Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 09:21 AM UTC

PDB ID	:	7CJJ / pdb_00007cjj
Title	:	Photosystem II structure in the S2 state
Authors	:	Li, H.; Shen, J.-R.; Suga, M.
Deposited on	:	2020-07-11
Resolution	:	2.40 Å(reported)

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

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

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

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

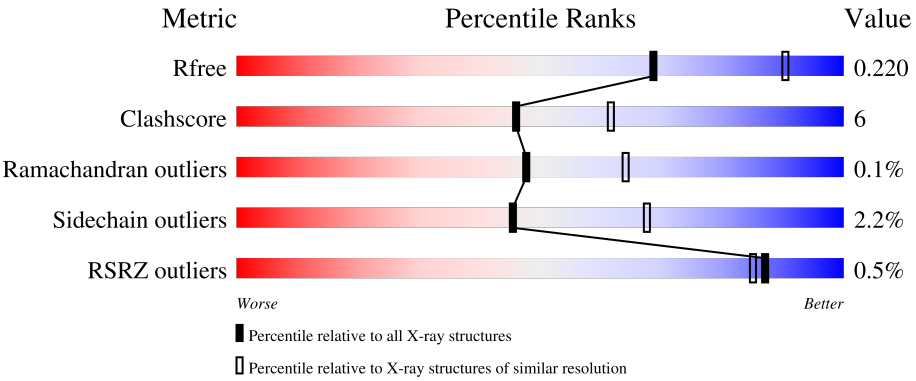
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

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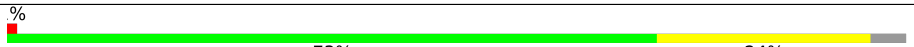
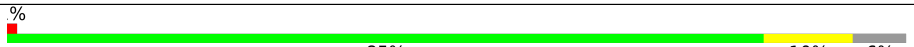
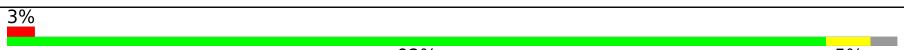
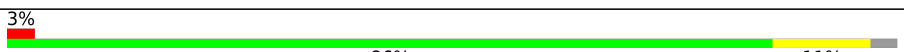
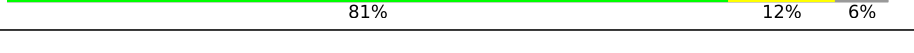
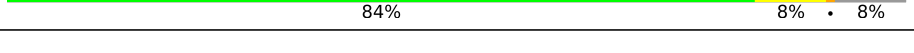
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	94% 5%
16	v	137	91% 8%
17	X	40	82% 12% 5%
17	x	40	90% 5% 5%
18	Y	30	7% 77% 20%
18	y	30	77% 17%
19	Z	62	84% 15%
19	z	62	3% 82% 18%
20	R	34	3% 94% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	C	515	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53612 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	18	0
			2773	1805	459	494	15			
1	a	334	Total	C	N	O	S	0	19	0
			2781	1811	460	495	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	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	5	0
			3522	2300	589	620	13			
3	c	455	Total	C	N	O	S	0	3	0
			3543	2316	592	622	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	4	0
			2764	1828	454	470	12			
4	d	341	Total	C	N	O	S	0	4	0
			2755	1823	453	467	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			668	435	108	125			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	3	0
			1886	1177	318	386	5			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	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 281	C 188	N 45	O 48	0	0	0
17	x	38	Total 281	C 188	N 45	O 48	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total 1	Cl 1	0	0
22	C	1	Total 1	Cl 1	0	0

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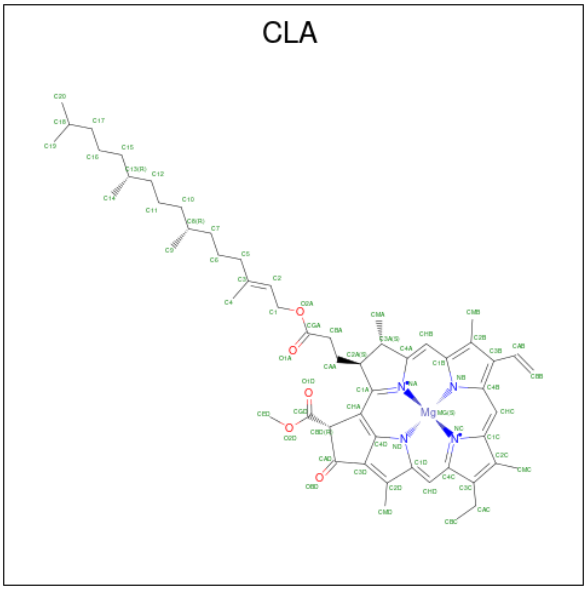
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	1	Total Cl 1 1	0	0
22	c	1	Total Cl 1 1	0	0

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

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

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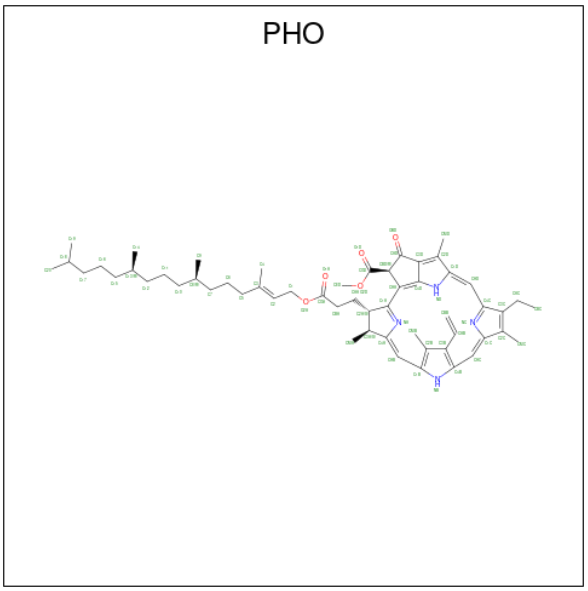
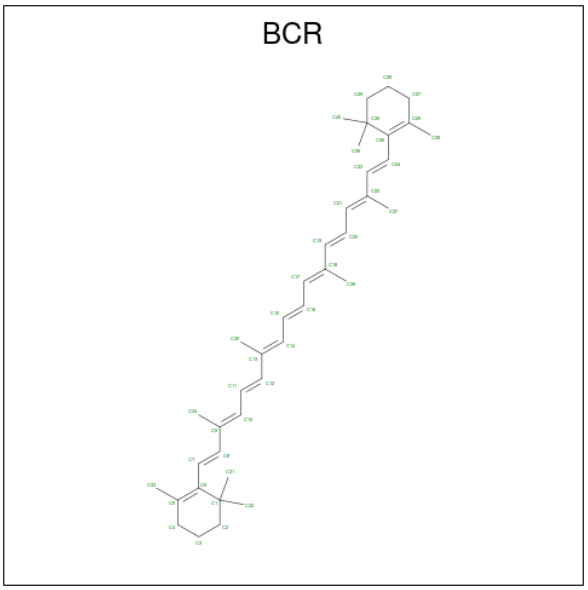
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



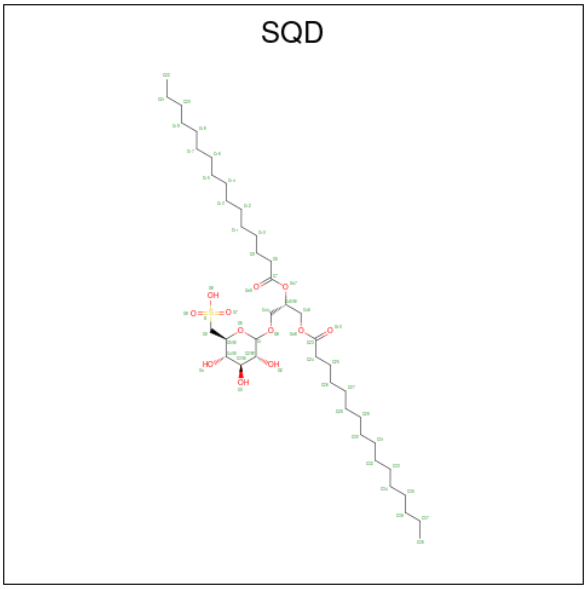
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



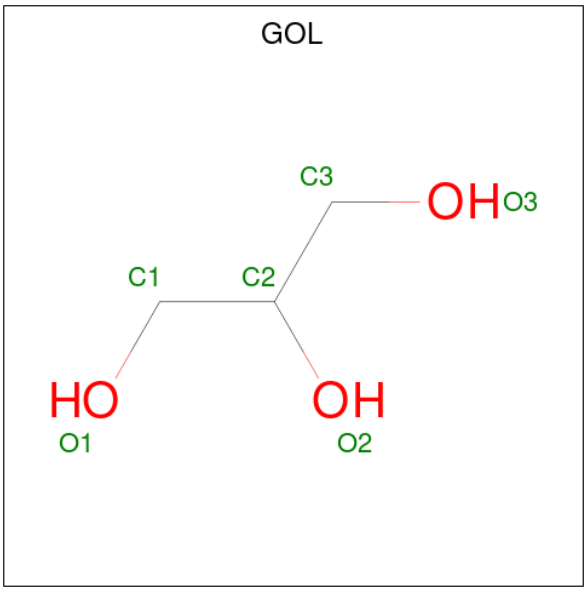
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total 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
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	k	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: $C_{41}H_{78}O_{12}S$).



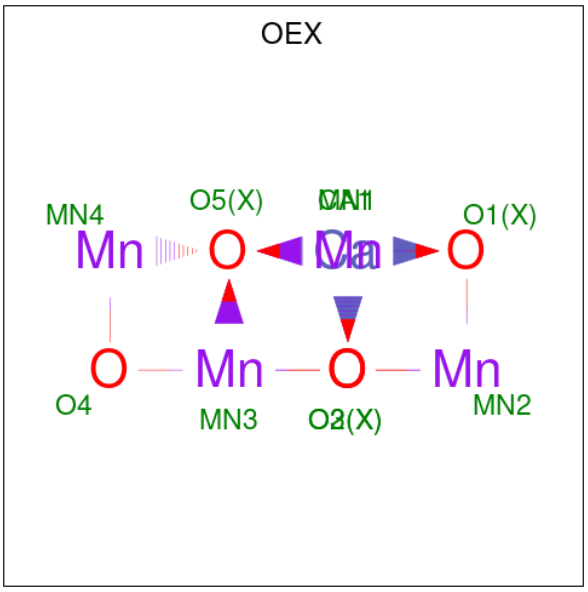
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0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

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



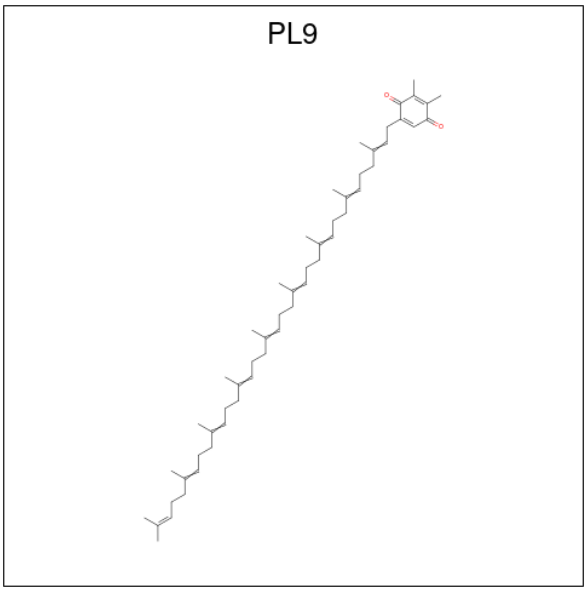
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27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

- 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	0	1
			20	2	8	10		
28	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- 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	0	1
			110	106	4		

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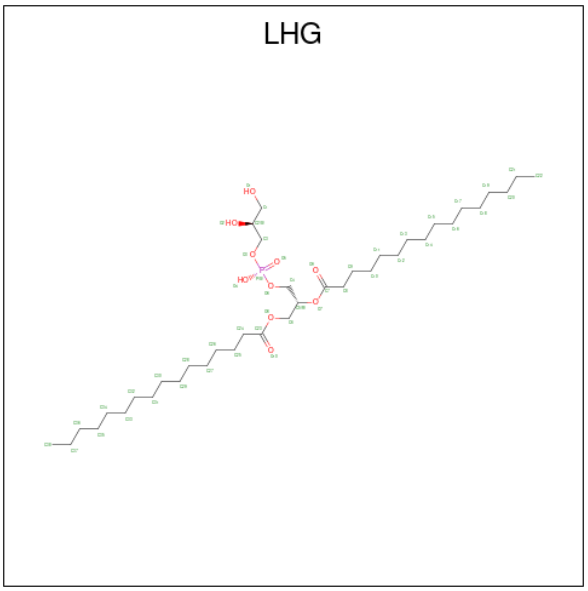
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total C O 55 53 2	0	0
29	a	1	Total C O 110 106 4	0	1
29	d	1	Total C O 55 53 2	0	0

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

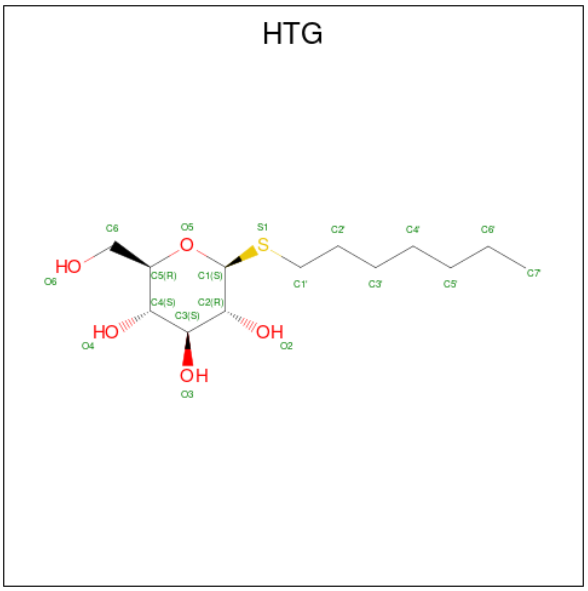
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	C	1	Total C O 34 29 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	3	Total C O 71 63 8	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0

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



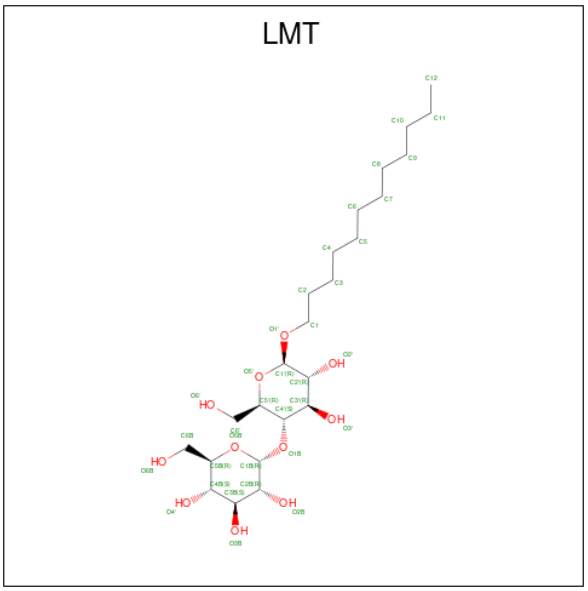
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



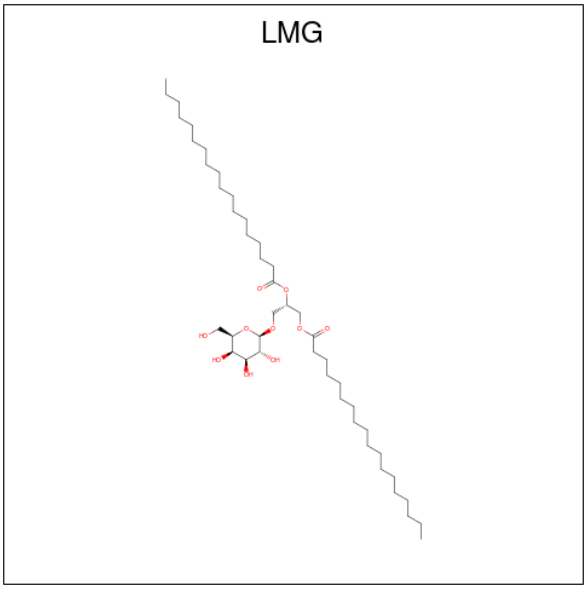
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	D	1	Total C O S 16 10 5 1	0	0
32	V	1	Total C O 11 6 5	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32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

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



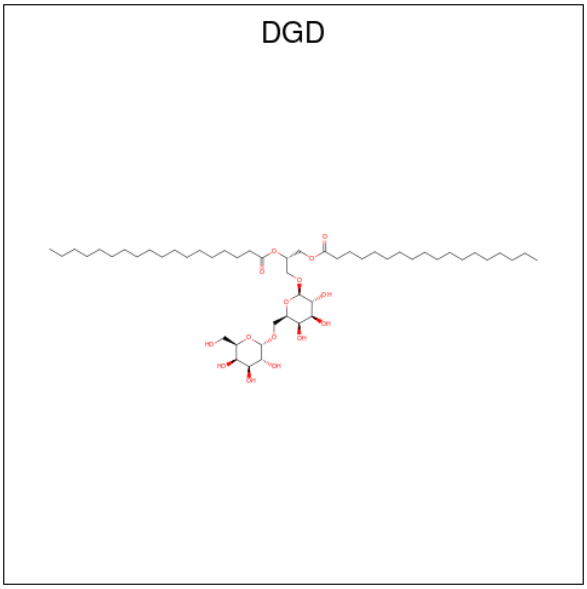
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			25	19	6		
33	B	1	Total	C	O	0	0
			26	19	7		
33	C	1	Total	C	O	0	0
			35	24	11		
33	D	1	Total	C	O	0	0
			35	24	11		
33	F	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	a	1	Total	C	O	0	0
			35	24	11		
33	a	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			25	19	6		
33	b	1	Total	C	O	0	0
			25	19	6		
33	e	1	Total	C	O	0	0
			35	24	11		
33	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	M	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0

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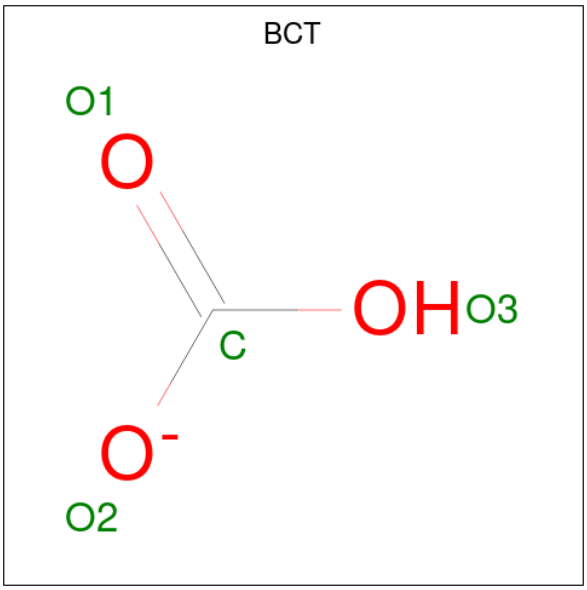
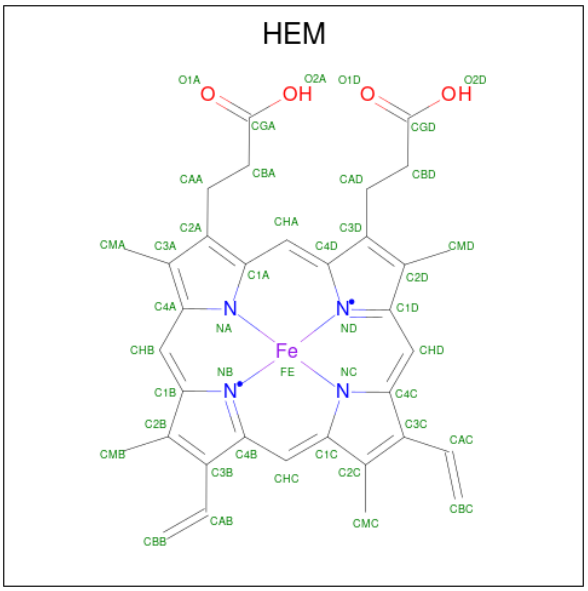
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Ca 1 1	0	0
36	a	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 8 2 6	0	1
37	d	1	Total C O 8 2 6	0	1

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

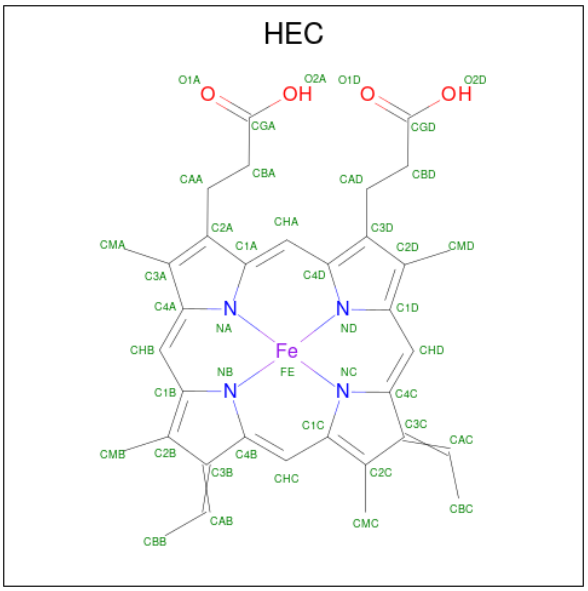


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	147	Total	O	0	11
			157	157		
41	B	218	Total	O	0	0
			218	218		
41	C	188	Total	O	0	4
			191	191		
41	D	124	Total	O	0	2
			126	126		
41	E	24	Total	O	0	0
			24	24		
41	F	8	Total	O	0	0
			8	8		
41	H	28	Total	O	0	0
			28	28		
41	I	4	Total	O	0	0
			4	4		
41	J	6	Total	O	0	0
			6	6		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 8 8	0	0
41	M	18	Total O 18 18	0	0
41	O	118	Total O 118 118	0	0
41	T	14	Total O 14 14	0	0
41	U	56	Total O 56 56	0	0
41	V	95	Total O 95 95	0	0
41	X	10	Total O 10 10	0	0
41	Y	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	139	Total O 150 150	0	12
41	b	220	Total O 220 220	0	0
41	c	169	Total O 172 172	0	4
41	d	129	Total O 129 129	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	22	Total O 22 22	0	0
41	i	1	Total O 1 1	0	0
41	j	4	Total O 4 4	0	0
41	k	5	Total O 5 5	0	0
41	l	8	Total O 8 8	0	0
41	m	10	Total O 10 10	0	0

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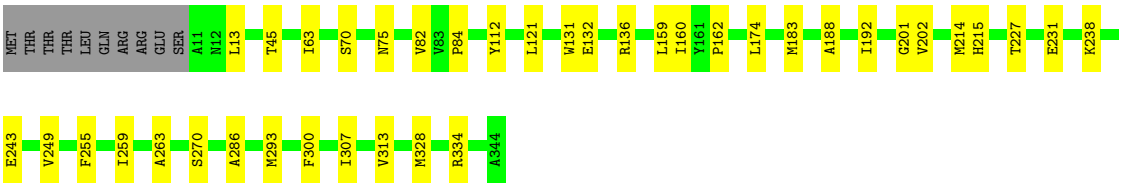
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	99	Total O 99 99	0	0
41	t	10	Total O 10 10	0	0
41	u	68	Total O 68 68	0	0
41	v	57	Total O 57 57	0	0
41	x	10	Total O 10 10	0	0
41	y	4	Total O 4 4	0	0

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.

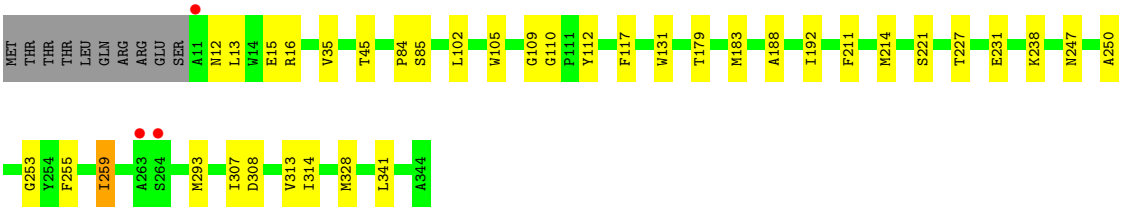
• Molecule 1: Photosystem II protein D1

Chain A:



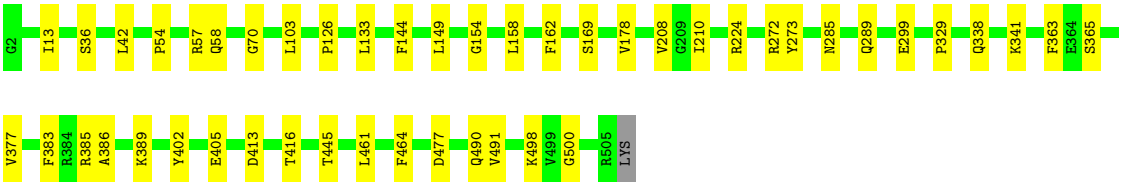
• Molecule 1: Photosystem II protein D1

Chain a:



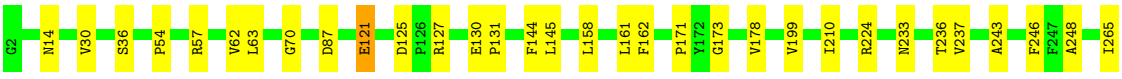
• Molecule 2: Photosystem II CP47 reaction center protein

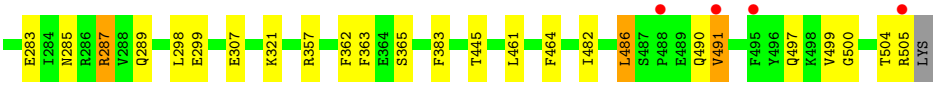
Chain B:



• Molecule 2: Photosystem II CP47 reaction center protein

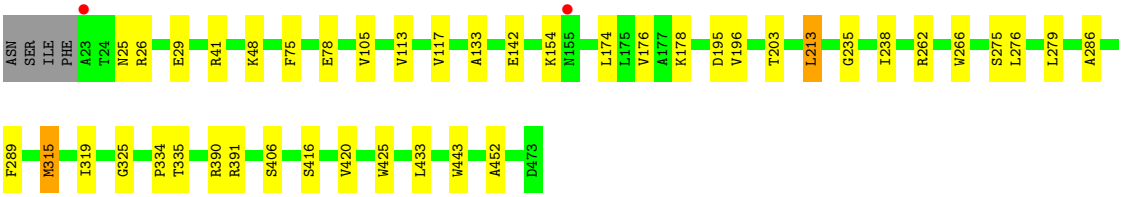
Chain b:





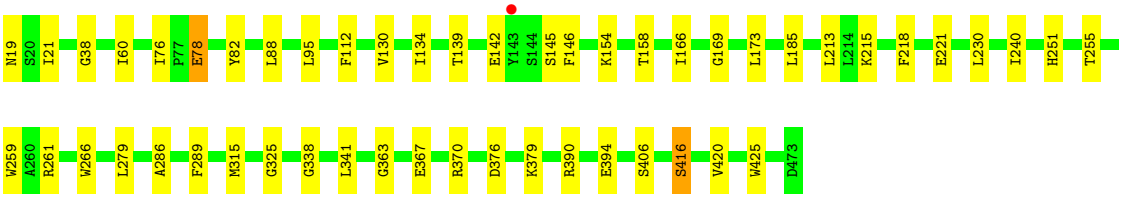
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



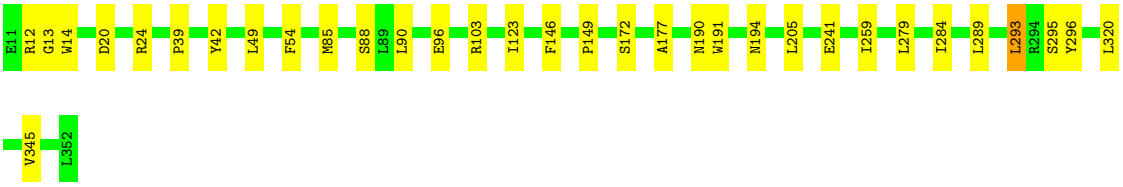
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



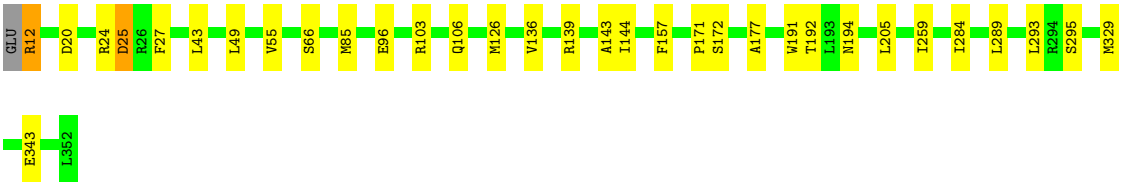
• Molecule 4: Photosystem II D2 protein

Chain D:



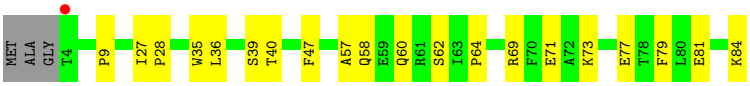
• Molecule 4: Photosystem II D2 protein

Chain d:

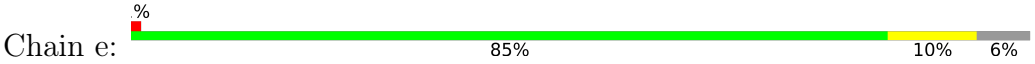


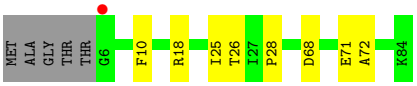
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

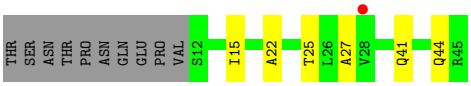


• Molecule 5: Cytochrome b559 subunit alpha

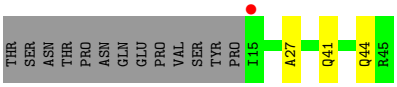




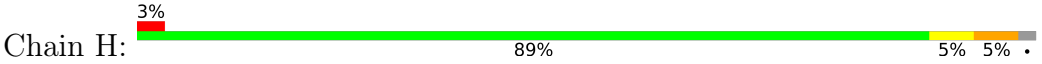
• Molecule 6: Cytochrome b559 subunit beta

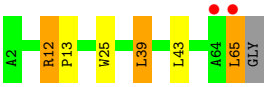


• Molecule 6: Cytochrome b559 subunit beta

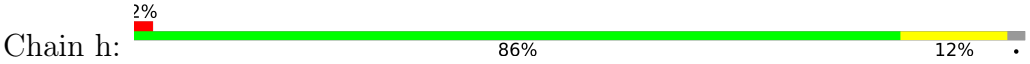


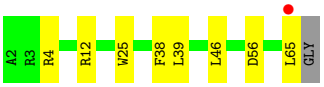
• Molecule 7: Photosystem II reaction center protein H



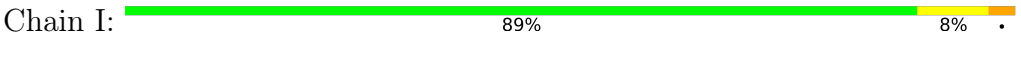


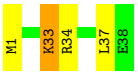
• Molecule 7: Photosystem II reaction center protein H





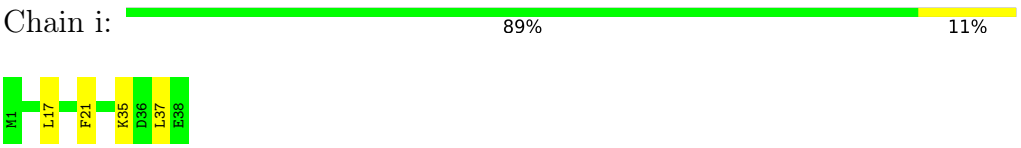
• Molecule 8: Photosystem II reaction center protein I





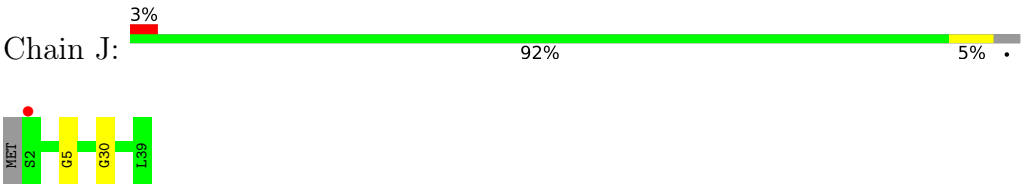
• Molecule 8: Photosystem II reaction center protein I

Chain i:



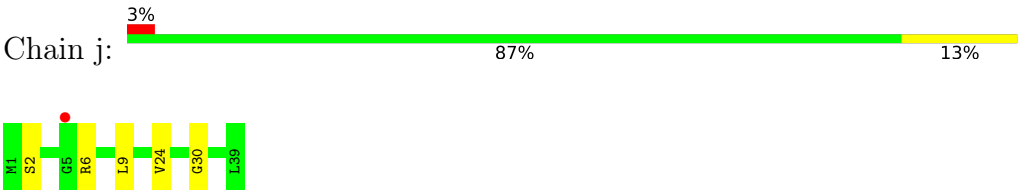
• Molecule 9: Photosystem II reaction center protein J

Chain J:



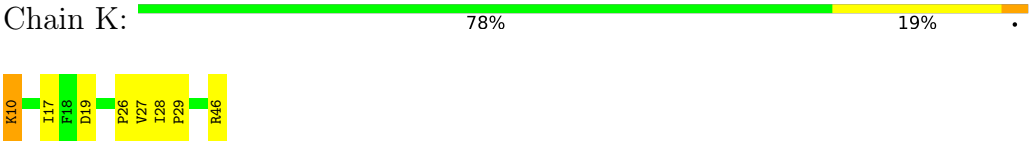
• Molecule 9: Photosystem II reaction center protein J

Chain j:



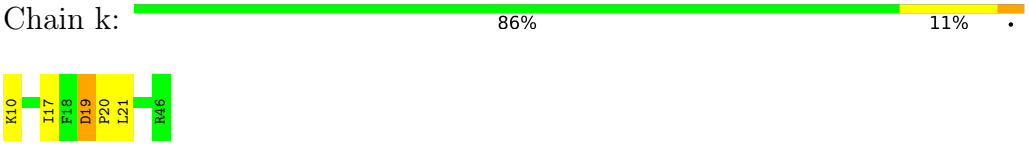
• Molecule 10: Photosystem II reaction center protein K

Chain K:



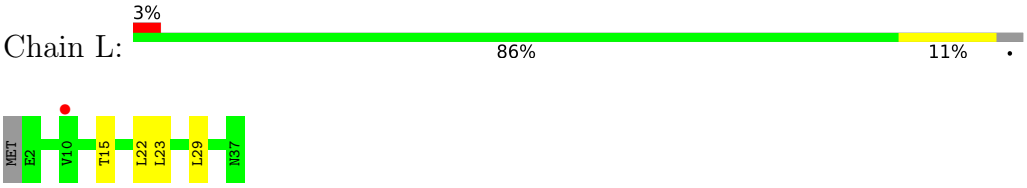
• Molecule 10: Photosystem II reaction center protein K

Chain k:



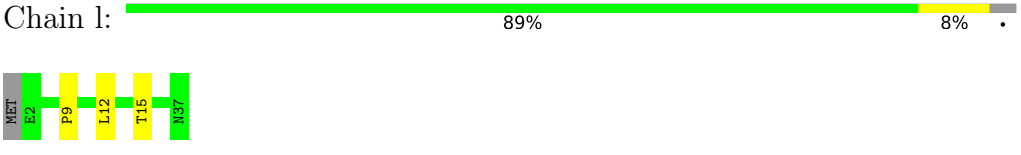
• Molecule 11: Photosystem II reaction center protein L

Chain L:



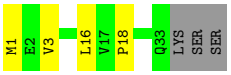
• Molecule 11: Photosystem II reaction center protein L

Chain l:



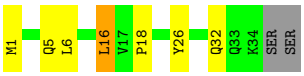
• Molecule 12: Photosystem II reaction center protein M

Chain M:



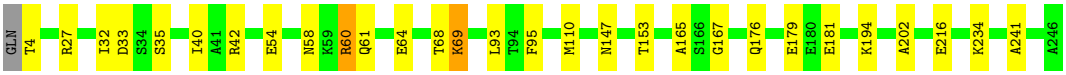
• Molecule 12: Photosystem II reaction center protein M

Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

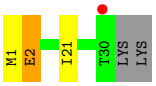


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

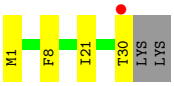
• Molecule 14: Photosystem II reaction center protein T

Chain T:



• Molecule 14: Photosystem II reaction center protein T

Chain t:

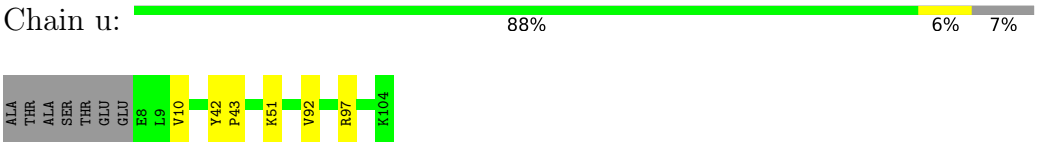


• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

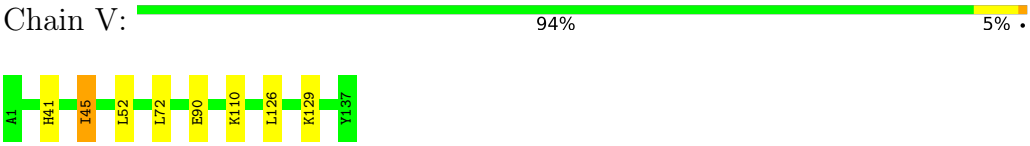
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



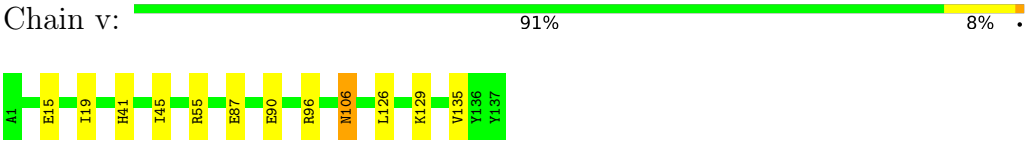
• Molecule 16: Cytochrome c-550

Chain V:



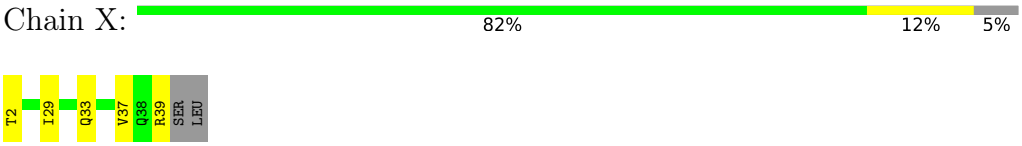
• Molecule 16: Cytochrome c-550

Chain v:



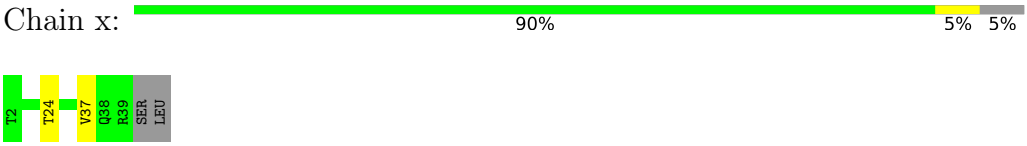
• Molecule 17: Photosystem II reaction center protein X

Chain X:



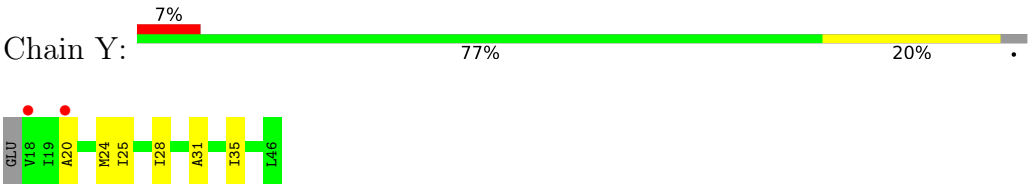
• Molecule 17: Photosystem II reaction center protein X

Chain x:



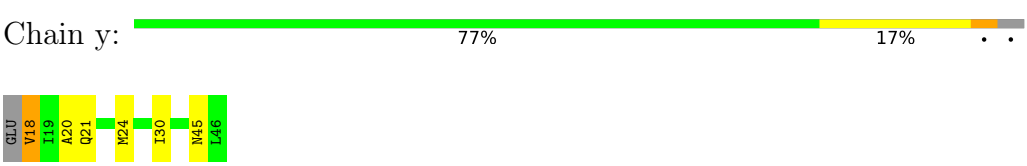
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



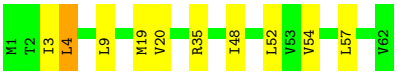
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



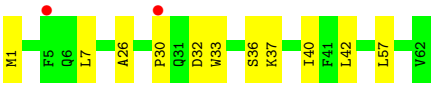
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



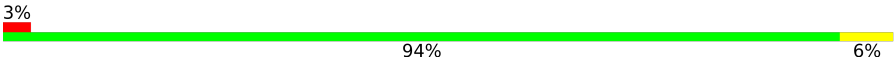
• Molecule 19: Photosystem II reaction center protein Z

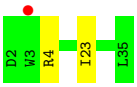
Chain z:



