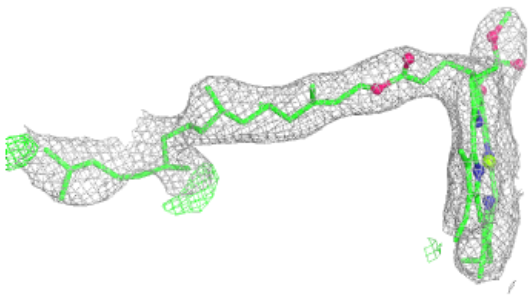


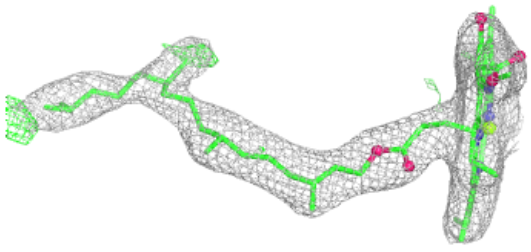


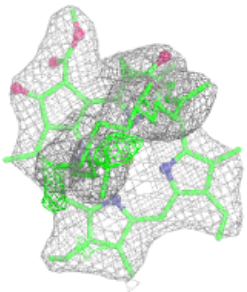


Electron density around CLA B 606:

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

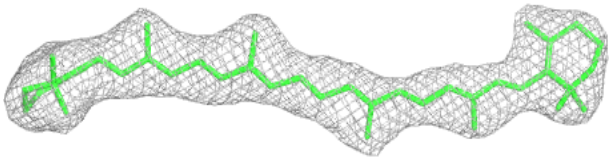


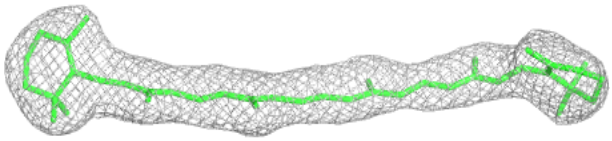


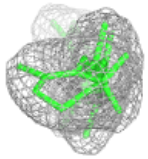


Electron density around BCR b 617:

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

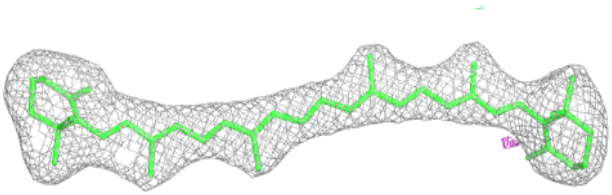


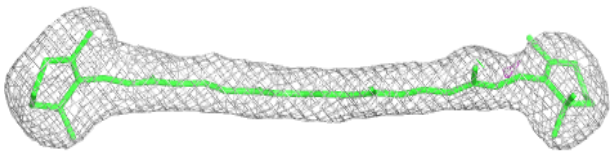


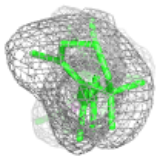


Electron density around BCR b 618:

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

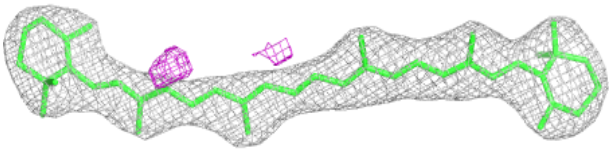




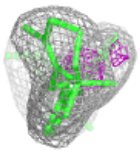


Electron density around BCR b 619:

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

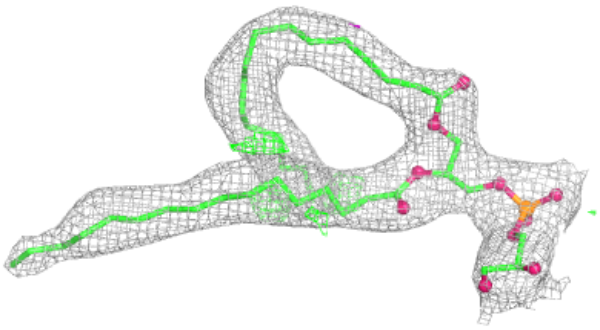


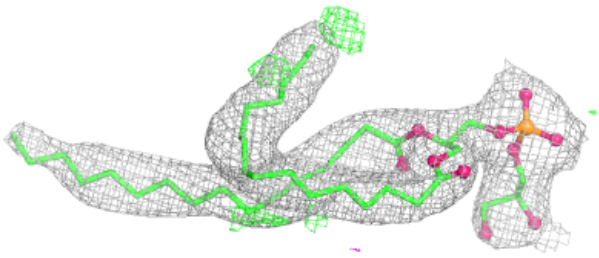


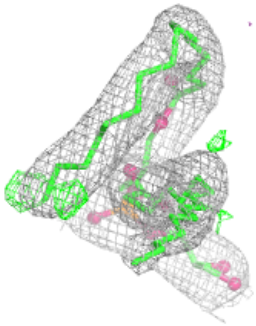


Electron density around LHG d 407:

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

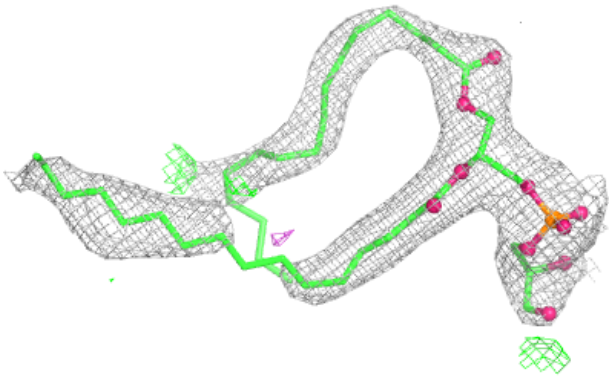


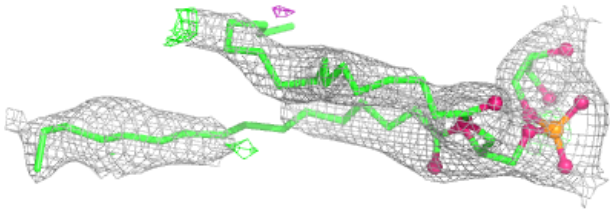


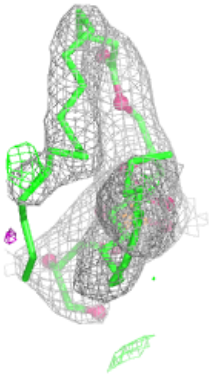


Electron density around LHG d 409:

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

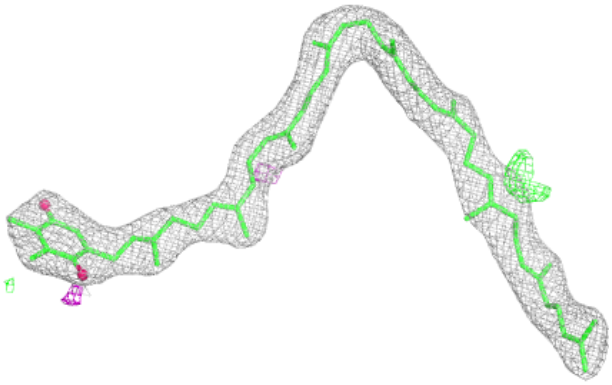


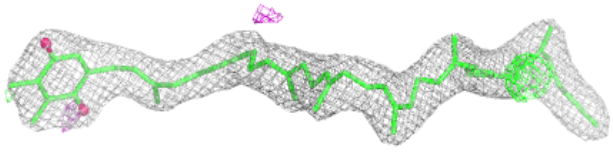


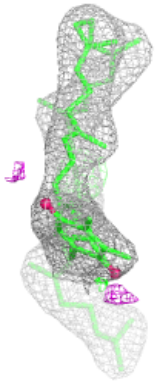


Electron density around PL9 D 407:

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

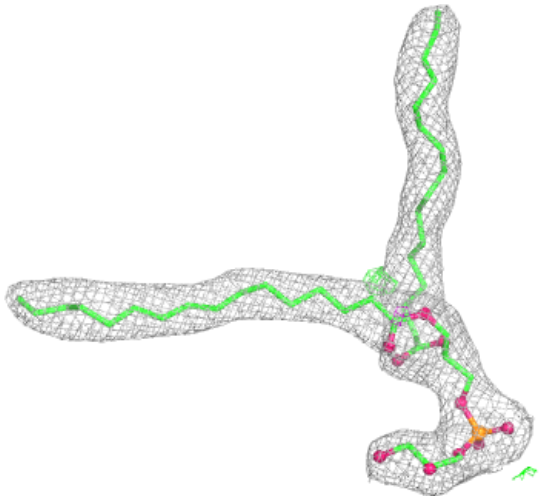


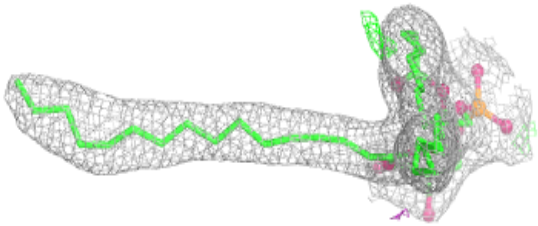


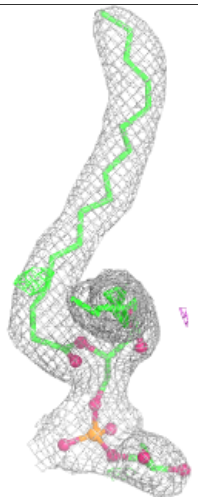


Electron density around LHG l 101:

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

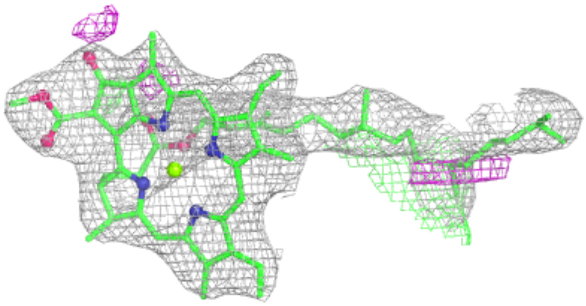


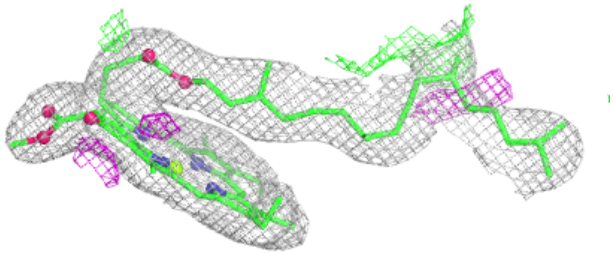


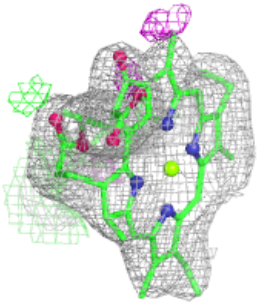


Electron density around CLA B 614:

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

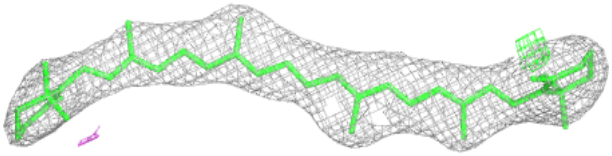


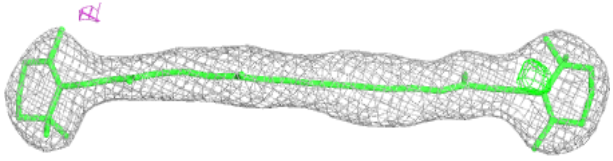


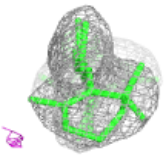


Electron density around BCR c 515:

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

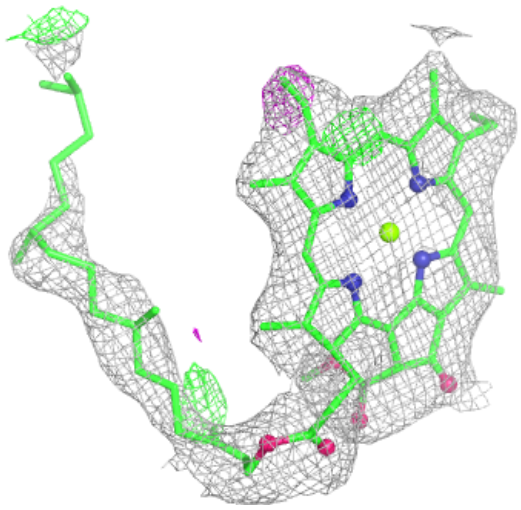


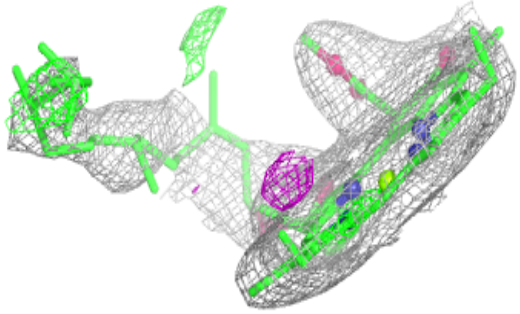


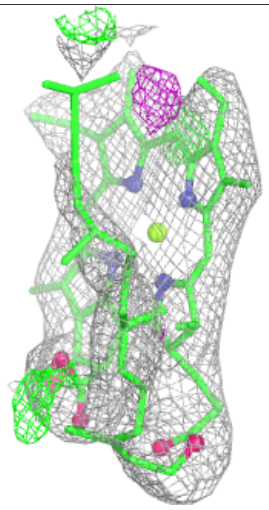


Electron density around CLA B 616:

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

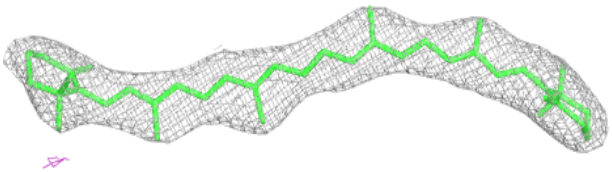


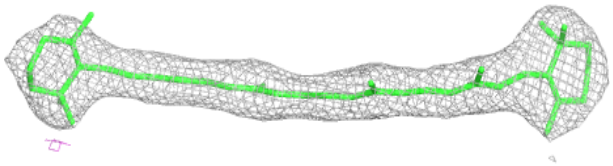


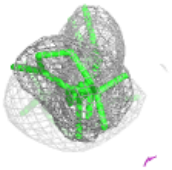


Electron density around BCR h 101:

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

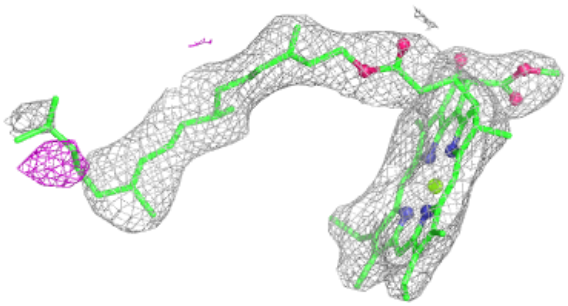


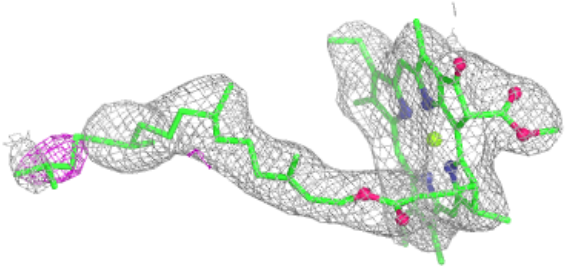


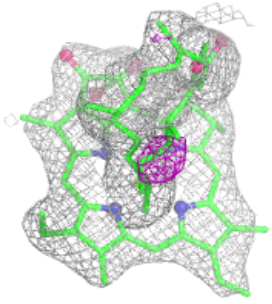


Electron density around CLA c 508:

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

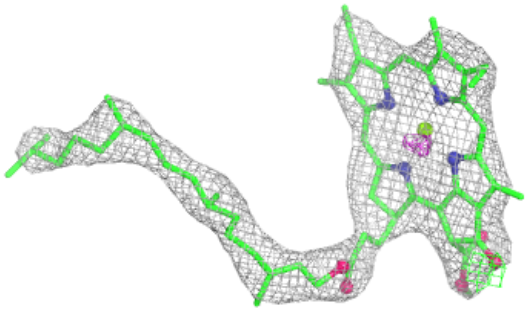


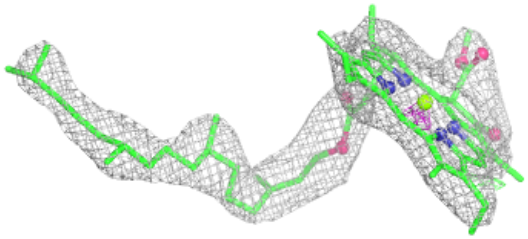


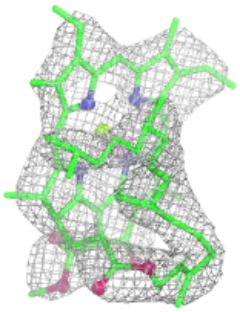


Electron density around CLA c 511:

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

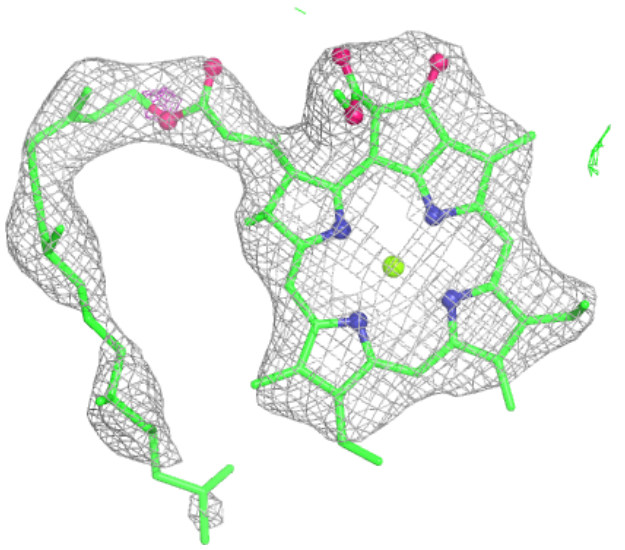


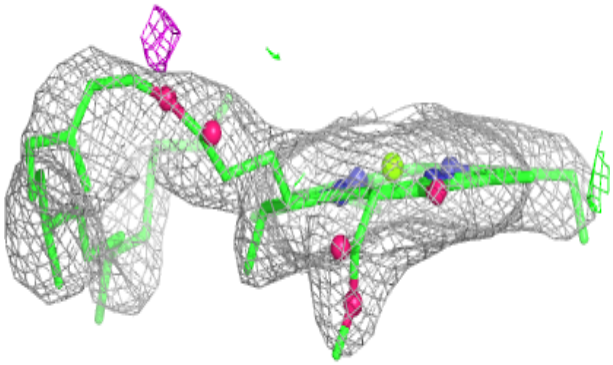


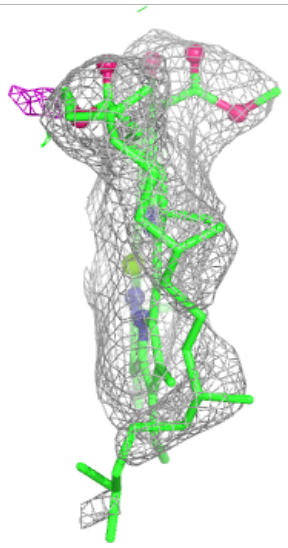


Electron density around CLA c 512:

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

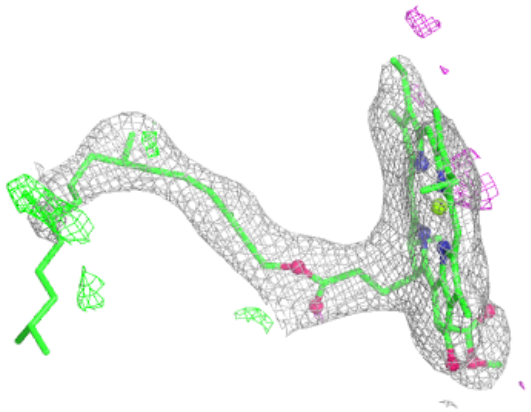


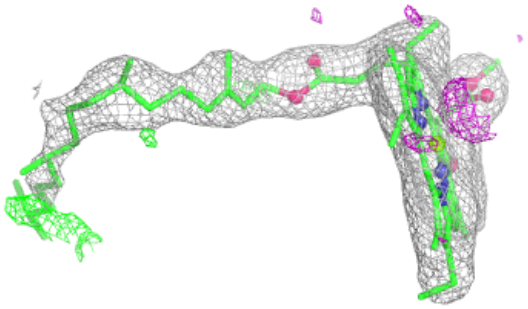


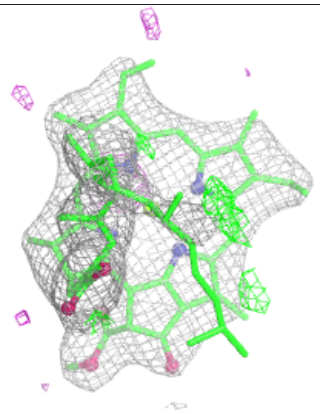


Electron density around CLA D 405:

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

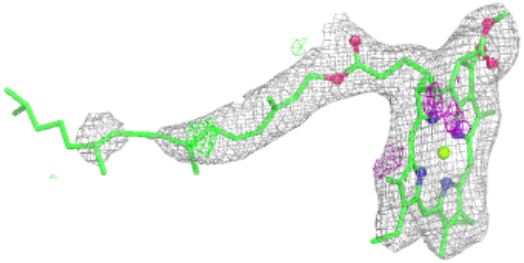


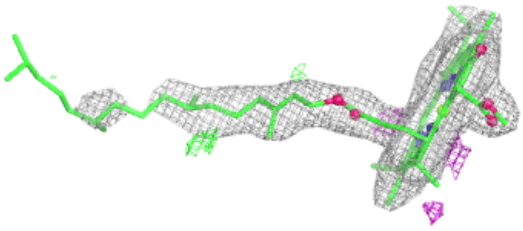


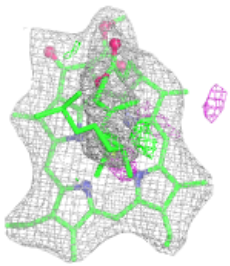


Electron density around CLA d 404:

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

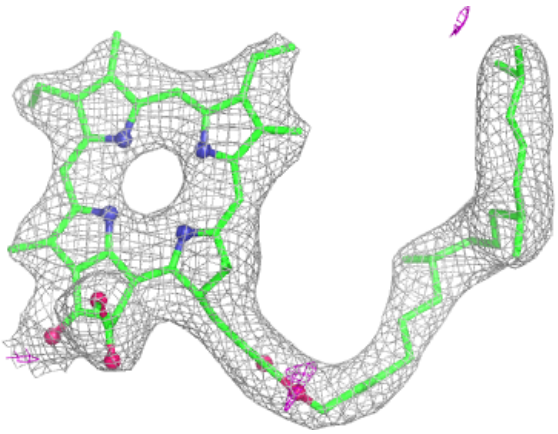


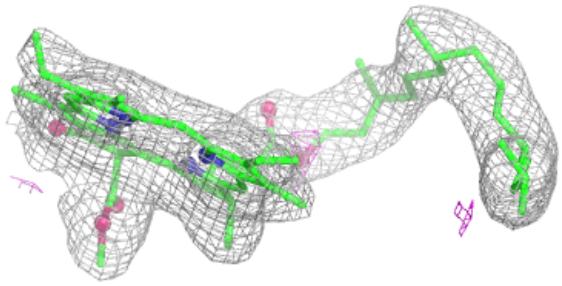


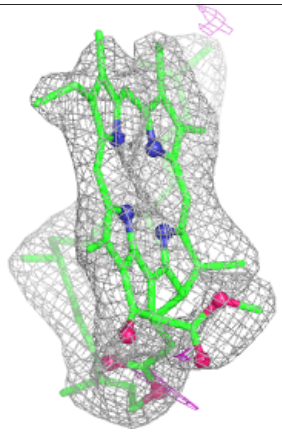


Electron density around PHO a 407:

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

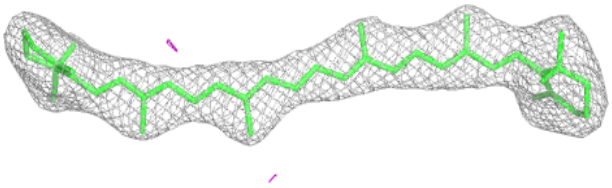


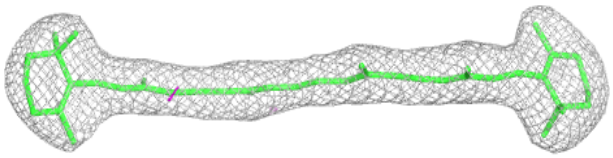


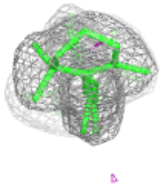


Electron density around BCR A 409:

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

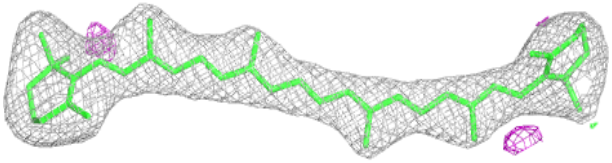


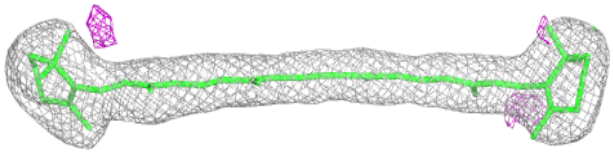


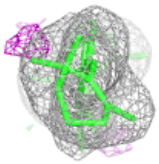


Electron density around BCR B 618:

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

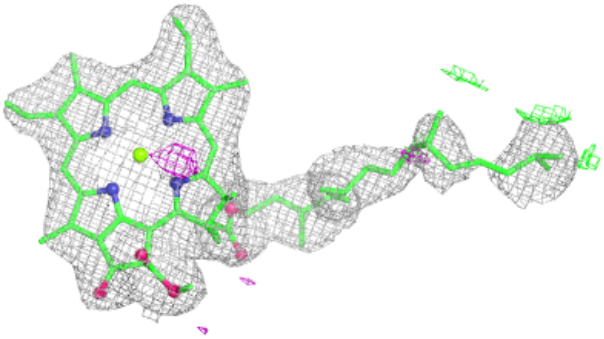


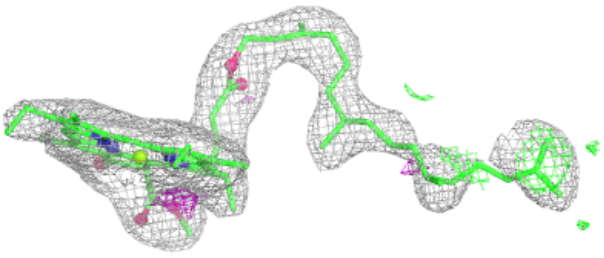


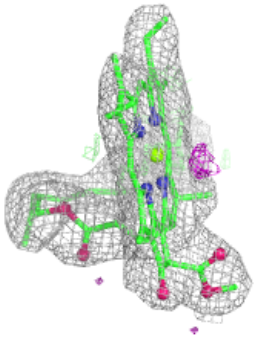


Electron density around CLA a 405:

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

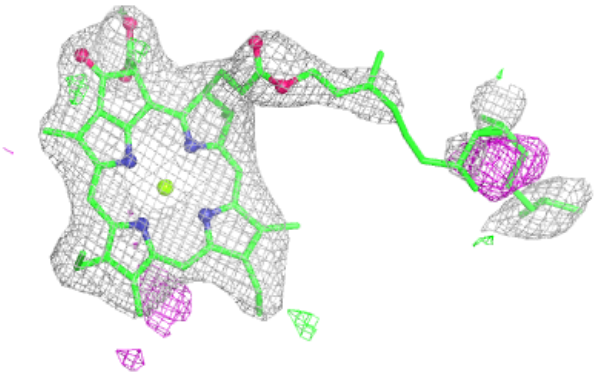


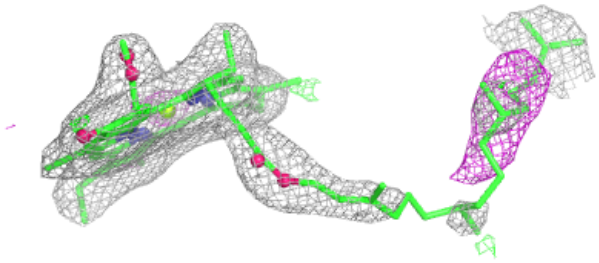




Electron density around CLA a 408:

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

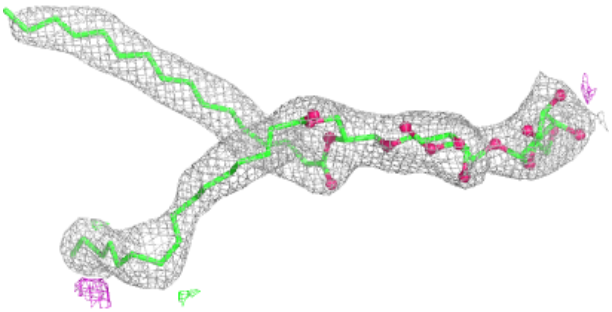


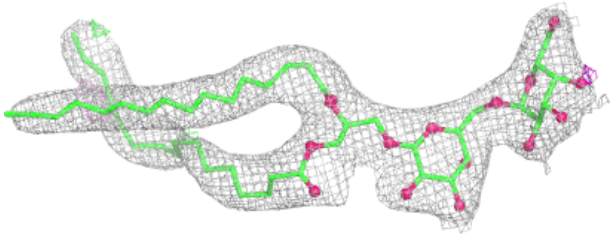


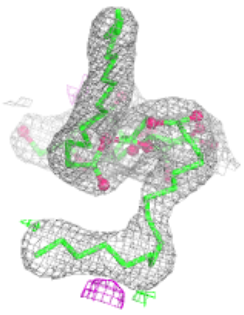


Electron density around DGD C 517:

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

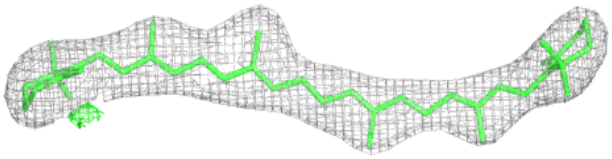


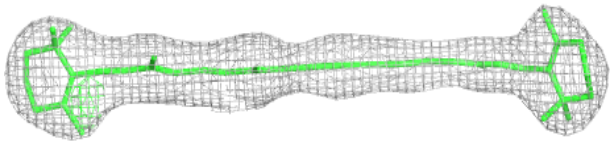


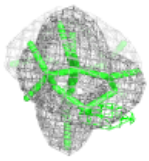


Electron density around BCR C 516:

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

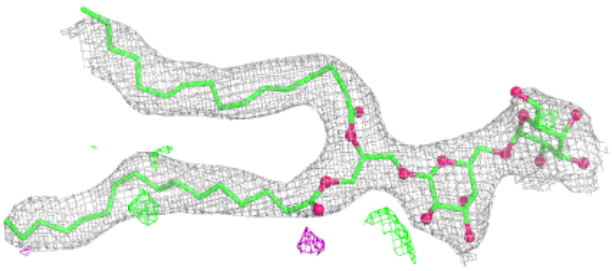


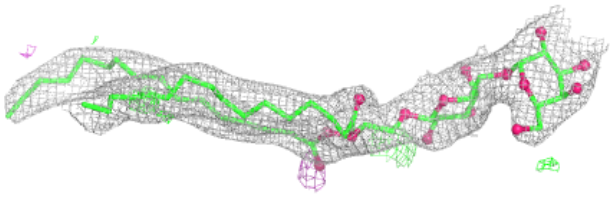


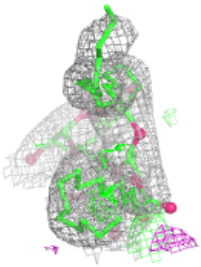


Electron density around DGD C 519:

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

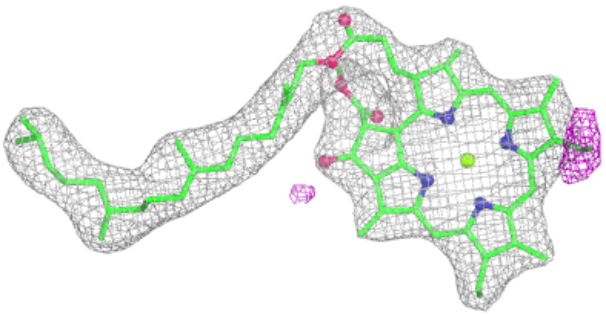


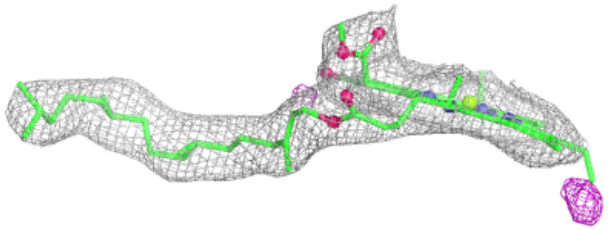


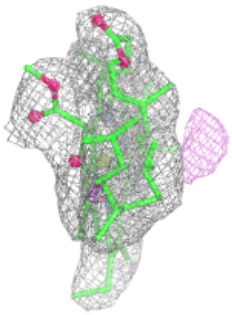


Electron density around CLA B 602:

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

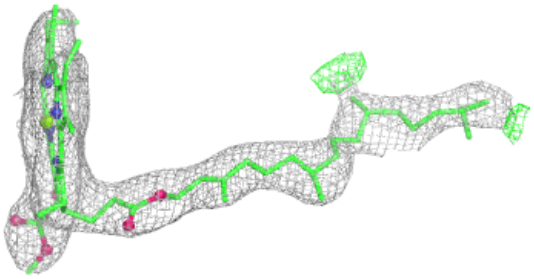


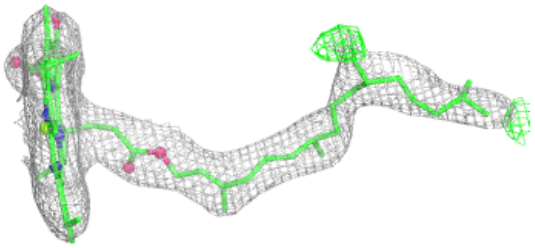


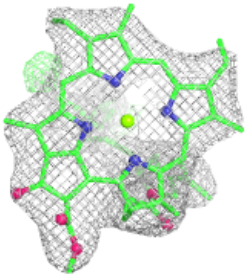


Electron density around CLA b 606:

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

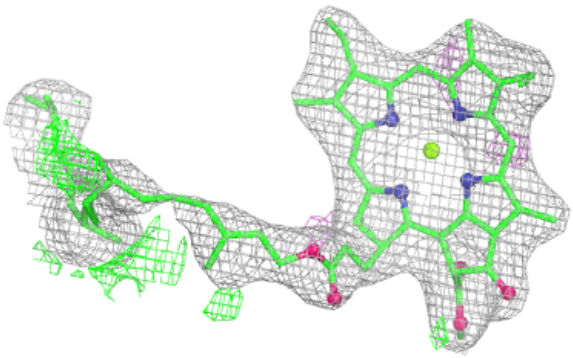


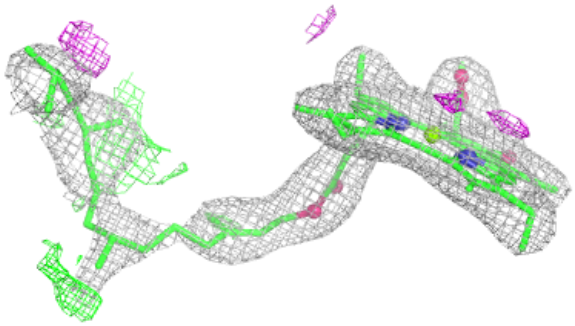


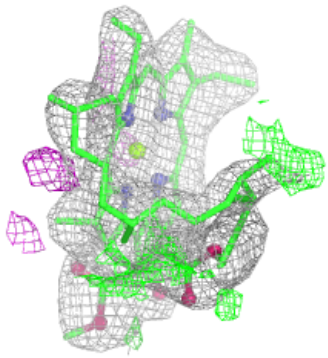


Electron density around CLA A 408:

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

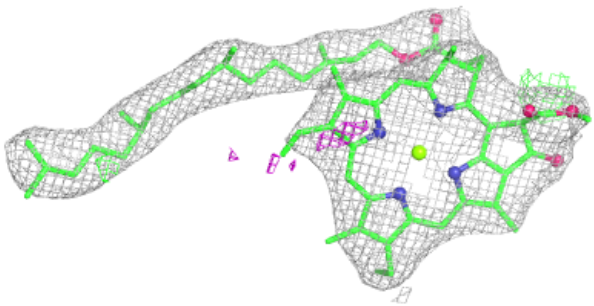


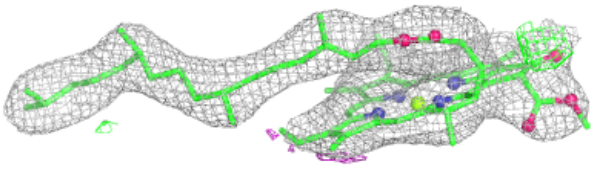


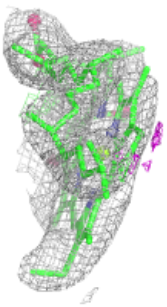


Electron density around CLA c 501:

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

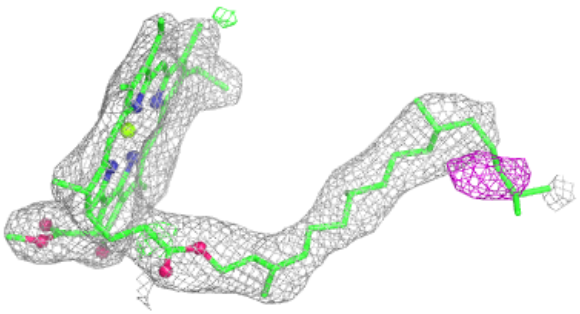


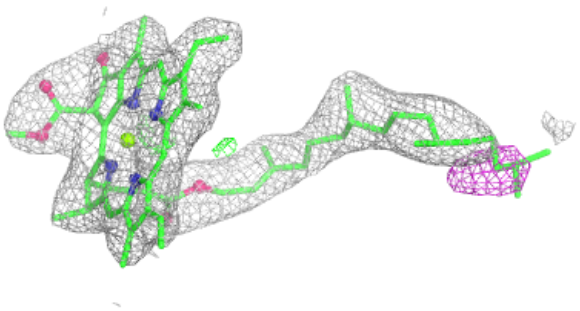


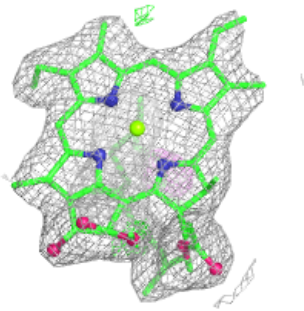


Electron density around CLA C 509:

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

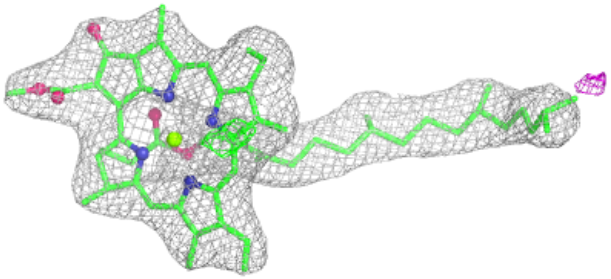


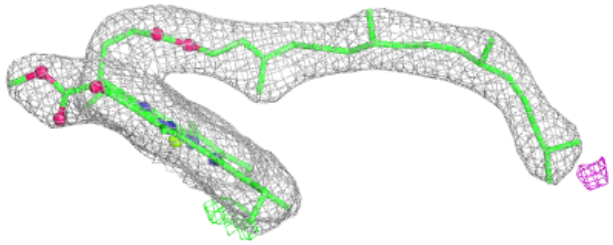


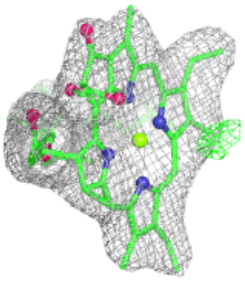


Electron density around CLA b 608:

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

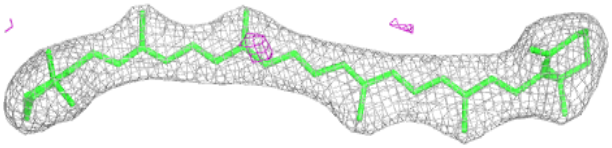


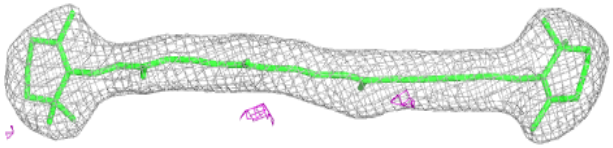


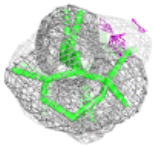


Electron density around BCR a 409:

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

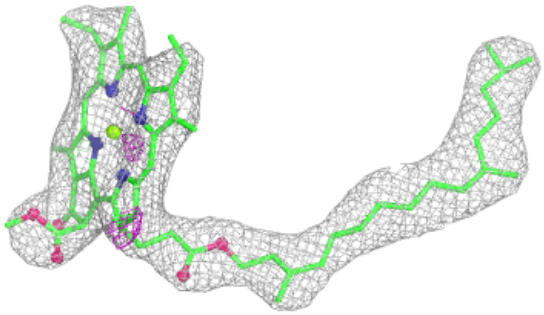


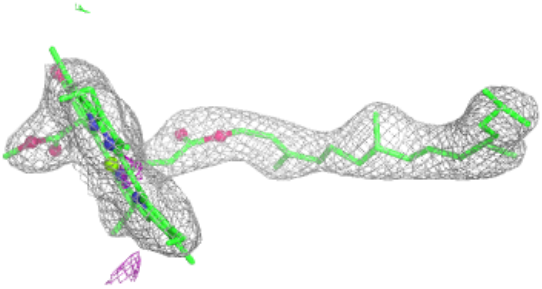


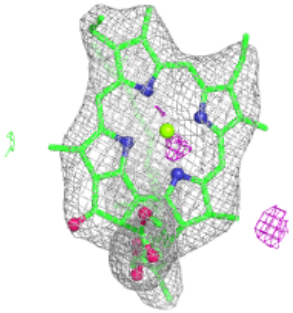


Electron density around CLA b 609:

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

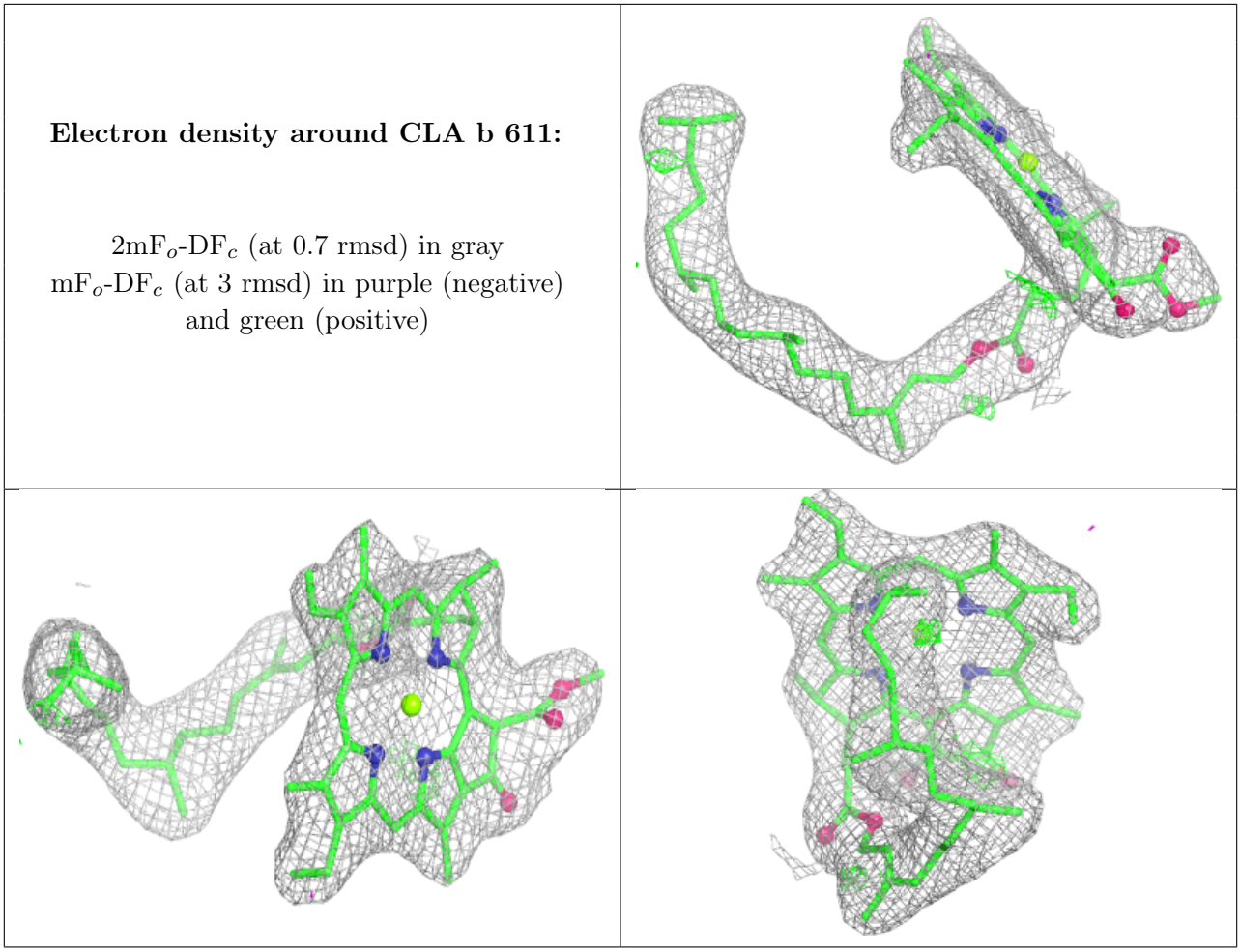






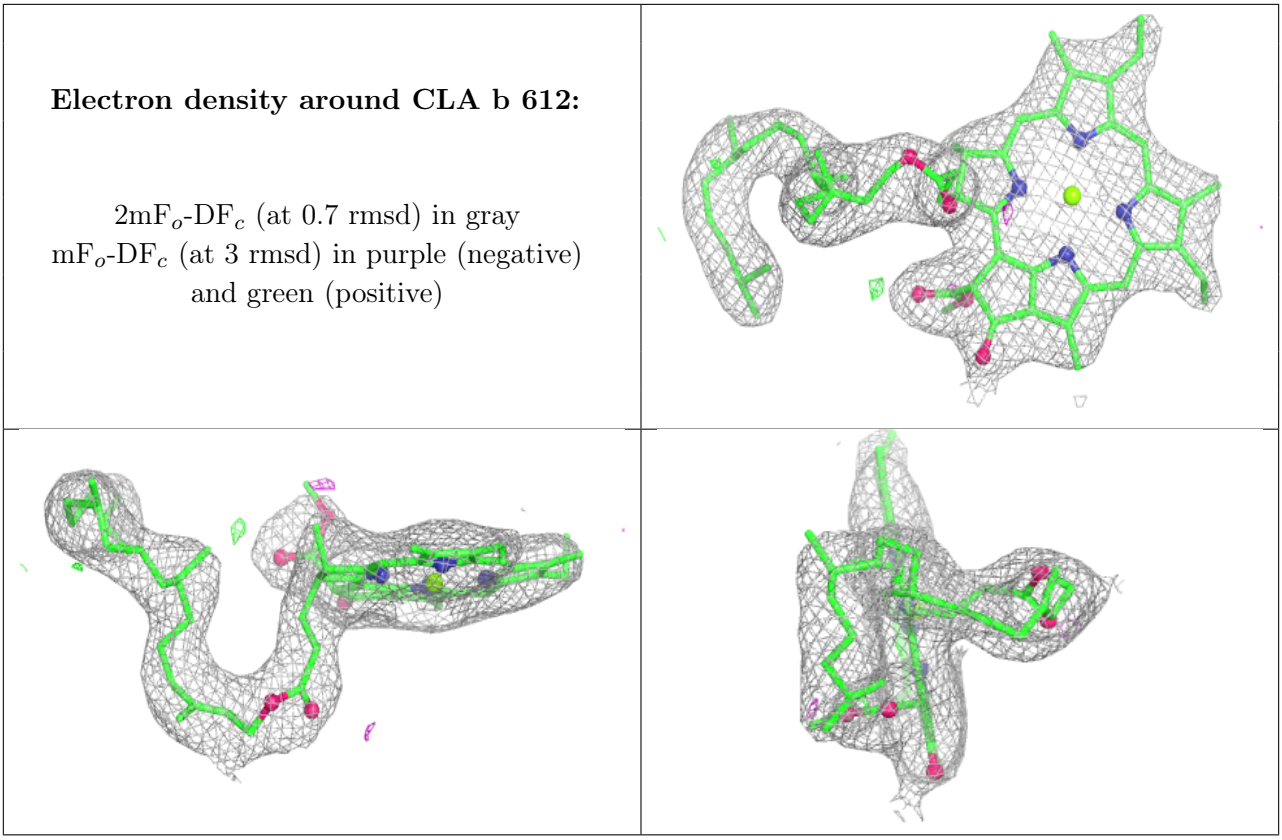
Electron density around CLA b 611:

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



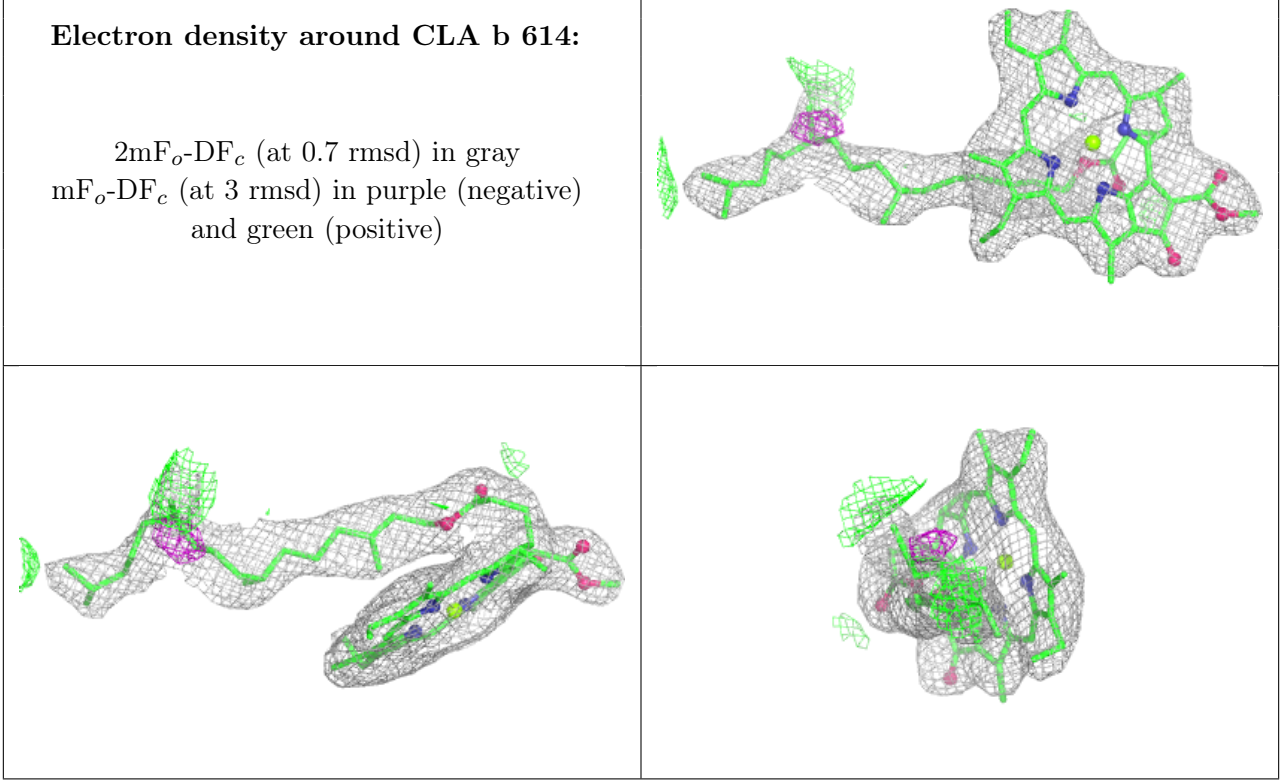
Electron density around CLA b 612:

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



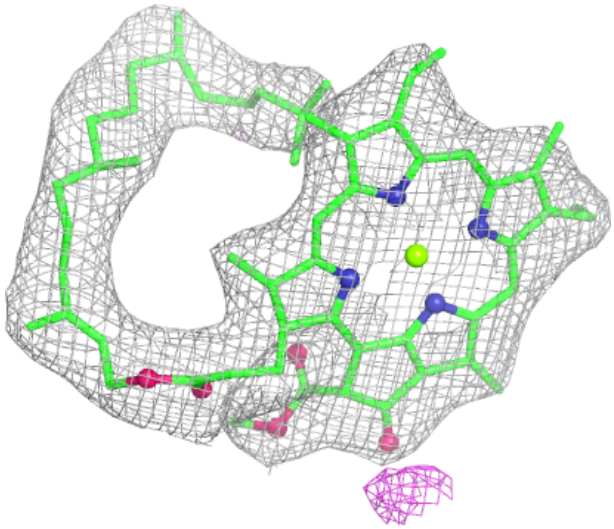
Electron density around CLA b 614:

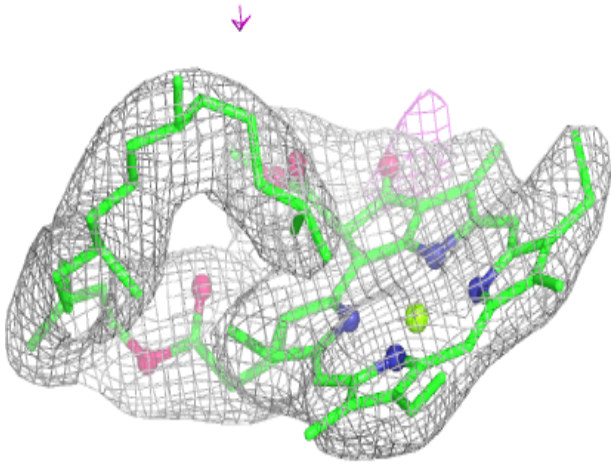
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

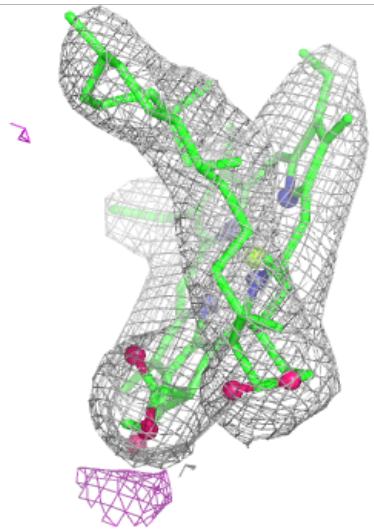


Electron density around CLA b 615:

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

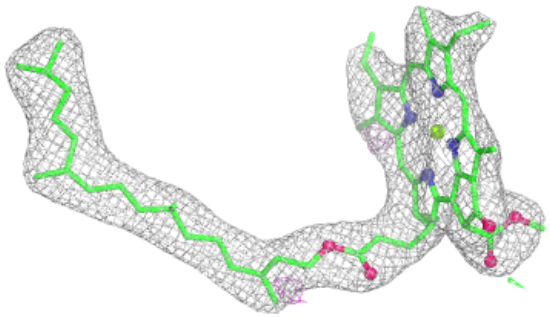


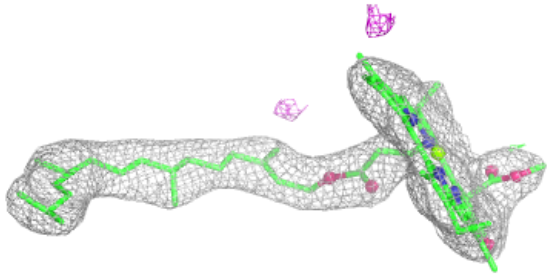


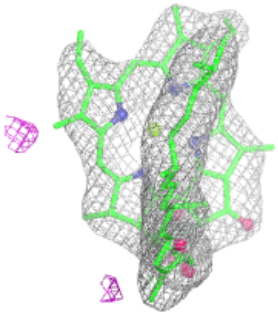


Electron density around CLA B 609:

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

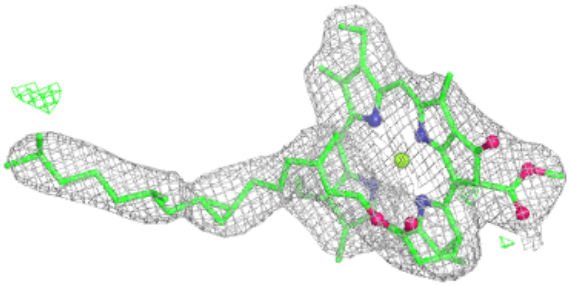


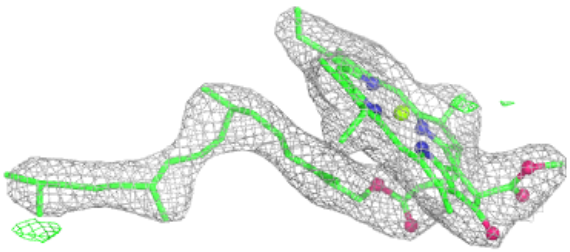


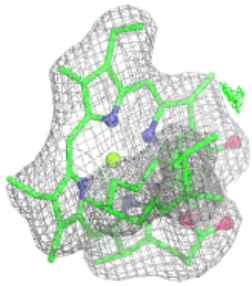


Electron density around CLA C 506:

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

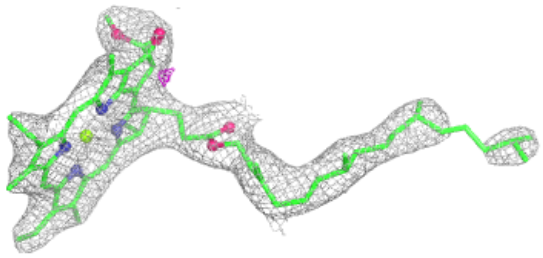


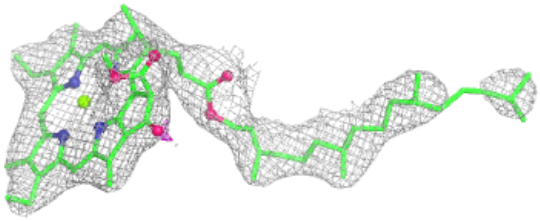


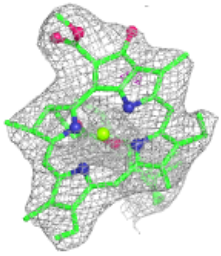


Electron density around CLA c 502:

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

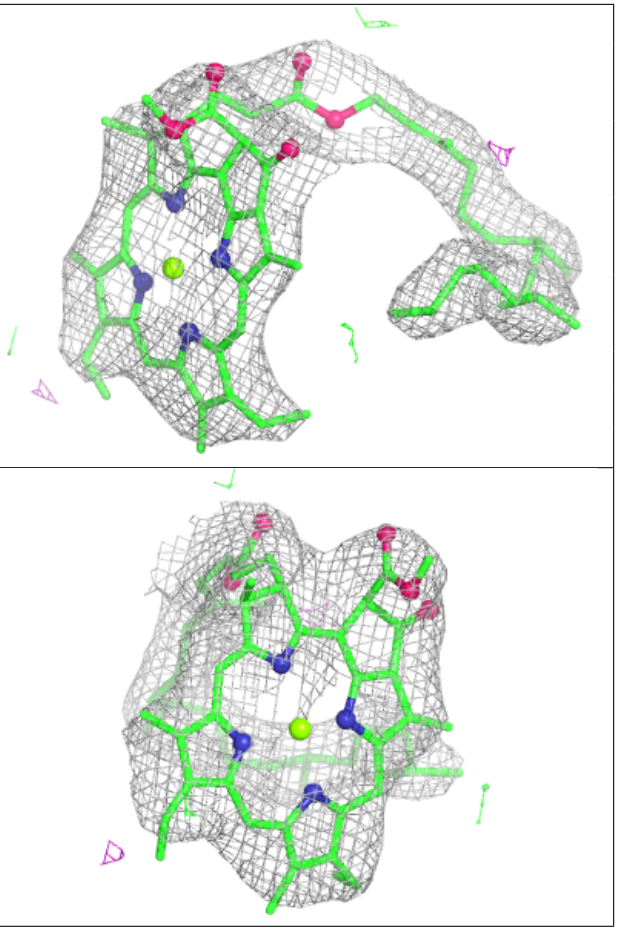






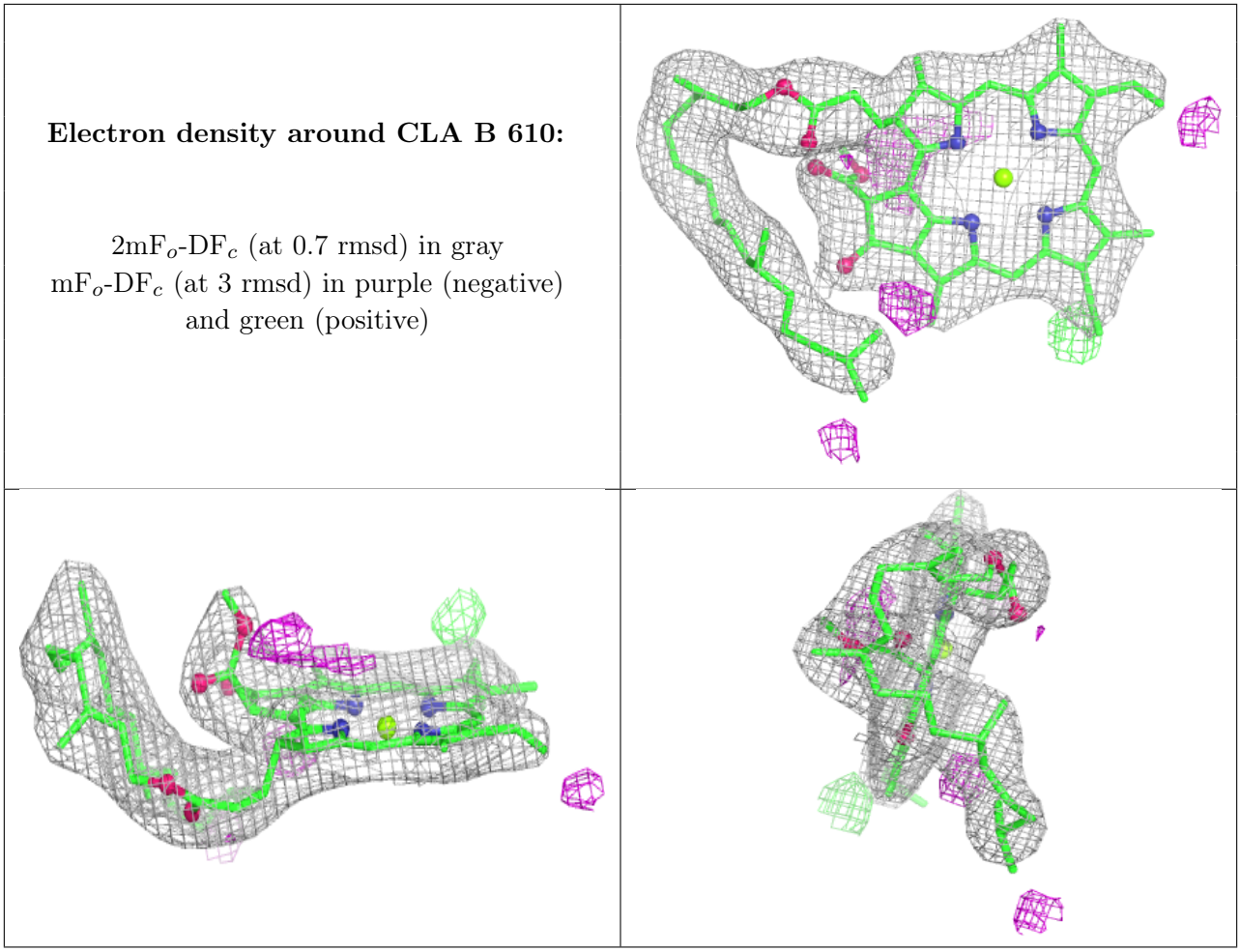
Electron density around CLA c 503:

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



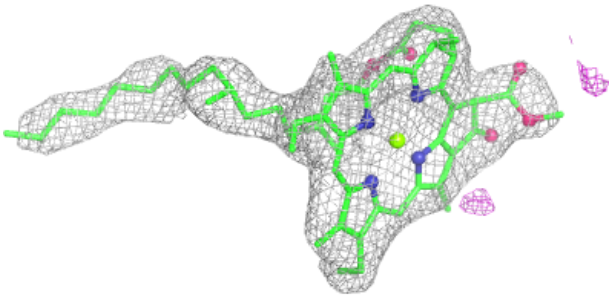
Electron density around CLA B 610:

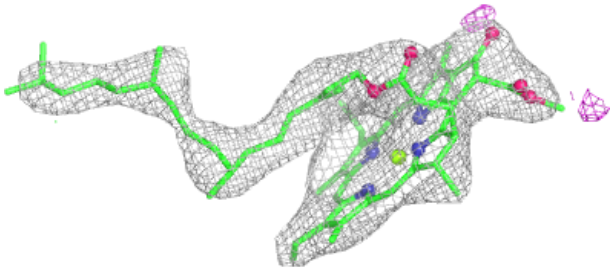
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

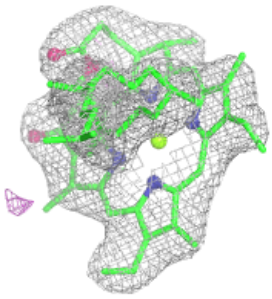


Electron density around CLA c 505:

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

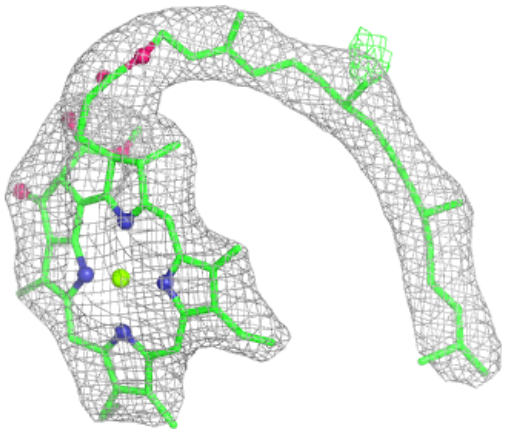


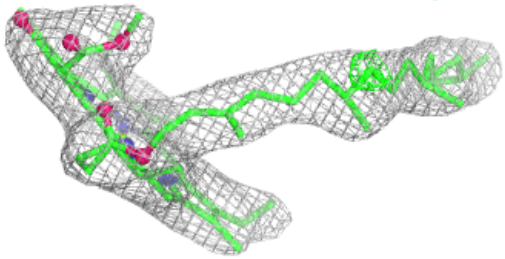


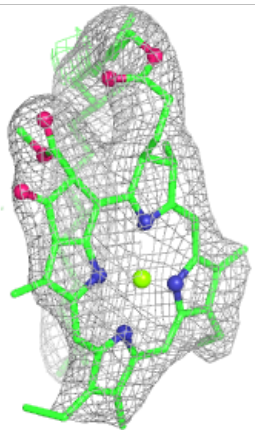


Electron density around CLA C 508:

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

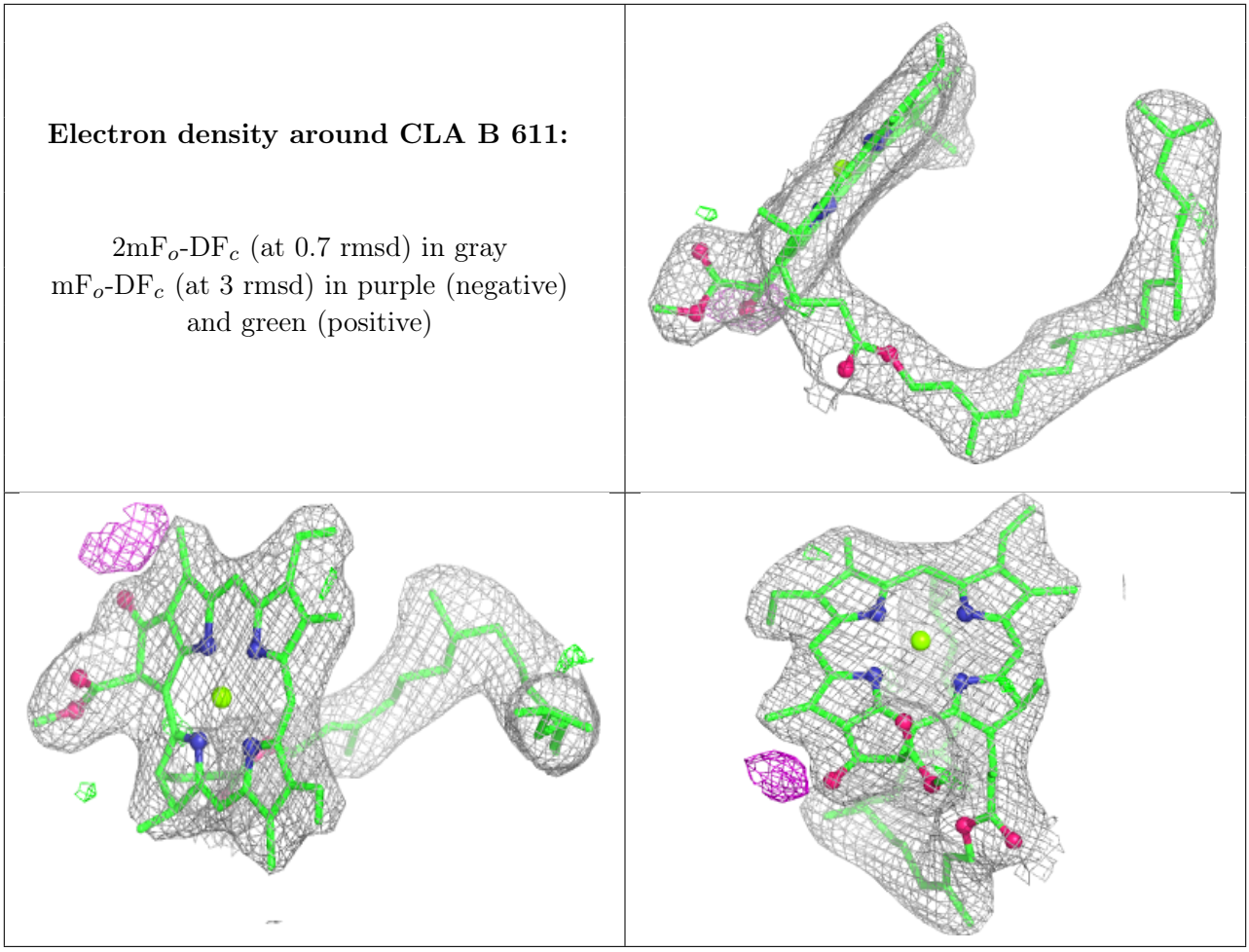






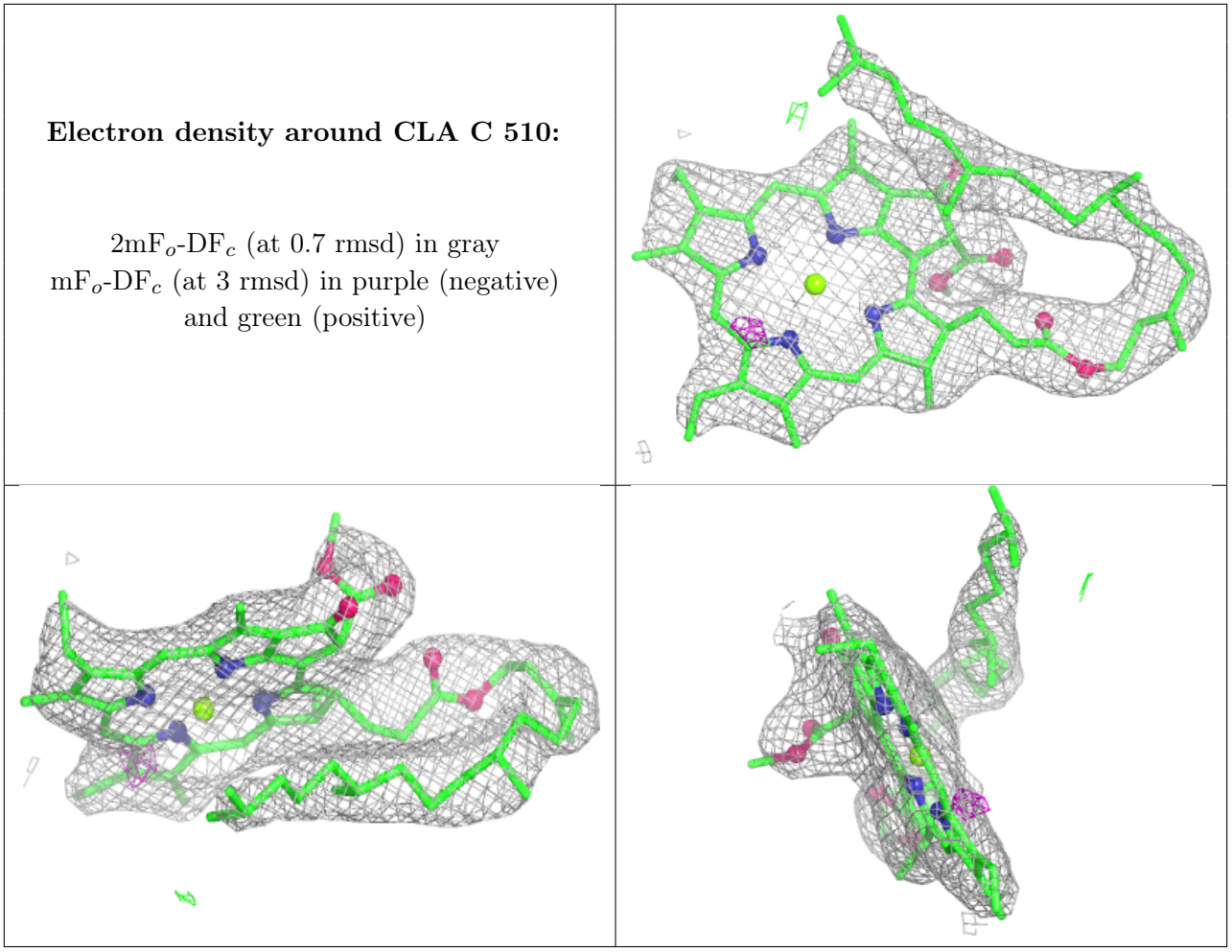
Electron density around CLA B 611:

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



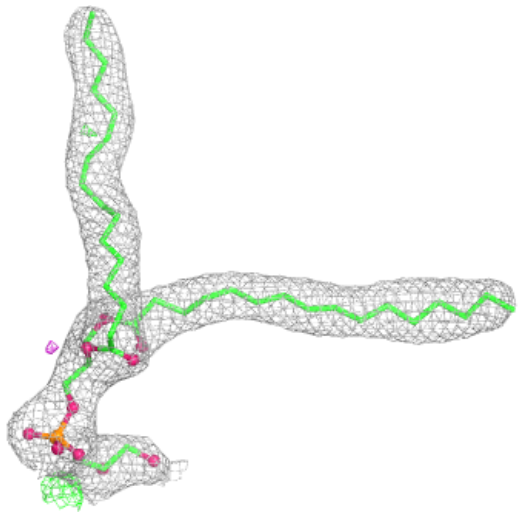
Electron density around CLA C 510:

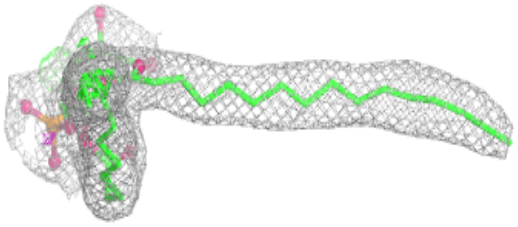
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

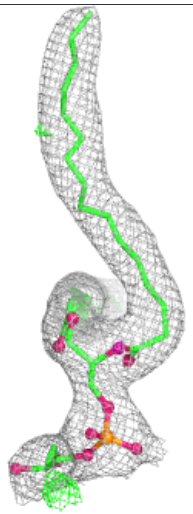


Electron density around LHG A 417:

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

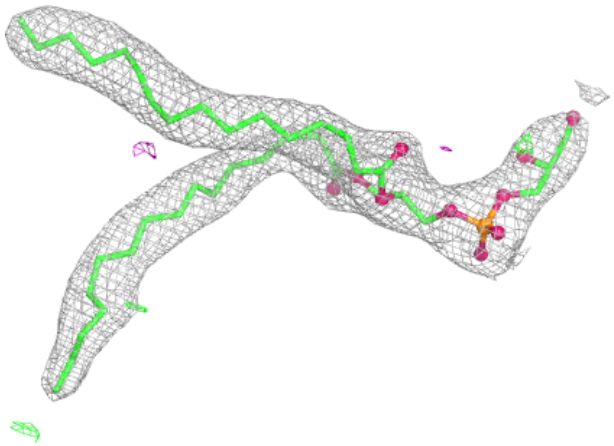


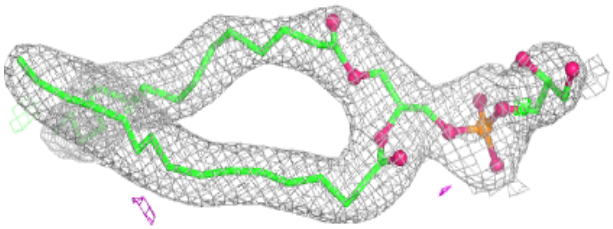


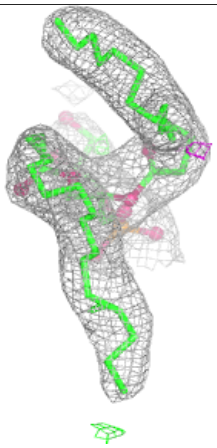


Electron density around LHG D 408:

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

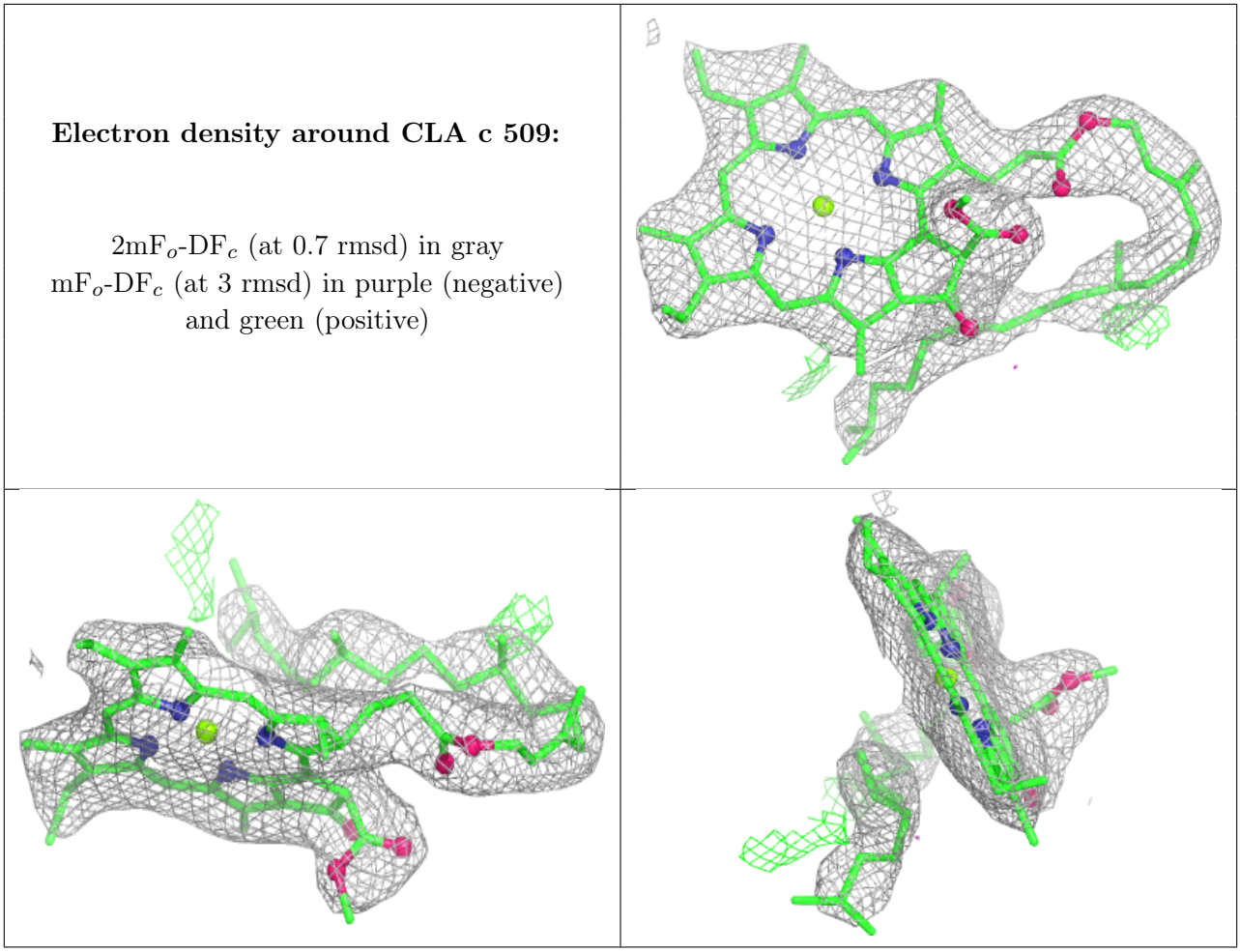






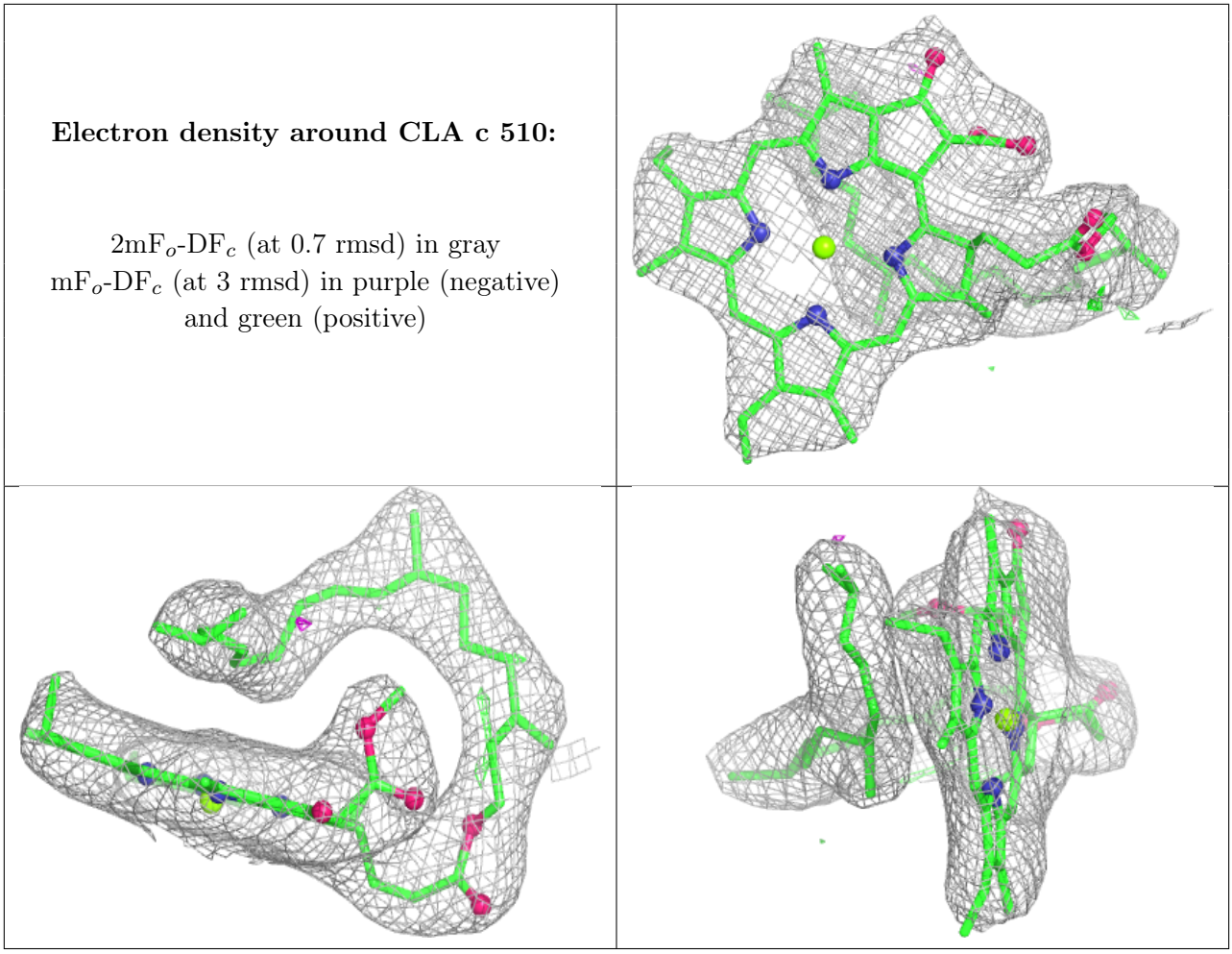
Electron density around CLA c 509:

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



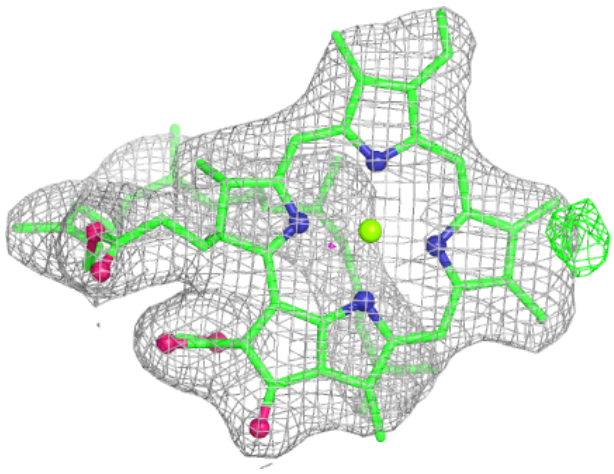
Electron density around CLA c 510:

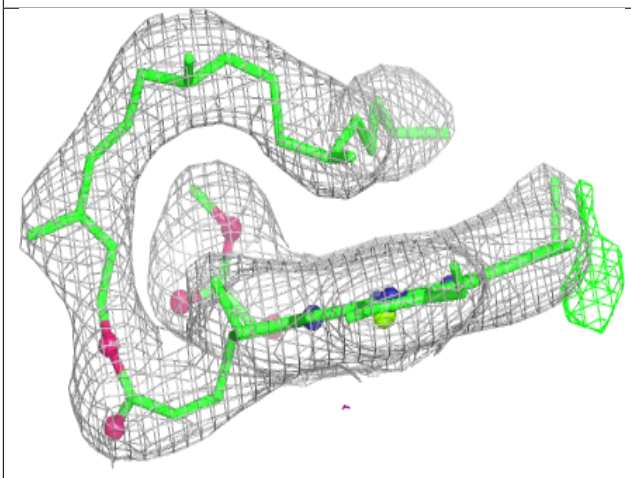
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

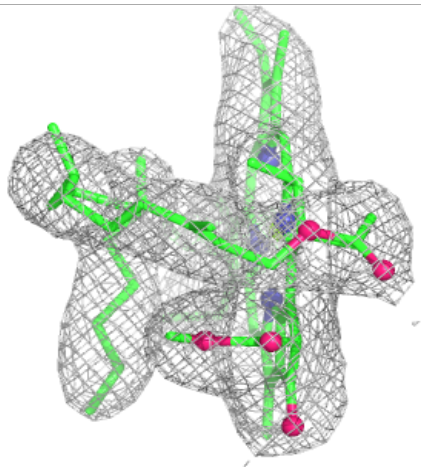


Electron density around CLA C 511:

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

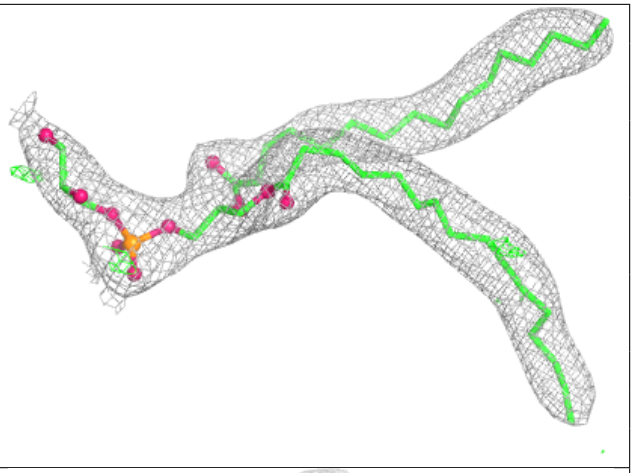


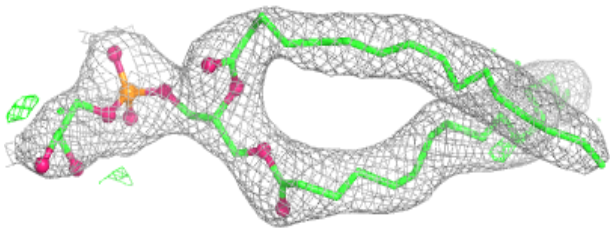


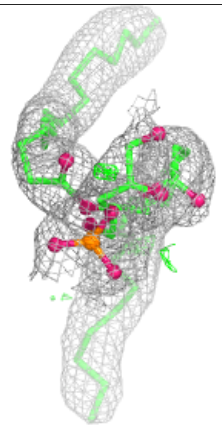


Electron density around LHG d 408:

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

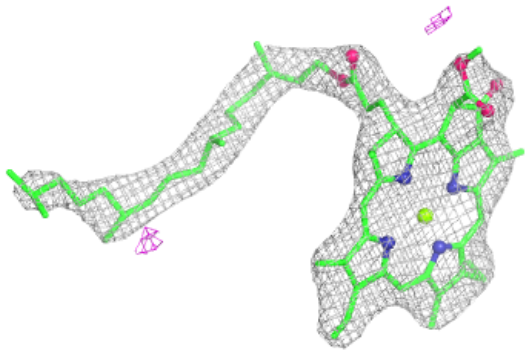


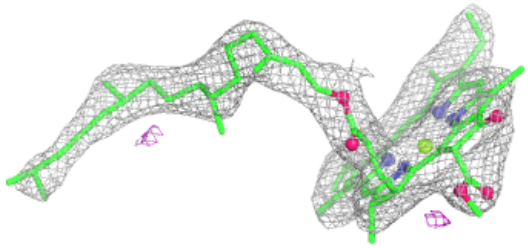


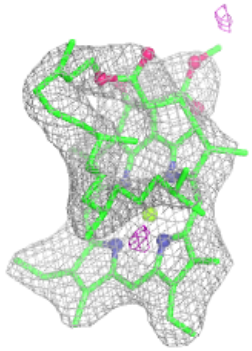


Electron density around CLA C 512:

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

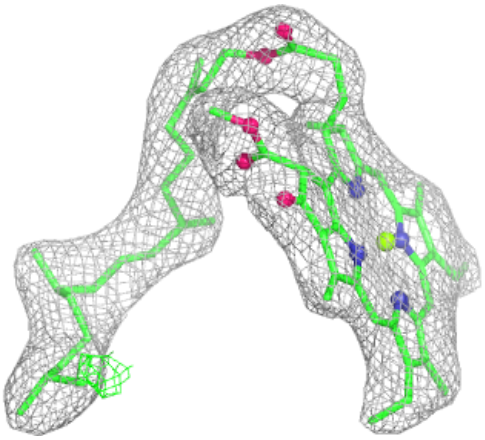


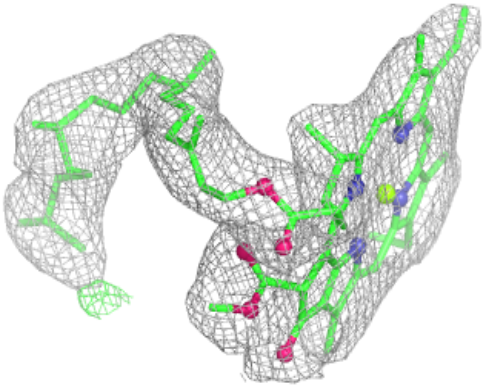


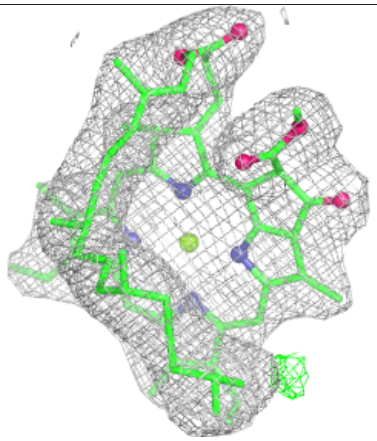


Electron density around CLA B 613:

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

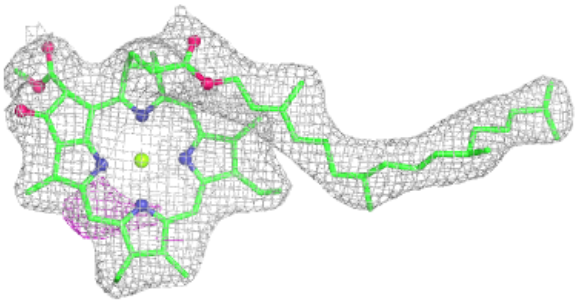


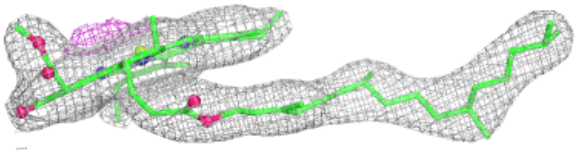


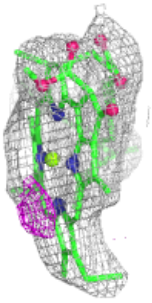


Electron density around CLA B 603:

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

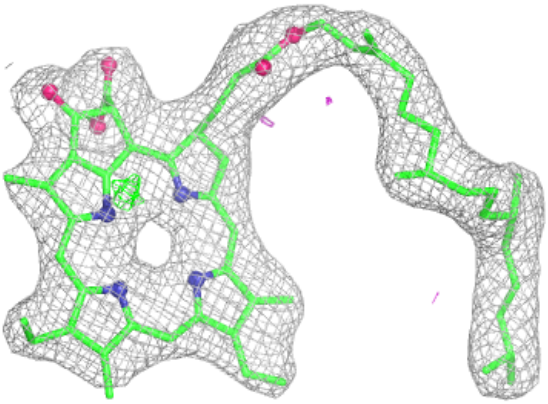


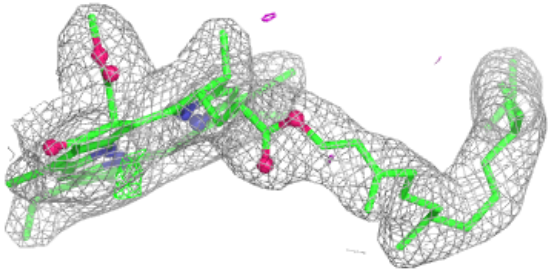


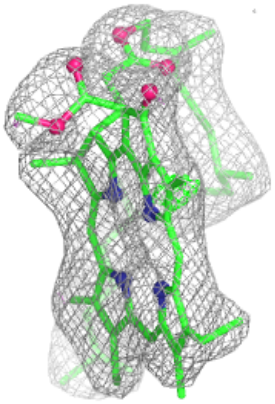


Electron density around PHO A 407:

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

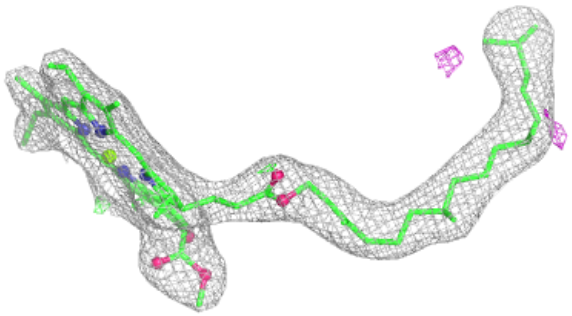


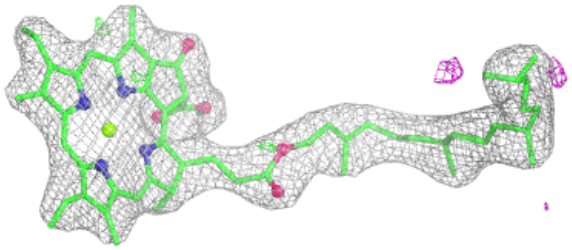


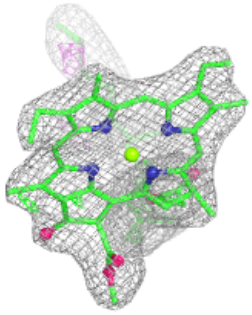


Electron density around CLA D 404:

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

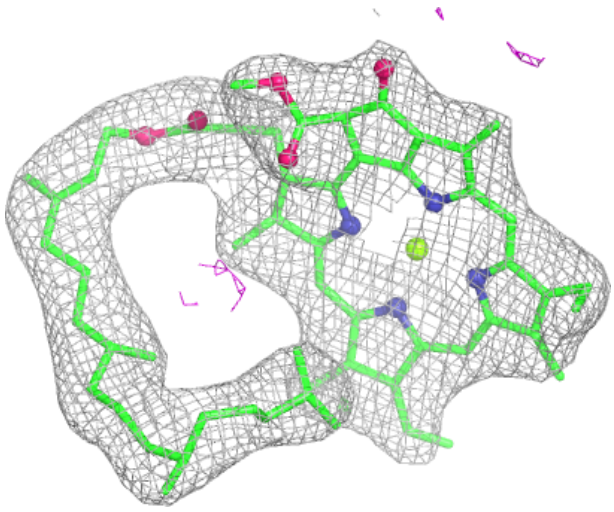


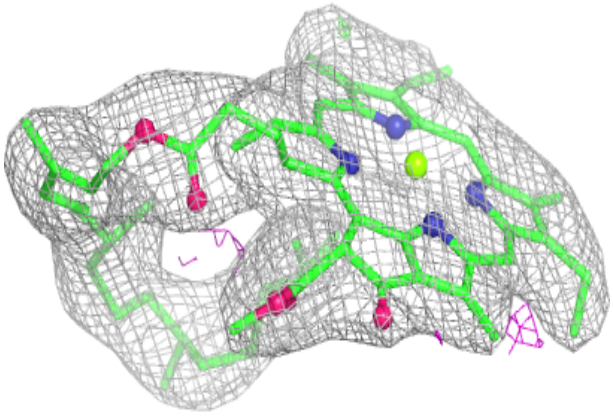


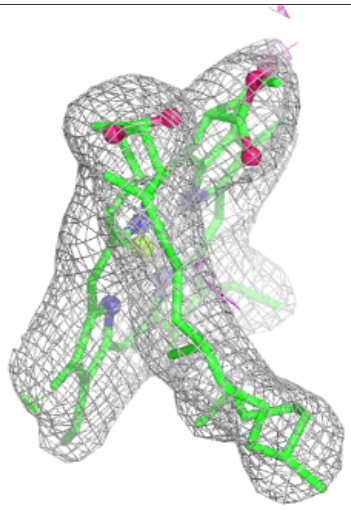


Electron density around CLA B 615:

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

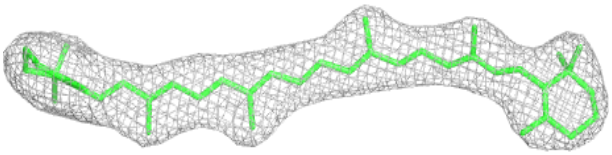


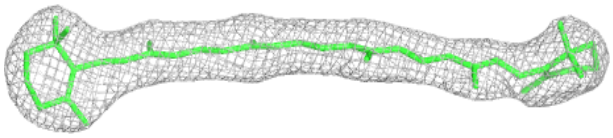


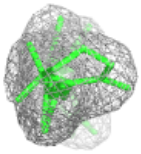


Electron density around BCR B 617:

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

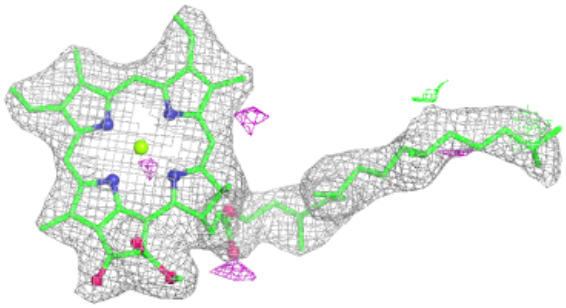


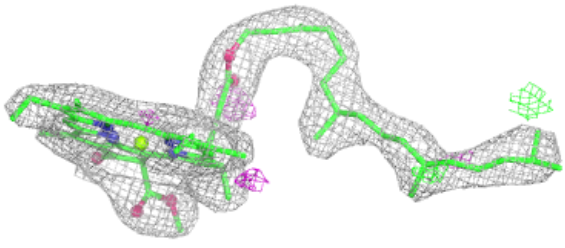


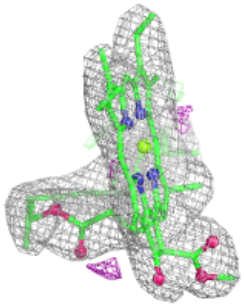


Electron density around CLA A 406:

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

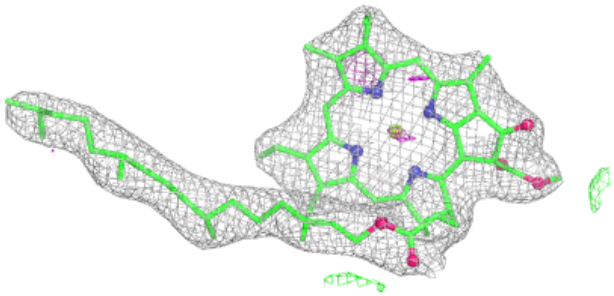


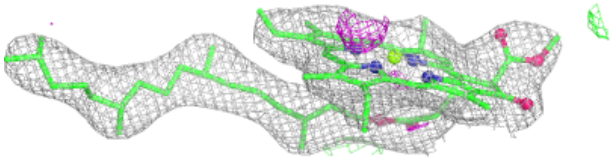


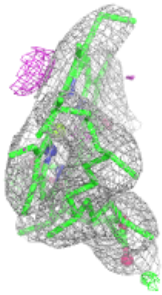


Electron density around CLA C 502:

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

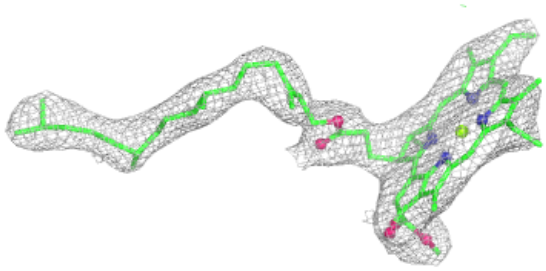


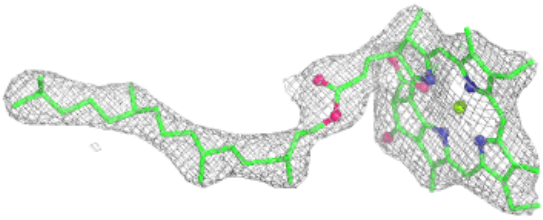


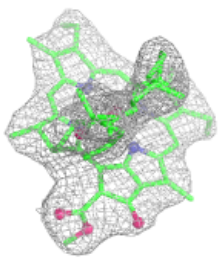


Electron density around CLA C 503:

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

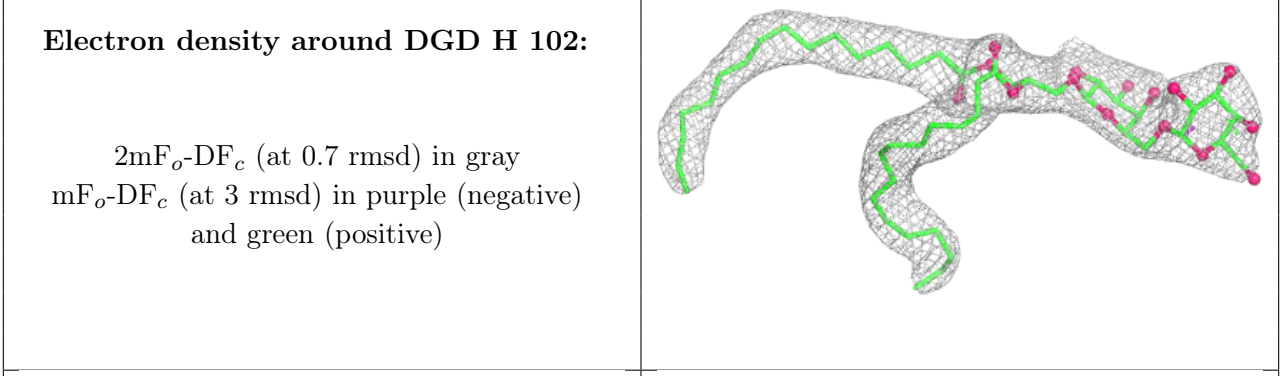


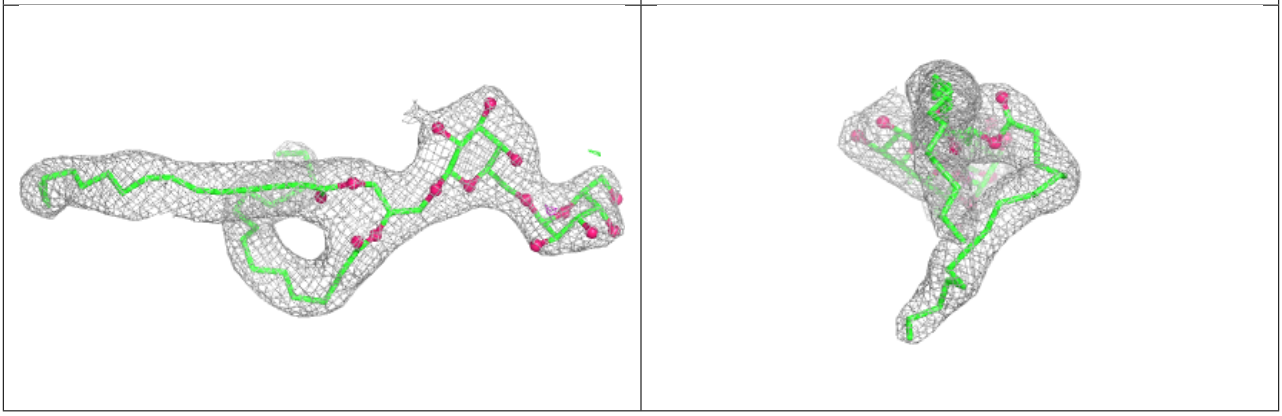




Electron density around DGD H 102:

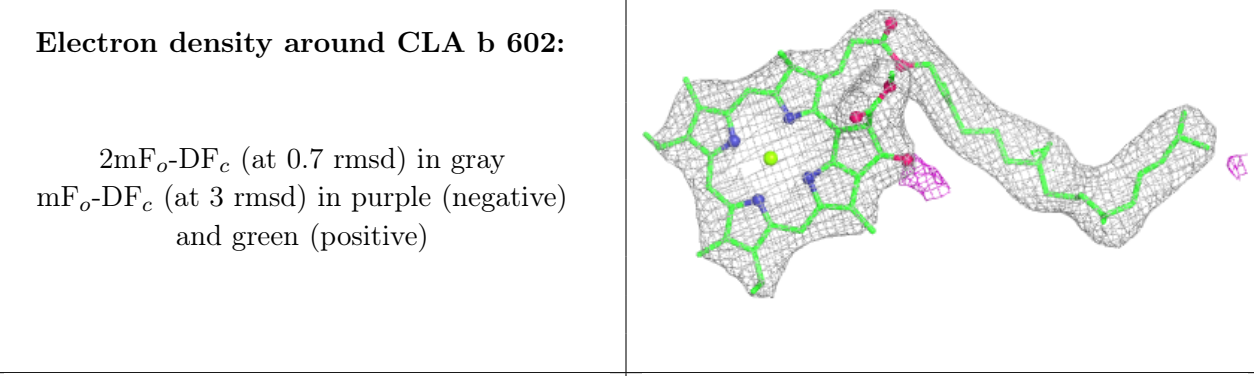
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

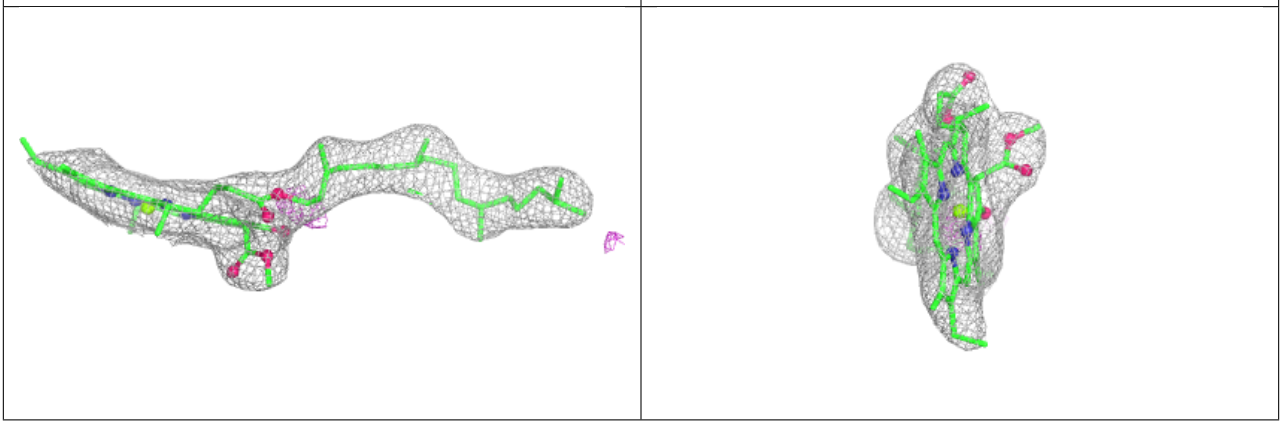




Electron density around CLA b 602:

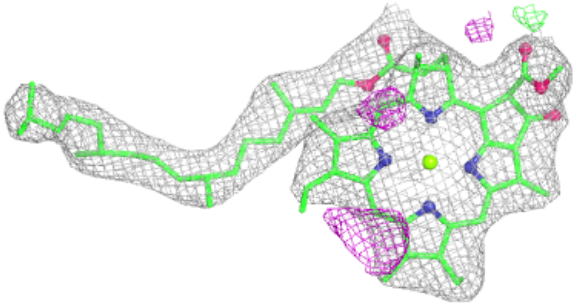
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

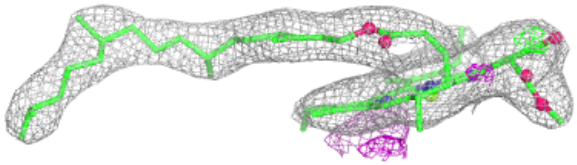


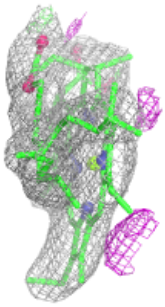


Electron density around CLA b 603:

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

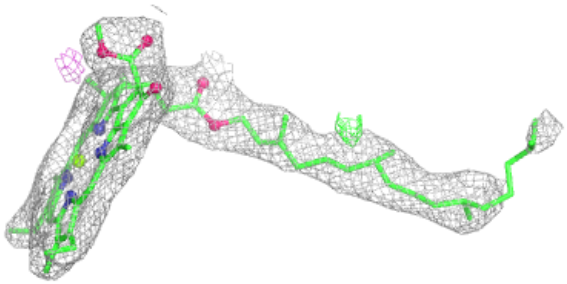


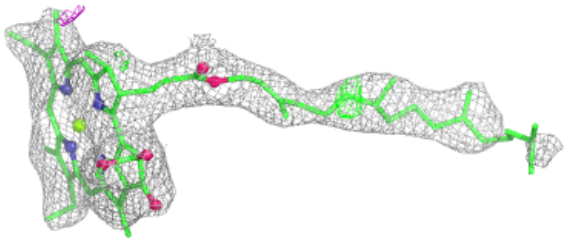


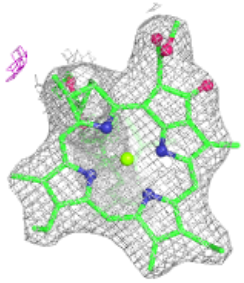


Electron density around CLA b 604:

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

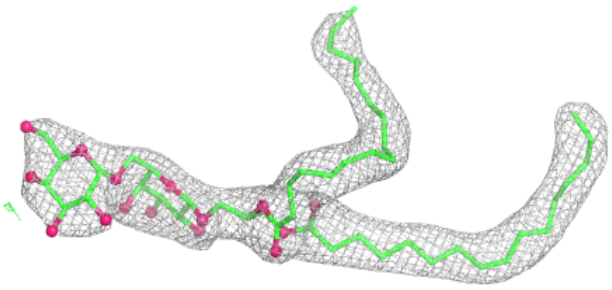


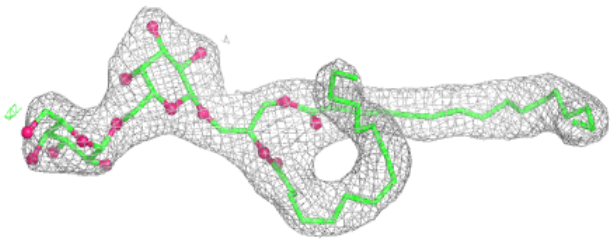




Electron density around DGD h 102:

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

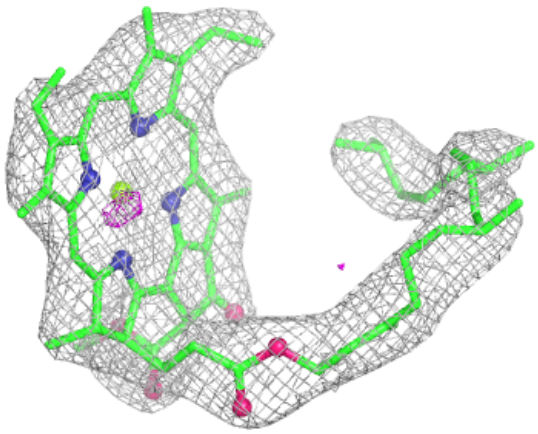


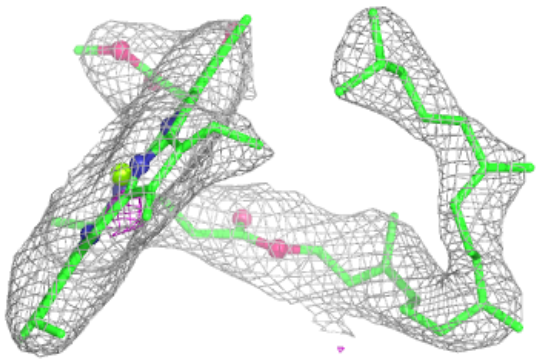


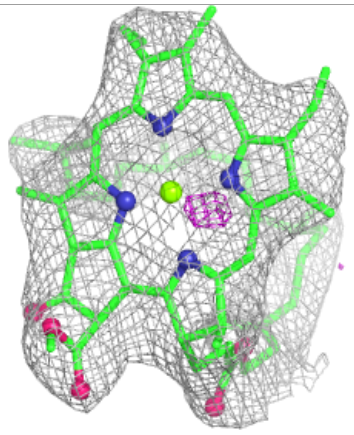


Electron density around CLA C 504:

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

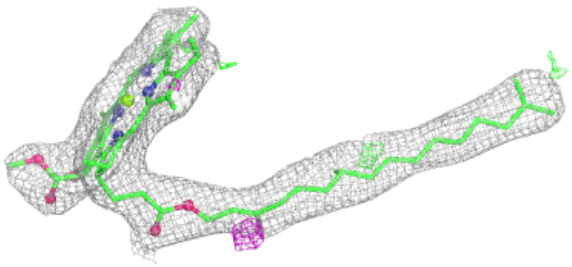


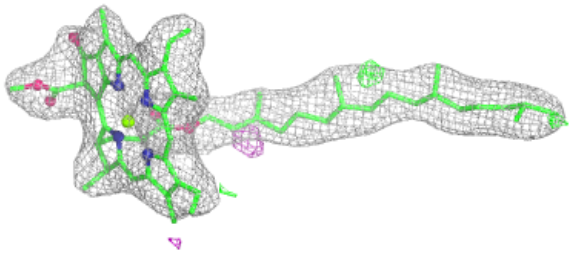


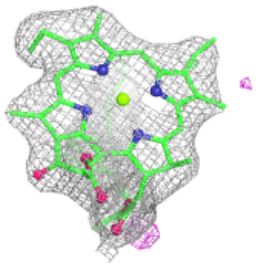


Electron density around CLA b 607:

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

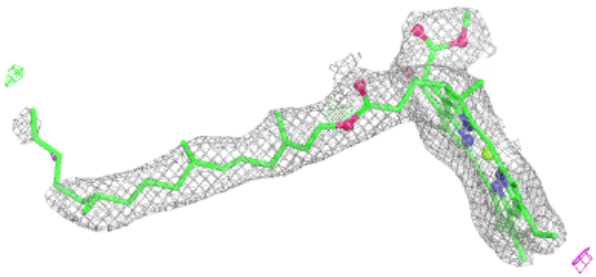


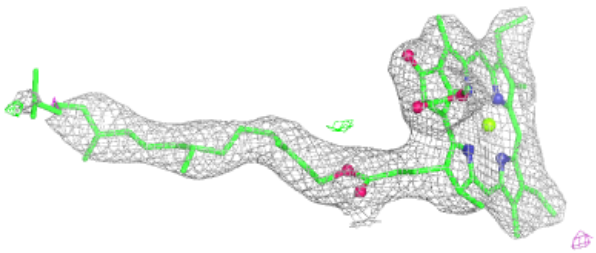


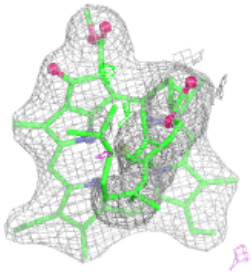


Electron density around CLA B 604:

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

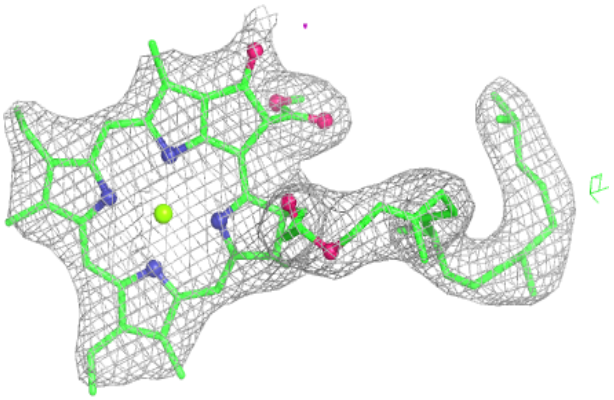


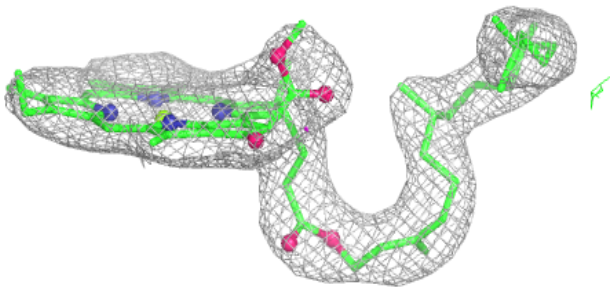


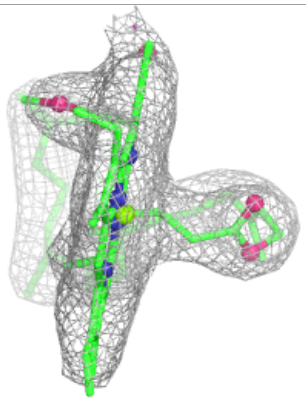


Electron density around CLA B 612:

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

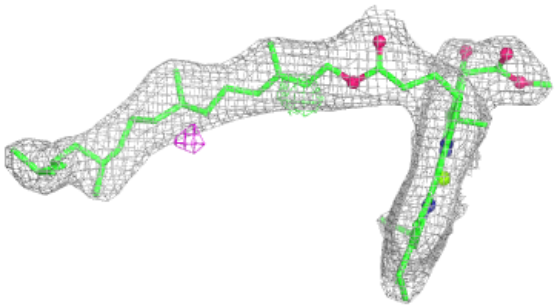


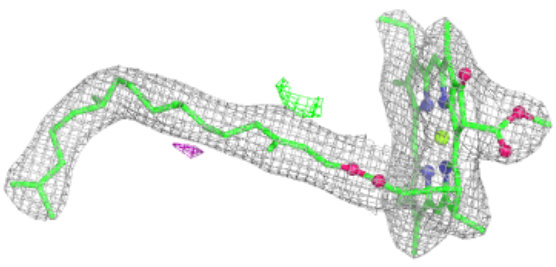


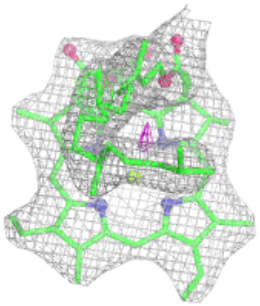


Electron density around CLA B 605:

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

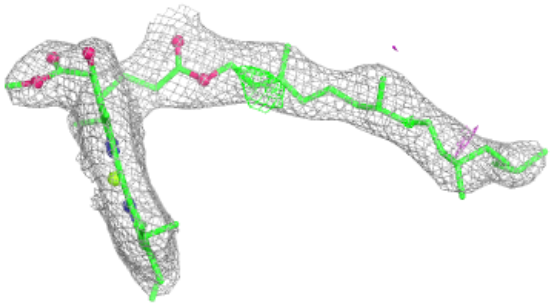


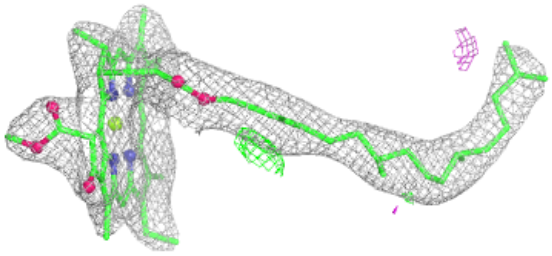


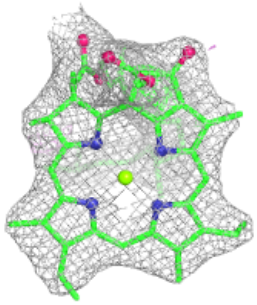


Electron density around CLA b 605:

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

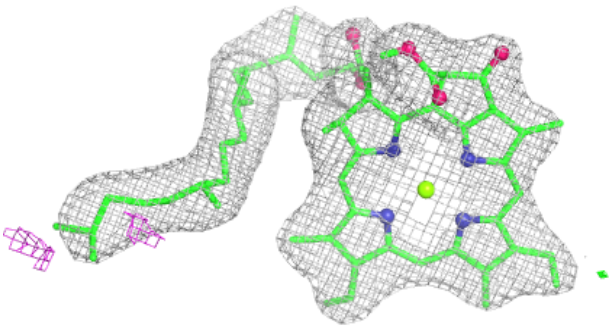


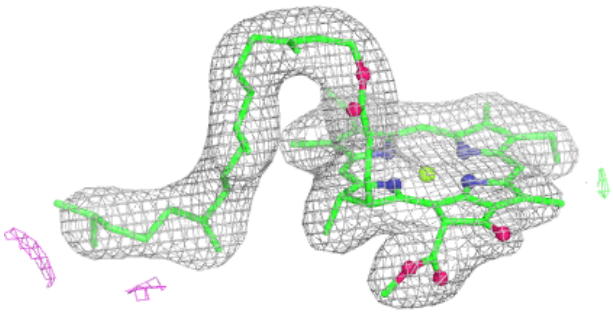




Electron density around CLA d 401:

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

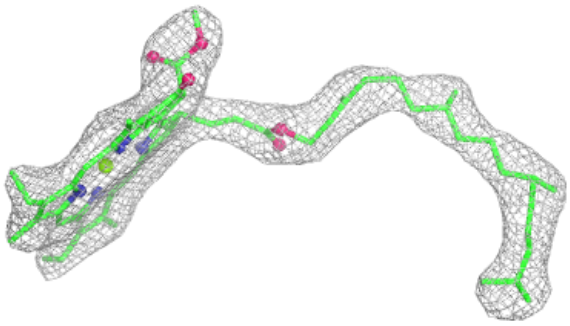


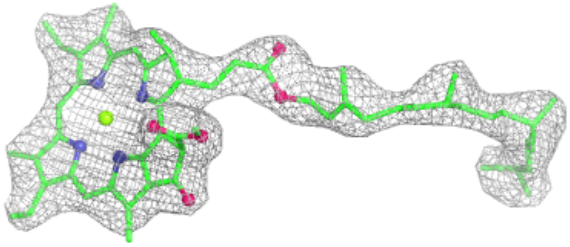


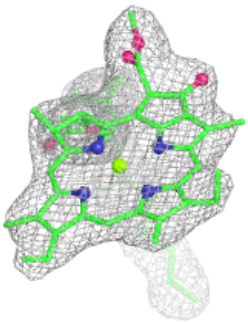


Electron density around CLA d 403:

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

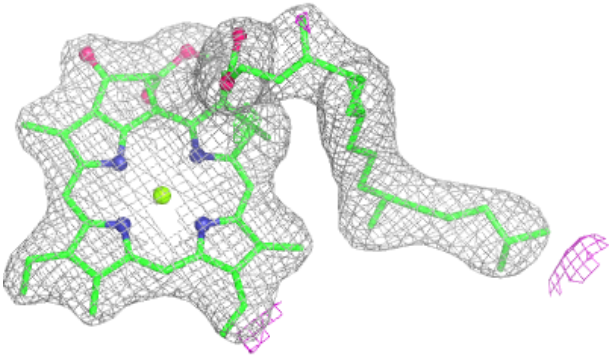


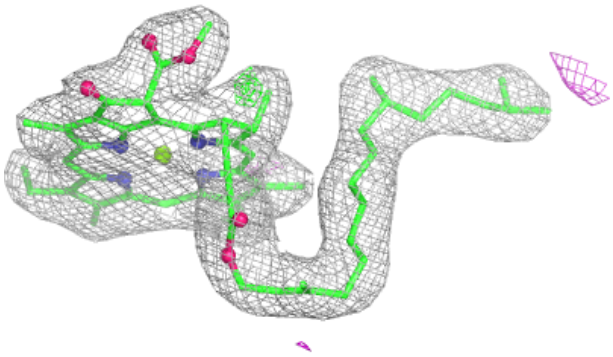


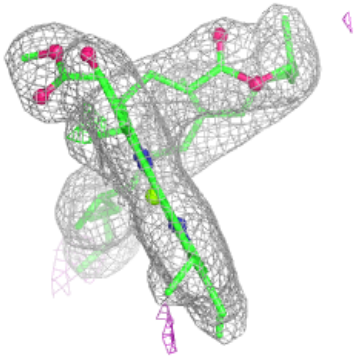


Electron density around CLA A 405:

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

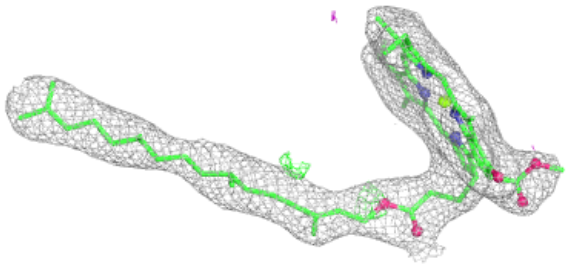


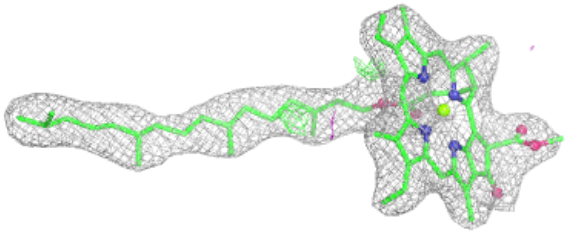


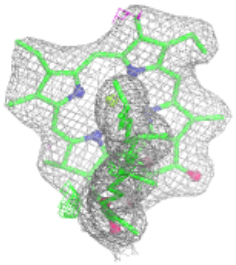


Electron density around CLA B 607:

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

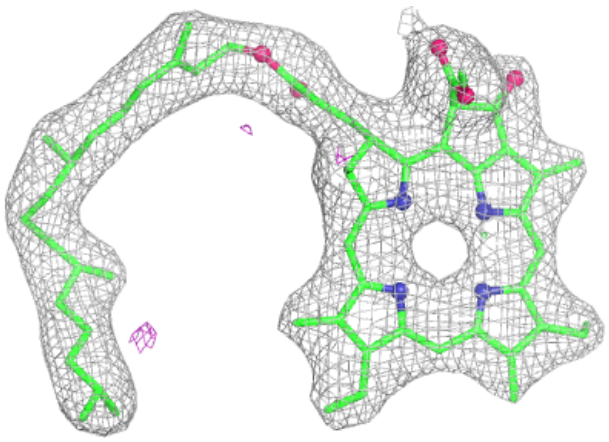


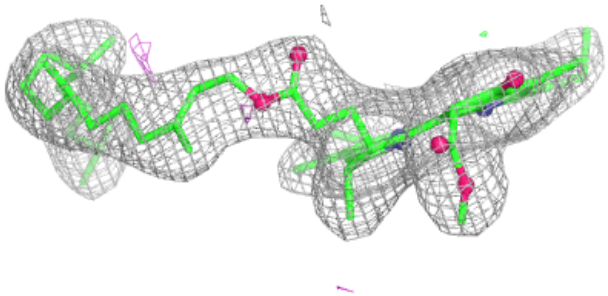




Electron density around PHO D 401:

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

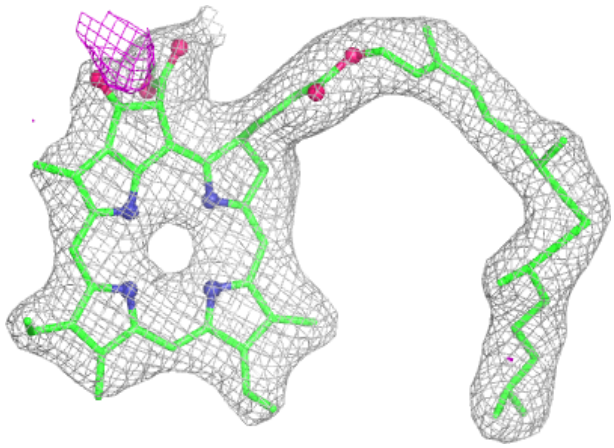


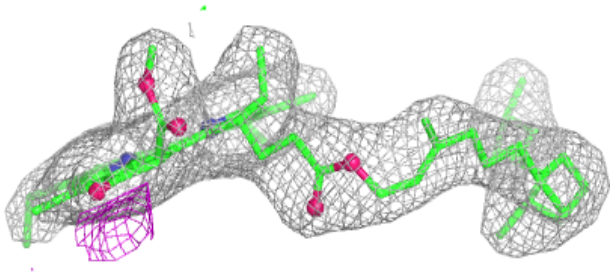




Electron density around PHO a 406:

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

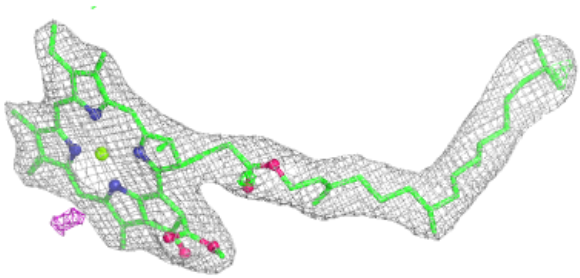


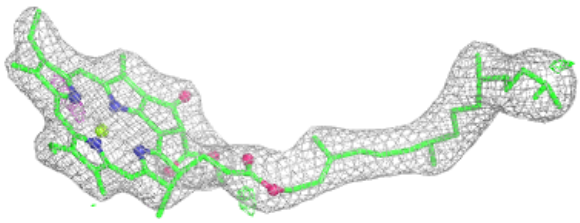




Electron density around CLA a 404:

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

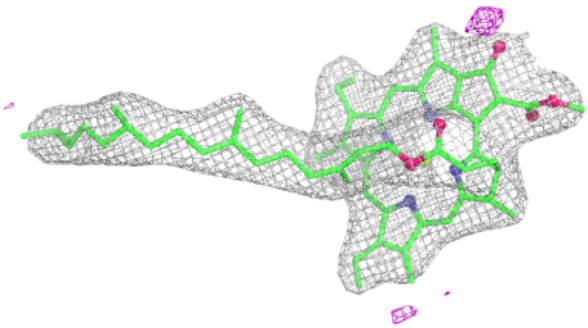


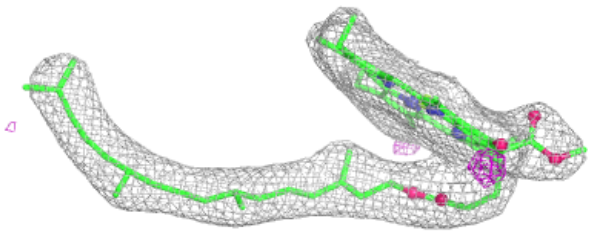


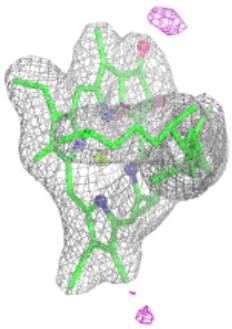


Electron density around CLA B 608:

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

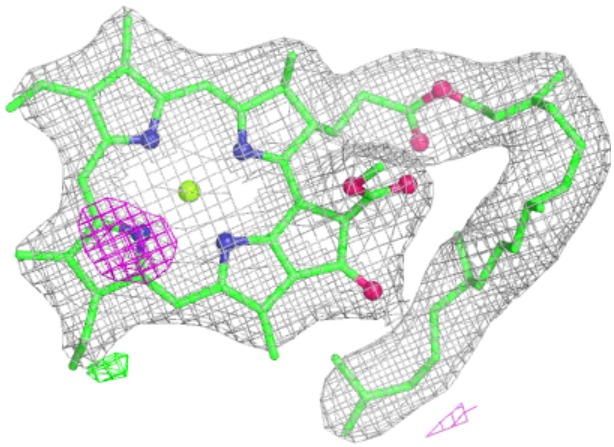


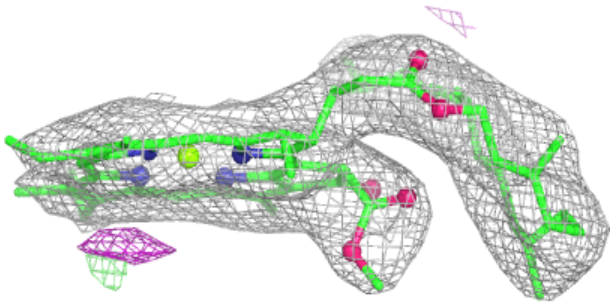


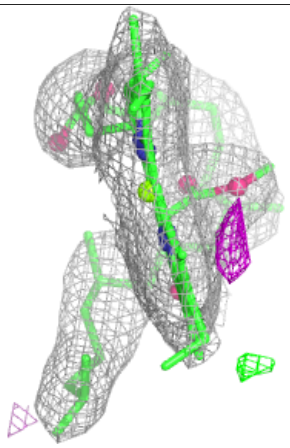


Electron density around CLA b 610:

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

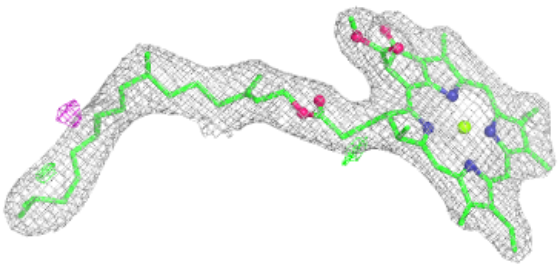


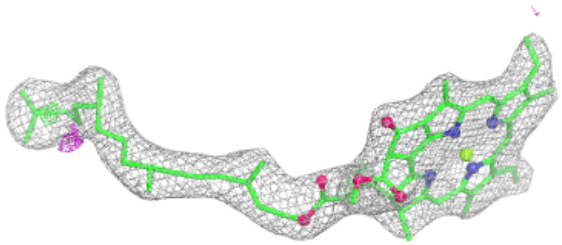




Electron density around CLA A 404:

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

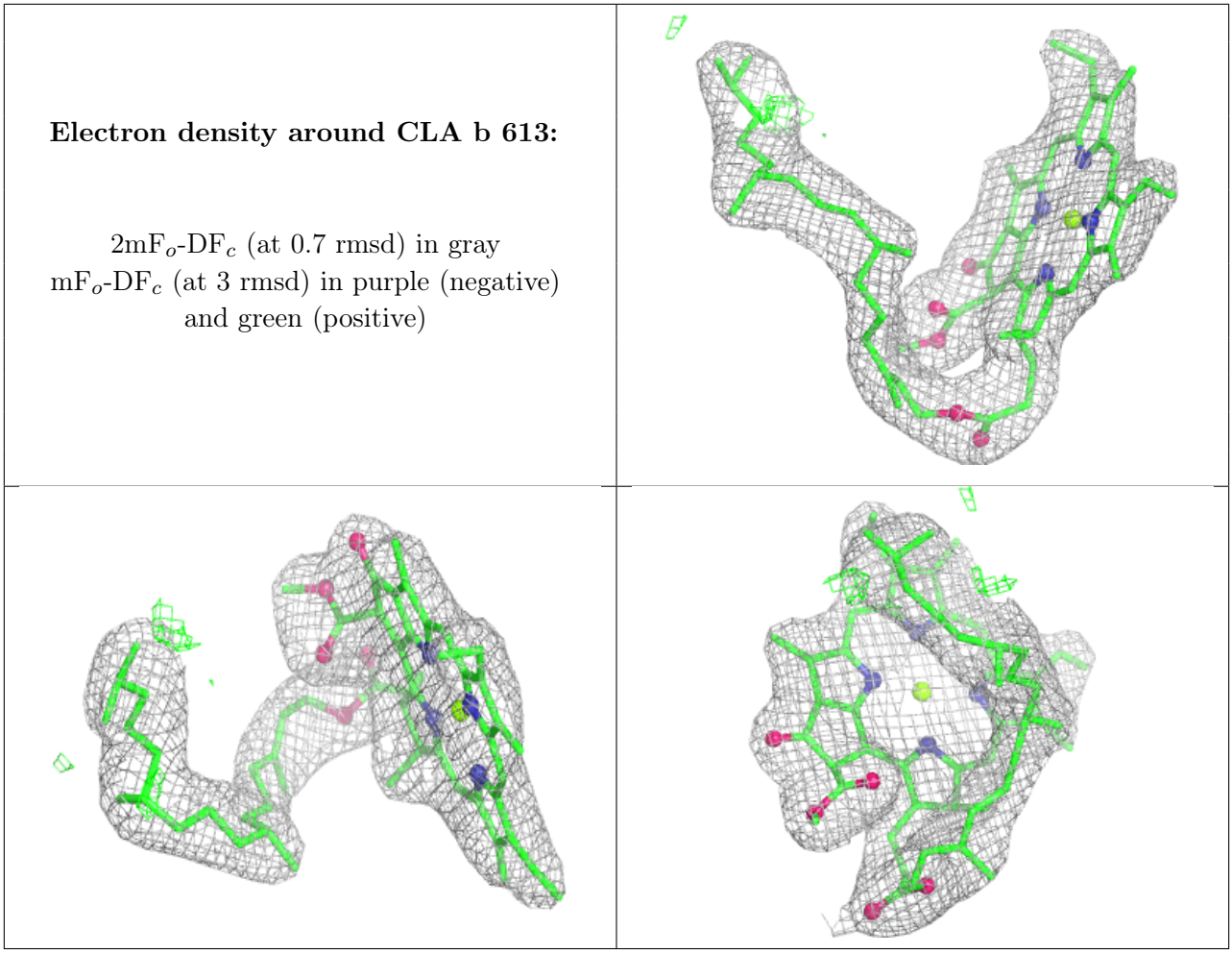






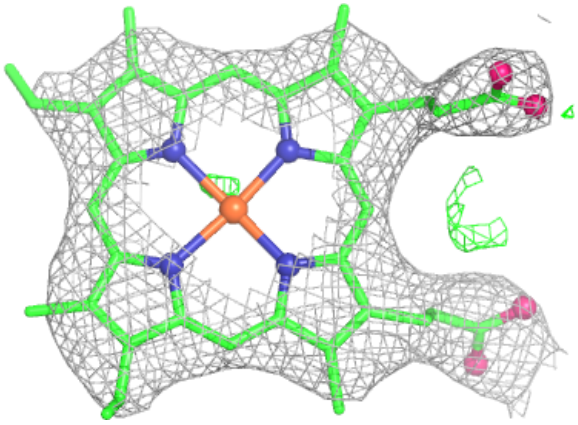
Electron density around CLA b 613:

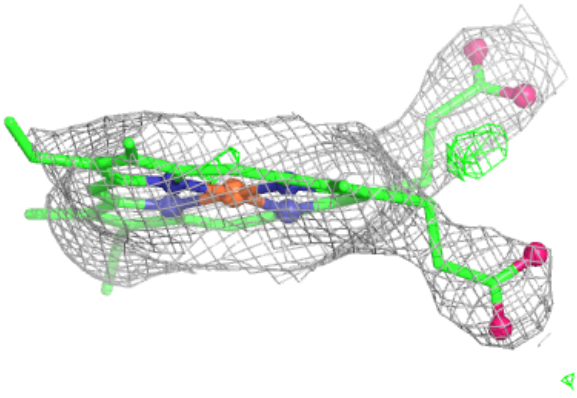
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

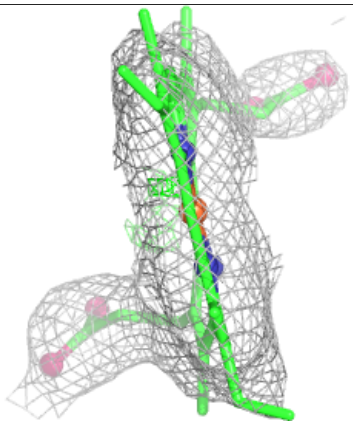


Electron density around HEM E 103:

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

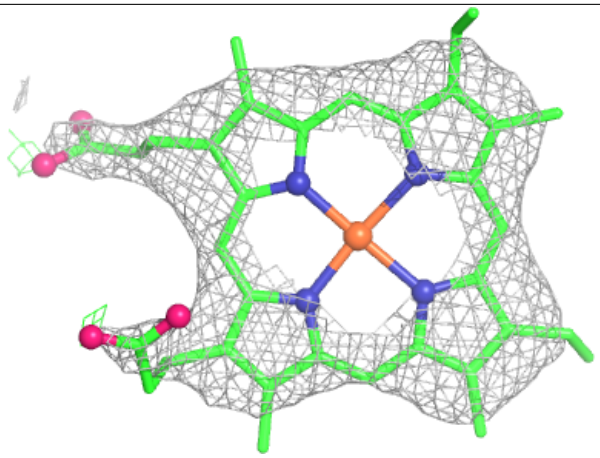


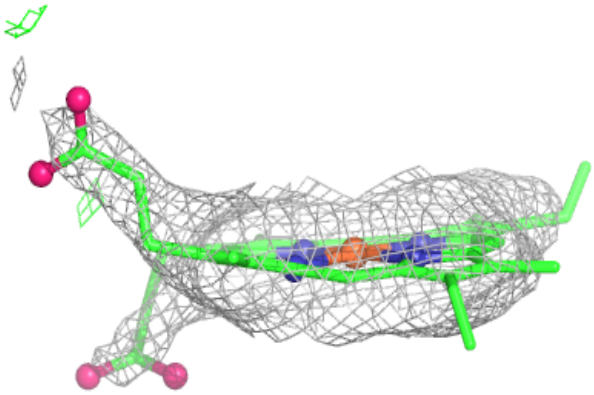


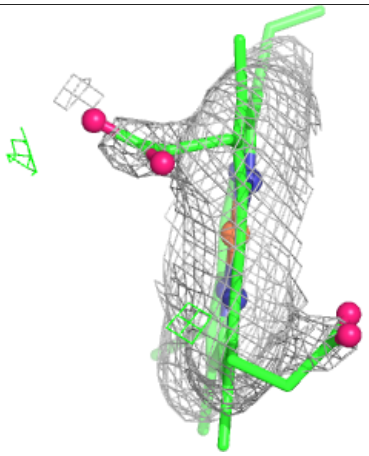


Electron density around HEM e 103:

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

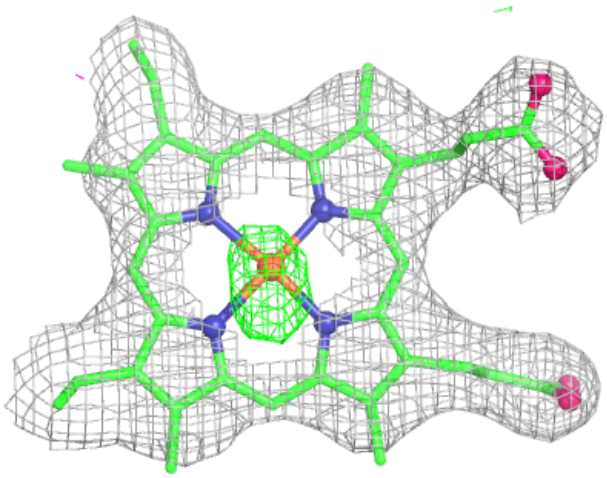


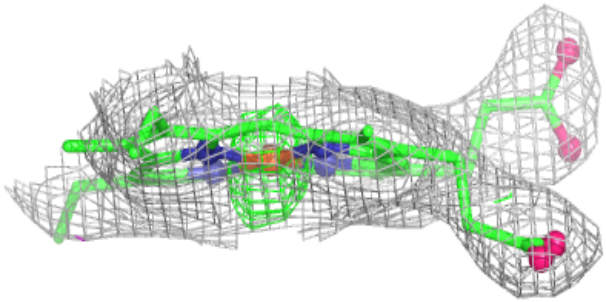


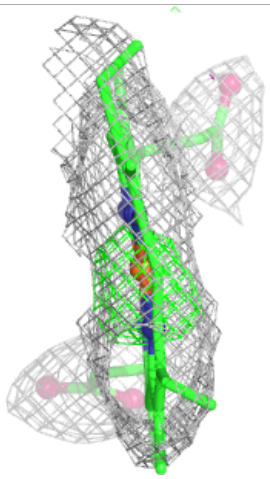


Electron density around HEC v 201:

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

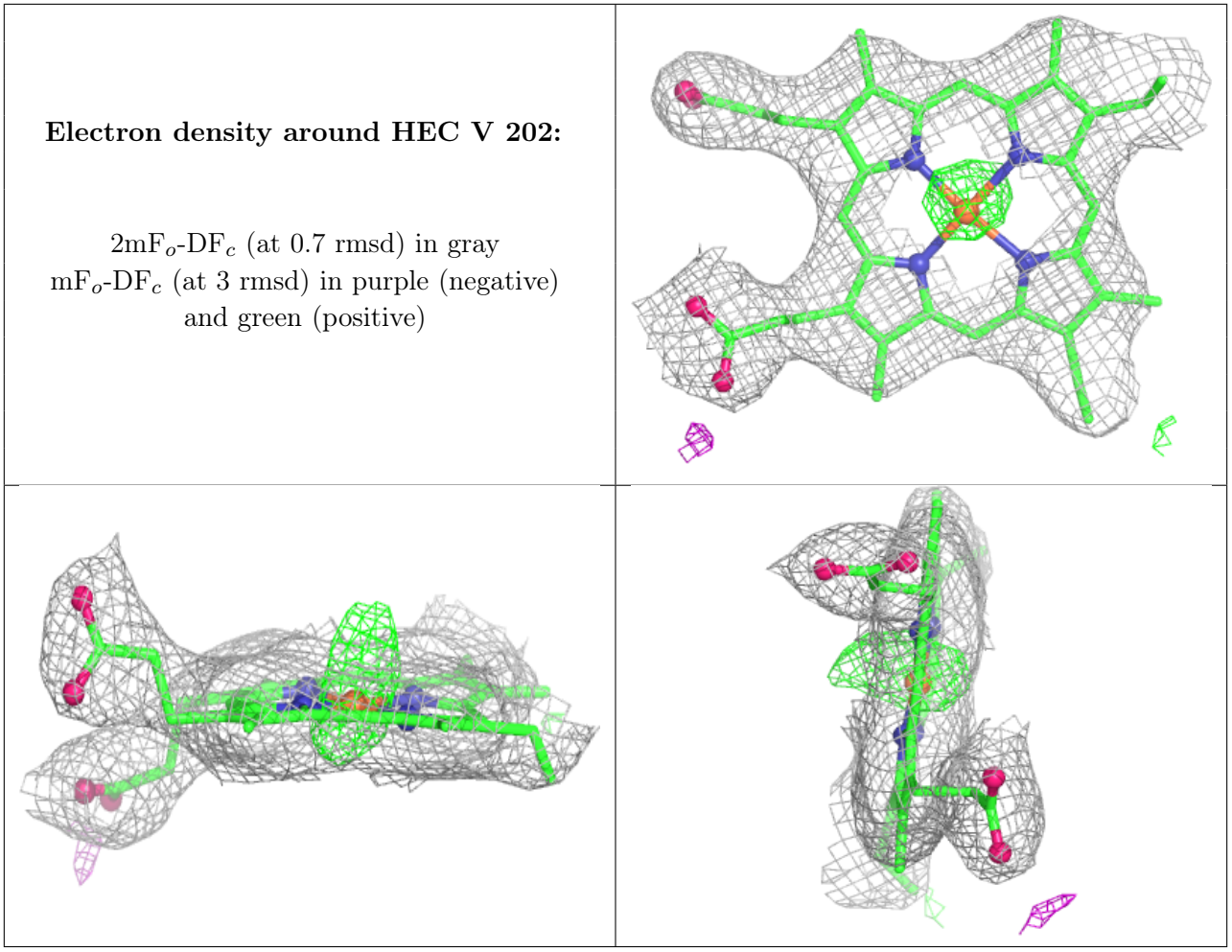






Electron density around HEC V 202:

$2mF_o$-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.