• 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	125.75Å 231.63Å 288.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.40 39.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.90-2.40) 82.1 (39.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.168 , 0.218 0.169 , 0.220	Depositor DCC
R_{free} test set	16450 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53612	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/2861	0.53	0/3897
1	a	0.32	0/2869	0.51	0/3908
2	B	0.33	0/4190	0.50	0/5708
2	b	0.31	0/4138	0.49	0/5640
3	C	0.29	0/3635	0.47	0/4948
3	c	0.27	0/3657	0.45	0/4978
4	D	0.35	0/2861	0.52	0/3897
4	d	0.32	0/2852	0.50	0/3885
5	E	0.26	0/687	0.46	0/936
5	e	0.27	0/667	0.45	0/908
6	F	0.28	0/284	0.45	0/387
6	f	0.23	0/257	0.45	0/349
7	H	0.27	0/530	0.49	0/723
7	h	0.27	0/519	0.48	0/708
8	I	0.24	0/311	0.38	0/419
8	i	0.27	0/311	0.42	0/419
9	J	0.27	0/278	0.46	0/376
9	j	0.25	0/283	0.41	0/383
10	K	0.25	0/303	0.44	0/416
10	k	0.27	0/303	0.48	0/416
11	L	0.40	0/311	0.50	0/423
11	l	0.33	0/311	0.53	0/423
12	M	0.40	0/261	0.52	0/357
12	m	0.32	0/262	0.49	0/357
13	O	0.32	0/1917	0.49	0/2599
13	o	0.29	0/1910	0.48	0/2589
14	T	0.35	0/257	0.46	0/349
14	t	0.34	0/257	0.43	0/349
15	U	0.33	0/776	0.54	0/1052
15	u	0.29	0/785	0.51	0/1064
16	V	0.31	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.27	0/1085	0.44	0/1473
17	X	0.23	0/284	0.37	0/384
17	x	0.20	0/284	0.37	0/384
18	Y	0.19	0/216	0.38	0/289
18	y	0.22	0/216	0.38	0/289
19	Z	0.20	0/490	0.37	0/669
19	z	0.21	0/490	0.34	0/669
20	R	0.20	0/279	0.37	0/383
All	All	0.31	0/43272	0.48	0/58876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2773	0	2626	27	0
1	a	2781	0	2636	28	0
2	B	4050	0	3894	35	0
2	b	3998	0	3852	39	0
3	C	3522	0	3429	32	0
3	c	3543	0	3451	34	0
4	D	2764	0	2656	28	0
4	d	2755	0	2650	23	0
5	E	668	0	652	15	0
5	e	648	0	634	5	0
6	F	275	0	282	6	0
6	f	250	0	261	3	0
7	H	517	0	542	7	0
7	h	506	0	529	8	0
8	I	314	0	328	3	0
8	i	314	0	328	2	0
9	J	272	0	279	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	3	0
10	K	293	0	305	5	0
10	k	293	0	305	3	0
11	L	304	0	314	4	0
11	l	304	0	314	3	0
12	M	268	0	283	3	0
12	m	269	0	288	6	0
13	O	1886	0	1856	17	0
13	o	1879	0	1850	13	0
14	T	258	0	261	2	0
14	t	258	0	261	3	0
15	U	765	0	767	5	0
15	u	774	0	773	3	0
16	V	1064	0	1073	6	0
16	v	1064	0	1073	9	0
17	X	281	0	312	4	0
17	x	281	0	312	3	0
18	Y	215	0	246	4	0
18	y	215	0	246	4	0
19	Z	479	0	516	5	0
19	z	479	0	516	4	0
20	R	273	0	305	2	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	1	0	0	0	0
22	C	1	0	0	0	0
22	a	1	0	0	0	0
22	c	1	0	0	0	0
23	A	260	0	288	14	0
23	B	1040	0	1152	33	0
23	C	845	0	936	36	0
23	D	130	0	144	4	0
23	a	260	0	288	12	0
23	b	1040	0	1152	36	0
23	c	845	0	936	45	0
23	d	130	0	144	5	0
24	A	128	0	148	2	0
24	a	128	0	148	2	0
25	A	40	0	56	2	0
25	B	160	0	224	14	0
25	C	80	0	112	5	0
25	D	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	T	40	0	56	8	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	11	0
25	c	80	0	112	7	0
25	d	40	0	56	4	0
25	h	40	0	56	5	0
25	k	80	0	112	4	0
26	A	108	0	155	3	0
26	B	54	0	78	3	0
26	D	43	0	53	3	0
26	L	54	0	78	1	0
26	a	108	0	155	4	0
26	f	43	0	53	3	0
27	A	6	0	8	0	0
27	B	18	0	24	1	0
27	C	6	0	8	0	0
27	O	6	0	8	0	0
27	a	6	0	8	1	0
27	b	12	0	16	1	0
27	c	12	0	16	1	0
27	v	6	0	8	1	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	13	0
29	D	55	0	80	3	0
29	a	110	0	160	12	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	C	34	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	32	0	0	1	0
30	d	71	0	0	0	0
30	i	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
31	A	49	0	74	4	0
31	D	98	0	148	6	0
31	E	42	0	57	5	0
31	L	49	0	74	3	0
31	a	42	0	57	3	0
31	b	49	0	74	0	0
31	d	147	0	222	13	0
32	B	57	0	78	6	0
32	C	19	0	26	0	0
32	D	16	0	17	2	0
32	V	11	0	10	0	0
32	b	57	0	78	2	0
32	c	19	0	26	1	0
32	h	16	0	17	1	0
33	B	86	0	116	1	0
33	C	35	0	46	1	0
33	D	35	0	46	2	0
33	F	35	0	46	1	0
33	M	70	0	92	3	0
33	a	70	0	92	4	0
33	b	50	0	70	1	0
33	e	35	0	46	0	0
33	m	35	0	46	0	0
34	C	153	0	216	10	0
34	D	51	0	72	0	0
34	M	51	0	72	2	0
34	Z	37	0	44	2	0
34	a	51	0	72	4	0
34	c	102	0	144	0	0
34	d	51	0	72	4	0
34	m	51	0	72	0	0
34	z	39	0	48	2	0
35	C	186	0	246	12	0
35	H	62	0	82	1	0
35	c	186	0	246	4	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
36	c	2	0	0	0	0
36	o	1	0	0	0	0
37	D	8	0	0	0	0
37	d	8	0	0	0	0
38	E	43	0	30	3	0
38	e	43	0	30	4	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	2	0
40	v	43	0	30	1	0
41	A	157	0	0	0	0
41	B	218	0	0	4	0
41	C	191	0	0	2	0
41	D	126	0	0	1	0
41	E	24	0	0	1	0
41	F	8	0	0	1	0
41	H	28	0	0	1	0
41	I	4	0	0	0	0
41	J	6	0	0	0	0
41	K	8	0	0	0	0
41	L	8	0	0	0	0
41	M	18	0	0	0	0
41	O	118	0	0	1	0
41	R	1	0	0	0	0
41	T	14	0	0	0	0
41	U	56	0	0	1	0
41	V	95	0	0	0	0
41	X	10	0	0	0	0
41	Y	1	0	0	0	0
41	a	150	0	0	1	0
41	b	220	0	0	2	0
41	c	172	0	0	6	0
41	d	129	0	0	0	0
41	e	15	0	0	1	0
41	f	5	0	0	1	0
41	h	22	0	0	0	0
41	i	1	0	0	0	0
41	j	4	0	0	0	0
41	k	5	0	0	1	0
41	l	8	0	0	0	0
41	m	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	o	99	0	0	0	0
41	t	10	0	0	0	0
41	u	68	0	0	0	0
41	v	57	0	0	1	0
41	x	10	0	0	0	0
41	y	4	0	0	1	0
All	All	53612	0	52351	600	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 (600) 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)
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.42	1.02
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.53	0.88
23:c:515:CLA:HBB1	25:c:516:BCR:H24C	1.58	0.84
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.60	0.83
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.63	0.81
23:B:604:CLA:H42	23:B:605:CLA:H2	1.64	0.80
23:b:604:CLA:H42	23:b:605:CLA:H2	1.63	0.79
1:A:214:MET:HG2	29:A:413[B]:PL9:H102	1.62	0.79
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.64	0.77
23:B:601:CLA:H12	23:B:601:CLA:H71	1.67	0.77
1:a:214:MET:HG2	29:a:414[B]:PL9:H102	1.66	0.76
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.72	0.71
1:A:214:MET:HG2	29:A:413[A]:PL9:H102	1.72	0.70
3:C:174:LEU:HB3	23:C:504:CLA:H152	1.76	0.68
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.74	0.68
2:B:341:LYS:NZ	32:B:622:HTG:O2	2.24	0.67
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.77	0.67
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.77	0.67
35:C:518:DGD:O1A	41:C:601:HOH:O	2.11	0.67
13:O:27:ARG:NH1	13:O:202:ALA:O	2.28	0.66
2:b:171:PRO:HD3	7:h:65:LEU:HD13	1.78	0.66
13:o:39:ARG:HG3	13:o:246:ALA:HB2	1.78	0.66
23:a:405:CLA:H203	34:d:411:LMG:H412	1.78	0.66
23:C:512:CLA:H52	31:D:408:LHG:H371	1.79	0.65
23:A:405:CLA:H202	31:E:101:LHG:H172	1.77	0.65
34:z:101:LMG:H302	34:z:101:LMG:H141	1.78	0.65
23:c:510:CLA:HBC3	23:c:512:CLA:H71	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:407:LHG:HC62	11:l:15:THR:HG23	1.79	0.64
16:v:106:ASN:OD1	16:v:106:ASN:N	2.29	0.64
32:B:624:HTG:H61	1:a:102:LEU:HD12	1.81	0.63
6:F:44:GLN:NE2	41:F:201:HOH:O	2.23	0.63
18:y:18:VAL:N	41:y:101:HOH:O	2.31	0.63
30:c:526:UNL:O6	41:c:601:HOH:O	2.16	0.63
25:B:631:BCR:HC8	25:B:631:BCR:H311	1.80	0.62
3:c:95:LEU:HD13	23:c:504:CLA:H142	1.82	0.62
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.81	0.62
32:B:621:HTG:H1	33:a:412:LMT:H12	1.82	0.61
23:c:505:CLA:HBB1	23:c:514:CLA:H41	1.82	0.61
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.35	0.61
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.82	0.61
3:C:433:LEU:HD22	23:C:504:CLA:HMC3	1.82	0.61
23:C:503:CLA:HBB1	23:C:503:CLA:HHC	1.81	0.61
1:A:227:THR:HB	1:A:231:GLU:HG3	1.83	0.61
13:O:58:ASN:ND2	41:O:401:HOH:O	2.23	0.60
3:C:262:ARG:NH2	33:C:526:LMT:O2'	2.30	0.60
26:L:102:SQD:H223	25:T:101:BCR:H351	1.83	0.60
2:b:482:ILE:HD12	2:b:486:LEU:HD12	1.84	0.60
1:a:259:ILE:HD12	29:a:414[B]:PL9:H222	1.82	0.60
26:a:409:SQD:H141	31:d:408:LHG:H152	1.83	0.59
3:c:19:ASN:ND2	41:c:609:HOH:O	2.35	0.59
3:C:176:VAL:HG21	3:C:238:ILE:HG13	1.84	0.59
38:E:102:HEM:O2A	41:E:201:HOH:O	2.17	0.59
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.84	0.59
23:A:407:CLA:H171	23:C:508:CLA:H121	1.85	0.59
3:C:275:SER:HB3	23:C:511:CLA:HED3	1.85	0.59
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.84	0.59
5:E:40:THR:HB	20:R:4:ARG:HD2	1.85	0.59
24:a:406:PHO:HAB	4:d:205:LEU:HD13	1.84	0.58
23:d:402:CLA:H191	34:d:411:LMG:H222	1.85	0.58
23:b:601:CLA:H72	23:b:601:CLA:H2	1.85	0.58
23:B:614:CLA:H43	26:B:620:SQD:H102	1.85	0.57
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.84	0.57
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.87	0.57
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.87	0.57
23:c:513:CLA:HBB1	23:c:513:CLA:HMB3	1.87	0.57
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.05	0.57
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.86	0.57
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:GLN:O	13:o:58:ASN:ND2	2.38	0.56
23:B:604:CLA:HBB1	23:B:604:CLA:HMB1	1.87	0.56
5:e:18:ARG:HH11	38:e:102:HEM:HBA2	1.69	0.56
33:D:402:LMT:H21	32:b:621:HTG:H3	1.87	0.56
23:C:505:CLA:HBB1	23:C:514:CLA:H41	1.86	0.56
23:c:503:CLA:C3D	23:c:505:CLA:H2	2.36	0.56
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.85	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.87	0.56
4:d:103:ARG:NH1	4:d:106:GLN:OE1	2.37	0.56
3:C:325:GLY:O	15:U:51:LYS:NZ	2.37	0.56
25:H:101:BCR:HC8	25:H:101:BCR:H331	1.88	0.56
3:c:146:PHE:HZ	23:c:514:CLA:HBB2	1.71	0.56
3:c:370:ARG:NH1	41:c:605:HOH:O	2.34	0.56
33:M:102:LMT:H6'1	12:m:32:GLN:HG2	1.88	0.56
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.87	0.56
29:A:413[B]:PL9:H28	31:E:101:LHG:H223	1.88	0.55
3:C:391:ARG:NH1	41:C:604:HOH:O	2.39	0.55
3:C:276:LEU:HD23	23:C:511:CLA:HED1	1.89	0.55
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.42	0.55
11:L:22:LEU:HD23	31:L:101:LHG:H172	1.89	0.55
10:k:19:ASP:OD2	41:k:201:HOH:O	2.17	0.55
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.88	0.55
34:a:417:LMG:H122	3:c:218:PHE:HE2	1.72	0.55
23:C:510:CLA:H203	35:C:519:DGD:HA92	1.89	0.55
23:a:404:CLA:HHC	23:a:404:CLA:HBB1	1.89	0.55
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.71	0.55
29:a:414[B]:PL9:H453	26:f:101:SQD:H262	1.89	0.54
32:B:621:HTG:H1'1	27:a:410:GOL:H12	1.89	0.54
15:U:86:GLU:H	15:U:86:GLU:CD	2.14	0.54
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.90	0.54
4:D:14:TRP:CD1	32:D:411:HTG:H61	2.43	0.54
3:c:325:GLY:O	15:u:51:LYS:NZ	2.39	0.54
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.90	0.54
23:C:508:CLA:HMC2	23:C:509:CLA:H102	1.89	0.54
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.54
38:e:102:HEM:HAC	6:f:27:ALA:HB1	1.90	0.54
23:a:407:CLA:H192	23:c:507:CLA:H142	1.89	0.53
3:c:286:ALA:HB2	23:c:504:CLA:HMD1	1.89	0.53
26:a:409:SQD:H271	31:d:408:LHG:H141	1.90	0.53
3:c:406:SER:HA	3:c:420:VAL:HG23	1.90	0.53
3:C:195:ASP:OD2	3:C:196:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:29:ILE:O	17:X:33:GLN:HG2	2.08	0.53
31:a:419:LHG:O5	5:e:10:PHE:HB2	2.08	0.53
2:b:283:GLU:OE2	2:b:287:ARG:NH1	2.37	0.53
31:A:416:LHG:H142	23:B:607:CLA:H201	1.90	0.53
23:A:404:CLA:HHC	23:A:404:CLA:HBB1	1.91	0.53
3:C:178:LYS:HB2	23:C:504:CLA:H172	1.90	0.52
34:C:521:LMG:H181	18:Y:25:ILE:HG12	1.91	0.52
25:H:101:BCR:H331	25:H:101:BCR:C8	2.38	0.52
34:M:101:LMG:HC71	34:M:101:LMG:O9	2.10	0.52
1:a:214:MET:HG2	29:a:414[B]:PL9:C10	2.37	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.52
13:O:68:THR:HG22	13:O:110[A]:MET:HG2	1.91	0.52
24:A:406:PHO:HAB	4:D:205:LEU:HD13	1.90	0.52
13:O:42:ARG:O	13:O:241:ALA:HA	2.10	0.52
10:k:21:LEU:HD13	18:y:24:MET:HE2	1.91	0.52
1:A:270:SER:HB2	26:A:409:SQD:O49	2.08	0.52
23:b:602:CLA:H101	23:b:609:CLA:H193	1.90	0.52
4:d:24:ARG:HD3	17:x:37:VAL:HG22	1.90	0.52
29:A:413[B]:PL9:H453	26:D:413:SQD:H282	1.91	0.52
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.27	0.52
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.45	0.52
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.92	0.52
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.91	0.52
2:b:87:ASP:OD2	32:b:624:HTG:O4	2.21	0.52
6:f:44:GLN:HG3	41:f:205:HOH:O	2.09	0.52
5:E:58:GLN:H	5:E:84:LYS:HZ2	1.58	0.51
2:b:357:ARG:NH1	27:b:627:GOL:O3	2.43	0.51
3:c:215:LYS:HD3	3:c:221:GLU:O	2.10	0.51
23:c:513:CLA:H191	34:z:101:LMG:H242	1.92	0.51
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.74	0.51
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.92	0.51
3:c:390:ARG:NH1	16:v:90:GLU:O	2.43	0.51
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.11	0.51
2:b:285:ASN:O	2:b:289:GLN:HG2	2.09	0.51
3:C:452:ALA:O	8:I:34:ARG:NH2	2.43	0.51
25:B:619:BCR:H331	25:B:619:BCR:C8	2.41	0.51
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.46	0.51
23:c:514:CLA:HHC	23:c:514:CLA:HBB1	1.92	0.51
1:A:300:PHE:HZ	35:C:520:DGD:HB61	1.76	0.51
23:B:616:CLA:HHC	23:B:616:CLA:HBB1	1.93	0.51
23:a:405:CLA:H122	29:a:414[B]:PL9:H203	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:507:CLA:CMD	23:c:509:CLA:HAB	2.40	0.51
1:a:227:THR:HB	1:a:231:GLU:HG3	1.91	0.51
1:a:45:THR:HG23	23:a:404:CLA:H201	1.93	0.51
3:c:425:TRP:CD1	23:c:506:CLA:HMA2	2.46	0.51
29:D:406:PL9:H411	11:L:29:LEU:HD23	1.93	0.50
1:a:15:GLU:HB2	33:a:418:LMT:H6'2	1.94	0.50
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.76	0.50
13:o:193:THR:HG21	13:o:220:LEU:HD12	1.92	0.50
23:B:602:CLA:HHC	23:B:602:CLA:HBB1	1.94	0.50
1:A:183:MET:HA	23:A:403:CLA:HMD1	1.92	0.50
2:b:464:PHE:CZ	31:d:406:LHG:H251	2.46	0.50
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	1.92	0.50
23:c:512:CLA:H52	31:d:408:LHG:H383	1.93	0.50
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.46	0.50
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.92	0.50
31:A:416:LHG:H361	23:B:613:CLA:H51	1.94	0.50
2:B:133:LEU:H	27:B:626:GOL:H31	1.76	0.50
3:C:425:TRP:CD1	23:C:506:CLA:HMA2	2.47	0.50
29:a:414[A]:PL9:H453	26:f:101:SQD:H262	1.93	0.50
31:d:408:LHG:H382	31:d:408:LHG:H122	1.93	0.50
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.93	0.50
2:b:125:ASP:OD1	2:b:127:ARG:NH1	2.45	0.50
41:c:610:HOH:O	34:d:411:LMG:H111	2.12	0.50
4:d:126:MET:HE3	4:d:143:ALA:O	2.12	0.50
29:D:406:PL9:H311	31:L:101:LHG:H201	1.93	0.49
2:b:491:VAL:HG13	4:d:136:VAL:HG13	1.93	0.49
3:C:279:LEU:HD22	23:C:511:CLA:HED2	1.93	0.49
38:E:102:HEM:HAC	6:F:27:ALA:HB1	1.94	0.49
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.48	0.49
23:A:405:CLA:H152	29:A:413[A]:PL9:H262	1.94	0.49
23:A:407:CLA:H193	23:C:508:CLA:H91	1.94	0.49
2:B:377:VAL:O	41:B:701:HOH:O	2.20	0.49
23:c:504:CLA:H193	32:c:523:HTG:H4'2	1.93	0.49
5:E:64:PRO:HB2	5:E:79:PHE:CD1	2.48	0.49
35:c:518:DGD:HG11	41:c:603:HOH:O	2.11	0.49
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.93	0.49
23:B:601:CLA:H72	23:B:601:CLA:C3D	2.42	0.49
23:B:616:CLA:H121	25:B:619:BCR:H12C	1.95	0.49
1:a:183:MET:HA	23:a:403:CLA:HMD1	1.95	0.49
29:A:413[A]:PL9:H453	26:D:413:SQD:H282	1.93	0.49
23:B:610:CLA:H122	23:B:615:CLA:HAA1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:619:BCR:H382	26:a:411:SQD:H241	1.95	0.49
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.59	0.49
31:A:416:LHG:H151	11:L:23:LEU:HD21	1.95	0.49
2:B:58:GLN:C	2:B:329:PRO:HB3	2.38	0.49
25:k:102:BCR:H321	25:k:102:BCR:HC8	1.94	0.49
19:z:1:MET:HE3	19:z:57:LEU:HD22	1.95	0.49
2:B:154:GLY:HA2	2:B:158:LEU:HD12	1.95	0.49
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.94	0.49
2:b:490:GLN:HG3	2:b:500:GLY:HA2	1.94	0.49
31:d:406:LHG:H212	12:m:18:PRO:HG3	1.94	0.49
2:B:149:LEU:HD13	23:B:604:CLA:H172	1.94	0.48
2:B:285:ASN:O	2:B:289:GLN:HG2	2.13	0.48
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.95	0.48
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.94	0.48
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.48	0.48
23:b:606:CLA:H72	25:b:619:BCR:H311	1.94	0.48
3:C:452:ALA:HB1	8:I:37:LEU:HD22	1.96	0.48
23:c:507:CLA:HBB1	23:c:507:CLA:HHC	1.95	0.48
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.95	0.48
31:D:408:LHG:H382	31:D:408:LHG:H112	1.95	0.48
13:O:33:ASP:OD2	13:O:35:SER:OG	2.25	0.48
3:c:76:ILE:HG22	3:c:78:GLU:HG2	1.96	0.48
23:c:510:CLA:H122	23:c:510:CLA:H162	1.53	0.48
34:C:502:LMG:H161	35:C:518:DGD:HA82	1.95	0.48
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.94	0.48
31:a:419:LHG:HC91	4:d:27:PHE:HZ	1.78	0.48
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.49	0.48
23:D:403:CLA:HBC3	23:D:403:CLA:HHD	1.96	0.48
16:v:45:ILE:HD13	27:v:201:GOL:H11	1.96	0.48
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.14	0.47
23:a:404:CLA:H52	29:d:405:PL9:H151	1.96	0.47
23:b:614:CLA:H62	23:b:614:CLA:H41	1.57	0.47
3:c:376:ASP:HB3	3:c:379:LYS:HB2	1.96	0.47
23:c:503:CLA:C4D	23:c:505:CLA:H2	2.45	0.47
3:C:443:TRP:CE2	23:C:510:CLA:HMD2	2.49	0.47
5:E:57:ALA:HB1	5:E:84:LYS:NZ	2.30	0.47
23:b:616:CLA:H152	23:b:616:CLA:H102	1.96	0.47
23:b:604:CLA:HMB1	23:b:604:CLA:HBB1	1.96	0.47
19:z:26:ALA:HB3	19:z:40:ILE:HD11	1.97	0.47
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.95	0.47
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:GLY:HA3	32:D:411:HTG:H62	1.96	0.47
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.78	0.47
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.49	0.47
23:b:613:CLA:H18	31:d:406:LHG:H202	1.96	0.47
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.50	0.47
2:b:130[B]:GLU:HG3	2:b:131:PRO:HD2	1.97	0.47
1:A:121[A]:LEU:HG	34:C:502:LMG:H182	1.97	0.47
23:a:404:CLA:HBA1	23:a:404:CLA:C4A	2.45	0.47
3:C:286:ALA:HB2	23:C:504:CLA:HMD2	1.97	0.47
31:L:101:LHG:H312	12:M:18:PRO:HB3	1.97	0.47
29:A:413[B]:PL9:H502	4:D:39:PRO:HG3	1.97	0.46
29:a:414[B]:PL9:H251	29:a:414[B]:PL9:H272	1.55	0.46
35:c:520:DGD:HAH1	34:d:411:LMG:H201	1.97	0.46
19:z:33:TRP:O	19:z:37:LYS:N	2.45	0.46
29:A:413[B]:PL9:H101	29:A:413[B]:PL9:C13	2.46	0.46
23:B:605:CLA:H61	23:B:605:CLA:H41	1.77	0.46
2:b:121:GLU:OE1	7:h:12:ARG:HD2	2.15	0.46
3:c:213:LEU:HD21	25:c:517:BCR:C19	2.45	0.46
31:d:407:LHG:H321	14:t:21:ILE:HD11	1.97	0.46
5:e:26:THR:HB	38:e:102:HEM:HAB	1.97	0.46
2:B:162:PHE:O	23:B:606:CLA:HHD	2.14	0.46
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.97	0.46
23:a:404:CLA:H143	23:a:404:CLA:H161	1.64	0.46
23:b:604:CLA:C4	23:b:605:CLA:H2	2.39	0.46
25:k:101:BCR:H371	25:k:101:BCR:H24C	1.63	0.46
3:C:433:LEU:HD13	23:C:504:CLA:CHC	2.46	0.46
4:D:194:ASN:HA	4:D:295:SER:OG	2.15	0.46
33:D:402:LMT:O4'	41:D:501:HOH:O	2.21	0.46
23:D:403:CLA:HBC3	23:D:403:CLA:CHD	2.44	0.46
2:B:386:ALA:HA	41:U:216:HOH:O	2.16	0.46
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.72	0.46
23:C:506:CLA:H42	35:C:519:DGD:HB52	1.98	0.46
3:c:95:LEU:HD21	23:c:503:CLA:OBD	2.16	0.46
4:D:146:PHE:O	4:D:149:PRO:HD2	2.14	0.46
23:B:613:CLA:H121	23:B:613:CLA:H162	1.52	0.46
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.15	0.46
4:d:194:ASN:HA	4:d:295:SER:OG	2.15	0.46
4:D:12:ARG:HH22	17:X:39:ARG:HH12	1.64	0.46
23:a:407:CLA:H102	23:a:407:CLA:H62	1.41	0.46
2:B:13:ILE:HG12	23:B:612:CLA:HAC2	1.98	0.46
23:B:602:CLA:H203	23:B:602:CLA:H162	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:506:CLA:H41	23:C:506:CLA:H62	1.70	0.46
23:C:510:CLA:HBC3	23:C:512:CLA:H71	1.97	0.46
2:b:233:ASN:O	2:b:236:THR:HG22	2.16	0.46
23:b:603:CLA:HAB	23:b:605:CLA:H152	1.98	0.46
16:v:41:HIS:HA	16:v:45:ILE:O	2.16	0.46
23:B:615:CLA:H152	23:B:615:CLA:H112	1.65	0.45
2:b:30:VAL:HG12	23:b:605:CLA:HHD	1.97	0.45
3:c:38:GLY:HA3	23:c:513:CLA:HMD2	1.97	0.45
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.45
1:a:117:PHE:HB3	34:a:417:LMG:H162	1.98	0.45
2:b:307:GLU:OE2	41:b:701:HOH:O	2.21	0.45
23:b:604:CLA:H13	23:b:604:CLA:H172	1.69	0.45
3:c:338:GLY:HA3	3:c:341:LEU:O	2.16	0.45
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.81	0.45
1:A:160:ILE:HD11	35:C:518:DGD:HBT2	1.98	0.45
1:A:307:ILE:HD13	1:A:313:VAL:HA	1.98	0.45
35:C:519:DGD:HBF2	35:C:519:DGD:HBE2	1.66	0.45
5:E:35:TRP:HZ2	33:F:101:LMT:H1'	1.81	0.45
13:O:216:GLU:CD	13:O:234:LYS:HD2	2.41	0.45
23:B:606:CLA:H161	23:B:606:CLA:H122	1.54	0.45
34:C:502:LMG:H391	35:C:518:DGD:HB51	1.99	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.45
25:k:102:BCR:H15C	25:k:102:BCR:H351	1.83	0.45
26:B:620:SQD:H351	26:B:620:SQD:H383	1.85	0.45
3:C:390:ARG:NH1	16:V:90:GLU:O	2.47	0.45
19:Z:19:MET:HE2	34:Z:101:LMG:H241	1.97	0.45
3:c:363:GLY:O	3:c:367:GLU:HG2	2.17	0.45
11:l:12:LEU:HD23	12:m:26:TYR:HB2	1.99	0.45
2:B:103:LEU:HD21	23:B:605:CLA:HMC3	1.99	0.45
23:C:507:CLA:HAA1	23:C:507:CLA:HBD	1.99	0.45
23:C:512:CLA:HBB1	23:C:512:CLA:HMB1	1.97	0.45
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.97	0.45
1:a:211:PHE:CD2	29:a:414[A]:PL9:H101	2.52	0.45
33:a:418:LMT:O4'	41:a:501:HOH:O	2.21	0.45
3:c:154:LYS:HE3	3:c:266:TRP:CD2	2.52	0.45
4:d:20:ASP:HB3	17:x:37:VAL:HG21	1.99	0.45
13:o:68:THR:HB	13:o:108:VAL:HB	1.97	0.45
23:B:616:CLA:H41	23:B:616:CLA:H62	1.46	0.45
5:E:9:PRO:HA	31:E:101:LHG:HC31	1.98	0.45
26:a:409:SQD:H132	26:a:409:SQD:H162	1.77	0.45
23:c:512:CLA:H61	23:c:512:CLA:H102	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.98	0.45
41:B:884:HOH:O	13:O:179:GLU:HG3	2.15	0.45
23:b:616:CLA:H92	23:b:616:CLA:H62	1.78	0.45
3:C:113:VAL:HG12	34:C:522:LMG:H161	1.99	0.45
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.99	0.45
16:V:52:LEU:HD12	40:V:201:HEC:HAD2	1.99	0.45
29:a:414[B]:PL9:H503	17:x:24:THR:OG1	2.17	0.45
33:a:418:LMT:H11	3:c:259:TRP:HB2	1.98	0.45
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.97	0.45
3:c:112:PHE:HE2	25:c:516:BCR:HC31	1.82	0.45
23:c:510:CLA:H92	31:d:408:LHG:H162	1.98	0.45
4:D:49:LEU:HD13	25:D:405:BCR:C15	2.47	0.44
31:a:419:LHG:HC91	4:d:27:PHE:CZ	2.52	0.44
23:b:604:CLA:HMD1	23:b:612:CLA:H203	1.99	0.44
23:c:505:CLA:HBB1	23:c:505:CLA:HHC	1.99	0.44
23:A:405:CLA:H172	29:A:413[A]:PL9:H261	1.99	0.44
2:B:477:ASP:OD1	2:B:477:ASP:N	2.50	0.44
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.98	0.44
25:B:618:BCR:H363	25:B:631:BCR:H19C	1.99	0.44
33:B:629:LMT:H123	14:t:8:PHE:HA	1.99	0.44
29:a:414[B]:PL9:H201	29:a:414[B]:PL9:H23	1.98	0.44
2:b:445:THR:HA	41:b:705:HOH:O	2.17	0.44
23:b:610:CLA:H122	23:b:615:CLA:HAA1	1.99	0.44
23:c:510:CLA:HMB1	23:c:510:CLA:HBB1	1.99	0.44
13:o:42:ARG:O	13:o:241:ALA:HA	2.17	0.44
23:C:504:CLA:H143	23:C:504:CLA:H161	1.89	0.44
35:C:520:DGD:HB91	35:C:520:DGD:HB62	1.80	0.44
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.86	0.44
25:d:404:BCR:H15C	25:d:404:BCR:H351	1.81	0.44
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.44
23:b:613:CLA:H72	23:b:613:CLA:H111	1.73	0.44
3:c:261:ARG:NH2	41:c:617:HOH:O	2.51	0.44
2:B:363:PHE:HB3	2:B:365:SER:O	2.18	0.44
23:C:508:CLA:H152	23:C:508:CLA:H18	1.70	0.44
5:E:77:GLU:O	5:E:81:GLU:HG2	2.18	0.44
25:K:101:BCR:H371	25:K:101:BCR:H24C	1.60	0.44
23:b:603:CLA:H141	23:b:603:CLA:H161	1.80	0.44
23:b:613:CLA:H151	23:b:613:CLA:H112	1.68	0.44
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.99	0.44
25:A:408:BCR:H24C	25:A:408:BCR:H371	1.63	0.44
3:C:26:ARG:HE	10:K:46:ARG:NH1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.52	0.44
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.87	0.44
23:c:508:CLA:H162	23:c:508:CLA:H122	1.77	0.44
29:A:413[B]:PL9:H403	6:F:22:ALA:HB2	2.00	0.44
23:B:607:CLA:H192	29:D:406:PL9:H303	2.00	0.44
31:D:408:LHG:H121	31:D:408:LHG:H361	1.99	0.44
13:O:40:ILE:HG13	13:O:95:PHE:CD1	2.52	0.44
1:a:85:SER:HA	1:a:109:GLY:HA3	2.00	0.44
1:a:179:THR:O	1:a:183:MET:HG3	2.18	0.44
23:b:604:CLA:H62	23:b:604:CLA:H92	1.68	0.44
2:b:62:VAL:HB	23:b:605:CLA:HED3	2.00	0.44
23:c:506:CLA:H203	31:d:408:LHG:H191	1.99	0.44
35:c:519:DGD:HAT1	35:c:520:DGD:HBE2	2.00	0.44
12:m:16:LEU:HD12	12:m:16:LEU:HA	1.81	0.44
2:B:385:ARG:HG2	13:O:165:ALA:O	2.18	0.43
2:B:413:ASP:OD2	2:B:416:THR:OG1	2.27	0.43
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.00	0.43
1:a:247:ASN:HB3	2:b:482:ILE:HD11	2.00	0.43
1:a:308:ASP:HB3	1:a:314:ILE:HD11	2.00	0.43
3:c:82:TYR:OH	3:c:394:GLU:OE2	2.31	0.43
26:B:620:SQD:H332	26:B:620:SQD:H301	1.89	0.43
41:B:777:HOH:O	7:H:65:LEU:HD21	2.17	0.43
23:C:508:CLA:H93	23:C:508:CLA:H61	1.83	0.43
23:D:404:CLA:H92	7:H:39:LEU:HD12	2.00	0.43
13:O:58:ASN:C	13:O:60:ARG:H	2.26	0.43
25:a:408:BCR:H24C	25:a:408:BCR:H371	1.61	0.43
16:v:41:HIS:CD2	40:v:202:HEC:NB	2.85	0.43
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	2.01	0.43
25:A:408:BCR:H11C	25:A:408:BCR:H341	1.93	0.43
23:C:503:CLA:C3D	23:C:505:CLA:H2	2.48	0.43
4:D:12:ARG:HH22	17:X:39:ARG:NH1	2.16	0.43
1:a:12:ASN:O	1:a:16:ARG:HG3	2.18	0.43
3:c:213:LEU:HD23	23:c:508:CLA:H202	2.01	0.43
25:c:516:BCR:H15C	25:c:516:BCR:H351	1.85	0.43
23:B:612:CLA:H61	23:B:612:CLA:H102	1.89	0.43
2:B:126:PRO:HB3	7:H:12[B]:ARG:HH21	1.84	0.43
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	1.99	0.43
25:B:618:BCR:H331	25:B:618:BCR:C8	2.48	0.43
31:D:407:LHG:HC62	11:L:15:THR:HG23	2.01	0.43
23:b:612:CLA:H61	23:b:612:CLA:H102	1.84	0.43
23:c:507:CLA:H61	23:c:507:CLA:H101	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:403:CLA:H191	31:D:407:LHG:H332	2.00	0.43
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.54	0.43
23:B:616:CLA:H41	23:B:616:CLA:H92	2.01	0.43
7:H:12[B]:ARG:HD2	41:H:219:HOH:O	2.18	0.43
7:H:12[B]:ARG:HB3	7:H:13:PRO:HD3	2.00	0.43
15:U:73:GLN:O	15:U:77:GLU:HG3	2.18	0.43
2:b:145:LEU:HD22	23:b:604:CLA:H192	2.00	0.43
23:b:605:CLA:H41	23:b:605:CLA:H62	1.73	0.43
5:e:25:ILE:O	5:e:28:PRO:HD2	2.17	0.43
25:h:102:BCR:H331	25:h:102:BCR:C8	2.48	0.43
1:A:263:ALA:HA	31:E:101:LHG:H282	1.99	0.43
25:B:631:BCR:H382	25:B:631:BCR:H23C	2.00	0.43
5:E:27:ILE:HD11	38:E:102:HEM:HBC2	2.01	0.43
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.73	0.43
23:c:511:CLA:HBB1	23:c:511:CLA:HMB1	1.99	0.43
23:B:613:CLA:H143	23:B:613:CLA:H111	1.89	0.43
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.82	0.43
1:a:221[A]:SER:HA	4:d:139:ARG:HB2	2.00	0.43
23:c:515:CLA:HBB1	25:c:516:BCR:H371	2.00	0.43
7:h:25:TRP:CD1	32:h:101:HTG:H1	2.54	0.43
3:C:117:VAL:HG11	34:C:522:LMG:H361	2.00	0.43
13:O:32:ILE:HG13	13:O:93:LEU:HD11	2.01	0.43
29:a:414[A]:PL9:H251	29:a:414[A]:PL9:H272	1.47	0.43
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.01	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.43
25:C:517:BCR:H24C	25:C:517:BCR:H371	1.85	0.43
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.94	0.43
3:c:185:LEU:HB2	3:c:230:LEU:HD13	2.01	0.43
23:d:403:CLA:H41	23:d:403:CLA:H61	1.67	0.43
1:A:215[A]:HIS:HA	29:A:413[A]:PL9:O1	2.18	0.42
1:a:84:PRO:HA	1:a:112:TYR:CG	2.54	0.42
1:a:221[B]:SER:HA	4:d:139:ARG:HB2	2.01	0.42
38:e:102:HEM:O2A	41:e:201:HOH:O	2.22	0.42
1:A:202:VAL:HG11	23:A:405:CLA:C3D	2.49	0.42
23:A:407:CLA:H61	23:A:407:CLA:H41	1.78	0.42
4:D:146:PHE:C	4:D:149:PRO:HD2	2.43	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.56	0.42
4:d:55:VAL:O	4:d:66:SER:HB3	2.19	0.42
7:h:38:PHE:HB2	25:h:102:BCR:C10	2.49	0.42
23:C:510:CLA:H142	23:C:510:CLA:H111	1.85	0.42
23:C:512:CLA:H152	23:C:512:CLA:H112	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:618:BCR:H371	25:b:618:BCR:H24C	1.67	0.42
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.43	0.42
23:B:607:CLA:H122	34:M:101:LMG:H241	2.00	0.42
25:C:517:BCR:H11C	25:C:517:BCR:H341	1.91	0.42
31:D:407:LHG:H322	14:T:21:ILE:HD11	2.00	0.42
25:T:101:BCR:HC8	25:T:101:BCR:H321	2.01	0.42
1:a:131:TRP:CH2	23:c:507:CLA:HAA2	2.54	0.42
23:C:503:CLA:C4D	23:C:505:CLA:H2	2.50	0.42
10:K:26:PRO:O	10:K:29:PRO:HD2	2.19	0.42
12:M:16[B]:LEU:HD23	12:m:16:LEU:HD23	2.02	0.42
25:T:101:BCR:H311	25:T:101:BCR:C8	2.50	0.42
29:a:414[B]:PL9:H471	26:f:101:SQD:H291	2.02	0.42
23:c:515:CLA:H203	23:c:515:CLA:H161	1.82	0.42
13:o:10:ILE:HG23	13:o:15:LEU:HB2	2.01	0.42
13:o:40:ILE:HG12	13:o:243:ILE:CD1	2.48	0.42
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.20	0.42
1:A:45:THR:HG23	23:A:404:CLA:H201	2.01	0.42
23:A:404:CLA:C4A	23:A:404:CLA:HBA1	2.50	0.42
33:M:103:LMT:O2'	12:m:6:LEU:HD11	2.19	0.42
23:B:601:CLA:H62	25:H:101:BCR:H402	2.01	0.42
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.02	0.42
3:C:315:MET:O	3:C:319:ILE:HG13	2.19	0.42
23:C:512:CLA:HED2	23:C:512:CLA:H2	2.01	0.42
34:C:521:LMG:H191	10:K:27:VAL:HG11	2.00	0.42
5:E:36:LEU:HA	5:E:39:SER:OG	2.19	0.42
10:K:28:ILE:HD11	18:Y:28:ILE:HD13	2.01	0.42
13:O:69:LYS:HE2	13:O:69:LYS:HB2	1.74	0.42
19:Z:48:ILE:HD11	34:Z:101:LMG:H191	2.00	0.42
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.79	0.42
23:c:507:CLA:HAA1	23:c:507:CLA:HBD	2.00	0.42
16:v:55:ARG:HD2	41:v:339:HOH:O	2.18	0.42
1:A:159:LEU:C	1:A:162:PRO:HD2	2.44	0.42
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.42
25:B:631:BCR:H24C	25:B:631:BCR:H371	1.84	0.42
3:C:41:ARG:NH1	23:C:513:CLA:HMD1	2.35	0.42
33:M:102:LMT:H6D	11:l:9:PRO:HA	2.02	0.42
16:V:72:LEU:HD23	16:V:72:LEU:HA	1.93	0.42
23:a:403:CLA:CBD	23:a:404:CLA:HAC2	2.49	0.42
2:b:248:ALA:HB2	23:b:603:CLA:H52	2.01	0.42
3:c:166:ILE:HG21	23:c:514:CLA:H171	2.02	0.42
7:h:38:PHE:HB2	25:h:102:BCR:H10C	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:407:CLA:H192	23:A:407:CLA:H161	1.80	0.42
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.95	0.42
32:B:621:HTG:H6'2	32:B:621:HTG:H3'1	1.90	0.42
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.42
35:C:519:DGD:HA81	35:C:519:DGD:HAE2	1.74	0.42
23:D:404:CLA:HHC	23:D:404:CLA:HBB1	2.00	0.42
2:b:237:VAL:HG22	23:b:610:CLA:HBC2	2.01	0.42
25:b:619:BCR:H20C	25:b:619:BCR:H361	1.85	0.42
3:c:130:VAL:O	3:c:134:ILE:HG12	2.20	0.42
23:c:507:CLA:HMD3	23:c:509:CLA:HAB	2.02	0.42
18:y:20:ALA:O	18:y:24:MET:HG2	2.20	0.42
24:A:415:PHO:HBC3	4:D:279:LEU:HD22	2.02	0.42
13:O:54:GLU:HG2	13:O:64:GLU:H	1.85	0.42
16:V:41:HIS:CD2	40:V:201:HEC:NB	2.88	0.42
23:c:513:CLA:H91	23:c:513:CLA:H111	1.80	0.42
23:c:514:CLA:O2D	23:c:515:CLA:HBB2	2.20	0.42
4:d:12:ARG:NH2	4:d:12:ARG:HB2	2.35	0.42
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.84	0.41
25:T:101:BCR:H382	25:T:101:BCR:H23C	2.01	0.41
18:Y:31:ALA:O	18:Y:35:ILE:HG13	2.19	0.41
3:c:169:GLY:O	3:c:173:LEU:HG	2.20	0.41
23:c:514:CLA:H142	23:c:514:CLA:H111	1.91	0.41
1:A:201:GLY:HA3	1:A:286:ALA:HB2	2.02	0.41
23:B:603:CLA:CGA	23:B:603:CLA:H3A	2.50	0.41
34:C:502:LMG:H232	23:C:507:CLA:H92	2.01	0.41
23:C:504:CLA:H192	23:C:504:CLA:H162	1.76	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.75	0.41
31:E:101:LHG:H261	31:E:101:LHG:H291	1.72	0.41
23:a:407:CLA:H203	23:c:508:CLA:H101	2.01	0.41
2:b:499:VAL:HG22	4:d:25:ASP:CG	2.45	0.41
23:c:512:CLA:H111	23:c:512:CLA:H142	1.78	0.41
4:d:43:LEU:HD22	25:d:404:BCR:H323	2.03	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.88	0.41
13:o:23:ASP:HB3	13:o:25:THR:HG23	2.01	0.41
13:o:142:PHE:HB2	13:o:199:LEU:HB2	2.02	0.41
25:B:631:BCR:HC7	25:B:631:BCR:H331	1.68	0.41
16:V:41:HIS:HA	16:V:45:ILE:O	2.20	0.41
24:a:416:PHO:NC	24:a:416:PHO:ND	2.67	0.41
16:v:87:GLU:CD	16:v:96:ARG:HH12	2.27	0.41
23:A:403:CLA:CBD	23:A:404:CLA:HAC2	2.51	0.41
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:404:BCR:H403	9:j:24:VAL:HG21	2.01	0.41
26:A:409:SQD:H81	26:A:409:SQD:H112	1.59	0.41
35:C:518:DGD:HA81	35:C:518:DGD:HAE1	1.87	0.41
1:a:238:LYS:HE3	14:t:30:THR:OG1	2.20	0.41
3:c:60:ILE:HG22	23:c:505:CLA:HHD	2.02	0.41
3:c:88:LEU:HB3	23:c:505:CLA:HED3	2.02	0.41
25:h:102:BCR:H24C	25:h:102:BCR:H371	1.68	0.41
29:A:413[B]:PL9:H151	29:A:413[B]:PL9:H171	1.80	0.41
31:A:416:LHG:H251	2:B:464:PHE:CZ	2.55	0.41
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.88	0.41
2:B:272:ARG:HG3	2:B:273:TYR:N	2.34	0.41
2:B:490:GLN:HE21	2:B:500:GLY:HA2	1.85	0.41
34:C:522:LMG:H422	34:C:522:LMG:H392	1.84	0.41
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.56	0.41
15:U:59:GLU:OE1	15:U:59:GLU:N	2.43	0.41
2:b:363:PHE:HB3	2:b:365:SER:O	2.21	0.41
23:b:605:CLA:H192	23:b:609:CLA:HBB2	2.03	0.41
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.55	0.41
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	2.01	0.41
25:b:619:BCR:H341	25:b:619:BCR:H11C	1.74	0.41
25:c:517:BCR:H15C	25:c:517:BCR:H351	1.85	0.41
15:u:42:TYR:HA	15:u:43:PRO:HA	1.87	0.41
2:B:149:LEU:HD12	2:B:149:LEU:HA	1.88	0.41
2:B:445:THR:HA	41:B:715:HOH:O	2.19	0.41
25:B:619:BCR:H331	25:B:619:BCR:HC8	2.03	0.41
32:B:622:HTG:O6	13:O:176:GLN:OE1	2.33	0.41
3:C:25:ASN:O	3:C:41:ARG:HD3	2.20	0.41
3:C:48:LYS:HG2	3:C:133:ALA:O	2.21	0.41
3:C:213:LEU:HD21	25:C:517:BCR:C20	2.51	0.41
23:C:508:CLA:HBA1	23:C:508:CLA:H3A	1.76	0.41
35:C:519:DGD:HA81	35:C:519:DGD:HA51	1.80	0.41
34:C:521:LMG:H202	34:C:521:LMG:H171	1.74	0.41
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.03	0.41
23:b:608:CLA:H192	23:d:403:CLA:HAA2	2.03	0.41
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.53	0.41
26:A:409:SQD:H181	26:A:409:SQD:H212	1.83	0.41
4:D:12:ARG:NH2	4:D:20:ASP:OD2	2.54	0.41
4:D:42:TYR:OH	6:F:25:THR:O	2.36	0.41
26:D:413:SQD:H342	26:D:413:SQD:H311	1.96	0.41
10:K:10:LYS:HB3	10:K:10:LYS:HE3	1.65	0.41
1:a:341:LEU:HD22	27:c:502:GOL:H31	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:626:LMT:H82	33:b:626:LMT:H112	1.84	0.41
31:d:408:LHG:H131	31:d:408:LHG:H102	1.94	0.41
23:b:602:CLA:H41	7:h:46:LEU:HA	2.04	0.40
23:b:605:CLA:H141	23:b:605:CLA:H161	1.77	0.40
25:b:619:BCR:C8	25:b:619:BCR:H331	2.51	0.40
23:c:509:CLA:H161	23:c:509:CLA:H203	1.67	0.40
25:c:516:BCR:H11C	25:c:516:BCR:H341	1.81	0.40
8:i:35:LYS:O	8:i:37:LEU:N	2.55	0.40
9:j:6:ARG:HH21	9:j:6:ARG:HA	1.86	0.40
1:A:63:ILE:HB	3:C:335:THR:HG21	2.03	0.40
1:A:121[B]:LEU:HD23	1:A:121[B]:LEU:HA	1.92	0.40
23:C:505:CLA:H192	23:C:505:CLA:H161	1.94	0.40
23:C:515:CLA:HBB1	25:C:516:BCR:H24C	2.03	0.40
3:c:154:LYS:HE3	3:c:266:TRP:CG	2.56	0.40
23:c:512:CLA:HBA1	23:c:512:CLA:H3A	1.77	0.40
23:d:403:CLA:HHC	23:d:403:CLA:HBB1	2.03	0.40
13:O:147:ASN:OD1	13:O:194:LYS:HE3	2.20	0.40
34:a:417:LMG:H172	34:a:417:LMG:H201	1.87	0.40
34:a:417:LMG:H402	35:c:518:DGD:HB71	2.03	0.40
2:b:162:PHE:O	23:b:606:CLA:HHD	2.21	0.40
2:b:321:LYS:HB3	2:b:321:LYS:HE3	1.74	0.40
23:b:613:CLA:H203	23:b:613:CLA:H161	1.93	0.40
3:c:158:THR:O	3:c:251:HIS:HB3	2.21	0.40
4:d:49:LEU:HD13	25:d:404:BCR:C15	2.52	0.40
4:d:157:PHE:CE2	4:d:171:PRO:HG2	2.56	0.40
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.56	0.40
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.03	0.40
1:A:70:SER:O	1:A:75:ASN:HB2	2.21	0.40
1:A:131:TRP:CD2	1:A:131:TRP:C	2.96	0.40
1:A:132:GLU:O	1:A:136:ARG:HG2	2.22	0.40
2:B:498:LYS:HD2	4:D:20:ASP:HA	2.03	0.40
25:C:516:BCR:H11C	25:C:516:BCR:H341	1.88	0.40
2:b:497:GLN:HB2	2:b:504:THR:HB	2.03	0.40
25:b:618:BCR:H20C	25:b:618:BCR:H361	1.96	0.40
31:d:407:LHG:H351	31:d:407:LHG:H382	1.84	0.40
29:A:413[B]:PL9:H372	29:A:413[B]:PL9:H351	1.81	0.40
19:Z:52:LEU:H	19:Z:52:LEU:HG	1.74	0.40
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.57	0.40
23:c:505:CLA:H192	23:c:505:CLA:H161	1.88	0.40
25:h:102:BCR:H11C	25:h:102:BCR:H341	1.96	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	349/344 (102%)	345 (99%)	3 (1%)	1 (0%)	36 50
1	a	350/344 (102%)	345 (99%)	4 (1%)	1 (0%)	36 50
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100 100
2	b	506/505 (100%)	496 (98%)	10 (2%)	0	100 100
3	C	454/455 (100%)	447 (98%)	5 (1%)	2 (0%)	30 43
3	c	456/455 (100%)	445 (98%)	10 (2%)	1 (0%)	43 58
4	D	344/342 (101%)	334 (97%)	10 (3%)	0	100 100
4	d	343/342 (100%)	331 (96%)	12 (4%)	0	100 100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100 100
5	e	77/84 (92%)	74 (96%)	3 (4%)	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%)	61 (97%)	2 (3%)	0	100 100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
9	J	36/39 (92%)	32 (89%)	3 (8%)	1 (3%)	4 3
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%)	32 (100%)	0	0	100 100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100 100
13	O	244/244 (100%)	236 (97%)	7 (3%)	1 (0%)	30 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	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%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	10
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5286/5384 (98%)	5165 (98%)	113 (2%)	8 (0%)	48	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
13	O	61	GLN
19	z	30	PRO
9	J	5	GLY
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	286/279 (102%)	283 (99%)	3 (1%)	68 84
1	a	287/279 (103%)	285 (99%)	2 (1%)	76 88
2	B	412/403 (102%)	409 (99%)	3 (1%)	76 88
2	b	406/403 (101%)	394 (97%)	12 (3%)	36 58
3	C	357/356 (100%)	351 (98%)	6 (2%)	53 74
3	c	359/356 (101%)	351 (98%)	8 (2%)	45 67
4	D	281/277 (101%)	277 (99%)	4 (1%)	59 79
4	d	280/277 (101%)	274 (98%)	6 (2%)	47 69
5	E	73/73 (100%)	72 (99%)	1 (1%)	59 79
5	e	70/73 (96%)	69 (99%)	1 (1%)	59 79
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	25/38 (66%)	25 (100%)	0	100 100
7	H	55/54 (102%)	50 (91%)	5 (9%)	9 14
7	h	54/54 (100%)	52 (96%)	2 (4%)	30 51
8	I	34/34 (100%)	33 (97%)	1 (3%)	37 60
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	26/27 (96%)	24 (92%)	2 (8%)	12 20
10	K	30/30 (100%)	27 (90%)	3 (10%)	7 11
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 11
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%)	30 (100%)	0	100 100
12	m	30/32 (94%)	28 (93%)	2 (7%)	15 26
13	O	209/207 (101%)	205 (98%)	4 (2%)	50 71
13	o	208/207 (100%)	203 (98%)	5 (2%)	43 65
14	T	26/28 (93%)	25 (96%)	1 (4%)	29 49
14	t	26/28 (93%)	26 (100%)	0	100 100
15	U	83/89 (93%)	80 (96%)	3 (4%)	31 52
15	u	84/89 (94%)	83 (99%)	1 (1%)	63 81
16	V	117/117 (100%)	115 (98%)	2 (2%)	53 74
16	v	117/117 (100%)	114 (97%)	3 (3%)	40 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	X	31/33 (94%)	30 (97%)	1 (3%)	34 56
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3 5
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12 20
19	z	52/52 (100%)	49 (94%)	3 (6%)	18 32
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4392/4403 (100%)	4298 (98%)	94 (2%)	45 69

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	238	LYS
1	A	243	GLU
2	B	169	SER
2	B	208	VAL
2	B	389	LYS
3	C	29	GLU
3	C	78	GLU
3	C	142	GLU
3	C	213	LEU
3	C	289	PHE
3	C	315	MET
4	D	241	GLU
4	D	259	ILE
4	D	293	LEU
4	D	345	VAL
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	39	LEU
7	H	43	LEU
7	H	65	LEU
8	I	33	LYS
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
13	O	4	THR
13	O	60	ARG

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Mol	Chain	Res	Type
13	O	69	LYS
13	O	181	GLU
14	T	2	GLU
15	U	56	GLU
15	U	70	ARG
15	U	86	GLU
16	V	45	ILE
16	V	110	LYS
17	X	2	THR
19	Z	3	ILE
19	Z	4	LEU
19	Z	20	VAL
19	Z	35	ARG
1	a	13	LEU
1	a	35	VAL
2	b	14	ASN
2	b	36	SER
2	b	63	LEU
2	b	121	GLU
2	b	161	LEU
2	b	287	ARG
2	b	298	LEU
2	b	299	GLU
2	b	362	PHE
2	b	486	LEU
2	b	491	VAL
2	b	505	ARG
3	c	21	ILE
3	c	78	GLU
3	c	145	SER
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	416	SER
4	d	12	ARG
4	d	25	ASP
4	d	144	ILE
4	d	259	ILE
4	d	293	LEU
4	d	329	MET
5	e	71	GLU

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Mol	Chain	Res	Type
7	h	39	LEU
7	h	56	ASP
9	j	2	SER
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
12	m	16	LEU
13	o	25	THR
13	o	37	THR
13	o	69	LYS
13	o	80	GLN
13	o	118	LEU
15	u	10	VAL
16	v	15	GLU
16	v	19	ILE
16	v	106	ASN
18	y	18	VAL
18	y	30	ILE
18	y	45	ASN
19	z	7	LEU
19	z	32	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	331	ASN
3	C	44	ASN
3	C	322	GLN
3	C	415	ASN
4	D	186	GLN
13	O	80	GLN
13	O	130	GLN
13	O	132	ASN
15	U	78	ASN
15	U	81	HIS
1	a	165	GLN
2	b	14	ASN
2	b	281	GLN
2	b	331	ASN

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Mol	Chain	Res	Type
3	c	28	GLN
3	c	322	GLN
3	c	373	ASN
3	c	415	ASN
13	o	196	GLN
15	u	78	ASN
19	z	58	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	0.65	0	8,9,11	1.44	2 (25%)
14	FME	T	1	14	8,9,10	0.67	0	8,9,11	1.15	1 (12%)
12	FME	M	1	12	8,9,10	0.64	0	8,9,11	1.46	3 (37%)
12	FME	m	1	12	8,9,10	0.65	0	8,9,11	1.19	1 (12%)
8	FME	i	1	8	8,9,10	0.63	0	8,9,11	0.88	0
8	FME	I	1	8	8,9,10	0.67	0	8,9,11	1.09	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	O-C-CA	-2.77	117.65	124.77
12	M	1	FME	CA-N-CN	-2.68	118.70	122.82
14	t	1	FME	O-C-CA	-2.60	118.08	124.77
14	t	1	FME	CA-N-CN	-2.42	119.10	122.82
12	M	1	FME	O-C-CA	-2.25	118.99	124.77
8	I	1	FME	O-C-CA	-2.14	119.28	124.77
12	m	1	FME	O-C-CA	-2.13	119.31	124.77
12	M	1	FME	O1-CN-N	-2.05	120.03	125.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 224 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 189 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	$\#\|Z\| > 2$
31	LHG	d	406	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	5 (9%)
23	CLA	c	509	41	69,73,73	2.08	19 (27%)	82,113,113	2.72	30 (36%)
23	CLA	C	505	-	69,73,73	2.02	20 (28%)	82,113,113	2.71	29 (35%)
23	CLA	b	603	-	69,73,73	2.06	20 (28%)	82,113,113	2.77	32 (39%)
23	CLA	C	510	-	69,73,73	1.99	20 (28%)	82,113,113	2.72	28 (34%)
26	SQD	D	413	-	41,43,54	1.09	2 (4%)	51,54,65	1.83	10 (19%)
23	CLA	A	404	41	69,73,73	2.00	20 (28%)	82,113,113	2.80	33 (40%)
28	OEX	A	412[B]	41,1,3	0,15,15	-	-	-		
23	CLA	b	610	41	69,73,73	1.98	18 (26%)	82,113,113	2.72	32 (39%)
23	CLA	b	611	-	69,73,73	1.95	20 (28%)	82,113,113	2.71	30 (36%)
40	HEC	v	202	16	46,50,50	1.88	5 (10%)	58,82,82	1.87	7 (12%)
31	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.07	2 (4%)
24	PHO	A	406	-	58,69,69	2.67	12 (20%)	55,99,99	2.86	16 (29%)
27	GOL	B	626	-	5,5,5	0.92	0	5,5,5	1.21	0
33	LMT	B	627	-	36,36,36	0.43	0	47,47,47	1.14	4 (8%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.86	14 (25%)
34	LMG	C	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.03	2 (3%)
33	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.94	3 (6%)
23	CLA	C	509	41	69,73,73	1.98	19 (27%)	82,113,113	2.65	29 (35%)
31	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	1.01	4 (7%)
23	CLA	b	605	-	69,73,73	1.99	21 (30%)	82,113,113	2.80	32 (39%)
32	HTG	D	411	-	16,16,19	0.97	2 (12%)	20,21,24	1.22	1 (5%)
31	LHG	A	416	-	48,48,48	0.88	2 (4%)	51,54,54	1.24	5 (9%)
23	CLA	c	510	-	69,73,73	2.09	21 (30%)	82,113,113	2.72	30 (36%)
23	CLA	d	402	-	69,73,73	1.88	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	B	616	-	69,73,73	2.00	19 (27%)	82,113,113	2.73	31 (37%)
23	CLA	B	614	-	69,73,73	1.99	18 (26%)	82,113,113	2.90	32 (39%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.06	4 (5%)
33	LMT	a	412	-	36,36,36	0.65	1 (2%)	47,47,47	1.31	5 (10%)
33	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	0.94	3 (6%)
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.37	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	508	-	69,73,73	2.05	20 (28%)	82,113,113	2.64	30 (36%)
28	OEX	a	413[A]	41,1,3	0,15,15	-	-	-		
34	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.03	3 (5%)
34	LMG	M	101	-	51,51,55	1.03	2 (3%)	59,59,63	1.08	3 (5%)
25	BCR	h	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
27	GOL	b	623	-	5,5,5	0.99	0	5,5,5	1.19	1 (20%)
37	BCT	d	401[B]	21	3,3,3	0.50	0	2,3,3	1.50	0
23	CLA	b	612	-	69,73,73	1.98	18 (26%)	82,113,113	2.78	30 (36%)
25	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	6 (10%)
34	LMG	d	411	39	51,51,55	0.92	2 (3%)	59,59,63	0.92	1 (1%)
25	BCR	b	619	-	41,41,41	1.20	2 (4%)	56,56,56	1.64	12 (21%)
29	PL9	A	413[A]	-	55,55,55	0.67	2 (3%)	68,69,69	2.01	22 (32%)
27	GOL	b	627	-	5,5,5	1.00	0	5,5,5	1.10	1 (20%)
25	BCR	C	517	-	41,41,41	1.04	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	d	403	-	69,73,73	2.09	22 (31%)	82,113,113	2.76	32 (39%)
31	LHG	D	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	4 (7%)
35	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.01	4 (5%)
23	CLA	B	606	-	69,73,73	2.00	21 (30%)	82,113,113	2.77	31 (37%)
23	CLA	C	513	3	69,73,73	2.06	22 (31%)	82,113,113	2.60	29 (35%)
32	HTG	c	523	-	19,19,19	0.91	2 (10%)	23,24,24	1.17	1 (4%)
25	BCR	k	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.68	12 (21%)
27	GOL	O	302	-	5,5,5	0.93	0	5,5,5	1.06	0
33	LMT	B	630	-	26,26,36	0.51	1 (3%)	31,31,47	1.02	2 (6%)
33	LMT	M	103	-	36,36,36	0.52	0	47,47,47	1.09	3 (6%)
23	CLA	a	405	41	69,73,73	1.92	20 (28%)	82,113,113	2.71	32 (39%)
23	CLA	b	607	41	69,73,73	2.01	19 (27%)	82,113,113	2.70	32 (39%)
34	LMG	C	522	-	51,51,55	1.04	3 (5%)	59,59,63	1.39	7 (11%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.10	3 (5%)
26	SQD	L	102	-	52,54,54	0.98	2 (3%)	62,65,65	1.62	10 (16%)
38	HEM	e	102	5,6	50,50,50	1.55	8 (16%)	67,82,82	1.61	11 (16%)
23	CLA	c	512	-	69,73,73	1.95	19 (27%)	82,113,113	2.65	33 (40%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	3 (6%)
23	CLA	A	403	-	69,73,73	1.93	19 (27%)	82,113,113	2.72	33 (40%)
23	CLA	C	515	-	69,73,73	2.02	20 (28%)	82,113,113	2.69	29 (35%)
23	CLA	B	601	41	69,73,73	2.08	20 (28%)	82,113,113	2.66	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMT	b	626	-	25,25,36	0.57	1 (4%)	30,30,47	1.13	3 (10%)
25	BCR	a	408	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)
37	BCT	D	401[B]	21	3,3,3	0.53	0	2,3,3	0.65	0
29	PL9	A	413[B]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
32	HTG	b	624	-	19,19,19	0.94	2 (10%)	23,24,24	1.33	5 (21%)
23	CLA	b	609	-	69,73,73	2.00	21 (30%)	82,113,113	2.64	30 (36%)
23	CLA	b	608	-	69,73,73	2.06	21 (30%)	82,113,113	2.69	34 (41%)
32	HTG	B	624	-	19,19,19	1.02	2 (10%)	23,24,24	1.33	3 (13%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
23	CLA	c	506	41	69,73,73	2.08	21 (30%)	82,113,113	2.70	33 (40%)
29	PL9	a	414[A]	-	55,55,55	0.66	2 (3%)	68,69,69	2.04	20 (29%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	10 (17%)
25	BCR	B	631	-	41,41,41	1.08	1 (2%)	56,56,56	1.46	11 (19%)
25	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.54	10 (17%)
26	SQD	a	409	-	52,54,54	0.93	2 (3%)	62,65,65	1.65	12 (19%)
35	DGD	c	518	-	63,63,67	0.91	2 (3%)	77,77,81	1.09	5 (6%)
23	CLA	B	609	-	69,73,73	2.00	19 (27%)	82,113,113	2.69	26 (31%)
23	CLA	B	604	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	29 (35%)
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.14	5 (6%)
33	LMT	B	629	-	25,25,36	0.42	0	30,30,47	1.10	2 (6%)
34	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.49	6 (13%)
23	CLA	c	513	3	69,73,73	1.98	19 (27%)	82,113,113	2.70	32 (39%)
32	HTG	h	101	-	16,16,19	1.06	1 (6%)	20,21,24	1.90	6 (30%)
33	LMT	C	526	-	36,36,36	0.52	1 (2%)	47,47,47	1.14	3 (6%)
23	CLA	A	405	41	69,73,73	2.02	18 (26%)	82,113,113	2.66	29 (35%)
25	BCR	D	405	-	41,41,41	1.02	1 (2%)	56,56,56	1.81	16 (28%)
23	CLA	B	608	-	69,73,73	1.96	20 (28%)	82,113,113	2.67	31 (37%)
24	PHO	A	415	-	58,69,69	2.70	13 (22%)	55,99,99	3.06	16 (29%)
23	CLA	b	601	41	69,73,73	2.09	20 (28%)	82,113,113	2.69	30 (36%)
23	CLA	c	507	-	69,73,73	2.06	19 (27%)	82,113,113	2.63	29 (35%)
40	HEC	V	201	16	46,50,50	1.89	6 (13%)	58,82,82	1.77	7 (12%)
23	CLA	A	407	-	69,73,73	2.04	20 (28%)	82,113,113	2.75	31 (37%)
33	LMT	m	103	-	36,36,36	0.45	0	47,47,47	1.07	3 (6%)
28	OEX	A	412[A]	41,1,3	0,15,15	-	-	-		
28	OEX	a	413[B]	41,1,3	0,15,15	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	612	-	69,73,73	1.90	18 (26%)	82,113,113	2.81	28 (34%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.76	17 (30%)
29	PL9	d	405	-	55,55,55	0.70	2 (3%)	68,69,69	1.58	15 (22%)
27	GOL	c	502	-	5,5,5	1.09	0	5,5,5	0.97	0
23	CLA	B	602	-	69,73,73	2.06	19 (27%)	82,113,113	2.74	34 (41%)
26	SQD	A	409	-	52,54,54	0.89	2 (3%)	62,65,65	2.03	11 (17%)
33	LMT	b	620	-	25,25,36	0.52	0	30,30,47	0.60	0
32	HTG	B	621	-	19,19,19	0.91	1 (5%)	23,24,24	1.54	4 (17%)
23	CLA	D	403	-	69,73,73	1.98	19 (27%)	82,113,113	2.80	32 (39%)
25	BCR	K	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	8 (14%)
32	HTG	b	622	-	19,19,19	0.94	1 (5%)	23,24,24	1.44	2 (8%)
35	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.06	7 (9%)
26	SQD	f	101	-	41,43,54	1.08	2 (4%)	51,54,65	1.25	5 (9%)
23	CLA	b	602	-	69,73,73	2.07	20 (28%)	82,113,113	2.78	34 (41%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.97	2 (4%)
26	SQD	B	620	-	52,54,54	0.95	2 (3%)	62,65,65	1.49	9 (14%)
34	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.07	5 (8%)
31	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.00	3 (5%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.17	5 (6%)
32	HTG	V	202	-	11,11,19	0.19	0	15,15,24	1.20	1 (6%)
27	GOL	C	524	-	5,5,5	1.14	0	5,5,5	1.17	1 (20%)
23	CLA	b	606	-	69,73,73	1.93	19 (27%)	82,113,113	2.81	32 (39%)
23	CLA	b	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.84	33 (40%)
23	CLA	c	504	-	69,73,73	1.99	19 (27%)	82,113,113	2.61	30 (36%)
23	CLA	B	610	41	69,73,73	2.04	20 (28%)	82,113,113	2.73	33 (40%)
23	CLA	c	515	-	69,73,73	2.09	21 (30%)	82,113,113	2.72	31 (37%)
29	PL9	D	406	-	55,55,55	0.70	2 (3%)	68,69,69	1.67	19 (27%)
26	SQD	a	411	-	52,54,54	0.99	2 (3%)	62,65,65	1.21	7 (11%)
24	PHO	a	416	-	58,69,69	2.81	12 (20%)	55,99,99	3.14	15 (27%)
23	CLA	C	504	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	28 (34%)
23	CLA	c	514	-	69,73,73	2.04	19 (27%)	82,113,113	2.66	33 (40%)
32	HTG	B	622	-	19,19,19	0.79	1 (5%)	23,24,24	1.25	1 (4%)
38	HEM	E	102	5,6	50,50,50	1.56	7 (14%)	67,82,82	1.63	17 (25%)
37	BCT	d	401[A]	21	3,3,3	0.43	0	2,3,3	1.94	1 (50%)
33	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	k	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.60	12 (21%)
23	CLA	C	507	-	69,73,73	2.00	19 (27%)	82,113,113	2.61	30 (36%)
23	CLA	a	404	41	69,73,73	2.03	19 (27%)	82,113,113	2.67	33 (40%)
23	CLA	c	505	-	69,73,73	2.01	19 (27%)	82,113,113	2.68	31 (37%)
23	CLA	C	512	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	29 (35%)
23	CLA	b	614	-	69,73,73	1.97	20 (28%)	82,113,113	2.75	31 (37%)
23	CLA	C	508	-	69,73,73	2.04	20 (28%)	82,113,113	2.66	34 (41%)
23	CLA	B	603	-	69,73,73	1.99	20 (28%)	82,113,113	2.75	30 (36%)
25	BCR	b	617	-	41,41,41	1.13	1 (2%)	56,56,56	1.49	8 (14%)
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	5 (9%)
23	CLA	D	404	-	69,73,73	2.03	19 (27%)	82,113,113	2.72	33 (40%)
29	PL9	a	414[B]	-	55,55,55	0.68	2 (3%)	68,69,69	1.96	18 (26%)
25	BCR	B	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.16	5 (8%)
23	CLA	B	607	41	69,73,73	1.99	18 (26%)	82,113,113	2.68	31 (37%)
25	BCR	A	408	-	41,41,41	1.11	2 (4%)	56,56,56	1.39	7 (12%)
23	CLA	B	611	-	69,73,73	1.99	20 (28%)	82,113,113	2.74	32 (39%)
23	CLA	B	613	-	69,73,73	1.95	17 (24%)	82,113,113	2.71	28 (34%)
23	CLA	B	615	-	69,73,73	1.94	17 (24%)	82,113,113	2.74	31 (37%)
23	CLA	C	514	-	69,73,73	2.05	20 (28%)	82,113,113	2.61	31 (37%)
25	BCR	c	517	-	41,41,41	1.08	1 (2%)	56,56,56	1.60	11 (19%)
23	CLA	b	604	-	69,73,73	1.96	19 (27%)	82,113,113	2.66	31 (37%)
24	PHO	a	406	-	58,69,69	2.72	13 (22%)	55,99,99	2.86	14 (25%)
23	CLA	a	407	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	33 (40%)
26	SQD	A	411	-	52,54,54	1.00	2 (3%)	62,65,65	1.26	8 (12%)
27	GOL	a	410	-	5,5,5	0.93	0	5,5,5	1.12	1 (20%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.59	13 (23%)
32	HTG	b	621	-	19,19,19	0.95	1 (5%)	23,24,24	1.31	4 (17%)
23	CLA	a	403	-	69,73,73	1.98	20 (28%)	82,113,113	2.74	34 (41%)
23	CLA	b	615	-	69,73,73	1.97	17 (24%)	82,113,113	2.67	29 (35%)
27	GOL	B	623	-	5,5,5	0.89	0	5,5,5	1.12	1 (20%)
32	HTG	C	523	-	19,19,19	0.85	1 (5%)	23,24,24	1.28	2 (8%)
35	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.07	7 (9%)
23	CLA	C	506	41	69,73,73	1.99	21 (30%)	82,113,113	2.65	35 (42%)
27	GOL	B	628	-	5,5,5	1.09	0	5,5,5	0.98	0
33	LMT	D	402	-	36,36,36	0.56	1 (2%)	47,47,47	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	503	-	69,73,73	2.02	21 (30%)	82,113,113	2.63	32 (39%)
23	CLA	B	605	-	69,73,73	2.06	18 (26%)	82,113,113	2.77	30 (36%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	11 (19%)
27	GOL	c	527	-	5,5,5	0.85	0	5,5,5	1.15	1 (20%)
31	LHG	L	101	-	48,48,48	0.90	3 (6%)	51,54,54	1.17	5 (9%)
34	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.20	7 (11%)
23	CLA	b	613	-	69,73,73	1.97	18 (26%)	82,113,113	2.68	31 (37%)
25	BCR	d	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.84	14 (25%)
27	GOL	A	410	-	5,5,5	1.14	0	5,5,5	0.98	0
23	CLA	c	511	-	69,73,73	2.09	20 (28%)	82,113,113	2.70	29 (35%)
34	LMG	D	412	39	51,51,55	0.88	3 (5%)	59,59,63	1.08	5 (8%)
23	CLA	C	511	-	69,73,73	2.07	20 (28%)	82,113,113	2.67	29 (35%)
37	BCT	D	401[A]	21	3,3,3	0.54	0	2,3,3	0.93	0
34	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	6 (10%)
27	GOL	v	201	-	5,5,5	1.26	1 (20%)	5,5,5	0.91	0
31	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	3 (5%)
33	LMT	F	101	-	36,36,36	0.55	1 (2%)	47,47,47	1.20	5 (10%)
23	CLA	C	503	-	69,73,73	1.99	19 (27%)	82,113,113	2.74	32 (39%)

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
31	LHG	d	406	-	-	20/53/53/53	-
23	CLA	c	509	41	1/1/15/20	10/39/115/115	-
23	CLA	C	505	-	1/1/15/20	4/39/115/115	-
23	CLA	b	603	-	1/1/15/20	7/39/115/115	-
23	CLA	C	510	-	1/1/15/20	5/39/115/115	-
26	SQD	D	413	-	-	12/38/58/69	0/1/1/1
23	CLA	A	404	41	1/1/15/20	2/39/115/115	-
23	CLA	b	610	41	1/1/15/20	7/39/115/115	-
23	CLA	b	611	-	1/1/15/20	3/39/115/115	-
40	HEC	v	202	16	-	6/14/54/54	-
31	LHG	E	101	-	-	16/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	406	-	-	1/37/103/103	0/5/6/6
27	GOL	B	626	-	-	3/4/4/4	-
33	LMT	B	627	-	-	9/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
34	LMG	C	502	-	-	24/46/66/70	0/1/1/1
33	LMT	M	102	-	-	6/21/61/61	0/2/2/2
23	CLA	C	509	41	1/1/15/20	6/39/115/115	-
31	LHG	d	407	-	-	23/53/53/53	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
32	HTG	D	411	-	-	2/7/27/30	0/1/1/1
31	LHG	A	416	-	-	16/53/53/53	-
23	CLA	c	510	-	1/1/15/20	8/39/115/115	-
23	CLA	d	402	-	1/1/15/20	3/39/115/115	-
23	CLA	B	616	-	1/1/15/20	8/39/115/115	-
23	CLA	B	614	-	1/1/15/20	9/39/115/115	-
35	DGD	h	103	-	-	12/51/91/95	0/2/2/2
33	LMT	a	412	-	-	7/21/61/61	0/2/2/2
33	LMT	e	101	-	-	9/21/61/61	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	508	-	1/1/15/20	10/39/115/115	-
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
34	LMG	M	101	-	-	21/46/66/70	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
27	GOL	b	623	-	-	2/4/4/4	-
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
34	LMG	d	411	39	-	8/46/66/70	0/1/1/1
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
29	PL9	A	413[A]	-	-	16/53/73/73	0/1/1/1
27	GOL	b	627	-	-	0/4/4/4	-
25	BCR	C	517	-	-	3/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	5/39/115/115	-
31	LHG	D	408	-	-	11/53/53/53	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	B	606	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	513	3	1/1/15/20	3/39/115/115	-
32	HTG	c	523	-	-	4/10/30/30	0/1/1/1
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
27	GOL	O	302	-	-	4/4/4/4	-
33	LMT	B	630	-	-	8/17/38/61	0/1/1/2
33	LMT	M	103	-	-	8/21/61/61	0/2/2/2
23	CLA	a	405	41	-	8/39/115/115	-
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
34	LMG	C	522	-	-	12/46/66/70	0/1/1/1
34	LMG	m	101	-	-	9/46/66/70	0/1/1/1
26	SQD	L	102	-	-	17/49/69/69	0/1/1/1
38	HEM	e	102	5,6	-	9/14/54/54	-
23	CLA	c	512	-	1/1/15/20	8/39/115/115	-
34	LMG	z	101	-	-	7/34/54/70	0/1/1/1
23	CLA	A	403	-	1/1/15/20	3/39/115/115	-
23	CLA	C	515	-	1/1/15/20	9/39/115/115	-
23	CLA	B	601	41	1/1/15/20	9/39/115/115	-
33	LMT	b	626	-	-	9/17/37/61	0/1/1/2
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
29	PL9	A	413[B]	-	-	16/53/73/73	0/1/1/1
32	HTG	b	624	-	-	2/10/30/30	0/1/1/1
23	CLA	b	609	-	1/1/15/20	10/39/115/115	-
23	CLA	b	608	-	1/1/15/20	5/39/115/115	-
32	HTG	B	624	-	-	5/10/30/30	0/1/1/1
35	DGD	C	520	-	-	8/51/91/95	0/2/2/2
23	CLA	c	506	41	1/1/15/20	4/39/115/115	-
29	PL9	a	414[A]	-	-	18/53/73/73	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
25	BCR	B	631	-	-	4/29/63/63	0/2/2/2
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
26	SQD	a	409	-	-	12/49/69/69	0/1/1/1
35	DGD	c	518	-	-	19/51/91/95	0/2/2/2
23	CLA	B	609	-	1/1/15/20	6/39/115/115	-
23	CLA	B	604	-	1/1/15/20	7/39/115/115	-
35	DGD	C	518	-	-	17/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	B	629	-	-	4/17/37/61	0/1/1/2
34	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
23	CLA	c	513	3	1/1/15/20	6/39/115/115	-
32	HTG	h	101	-	-	2/7/27/30	0/1/1/1
33	LMT	C	526	-	-	8/21/61/61	0/2/2/2
23	CLA	A	405	41	-	5/39/115/115	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	B	608	-	-	2/39/115/115	-
24	PHO	A	415	-	-	2/37/103/103	0/5/6/6
23	CLA	b	601	41	1/1/15/20	16/39/115/115	-
23	CLA	c	507	-	1/1/15/20	4/39/115/115	-
40	HEC	V	201	16	-	6/14/54/54	-
23	CLA	A	407	-	1/1/15/20	8/39/115/115	-
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	7/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
27	GOL	c	502	-	-	0/4/4/4	-
23	CLA	B	602	-	1/1/15/20	10/39/115/115	-
26	SQD	A	409	-	-	13/49/69/69	0/1/1/1
33	LMT	b	620	-	-	6/17/37/61	0/1/1/2
32	HTG	B	621	-	-	4/10/30/30	0/1/1/1
23	CLA	D	403	-	1/1/15/20	6/39/115/115	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
32	HTG	b	622	-	-	2/10/30/30	0/1/1/1
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
26	SQD	f	101	-	-	14/38/58/69	0/1/1/1
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
31	LHG	a	419	-	-	18/46/46/53	-
26	SQD	B	620	-	-	19/49/69/69	0/1/1/1
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
31	LHG	D	407	-	-	15/53/53/53	-
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
32	HTG	V	202	-	-	1/2/19/30	0/1/1/1
27	GOL	C	524	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	-	1/1/15/20	9/39/115/115	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	c	504	-	1/1/15/20	6/39/115/115	-
23	CLA	B	610	41	1/1/15/20	6/39/115/115	-
23	CLA	c	515	-	1/1/15/20	11/39/115/115	-
29	PL9	D	406	-	-	7/53/73/73	0/1/1/1
26	SQD	a	411	-	-	17/49/69/69	0/1/1/1
24	PHO	a	416	-	-	5/37/103/103	0/5/6/6
23	CLA	C	504	-	-	9/39/115/115	-
23	CLA	c	514	-	1/1/15/20	8/39/115/115	-
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
38	HEM	E	102	5,6	-	5/14/54/54	-
33	LMT	a	418	-	-	4/21/61/61	0/2/2/2
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/15/20	8/39/115/115	-
23	CLA	a	404	41	1/1/15/20	8/39/115/115	-
23	CLA	c	505	-	1/1/15/20	1/39/115/115	-
23	CLA	C	512	-	1/1/15/20	9/39/115/115	-
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
23	CLA	C	508	-	1/1/15/20	11/39/115/115	-
23	CLA	B	603	-	1/1/15/20	5/39/115/115	-
25	BCR	b	617	-	-	4/29/63/63	0/2/2/2
31	LHG	d	408	-	-	9/53/53/53	-
23	CLA	D	404	-	1/1/15/20	9/39/115/115	-
29	PL9	a	414[B]	-	-	17/53/73/73	0/1/1/1
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
23	CLA	B	607	41	1/1/15/20	3/39/115/115	-
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	B	613	-	1/1/15/20	9/39/115/115	-
23	CLA	B	615	-	1/1/15/20	7/39/115/115	-
23	CLA	C	514	-	1/1/15/20	16/39/115/115	-
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/15/20	11/39/115/115	-
24	PHO	a	406	-	-	4/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	407	-	1/1/15/20	12/39/115/115	-
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
27	GOL	a	410	-	-	4/4/4/4	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	HTG	b	621	-	-	5/10/30/30	0/1/1/1
23	CLA	a	403	-	1/1/15/20	5/39/115/115	-
23	CLA	b	615	-	1/1/15/20	11/39/115/115	-
27	GOL	B	623	-	-	2/4/4/4	-
32	HTG	C	523	-	-	2/10/30/30	0/1/1/1
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	C	506	41	1/1/15/20	7/39/115/115	-
27	GOL	B	628	-	-	0/4/4/4	-
33	LMT	D	402	-	-	10/21/61/61	0/2/2/2
23	CLA	c	503	-	1/1/15/20	5/39/115/115	-
23	CLA	B	605	-	1/1/15/20	9/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	GOL	c	527	-	-	0/4/4/4	-
31	LHG	L	101	-	-	16/53/53/53	-
34	LMG	a	417	-	-	12/46/66/70	0/1/1/1
23	CLA	b	613	-	1/1/15/20	2/39/115/115	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
27	GOL	A	410	-	-	3/4/4/4	-
23	CLA	c	511	-	1/1/15/20	12/39/115/115	-
34	LMG	D	412	39	-	9/46/66/70	0/1/1/1
23	CLA	C	511	-	1/1/15/20	4/39/115/115	-
34	LMG	c	522	-	-	9/46/66/70	0/1/1/1
27	GOL	v	201	-	-	2/4/4/4	-
31	LHG	b	628	-	-	13/53/53/53	-
33	LMT	F	101	-	-	5/21/61/61	0/2/2/2
23	CLA	C	503	-	1/1/15/20	5/39/115/115	-

All (1585) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416	PHO	C1B-C2B	10.03	1.50	1.39
24	a	406	PHO	C1D-C2D	8.92	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	415	PHO	C1D-C2D	8.82	1.49	1.39
24	A	406	PHO	C1D-C2D	8.81	1.49	1.39
24	A	406	PHO	C1B-C2B	8.75	1.49	1.39
24	a	406	PHO	C1B-C2B	8.70	1.49	1.39
24	A	415	PHO	C1B-C2B	8.29	1.48	1.39
24	a	416	PHO	C1D-C2D	8.26	1.48	1.39
24	a	416	PHO	C3B-C4B	7.89	1.49	1.41
24	A	406	PHO	C3B-C4B	7.10	1.48	1.41
24	A	415	PHO	C4D-CHA	6.96	1.49	1.39
24	A	415	PHO	C3B-C4B	6.96	1.48	1.41
40	V	201	HEC	CAC-C3C	6.82	1.57	1.35
24	a	416	PHO	C4D-CHA	6.79	1.49	1.39
24	a	406	PHO	C3B-C2B	6.76	1.49	1.40
40	v	202	HEC	CAC-C3C	6.73	1.56	1.35
40	V	201	HEC	CAB-C3B	6.53	1.56	1.35
24	a	406	PHO	C4D-CHA	6.51	1.49	1.39
24	A	415	PHO	C3B-C2B	6.46	1.49	1.40
24	A	406	PHO	C3B-C2B	6.45	1.49	1.40
24	a	406	PHO	C3D-C2D	6.36	1.50	1.39
24	a	416	PHO	C3B-C2B	6.31	1.48	1.40
24	a	406	PHO	C3B-C4B	6.29	1.47	1.41
24	A	406	PHO	C4D-CHA	6.25	1.48	1.39
40	v	202	HEC	CAB-C3B	6.12	1.54	1.35
23	C	510	CLA	C3C-C2C	5.83	1.49	1.36
24	a	416	PHO	C3D-C2D	5.77	1.49	1.39
40	v	202	HEC	C3D-C2D	5.75	1.53	1.38
25	d	404	BCR	C23-C22	-5.71	1.33	1.46
24	A	415	PHO	C3D-C2D	5.67	1.49	1.39
23	B	610	CLA	C3C-C2C	5.66	1.49	1.36
23	c	507	CLA	C3C-C2C	5.66	1.49	1.36
23	b	601	CLA	C3C-C2C	5.55	1.48	1.36
23	c	510	CLA	C1D-ND	5.53	1.45	1.37
23	C	513	CLA	O2D-CGD	5.50	1.46	1.33
23	B	611	CLA	C3C-C2C	5.49	1.48	1.36
23	c	510	CLA	C3C-C2C	5.49	1.48	1.36
23	B	602	CLA	CHC-C1C	5.48	1.49	1.38
23	B	605	CLA	CHC-C1C	5.48	1.49	1.38
23	a	404	CLA	C1D-ND	5.44	1.45	1.37
23	C	514	CLA	C3C-C2C	5.40	1.48	1.36
23	a	407	CLA	C3C-C2C	5.39	1.48	1.36
38	E	102	HEM	FE-NB	5.39	2.11	1.94
23	b	605	CLA	C3C-C2C	5.38	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C3C-C2C	5.37	1.48	1.36
23	D	403	CLA	C3C-C2C	5.37	1.48	1.36
23	B	601	CLA	C3C-C2C	5.36	1.48	1.36
23	C	509	CLA	C3C-C2C	5.35	1.48	1.36
25	b	619	BCR	C23-C22	-5.34	1.34	1.46
23	A	407	CLA	C3C-C2C	5.34	1.48	1.36
23	C	503	CLA	C3C-C2C	5.33	1.48	1.36
23	b	607	CLA	C3C-C2C	5.33	1.48	1.36
23	b	612	CLA	C3C-C2C	5.32	1.48	1.36
23	C	515	CLA	C3C-C2C	5.32	1.48	1.36
25	k	101	BCR	C23-C22	-5.31	1.34	1.46
23	a	404	CLA	C3C-C2C	5.31	1.48	1.36
23	A	405	CLA	C3C-C2C	5.31	1.48	1.36
24	a	406	PHO	OBD-CAD	5.30	1.29	1.22
23	b	603	CLA	C3C-C2C	5.29	1.48	1.36
23	A	404	CLA	C3C-C2C	5.29	1.48	1.36
23	C	505	CLA	C3C-C2C	5.29	1.48	1.36
23	c	515	CLA	C1D-ND	5.28	1.44	1.37
23	d	403	CLA	CHC-C1C	5.27	1.49	1.38
23	C	511	CLA	C3C-C2C	5.27	1.48	1.36
23	c	515	CLA	C3C-C2C	5.27	1.48	1.36
23	d	403	CLA	C3C-C2C	5.27	1.48	1.36
23	c	511	CLA	O2D-CGD	5.27	1.46	1.33
38	e	102	HEM	FE-NB	5.26	2.11	1.94
23	c	504	CLA	C3C-C2C	5.25	1.48	1.36
23	c	509	CLA	C1D-ND	5.25	1.44	1.37
23	B	614	CLA	C3C-C2C	5.25	1.48	1.36
23	b	601	CLA	C1D-ND	5.25	1.44	1.37
23	D	404	CLA	C3C-C2C	5.25	1.48	1.36
23	B	605	CLA	O2D-CGD	5.24	1.46	1.33
23	b	603	CLA	O2D-CGD	5.21	1.46	1.33
23	c	506	CLA	C3C-C2C	5.20	1.48	1.36
23	c	511	CLA	C3C-C2C	5.17	1.47	1.36
23	c	509	CLA	CHC-C1C	5.17	1.48	1.38
23	c	514	CLA	O2D-CGD	5.17	1.45	1.33
23	c	514	CLA	C3C-C2C	5.17	1.47	1.36
25	A	408	BCR	C23-C22	-5.16	1.34	1.46
23	C	511	CLA	C1D-ND	5.15	1.44	1.37
23	c	508	CLA	C3C-C2C	5.14	1.47	1.36
23	b	613	CLA	C3C-C2C	5.14	1.47	1.36
23	A	407	CLA	O2D-CGD	5.14	1.45	1.33
23	c	510	CLA	O2D-CGD	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	CHC-C1C	5.12	1.48	1.38
23	b	614	CLA	O2D-CGD	5.12	1.45	1.33
23	C	512	CLA	C1D-ND	5.11	1.44	1.37
23	B	609	CLA	O2D-CGD	5.11	1.45	1.33
23	b	610	CLA	C3C-C2C	5.10	1.47	1.36
23	B	607	CLA	CHC-C1C	5.10	1.48	1.38
23	c	504	CLA	O2D-CGD	5.10	1.45	1.33
23	c	505	CLA	C3C-C2C	5.10	1.47	1.36
23	c	506	CLA	C1D-ND	5.10	1.44	1.37
23	B	611	CLA	O2D-CGD	5.09	1.45	1.33
23	B	601	CLA	O2D-CGD	5.09	1.45	1.33
24	A	406	PHO	C3D-C2D	5.09	1.48	1.39
23	c	514	CLA	CHC-C1C	5.09	1.48	1.38
25	B	631	BCR	C23-C22	-5.09	1.35	1.46
23	b	606	CLA	C3C-C2C	5.09	1.47	1.36
25	b	617	BCR	C23-C22	-5.08	1.35	1.46
23	B	605	CLA	C3C-C2C	5.08	1.47	1.36
40	V	201	HEC	C3D-C2D	5.07	1.52	1.38
23	B	603	CLA	C3C-C2C	5.07	1.47	1.36
23	C	506	CLA	O2D-CGD	5.07	1.45	1.33
23	c	512	CLA	C3C-C2C	5.07	1.47	1.36
25	K	101	BCR	C23-C22	-5.06	1.35	1.46
23	C	507	CLA	C3C-C2C	5.06	1.47	1.36
23	b	602	CLA	C3C-C2C	5.06	1.47	1.36
23	B	615	CLA	C3C-C2C	5.05	1.47	1.36
23	B	616	CLA	C3C-C2C	5.05	1.47	1.36
23	d	403	CLA	C1D-ND	5.04	1.44	1.37
23	b	616	CLA	O2D-CGD	5.04	1.45	1.33
23	b	611	CLA	O2D-CGD	5.04	1.45	1.33
23	b	609	CLA	C3C-C2C	5.03	1.47	1.36
23	B	602	CLA	C3C-C2C	5.03	1.47	1.36
25	k	102	BCR	C23-C22	-5.03	1.35	1.46
23	c	503	CLA	C3C-C2C	5.03	1.47	1.36
23	B	604	CLA	C3C-C2C	5.02	1.47	1.36
23	B	606	CLA	C3C-C2C	5.02	1.47	1.36
23	C	504	CLA	C3C-C2C	5.02	1.47	1.36
23	c	515	CLA	CHC-C1C	5.01	1.48	1.38
23	b	604	CLA	C3C-C2C	5.01	1.47	1.36
23	b	602	CLA	O2D-CGD	5.01	1.45	1.33
23	a	403	CLA	C3C-C2C	5.01	1.47	1.36
23	C	504	CLA	CHC-C1C	5.00	1.48	1.38
23	c	515	CLA	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2D-CGD	4.97	1.45	1.33
24	a	416	PHO	O2D-CGD	4.97	1.45	1.33
23	b	608	CLA	C3C-C2C	4.97	1.47	1.36
23	c	503	CLA	C1D-ND	4.96	1.44	1.37
23	C	504	CLA	O2D-CGD	4.96	1.45	1.33
23	c	508	CLA	O2D-CGD	4.96	1.45	1.33
23	A	405	CLA	O2D-CGD	4.96	1.45	1.33
23	B	615	CLA	O2D-CGD	4.96	1.45	1.33
23	B	608	CLA	C3C-C2C	4.95	1.47	1.36
24	A	406	PHO	OBD-CAD	4.95	1.28	1.22
23	b	608	CLA	CHC-C1C	4.95	1.48	1.38
23	b	611	CLA	C3C-C2C	4.94	1.47	1.36
23	B	601	CLA	CHC-C1C	4.94	1.48	1.38
23	A	405	CLA	CHC-C1C	4.94	1.48	1.38
23	c	507	CLA	CHC-C1C	4.93	1.48	1.38
23	D	404	CLA	O2D-CGD	4.93	1.45	1.33
25	c	517	BCR	C23-C22	-4.93	1.35	1.46
23	C	514	CLA	CHC-C1C	4.93	1.48	1.38
23	C	508	CLA	O2D-CGD	4.93	1.45	1.33
25	C	516	BCR	C23-C22	-4.93	1.35	1.46
23	a	403	CLA	C1D-ND	4.93	1.44	1.37
23	C	512	CLA	C3C-C2C	4.93	1.47	1.36
23	c	513	CLA	C3C-C2C	4.92	1.47	1.36
23	B	613	CLA	O2D-CGD	4.92	1.45	1.33
23	b	616	CLA	C3C-C2C	4.92	1.47	1.36
23	c	511	CLA	C1D-ND	4.91	1.44	1.37
24	a	416	PHO	OBD-CAD	4.90	1.28	1.22
23	c	506	CLA	O2D-CGD	4.90	1.45	1.33
23	D	404	CLA	CHC-C1C	4.89	1.48	1.38
23	B	602	CLA	O2D-CGD	4.89	1.45	1.33
25	b	618	BCR	C23-C22	-4.89	1.35	1.46
23	b	613	CLA	O2D-CGD	4.88	1.45	1.33
23	b	608	CLA	O2D-CGD	4.87	1.45	1.33
25	c	516	BCR	C23-C22	-4.87	1.35	1.46
23	c	508	CLA	C1D-ND	4.87	1.44	1.37
23	C	515	CLA	C1D-ND	4.87	1.44	1.37
23	C	505	CLA	O2D-CGD	4.86	1.45	1.33
23	B	613	CLA	CHC-C1C	4.86	1.48	1.38
23	b	602	CLA	CHC-C1C	4.86	1.48	1.38
23	C	512	CLA	CHC-C1C	4.86	1.48	1.38
23	A	404	CLA	CHC-C1C	4.85	1.48	1.38
24	A	415	PHO	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	O2D-CGD	4.85	1.45	1.33
23	c	507	CLA	O2D-CGD	4.85	1.45	1.33
23	C	507	CLA	O2D-CGD	4.84	1.45	1.33
23	C	515	CLA	CHC-C1C	4.84	1.48	1.38
23	B	615	CLA	C1D-ND	4.83	1.44	1.37
24	A	415	PHO	OBD-CAD	4.83	1.28	1.22
23	b	616	CLA	CHC-C1C	4.83	1.48	1.38
23	b	604	CLA	O2D-CGD	4.83	1.45	1.33
25	T	101	BCR	C23-C22	-4.82	1.35	1.46
23	b	614	CLA	C3C-C2C	4.82	1.47	1.36
23	a	407	CLA	CHC-C1C	4.82	1.48	1.38
23	B	605	CLA	C1D-ND	4.82	1.44	1.37
23	B	610	CLA	CHC-C1C	4.82	1.48	1.38
23	C	507	CLA	CHC-C1C	4.81	1.48	1.38
23	A	403	CLA	C3C-C2C	4.80	1.47	1.36
23	A	403	CLA	C1D-ND	4.79	1.44	1.37
23	d	402	CLA	C3C-C2C	4.79	1.47	1.36
23	B	609	CLA	C1D-ND	4.79	1.44	1.37
23	C	506	CLA	C3C-C2C	4.79	1.47	1.36
25	H	101	BCR	C23-C22	-4.79	1.35	1.46
23	b	609	CLA	O2D-CGD	4.79	1.45	1.33
23	b	607	CLA	O2D-CGD	4.78	1.45	1.33
23	C	508	CLA	C3C-C2C	4.78	1.47	1.36
23	c	509	CLA	C3C-C2C	4.78	1.47	1.36
25	h	102	BCR	C23-C22	-4.78	1.35	1.46
23	b	615	CLA	O2D-CGD	4.78	1.45	1.33
23	c	505	CLA	C1D-ND	4.77	1.44	1.37
23	a	403	CLA	CHC-C1C	4.77	1.48	1.38
23	C	505	CLA	C1D-ND	4.77	1.44	1.37
23	c	508	CLA	CHC-C1C	4.77	1.48	1.38
23	B	601	CLA	O2A-CGA	4.77	1.47	1.33
23	B	609	CLA	C3C-C2C	4.77	1.47	1.36
23	c	513	CLA	C1D-ND	4.76	1.44	1.37
23	C	513	CLA	CHC-C1C	4.76	1.48	1.38
23	C	508	CLA	CHD-C1D	4.76	1.47	1.38
23	B	606	CLA	O2D-CGD	4.76	1.44	1.33
34	M	101	LMG	O8-C28	4.75	1.47	1.33
23	c	510	CLA	CHC-C1C	4.75	1.48	1.38
23	a	404	CLA	O2D-CGD	4.75	1.44	1.33
23	B	616	CLA	CHC-C1C	4.75	1.48	1.38
23	B	604	CLA	CHC-C1C	4.75	1.48	1.38
23	b	601	CLA	CHC-C1C	4.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	O2D-CGD	4.73	1.44	1.33
23	C	509	CLA	O2D-CGD	4.73	1.44	1.33
23	D	404	CLA	C1D-ND	4.72	1.44	1.37
23	b	601	CLA	O2D-CGD	4.72	1.44	1.33
23	b	606	CLA	CHC-C1C	4.72	1.47	1.38
23	a	405	CLA	C3C-C2C	4.71	1.46	1.36
23	c	505	CLA	CHC-C1C	4.71	1.47	1.38
23	B	612	CLA	CHC-C1C	4.71	1.47	1.38
23	B	605	CLA	CHC-C4B	4.71	1.50	1.39
23	b	601	CLA	O2A-CGA	4.71	1.47	1.33
23	B	606	CLA	C1D-ND	4.69	1.44	1.37
23	b	610	CLA	CHC-C1C	4.69	1.47	1.38
23	b	605	CLA	O2D-CGD	4.69	1.44	1.33
25	a	408	BCR	C23-C22	-4.69	1.35	1.46
23	B	609	CLA	CHC-C1C	4.68	1.47	1.38
23	a	404	CLA	C3D-C2D	4.68	1.51	1.39
23	C	510	CLA	CHC-C1C	4.68	1.47	1.38
23	a	407	CLA	O2D-CGD	4.68	1.44	1.33
23	C	508	CLA	C1D-ND	4.67	1.44	1.37
23	C	511	CLA	O2D-CGD	4.67	1.44	1.33
23	C	508	CLA	CHC-C1C	4.67	1.47	1.38
25	B	619	BCR	C23-C22	-4.67	1.36	1.46
23	C	506	CLA	CHC-C1C	4.67	1.47	1.38
23	B	606	CLA	CHC-C1C	4.67	1.47	1.38
25	B	617	BCR	C23-C22	-4.66	1.36	1.46
23	b	603	CLA	CHC-C1C	4.66	1.47	1.38
23	B	611	CLA	C1D-ND	4.66	1.44	1.37
23	B	614	CLA	C1D-ND	4.66	1.44	1.37
23	A	407	CLA	CHC-C1C	4.65	1.47	1.38
23	b	605	CLA	CHC-C1C	4.65	1.47	1.38
23	B	614	CLA	O2D-CGD	4.65	1.44	1.33
23	c	503	CLA	O2D-CGD	4.64	1.44	1.33
23	C	515	CLA	O2D-CGD	4.64	1.44	1.33
23	c	504	CLA	C1D-ND	4.64	1.44	1.37
23	b	607	CLA	CHC-C1C	4.64	1.47	1.38
23	b	613	CLA	C1D-ND	4.64	1.44	1.37
23	A	404	CLA	C1D-ND	4.63	1.43	1.37
23	c	513	CLA	CHC-C1C	4.63	1.47	1.38
23	c	515	CLA	CHD-C1D	4.62	1.47	1.38
23	B	603	CLA	O2D-CGD	4.62	1.44	1.33
23	B	603	CLA	CHC-C1C	4.62	1.47	1.38
23	a	405	CLA	CHC-C1C	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1D-ND	4.61	1.43	1.37
23	B	615	CLA	C3D-C2D	4.61	1.51	1.39
23	C	505	CLA	CHC-C1C	4.60	1.47	1.38
25	C	517	BCR	C23-C22	-4.59	1.36	1.46
23	c	511	CLA	CHC-C1C	4.59	1.47	1.38
23	A	407	CLA	C1D-ND	4.58	1.43	1.37
23	b	615	CLA	C1D-ND	4.58	1.43	1.37
23	B	614	CLA	CHC-C1C	4.58	1.47	1.38
23	B	612	CLA	O2D-CGD	4.58	1.44	1.33
26	A	411	SQD	O48-C23	4.58	1.46	1.33
23	b	603	CLA	C1D-ND	4.57	1.43	1.37
23	A	405	CLA	CHD-C4C	4.57	1.49	1.39
23	d	403	CLA	O2D-CGD	4.57	1.44	1.33
23	D	403	CLA	CHB-C1B	4.57	1.49	1.39
23	b	602	CLA	CHD-C1D	4.56	1.47	1.38
23	b	612	CLA	O2D-CGD	4.56	1.44	1.33
23	C	513	CLA	C3C-C2C	4.56	1.46	1.36
23	B	612	CLA	C3C-C2C	4.55	1.46	1.36
23	B	613	CLA	C3C-C2C	4.55	1.46	1.36
23	B	605	CLA	CHD-C1D	4.55	1.47	1.38
23	b	602	CLA	C1D-ND	4.55	1.43	1.37
23	C	513	CLA	C1D-ND	4.55	1.43	1.37
23	A	407	CLA	CHD-C1D	4.55	1.47	1.38
23	B	616	CLA	C1D-ND	4.54	1.43	1.37
23	B	604	CLA	C1D-ND	4.54	1.43	1.37
23	B	601	CLA	C1D-ND	4.54	1.43	1.37
23	b	615	CLA	CHC-C1C	4.54	1.47	1.38
23	B	607	CLA	C3C-C2C	4.53	1.46	1.36
23	A	404	CLA	O2D-CGD	4.53	1.44	1.33
34	M	101	LMG	O7-C10	4.52	1.47	1.34
23	C	509	CLA	CHC-C1C	4.52	1.47	1.38
23	b	604	CLA	C1D-ND	4.52	1.43	1.37
23	c	508	CLA	CHD-C1D	4.51	1.47	1.38
23	c	513	CLA	CHB-C1B	4.51	1.49	1.39
24	a	406	PHO	O2D-CGD	4.51	1.44	1.33
23	B	602	CLA	CHD-C1D	4.51	1.47	1.38
23	b	614	CLA	CHC-C1C	4.50	1.47	1.38
24	A	406	PHO	O2D-CGD	4.50	1.44	1.33
23	C	503	CLA	O2D-CGD	4.50	1.44	1.33
23	B	609	CLA	O2A-CGA	4.50	1.46	1.33
25	D	405	BCR	C23-C22	-4.49	1.36	1.46
23	c	513	CLA	O2D-CGD	4.49	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	CHD-C1D	4.49	1.47	1.38
23	a	404	CLA	CHC-C1C	4.48	1.47	1.38
23	B	602	CLA	CHC-C4B	4.48	1.49	1.39
23	B	615	CLA	CHC-C1C	4.48	1.47	1.38
34	C	521	LMG	O8-C28	4.47	1.46	1.33
23	C	514	CLA	C1D-ND	4.47	1.43	1.37
34	C	522	LMG	O7-C10	4.46	1.46	1.34
23	c	503	CLA	CHC-C1C	4.46	1.47	1.38
23	c	512	CLA	O2D-CGD	4.46	1.44	1.33
23	c	514	CLA	O2A-CGA	4.46	1.46	1.33
23	B	606	CLA	CHD-C1D	4.46	1.47	1.38
23	C	512	CLA	O2D-CGD	4.46	1.44	1.33
34	C	522	LMG	O8-C28	4.45	1.46	1.33
23	c	504	CLA	CHC-C1C	4.45	1.47	1.38
23	A	403	CLA	O2D-CGD	4.45	1.44	1.33
23	D	403	CLA	CHC-C1C	4.45	1.47	1.38
23	a	407	CLA	O2A-CGA	4.45	1.46	1.33
23	C	510	CLA	O2D-CGD	4.44	1.44	1.33
31	E	101	LHG	O8-C23	4.44	1.46	1.33
23	b	610	CLA	O2D-CGD	4.44	1.44	1.33
23	B	607	CLA	O2D-CGD	4.43	1.44	1.33
23	c	505	CLA	O2D-CGD	4.43	1.44	1.33
23	C	511	CLA	CHD-C1D	4.43	1.47	1.38
23	c	513	CLA	O2A-CGA	4.43	1.46	1.33
23	c	506	CLA	CHC-C1C	4.43	1.47	1.38
23	b	604	CLA	CHC-C1C	4.43	1.47	1.38
23	b	601	CLA	CHD-C1D	4.42	1.47	1.38
23	B	602	CLA	C1D-ND	4.42	1.43	1.37
23	b	611	CLA	C1D-ND	4.41	1.43	1.37
23	B	609	CLA	CHD-C1D	4.41	1.47	1.38
23	d	403	CLA	CHD-C1D	4.41	1.47	1.38
23	c	514	CLA	CHD-C1D	4.41	1.47	1.38
23	c	514	CLA	C1D-ND	4.40	1.43	1.37
26	D	413	SQD	O47-C7	4.40	1.46	1.34
23	B	604	CLA	O2D-CGD	4.39	1.44	1.33
31	a	419	LHG	O8-C23	4.39	1.46	1.33
23	B	610	CLA	C1D-ND	4.38	1.43	1.37
23	c	510	CLA	O2A-CGA	4.38	1.46	1.33
34	z	101	LMG	O8-C28	4.38	1.46	1.33
23	C	506	CLA	O2A-CGA	4.38	1.46	1.33
23	c	509	CLA	CHD-C4C	4.38	1.49	1.39
23	B	612	CLA	CHB-C1B	4.38	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	403	CLA	O2D-CGD	4.38	1.44	1.33
23	a	403	CLA	CHD-C1D	4.37	1.47	1.38
23	C	511	CLA	CHC-C1C	4.37	1.47	1.38
23	D	403	CLA	O2D-CGD	4.37	1.44	1.33
23	c	507	CLA	CHD-C1D	4.37	1.47	1.38
26	L	102	SQD	O48-C23	4.37	1.46	1.33
23	c	515	CLA	CHD-C4C	4.37	1.49	1.39
23	C	514	CLA	CHD-C1D	4.36	1.46	1.38
23	b	605	CLA	C1D-ND	4.36	1.43	1.37
31	a	419	LHG	O7-C7	4.36	1.46	1.34
23	C	513	CLA	O2A-CGA	4.36	1.46	1.33
23	d	402	CLA	O2D-CGD	4.36	1.43	1.33
34	c	522	LMG	O8-C28	4.36	1.46	1.33
23	c	512	CLA	C1D-ND	4.35	1.43	1.37
23	B	614	CLA	C4B-NB	-4.34	1.32	1.37
23	B	613	CLA	C1D-ND	4.34	1.43	1.37
23	d	403	CLA	CHD-C4C	4.33	1.49	1.39
23	c	511	CLA	CHD-C1D	4.33	1.46	1.38
23	c	506	CLA	CHD-C1D	4.33	1.46	1.38
23	b	607	CLA	CHD-C1D	4.32	1.46	1.38
35	c	520	DGD	O1G-C1A	4.32	1.45	1.33
26	B	620	SQD	O47-C7	4.32	1.46	1.34
26	f	101	SQD	O47-C7	4.32	1.46	1.34
35	c	518	DGD	O1G-C1A	4.32	1.45	1.33
23	c	515	CLA	O2A-CGA	4.32	1.45	1.33
23	c	511	CLA	O2A-CGA	4.32	1.45	1.33
23	a	405	CLA	O2D-CGD	4.32	1.43	1.33
23	c	512	CLA	CHC-C1C	4.31	1.47	1.38
23	C	508	CLA	O2A-CGA	4.31	1.45	1.33
23	b	602	CLA	O2A-CGA	4.31	1.45	1.33
23	c	509	CLA	CHD-C1D	4.30	1.46	1.38
23	C	514	CLA	O2A-CGA	4.30	1.45	1.33
23	C	507	CLA	CHD-C1D	4.30	1.46	1.38
23	b	608	CLA	O2A-CGA	4.29	1.45	1.33
23	B	610	CLA	CHD-C1D	4.29	1.46	1.38
26	a	411	SQD	O48-C23	4.29	1.45	1.33
23	b	613	CLA	CHC-C1C	4.29	1.47	1.38
23	C	508	CLA	CHD-C4C	4.29	1.49	1.39
23	c	507	CLA	O2A-CGA	4.29	1.45	1.33
25	Y	101	BCR	C23-C22	-4.28	1.36	1.46
23	B	611	CLA	CHC-C1C	4.28	1.47	1.38
23	B	601	CLA	CHD-C1D	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	522	LMG	O7-C10	4.28	1.46	1.34
23	B	608	CLA	O2A-CGA	4.28	1.45	1.33
23	b	602	CLA	CHD-C4C	4.27	1.48	1.39
23	d	402	CLA	O2A-CGA	4.27	1.45	1.33
23	C	503	CLA	CHD-C1D	4.27	1.46	1.38
23	D	403	CLA	O2A-CGA	4.27	1.45	1.33
23	b	601	CLA	C3D-C2D	4.27	1.50	1.39
23	b	614	CLA	C1D-ND	4.27	1.43	1.37
23	C	503	CLA	CHC-C1C	4.26	1.47	1.38
23	b	611	CLA	CHC-C1C	4.26	1.47	1.38
23	c	503	CLA	CHB-C1B	4.26	1.49	1.39
23	c	509	CLA	OBD-CAD	4.26	1.29	1.22
35	C	520	DGD	O1G-C1A	4.25	1.45	1.33
23	a	404	CLA	O2A-CGA	4.25	1.45	1.33
23	b	608	CLA	C1D-ND	4.25	1.43	1.37
23	b	612	CLA	CHC-C1C	4.25	1.47	1.38
23	D	403	CLA	CHD-C4C	4.24	1.48	1.39
34	Z	101	LMG	O7-C10	4.24	1.46	1.34
23	d	402	CLA	CHC-C1C	4.23	1.47	1.38
34	d	411	LMG	O8-C28	4.23	1.45	1.33
23	b	611	CLA	O2A-CGA	4.23	1.45	1.33
23	b	612	CLA	O2A-CGA	4.23	1.45	1.33
23	b	609	CLA	C1D-ND	4.23	1.43	1.37
23	C	510	CLA	C1D-ND	4.23	1.43	1.37
23	C	515	CLA	CHD-C1D	4.23	1.46	1.38
23	B	616	CLA	CHC-C4B	4.22	1.48	1.39
23	C	504	CLA	O2A-CGA	4.22	1.45	1.33
23	b	601	CLA	CHD-C4C	4.22	1.48	1.39
23	b	607	CLA	CHB-C1B	4.22	1.48	1.39
35	h	103	DGD	O1G-C1A	4.21	1.45	1.33
26	a	411	SQD	O47-C7	4.21	1.46	1.34
23	B	608	CLA	C1D-ND	4.21	1.43	1.37
34	C	521	LMG	O7-C10	4.21	1.46	1.34
34	m	101	LMG	O8-C28	4.21	1.45	1.33
31	b	628	LHG	O8-C23	4.21	1.45	1.33
23	C	515	CLA	O2A-CGA	4.21	1.45	1.33
23	d	403	CLA	C3D-C2D	4.20	1.50	1.39
23	B	601	CLA	CHC-C4B	4.20	1.48	1.39
23	B	608	CLA	CHC-C1C	4.20	1.46	1.38
23	A	407	CLA	O2A-CGA	4.20	1.45	1.33
26	a	409	SQD	O48-C23	4.20	1.45	1.33
23	c	507	CLA	C1D-ND	4.20	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	CHB-C1B	4.20	1.48	1.39
23	c	508	CLA	CHD-C4C	4.20	1.48	1.39
23	B	607	CLA	O2A-CGA	4.19	1.45	1.33
23	b	610	CLA	CHB-C1B	4.19	1.48	1.39
23	d	403	CLA	O2A-CGA	4.19	1.45	1.33
23	C	509	CLA	C1D-ND	4.19	1.43	1.37
23	A	404	CLA	CHC-C4B	4.19	1.48	1.39
23	C	503	CLA	C1D-ND	4.19	1.43	1.37
23	A	404	CLA	CHD-C1D	4.19	1.46	1.38
23	c	506	CLA	C3D-C2D	4.19	1.50	1.39
26	L	102	SQD	O47-C7	4.18	1.46	1.34
23	c	503	CLA	CHD-C1D	4.18	1.46	1.38
23	b	610	CLA	CHD-C1D	4.18	1.46	1.38
23	b	613	CLA	C3D-C2D	4.17	1.50	1.39
23	b	616	CLA	CHC-C4B	4.17	1.48	1.39
23	C	513	CLA	CHD-C1D	4.17	1.46	1.38
23	b	608	CLA	CHD-C4C	4.16	1.48	1.39
23	C	504	CLA	C1D-ND	4.16	1.43	1.37
23	b	609	CLA	CHD-C1D	4.16	1.46	1.38
26	a	409	SQD	O47-C7	4.16	1.46	1.34
23	a	407	CLA	C1D-ND	4.16	1.43	1.37
23	c	511	CLA	CHD-C4C	4.16	1.48	1.39
34	c	521	LMG	O8-C28	4.15	1.45	1.33
23	c	505	CLA	CHD-C1D	4.15	1.46	1.38
26	A	411	SQD	O47-C7	4.15	1.46	1.34
23	B	607	CLA	C1D-ND	4.15	1.43	1.37
23	C	509	CLA	O2A-CGA	4.14	1.45	1.33
23	B	604	CLA	CHD-C1D	4.14	1.46	1.38
23	b	605	CLA	OBD-CAD	4.14	1.29	1.22
34	c	521	LMG	O7-C10	4.13	1.46	1.34
34	C	502	LMG	O8-C28	4.13	1.45	1.33
23	C	510	CLA	O2A-CGA	4.13	1.45	1.33
23	B	606	CLA	O2A-CGA	4.13	1.45	1.33
24	A	406	PHO	O2A-CGA	4.13	1.45	1.33
23	c	509	CLA	CHC-C4B	4.13	1.48	1.39
23	a	405	CLA	C3D-C2D	4.12	1.50	1.39
23	B	607	CLA	CHB-C1B	4.12	1.48	1.39
23	c	510	CLA	CHD-C1D	4.12	1.46	1.38
23	C	511	CLA	CHD-C4C	4.11	1.48	1.39
23	c	507	CLA	CHC-C4B	4.11	1.48	1.39
23	c	514	CLA	CHC-C4B	4.11	1.48	1.39
35	c	518	DGD	O2G-C1B	4.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	O2A-CGA	4.11	1.45	1.33
26	B	620	SQD	O48-C23	4.11	1.45	1.33
23	b	610	CLA	CHC-C4B	4.11	1.48	1.39
34	C	502	LMG	O7-C10	4.11	1.45	1.34
23	B	603	CLA	C1B-NB	-4.11	1.32	1.37
23	A	407	CLA	CHD-C4C	4.11	1.48	1.39
23	B	604	CLA	CHD-C4C	4.10	1.48	1.39
35	c	519	DGD	O1G-C1A	4.10	1.45	1.33
23	C	505	CLA	O2A-CGA	4.10	1.45	1.33
34	a	417	LMG	O8-C28	4.10	1.45	1.33
23	A	403	CLA	CHC-C1C	4.10	1.46	1.38
23	C	513	CLA	CHD-C4C	4.10	1.48	1.39
23	c	509	CLA	O2A-CGA	4.09	1.45	1.33
23	c	503	CLA	CHD-C4C	4.09	1.48	1.39
23	b	607	CLA	C1D-ND	4.09	1.43	1.37
23	b	603	CLA	OBD-CAD	4.09	1.29	1.22
26	D	413	SQD	O48-C23	4.08	1.45	1.33
23	B	614	CLA	CHC-C4B	4.08	1.48	1.39
31	D	408	LHG	O7-C7	4.08	1.45	1.34
23	C	503	CLA	CHC-C4B	4.08	1.48	1.39
31	L	101	LHG	O8-C23	4.08	1.45	1.33
23	b	615	CLA	OBD-CAD	4.08	1.29	1.22
23	A	405	CLA	C1D-ND	4.08	1.43	1.37
23	B	603	CLA	O2A-CGA	4.08	1.45	1.33
31	b	628	LHG	O7-C7	4.07	1.45	1.34
23	C	512	CLA	C3D-C2D	4.07	1.50	1.39
23	B	607	CLA	CHC-C4B	4.07	1.48	1.39
34	z	101	LMG	O7-C10	4.07	1.45	1.34
23	C	506	CLA	C1D-ND	4.06	1.43	1.37
23	b	603	CLA	CHD-C1D	4.06	1.46	1.38
23	C	514	CLA	C3D-C2D	4.06	1.50	1.39
35	C	519	DGD	O1G-C1A	4.06	1.45	1.33
23	D	404	CLA	CHD-C1D	4.05	1.46	1.38
23	c	512	CLA	CHD-C1D	4.05	1.46	1.38
23	B	608	CLA	O2D-CGD	4.05	1.43	1.33
31	E	101	LHG	O7-C7	4.05	1.45	1.34
35	C	518	DGD	O1G-C1A	4.05	1.45	1.33
23	A	405	CLA	CHD-C1D	4.05	1.46	1.38
23	b	605	CLA	CHD-C1D	4.05	1.46	1.38
23	B	610	CLA	OBD-CAD	4.04	1.29	1.22
23	a	404	CLA	CHD-C1D	4.04	1.46	1.38
23	c	506	CLA	CHB-C1B	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	O2A-CGA	4.04	1.45	1.33
23	a	403	CLA	CHD-C4C	4.04	1.48	1.39
23	c	504	CLA	O2A-CGA	4.03	1.45	1.33
23	B	607	CLA	CHD-C1D	4.03	1.46	1.38
23	b	612	CLA	CHD-C1D	4.03	1.46	1.38
23	A	407	CLA	CHC-C4B	4.03	1.48	1.39
23	C	504	CLA	C3D-C2D	4.03	1.50	1.39
23	c	510	CLA	C3D-C2D	4.03	1.50	1.39
23	C	512	CLA	CHD-C1D	4.03	1.46	1.38
23	B	604	CLA	CHB-C1B	4.03	1.48	1.39
26	f	101	SQD	O48-C23	4.03	1.45	1.33
31	d	408	LHG	O8-C23	4.02	1.45	1.33
23	B	613	CLA	O2A-CGA	4.02	1.45	1.33
23	D	404	CLA	C3D-C2D	4.02	1.49	1.39
23	B	610	CLA	O2D-CGD	4.02	1.43	1.33
23	B	603	CLA	CHB-C1B	4.01	1.48	1.39
23	C	513	CLA	CHB-C1B	4.01	1.48	1.39
23	c	506	CLA	CHD-C4C	4.01	1.48	1.39
23	c	508	CLA	O2A-CGA	4.01	1.45	1.33
23	C	504	CLA	CHB-C1B	4.01	1.48	1.39
23	b	612	CLA	C1B-NB	-4.01	1.32	1.37
23	c	506	CLA	O2A-CGA	4.01	1.45	1.33
25	B	618	BCR	C23-C22	-4.00	1.37	1.46
23	b	605	CLA	CHC-C4B	3.99	1.48	1.39
23	C	507	CLA	CHD-C4C	3.99	1.48	1.39
23	C	511	CLA	O2A-CGA	3.99	1.45	1.33
23	C	505	CLA	CHD-C4C	3.99	1.48	1.39
23	C	506	CLA	C3D-C2D	3.99	1.49	1.39
23	c	507	CLA	C3D-C2D	3.99	1.49	1.39
23	B	605	CLA	O2A-CGA	3.99	1.45	1.33
23	d	403	CLA	CHC-C4B	3.98	1.48	1.39
34	a	417	LMG	O7-C10	3.98	1.45	1.34
23	c	505	CLA	O2A-CGA	3.98	1.45	1.33
35	C	518	DGD	O2G-C1B	3.98	1.45	1.34
23	B	610	CLA	C3D-C2D	3.98	1.49	1.39
23	C	510	CLA	CHB-C1B	3.98	1.48	1.39
23	B	614	CLA	CHB-C1B	3.98	1.48	1.39
23	C	503	CLA	OBD-CAD	3.97	1.29	1.22
23	A	405	CLA	C3D-C2D	3.97	1.49	1.39
23	c	509	CLA	C3D-C2D	3.97	1.49	1.39
38	E	102	HEM	FE-NC	3.97	2.08	1.95
23	B	613	CLA	CHB-C1B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C3D-C2D	3.97	1.49	1.39
23	c	503	CLA	C3D-C2D	3.97	1.49	1.39
23	b	606	CLA	O2D-CGD	3.96	1.43	1.33
31	d	408	LHG	O7-C7	3.96	1.45	1.34
23	b	615	CLA	O2A-CGA	3.96	1.44	1.33
23	C	512	CLA	CHD-C4C	3.96	1.48	1.39
23	c	505	CLA	CHD-C4C	3.96	1.48	1.39
23	B	606	CLA	CHB-C1B	3.95	1.48	1.39
23	b	614	CLA	C3D-C2D	3.95	1.49	1.39
23	C	507	CLA	C1D-ND	3.95	1.43	1.37
23	B	610	CLA	CHC-C4B	3.95	1.48	1.39
23	B	601	CLA	CHD-C4C	3.95	1.48	1.39
23	c	512	CLA	CHD-C4C	3.95	1.48	1.39
23	B	615	CLA	O2A-CGA	3.95	1.44	1.33
23	b	607	CLA	C1B-NB	-3.95	1.32	1.37
23	C	503	CLA	CHD-C4C	3.94	1.48	1.39
23	B	602	CLA	C3D-C2D	3.94	1.49	1.39
23	C	514	CLA	CHD-C4C	3.94	1.48	1.39
23	C	512	CLA	CHB-C1B	3.94	1.48	1.39
23	B	610	CLA	CHD-C4C	3.94	1.48	1.39
23	b	604	CLA	CHC-C4B	3.94	1.48	1.39
34	m	101	LMG	O7-C10	3.93	1.45	1.34
23	a	405	CLA	O2A-CGA	3.93	1.44	1.33
23	b	611	CLA	CHD-C4C	3.93	1.48	1.39
31	A	416	LHG	O7-C7	3.93	1.45	1.34
23	A	404	CLA	O2A-CGA	3.93	1.44	1.33
38	e	102	HEM	FE-NC	3.93	2.08	1.95
23	C	511	CLA	C3D-C2D	3.93	1.49	1.39
23	c	512	CLA	CHB-C1B	3.92	1.48	1.39
35	h	103	DGD	O2G-C1B	3.92	1.45	1.34
23	B	611	CLA	OBD-CAD	3.92	1.29	1.22
26	A	409	SQD	O48-C23	3.92	1.44	1.33
23	B	616	CLA	O2A-CGA	3.92	1.44	1.33
23	B	602	CLA	CHD-C4C	3.92	1.48	1.39
23	b	613	CLA	CHB-C1B	3.92	1.48	1.39
23	b	614	CLA	CHD-C1D	3.92	1.46	1.38
23	b	611	CLA	CHD-C1D	3.92	1.46	1.38
35	C	519	DGD	O2G-C1B	3.91	1.45	1.34
23	B	608	CLA	CHD-C1D	3.91	1.46	1.38
23	D	403	CLA	CHD-C1D	3.91	1.46	1.38
23	b	616	CLA	O2A-CGA	3.91	1.44	1.33
23	C	503	CLA	O2A-CGA	3.91	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	CHC-C4B	3.91	1.48	1.39
23	C	513	CLA	C3D-C2D	3.90	1.49	1.39
34	d	411	LMG	O7-C10	3.90	1.45	1.34
23	b	616	CLA	CHD-C1D	3.90	1.46	1.38
23	c	505	CLA	CHB-C1B	3.90	1.48	1.39
23	C	515	CLA	C3D-C2D	3.90	1.49	1.39
23	D	404	CLA	O2A-CGA	3.90	1.44	1.33
23	b	608	CLA	CHB-C1B	3.90	1.48	1.39
23	B	614	CLA	O2A-CGA	3.89	1.44	1.33
23	a	404	CLA	CHC-C4B	3.89	1.48	1.39
35	c	519	DGD	O2G-C1B	3.88	1.45	1.34
23	a	404	CLA	CHD-C4C	3.88	1.48	1.39
23	C	515	CLA	CHB-C1B	3.88	1.48	1.39
23	D	404	CLA	OBD-CAD	3.88	1.29	1.22
23	b	608	CLA	OBD-CAD	3.87	1.29	1.22
23	b	610	CLA	C3D-C2D	3.87	1.49	1.39
23	B	609	CLA	CHD-C4C	3.87	1.48	1.39
23	b	616	CLA	C1D-ND	3.87	1.42	1.37
23	C	504	CLA	CHC-C4B	3.87	1.48	1.39
23	b	612	CLA	CHB-C1B	3.87	1.48	1.39
23	b	606	CLA	CHD-C4C	3.87	1.48	1.39
23	B	611	CLA	C3D-C2D	3.87	1.49	1.39
23	C	515	CLA	CHD-C4C	3.87	1.48	1.39
23	B	611	CLA	CHB-C1B	3.87	1.48	1.39
31	D	407	LHG	O8-C23	3.87	1.44	1.33
23	b	615	CLA	C3D-C2D	3.87	1.49	1.39
23	C	511	CLA	OBD-CAD	3.87	1.29	1.22
23	b	604	CLA	O2A-CGA	3.86	1.44	1.33
23	c	513	CLA	CHD-C4C	3.86	1.48	1.39
23	C	512	CLA	CHC-C4B	3.86	1.48	1.39
23	b	615	CLA	CHD-C4C	3.86	1.48	1.39
23	b	610	CLA	C1D-ND	3.86	1.42	1.37
23	b	603	CLA	O2A-CGA	3.86	1.44	1.33
23	c	508	CLA	C3D-C2D	3.86	1.49	1.39
23	b	604	CLA	C3D-C2D	3.86	1.49	1.39
23	C	512	CLA	O2A-CGA	3.85	1.44	1.33
23	C	506	CLA	CHD-C1D	3.85	1.45	1.38
23	C	505	CLA	C3D-C2D	3.85	1.49	1.39
23	a	403	CLA	C3D-C2D	3.85	1.49	1.39
23	b	606	CLA	OBD-CAD	3.85	1.29	1.22
23	c	514	CLA	C3D-C2D	3.85	1.49	1.39
23	b	613	CLA	O2A-CGA	3.85	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	O2A-CGA	3.84	1.44	1.33
23	c	515	CLA	C3D-C2D	3.84	1.49	1.39
23	c	504	CLA	CHB-C1B	3.84	1.48	1.39
23	C	510	CLA	C3D-C2D	3.84	1.49	1.39
23	b	609	CLA	C3D-C2D	3.83	1.49	1.39
23	C	507	CLA	O2A-CGA	3.83	1.44	1.33
23	C	510	CLA	CHD-C1D	3.83	1.45	1.38
23	b	603	CLA	CHD-C4C	3.83	1.47	1.39
23	C	507	CLA	C3D-C2D	3.83	1.49	1.39
23	c	504	CLA	CHD-C4C	3.83	1.47	1.39
23	B	612	CLA	O2A-CGA	3.83	1.44	1.33
23	A	405	CLA	CHC-C4B	3.83	1.48	1.39
23	B	607	CLA	CHD-C4C	3.82	1.47	1.39
31	d	406	LHG	O7-C7	3.82	1.45	1.34
31	d	406	LHG	O8-C23	3.82	1.44	1.33
23	b	604	CLA	CHD-C1D	3.82	1.45	1.38
23	B	603	CLA	C3D-C2D	3.82	1.49	1.39
23	b	602	CLA	C3D-C2D	3.82	1.49	1.39
23	c	511	CLA	C3D-C2D	3.82	1.49	1.39
23	A	407	CLA	C3D-C2D	3.82	1.49	1.39
23	c	504	CLA	CHD-C1D	3.82	1.45	1.38
23	C	511	CLA	CHB-C1B	3.82	1.48	1.39
23	C	506	CLA	CHB-C1B	3.82	1.48	1.39
23	c	505	CLA	CHC-C4B	3.82	1.48	1.39
23	c	514	CLA	CHD-C4C	3.81	1.47	1.39
23	B	603	CLA	C1D-ND	3.81	1.42	1.37
23	c	510	CLA	CHD-C4C	3.81	1.47	1.39
23	B	601	CLA	C3D-C2D	3.81	1.49	1.39
23	c	507	CLA	CHD-C4C	3.81	1.47	1.39
31	D	408	LHG	O8-C23	3.81	1.44	1.33
23	c	514	CLA	OBD-CAD	3.80	1.29	1.22
23	B	604	CLA	C3D-C2D	3.80	1.49	1.39
23	C	504	CLA	OBD-CAD	3.80	1.29	1.22
35	C	520	DGD	O2G-C1B	3.80	1.45	1.34
23	B	613	CLA	C3D-C2D	3.80	1.49	1.39
23	b	611	CLA	CHB-C1B	3.80	1.47	1.39
23	B	611	CLA	CHD-C1D	3.80	1.45	1.38
23	C	504	CLA	CHD-C1D	3.80	1.45	1.38
23	c	513	CLA	CHD-C1D	3.80	1.45	1.38
23	C	514	CLA	OBD-CAD	3.80	1.29	1.22
23	b	602	CLA	CHC-C4B	3.80	1.47	1.39
23	b	609	CLA	CHC-C4B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3D-C2D	3.79	1.49	1.39
23	C	508	CLA	C3D-C2D	3.79	1.49	1.39
34	D	412	LMG	O8-C28	3.79	1.44	1.33
23	b	615	CLA	CHD-C1D	3.79	1.45	1.38
23	b	605	CLA	CHD-C4C	3.79	1.47	1.39
31	d	407	LHG	O8-C23	3.79	1.44	1.33
23	B	609	CLA	C3D-C2D	3.79	1.49	1.39
23	B	604	CLA	O2A-CGA	3.79	1.44	1.33
23	C	506	CLA	CHD-C4C	3.79	1.47	1.39
23	c	511	CLA	OBD-CAD	3.78	1.29	1.22
23	a	407	CLA	CHB-C1B	3.78	1.47	1.39
23	b	612	CLA	C1D-ND	3.78	1.42	1.37
23	C	507	CLA	CHB-C1B	3.78	1.47	1.39
23	c	510	CLA	OBD-CAD	3.77	1.29	1.22
23	c	512	CLA	OBD-CAD	3.77	1.29	1.22
23	C	507	CLA	CHC-C4B	3.77	1.47	1.39
23	b	605	CLA	C1B-NB	-3.77	1.32	1.37
23	C	505	CLA	CHB-C1B	3.77	1.47	1.39
23	b	603	CLA	CHB-C1B	3.77	1.47	1.39
35	H	102	DGD	O1G-C1A	3.76	1.44	1.33
23	b	613	CLA	CHD-C1D	3.76	1.45	1.38
23	A	405	CLA	OBD-CAD	3.76	1.29	1.22
23	B	612	CLA	C3D-C2D	3.76	1.49	1.39
23	B	605	CLA	C3D-C2D	3.76	1.49	1.39
23	b	612	CLA	CHC-C4B	3.75	1.47	1.39
23	b	611	CLA	C3D-C2D	3.75	1.49	1.39
23	C	509	CLA	CHD-C1D	3.75	1.45	1.38
23	B	604	CLA	CHC-C4B	3.75	1.47	1.39
23	c	508	CLA	CHC-C4B	3.75	1.47	1.39
26	A	409	SQD	O47-C7	3.75	1.44	1.34
23	C	515	CLA	CHC-C4B	3.75	1.47	1.39
23	a	407	CLA	CHD-C1D	3.74	1.45	1.38
24	a	406	PHO	O2A-CGA	3.74	1.44	1.33
23	B	608	CLA	C3D-C2D	3.74	1.49	1.39
23	a	403	CLA	O2A-CGA	3.74	1.44	1.33
23	A	404	CLA	CHD-C4C	3.74	1.47	1.39
23	B	613	CLA	CHD-C1D	3.74	1.45	1.38
23	b	609	CLA	CHD-C4C	3.74	1.47	1.39
23	D	404	CLA	CHC-C4B	3.74	1.47	1.39
23	B	609	CLA	CHB-C1B	3.74	1.47	1.39
23	B	615	CLA	CHC-C4B	3.73	1.47	1.39
24	a	416	PHO	O2A-CGA	3.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	520	DGD	O2G-C1B	3.73	1.44	1.34
23	c	513	CLA	C3D-C2D	3.73	1.49	1.39
23	b	604	CLA	CHB-C1B	3.73	1.47	1.39
23	A	403	CLA	C3D-C2D	3.72	1.49	1.39
23	B	616	CLA	CHB-C1B	3.72	1.47	1.39
23	C	511	CLA	CHC-C4B	3.72	1.47	1.39
23	C	505	CLA	CHD-C1D	3.72	1.45	1.38
23	B	601	CLA	OBD-CAD	3.72	1.28	1.22
23	b	606	CLA	O2A-CGA	3.72	1.44	1.33
23	B	614	CLA	C3D-C2D	3.72	1.49	1.39
23	B	602	CLA	CHB-C1B	3.72	1.47	1.39
23	b	607	CLA	C3D-C2D	3.71	1.49	1.39
23	b	614	CLA	CHB-C1B	3.71	1.47	1.39
23	B	616	CLA	CHD-C4C	3.71	1.47	1.39
24	A	415	PHO	O2A-CGA	3.71	1.44	1.33
31	d	407	LHG	O7-C7	3.71	1.44	1.34
23	A	403	CLA	CHB-C1B	3.70	1.47	1.39
23	b	604	CLA	CHD-C4C	3.70	1.47	1.39
23	b	612	CLA	C3D-C2D	3.70	1.49	1.39
23	b	616	CLA	CHB-C1B	3.70	1.47	1.39
23	C	509	CLA	C3D-C2D	3.70	1.49	1.39
23	B	614	CLA	CHD-C4C	3.70	1.47	1.39
23	d	402	CLA	OBD-CAD	3.70	1.28	1.22
23	C	503	CLA	CHB-C1B	3.69	1.47	1.39
23	c	506	CLA	OBD-CAD	3.69	1.28	1.22
23	a	405	CLA	C1D-ND	3.69	1.42	1.37
23	b	608	CLA	CHC-C4B	3.69	1.47	1.39
23	B	616	CLA	CHD-C1D	3.69	1.45	1.38
23	a	407	CLA	C1B-NB	-3.69	1.33	1.37
23	c	503	CLA	CHC-C4B	3.68	1.47	1.39
23	B	615	CLA	OBD-CAD	3.68	1.28	1.22
23	C	514	CLA	CHC-C4B	3.68	1.47	1.39
23	b	614	CLA	CHC-C4B	3.68	1.47	1.39
23	B	606	CLA	C3D-C2D	3.68	1.49	1.39
23	A	403	CLA	O2A-CGA	3.67	1.44	1.33
23	d	402	CLA	C3D-C2D	3.67	1.49	1.39
23	B	610	CLA	O2A-CGA	3.67	1.44	1.33
23	c	514	CLA	CHB-C1B	3.66	1.47	1.39
23	B	606	CLA	CHD-C4C	3.66	1.47	1.39
23	c	512	CLA	C3D-C2D	3.65	1.49	1.39
23	B	615	CLA	CHB-C1B	3.65	1.47	1.39
23	B	613	CLA	C1B-NB	-3.64	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C3D-C2D	3.63	1.48	1.39
23	c	508	CLA	OBD-CAD	3.63	1.28	1.22
23	b	604	CLA	OBD-CAD	3.63	1.28	1.22
23	b	613	CLA	CHD-C4C	3.63	1.47	1.39
23	b	609	CLA	CHB-C1B	3.63	1.47	1.39
23	b	607	CLA	O2A-CGA	3.63	1.43	1.33
23	b	606	CLA	CHD-C1D	3.63	1.45	1.38
23	a	405	CLA	CHC-C4B	3.62	1.47	1.39
23	b	610	CLA	C1B-NB	-3.62	1.33	1.37
23	b	616	CLA	C3D-C2D	3.62	1.48	1.39
23	C	509	CLA	CHD-C4C	3.62	1.47	1.39
23	b	605	CLA	CHB-C1B	3.62	1.47	1.39
23	A	404	CLA	C3D-C2D	3.61	1.48	1.39
23	B	605	CLA	CHD-C4C	3.61	1.47	1.39
23	D	403	CLA	C1D-ND	3.61	1.42	1.37
23	b	607	CLA	CHD-C4C	3.61	1.47	1.39
23	b	603	CLA	C3D-C2D	3.61	1.48	1.39
23	B	601	CLA	C1B-NB	-3.61	1.33	1.37
23	B	608	CLA	CHD-C4C	3.61	1.47	1.39
23	B	610	CLA	CHB-C1B	3.60	1.47	1.39
34	D	412	LMG	O7-C10	3.60	1.44	1.34
23	C	505	CLA	CHC-C4B	3.60	1.47	1.39
23	c	511	CLA	CHB-C1B	3.60	1.47	1.39
23	a	405	CLA	CHD-C4C	3.59	1.47	1.39
23	B	602	CLA	O2A-CGA	3.59	1.43	1.33
23	c	507	CLA	OBD-CAD	3.59	1.28	1.22
23	C	503	CLA	C3D-C2D	3.58	1.48	1.39
23	B	604	CLA	OBD-CAD	3.58	1.28	1.22
23	B	611	CLA	O2A-CGA	3.58	1.43	1.33
23	A	404	CLA	OBD-CAD	3.58	1.28	1.22
23	C	509	CLA	CHC-C4B	3.57	1.47	1.39
23	c	512	CLA	CHC-C4B	3.57	1.47	1.39
23	b	601	CLA	CHC-C4B	3.57	1.47	1.39
35	H	102	DGD	O2G-C1B	3.57	1.44	1.34
31	A	416	LHG	O8-C23	3.57	1.43	1.33
23	c	510	CLA	CHB-C1B	3.57	1.47	1.39
23	B	609	CLA	CHC-C4B	3.57	1.47	1.39
23	c	504	CLA	CHC-C4B	3.57	1.47	1.39
23	c	507	CLA	CHB-C1B	3.57	1.47	1.39
23	C	504	CLA	CHD-C4C	3.56	1.47	1.39
23	c	508	CLA	CHB-C1B	3.56	1.47	1.39
23	C	510	CLA	CHD-C4C	3.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CHD-C4C	3.56	1.47	1.39
23	C	512	CLA	C1B-NB	-3.56	1.33	1.37
23	c	513	CLA	CHC-C4B	3.56	1.47	1.39
23	b	605	CLA	C3D-C2D	3.55	1.48	1.39
23	b	616	CLA	CHD-C4C	3.55	1.47	1.39
23	b	601	CLA	CHB-C1B	3.54	1.47	1.39
23	c	508	CLA	C1B-NB	-3.54	1.33	1.37
23	B	612	CLA	CHC-C4B	3.54	1.47	1.39
23	C	510	CLA	OBD-CAD	3.54	1.28	1.22
23	c	512	CLA	O2A-CGA	3.53	1.43	1.33
23	b	614	CLA	C1B-NB	-3.53	1.33	1.37
23	B	616	CLA	C1B-NB	-3.53	1.33	1.37
23	D	404	CLA	CHD-C4C	3.53	1.47	1.39
23	b	611	CLA	CHC-C4B	3.53	1.47	1.39
23	a	403	CLA	OBD-CAD	3.53	1.28	1.22
23	a	405	CLA	OBD-CAD	3.53	1.28	1.22
23	b	601	CLA	OBD-CAD	3.52	1.28	1.22
23	C	509	CLA	CHB-C1B	3.52	1.47	1.39
23	a	405	CLA	CHB-C1B	3.52	1.47	1.39
23	B	611	CLA	CHD-C4C	3.51	1.47	1.39
23	B	608	CLA	CHC-C4B	3.51	1.47	1.39
23	a	407	CLA	CHD-C4C	3.51	1.47	1.39
23	C	505	CLA	OBD-CAD	3.51	1.28	1.22
23	C	509	CLA	OBD-CAD	3.51	1.28	1.22
31	D	407	LHG	O7-C7	3.50	1.44	1.34
23	C	508	CLA	CHB-C1B	3.49	1.47	1.39
23	c	506	CLA	CHC-C4B	3.49	1.47	1.39
23	b	612	CLA	C4B-NB	-3.49	1.33	1.37
23	A	405	CLA	O2A-CGA	3.49	1.43	1.33
23	b	608	CLA	C3D-C2D	3.49	1.48	1.39
23	c	515	CLA	CHB-C1B	3.48	1.47	1.39
23	C	513	CLA	CHC-C4B	3.48	1.47	1.39
23	b	602	CLA	OBD-CAD	3.48	1.28	1.22
23	B	608	CLA	CHB-C1B	3.48	1.47	1.39
31	L	101	LHG	O7-C7	3.47	1.44	1.34
23	b	614	CLA	CHD-C4C	3.47	1.47	1.39
23	b	605	CLA	O2A-CGA	3.47	1.43	1.33
23	b	610	CLA	OBD-CAD	3.47	1.28	1.22
32	h	101	HTG	C1'-S1	-3.46	1.76	1.81
23	d	403	CLA	OBD-CAD	3.46	1.28	1.22
23	c	511	CLA	C1B-NB	-3.45	1.33	1.37
23	A	403	CLA	CHD-C4C	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C3D-C2D	3.45	1.48	1.39
23	c	510	CLA	CHC-C4B	3.45	1.47	1.39
23	B	603	CLA	OBD-CAD	3.45	1.28	1.22
23	b	616	CLA	C1B-NB	-3.45	1.33	1.37
23	B	605	CLA	C1B-NB	-3.44	1.33	1.37
23	b	614	CLA	C1B-C2B	3.44	1.51	1.43
23	B	607	CLA	C3D-C2D	3.44	1.48	1.39
23	c	509	CLA	CHB-C1B	3.44	1.47	1.39
38	e	102	HEM	C4D-ND	-3.44	1.34	1.40
23	C	510	CLA	CHC-C4B	3.44	1.47	1.39
23	B	612	CLA	C1D-ND	3.43	1.42	1.37
23	b	607	CLA	CHC-C4B	3.43	1.47	1.39
23	d	402	CLA	C1B-NB	-3.43	1.33	1.37
23	A	403	CLA	CHC-C4B	3.43	1.47	1.39
23	A	404	CLA	C1B-NB	-3.43	1.33	1.37
23	B	608	CLA	OBD-CAD	3.43	1.28	1.22
23	B	606	CLA	CHC-C4B	3.43	1.47	1.39
23	B	611	CLA	C1B-NB	-3.42	1.33	1.37
23	A	407	CLA	CHB-C1B	3.42	1.47	1.39
23	d	402	CLA	CHB-C1B	3.42	1.47	1.39
23	a	403	CLA	CHC-C4B	3.41	1.47	1.39
23	B	616	CLA	OBD-CAD	3.41	1.28	1.22
23	C	508	CLA	OBD-CAD	3.41	1.28	1.22
23	d	402	CLA	CHC-C4B	3.41	1.47	1.39
23	B	603	CLA	CHC-C4B	3.41	1.47	1.39
23	b	603	CLA	CHC-C4B	3.41	1.47	1.39
23	C	514	CLA	CHB-C1B	3.41	1.47	1.39
23	B	603	CLA	CHD-C1D	3.41	1.45	1.38
23	A	404	CLA	CHB-C1B	3.40	1.47	1.39
23	d	403	CLA	CHB-C1B	3.40	1.47	1.39
23	b	606	CLA	CHC-C4B	3.40	1.47	1.39
23	D	403	CLA	OBD-CAD	3.40	1.28	1.22
23	B	612	CLA	CHD-C1D	3.40	1.45	1.38
23	c	511	CLA	CHC-C4B	3.40	1.47	1.39
23	B	612	CLA	C1C-C2C	3.39	1.51	1.44
23	B	613	CLA	CHD-C4C	3.39	1.46	1.39
23	b	602	CLA	CHB-C1B	3.39	1.47	1.39
23	c	515	CLA	CHC-C4B	3.39	1.47	1.39
23	C	506	CLA	CHC-C4B	3.38	1.47	1.39
23	b	610	CLA	CHD-C4C	3.38	1.46	1.39
23	B	615	CLA	CHD-C4C	3.38	1.46	1.39
23	b	613	CLA	OBD-CAD	3.38	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	622	HTG	C1'-S1	-3.37	1.76	1.81
23	b	615	CLA	CHB-C1B	3.37	1.47	1.39
23	A	403	CLA	C4B-NB	-3.37	1.33	1.37
23	A	403	CLA	CHD-C1D	3.37	1.45	1.38
23	B	608	CLA	C4B-NB	-3.36	1.33	1.37
23	C	513	CLA	OBD-CAD	3.36	1.28	1.22
23	c	511	CLA	C4C-C3C	3.36	1.50	1.45
23	C	507	CLA	C1B-C2B	3.36	1.51	1.43
23	A	405	CLA	C1B-NB	-3.36	1.33	1.37
23	a	405	CLA	CHD-C1D	3.35	1.44	1.38
23	B	607	CLA	OBD-CAD	3.35	1.28	1.22
23	B	602	CLA	OBD-CAD	3.35	1.28	1.22
23	c	504	CLA	OBD-CAD	3.35	1.28	1.22
23	B	602	CLA	C1C-C2C	3.35	1.51	1.44
23	a	404	CLA	CHB-C1B	3.34	1.46	1.39
23	a	404	CLA	OBD-CAD	3.34	1.28	1.22
23	b	606	CLA	CHB-C1B	3.34	1.46	1.39
23	C	508	CLA	CHC-C4B	3.34	1.46	1.39
23	a	407	CLA	C3D-C2D	3.34	1.48	1.39
23	C	514	CLA	C1B-NB	-3.33	1.33	1.37
23	B	613	CLA	CHC-C4B	3.32	1.46	1.39
23	B	612	CLA	OBD-CAD	3.32	1.28	1.22
23	b	603	CLA	C1B-C2B	3.32	1.50	1.43
23	D	404	CLA	C1B-NB	-3.32	1.33	1.37
23	B	608	CLA	C1B-NB	-3.30	1.33	1.37
38	E	102	HEM	C4D-ND	-3.30	1.34	1.40
23	b	610	CLA	O2A-CGA	3.29	1.42	1.33
23	b	609	CLA	OBD-CAD	3.29	1.28	1.22
23	c	509	CLA	C1B-NB	-3.29	1.33	1.37
23	b	616	CLA	OBD-CAD	3.28	1.28	1.22
23	a	403	CLA	CHB-C1B	3.28	1.46	1.39
23	b	606	CLA	C1B-NB	-3.28	1.33	1.37
23	B	615	CLA	CHD-C1D	3.27	1.44	1.38
23	C	507	CLA	C1B-NB	-3.25	1.33	1.37
38	E	102	HEM	C1B-NB	-3.25	1.34	1.40
32	B	621	HTG	C1'-S1	-3.25	1.76	1.81
23	c	503	CLA	C4B-NB	-3.25	1.33	1.37
23	d	402	CLA	CHD-C1D	3.25	1.44	1.38
23	B	611	CLA	CHC-C4B	3.25	1.46	1.39
23	c	515	CLA	OBD-CAD	3.25	1.28	1.22
23	D	403	CLA	C3D-C2D	3.24	1.47	1.39
23	b	612	CLA	OBD-CAD	3.24	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C1D-ND	3.24	1.42	1.37
23	C	506	CLA	OBD-CAD	3.24	1.28	1.22
23	B	605	CLA	OBD-CAD	3.24	1.28	1.22
23	b	615	CLA	CHC-C4B	3.23	1.46	1.39
23	D	403	CLA	CHC-C4B	3.22	1.46	1.39
23	c	506	CLA	C4B-NB	-3.22	1.33	1.37
23	B	612	CLA	C1B-NB	-3.22	1.33	1.37
23	B	601	CLA	CHB-C1B	3.21	1.46	1.39
23	b	614	CLA	OBD-CAD	3.21	1.28	1.22
32	B	624	HTG	C1'-S1	-3.19	1.76	1.81
23	c	510	CLA	C1B-NB	-3.19	1.33	1.37
23	b	601	CLA	C1B-NB	-3.18	1.33	1.37
23	C	508	CLA	C1B-NB	-3.18	1.33	1.37
23	b	612	CLA	CHD-C4C	3.17	1.46	1.39
23	C	504	CLA	C4B-NB	-3.17	1.33	1.37
23	B	609	CLA	OBD-CAD	3.17	1.27	1.22
38	e	102	HEM	C1B-NB	-3.17	1.34	1.40
23	d	402	CLA	CHD-C4C	3.16	1.46	1.39
23	B	607	CLA	C1B-NB	-3.16	1.33	1.37
23	D	403	CLA	C4B-NB	-3.15	1.33	1.37
23	C	507	CLA	OBD-CAD	3.15	1.27	1.22
23	C	513	CLA	C4B-NB	-3.15	1.33	1.37
23	c	513	CLA	OBD-CAD	3.14	1.27	1.22
23	b	613	CLA	C1B-NB	-3.14	1.33	1.37
23	B	604	CLA	C1B-NB	-3.14	1.33	1.37
23	C	511	CLA	C4B-NB	-3.14	1.33	1.37
23	B	606	CLA	C1B-NB	-3.13	1.33	1.37
23	C	512	CLA	OBD-CAD	3.13	1.27	1.22
23	b	613	CLA	C4B-NB	-3.13	1.33	1.37
23	A	405	CLA	CHB-C1B	3.13	1.46	1.39
23	C	506	CLA	C1B-NB	-3.12	1.33	1.37
32	b	624	HTG	C1'-S1	-3.12	1.77	1.81
23	c	503	CLA	OBD-CAD	3.12	1.27	1.22
23	c	512	CLA	C1B-NB	-3.12	1.33	1.37
23	C	509	CLA	C1B-NB	-3.10	1.33	1.37
23	b	604	CLA	C1B-NB	-3.08	1.33	1.37
23	b	613	CLA	CHC-C4B	3.08	1.46	1.39
23	d	402	CLA	C1B-C2B	3.08	1.50	1.43
32	b	621	HTG	C1'-S1	-3.08	1.77	1.81
23	b	608	CLA	C1B-NB	-3.08	1.33	1.37
23	B	605	CLA	CHB-C1B	3.08	1.46	1.39
23	C	511	CLA	C1B-NB	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1B-C2B	3.07	1.50	1.43
23	C	510	CLA	C4B-NB	-3.06	1.33	1.37
23	c	506	CLA	C4C-C3C	3.06	1.50	1.45
23	A	403	CLA	OBD-CAD	3.06	1.27	1.22
23	C	509	CLA	C4B-NB	-3.05	1.33	1.37
23	B	610	CLA	C4B-NB	-3.05	1.33	1.37
23	d	403	CLA	C4B-NB	-3.05	1.33	1.37
23	B	614	CLA	OBD-CAD	3.04	1.27	1.22
23	c	505	CLA	C1B-C2B	3.04	1.50	1.43
23	A	407	CLA	OBD-CAD	3.03	1.27	1.22
23	b	607	CLA	C1B-C2B	3.02	1.50	1.43
23	C	506	CLA	C4B-NB	-3.02	1.33	1.37
23	B	606	CLA	OBD-CAD	3.02	1.27	1.22
23	A	407	CLA	C1B-NB	-3.02	1.33	1.37
23	B	613	CLA	C1B-C2B	3.02	1.50	1.43
32	c	523	HTG	C1'-S1	-3.02	1.77	1.81
23	D	403	CLA	C1B-NB	-3.01	1.33	1.37
23	B	603	CLA	C1B-C2B	3.01	1.50	1.43
23	b	612	CLA	C1B-C2B	3.00	1.50	1.43
23	B	614	CLA	C4D-CHA	3.00	1.48	1.38
23	C	506	CLA	C4D-CHA	3.00	1.48	1.38
23	b	604	CLA	C1B-C2B	3.00	1.50	1.43
23	c	510	CLA	C4B-NB	-2.99	1.33	1.37
23	d	403	CLA	C1B-NB	-2.99	1.33	1.37
23	c	504	CLA	C4B-NB	-2.99	1.33	1.37
23	b	613	CLA	C1B-C2B	2.99	1.50	1.43
23	B	604	CLA	C4D-CHA	2.98	1.48	1.38
23	C	513	CLA	C4D-CHA	2.97	1.48	1.38
23	b	608	CLA	C4B-NB	-2.97	1.34	1.37
23	c	505	CLA	OBD-CAD	2.96	1.27	1.22
23	c	515	CLA	C4B-NB	-2.96	1.34	1.37
23	b	609	CLA	C1B-NB	-2.96	1.34	1.37
23	C	513	CLA	C1B-C2B	2.96	1.50	1.43
23	b	611	CLA	OBD-CAD	2.95	1.27	1.22
23	b	602	CLA	C1B-NB	-2.95	1.34	1.37
23	c	510	CLA	C4D-CHA	2.95	1.48	1.38
23	a	405	CLA	C1C-C2C	2.95	1.50	1.44
23	b	610	CLA	C1B-C2B	2.95	1.50	1.43
23	D	404	CLA	C1B-C2B	2.95	1.50	1.43
23	b	615	CLA	C1B-C2B	2.95	1.50	1.43
23	b	607	CLA	OBD-CAD	2.94	1.27	1.22
23	A	403	CLA	C1B-NB	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C4D-CHA	2.93	1.48	1.38
23	C	511	CLA	C1B-C2B	2.93	1.50	1.43
23	c	512	CLA	C1B-C2B	2.93	1.50	1.43
23	c	514	CLA	C1B-NB	-2.92	1.34	1.37
23	b	604	CLA	C4D-CHA	2.91	1.48	1.38
23	C	508	CLA	C4B-NB	-2.91	1.34	1.37
23	C	509	CLA	C4D-CHA	2.91	1.48	1.38
23	B	607	CLA	C1B-C2B	2.91	1.49	1.43
23	C	515	CLA	OBD-CAD	2.91	1.27	1.22
23	B	611	CLA	C1C-C2C	2.90	1.50	1.44
23	c	505	CLA	C4C-C3C	2.90	1.50	1.45
23	B	611	CLA	C1B-C2B	2.90	1.49	1.43
23	B	613	CLA	OBD-CAD	2.90	1.27	1.22
23	B	603	CLA	C1C-C2C	2.89	1.50	1.44
23	a	407	CLA	C1C-C2C	2.89	1.50	1.44
23	B	614	CLA	CHD-C1D	2.89	1.44	1.38
23	B	614	CLA	C1B-C2B	2.88	1.49	1.43
23	B	608	CLA	C4D-CHA	2.88	1.48	1.38
23	a	405	CLA	C1B-NB	-2.88	1.34	1.37
32	D	411	HTG	C1'-S1	-2.88	1.77	1.81
23	C	512	CLA	C4B-NB	-2.87	1.34	1.37
23	B	606	CLA	C1B-C2B	2.87	1.49	1.43
23	b	603	CLA	C4B-NB	-2.87	1.34	1.37
23	B	610	CLA	C1B-NB	-2.87	1.34	1.37
23	B	610	CLA	C4C-C3C	2.87	1.49	1.45
23	c	511	CLA	C4D-CHA	2.87	1.48	1.38
23	b	601	CLA	C1B-C2B	2.87	1.49	1.43
23	c	512	CLA	C4D-CHA	2.87	1.48	1.38
23	B	615	CLA	C1B-C2B	2.87	1.49	1.43
23	c	515	CLA	C1B-NB	-2.86	1.34	1.37
23	a	404	CLA	C1B-C2B	2.86	1.49	1.43
29	A	413[B]	PL9	C6-C5	2.86	1.49	1.35
23	C	514	CLA	C4D-CHA	2.86	1.48	1.38
23	a	407	CLA	C1B-C2B	2.86	1.49	1.43
23	b	602	CLA	C4B-NB	-2.85	1.34	1.37
23	c	510	CLA	C1B-C2B	2.85	1.49	1.43
23	c	505	CLA	C4D-CHA	2.85	1.48	1.38
23	c	505	CLA	C1C-C2C	2.85	1.50	1.44
23	a	405	CLA	C1B-C2B	2.84	1.49	1.43
23	B	609	CLA	C1B-C2B	2.84	1.49	1.43
23	B	604	CLA	C1B-C2B	2.84	1.49	1.43
29	A	413[A]	PL9	C6-C5	2.84	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C1C-C2C	2.84	1.50	1.44
23	c	507	CLA	C4D-CHA	2.83	1.48	1.38
23	b	616	CLA	C4D-CHA	2.83	1.48	1.38
23	C	505	CLA	C1B-C2B	2.83	1.49	1.43
23	B	602	CLA	C1B-NB	-2.83	1.34	1.37
23	B	612	CLA	CHD-C4C	2.83	1.45	1.39
23	D	403	CLA	C1B-C2B	2.83	1.49	1.43
23	b	615	CLA	C4C-C3C	2.83	1.49	1.45
32	C	523	HTG	C1'-S1	-2.83	1.77	1.81
23	C	503	CLA	C4D-CHA	2.83	1.48	1.38
23	c	506	CLA	C1B-C2B	2.83	1.49	1.43
23	C	507	CLA	C4D-CHA	2.82	1.48	1.38
33	a	412	LMT	O1'-C1'	2.82	1.44	1.40
23	c	509	CLA	C4D-CHA	2.82	1.48	1.38
23	C	504	CLA	C1B-C2B	2.82	1.49	1.43
23	b	602	CLA	C4D-CHA	2.82	1.48	1.38
23	c	511	CLA	C1B-C2B	2.81	1.49	1.43
29	a	414[A]	PL9	C6-C5	2.81	1.49	1.35
23	b	615	CLA	C1B-NB	-2.81	1.34	1.37
23	b	609	CLA	C4D-CHA	2.81	1.48	1.38
23	B	607	CLA	C1C-C2C	2.81	1.50	1.44
29	a	414[B]	PL9	C6-C5	2.80	1.49	1.35
23	c	509	CLA	C1C-C2C	2.80	1.50	1.44
23	C	503	CLA	C1B-NB	-2.80	1.34	1.37
23	C	515	CLA	C1B-NB	-2.80	1.34	1.37
23	d	403	CLA	C3B-C4B	2.80	1.50	1.42
23	b	602	CLA	C1B-C2B	2.79	1.49	1.43
23	C	506	CLA	C1C-C2C	2.79	1.50	1.44
23	C	508	CLA	C4D-CHA	2.79	1.48	1.38
24	A	415	PHO	CHA-CBD	-2.79	1.48	1.51
23	b	614	CLA	C4D-CHA	2.79	1.48	1.38
23	b	610	CLA	C1C-C2C	2.78	1.50	1.44
23	b	602	CLA	C4C-C3C	2.78	1.49	1.45
23	A	407	CLA	C4D-CHA	2.78	1.47	1.38
23	A	404	CLA	C4D-CHA	2.78	1.47	1.38
23	B	611	CLA	C4D-CHA	2.78	1.47	1.38
23	b	615	CLA	C4D-CHA	2.78	1.47	1.38
23	c	505	CLA	C1B-NB	-2.76	1.34	1.37
23	C	515	CLA	C1C-C2C	2.76	1.50	1.44
23	b	610	CLA	C4B-NB	-2.76	1.34	1.37
23	b	603	CLA	C1C-C2C	2.76	1.50	1.44
23	C	503	CLA	C3B-C4B	2.76	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	515	CLA	C1B-C2B	2.76	1.49	1.43
23	C	510	CLA	C4D-CHA	2.76	1.47	1.38
23	C	511	CLA	C1C-C2C	2.75	1.50	1.44
23	A	405	CLA	C3B-C4B	2.75	1.50	1.42
23	b	608	CLA	C4D-CHA	2.75	1.47	1.38
23	A	405	CLA	C4C-C3C	2.75	1.49	1.45
23	B	616	CLA	C1B-C2B	2.75	1.49	1.43
23	B	609	CLA	C1B-NB	-2.74	1.34	1.37
23	C	510	CLA	C3B-C2B	2.74	1.50	1.41
23	C	505	CLA	C1B-NB	-2.74	1.34	1.37
23	b	611	CLA	C4B-NB	-2.74	1.34	1.37
23	C	506	CLA	C1B-C2B	2.74	1.49	1.43
23	C	515	CLA	C4B-NB	-2.73	1.34	1.37
23	c	511	CLA	C4B-NB	-2.73	1.34	1.37
25	b	619	BCR	C30-C25	-2.73	1.50	1.53
23	c	513	CLA	C4D-CHA	2.73	1.47	1.38
23	c	506	CLA	C4D-CHA	2.72	1.47	1.38
23	B	615	CLA	C4D-CHA	2.72	1.47	1.38
23	D	403	CLA	C4C-C3C	2.72	1.49	1.45
23	c	515	CLA	C1C-C2C	2.72	1.50	1.44
32	B	624	HTG	C1-S1	-2.72	1.76	1.80
23	B	610	CLA	C4D-CHA	2.72	1.47	1.38
23	C	508	CLA	C4C-C3C	2.72	1.49	1.45
23	b	603	CLA	C4C-C3C	2.72	1.49	1.45
23	C	503	CLA	C1C-C2C	2.72	1.50	1.44
23	b	601	CLA	C4B-NB	-2.71	1.34	1.37
23	c	506	CLA	C3B-C2B	2.71	1.50	1.41
23	B	613	CLA	C4D-CHA	2.71	1.47	1.38
23	b	603	CLA	C1B-NB	-2.71	1.34	1.37
23	b	608	CLA	C1B-C2B	2.71	1.49	1.43
23	C	512	CLA	C1C-C2C	2.70	1.50	1.44
23	b	610	CLA	C4D-CHA	2.70	1.47	1.38
23	C	512	CLA	C4D-CHA	2.70	1.47	1.38
23	a	405	CLA	C4B-NB	-2.70	1.34	1.37
23	B	610	CLA	C3D-C4D	-2.70	1.38	1.44
23	C	515	CLA	C4D-CHA	2.70	1.47	1.38
23	C	507	CLA	C4C-C3C	2.69	1.49	1.45
23	c	515	CLA	C4C-C3C	2.69	1.49	1.45
23	c	504	CLA	C1B-C2B	2.69	1.49	1.43
23	C	503	CLA	C1B-C2B	2.69	1.49	1.43
23	b	611	CLA	C1B-C2B	2.69	1.49	1.43
23	B	605	CLA	C4D-CHA	2.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C4D-CHA	2.69	1.47	1.38
23	a	407	CLA	C4D-CHA	2.69	1.47	1.38
23	c	507	CLA	C1B-NB	-2.68	1.34	1.37
23	d	402	CLA	C4B-NB	-2.68	1.34	1.37
23	b	611	CLA	C4D-CHA	2.68	1.47	1.38
23	c	514	CLA	C4D-CHA	2.68	1.47	1.38
23	c	508	CLA	C4B-NB	-2.68	1.34	1.37
23	B	608	CLA	C1B-C2B	2.68	1.49	1.43
23	B	612	CLA	C1B-C2B	2.67	1.49	1.43
23	B	602	CLA	C3B-C4B	2.67	1.50	1.42
23	A	407	CLA	C1C-C2C	2.67	1.49	1.44
23	A	403	CLA	C1B-C2B	2.66	1.49	1.43
23	A	405	CLA	C4B-NB	-2.66	1.34	1.37
23	b	603	CLA	C4D-CHA	2.66	1.47	1.38
23	b	609	CLA	C1C-C2C	2.66	1.49	1.44
23	b	616	CLA	C3B-C4B	2.66	1.50	1.42
23	b	607	CLA	C4D-CHA	2.66	1.47	1.38
23	d	402	CLA	C4D-CHA	2.66	1.47	1.38
38	e	102	HEM	C1C-C2C	-2.66	1.40	1.45
23	a	403	CLA	C1B-NB	-2.65	1.34	1.37
23	a	403	CLA	C4B-NB	-2.65	1.34	1.37
23	B	607	CLA	C4C-C3C	2.65	1.49	1.45
23	b	602	CLA	C1C-C2C	2.65	1.49	1.44
23	a	404	CLA	C1C-C2C	2.65	1.49	1.44
23	C	511	CLA	C4D-CHA	2.64	1.47	1.38
23	A	407	CLA	C4B-NB	-2.64	1.34	1.37
23	B	612	CLA	C4B-NB	-2.64	1.34	1.37
24	a	416	PHO	C3A-C2A	-2.64	1.52	1.54
23	B	609	CLA	C3B-C4B	2.64	1.50	1.42
23	c	507	CLA	C4B-NB	-2.64	1.34	1.37
23	B	615	CLA	C1C-C2C	2.64	1.49	1.44
23	c	503	CLA	C4D-CHA	2.64	1.47	1.38
23	B	602	CLA	C4D-CHA	2.63	1.47	1.38
23	D	404	CLA	C1C-C2C	2.63	1.49	1.44
23	c	507	CLA	C3B-C4B	2.63	1.50	1.42
23	b	601	CLA	C3B-C4B	2.63	1.50	1.42
23	B	606	CLA	C3D-C4D	-2.63	1.38	1.44
23	C	511	CLA	C4C-C3C	2.63	1.49	1.45
32	B	622	HTG	C1'-S1	-2.62	1.77	1.81
23	c	507	CLA	C1B-C2B	2.62	1.49	1.43
23	A	403	CLA	C1C-C2C	2.62	1.49	1.44
23	b	616	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C1B-C2B	2.61	1.49	1.43
23	C	504	CLA	C4D-CHA	2.61	1.47	1.38
23	c	513	CLA	C1B-NB	-2.61	1.34	1.37
23	a	403	CLA	C3B-C2B	2.61	1.50	1.41
23	c	515	CLA	C1B-C2B	2.61	1.49	1.43
23	a	404	CLA	C1B-NB	-2.61	1.34	1.37
38	e	102	HEM	C1D-ND	-2.61	1.33	1.38
23	B	616	CLA	C3B-C4B	2.60	1.50	1.42
34	Z	101	LMG	O8-C28	2.60	1.45	1.33
23	b	606	CLA	C4D-CHA	2.60	1.47	1.38
23	a	405	CLA	C4D-CHA	2.60	1.47	1.38
23	A	403	CLA	C3B-C2B	2.60	1.49	1.41
23	B	603	CLA	C4D-CHA	2.60	1.47	1.38
23	B	601	CLA	C4D-CHA	2.60	1.47	1.38
23	c	511	CLA	C3B-C2B	2.60	1.49	1.41
23	b	603	CLA	C3D-C4D	-2.60	1.38	1.44
23	C	514	CLA	C4B-NB	-2.60	1.34	1.37
23	c	509	CLA	C1B-C2B	2.59	1.49	1.43
23	B	609	CLA	C4D-CHA	2.59	1.47	1.38
23	C	505	CLA	C4D-CHA	2.59	1.47	1.38
23	c	507	CLA	C4C-C3C	2.59	1.49	1.45
23	c	513	CLA	C4B-NB	-2.58	1.34	1.37
23	C	510	CLA	C1B-NB	-2.58	1.34	1.37
23	b	616	CLA	C1B-C2B	2.58	1.49	1.43
23	c	503	CLA	C1C-C2C	2.58	1.49	1.44
23	B	616	CLA	C4D-CHA	2.58	1.47	1.38
23	D	404	CLA	C4D-CHA	2.58	1.47	1.38
23	b	612	CLA	C3B-C2B	2.57	1.49	1.41
23	c	515	CLA	C4D-CHA	2.57	1.47	1.38
23	B	601	CLA	C3B-C4B	2.56	1.50	1.42
23	C	513	CLA	C1B-NB	-2.56	1.34	1.37
23	b	608	CLA	C3D-C4D	-2.56	1.38	1.44
29	d	405	PL9	C6-C5	2.56	1.47	1.35
23	a	407	CLA	C4B-NB	-2.56	1.34	1.37
23	C	509	CLA	C1B-C2B	2.55	1.49	1.43
23	c	510	CLA	C3B-C2B	2.55	1.49	1.41
23	c	503	CLA	C1B-NB	-2.55	1.34	1.37
23	C	505	CLA	C3B-C4B	2.55	1.50	1.42
23	b	609	CLA	C4B-NB	-2.55	1.34	1.37
23	c	508	CLA	C1B-C2B	2.55	1.49	1.43
23	B	616	CLA	C1C-C2C	2.55	1.49	1.44
23	C	510	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	C4D-CHA	2.54	1.47	1.38
23	A	404	CLA	C3B-C4B	2.54	1.50	1.42
23	a	403	CLA	C1B-C2B	2.54	1.49	1.43
23	b	601	CLA	C4D-CHA	2.53	1.47	1.38
23	A	404	CLA	C1B-C2B	2.53	1.49	1.43
23	c	504	CLA	C4D-CHA	2.53	1.47	1.38
23	b	605	CLA	C4D-CHA	2.53	1.47	1.38
23	A	405	CLA	C4D-CHA	2.53	1.47	1.38
23	C	513	CLA	C1C-C2C	2.53	1.49	1.44
24	a	416	PHO	C1B-NB	-2.53	1.34	1.38
23	B	613	CLA	C1C-C2C	2.53	1.49	1.44
23	c	503	CLA	C1B-C2B	2.52	1.49	1.43
23	c	514	CLA	C3B-C4B	2.52	1.50	1.42
23	A	407	CLA	C1B-C2B	2.52	1.49	1.43
23	c	508	CLA	C4D-CHA	2.52	1.47	1.38
23	c	503	CLA	C3D-C4D	-2.52	1.38	1.44
23	C	514	CLA	C1C-C2C	2.52	1.49	1.44
23	b	606	CLA	C1C-C2C	2.52	1.49	1.44
23	C	507	CLA	C1C-C2C	2.52	1.49	1.44
23	D	403	CLA	C1C-C2C	2.52	1.49	1.44
23	c	515	CLA	C3B-C4B	2.52	1.50	1.42
23	B	614	CLA	C3D-C4D	-2.52	1.38	1.44
23	A	404	CLA	C1C-C2C	2.52	1.49	1.44
23	C	509	CLA	C1C-C2C	2.51	1.49	1.44
23	c	505	CLA	C4B-NB	-2.51	1.34	1.37
23	C	514	CLA	C1B-C2B	2.51	1.49	1.43
24	a	406	PHO	C4B-NB	-2.51	1.34	1.38
23	b	612	CLA	C4D-CHA	2.51	1.47	1.38
23	B	601	CLA	C4B-NB	-2.51	1.34	1.37
23	c	506	CLA	C1B-NB	-2.51	1.34	1.37
23	B	610	CLA	C3B-C4B	2.50	1.50	1.42
23	C	512	CLA	C1B-C2B	2.50	1.49	1.43
23	B	606	CLA	C4B-NB	-2.50	1.34	1.37
24	a	416	PHO	C4B-NB	-2.50	1.34	1.38
23	C	509	CLA	C4C-C3C	2.50	1.49	1.45
23	c	514	CLA	C4C-C3C	2.50	1.49	1.45
23	b	611	CLA	C1B-NB	-2.49	1.34	1.37
23	b	608	CLA	C3B-C4B	2.49	1.50	1.42
23	C	505	CLA	C4C-C3C	2.49	1.49	1.45
23	B	604	CLA	C1C-C2C	2.49	1.49	1.44
23	a	407	CLA	OBD-CAD	2.49	1.26	1.22
23	b	609	CLA	C3B-C4B	2.49	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	522	LMG	O1-C1	2.48	1.44	1.40
23	c	503	CLA	C4C-C3C	2.48	1.49	1.45
23	b	606	CLA	C4B-NB	-2.48	1.34	1.37
23	c	506	CLA	C1C-C2C	2.48	1.49	1.44
23	C	511	CLA	C3B-C2B	2.48	1.49	1.41
23	c	514	CLA	C1C-C2C	2.48	1.49	1.44
23	C	503	CLA	C3D-C4D	-2.48	1.38	1.44
23	b	616	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	504	CLA	C1C-C2C	2.48	1.49	1.44
23	c	515	CLA	C3D-C4D	-2.48	1.38	1.44
25	d	404	BCR	C30-C25	-2.47	1.50	1.53
23	d	402	CLA	C4C-C3C	2.47	1.49	1.45
23	b	616	CLA	C4B-NB	-2.47	1.34	1.37
23	C	513	CLA	C4C-C3C	2.47	1.49	1.45
23	C	512	CLA	C4C-C3C	2.47	1.49	1.45
23	C	505	CLA	C1C-C2C	2.46	1.49	1.44
23	c	505	CLA	C3B-C4B	2.46	1.49	1.42
23	B	614	CLA	C3B-C4B	2.46	1.49	1.42
23	a	403	CLA	C4D-CHA	2.46	1.46	1.38
38	E	102	HEM	C1C-C2C	-2.46	1.40	1.45
23	B	613	CLA	C3B-C2B	2.46	1.49	1.41
23	A	405	CLA	C1B-C2B	2.46	1.48	1.43
23	B	601	CLA	C1C-C2C	2.46	1.49	1.44
23	A	404	CLA	C4B-NB	-2.46	1.34	1.37
31	D	407	LHG	O7-C5	-2.46	1.40	1.46
23	b	605	CLA	C1B-C2B	2.45	1.48	1.43
31	L	101	LHG	O7-C5	-2.45	1.40	1.46
23	b	613	CLA	C1C-C2C	2.45	1.49	1.44
23	b	611	CLA	C3D-C4D	-2.45	1.38	1.44
24	A	415	PHO	C1B-NB	-2.45	1.34	1.38
23	B	608	CLA	C1C-C2C	2.45	1.49	1.44
23	C	505	CLA	C4B-NB	-2.45	1.34	1.37
23	d	402	CLA	C1C-C2C	2.44	1.49	1.44
24	A	415	PHO	C4B-NB	-2.44	1.34	1.38
23	A	403	CLA	C4D-CHA	2.44	1.46	1.38
23	B	603	CLA	C4B-NB	-2.44	1.34	1.37
23	b	610	CLA	C3D-C4D	-2.44	1.38	1.44
29	D	406	PL9	C6-C5	2.44	1.47	1.35
23	B	614	CLA	C1B-NB	-2.44	1.34	1.37
23	C	506	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	605	CLA	C3B-C4B	2.44	1.49	1.42
23	C	504	CLA	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	402	LMT	O1'-C1'	2.44	1.44	1.40
23	a	403	CLA	C1C-C2C	2.43	1.49	1.44
23	B	615	CLA	C1B-NB	-2.43	1.34	1.37
23	B	614	CLA	C1C-C2C	2.43	1.49	1.44
23	b	602	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	508	CLA	C1B-C2B	2.43	1.48	1.43
23	b	607	CLA	C4B-NB	-2.43	1.34	1.37
23	B	609	CLA	C1C-C2C	2.43	1.49	1.44
23	c	508	CLA	C3D-C4D	-2.43	1.38	1.44
23	b	613	CLA	C4C-C3C	2.43	1.49	1.45
23	B	612	CLA	C3B-C2B	2.43	1.49	1.41
23	c	507	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	507	CLA	C3D-C4D	-2.43	1.38	1.44
23	b	608	CLA	C1C-C2C	2.43	1.49	1.44
23	D	403	CLA	C4D-CHA	2.42	1.46	1.38
23	B	612	CLA	C4D-CHA	2.42	1.46	1.38
23	b	603	CLA	C3B-C2B	2.42	1.49	1.41
23	B	613	CLA	C4C-C3C	2.41	1.49	1.45
23	a	404	CLA	C3B-C4B	2.41	1.49	1.42
23	b	613	CLA	C3B-C2B	2.41	1.49	1.41
23	b	605	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	603	CLA	C3B-C2B	2.40	1.49	1.41
23	a	405	CLA	C3B-C4B	2.40	1.49	1.42
23	B	601	CLA	C1B-C2B	2.40	1.48	1.43
23	d	403	CLA	C1B-C2B	2.39	1.48	1.43
23	B	608	CLA	C3D-C4D	-2.39	1.38	1.44
32	b	624	HTG	C1-S1	-2.39	1.76	1.80
23	C	508	CLA	C1C-C2C	2.39	1.49	1.44
23	C	509	CLA	C3B-C2B	2.39	1.49	1.41
23	B	605	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	613	CLA	C4D-CHA	2.38	1.46	1.38
40	V	201	HEC	CMB-C2B	2.38	1.55	1.50
23	C	503	CLA	C4B-NB	-2.38	1.34	1.37
23	C	512	CLA	C3D-C4D	-2.38	1.38	1.44
23	A	407	CLA	C4C-C3C	2.38	1.49	1.45
35	h	103	DGD	O5D-C1E	2.38	1.44	1.40
23	c	505	CLA	C3D-C4D	-2.38	1.38	1.44
23	c	511	CLA	C1C-C2C	2.37	1.49	1.44
23	b	607	CLA	C4C-C3C	2.37	1.49	1.45
23	b	606	CLA	C1B-C2B	2.37	1.48	1.43
23	c	509	CLA	C4B-NB	-2.37	1.34	1.37
23	b	609	CLA	C3B-C2B	2.37	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C3B-C2B	2.36	1.49	1.41
29	D	406	PL9	C2-C3	2.36	1.40	1.34
23	C	513	CLA	C3B-C4B	2.36	1.49	1.42
23	B	608	CLA	C3B-C2B	2.36	1.49	1.41
23	c	513	CLA	C3B-C2B	2.36	1.49	1.41
23	C	510	CLA	C3D-C4D	-2.36	1.38	1.44
23	a	405	CLA	C3D-C4D	-2.36	1.38	1.44
23	c	514	CLA	C1B-C2B	2.36	1.48	1.43
23	C	514	CLA	C4C-C3C	2.35	1.49	1.45
23	b	612	CLA	C4C-C3C	2.35	1.49	1.45
23	B	609	CLA	C3D-C4D	-2.35	1.38	1.44
23	C	514	CLA	C3B-C2B	2.35	1.49	1.41
23	d	403	CLA	C4D-CHA	2.35	1.46	1.38
23	c	512	CLA	C3D-C4D	-2.35	1.38	1.44
23	A	403	CLA	C4C-C3C	2.35	1.49	1.45
23	B	608	CLA	C4C-C3C	2.35	1.49	1.45
23	b	610	CLA	C4C-C3C	2.35	1.49	1.45
23	D	404	CLA	C3B-C4B	2.35	1.49	1.42
23	c	504	CLA	C1B-NB	-2.35	1.34	1.37
23	A	407	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	610	CLA	C1B-C2B	2.35	1.48	1.43
23	b	608	CLA	C4C-C3C	2.34	1.49	1.45
23	B	604	CLA	C3B-C2B	2.34	1.49	1.41
23	a	407	CLA	C4C-C3C	2.34	1.49	1.45
23	d	403	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	504	CLA	C3B-C4B	2.34	1.49	1.42
23	b	602	CLA	C3B-C4B	2.34	1.49	1.42
23	B	605	CLA	C1C-C2C	2.34	1.49	1.44
23	c	508	CLA	C1C-C2C	2.34	1.49	1.44
23	b	615	CLA	C3B-C4B	2.33	1.49	1.42
23	b	614	CLA	C3B-C2B	2.33	1.49	1.41
33	C	526	LMT	O1'-C1'	2.32	1.44	1.40
35	H	102	DGD	O5D-C1E	2.32	1.44	1.40
29	A	413[A]	PL9	C2-C3	2.32	1.40	1.34
23	C	508	CLA	C1D-C2D	2.32	1.49	1.45
23	B	612	CLA	C4C-C3C	2.32	1.49	1.45
23	c	512	CLA	C1C-C2C	2.32	1.49	1.44
23	B	602	CLA	C3D-C4D	-2.32	1.39	1.44
24	a	406	PHO	C1B-NB	-2.31	1.34	1.38
23	b	604	CLA	C4B-NB	-2.31	1.34	1.37
23	a	407	CLA	C3D-C4D	-2.31	1.39	1.44
23	c	512	CLA	C4C-C3C	2.30	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C3B-C4B	2.30	1.49	1.42
23	b	607	CLA	C1C-C2C	2.30	1.49	1.44
23	B	611	CLA	C4B-NB	-2.30	1.34	1.37
23	a	404	CLA	C4B-NB	-2.30	1.34	1.37
23	B	609	CLA	C4C-C3C	2.30	1.48	1.45
23	B	615	CLA	C3B-C4B	2.30	1.49	1.42
23	C	508	CLA	C3D-C4D	-2.30	1.39	1.44
40	V	201	HEC	CMC-C2C	2.29	1.55	1.50
23	C	509	CLA	C3D-C4D	-2.29	1.39	1.44
23	C	513	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	603	CLA	C3B-C4B	2.29	1.49	1.42
23	C	506	CLA	C3B-C2B	2.29	1.48	1.41
23	c	506	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	616	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	616	CLA	C4B-NB	-2.28	1.34	1.37
23	b	609	CLA	C3D-C4D	-2.28	1.39	1.44
29	d	405	PL9	C2-C3	2.28	1.40	1.34
23	c	509	CLA	C3B-C4B	2.28	1.49	1.42
23	B	608	CLA	C3B-C4B	2.27	1.49	1.42
23	b	606	CLA	C3D-C4D	-2.27	1.39	1.44
23	C	503	CLA	C4C-C3C	2.27	1.48	1.45
23	C	510	CLA	C4C-C3C	2.27	1.48	1.45
23	D	404	CLA	C4B-NB	-2.26	1.34	1.37
23	C	504	CLA	C3B-C2B	2.26	1.48	1.41
23	b	604	CLA	C3B-C2B	2.26	1.48	1.41
29	A	413[B]	PL9	C2-C3	2.26	1.40	1.34
23	d	402	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	602	CLA	C4C-C3C	2.26	1.48	1.45
23	b	602	CLA	C3B-C2B	2.26	1.48	1.41
23	c	508	CLA	C3B-C2B	2.25	1.48	1.41
23	c	510	CLA	C4C-C3C	2.25	1.48	1.45
34	Z	101	LMG	O1-C1	2.25	1.44	1.40
23	c	503	CLA	C3B-C4B	2.25	1.49	1.42
23	D	403	CLA	C3D-C4D	-2.25	1.39	1.44
23	c	504	CLA	C3B-C2B	2.25	1.48	1.41
23	C	507	CLA	C4B-NB	-2.25	1.34	1.37
23	b	614	CLA	C1C-C2C	2.25	1.49	1.44
23	C	515	CLA	C3B-C4B	2.25	1.49	1.42
38	E	102	HEM	C1D-ND	-2.24	1.34	1.38
23	c	504	CLA	C3B-C4B	2.24	1.49	1.42
23	c	512	CLA	C3B-C2B	2.24	1.48	1.41
23	B	606	CLA	C3B-C2B	2.24	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C4C-C3C	2.24	1.48	1.45
23	C	513	CLA	C1C-NC	-2.24	1.34	1.37
24	a	406	PHO	C1D-ND	-2.24	1.34	1.38
23	c	510	CLA	C1C-C2C	2.24	1.49	1.44
38	E	102	HEM	C3B-C4B	2.23	1.49	1.44
23	C	507	CLA	C3B-C4B	2.23	1.49	1.42
23	c	506	CLA	C1D-C2D	2.23	1.49	1.45
23	b	604	CLA	C1C-C2C	2.23	1.49	1.44
23	C	515	CLA	C4C-C3C	2.23	1.48	1.45
23	B	606	CLA	C1C-C2C	2.23	1.49	1.44
23	B	603	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	607	CLA	C3B-C2B	2.23	1.48	1.41
23	b	609	CLA	C1C-NC	-2.22	1.34	1.37
23	d	403	CLA	C1C-C2C	2.22	1.49	1.44
23	b	611	CLA	C3B-C2B	2.22	1.48	1.41
23	a	404	CLA	C4C-C3C	2.22	1.48	1.45
23	b	601	CLA	C1C-C2C	2.21	1.49	1.44
23	a	404	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	514	CLA	C3D-C4D	-2.21	1.39	1.44
33	F	101	LMT	O1'-C1'	2.21	1.43	1.40
23	b	601	CLA	C3B-C2B	2.21	1.48	1.41
23	c	510	CLA	C1C-NC	-2.21	1.34	1.37
23	B	603	CLA	C4C-C3C	2.21	1.48	1.45
23	b	605	CLA	C1D-C2D	2.21	1.49	1.45
23	d	402	CLA	C3B-C2B	2.20	1.48	1.41
23	c	509	CLA	C1D-C2D	2.20	1.49	1.45
24	a	406	PHO	CBD-CGD	-2.20	1.49	1.52
23	c	504	CLA	C1C-C2C	2.20	1.49	1.44
23	c	510	CLA	C3D-C4D	-2.20	1.39	1.44
23	C	514	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	605	CLA	C3B-C4B	2.20	1.49	1.42
23	b	615	CLA	C4B-NB	-2.20	1.35	1.37
23	C	508	CLA	C3B-C4B	2.19	1.49	1.42
23	c	511	CLA	C3B-C4B	2.19	1.49	1.42
23	A	407	CLA	C3B-C2B	2.19	1.48	1.41
23	C	504	CLA	C1B-NB	-2.18	1.35	1.37
34	D	412	LMG	O7-C8	-2.18	1.41	1.46
23	c	506	CLA	C1C-NC	-2.18	1.34	1.37
23	B	602	CLA	C1B-C2B	2.18	1.48	1.43
23	c	511	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	601	CLA	C3B-C2B	2.18	1.48	1.41
23	c	503	CLA	C1C-NC	-2.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	515	CLA	C3B-C2B	2.18	1.48	1.41
23	B	606	CLA	C3B-C4B	2.18	1.49	1.42
23	d	403	CLA	CHB-C4A	-2.18	1.32	1.37
23	B	604	CLA	C4C-C3C	2.17	1.48	1.45
33	e	101	LMT	O1'-C1'	2.17	1.43	1.40
29	a	414[B]	PL9	C2-C3	2.17	1.40	1.34
23	B	611	CLA	C3B-C2B	2.16	1.48	1.41
23	b	605	CLA	C1C-C2C	2.16	1.48	1.44
23	D	403	CLA	C3B-C2B	2.16	1.48	1.41
24	A	415	PHO	C1D-ND	-2.16	1.34	1.38
23	b	611	CLA	C1C-C2C	2.16	1.48	1.44
23	B	604	CLA	MG-NA	2.16	2.11	2.06
23	b	606	CLA	C3B-C2B	2.16	1.48	1.41
23	C	514	CLA	C3B-C4B	2.16	1.49	1.42
25	A	408	BCR	C1-C6	-2.16	1.51	1.53
32	D	411	HTG	C1-S1	-2.15	1.77	1.80
23	b	611	CLA	C3B-C4B	2.15	1.49	1.42
23	C	512	CLA	C3B-C2B	2.15	1.48	1.41
23	A	407	CLA	C3B-C4B	2.15	1.49	1.42
23	c	514	CLA	C4B-NB	-2.15	1.35	1.37
23	b	614	CLA	C4C-C3C	2.15	1.48	1.45
23	a	407	CLA	C3B-C2B	2.15	1.48	1.41
23	A	403	CLA	C3D-C4D	-2.15	1.39	1.44
23	c	512	CLA	C4B-NB	-2.15	1.35	1.37
23	c	503	CLA	C3B-C2B	2.14	1.48	1.41
23	b	601	CLA	C1C-NC	-2.14	1.34	1.37
33	b	626	LMT	O1'-C1'	2.14	1.43	1.40
23	c	508	CLA	C3B-C4B	2.14	1.49	1.42
23	B	610	CLA	C1C-C2C	2.14	1.48	1.44
23	D	404	CLA	C1D-C2D	2.14	1.49	1.45
23	b	601	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	611	CLA	C4C-C3C	2.14	1.48	1.45
23	a	403	CLA	C4C-C3C	2.14	1.48	1.45
23	B	606	CLA	MG-NA	2.14	2.11	2.06
23	c	515	CLA	C3B-C2B	2.14	1.48	1.41
23	C	505	CLA	C3D-C4D	-2.13	1.39	1.44
23	b	608	CLA	C3B-C2B	2.13	1.48	1.41
23	B	602	CLA	C4B-NB	-2.13	1.35	1.37
23	a	403	CLA	C3D-C4D	-2.13	1.39	1.44
23	c	513	CLA	C4C-C3C	2.12	1.48	1.45
40	v	202	HEC	CMC-C2C	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	617	BCR	C1-C6	-2.12	1.51	1.53
23	B	609	CLA	C1D-C2D	2.12	1.49	1.45
23	a	403	CLA	C3B-C4B	2.11	1.48	1.42
38	e	102	HEM	C4B-NB	-2.11	1.34	1.38
23	A	404	CLA	C4C-C3C	2.11	1.48	1.45
23	B	607	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	616	CLA	C3B-C2B	2.10	1.48	1.41
23	B	615	CLA	C4B-NB	-2.10	1.35	1.37
24	A	406	PHO	C3D-C4D	-2.10	1.38	1.41
23	C	515	CLA	C3D-C4D	-2.10	1.39	1.44
23	a	405	CLA	C3B-C2B	2.09	1.48	1.41
23	B	606	CLA	C1D-C2D	2.09	1.49	1.45
40	V	201	HEC	CMA-C3A	2.09	1.55	1.50
23	b	614	CLA	C4B-NB	-2.09	1.35	1.37
24	A	406	PHO	C1D-ND	-2.09	1.34	1.38
23	b	604	CLA	C1A-CHA	2.09	1.51	1.43
29	a	414[A]	PL9	C2-C3	2.09	1.39	1.34
23	B	610	CLA	C3B-C2B	2.08	1.48	1.41
23	C	510	CLA	C1C-NC	-2.08	1.34	1.37
23	d	403	CLA	C1D-C2D	2.08	1.49	1.45
23	c	508	CLA	C4C-C3C	2.08	1.48	1.45
23	B	604	CLA	C3D-C4D	-2.07	1.39	1.44
23	C	511	CLA	C1C-NC	-2.07	1.34	1.37
35	C	519	DGD	O3G-C1D	2.07	1.43	1.40
23	b	614	CLA	C3D-C4D	-2.07	1.39	1.44
33	a	418	LMT	O1'-C1'	2.07	1.43	1.40
23	b	605	CLA	C4B-NB	-2.07	1.35	1.37
23	b	605	CLA	C4C-C3C	2.07	1.48	1.45
23	c	509	CLA	C4C-C3C	2.07	1.48	1.45
23	d	403	CLA	C4C-C3C	2.07	1.48	1.45
23	b	609	CLA	C1B-C2B	2.07	1.48	1.43
23	B	611	CLA	C3D-C4D	-2.07	1.39	1.44
23	b	611	CLA	C4C-C3C	2.06	1.48	1.45
23	C	511	CLA	C3D-C4D	-2.06	1.39	1.44
23	A	404	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	601	CLA	C4C-C3C	2.06	1.48	1.45
32	c	523	HTG	C1-S1	-2.05	1.77	1.80
23	B	603	CLA	C3B-C4B	2.05	1.48	1.42
23	C	506	CLA	C4C-C3C	2.05	1.48	1.45
40	v	202	HEC	C3B-C2B	-2.04	1.34	1.41
23	C	505	CLA	C3B-C2B	2.04	1.48	1.41
23	A	404	CLA	C1D-C2D	2.04	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	515	CLA	C1D-C2D	2.04	1.49	1.45
23	c	510	CLA	C3B-C4B	2.03	1.48	1.42
23	b	612	CLA	C3B-C4B	2.03	1.48	1.42
23	b	607	CLA	C1A-CHA	2.03	1.51	1.43
27	v	201	GOL	C3-C2	2.03	1.59	1.51
23	C	506	CLA	C3B-C4B	2.03	1.48	1.42
23	a	405	CLA	C4C-C3C	2.03	1.48	1.45
38	e	102	HEM	C3B-C4B	2.03	1.48	1.44
24	A	406	PHO	C4B-NB	-2.02	1.35	1.38
23	C	510	CLA	C1C-C2C	2.02	1.48	1.44
23	d	403	CLA	C3B-C2B	2.02	1.48	1.41
33	B	630	LMT	O1'-C1'	2.02	1.43	1.40
23	c	513	CLA	C1C-C2C	2.02	1.48	1.44
23	b	605	CLA	C3B-C2B	2.02	1.48	1.41
35	c	520	DGD	O2G-C2G	-2.02	1.41	1.46
23	C	506	CLA	C1A-CHA	2.02	1.51	1.43
23	b	609	CLA	C4C-C3C	2.02	1.48	1.45
23	c	513	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	513	CLA	C1D-C2D	2.01	1.49	1.45
23	b	604	CLA	C3B-C4B	2.01	1.48	1.42
23	b	608	CLA	C1D-C2D	2.01	1.49	1.45
23	B	605	CLA	C4C-C3C	2.01	1.48	1.45
23	B	616	CLA	C3B-C2B	2.01	1.47	1.41
23	A	405	CLA	C3D-C4D	-2.01	1.39	1.44
23	b	614	CLA	C3B-C4B	2.01	1.48	1.42
23	B	611	CLA	C3B-C4B	2.01	1.48	1.42
23	C	512	CLA	C3B-C4B	2.01	1.48	1.42
23	b	607	CLA	C3D-C4D	-2.01	1.39	1.44
23	D	404	CLA	C3D-C4D	-2.00	1.39	1.44

All (2904) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	415	PHO	C2D-C1D-ND	12.52	118.48	109.43
24	a	416	PHO	C2D-C1D-ND	12.34	118.35	109.43
23	B	614	CLA	C1D-ND-C4D	-10.41	99.01	106.31
24	a	406	PHO	C2D-C1D-ND	10.34	116.91	109.43
23	b	605	CLA	C1D-ND-C4D	-10.34	99.05	106.31
24	A	406	PHO	C2D-C1D-ND	10.27	116.85	109.43
23	A	404	CLA	C1D-ND-C4D	-10.27	99.11	106.31
23	B	612	CLA	C1D-ND-C4D	-10.11	99.22	106.31
23	a	405	CLA	C1D-ND-C4D	-10.11	99.22	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C1D-ND-C4D	-10.03	99.28	106.31
23	D	403	CLA	C1D-ND-C4D	-9.92	99.35	106.31
23	B	607	CLA	C1D-ND-C4D	-9.92	99.35	106.31
23	B	613	CLA	C1D-ND-C4D	-9.87	99.39	106.31
23	C	503	CLA	C1D-ND-C4D	-9.79	99.44	106.31
23	b	615	CLA	C1D-ND-C4D	-9.79	99.45	106.31
23	b	606	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	A	403	CLA	C1D-ND-C4D	-9.77	99.45	106.31
23	B	609	CLA	C1D-ND-C4D	-9.77	99.46	106.31
23	B	605	CLA	C1D-ND-C4D	-9.75	99.47	106.31
23	c	513	CLA	C1D-ND-C4D	-9.73	99.48	106.31
23	B	601	CLA	C1D-ND-C4D	-9.70	99.50	106.31
23	a	407	CLA	C1D-ND-C4D	-9.70	99.51	106.31
23	A	405	CLA	C1D-ND-C4D	-9.68	99.52	106.31
23	C	515	CLA	C1D-ND-C4D	-9.66	99.53	106.31
23	D	404	CLA	C1D-ND-C4D	-9.65	99.54	106.31
23	B	603	CLA	C1D-ND-C4D	-9.64	99.55	106.31
23	B	615	CLA	C1D-ND-C4D	-9.60	99.58	106.31
23	c	505	CLA	C1D-ND-C4D	-9.60	99.58	106.31
23	b	603	CLA	C1D-ND-C4D	-9.50	99.65	106.31
23	B	616	CLA	C1D-ND-C4D	-9.50	99.65	106.31
23	B	608	CLA	C1D-ND-C4D	-9.48	99.66	106.31
23	C	510	CLA	C1D-ND-C4D	-9.45	99.68	106.31
23	C	505	CLA	C1D-ND-C4D	-9.43	99.69	106.31
23	c	515	CLA	C1D-ND-C4D	-9.43	99.69	106.31
23	d	403	CLA	C1D-ND-C4D	-9.43	99.69	106.31
23	B	602	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	C	504	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	b	614	CLA	C1D-ND-C4D	-9.36	99.75	106.31
23	b	612	CLA	C1D-ND-C4D	-9.36	99.75	106.31
24	a	406	PHO	O2D-CGD-CBD	9.36	121.23	110.95
23	A	407	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	b	607	CLA	C1D-ND-C4D	-9.31	99.78	106.31
24	a	416	PHO	O2D-CGD-CBD	9.27	121.13	110.95
23	c	512	CLA	C1D-ND-C4D	-9.19	99.87	106.31
23	c	503	CLA	C1D-ND-C4D	-9.17	99.88	106.31
40	v	202	HEC	CBB-CAB-C3B	-9.15	109.15	127.43
23	b	601	CLA	C1D-ND-C4D	-9.15	99.89	106.31
23	C	513	CLA	C1D-ND-C4D	-9.14	99.90	106.31
23	C	511	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	b	609	CLA	C1D-ND-C4D	-9.09	99.94	106.31
23	c	509	CLA	C1D-ND-C4D	-9.06	99.95	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	C1D-ND-C4D	-9.03	99.98	106.31
23	b	604	CLA	C1D-ND-C4D	-9.02	99.98	106.31
23	b	608	CLA	C1D-ND-C4D	-9.02	99.99	106.31
23	b	616	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	B	611	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	b	602	CLA	C1D-ND-C4D	-8.95	100.03	106.31
23	c	514	CLA	C1D-ND-C4D	-8.95	100.03	106.31
23	d	402	CLA	C1D-ND-C4D	-8.95	100.03	106.31
23	c	508	CLA	C1D-ND-C4D	-8.92	100.06	106.31
23	b	610	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	c	511	CLA	C1D-ND-C4D	-8.89	100.08	106.31
23	C	509	CLA	C1D-ND-C4D	-8.86	100.10	106.31
23	b	611	CLA	C1D-ND-C4D	-8.84	100.11	106.31
23	C	508	CLA	C1D-ND-C4D	-8.80	100.14	106.31
23	C	507	CLA	C1D-ND-C4D	-8.77	100.16	106.31
23	c	507	CLA	C1D-ND-C4D	-8.75	100.17	106.31
23	a	404	CLA	C1D-ND-C4D	-8.73	100.19	106.31
23	b	613	CLA	C1D-ND-C4D	-8.73	100.19	106.31
23	C	512	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	a	403	CLA	C1D-ND-C4D	-8.66	100.23	106.31
24	A	415	PHO	O2D-CGD-CBD	8.65	120.45	110.95
23	C	506	CLA	C1D-ND-C4D	-8.64	100.25	106.31
23	B	610	CLA	C1D-ND-C4D	-8.64	100.25	106.31
23	B	606	CLA	C1D-ND-C4D	-8.54	100.32	106.31
23	C	514	CLA	C1D-ND-C4D	-8.51	100.34	106.31
23	c	510	CLA	C1D-ND-C4D	-8.40	100.42	106.31
23	B	604	CLA	C1D-ND-C4D	-8.35	100.46	106.31
24	A	406	PHO	C3B-C4B-NB	8.15	112.77	107.46
40	V	201	HEC	CBB-CAB-C3B	-8.08	111.29	127.43
23	B	606	CLA	CMD-C2D-C1D	8.02	138.85	124.73
23	D	403	CLA	C4A-NA-C1A	-7.96	103.05	106.68
24	a	406	PHO	C3B-C4B-NB	7.89	112.61	107.46
24	A	415	PHO	C3B-C4B-NB	7.74	112.51	107.46
23	b	616	CLA	C4A-NA-C1A	-7.54	103.24	106.68
26	A	409	SQD	O6-C1-C2	7.48	119.64	108.27
23	B	615	CLA	CHD-C4C-C3C	-7.47	113.88	124.77
23	B	614	CLA	C2D-C1D-ND	7.47	117.52	110.13
23	b	616	CLA	CHD-C4C-C3C	-7.37	114.03	124.77
24	a	416	PHO	C3B-C4B-NB	7.28	112.21	107.46
23	B	612	CLA	C2D-C1D-ND	7.28	117.33	110.13
24	A	406	PHO	O2D-CGD-CBD	7.28	118.94	110.95
23	B	602	CLA	C4A-NA-C1A	-7.24	103.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	C4A-NA-C1A	-7.22	103.38	106.68
23	B	614	CLA	CHD-C4C-C3C	-7.19	114.28	124.77
23	B	615	CLA	C2D-C1D-ND	7.18	117.23	110.13
23	B	612	CLA	CHD-C4C-C3C	-7.14	114.37	124.77
23	B	613	CLA	C2D-C1D-ND	7.12	117.17	110.13
23	B	610	CLA	CMD-C2D-C1D	7.03	137.11	124.73
23	A	404	CLA	C2D-C1D-ND	7.02	117.08	110.13
23	c	515	CLA	CMD-C2D-C1D	7.02	137.09	124.73
23	B	606	CLA	O2D-CGD-CBD	7.01	123.48	111.23
23	b	611	CLA	CMD-C2D-C1D	7.00	137.06	124.73
23	b	602	CLA	C4A-NA-C1A	-7.00	103.48	106.68
23	C	508	CLA	CMD-C2D-C1D	7.00	137.05	124.73
23	b	608	CLA	CMD-C2D-C1D	7.00	137.05	124.73
23	b	603	CLA	CMD-C2D-C1D	6.99	137.03	124.73
23	b	606	CLA	CMD-C2D-C1D	6.95	136.97	124.73
23	b	605	CLA	CMD-C2D-C1D	6.94	136.94	124.73
23	c	509	CLA	CMD-C2D-C1D	6.87	136.83	124.73
23	A	407	CLA	CMD-C2D-C1D	6.87	136.83	124.73
23	B	605	CLA	C4A-NA-C1A	-6.87	103.54	106.68
23	a	405	CLA	C2D-C1D-ND	6.86	116.92	110.13
23	c	506	CLA	CMD-C2D-C1D	6.82	136.73	124.73
23	B	609	CLA	CMD-C2D-C1D	6.80	136.70	124.73
23	C	509	CLA	CMD-C2D-C1D	6.79	136.68	124.73
23	b	607	CLA	C2D-C1D-ND	6.77	116.83	110.13
23	C	505	CLA	C4A-NA-C1A	-6.77	103.59	106.68
23	B	603	CLA	C2D-C1D-ND	6.77	116.82	110.13
23	D	403	CLA	CMD-C2D-C1D	6.75	136.61	124.73
23	B	616	CLA	CHD-C4C-C3C	-6.72	114.97	124.77
23	B	614	CLA	CMD-C2D-C1D	6.71	136.55	124.73
23	b	614	CLA	C2D-C1D-ND	6.71	116.77	110.13
23	b	616	CLA	C2D-C1D-ND	6.68	116.74	110.13
23	B	603	CLA	CHD-C4C-C3C	-6.65	115.07	124.77
23	b	616	CLA	O2D-CGD-CBD	6.65	122.86	111.23
23	a	407	CLA	C2D-C1D-ND	6.64	116.70	110.13
23	b	604	CLA	O2D-CGD-CBD	6.64	122.84	111.23
23	C	504	CLA	CHD-C4C-C3C	-6.63	115.11	124.77
23	a	405	CLA	CHD-C4C-C3C	-6.63	115.11	124.77
23	b	610	CLA	CHD-C4C-C3C	-6.61	115.13	124.77
23	b	605	CLA	CHD-C4C-C3C	-6.60	115.15	124.77
23	B	602	CLA	CHD-C4C-C3C	-6.60	115.15	124.77
23	B	607	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	B	605	CLA	CHD-C4C-C3C	-6.58	115.18	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMD-C2D-C1D	6.56	136.28	124.73
23	c	507	CLA	C4A-NA-C1A	-6.56	103.69	106.68
23	B	614	CLA	O2D-CGD-CBD	6.55	122.69	111.23
23	c	513	CLA	C2D-C1D-ND	6.55	116.61	110.13
23	A	404	CLA	CMD-C2D-C1D	6.53	136.22	124.73
29	a	414[B]	PL9	C7-C3-C4	6.52	122.28	116.91
23	b	602	CLA	CMD-C2D-C1D	6.52	136.21	124.73
23	B	616	CLA	O2D-CGD-CBD	6.46	122.53	111.23
23	B	616	CLA	C4A-NA-C1A	-6.45	103.74	106.68
23	B	611	CLA	CHD-C4C-C3C	-6.45	115.37	124.77
23	C	515	CLA	CHD-C4C-C3C	-6.44	115.38	124.77
23	b	613	CLA	C2D-C1D-ND	6.44	116.50	110.13
23	a	403	CLA	CMD-C2D-C1D	6.44	136.07	124.73
23	A	403	CLA	CMD-C2D-C1D	6.44	136.06	124.73
23	b	601	CLA	CHD-C4C-C3C	-6.43	115.40	124.77
23	C	504	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	c	503	CLA	CMD-C2D-C1D	6.43	136.05	124.73
23	c	510	CLA	CHD-C4C-C3C	-6.43	115.40	124.77
23	C	510	CLA	C2D-C1D-ND	6.42	116.48	110.13
23	C	505	CLA	CMD-C2D-C1D	6.42	136.03	124.73
23	b	604	CLA	C2D-C1D-ND	6.41	116.47	110.13
23	B	616	CLA	C2D-C1D-ND	6.41	116.47	110.13
23	C	510	CLA	CHD-C4C-C3C	-6.40	115.44	124.77
23	b	609	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
23	C	505	CLA	C2D-C1D-ND	6.35	116.41	110.13
23	C	503	CLA	CMD-C2D-C1D	6.34	135.89	124.73
23	C	509	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	b	614	CLA	O2D-CGD-CBD	6.32	122.28	111.23
23	D	404	CLA	CMD-C2D-C1D	6.32	135.85	124.73
23	D	403	CLA	C2D-C1D-ND	6.32	116.38	110.13
23	b	615	CLA	C2D-C1D-ND	6.31	116.37	110.13
23	A	407	CLA	C4A-NA-C1A	-6.31	103.80	106.68
23	B	604	CLA	O2D-CGD-CBD	6.31	122.26	111.23
23	B	601	CLA	CMD-C2D-C1D	6.29	135.80	124.73
23	c	505	CLA	C2D-C1D-ND	6.28	116.34	110.13
23	C	511	CLA	CMD-C2D-C1D	6.28	135.79	124.73
23	B	610	CLA	O2D-CGD-CBD	6.28	122.20	111.23
23	B	611	CLA	C2D-C1D-ND	6.28	116.34	110.13
23	a	407	CLA	CHD-C4C-C3C	-6.26	115.64	124.77
23	b	601	CLA	O2D-CGD-CBD	6.26	122.17	111.23
23	C	513	CLA	CMD-C2D-C1D	6.26	135.75	124.73
23	B	616	CLA	CMD-C2D-C1D	6.25	135.74	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	416	PHO	C4D-ND-C1D	-6.25	101.38	108.87
23	B	612	CLA	O2D-CGD-CBD	6.25	122.15	111.23
23	b	608	CLA	C4A-NA-C1A	-6.25	103.83	106.68
23	B	604	CLA	CHD-C4C-C3C	-6.24	115.67	124.77
23	c	515	CLA	C4A-NA-C1A	-6.24	103.83	106.68
23	C	505	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	C	515	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	c	504	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	a	404	CLA	C2D-C1D-ND	6.22	116.28	110.13
23	c	513	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
23	c	505	CLA	CMD-C2D-C1D	6.19	135.62	124.73
23	b	602	CLA	O2D-CGD-CBD	6.18	122.04	111.23
24	A	415	PHO	C2B-C1B-NB	6.18	113.90	109.43
23	c	511	CLA	CMD-C2D-C1D	6.18	135.60	124.73
23	b	610	CLA	C2D-C1D-ND	6.17	116.24	110.13
23	D	404	CLA	CHD-C4C-C3C	-6.17	115.77	124.77
23	b	615	CLA	CMD-C2D-C1D	6.16	135.58	124.73
23	d	402	CLA	C2D-C1D-ND	6.16	116.22	110.13
23	B	607	CLA	CHD-C4C-C3C	-6.16	115.80	124.77
23	C	509	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
23	d	403	CLA	C2B-C1B-NB	6.14	116.69	110.33
23	A	404	CLA	CHD-C4C-C3C	-6.13	115.83	124.77
23	B	608	CLA	C2D-C1D-ND	6.13	116.20	110.13
23	c	510	CLA	C2D-C1D-ND	6.13	116.20	110.13
23	b	606	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
23	B	608	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
23	C	503	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	D	404	CLA	C2D-C1D-ND	6.11	116.18	110.13
23	b	609	CLA	CMD-C2D-C1D	6.11	135.49	124.73
23	b	614	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
23	d	403	CLA	CMD-C2D-C1D	6.11	135.49	124.73
25	Y	101	BCR	C33-C5-C6	-6.11	117.82	124.48
23	c	512	CLA	CMD-C2D-C1D	6.11	135.48	124.73
23	B	606	CLA	C4A-NA-C1A	-6.10	103.89	106.68
23	A	403	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	c	514	CLA	C4A-NA-C1A	-6.08	103.90	106.68
23	c	509	CLA	O2D-CGD-CBD	6.08	121.86	111.23
23	a	404	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	C	506	CLA	C2D-C1D-ND	6.08	116.14	110.13
26	D	413	SQD	O6-C1-C2	6.08	117.50	108.27
23	c	507	CLA	O2D-CGD-CBD	6.07	121.85	111.23
23	B	605	CLA	CMD-C2D-C1D	6.07	135.42	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
23	A	405	CLA	C2D-C1D-ND	6.04	116.10	110.13
24	A	415	PHO	C4D-ND-C1D	-6.04	101.64	108.87
23	a	407	CLA	CMD-C2D-C1D	6.04	135.36	124.73
23	b	607	CLA	CHD-C4C-C3C	-6.03	115.97	124.77
23	b	606	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	b	611	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
23	b	609	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	B	601	CLA	O2D-CGD-CBD	6.02	121.76	111.23
23	C	509	CLA	O2D-CGD-CBD	6.01	121.74	111.23
23	b	612	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	b	603	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
24	a	416	PHO	C2B-C1B-NB	6.00	113.77	109.43
23	b	616	CLA	CMD-C2D-C1D	6.00	135.30	124.73
23	B	601	CLA	CHD-C4C-C3C	-6.00	116.03	124.77
23	C	515	CLA	CMD-C2D-C1D	5.99	135.28	124.73
23	B	611	CLA	CMD-C2D-C1D	5.99	135.28	124.73
23	c	508	CLA	CMD-C2D-C1D	5.99	135.27	124.73
23	b	606	CLA	C2D-C1D-ND	5.99	116.05	110.13
23	C	503	CLA	C2D-C1D-ND	5.99	116.05	110.13
23	C	511	CLA	CHD-C4C-C3C	-5.98	116.06	124.77
23	b	607	CLA	CMD-C2D-C1D	5.97	135.25	124.73
26	L	102	SQD	O6-C1-C2	5.97	117.33	108.27
23	c	504	CLA	CHD-C4C-C3C	-5.97	116.07	124.77
23	b	605	CLA	C2D-C1D-ND	5.97	116.03	110.13
23	b	604	CLA	CHD-C4C-C3C	-5.96	116.09	124.77
23	C	514	CLA	O2D-CGD-CBD	5.95	121.63	111.23
24	a	406	PHO	C2B-C1B-NB	5.95	113.73	109.43
23	A	407	CLA	C2D-C1D-ND	5.95	116.01	110.13
23	B	609	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
23	B	605	CLA	C2D-C1D-ND	5.94	116.01	110.13
23	b	613	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
23	b	609	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	B	601	CLA	C2D-C1D-ND	5.93	116.00	110.13
26	A	409	SQD	C1-C2-C3	-5.93	97.54	110.01
23	c	513	CLA	CMD-C2D-C1D	5.93	135.16	124.73
23	C	514	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
23	c	503	CLA	C2D-C1D-ND	5.91	115.97	110.13
40	v	202	HEC	CBC-CAC-C3C	-5.90	115.64	127.43
23	b	611	CLA	C4A-NA-C1A	-5.89	103.99	106.68
23	B	609	CLA	C2D-C1D-ND	5.89	115.95	110.13
23	C	510	CLA	CMD-C2D-C1D	5.88	135.09	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	603	CLA	O2D-CGD-CBD	5.88	121.51	111.23
23	C	514	CLA	C4A-NA-C1A	-5.87	104.00	106.68
23	b	611	CLA	C2D-C1D-ND	5.87	115.94	110.13
23	B	606	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
23	c	512	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
23	C	512	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
24	A	406	PHO	C2B-C1B-NB	5.86	113.66	109.43
23	B	614	CLA	C3D-C2D-C1D	-5.85	97.84	105.83
23	b	606	CLA	O2D-CGD-CBD	5.85	121.46	111.23
24	A	406	PHO	C4D-ND-C1D	-5.85	101.86	108.87
23	c	508	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
23	c	507	CLA	CMD-C2D-C1D	5.85	135.03	124.73
23	c	505	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
23	c	514	CLA	O2D-CGD-CBD	5.84	121.44	111.23
23	B	602	CLA	CMD-C2D-C1D	5.84	135.01	124.73
23	b	601	CLA	CMD-C2D-C1D	5.84	135.01	124.73
23	B	613	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
23	c	510	CLA	O2D-CGD-CBD	5.84	121.44	111.23
23	b	601	CLA	C2D-C1D-ND	5.82	115.89	110.13
23	A	405	CLA	C4A-NA-C1A	-5.82	104.03	106.68
23	C	503	CLA	O2D-CGD-CBD	5.82	121.40	111.23
23	B	613	CLA	C1-C2-C3	-5.81	116.67	126.20
23	C	510	CLA	O2D-CGD-CBD	5.81	121.38	111.23
23	C	503	CLA	C4A-NA-C1A	-5.80	104.03	106.68
23	b	612	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
23	C	507	CLA	C4A-NA-C1A	-5.78	104.04	106.68
23	c	506	CLA	O2D-CGD-CBD	5.78	121.33	111.23
23	C	513	CLA	C2D-C1D-ND	5.77	115.84	110.13
23	C	506	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
23	c	509	CLA	C2D-C1D-ND	5.76	115.83	110.13
23	c	507	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
23	c	503	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
23	B	613	CLA	CMD-C2D-C1D	5.74	134.84	124.73
23	b	613	CLA	C2C-C1C-NC	5.74	116.01	109.98
23	c	514	CLA	CHD-C4C-C3C	-5.73	116.41	124.77
23	C	504	CLA	CMD-C2D-C1D	5.72	134.80	124.73
23	B	607	CLA	CMD-C2D-C1D	5.70	134.77	124.73
23	d	402	CLA	C2C-C1C-NC	5.70	115.97	109.98
23	B	608	CLA	CMD-C2D-C1D	5.70	134.76	124.73
24	A	406	PHO	C3D-C4D-ND	5.70	115.01	107.71
23	C	512	CLA	C2D-C1D-ND	5.69	115.76	110.13
23	b	612	CLA	O2D-CGD-CBD	5.69	121.17	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C4A-NA-C1A	-5.68	104.09	106.68
26	A	409	SQD	C1-O5-C5	-5.68	102.64	113.72
23	C	508	CLA	C4A-NA-C1A	-5.67	104.09	106.68
23	c	506	CLA	C2D-C1D-ND	5.67	115.74	110.13
26	a	409	SQD	O6-C1-C2	5.67	116.89	108.27
23	C	506	CLA	CMD-C2D-C1D	5.67	134.71	124.73
23	C	507	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
23	b	612	CLA	CMD-C2D-C1D	5.66	134.70	124.73
23	d	403	CLA	C3B-C2B-C1B	-5.65	100.51	107.17
23	b	610	CLA	O2D-CGD-CBD	5.64	121.08	111.23
23	c	511	CLA	C2D-C1D-ND	5.62	115.69	110.13
23	C	507	CLA	CMD-C2D-C1D	5.61	134.62	124.73
23	c	508	CLA	C2D-C1D-ND	5.60	115.67	110.13
23	C	511	CLA	C2D-C1D-ND	5.60	115.67	110.13
23	d	402	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
23	c	506	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
23	C	513	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
23	c	514	CLA	C2D-C1D-ND	5.57	115.64	110.13
23	A	404	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
23	A	405	CLA	CMD-C2D-C1D	5.57	134.54	124.73
23	B	602	CLA	C2D-C1D-ND	5.57	115.63	110.13
23	B	603	CLA	CMD-C2D-C1D	5.56	134.52	124.73
23	B	604	CLA	C2D-C1D-ND	5.56	115.63	110.13
23	c	514	CLA	CMD-C2D-C1D	5.55	134.51	124.73
23	d	403	CLA	C2D-C1D-ND	5.55	115.62	110.13
23	C	514	CLA	C2D-C1D-ND	5.55	115.62	110.13
23	b	603	CLA	C2D-C1D-ND	5.55	115.62	110.13
23	c	510	CLA	C2C-C1C-NC	5.54	115.80	109.98
23	B	606	CLA	C2D-C1D-ND	5.53	115.60	110.13
23	A	405	CLA	O2D-CGD-CBD	5.52	120.89	111.23
29	a	414[A]	PL9	C7-C3-C4	5.52	121.45	116.91
23	B	615	CLA	CMD-C2D-C1D	5.51	134.42	124.73
23	a	405	CLA	C4A-NA-C1A	-5.50	104.17	106.68
23	c	515	CLA	C2D-C1D-ND	5.50	115.57	110.13
23	C	512	CLA	O2D-CGD-CBD	5.49	120.83	111.23
23	b	601	CLA	C4A-NA-C1A	-5.49	104.17	106.68
23	C	511	CLA	O2D-CGD-CBD	5.49	120.82	111.23
23	B	611	CLA	O2D-CGD-CBD	5.49	120.82	111.23
23	C	507	CLA	C2D-C1D-ND	5.49	115.56	110.13
23	D	404	CLA	O2D-CGD-CBD	5.49	120.82	111.23
23	C	506	CLA	C2C-C1C-NC	5.48	115.73	109.98
24	a	416	PHO	C3D-C4D-ND	5.47	114.72	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	416	PHO	C1-C2-C3	-5.47	117.23	126.20
23	C	510	CLA	C2C-C1C-NC	5.47	115.73	109.98
23	B	604	CLA	CMD-C2D-C1D	5.47	134.36	124.73
23	C	507	CLA	O2D-CGD-CBD	5.46	120.78	111.23
23	A	407	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
23	c	510	CLA	CMD-C2D-C1D	5.46	134.34	124.73
23	a	403	CLA	C4A-NA-C1A	-5.46	104.19	106.68
23	b	605	CLA	C4A-NA-C1A	-5.43	104.20	106.68
23	c	507	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	a	403	CLA	CHD-C4C-C3C	-5.42	116.88	124.77
23	c	508	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	b	613	CLA	CMD-C2D-C1D	5.41	134.26	124.73
23	b	612	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	c	512	CLA	C2D-C1D-ND	5.41	115.48	110.13
23	d	403	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
23	D	403	CLA	C2C-C1C-NC	5.39	115.64	109.98
23	B	605	CLA	O2D-CGD-CBD	5.38	120.64	111.23
25	k	102	BCR	C33-C5-C6	-5.38	118.62	124.48
23	B	610	CLA	C2D-C1D-ND	5.37	115.44	110.13
23	d	403	CLA	O2D-CGD-CBD	5.36	120.60	111.23
23	a	404	CLA	CMD-C2D-C1D	5.36	134.16	124.73
23	B	614	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
26	B	620	SQD	O47-C7-C8	5.35	123.04	111.48
23	c	509	CLA	C4A-NA-C1A	-5.34	104.24	106.68
23	c	515	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
23	b	604	CLA	CMD-C2D-C1D	5.32	134.10	124.73
23	c	504	CLA	CMD-C2D-C1D	5.32	134.10	124.73
23	b	615	CLA	C2C-C1C-NC	5.31	115.56	109.98
23	b	612	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
32	b	622	HTG	C1'-S1-C1	5.31	111.91	100.45
23	b	607	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
23	c	515	CLA	C2B-C1B-NB	5.29	115.82	110.33
23	b	616	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
23	b	610	CLA	CMD-C2D-C1D	5.29	134.04	124.73
23	c	511	CLA	C2C-C1C-NC	5.29	115.53	109.98
23	A	403	CLA	C2C-C1C-NC	5.27	115.52	109.98
23	d	402	CLA	C4A-NA-C1A	-5.27	104.27	106.68
25	D	405	BCR	C7-C8-C9	-5.26	118.46	126.23
23	B	613	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
23	c	510	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
23	a	403	CLA	C2C-C1C-NC	5.24	115.48	109.98
24	a	406	PHO	C3D-C4D-ND	5.23	114.41	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	404	CLA	C4A-NA-C1A	-5.23	104.29	106.68
23	b	603	CLA	O2D-CGD-CBD	5.22	120.36	111.23
23	c	510	CLA	C3B-C2B-C1B	-5.22	101.01	107.17
23	a	407	CLA	O2D-CGD-CBD	5.22	120.35	111.23
23	b	613	CLA	C1-C2-C3	-5.21	117.65	126.20
23	B	604	CLA	C4A-NA-C1A	-5.21	104.30	106.68
23	B	615	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
29	A	413[A]	PL9	C7-C3-C4	5.20	121.19	116.91
23	c	509	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
23	a	407	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	B	610	CLA	C4A-NA-C1A	-5.18	104.31	106.68
23	B	606	CLA	CHD-C1D-ND	-5.18	117.51	124.80
23	c	514	CLA	C2B-C1B-NB	5.18	115.69	110.33
23	c	511	CLA	C4A-NA-C1A	-5.18	104.32	106.68
23	C	514	CLA	CMD-C2D-C1D	5.17	133.84	124.73
23	b	611	CLA	C2C-C1C-NC	5.17	115.41	109.98
23	b	602	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
23	c	506	CLA	C2C-C1C-NC	5.16	115.40	109.98
32	C	523	HTG	C1'-S1-C1	5.16	111.58	100.45
23	c	513	CLA	O2D-CGD-CBD	5.15	120.24	111.23
23	A	407	CLA	C2B-C1B-NB	5.14	115.66	110.33
23	b	607	CLA	O2D-CGD-CBD	5.14	120.22	111.23
23	b	602	CLA	C2D-C1D-ND	5.13	115.21	110.13
23	A	403	CLA	CHD-C4C-C3C	-5.13	117.29	124.77
23	c	504	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	A	405	CLA	CHD-C4C-C3C	-5.12	117.31	124.77
23	a	405	CLA	CMD-C2D-C1D	5.12	133.74	124.73
23	c	505	CLA	O2D-CGD-CBD	5.11	120.17	111.23
23	a	404	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
26	A	409	SQD	O47-C7-C8	5.11	122.53	111.48
23	b	614	CLA	CMD-C2D-C1D	5.10	133.70	124.73
23	b	612	CLA	C2C-C1C-NC	5.10	115.33	109.98
23	b	606	CLA	C2B-C1B-NB	5.09	115.61	110.33
23	A	407	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
23	b	614	CLA	C2C-C1C-NC	5.09	115.32	109.98
23	B	609	CLA	CMB-C2B-C1B	5.08	133.16	125.42
23	b	608	CLA	CHD-C4C-C3C	-5.08	117.37	124.77
23	b	615	CLA	C4A-NA-C1A	-5.08	104.36	106.68
23	b	603	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	a	404	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	C	511	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
23	c	511	CLA	O2D-CGD-CBD	5.07	120.09	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2C-C1C-NC	5.06	115.30	109.98
23	b	615	CLA	CHD-C4C-C3C	-5.06	117.39	124.77
23	A	405	CLA	C3D-C4D-ND	5.04	118.19	109.99
23	B	607	CLA	C2C-C1C-NC	5.04	115.28	109.98
23	b	605	CLA	C3D-C4D-ND	5.04	118.18	109.99
23	b	604	CLA	C2C-C1C-NC	5.04	115.28	109.98
23	c	506	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
26	f	101	SQD	O47-C7-C8	5.04	122.38	111.48
23	a	403	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
23	C	504	CLA	C3B-C2B-C1B	-5.03	101.23	107.17
23	C	509	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
24	A	415	PHO	C3D-C4D-ND	5.03	114.16	107.71
23	a	403	CLA	C2B-C1B-NB	5.03	115.54	110.33
23	B	612	CLA	C3C-C4C-NC	5.02	116.86	110.43
23	C	508	CLA	C2D-C1D-ND	5.02	115.10	110.13
23	b	602	CLA	C2B-C1B-NB	5.02	115.53	110.33
23	B	613	CLA	C2C-C1C-NC	5.02	115.25	109.98
23	A	404	CLA	O2D-CGD-CBD	5.02	120.00	111.23
23	A	403	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
23	B	606	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
23	C	511	CLA	C2C-C1C-NC	5.01	115.24	109.98
23	b	611	CLA	O2D-CGD-CBD	5.01	119.98	111.23
23	c	512	CLA	C2C-C1C-NC	5.01	115.24	109.98
23	a	403	CLA	C2D-C1D-ND	5.00	115.08	110.13
23	A	403	CLA	CAA-C2A-C3A	-5.00	99.49	113.00
23	b	613	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	c	515	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
23	b	614	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	B	610	CLA	CHD-C4C-C3C	-4.99	117.49	124.77
23	c	503	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	b	602	CLA	CHD-C4C-C3C	-4.99	117.50	124.77
23	b	607	CLA	C4A-NA-C1A	-4.98	104.41	106.68
23	B	603	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	b	601	CLA	C2B-C1B-NB	4.97	115.48	110.33
23	B	615	CLA	C4A-NA-C1A	-4.97	104.41	106.68
23	B	604	CLA	C2C-C1C-NC	4.97	115.20	109.98
23	b	611	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	C	512	CLA	C4A-NA-C1A	-4.95	104.42	106.68
23	D	403	CLA	CHD-C4C-C3C	-4.95	117.56	124.77
23	b	605	CLA	O2D-CGD-CBD	4.94	119.87	111.23
23	C	515	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
23	C	505	CLA	C3D-C2D-C1D	-4.94	99.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	CHD-C4C-C3C	-4.93	117.58	124.77
23	B	607	CLA	C4A-NA-C1A	-4.93	104.43	106.68
23	C	504	CLA	O2D-CGD-CBD	4.93	119.84	111.23
23	c	511	CLA	CHD-C4C-C3C	-4.93	117.59	124.77
23	C	513	CLA	C2C-C1C-NC	4.92	115.15	109.98
23	c	505	CLA	C4A-NA-C1A	-4.92	104.43	106.68
23	b	610	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
23	A	405	CLA	C2B-C1B-NB	4.92	115.42	110.33
23	c	504	CLA	C3D-C4D-ND	4.91	117.97	109.99
23	c	505	CLA	C2C-C1C-NC	4.91	115.14	109.98
23	B	608	CLA	C2C-C1C-NC	4.91	115.14	109.98
24	a	406	PHO	C4D-ND-C1D	-4.91	102.99	108.87
23	B	616	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
23	b	610	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	c	509	CLA	C2B-C1B-NB	4.90	115.41	110.33
23	c	505	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
26	L	102	SQD	O47-C7-C8	4.90	122.08	111.48
23	B	612	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
23	B	601	CLA	C2B-C1B-NB	4.89	115.40	110.33
23	b	604	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	a	405	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	C	508	CLA	O2D-CGD-CBD	4.88	119.75	111.23
23	b	608	CLA	C2D-C1D-ND	4.88	114.95	110.13
23	c	503	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	c	507	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
23	b	607	CLA	C2C-C1C-NC	4.87	115.09	109.98
25	b	617	BCR	C7-C8-C9	-4.87	119.03	126.23
24	A	415	PHO	C1-C2-C3	-4.87	118.22	126.20
23	C	514	CLA	C2B-C1B-NB	4.86	115.37	110.33
23	B	605	CLA	C3D-C4D-ND	4.86	117.88	109.99
23	d	402	CLA	CMD-C2D-C1D	4.85	133.28	124.73
23	b	612	CLA	C2B-C1B-NB	4.85	115.36	110.33
23	B	608	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
23	D	403	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
23	a	405	CLA	C3D-C4D-ND	4.84	117.85	109.99
23	A	407	CLA	CHD-C1D-ND	-4.84	117.99	124.80
23	c	513	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	C	512	CLA	C2C-C1C-NC	4.84	115.06	109.98
23	B	605	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
29	a	414[B]	PL9	C7-C3-C2	-4.83	117.70	123.39
23	c	507	CLA	C2B-C1B-NB	4.82	115.33	110.33
23	b	603	CLA	C3B-C2B-C1B	-4.82	101.48	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	C3D-C4D-ND	4.82	117.83	109.99
23	C	507	CLA	C2C-C1C-NC	4.82	115.05	109.98
23	c	511	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	c	510	CLA	C2B-C1B-NB	4.82	115.33	110.33
23	B	611	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	a	405	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	B	616	CLA	C2B-C1B-NB	4.82	115.32	110.33
32	D	411	HTG	C1'-S1-C1	4.81	110.85	100.45
23	c	514	CLA	C3B-C2B-C1B	-4.81	101.49	107.17
23	A	405	CLA	CHD-C1D-ND	-4.81	118.03	124.80
23	c	508	CLA	C2C-C1C-NC	4.80	115.03	109.98
23	C	509	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
23	b	608	CLA	C2B-C1B-NB	4.80	115.31	110.33
23	c	512	CLA	O2D-CGD-CBD	4.80	119.62	111.23
23	b	601	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
23	C	505	CLA	C2C-C1C-NC	4.79	115.02	109.98
29	a	414[A]	PL9	C37-C38-C39	-4.79	116.66	127.62
23	c	511	CLA	C2B-C1B-NB	4.79	115.29	110.33
23	C	514	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	B	608	CLA	O2D-CGD-CBD	4.79	119.60	111.23
23	A	407	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	c	515	CLA	CHD-C1D-ND	-4.79	118.06	124.80
23	C	506	CLA	O2D-CGD-CBD	4.78	119.59	111.23
23	C	506	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
23	B	602	CLA	C3D-C4D-ND	4.77	117.75	109.99
23	a	404	CLA	O2D-CGD-CBD	4.77	119.57	111.23
23	b	603	CLA	C4A-NA-C1A	-4.77	104.50	106.68
23	a	404	CLA	CMB-C2B-C1B	4.77	132.68	125.42
23	C	509	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	D	403	CLA	C1-C2-C3	-4.76	118.40	126.20
23	B	610	CLA	C2B-C1B-NB	4.76	115.26	110.33
23	C	506	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	a	407	CLA	C4A-NA-C1A	-4.76	104.51	106.68
23	C	504	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
23	B	602	CLA	O2D-CGD-CBD	4.75	119.53	111.23
23	c	506	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	C	510	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	C	515	CLA	O2D-CGD-CBD	4.75	119.53	111.23
23	B	607	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	b	608	CLA	O2D-CGD-CBD	4.74	119.52	111.23
23	B	603	CLA	C2C-C1C-NC	4.74	114.96	109.98
26	D	413	SQD	O47-C7-C8	4.74	121.73	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	B	612	CLA	O2D-CGD-O1D	-4.73	114.65	123.85
23	b	609	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	B	607	CLA	O2D-CGD-CBD	4.73	119.49	111.23
23	B	603	CLA	C4A-NA-C1A	-4.72	104.53	106.68
23	C	508	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	A	403	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	C	507	CLA	CMB-C2B-C1B	4.71	132.59	125.42
23	C	515	CLA	C4A-NA-C1A	-4.71	104.53	106.68
23	B	615	CLA	CMB-C2B-C1B	4.70	132.58	125.42
23	b	602	CLA	C3D-C4D-ND	4.70	117.63	109.99
23	b	610	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	508	CLA	C2B-C1B-NB	4.70	115.20	110.33
23	B	612	CLA	CMD-C2D-C1D	4.69	133.00	124.73
23	c	503	CLA	O2D-CGD-CBD	4.69	119.44	111.23
23	B	601	CLA	C3D-C4D-ND	4.69	117.62	109.99
23	B	610	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	b	611	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	B	605	CLA	C2B-C1B-NB	4.69	115.19	110.33
32	h	101	HTG	C1'-S1-C1	4.68	110.57	100.45
23	C	510	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	A	403	CLA	C3D-C4D-ND	4.68	117.60	109.99
23	B	610	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	B	611	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
23	b	606	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
23	B	611	CLA	C1-C2-C3	-4.67	118.55	126.20
23	B	608	CLA	C2B-C1B-NB	4.67	115.16	110.33
23	D	404	CLA	C3D-C4D-ND	4.66	117.57	109.99
23	B	609	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	b	615	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	b	613	CLA	C3B-C2B-C1B	-4.65	101.68	107.17
23	B	609	CLA	C2C-C1C-NC	4.65	114.87	109.98
23	C	515	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	C	512	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	c	509	CLA	CHD-C1D-ND	-4.65	118.26	124.80
23	B	609	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	C	508	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
23	C	508	CLA	C3D-C4D-ND	4.64	117.54	109.99
23	b	608	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
23	D	404	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	a	403	CLA	C1D-CHD-C4C	-4.64	116.16	126.02
23	c	511	CLA	C1-C2-C3	-4.64	118.59	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	B	616	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	C	512	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	c	504	CLA	O2D-CGD-CBD	4.63	119.33	111.23
23	c	508	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	b	601	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
23	B	613	CLA	C3B-C4B-NB	4.63	114.66	110.53
38	e	102	HEM	CHC-C4B-NB	4.62	129.40	124.42
23	B	610	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	B	601	CLA	C4A-NA-C1A	-4.62	104.57	106.68
23	b	602	CLA	C2C-C1C-NC	4.62	114.83	109.98
23	B	605	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
29	a	414[A]	PL9	C7-C3-C2	-4.61	117.95	123.39
23	b	614	CLA	C4A-NA-C1A	-4.61	104.58	106.68
23	b	613	CLA	C3B-C4B-NB	4.61	114.65	110.53
23	A	407	CLA	C2C-C1C-NC	4.61	114.82	109.98
25	b	619	BCR	C38-C26-C25	-4.61	119.46	124.48
23	c	515	CLA	C3D-C4D-ND	4.60	117.47	109.99
23	C	503	CLA	C3D-C4D-ND	4.60	117.47	109.99
23	c	515	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	B	603	CLA	C3C-C4C-NC	4.60	116.32	110.43
23	b	601	CLA	C3D-C4D-ND	4.59	117.45	109.99
23	C	513	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	d	402	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
23	B	601	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	d	402	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	D	403	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	C	503	CLA	C2B-C1B-NB	4.58	115.08	110.33
23	d	403	CLA	CHD-C1D-ND	-4.58	118.35	124.80
23	b	614	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	D	403	CLA	CHD-C1D-ND	-4.58	118.36	124.80
23	C	515	CLA	C2B-C1B-NB	4.58	115.08	110.33
23	C	504	CLA	C4A-NA-C1A	-4.58	104.59	106.68
23	A	407	CLA	C3D-C4D-ND	4.58	117.43	109.99
23	b	616	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
23	D	403	CLA	C1C-C2C-C3C	-4.57	102.17	106.98
23	b	609	CLA	C2B-C1B-NB	4.57	115.07	110.33
23	C	508	CLA	CHD-C1D-ND	-4.57	118.37	124.80
23	C	514	CLA	C2C-C1C-NC	4.57	114.78	109.98
23	b	606	CLA	CHD-C1D-ND	-4.56	118.38	124.80
29	a	414[A]	PL9	C15-C14-C16	4.56	123.14	115.23
23	b	616	CLA	C1D-CHD-C4C	-4.56	116.33	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	403	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	B	610	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	b	606	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	c	507	CLA	C2C-C1C-NC	4.55	114.76	109.98
23	a	404	CLA	C1C-C2C-C3C	-4.55	102.19	106.98
23	a	407	CLA	C2C-C1C-NC	4.55	114.76	109.98
23	C	511	CLA	C2B-C1B-NB	4.54	115.03	110.33
23	b	615	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	B	604	CLA	C1D-CHD-C4C	-4.54	116.38	126.02
23	b	603	CLA	C1D-CHD-C4C	-4.54	116.38	126.02
23	C	510	CLA	C3C-C4C-NC	4.54	116.24	110.43
23	c	503	CLA	C4A-NA-C1A	-4.54	104.61	106.68
26	B	620	SQD	O6-C1-C2	4.53	115.16	108.27
23	C	503	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	A	404	CLA	CHD-C1D-ND	-4.53	118.42	124.80
23	c	508	CLA	O2D-CGD-CBD	4.53	119.15	111.23
23	c	513	CLA	C2C-C1C-NC	4.52	114.73	109.98
23	c	512	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	b	605	CLA	C4-C3-C5	4.52	123.08	115.23
23	b	608	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	c	513	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
23	B	609	CLA	CHD-C1D-ND	-4.51	118.45	124.80
23	a	403	CLA	C1C-C2C-C3C	-4.51	102.23	106.98
23	b	605	CLA	C2B-C1B-NB	4.51	115.00	110.33
23	C	513	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
26	a	409	SQD	O47-C7-C8	4.51	121.24	111.48
23	C	515	CLA	C3D-C4D-ND	4.51	117.32	109.99
23	B	612	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
23	B	606	CLA	C2C-C1C-NC	4.51	114.72	109.98
23	b	615	CLA	C2B-C1B-NB	4.51	115.00	110.33
23	b	605	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
23	B	608	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
26	D	413	SQD	C44-O6-C1	-4.50	104.14	113.80
25	c	517	BCR	C7-C8-C9	-4.50	119.58	126.23
23	b	605	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	b	609	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
23	A	405	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
23	A	405	CLA	C2C-C1C-NC	4.49	114.70	109.98
23	B	615	CLA	C3C-C4C-NC	4.49	116.19	110.43
23	b	603	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	A	404	CLA	C3B-C2B-C1B	-4.49	101.87	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
23	C	507	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	b	609	CLA	O2D-CGD-CBD	4.49	119.08	111.23
23	C	505	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	B	614	CLA	C2B-C1B-NB	4.49	114.98	110.33
23	c	506	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	b	608	CLA	CHD-C1D-ND	-4.49	118.49	124.80
25	B	618	BCR	C15-C14-C13	-4.48	121.00	127.28
23	C	513	CLA	O2D-CGD-CBD	4.48	119.06	111.23
23	c	510	CLA	C1-C2-C3	-4.47	118.87	126.20
23	b	605	CLA	CHD-C1D-ND	-4.47	118.51	124.80
23	b	611	CLA	C2B-C1B-NB	4.47	114.96	110.33
23	c	515	CLA	C2C-C1C-NC	4.47	114.67	109.98
32	c	523	HTG	C1'-S1-C1	4.46	110.09	100.45
23	B	602	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
23	c	508	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	A	404	CLA	C3D-C4D-ND	4.46	117.23	109.99
23	B	609	CLA	C2B-C1B-NB	4.46	114.95	110.33
25	d	404	BCR	C7-C8-C9	-4.45	119.65	126.23
23	c	509	CLA	CMC-C2C-C1C	4.45	131.99	125.03
23	c	503	CLA	C3B-C2B-C1B	-4.45	101.93	107.17
23	c	511	CLA	CAC-C3C-C4C	4.45	130.58	124.79
23	C	512	CLA	C1-C2-C3	-4.44	118.92	126.20
23	B	601	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	a	404	CLA	C4A-NA-C1A	-4.44	104.65	106.68
23	c	508	CLA	C3B-C2B-C1B	-4.43	101.94	107.17
23	C	503	CLA	C1D-CHD-C4C	-4.43	116.60	126.02
23	B	614	CLA	CHD-C1D-ND	-4.43	118.57	124.80
23	C	506	CLA	C1C-C2C-C3C	-4.43	102.33	106.98
23	C	506	CLA	C4A-NA-C1A	-4.43	104.66	106.68
23	c	508	CLA	C3D-C4D-ND	4.42	117.18	109.99
23	C	513	CLA	C3D-C4D-ND	4.42	117.17	109.99
34	C	522	LMG	O6-C5-C4	4.42	117.67	109.70
23	b	613	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
23	C	503	CLA	C2C-C1C-NC	4.42	114.62	109.98
23	c	514	CLA	C3D-C4D-ND	4.41	117.16	109.99
23	c	505	CLA	C1D-CHD-C4C	-4.41	116.64	126.02
23	A	403	CLA	CHD-C1D-ND	-4.41	118.60	124.80
23	C	511	CLA	C4A-NA-C1A	-4.41	104.67	106.68
23	C	515	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	C	511	CLA	C3D-C4D-ND	4.40	117.14	109.99
23	a	403	CLA	C3D-C4D-ND	4.40	117.14	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	c	504	CLA	CHD-C1D-ND	-4.40	118.61	124.80
23	b	609	CLA	C3D-C4D-ND	4.39	117.13	109.99
23	b	604	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
23	C	511	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
29	a	414[B]	PL9	C37-C38-C39	-4.39	117.58	127.62
23	B	603	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	b	615	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	c	505	CLA	CMB-C2B-C1B	4.39	132.10	125.42
23	b	612	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	b	611	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	B	604	CLA	C3C-C4C-NC	4.39	116.05	110.43
23	c	507	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	b	610	CLA	C1-C2-C3	-4.38	119.01	126.20
23	B	608	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	B	613	CLA	C3C-C4C-NC	4.38	116.04	110.43
23	A	404	CLA	C2B-C1B-NB	4.38	114.87	110.33
23	c	505	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
23	B	612	CLA	CMC-C2C-C1C	4.37	131.86	125.03
23	B	612	CLA	C3D-C4D-ND	4.37	117.08	109.99
23	C	506	CLA	C2B-C1B-NB	4.37	114.85	110.33
23	c	503	CLA	C3D-C4D-ND	4.37	117.08	109.99
23	C	507	CLA	C3D-C4D-ND	4.36	117.08	109.99
25	d	404	BCR	C15-C14-C13	-4.36	121.16	127.28
23	C	504	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	d	403	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	C	512	CLA	C2B-C1B-NB	4.36	114.85	110.33
23	c	504	CLA	C1C-C2C-C3C	-4.36	102.40	106.98
23	B	607	CLA	C3D-C4D-ND	4.36	117.07	109.99
29	D	406	PL9	C42-C43-C44	-4.35	117.67	127.62
23	B	615	CLA	C2C-C1C-NC	4.35	114.55	109.98
23	B	602	CLA	CMC-C2C-C1C	4.35	131.83	125.03
23	C	510	CLA	O2D-CGD-O1D	-4.35	115.39	123.85
23	b	610	CLA	C3C-C4C-NC	4.34	116.00	110.43
23	b	613	CLA	C3C-C4C-NC	4.34	115.99	110.43
23	C	513	CLA	C3B-C4B-NB	4.34	114.40	110.53
23	b	603	CLA	C2B-C1B-NB	4.34	114.82	110.33
23	C	506	CLA	C3C-C4C-NC	4.33	115.98	110.43
23	b	606	CLA	O2D-CGD-O1D	-4.33	115.41	123.85
23	b	609	CLA	CHD-C1D-ND	-4.33	118.70	124.80
29	A	413[B]	PL9	C37-C38-C39	-4.33	117.71	127.62
23	c	513	CLA	C1-C2-C3	-4.33	119.10	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	a	405	CLA	C2B-C1B-NB	4.33	114.81	110.33
23	c	504	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
23	a	407	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
23	b	606	CLA	C3D-C4D-ND	4.32	117.01	109.99
23	B	613	CLA	C3D-C4D-ND	4.32	117.00	109.99
23	A	407	CLA	C1-C2-C3	-4.32	119.13	126.20
23	C	513	CLA	C2B-C1B-NB	4.31	114.79	110.33
23	b	604	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	B	606	CLA	C3B-C2B-C1B	-4.30	102.11	107.17
23	b	615	CLA	CHD-C1D-ND	-4.29	118.76	124.80
23	B	602	CLA	C2B-C1B-NB	4.29	114.78	110.33
23	A	404	CLA	CMB-C2B-C1B	4.29	131.96	125.42
23	C	504	CLA	C3C-C4C-NC	4.29	115.93	110.43
23	B	601	CLA	CHD-C1D-ND	-4.29	118.76	124.80
23	B	603	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	b	612	CLA	C1-C2-C3	-4.29	119.17	126.20
23	b	605	CLA	C2C-C1C-NC	4.29	114.48	109.98
23	A	404	CLA	CBC-CAC-C3C	-4.29	100.80	112.42
23	A	405	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
23	a	404	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
23	b	603	CLA	C3B-C4B-NB	4.28	114.35	110.53
23	C	514	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
29	A	413[A]	PL9	C15-C14-C16	4.28	122.66	115.23
23	C	503	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
23	c	505	CLA	C2B-C1B-NB	4.28	114.76	110.33
23	B	615	CLA	C3D-C4D-ND	4.28	116.94	109.99
25	T	101	BCR	C15-C16-C17	-4.28	114.77	123.52
34	M	101	LMG	O7-C10-C11	4.27	120.73	111.48
23	a	405	CLA	CHD-C1D-ND	-4.27	118.79	124.80
32	B	621	HTG	O5-C1-C2	4.27	116.20	110.32
23	c	514	CLA	C2C-C1C-NC	4.27	114.46	109.98
23	b	610	CLA	C4A-NA-C1A	-4.27	104.73	106.68
33	C	526	LMT	C1'-O5'-C5'	4.26	122.05	113.72
23	d	402	CLA	C3D-C4D-ND	4.26	116.92	109.99
23	C	508	CLA	CAC-C3C-C4C	4.26	130.33	124.79
34	Z	101	LMG	O7-C10-C11	4.26	120.69	111.48
23	b	603	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	c	506	CLA	C2B-C1B-NB	4.25	114.74	110.33
23	B	616	CLA	C3C-C4C-NC	4.25	115.88	110.43
23	B	604	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	c	505	CLA	C3C-C4C-NC	4.25	115.87	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	CMB-C2B-C1B	4.25	131.89	125.42
23	B	609	CLA	O2D-CGD-CBD	4.25	118.66	111.23
23	a	404	CLA	C3D-C4D-ND	4.25	116.89	109.99
23	b	610	CLA	C3D-C4D-ND	4.25	116.89	109.99
32	B	622	HTG	C1'-S1-C1	4.24	109.61	100.45
23	B	614	CLA	O2D-CGD-O1D	-4.24	115.59	123.85
23	c	509	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	c	506	CLA	CHD-C1D-ND	-4.24	118.84	124.80
23	C	509	CLA	C3C-C4C-NC	4.23	115.85	110.43
23	C	505	CLA	C1D-CHD-C4C	-4.23	117.03	126.02
23	c	505	CLA	C3D-C4D-ND	4.23	116.86	109.99
23	c	511	CLA	C3D-C4D-ND	4.23	116.86	109.99
23	b	601	CLA	C2C-C1C-NC	4.22	114.42	109.98
23	b	614	CLA	C3D-C4D-ND	4.22	116.85	109.99
34	C	522	LMG	O7-C10-C11	4.22	120.62	111.48
23	b	606	CLA	C1D-CHD-C4C	-4.22	117.04	126.02
23	c	506	CLA	C3B-C4B-NB	4.22	114.30	110.53
23	C	510	CLA	C1D-CHD-C4C	-4.22	117.04	126.02
23	B	610	CLA	CAC-C3C-C4C	4.22	130.28	124.79
23	C	505	CLA	C3D-C4D-ND	4.22	116.85	109.99
23	B	615	CLA	C1D-CHD-C4C	-4.22	117.05	126.02
31	A	416	LHG	O7-C7-C8	4.22	120.61	111.48
23	C	510	CLA	C3D-C4D-ND	4.22	116.84	109.99
23	b	610	CLA	C1D-CHD-C4C	-4.22	117.06	126.02
23	A	403	CLA	O2A-CGA-CBA	4.21	124.69	111.83
23	C	514	CLA	C3D-C4D-ND	4.21	116.83	109.99
23	C	508	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	c	510	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
23	B	614	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
25	b	617	BCR	C33-C5-C6	-4.21	119.89	124.48
23	B	611	CLA	C4A-NA-C1A	-4.21	104.76	106.68
33	F	101	LMT	C1B-O5B-C5B	4.20	121.93	113.72
23	c	513	CLA	C3D-C4D-ND	4.20	116.82	109.99
23	d	402	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	b	611	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	C	510	CLA	C3B-C4B-NB	4.20	114.28	110.53
23	c	514	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	A	403	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
23	c	510	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
23	b	612	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	C	515	CLA	C1-C2-C3	-4.19	119.34	126.20
23	B	611	CLA	C3B-C2B-C1B	-4.19	102.23	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	C3C-C4C-NC	4.18	115.79	110.43
23	B	616	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	a	403	CLA	CAA-C2A-C3A	-4.18	101.71	113.00
23	a	407	CLA	C3C-C4C-NC	4.17	115.78	110.43
23	b	612	CLA	C3B-C4B-NB	4.17	114.25	110.53
23	B	605	CLA	CHD-C1D-ND	-4.17	118.94	124.80
23	c	507	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	B	603	CLA	CHD-C1D-ND	-4.16	118.94	124.80
23	A	407	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
23	b	607	CLA	C3D-C4D-ND	4.16	116.74	109.99
33	a	412	LMT	C1B-O5B-C5B	4.16	121.83	113.72
23	b	604	CLA	C3D-C4D-ND	4.15	116.74	109.99
23	b	601	CLA	C1D-CHD-C4C	-4.15	117.19	126.02
23	d	402	CLA	O2D-CGD-CBD	4.15	118.49	111.23
23	b	602	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
29	A	413[A]	PL9	C37-C38-C39	-4.15	118.13	127.62
23	d	402	CLA	C2B-C1B-NB	4.15	114.63	110.33
34	a	417	LMG	O7-C10-C11	4.15	120.45	111.48
23	a	405	CLA	C2C-C1C-NC	4.14	114.33	109.98
23	A	404	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
29	A	413[B]	PL9	C15-C14-C16	4.14	122.42	115.23
23	B	607	CLA	C3C-C4C-NC	4.14	115.73	110.43
25	B	631	BCR	C33-C5-C6	-4.14	119.97	124.48
23	C	512	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
23	b	602	CLA	CHD-C1D-ND	-4.14	118.98	124.80
25	K	101	BCR	C7-C8-C9	-4.13	120.12	126.23
23	c	505	CLA	CAC-C3C-C4C	4.13	130.16	124.79
23	C	512	CLA	C3D-C4D-ND	4.13	116.70	109.99
23	b	608	CLA	C1-C2-C3	-4.13	119.43	126.20
25	d	404	BCR	C38-C26-C25	-4.13	119.98	124.48
29	A	413[A]	PL9	C27-C28-C29	-4.12	118.18	127.62
31	D	408	LHG	O7-C7-C8	4.12	120.40	111.48
23	B	615	CLA	CHD-C1D-ND	-4.12	119.00	124.80
23	C	515	CLA	C3C-C4C-NC	4.12	115.71	110.43
23	D	404	CLA	C3C-C4C-NC	4.12	115.71	110.43
23	D	404	CLA	C2B-C1B-NB	4.12	114.60	110.33
23	b	616	CLA	C3C-C4C-NC	4.12	115.70	110.43
23	c	512	CLA	C3B-C4B-NB	4.11	114.20	110.53
23	b	609	CLA	C3C-C4C-NC	4.11	115.69	110.43
23	C	505	CLA	O2D-CGD-CBD	4.11	118.41	111.23
23	B	602	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
40	V	201	HEC	CBC-CAC-C3C	-4.10	119.23	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C3C-C4C-NC	4.10	115.68	110.43
23	b	608	CLA	C2C-C1C-NC	4.10	114.29	109.98
23	C	507	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
23	C	504	CLA	C1-C2-C3	-4.10	119.48	126.20
23	C	511	CLA	C3B-C4B-NB	4.10	114.19	110.53
23	c	511	CLA	C3B-C4B-NB	4.09	114.19	110.53
23	a	407	CLA	C3D-C4D-ND	4.09	116.64	109.99
23	B	614	CLA	C2C-C1C-NC	4.09	114.28	109.98
23	b	610	CLA	CMB-C2B-C1B	4.08	131.64	125.42
23	B	606	CLA	C2B-C1B-NB	4.08	114.56	110.33
23	C	511	CLA	C1-C2-C3	-4.08	119.50	126.20
23	b	610	CLA	O2A-CGA-CBA	4.08	124.28	111.83
23	B	612	CLA	C2C-C1C-NC	4.08	114.27	109.98
23	b	606	CLA	C2C-C1C-NC	4.08	114.26	109.98
23	B	609	CLA	C3C-C4C-NC	4.07	115.65	110.43
23	b	613	CLA	C3D-C4D-ND	4.07	116.61	109.99
23	D	404	CLA	CMB-C2B-C1B	4.07	131.62	125.42
23	B	613	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
23	B	611	CLA	CHD-C1D-ND	-4.07	119.07	124.80
23	C	504	CLA	CMB-C2B-C1B	4.07	131.62	125.42
23	B	612	CLA	C4A-NA-C1A	-4.07	104.82	106.68
23	c	512	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
23	b	614	CLA	O2D-CGD-O1D	-4.07	115.93	123.85
23	B	607	CLA	CHD-C1D-ND	-4.07	119.08	124.80
23	B	604	CLA	C3D-C4D-ND	4.07	116.60	109.99
23	D	404	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
23	B	614	CLA	C3D-C4D-ND	4.06	116.59	109.99
23	c	503	CLA	CHD-C1D-ND	-4.06	119.09	124.80
23	a	404	CLA	C1D-CHD-C4C	-4.06	117.40	126.02
23	c	515	CLA	O2D-CGD-CBD	4.06	118.32	111.23
23	B	616	CLA	CHD-C1D-ND	-4.06	119.09	124.80
25	Y	101	BCR	C37-C22-C23	4.05	124.28	118.09
23	C	509	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	b	602	CLA	C1-C2-C3	-4.05	119.56	126.20
23	b	607	CLA	C3B-C2B-C1B	-4.05	102.40	107.17
23	b	614	CLA	C3C-C4C-NC	4.05	115.61	110.43
32	h	101	HTG	O5-C5-C4	4.05	116.99	109.70
23	c	512	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
23	c	513	CLA	O2D-CGD-O1D	-4.04	115.99	123.85
23	B	605	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	B	613	CLA	CHD-C1D-ND	-4.03	119.14	124.80
23	b	613	CLA	C2B-C1B-NB	4.03	114.50	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	O2A-CGA-CBA	4.02	124.11	111.83
23	d	402	CLA	C3B-C4B-NB	4.02	114.12	110.53
29	A	413[B]	PL9	C7-C3-C4	4.02	120.22	116.91
23	C	506	CLA	C3D-C4D-ND	4.02	116.52	109.99
23	c	503	CLA	C1C-C2C-C3C	-4.02	102.76	106.98
23	B	609	CLA	C3B-C2B-C1B	-4.02	102.44	107.17
23	B	614	CLA	C3C-C4C-NC	4.01	115.57	110.43
31	E	101	LHG	O7-C7-C8	4.01	120.16	111.48
23	b	601	CLA	CHD-C1D-ND	-4.01	119.16	124.80
25	C	517	BCR	C7-C8-C9	-4.01	120.30	126.23
23	c	508	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
23	B	612	CLA	C1-C2-C3	-4.01	119.62	126.20
23	C	504	CLA	CHD-C1D-ND	-4.01	119.16	124.80
23	a	405	CLA	C3C-C4C-NC	4.01	115.56	110.43
23	b	612	CLA	C3C-C4C-NC	4.01	115.56	110.43
23	D	404	CLA	CHD-C1D-ND	-4.00	119.17	124.80
23	c	506	CLA	C4A-NA-C1A	-4.00	104.85	106.68
38	E	102	HEM	CHC-C4B-NB	4.00	128.73	124.42
23	c	507	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
23	c	512	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
23	A	405	CLA	CMB-C2B-C1B	4.00	131.51	125.42
23	C	507	CLA	C2B-C1B-NB	4.00	114.47	110.33
23	B	606	CLA	O2D-CGD-O1D	-4.00	116.07	123.85
23	B	611	CLA	C3C-C4C-NC	4.00	115.55	110.43
34	C	502	LMG	O7-C10-C11	3.99	120.12	111.48
23	b	603	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	b	614	CLA	C2B-C1B-NB	3.99	114.47	110.33
23	C	510	CLA	C2B-C1B-NB	3.99	114.46	110.33
23	b	614	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
23	B	608	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	b	607	CLA	CHD-C1D-ND	-3.98	119.19	124.80
23	B	602	CLA	CAA-C2A-C3A	-3.98	102.24	113.00
23	B	607	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
23	c	511	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	B	602	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
23	B	602	CLA	C3C-C4C-NC	3.98	115.53	110.43
23	B	603	CLA	C2B-C1B-NB	3.98	114.45	110.33
23	B	611	CLA	C2B-C1B-NB	3.98	114.45	110.33
23	b	611	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
23	c	512	CLA	C4A-NA-C1A	-3.97	104.87	106.68
23	C	504	CLA	C2B-C1B-NB	3.97	114.44	110.33
23	B	611	CLA	C3D-C4D-ND	3.97	116.44	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	514	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
23	B	615	CLA	C3B-C2B-C1B	-3.97	102.49	107.17
23	b	613	CLA	O2A-CGA-O1A	-3.96	113.71	123.63
23	c	503	CLA	C2B-C1B-NB	3.96	114.44	110.33
23	C	513	CLA	C4A-NA-C1A	-3.96	104.87	106.68
23	c	508	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
23	c	509	CLA	C2C-C1C-NC	3.96	114.14	109.98
23	c	513	CLA	CHD-C1D-ND	-3.96	119.23	124.80
23	B	608	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
25	k	102	BCR	C15-C14-C13	-3.96	121.73	127.28
23	c	508	CLA	CHD-C1D-ND	-3.96	119.23	124.80
23	B	615	CLA	O2D-CGD-CBD	3.96	118.15	111.23
23	B	610	CLA	CHD-C1D-ND	-3.96	119.24	124.80
34	c	522	LMG	O7-C10-C11	3.96	120.04	111.48
23	b	614	CLA	C3B-C4B-NB	3.95	114.06	110.53
23	C	515	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
23	C	506	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
23	A	407	CLA	O2D-CGD-CBD	3.95	118.13	111.23
23	C	507	CLA	C3C-C4C-NC	3.94	115.48	110.43
23	c	512	CLA	C3D-C2D-C1D	-3.94	100.45	105.83
23	C	515	CLA	CHD-C1D-ND	-3.94	119.25	124.80
23	B	602	CLA	CHD-C1D-ND	-3.94	119.25	124.80
23	b	614	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
29	A	413[B]	PL9	C32-C33-C34	-3.94	118.61	127.62
23	b	606	CLA	C1-C2-C3	-3.94	119.75	126.20
23	d	402	CLA	C3C-C4C-NC	3.94	115.47	110.43
23	c	504	CLA	C4A-NA-C1A	-3.93	104.88	106.68
23	a	404	CLA	C2B-C1B-NB	3.93	114.41	110.33
23	a	407	CLA	C2B-C1B-NB	3.93	114.41	110.33
23	C	513	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	a	405	CLA	O2D-CGD-CBD	3.93	118.10	111.23
23	C	512	CLA	CHD-C1D-ND	-3.93	119.27	124.80
25	K	101	BCR	C24-C23-C22	-3.93	120.42	126.23
25	T	101	BCR	C11-C10-C9	-3.93	121.77	127.28
23	C	505	CLA	CHD-C1D-ND	-3.92	119.28	124.80
23	B	606	CLA	C3D-C4D-ND	3.92	116.36	109.99
23	B	604	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
23	A	403	CLA	C2B-C1B-NB	3.92	114.39	110.33
23	b	607	CLA	C3C-C4C-NC	3.91	115.44	110.43
23	c	514	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
23	C	513	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
23	b	610	CLA	C2B-C1B-NB	3.90	114.38	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	403	CLA	C3D-C2D-C1D	-3.90	100.50	105.83
23	D	403	CLA	C2B-C1B-NB	3.90	114.37	110.33
23	C	504	CLA	C2C-C1C-NC	3.90	114.08	109.98
25	D	405	BCR	C38-C26-C25	-3.90	120.23	124.48
23	b	604	CLA	C2B-C1B-NB	3.90	114.37	110.33
31	d	406	LHG	O7-C7-C8	3.90	119.91	111.48
23	b	604	CLA	C3C-C4C-NC	3.90	115.42	110.43
25	h	102	BCR	C7-C8-C9	-3.89	120.47	126.23
23	b	616	CLA	CHD-C4C-NC	3.89	130.27	124.23
23	C	505	CLA	C1-C2-C3	-3.89	119.82	126.20
23	B	607	CLA	C3B-C2B-C1B	-3.89	102.58	107.17
23	B	612	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
23	C	507	CLA	CHD-C1D-ND	-3.89	119.33	124.80
23	B	612	CLA	CAC-C3C-C4C	3.89	129.85	124.79
23	D	404	CLA	C2C-C1C-NC	3.89	114.06	109.98
35	C	518	DGD	O1G-C1A-C2A	3.89	123.68	111.83
23	b	612	CLA	C1D-CHD-C4C	-3.88	117.76	126.02
23	c	509	CLA	CMB-C2B-C1B	3.88	131.33	125.42
25	A	408	BCR	C24-C23-C22	-3.88	120.49	126.23
29	A	413[B]	PL9	C10-C9-C11	3.88	121.96	115.23
24	A	406	PHO	C1A-C2A-C3A	-3.88	99.15	102.84
34	Z	101	LMG	C1-C2-C3	3.88	118.16	110.01
23	a	403	CLA	CHD-C1D-ND	-3.87	119.35	124.80
23	a	403	CLA	O2D-CGD-CBD	3.87	118.00	111.23
29	a	414[A]	PL9	C27-C28-C29	-3.87	118.76	127.62
23	C	511	CLA	CHD-C1D-ND	-3.87	119.36	124.80
23	B	605	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
23	B	611	CLA	C3B-C4B-NB	3.87	113.98	110.53
23	c	512	CLA	C2B-C1B-NB	3.87	114.34	110.33
23	B	606	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
23	b	612	CLA	CHD-C1D-ND	-3.87	119.36	124.80
38	e	102	HEM	CHD-C4C-NC	3.86	128.66	124.45
23	a	403	CLA	C3B-C4B-NB	3.86	113.98	110.53
23	C	503	CLA	CHD-C1D-ND	-3.86	119.37	124.80
23	b	602	CLA	CAC-C3C-C4C	3.86	129.81	124.79
31	d	408	LHG	O7-C7-C8	3.86	119.82	111.48
23	C	511	CLA	C1D-CHD-C4C	-3.86	117.83	126.02
23	c	515	CLA	C1D-CHD-C4C	-3.86	117.83	126.02
23	b	612	CLA	O2D-CGD-O1D	-3.85	116.34	123.85
23	b	611	CLA	C3C-C4C-NC	3.85	115.37	110.43
23	B	606	CLA	C3C-C4C-NC	3.85	115.37	110.43
23	c	508	CLA	C1-C2-C3	-3.85	119.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
23	b	605	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
23	b	613	CLA	O2A-CGA-CBA	3.85	123.56	111.83
23	c	513	CLA	C1D-CHD-C4C	-3.85	117.85	126.02
23	B	610	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
23	c	503	CLA	C3C-C4C-NC	3.84	115.35	110.43
23	c	506	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	c	503	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
23	B	613	CLA	C2B-C1B-NB	3.84	114.31	110.33
23	D	403	CLA	O2D-CGD-CBD	3.84	117.94	111.23
23	c	510	CLA	C3B-C4B-NB	3.84	113.95	110.53
24	a	416	PHO	C4-C3-C5	3.83	121.88	115.23
23	b	616	CLA	C3D-C4D-ND	3.83	116.22	109.99
25	a	408	BCR	C24-C23-C22	-3.83	120.56	126.23
29	A	413[A]	PL9	C7-C3-C2	-3.83	118.87	123.39
23	C	509	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
23	b	609	CLA	C2C-C1C-NC	3.83	114.00	109.98
35	C	519	DGD	O2G-C1B-C2B	3.83	119.77	111.48
23	b	616	CLA	O2D-CGD-O1D	-3.82	116.40	123.85
23	c	511	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
23	b	604	CLA	C3B-C4B-NB	3.82	113.94	110.53
23	B	605	CLA	C2C-C1C-NC	3.82	113.99	109.98
23	C	512	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	B	608	CLA	CHD-C1D-ND	-3.81	119.44	124.80
23	b	614	CLA	C1-C2-C3	-3.81	119.95	126.20
23	B	604	CLA	C1-C2-C3	-3.81	119.95	126.20
25	H	101	BCR	C38-C26-C25	-3.81	120.33	124.48
23	B	606	CLA	C3B-C4B-NB	3.81	113.93	110.53
23	b	603	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
25	d	404	BCR	C28-C27-C26	-3.81	107.27	114.06
23	B	614	CLA	CHD-C4C-NC	3.80	130.13	124.23
23	c	507	CLA	CHD-C1D-ND	-3.80	119.46	124.80
24	A	406	PHO	CMA-C3A-C4A	-3.80	106.43	114.61
23	B	610	CLA	CAA-C2A-C3A	-3.79	102.75	113.00
25	C	516	BCR	C7-C8-C9	-3.79	120.63	126.23
38	E	102	HEM	CHD-C4C-NC	3.79	128.58	124.45
23	b	615	CLA	O2D-CGD-CBD	3.79	117.85	111.23
23	b	608	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
23	c	513	CLA	C4A-NA-C1A	-3.78	104.95	106.68
23	C	514	CLA	C3C-C4C-NC	3.78	115.27	110.43
23	b	615	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
23	B	607	CLA	CMB-C2B-C1B	3.78	131.17	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	404	CLA	C1D-CHD-C4C	-3.78	118.00	126.02
23	b	610	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
23	b	603	CLA	CHD-C1D-ND	-3.77	119.49	124.80
23	B	604	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
23	B	616	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
23	b	608	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
29	d	405	PL9	C42-C43-C44	-3.77	119.00	127.62
23	A	403	CLA	O2A-CGA-O1A	-3.77	114.20	123.63
23	b	605	CLA	C3C-C4C-NC	3.77	115.25	110.43
23	C	508	CLA	C1-C2-C3	-3.76	120.03	126.20
23	c	506	CLA	CAC-C3C-C4C	3.76	129.69	124.79
26	A	411	SQD	C3-C4-C5	3.76	117.05	110.23
23	b	605	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
23	A	404	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
23	a	407	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
23	B	608	CLA	C3B-C4B-NB	3.75	113.88	110.53
32	b	621	HTG	C1-O5-C5	3.75	119.29	112.56
35	c	519	DGD	O2G-C1B-C2B	3.75	119.59	111.48
23	B	613	CLA	C4A-NA-C1A	-3.75	104.97	106.68
23	b	607	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
23	c	510	CLA	C4A-NA-C1A	-3.75	104.97	106.68
23	b	607	CLA	C3B-C4B-NB	3.75	113.87	110.53
23	b	607	CLA	C1D-CHD-C4C	-3.74	118.06	126.02
23	c	504	CLA	C2B-C1B-NB	3.74	114.21	110.33
26	D	413	SQD	C1-O5-C5	-3.74	106.41	113.72
23	c	510	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
34	c	522	LMG	O6-C5-C4	3.73	116.43	109.70
23	b	612	CLA	CAC-C3C-C4C	3.73	129.65	124.79
23	b	606	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
23	a	404	CLA	CHD-C1D-ND	-3.73	119.56	124.80
26	a	411	SQD	O47-C7-C8	3.72	119.54	111.48
25	Y	101	BCR	C16-C17-C18	-3.72	122.06	127.28
25	C	516	BCR	C16-C17-C18	-3.72	122.06	127.28
23	c	513	CLA	C3B-C4B-NB	3.72	113.85	110.53
23	B	601	CLA	C2C-C1C-NC	3.72	113.89	109.98
33	M	103	LMT	C1'-O5'-C5'	3.72	120.98	113.72
23	b	615	CLA	C3B-C4B-NB	3.72	113.85	110.53
23	C	509	CLA	C3D-C4D-ND	3.72	116.03	109.99
23	c	514	CLA	C3C-C4C-NC	3.72	115.19	110.43
34	C	522	LMG	C3-C4-C5	3.72	116.97	110.23
23	c	512	CLA	CBC-CAC-C3C	-3.71	102.35	112.42
23	B	608	CLA	C3C-C4C-NC	3.71	115.19	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	603	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
23	B	601	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
23	a	407	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
23	b	615	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
23	B	612	CLA	C2B-C1B-NB	3.71	114.17	110.33
34	z	101	LMG	O7-C10-C11	3.71	119.50	111.48
23	b	613	CLA	O2D-CGD-CBD	3.71	117.71	111.23
23	c	509	CLA	C1C-C2C-C3C	-3.70	103.08	106.98
23	b	609	CLA	C1-C2-C3	-3.70	120.13	126.20
31	L	101	LHG	O7-C7-C8	3.70	119.48	111.48
23	d	402	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
23	C	510	CLA	C4C-C3C-C2C	-3.69	101.52	106.89
23	d	402	CLA	C1-C2-C3	-3.69	120.15	126.20
38	e	102	HEM	CAD-CBD-CGD	3.69	123.46	113.67
23	a	407	CLA	CHD-C1D-ND	-3.69	119.61	124.80
23	C	505	CLA	C3C-C4C-NC	3.69	115.16	110.43
23	c	510	CLA	C3D-C4D-ND	3.69	115.99	109.99
23	c	513	CLA	C3C-C4C-NC	3.69	115.16	110.43
23	b	612	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
23	B	605	CLA	C4-C3-C5	3.68	121.62	115.23
40	V	201	HEC	C4D-ND-C1D	3.68	111.82	105.82
23	A	404	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
23	B	613	CLA	C4B-C3B-C2B	-3.68	102.72	107.30
25	b	619	BCR	C11-C10-C9	-3.68	122.12	127.28
26	a	409	SQD	C1-C2-C3	-3.68	102.27	110.01
23	B	615	CLA	CHD-C4C-NC	3.68	129.93	124.23
23	a	405	CLA	C1D-CHD-C4C	-3.68	118.21	126.02
23	b	603	CLA	CAA-C2A-C3A	-3.68	103.06	113.00
23	C	504	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
40	v	202	HEC	C4D-ND-C1D	3.67	111.81	105.82
23	d	402	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
23	a	403	CLA	CAC-C3C-C4C	3.67	129.56	124.79
23	C	506	CLA	C3B-C4B-NB	3.67	113.81	110.53
23	B	615	CLA	CED-O2D-CGD	3.67	124.23	115.92
23	B	607	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
23	C	506	CLA	CHD-C1D-ND	-3.66	119.65	124.80
23	c	514	CLA	C1-C2-C3	-3.66	120.20	126.20
23	B	613	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	C	505	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	b	608	CLA	C3B-C4B-NB	3.65	113.79	110.53
23	C	509	CLA	C2B-C1B-NB	3.65	114.11	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
23	A	405	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	c	506	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	C	508	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
24	a	406	PHO	CMA-C3A-C4A	-3.65	106.75	114.61
34	c	521	LMG	O7-C10-C11	3.64	119.36	111.48
23	b	611	CLA	C3B-C4B-NB	3.64	113.78	110.53
26	a	409	SQD	C1-O5-C5	-3.64	106.61	113.72
29	A	413[B]	PL9	C27-C28-C29	-3.64	119.29	127.62
23	A	403	CLA	CAC-C3C-C4C	3.64	129.53	124.79
23	B	602	CLA	CMB-C2B-C1B	3.64	130.96	125.42
23	a	405	CLA	CMC-C2C-C1C	3.64	130.72	125.03
23	C	514	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
23	C	503	CLA	C3C-C4C-NC	3.63	115.09	110.43
25	C	516	BCR	C15-C14-C13	-3.63	122.18	127.28
25	d	404	BCR	C33-C5-C6	-3.63	120.52	124.48
34	m	101	LMG	O7-C10-C11	3.63	119.33	111.48
23	B	603	CLA	C3B-C4B-NB	3.63	113.77	110.53
35	C	518	DGD	O2G-C1B-C2B	3.63	119.33	111.48
23	D	404	CLA	CAC-C3C-C4C	3.63	129.51	124.79
23	C	503	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
23	c	508	CLA	C3B-C4B-NB	3.63	113.77	110.53
25	b	619	BCR	C39-C30-C25	-3.62	104.56	110.24
23	a	405	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
25	c	516	BCR	C11-C10-C9	-3.62	122.20	127.28
26	a	409	SQD	C44-O6-C1	-3.62	106.04	113.80
23	C	509	CLA	C4A-NA-C1A	-3.62	105.03	106.68
23	b	603	CLA	CMB-C2B-C1B	3.62	130.93	125.42
29	d	405	PL9	C40-C39-C41	3.62	121.51	115.23
23	C	513	CLA	CAC-C3C-C4C	3.62	129.50	124.79
23	b	604	CLA	C1-C2-C3	-3.62	120.27	126.20
23	B	615	CLA	C2B-C1B-NB	3.62	114.08	110.33
23	C	513	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
23	d	403	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
23	B	615	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	B	614	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
26	a	411	SQD	O48-C23-C24	3.60	122.82	111.83
23	b	604	CLA	C1D-CHD-C4C	-3.60	118.36	126.02
23	c	513	CLA	C2B-C1B-NB	3.60	114.06	110.33
23	B	613	CLA	CAC-C3C-C4C	3.60	129.47	124.79
23	b	601	CLA	C3C-C4C-NC	3.60	115.04	110.43
23	b	614	CLA	CHD-C1D-ND	-3.60	119.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
23	b	610	CLA	O2A-CGA-O1A	-3.60	114.63	123.63
23	A	404	CLA	CAA-C2A-C3A	-3.59	103.29	113.00
23	c	503	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
23	C	514	CLA	CHD-C1D-ND	-3.59	119.75	124.80
23	c	514	CLA	CAC-C3C-C4C	3.59	129.46	124.79
23	a	407	CLA	C3B-C4B-NB	3.59	113.73	110.53
23	B	604	CLA	O2A-CGA-O1A	-3.59	114.66	123.63
23	C	506	CLA	C1-C2-C3	-3.59	120.32	126.20
23	C	513	CLA	C3C-C4C-NC	3.59	115.02	110.43
23	A	403	CLA	C3C-C4C-NC	3.58	115.02	110.43
33	M	103	LMT	O5'-C5'-C4'	3.58	117.13	109.72
35	c	518	DGD	O2G-C1B-C2B	3.58	119.23	111.48
23	d	403	CLA	C2C-C1C-NC	3.58	113.74	109.98
23	C	507	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
23	c	507	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
31	A	416	LHG	O8-C23-O10	-3.58	114.67	123.63
25	b	619	BCR	C15-C14-C13	-3.58	122.26	127.28
35	C	520	DGD	O2G-C1B-C2B	3.57	119.21	111.48
34	C	521	LMG	O7-C10-C11	3.57	119.21	111.48
25	b	618	BCR	C29-C30-C25	3.57	115.63	110.44
23	B	608	CLA	C4A-NA-C1A	-3.57	105.05	106.68
23	b	611	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
23	C	512	CLA	C3C-C4C-NC	3.57	115.00	110.43
23	c	504	CLA	C3C-C4C-NC	3.57	115.00	110.43
23	b	607	CLA	O2D-CGD-O1D	-3.57	116.91	123.85
23	b	602	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
23	B	612	CLA	C4C-C3C-C2C	-3.56	101.71	106.89
23	B	616	CLA	C2C-C1C-NC	3.56	113.72	109.98
23	b	616	CLA	CHD-C1D-ND	-3.56	119.79	124.80
23	B	607	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
23	c	505	CLA	CHD-C1D-ND	-3.56	119.79	124.80
23	b	608	CLA	CBC-CAC-C3C	-3.56	102.78	112.42
33	b	626	LMT	C1'-O5'-C5'	3.56	120.66	113.72
23	c	515	CLA	C3B-C4B-NB	3.55	113.70	110.53
23	D	404	CLA	C3B-C4B-NB	3.55	113.70	110.53
25	C	517	BCR	C3-C4-C5	-3.55	107.73	114.06
23	c	512	CLA	CHD-C1D-ND	-3.55	119.81	124.80
23	c	506	CLA	C3C-C4C-NC	3.54	114.97	110.43
26	A	411	SQD	O47-C7-C8	3.54	119.14	111.48
24	a	416	PHO	O2D-CGD-O1D	-3.54	116.96	123.85
23	B	609	CLA	C1C-C2C-C3C	-3.54	103.26	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	403	CLA	C1D-CHD-C4C	-3.54	118.51	126.02
29	A	413[B]	PL9	C7-C3-C2	-3.53	119.23	123.39
23	b	602	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	C	507	CLA	CAC-C3C-C4C	3.53	129.38	124.79
23	B	602	CLA	CAC-C3C-C4C	3.52	129.38	124.79
29	a	414[B]	PL9	C32-C33-C34	-3.52	119.56	127.62
23	C	503	CLA	C1-C2-C3	-3.52	120.42	126.20
23	B	606	CLA	C1C-C2C-C3C	-3.52	103.27	106.98
23	C	507	CLA	C1C-C2C-C3C	-3.52	103.27	106.98
23	C	514	CLA	C3B-C4B-NB	3.52	113.67	110.53
23	B	612	CLA	CHD-C1D-ND	-3.52	119.85	124.80
23	c	515	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	B	603	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
23	b	609	CLA	C4C-C3C-C2C	-3.51	101.78	106.89
23	B	605	CLA	CMB-C2B-C1B	3.51	130.76	125.42
25	k	101	BCR	C24-C23-C22	-3.51	121.04	126.23
29	A	413[B]	PL9	C42-C43-C44	-3.50	119.61	127.62
23	a	404	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
23	B	610	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	B	602	CLA	C2C-C1C-NC	3.50	113.65	109.98
23	C	509	CLA	C4C-C3C-C2C	-3.50	101.80	106.89
23	C	510	CLA	CHD-C1D-ND	-3.49	119.89	124.80
23	c	514	CLA	CHD-C1D-ND	-3.49	119.89	124.80
32	V	202	HTG	C1-O5-C5	3.49	116.86	112.19
26	A	409	SQD	C44-O6-C1	-3.49	106.32	113.80
23	a	407	CLA	O2D-CGD-O1D	-3.48	117.06	123.85
23	b	605	CLA	O2A-CGA-O1A	-3.48	114.91	123.63
38	E	102	HEM	CAD-CBD-CGD	3.48	122.90	113.67
23	c	507	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	A	405	CLA	O2A-CGA-O1A	-3.47	114.94	123.63
23	B	611	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	d	402	CLA	CHD-C1D-ND	-3.47	119.92	124.80
25	Y	101	BCR	C15-C14-C13	-3.47	122.41	127.28
23	c	515	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	B	616	CLA	CMB-C2B-C1B	3.47	130.70	125.42
34	C	521	LMG	O8-C28-C29	3.47	122.41	111.83
23	c	515	CLA	C1-C2-C3	-3.47	120.52	126.20
26	A	409	SQD	O9-S-C6	3.46	111.93	106.76
29	A	413[A]	PL9	C20-C19-C21	3.46	121.24	115.23
26	L	102	SQD	C1-C2-C3	-3.46	102.72	110.01
23	b	606	CLA	C3C-C4C-NC	3.46	114.87	110.43
23	c	512	CLA	C3C-C4C-NC	3.46	114.86	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
29	A	413[A]	PL9	C25-C24-C26	3.46	121.23	115.23
23	b	605	CLA	CHD-C4C-NC	3.46	129.59	124.23
23	b	601	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
26	B	620	SQD	C3-C4-C5	3.46	116.50	110.23
24	A	415	PHO	C4-C3-C5	3.46	121.23	115.23
23	A	405	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
25	c	517	BCR	C33-C5-C6	-3.45	120.72	124.48
23	c	511	CLA	C3C-C4C-NC	3.45	114.85	110.43
34	D	412	LMG	O7-C10-C11	3.45	118.95	111.48
23	D	403	CLA	C3C-C4C-NC	3.45	114.85	110.43
23	C	508	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
23	c	505	CLA	C4C-C3C-C2C	-3.45	101.88	106.89
23	b	602	CLA	CAA-C2A-C3A	-3.44	103.69	113.00
23	A	403	CLA	C3B-C4B-NB	3.44	113.60	110.53
23	b	601	CLA	C3B-C4B-NB	3.44	113.60	110.53
25	D	405	BCR	C24-C23-C22	-3.44	121.15	126.23
23	b	613	CLA	CHD-C1D-ND	-3.44	119.97	124.80
23	A	404	CLA	CHD-C4C-NC	3.43	129.56	124.23
23	b	601	CLA	CHD-C4C-NC	3.43	129.56	124.23
23	b	606	CLA	C4-C3-C5	3.43	121.19	115.23
23	B	601	CLA	C3C-C4C-NC	3.43	114.83	110.43
35	C	519	DGD	O1G-C1A-C2A	3.43	122.30	111.83
23	c	511	CLA	C1D-CHD-C4C	-3.43	118.73	126.02
23	B	614	CLA	C4A-NA-C1A	-3.43	105.12	106.68
23	C	511	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
25	C	517	BCR	C33-C5-C6	-3.42	120.75	124.48
23	b	606	CLA	C3B-C4B-NB	3.42	113.58	110.53
23	b	607	CLA	C2B-C1B-NB	3.42	113.87	110.33
23	A	407	CLA	C3C-C4C-NC	3.42	114.81	110.43
23	B	607	CLA	CAA-C2A-C3A	-3.41	103.77	113.00
23	b	615	CLA	CHC-C1C-C2C	-3.41	117.26	126.95
23	c	508	CLA	C3C-C4C-NC	3.41	114.80	110.43
34	C	522	LMG	O8-C28-C29	3.41	122.23	111.83
23	C	509	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
23	d	402	CLA	C4-C3-C5	3.41	121.14	115.23
29	a	414[B]	PL9	C27-C28-C29	-3.41	119.82	127.62
23	c	505	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
23	c	503	CLA	O2A-CGA-O1A	-3.40	115.11	123.63
23	a	404	CLA	C3C-C4C-NC	3.40	114.79	110.43
23	B	613	CLA	O2D-CGD-CBD	3.40	117.17	111.23
23	d	403	CLA	C1-C2-C3	-3.40	120.63	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	BCR	C40-C30-C25	-3.40	104.91	110.24
23	C	504	CLA	C4C-C3C-C2C	-3.40	101.94	106.89
23	B	613	CLA	CMC-C2C-C1C	3.40	130.34	125.03
23	C	511	CLA	C4C-C3C-C2C	-3.40	101.95	106.89
23	a	403	CLA	O2A-CGA-CBA	3.40	122.19	111.83
24	A	415	PHO	O2D-CGD-O1D	-3.40	117.24	123.85
29	A	413[B]	PL9	C7-C8-C9	-3.40	120.98	126.83
25	b	618	BCR	C15-C14-C13	-3.40	122.52	127.28
23	b	602	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
40	V	201	HEC	CBD-CAD-C3D	-3.39	103.15	112.53
23	B	616	CLA	C4C-C3C-C2C	-3.39	101.95	106.89
31	b	628	LHG	O7-C7-C8	3.39	118.82	111.48
23	B	603	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
23	c	505	CLA	C3B-C4B-NB	3.39	113.56	110.53
23	b	616	CLA	CBC-CAC-C3C	-3.39	103.24	112.42
23	c	512	CLA	C1-C2-C3	-3.39	120.65	126.20
23	c	511	CLA	C4B-C3B-C2B	-3.38	103.09	107.30
23	c	512	CLA	C4B-C3B-C2B	-3.38	103.09	107.30
23	b	612	CLA	C4-C3-C5	3.38	121.10	115.23
23	C	510	CLA	C4A-NA-C1A	-3.38	105.14	106.68
29	a	414[B]	PL9	C25-C24-C26	3.38	121.10	115.23
25	H	101	BCR	C7-C8-C9	-3.38	121.23	126.23
23	b	604	CLA	C4A-NA-C1A	-3.38	105.14	106.68
25	b	619	BCR	C24-C23-C22	-3.38	121.23	126.23
23	b	609	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
23	D	404	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
34	Z	101	LMG	O6-C1-C2	3.38	117.31	110.37
23	b	616	CLA	C2C-C1C-NC	3.38	113.53	109.98
25	a	408	BCR	C11-C10-C9	-3.38	122.54	127.28
23	B	603	CLA	C4C-C3C-C2C	-3.38	101.98	106.89
23	c	504	CLA	C1-C2-C3	-3.38	120.67	126.20
23	a	403	CLA	C3C-C4C-NC	3.37	114.75	110.43
25	H	101	BCR	C24-C23-C22	-3.37	121.25	126.23
29	a	414[A]	PL9	C37-C36-C34	-3.37	102.02	113.19
23	C	508	CLA	C1D-CHD-C4C	-3.37	118.86	126.02
23	C	513	CLA	C4B-C3B-C2B	-3.37	103.12	107.30
23	C	508	CLA	C3B-C4B-NB	3.36	113.53	110.53
23	c	515	CLA	CAC-C3C-C4C	3.36	129.16	124.79
23	b	603	CLA	O2A-CGA-O1A	-3.36	115.23	123.63
25	D	405	BCR	C28-C27-C26	-3.35	108.08	114.06
23	A	407	CLA	C3B-C4B-NB	3.35	113.52	110.53
23	C	511	CLA	O2D-CGD-O1D	-3.35	117.32	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	CMC-C2C-C1C	3.35	130.27	125.03
23	c	509	CLA	C3C-C4C-NC	3.35	114.72	110.43
23	A	407	CLA	CAA-C2A-C3A	-3.35	103.95	113.00
23	b	607	CLA	CAA-C2A-C3A	-3.35	103.96	113.00
25	K	101	BCR	C38-C26-C25	-3.35	120.83	124.48
23	B	610	CLA	C3C-C4C-NC	3.34	114.71	110.43
23	c	507	CLA	C1D-CHD-C4C	-3.34	118.91	126.02
23	b	602	CLA	C3B-C4B-NB	3.34	113.51	110.53
24	a	416	PHO	C1A-C2A-C3A	-3.34	99.66	102.84
23	A	403	CLA	C4A-NA-C1A	-3.34	105.16	106.68
33	C	526	LMT	O1B-C4'-C3'	3.34	115.71	107.23
23	B	604	CLA	C2B-C1B-NB	3.34	113.79	110.33
25	T	101	BCR	C33-C5-C6	-3.34	120.84	124.48
23	C	515	CLA	C1C-C2C-C3C	-3.33	103.47	106.98
23	b	601	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
23	b	614	CLA	O2A-CGA-CBA	3.33	121.99	111.83
23	b	604	CLA	CHD-C1D-ND	-3.33	120.11	124.80
23	B	611	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
23	c	507	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
23	B	615	CLA	CMC-C2C-C1C	3.33	130.23	125.03
23	D	403	CLA	O2A-CGA-CBA	3.33	121.98	111.83
31	b	628	LHG	O8-C23-C24	3.33	121.98	111.83
23	C	509	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
23	c	509	CLA	C1D-CHD-C4C	-3.32	118.95	126.02
26	A	409	SQD	O48-C23-C24	3.32	121.97	111.83
23	B	609	CLA	C1D-CHD-C4C	-3.32	118.96	126.02
23	D	404	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
23	B	603	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
23	B	605	CLA	O2A-CGA-O1A	-3.32	115.33	123.63
23	b	602	CLA	C3C-C4C-NC	3.32	114.68	110.43
25	h	102	BCR	C16-C17-C18	-3.31	122.63	127.28
23	b	610	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
23	b	608	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
23	c	504	CLA	CMB-C2B-C1B	3.31	130.46	125.42
23	D	403	CLA	C3B-C4B-NB	3.31	113.49	110.53
23	b	607	CLA	CMB-C2B-C1B	3.31	130.46	125.42
23	b	616	CLA	CMC-C2C-C1C	3.31	130.21	125.03
23	C	515	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
23	C	503	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	b	605	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
23	b	612	CLA	O2A-CGA-CBA	3.30	121.90	111.83
23	A	405	CLA	CAA-C2A-C3A	-3.30	104.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	405	PL9	C37-C38-C39	-3.30	120.07	127.62
35	C	518	DGD	O1G-C1A-O1A	-3.30	115.38	123.63
23	b	613	CLA	C4B-C3B-C2B	-3.29	103.20	107.30
25	b	618	BCR	C24-C23-C22	-3.29	121.36	126.23
25	H	101	BCR	C11-C10-C9	-3.29	122.66	127.28
23	B	610	CLA	CMB-C2B-C1B	3.29	130.43	125.42
23	B	605	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
23	B	610	CLA	C1D-CHD-C4C	-3.29	119.03	126.02
29	D	406	PL9	C22-C23-C24	-3.29	120.10	127.62
23	c	507	CLA	CMB-C2B-C1B	3.29	130.42	125.42
23	c	509	CLA	CHD-C4C-NC	3.29	129.32	124.23
23	D	404	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
23	a	405	CLA	CHD-C4C-NC	3.28	129.32	124.23
23	c	508	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
23	A	407	CLA	C1D-CHD-C4C	-3.28	119.05	126.02
25	k	101	BCR	C29-C30-C25	3.28	115.20	110.44
23	a	403	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
23	B	602	CLA	CHD-C4C-NC	3.28	129.32	124.23
23	a	403	CLA	C4-C3-C5	3.28	120.92	115.23
23	b	612	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
23	b	605	CLA	C2A-C1A-CHA	-3.28	118.18	123.87
23	C	507	CLA	C3B-C4B-NB	3.28	113.45	110.53
34	m	101	LMG	O8-C28-C29	3.28	121.82	111.83
23	B	611	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
23	a	404	CLA	CHD-C4C-NC	3.27	129.30	124.23
23	b	616	CLA	OBD-CAD-C3D	-3.27	120.78	128.42
23	b	616	CLA	C4C-C3C-C2C	-3.27	102.14	106.89
23	c	510	CLA	C4C-C3C-C2C	-3.27	102.14	106.89
23	c	504	CLA	C1D-CHD-C4C	-3.26	119.08	126.02
23	b	606	CLA	CHD-C4C-NC	3.26	129.29	124.23
23	A	404	CLA	C3C-C4C-NC	3.26	114.60	110.43
23	B	606	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
23	B	605	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
23	d	403	CLA	CAA-C2A-C3A	-3.25	104.22	113.00
23	c	509	CLA	O2A-CGA-CBA	3.25	121.74	111.83
23	c	513	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
24	a	406	PHO	O1D-CGD-CBD	-3.25	119.80	124.72
23	b	608	CLA	C1D-CHD-C4C	-3.25	119.12	126.02
23	B	607	CLA	C4-C3-C5	3.25	120.86	115.23
23	c	514	CLA	C1C-C2C-C3C	-3.23	103.58	106.98
23	b	608	CLA	CMC-C2C-C1C	3.23	130.08	125.03
31	a	419	LHG	O7-C7-C8	3.23	118.47	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	619	BCR	C7-C8-C9	-3.23	121.46	126.23
26	A	411	SQD	O48-C23-C24	3.23	121.68	111.83
23	C	512	CLA	C3B-C4B-NB	3.23	113.41	110.53
26	D	413	SQD	C1-C2-C3	-3.22	103.23	110.01
23	B	605	CLA	CHD-C4C-NC	3.22	129.23	124.23
23	b	612	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
25	C	516	BCR	C33-C5-C6	-3.22	120.97	124.48
23	b	615	CLA	C3C-C4C-NC	3.22	114.56	110.43
23	c	511	CLA	O2A-CGA-CBA	3.22	121.65	111.83
23	B	609	CLA	O2A-CGA-CBA	3.21	121.64	111.83
26	a	411	SQD	C3-C4-C5	3.21	116.06	110.23
23	a	403	CLA	CHC-C1C-C2C	-3.21	117.82	126.95
23	a	407	CLA	OBD-CAD-C3D	-3.21	120.91	128.42
23	b	615	CLA	CAC-C3C-C4C	3.21	128.97	124.79
25	T	101	BCR	C39-C30-C25	-3.21	105.21	110.24
23	b	608	CLA	CAC-C3C-C4C	3.21	128.96	124.79
29	a	414[B]	PL9	C20-C19-C21	3.20	120.78	115.23
23	B	601	CLA	O2A-CGA-CBA	3.20	121.58	111.83
23	B	608	CLA	CBC-CAC-C3C	-3.19	103.76	112.42
23	b	601	CLA	C4-C3-C5	3.19	120.77	115.23
29	a	414[A]	PL9	C42-C43-C44	-3.19	120.32	127.62
25	B	619	BCR	C29-C30-C25	3.19	115.07	110.44
23	C	505	CLA	CMB-C2B-C1B	3.19	130.27	125.42
23	B	604	CLA	C3B-C4B-NB	3.19	113.38	110.53
23	c	506	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	C	510	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
25	B	631	BCR	C3-C4-C5	-3.19	108.37	114.06
29	A	413[A]	PL9	C42-C43-C44	-3.19	120.33	127.62
23	C	510	CLA	CHC-C1C-C2C	-3.19	117.89	126.95
23	c	512	CLA	C4-C3-C5	3.19	120.76	115.23
25	T	101	BCR	C15-C14-C13	3.19	131.75	127.28
31	d	406	LHG	O8-C23-O10	-3.18	115.66	123.63
25	K	101	BCR	C15-C14-C13	-3.18	122.81	127.28
29	A	413[B]	PL9	C20-C19-C21	3.18	120.75	115.23
25	k	101	BCR	C11-C10-C9	-3.18	122.82	127.28
35	h	103	DGD	O1G-C1A-C2A	3.18	121.53	111.83
23	B	616	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
23	C	505	CLA	CHD-C4C-NC	3.18	129.16	124.23
29	a	414[A]	PL9	C7-C8-C9	-3.17	121.36	126.83
23	B	611	CLA	CMC-C2C-C1C	3.17	129.99	125.03
23	b	611	CLA	O2A-CGA-CBA	3.17	121.51	111.83
23	B	616	CLA	CHD-C4C-NC	3.17	129.15	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	CMC-C2C-C1C	3.17	129.99	125.03
23	B	601	CLA	CHD-C4C-NC	3.17	129.14	124.23
23	a	407	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	B	608	CLA	C4B-C3B-C2B	-3.17	103.37	107.30
23	a	407	CLA	O2A-CGA-CBA	3.16	121.48	111.83
29	A	413[A]	PL9	C10-C9-C11	3.16	120.72	115.23
23	c	513	CLA	CAC-C3C-C4C	3.16	128.90	124.79
24	A	415	PHO	C1A-C2A-C3A	-3.16	99.83	102.84
25	k	102	BCR	C24-C23-C22	-3.16	121.56	126.23
23	C	505	CLA	C4-C3-C5	3.16	120.71	115.23
23	d	403	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	b	617	BCR	C16-C17-C18	-3.16	122.85	127.28
25	k	101	BCR	C3-C4-C5	-3.16	108.43	114.06
23	c	509	CLA	O2A-CGA-O1A	-3.15	115.74	123.63
23	A	405	CLA	C2A-C1A-CHA	-3.15	118.40	123.87
23	b	613	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
23	A	407	CLA	CMA-C3A-C2A	-3.15	101.81	113.98
23	B	614	CLA	O2A-CGA-O1A	-3.15	115.75	123.63
23	B	613	CLA	C4-C3-C5	3.15	120.69	115.23
23	C	514	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
26	a	411	SQD	O7-S-C6	3.15	111.45	106.76
33	a	412	LMT	O5'-C5'-C4'	3.15	116.23	109.72
23	a	407	CLA	CMC-C2C-C1C	3.15	129.95	125.03
29	a	414[A]	PL9	C32-C33-C34	-3.15	120.42	127.62
23	a	404	CLA	CBC-CAC-C3C	-3.14	103.90	112.42
23	B	606	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
23	b	611	CLA	C1-C2-C3	-3.14	121.05	126.20
23	c	513	CLA	CHD-C4C-NC	3.14	129.10	124.23
23	D	404	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
23	B	604	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
23	B	604	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
23	b	604	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
23	C	508	CLA	C3C-C4C-NC	3.14	114.45	110.43
25	B	618	BCR	C29-C30-C25	3.14	115.00	110.44
23	D	404	CLA	O2A-CGA-CBA	3.14	121.40	111.83
23	C	503	CLA	CMB-C2B-C1B	3.13	130.19	125.42
23	C	515	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
32	B	624	HTG	C1'-S1-C1	3.13	107.21	100.45
29	a	414[A]	PL9	C25-C24-C26	3.13	120.66	115.23
23	B	601	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	b	607	CLA	CHC-C1C-C2C	-3.13	118.05	126.95
23	b	604	CLA	C4B-C3B-C2B	-3.13	103.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	PHO	O2A-CGA-CBA	3.13	121.38	111.83
23	b	603	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
29	A	413[B]	PL9	C17-C18-C19	-3.13	120.46	127.62
29	a	414[A]	PL9	C22-C23-C24	-3.13	120.46	127.62
23	D	403	CLA	CBC-CAC-C3C	-3.13	103.94	112.42
23	B	608	CLA	CMA-C3A-C4A	-3.13	103.36	111.77
23	b	607	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	b	610	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	c	510	CLA	CHD-C1D-ND	-3.13	120.40	124.80
23	B	611	CLA	CHD-C4C-NC	3.12	129.07	124.23
23	B	609	CLA	C3B-C4B-NB	3.12	113.32	110.53
23	C	503	CLA	C4-C3-C5	3.12	120.65	115.23
29	A	413[A]	PL9	C53-C6-C1	3.12	121.67	115.28
23	B	610	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
23	c	503	CLA	C3B-C4B-NB	3.12	113.32	110.53
25	H	101	BCR	C31-C1-C6	-3.12	105.35	110.24
23	B	602	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
23	b	608	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
25	k	101	BCR	C15-C14-C13	-3.12	122.90	127.28
23	C	512	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
29	A	413[B]	PL9	C22-C23-C24	-3.11	120.50	127.62
23	B	615	CLA	C4C-C3C-C2C	-3.11	102.36	106.89
23	C	503	CLA	CHD-C4C-NC	3.11	129.06	124.23
23	B	610	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
24	A	406	PHO	CBC-CAC-C3C	-3.11	108.42	112.87
23	b	605	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	d	402	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
23	B	611	CLA	CMB-C2B-C1B	3.11	130.15	125.42
23	b	607	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
23	b	603	CLA	O2A-CGA-CBA	3.10	121.28	111.83
23	c	511	CLA	C1-O2A-CGA	3.10	124.15	116.65
38	E	102	HEM	C1B-NB-C4B	3.10	108.87	105.21
29	D	406	PL9	C30-C29-C31	3.09	120.60	115.23
25	D	405	BCR	C29-C30-C25	3.09	114.93	110.44
35	h	103	DGD	O2G-C1B-C2B	3.09	118.17	111.48
23	C	504	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
23	C	503	CLA	CMC-C2C-C1C	3.09	129.87	125.03
23	A	405	CLA	C3C-C4C-NC	3.09	114.39	110.43
23	B	604	CLA	C4-C3-C5	3.09	120.59	115.23
23	a	403	CLA	O2A-CGA-O1A	-3.09	115.90	123.63
23	c	508	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
31	d	407	LHG	C6-C5-C4	-3.09	104.58	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	O2A-CGA-CBA	3.09	121.25	111.83
23	a	405	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
23	B	601	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
23	C	510	CLA	C4-C3-C5	3.09	120.58	115.23
23	b	614	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	d	403	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
23	a	407	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
23	c	505	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
23	c	512	CLA	O2A-CGA-O1A	-3.08	115.92	123.63
23	b	616	CLA	C1-C2-C3	-3.08	121.16	126.20
23	b	610	CLA	CHD-C1D-ND	-3.08	120.47	124.80
23	B	612	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
23	d	402	CLA	CBC-CAC-C3C	-3.08	104.08	112.42
23	c	513	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
23	A	404	CLA	C4-C3-C5	3.07	120.56	115.23
23	b	616	CLA	O2A-CGA-CBA	3.07	121.21	111.83
23	A	403	CLA	O2D-CGD-CBD	3.07	116.60	111.23
23	b	609	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
32	h	101	HTG	C1-O5-C5	3.07	118.07	112.56
23	b	601	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
23	B	615	CLA	C4-C3-C5	3.07	120.56	115.23
23	a	405	CLA	CMB-C2B-C1B	3.07	130.09	125.42
23	b	614	CLA	CMC-C2C-C1C	3.07	129.83	125.03
25	D	405	BCR	C37-C22-C23	3.07	122.77	118.09
23	c	515	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
25	B	619	BCR	C24-C23-C22	-3.06	121.70	126.23
23	b	604	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
23	B	607	CLA	CBC-CAC-C3C	-3.06	104.12	112.42
23	b	607	CLA	C1-O2A-CGA	3.06	124.06	116.65
25	Y	101	BCR	C38-C26-C25	-3.06	121.14	124.48
23	C	514	CLA	C1-C2-C3	-3.06	121.19	126.20
26	L	102	SQD	C1-O5-C5	-3.06	107.75	113.72
25	k	102	BCR	C38-C26-C25	-3.06	121.15	124.48
23	B	608	CLA	CHD-C4C-NC	3.06	128.97	124.23
23	C	504	CLA	CHD-C4C-NC	3.05	128.97	124.23
23	c	508	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
34	c	522	LMG	O8-C28-C29	3.05	121.14	111.83
23	d	403	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
29	A	413[A]	PL9	C17-C18-C19	-3.05	120.64	127.62
23	B	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	d	403	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	b	606	CLA	CMC-C2C-C1C	3.05	129.80	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	508	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	C	515	CLA	C3B-C4B-NB	3.05	113.25	110.53
23	C	507	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
23	B	614	CLA	C1-C2-C3	-3.05	121.21	126.20
23	c	505	CLA	CMC-C2C-C1C	3.04	129.79	125.03
23	C	514	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	a	405	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
23	c	511	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
23	b	611	CLA	CMC-C2C-C1C	3.04	129.78	125.03
23	c	511	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
31	D	408	LHG	O8-C23-C24	3.04	121.10	111.83
26	A	409	SQD	O48-C23-O10	-3.04	116.03	123.63
23	b	616	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
23	b	611	CLA	CMB-C2B-C1B	3.03	130.04	125.42
23	C	504	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
23	b	603	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	c	503	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
32	B	621	HTG	C1-C2-C3	3.03	116.48	110.55
23	b	606	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
23	c	504	CLA	CHD-C4C-NC	3.03	128.93	124.23
25	b	617	BCR	C29-C30-C25	3.03	114.84	110.44
23	b	601	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
23	A	407	CLA	CBC-CAC-C3C	-3.03	104.22	112.42
23	B	612	CLA	C4-C3-C5	3.03	120.48	115.23
23	B	611	CLA	CBC-CAC-C3C	-3.02	104.22	112.42
25	C	517	BCR	C38-C26-C25	-3.02	121.19	124.48
25	k	101	BCR	C34-C9-C8	3.02	122.70	118.09
23	a	407	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
23	B	613	CLA	C1D-CHD-C4C	-3.02	119.60	126.02
26	A	409	SQD	C45-O47-C7	-3.02	110.57	117.80
23	c	515	CLA	O2A-CGA-CBA	3.02	121.04	111.83
23	c	509	CLA	C1-C2-C3	-3.02	121.25	126.20
23	B	614	CLA	C4-C3-C5	3.02	120.47	115.23
23	B	614	CLA	C3B-C4B-NB	3.02	113.22	110.53
23	C	515	CLA	CHD-C4C-NC	3.02	128.91	124.23
23	C	507	CLA	CMC-C2C-C1C	3.02	129.75	125.03
23	B	609	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
31	E	101	LHG	O8-C23-C24	3.02	121.03	111.83
23	c	512	CLA	CHD-C4C-NC	3.02	128.91	124.23
23	C	511	CLA	CAC-C3C-C4C	3.02	128.71	124.79
23	C	508	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
23	b	613	CLA	C4C-C3C-C2C	-3.01	102.50	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	CHC-C1C-C2C	-3.01	118.38	126.95
23	b	610	CLA	C4-C3-C5	3.01	120.46	115.23
23	A	405	CLA	O2A-CGA-CBA	3.01	121.02	111.83
23	B	601	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
23	b	612	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
23	a	407	CLA	C1-C2-C3	-3.01	121.26	126.20
23	a	403	CLA	CMC-C2C-C1C	3.01	129.74	125.03
23	b	608	CLA	C3C-C4C-NC	3.01	114.29	110.43
23	c	510	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
23	B	614	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
23	c	512	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
29	A	413[B]	PL9	C25-C24-C26	3.01	120.45	115.23
23	d	403	CLA	O2A-CGA-CBA	3.00	120.99	111.83
35	c	520	DGD	O2G-C1B-C2B	3.00	117.98	111.48
23	a	404	CLA	CMA-C3A-C2A	-3.00	102.38	113.98
23	B	607	CLA	C2B-C1B-NB	3.00	113.43	110.33
23	c	511	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
23	c	514	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
23	B	614	CLA	O2A-CGA-CBA	2.99	120.96	111.83
29	A	413[A]	PL9	C22-C23-C24	-2.99	120.77	127.62
25	B	618	BCR	C28-C27-C26	-2.99	108.72	114.06
23	d	402	CLA	O2A-CGA-CBA	2.99	120.96	111.83
38	E	102	HEM	CHB-C1B-NB	2.99	128.07	124.37
25	c	516	BCR	C20-C21-C22	-2.99	123.08	127.28
23	c	513	CLA	CBC-CAC-C3C	-2.99	104.31	112.42
23	B	609	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	b	610	CLA	CHD-C4C-NC	2.99	128.87	124.23
23	B	614	CLA	C2A-C1A-CHA	-2.99	118.68	123.87
23	b	611	CLA	O2A-CGA-O1A	-2.99	116.15	123.63
35	C	519	DGD	O1G-C1A-O1A	-2.99	116.15	123.63
38	e	102	HEM	C1B-NB-C4B	2.99	108.74	105.21
23	c	506	CLA	C4B-C3B-C2B	-2.99	103.59	107.30
25	c	516	BCR	C38-C26-C25	-2.98	121.23	124.48
23	C	511	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
23	B	601	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
29	a	414[B]	PL9	C37-C36-C34	-2.98	103.31	113.19
23	c	512	CLA	O2A-CGA-CBA	2.98	120.93	111.83
23	b	613	CLA	CAC-C3C-C4C	2.98	128.67	124.79
23	D	403	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
23	B	606	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
23	c	509	CLA	C4-C3-C5	2.98	120.40	115.23
31	A	416	LHG	O8-C23-C24	2.98	120.91	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	403	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
23	B	605	CLA	C2A-C1A-CHA	-2.98	118.70	123.87
24	A	406	PHO	C1-C2-C3	-2.98	121.32	126.20
23	C	505	CLA	C3B-C4B-NB	2.98	113.19	110.53
23	B	613	CLA	O2A-CGA-CBA	2.97	120.90	111.83
25	c	517	BCR	C15-C16-C17	-2.97	117.43	123.52
23	b	604	CLA	CMC-C2C-C1C	2.97	129.68	125.03
23	A	403	CLA	C2A-C1A-CHA	-2.97	118.71	123.87
34	D	412	LMG	O8-C28-O10	-2.96	116.21	123.63
23	C	514	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	c	514	CLA	CMB-C2B-C1B	2.96	129.93	125.42
31	d	408	LHG	O8-C23-C24	2.96	120.87	111.83
23	b	613	CLA	C4-C3-C5	2.96	120.37	115.23
23	b	609	CLA	CHD-C4C-NC	2.96	128.83	124.23
23	c	504	CLA	CBC-CAC-C3C	-2.96	104.39	112.42
23	A	407	CLA	C2A-C1A-CHA	-2.96	118.72	123.87
23	c	503	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
23	B	602	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
23	a	404	CLA	C1-C2-C3	-2.95	121.36	126.20
23	c	510	CLA	CHD-C4C-NC	2.95	128.81	124.23
23	B	601	CLA	CAC-C3C-C4C	2.95	128.63	124.79
23	b	611	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
23	a	405	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
23	C	503	CLA	C3B-C4B-NB	2.95	113.16	110.53
23	a	404	CLA	CAA-C2A-C3A	-2.95	105.04	113.00
29	a	414[B]	PL9	C42-C43-C44	-2.95	120.88	127.62
23	C	505	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	C	512	CLA	CMC-C2C-C1C	2.94	129.63	125.03
34	z	101	LMG	O8-C28-C29	2.94	120.80	111.83
34	c	521	LMG	O8-C28-C29	2.94	120.80	111.83
25	c	517	BCR	C15-C14-C13	-2.94	123.16	127.28
26	a	409	SQD	O8-S-C6	2.94	111.64	105.97
23	C	503	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
32	B	624	HTG	O5-C5-C4	2.94	114.99	109.70
23	C	506	CLA	C4B-C3B-C2B	-2.93	103.65	107.30
38	e	102	HEM	CHA-C4D-ND	2.93	128.00	124.37
23	B	612	CLA	O2A-CGA-CBA	2.93	120.77	111.83
23	A	405	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
29	A	413[A]	PL9	C32-C33-C34	-2.93	120.92	127.62
23	c	514	CLA	C4-C3-C5	2.93	120.31	115.23
23	c	514	CLA	O2A-CGA-CBA	2.93	120.75	111.83
23	C	512	CLA	CHD-C4C-NC	2.93	128.77	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	BCR	C24-C23-C22	-2.92	121.91	126.23
23	B	615	CLA	C3B-C4B-NB	2.92	113.14	110.53
26	a	409	SQD	O48-C23-C24	2.92	120.74	111.83
29	a	414[B]	PL9	C15-C14-C16	2.92	120.30	115.23
23	b	615	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
35	C	520	DGD	O1G-C1A-C2A	2.92	120.73	111.83
25	a	408	BCR	C33-C5-C6	-2.92	121.30	124.48
23	b	609	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
26	L	102	SQD	C3-C4-C5	2.91	115.52	110.23
23	C	514	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
23	a	405	CLA	C1-C2-C3	-2.91	121.43	126.20
23	C	512	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
23	C	513	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
23	b	602	CLA	CMC-C2C-C1C	2.91	129.58	125.03
25	c	516	BCR	C15-C14-C13	-2.91	123.20	127.28
23	B	612	CLA	CHD-C4C-NC	2.91	128.74	124.23
23	B	606	CLA	C4-C3-C5	2.90	120.27	115.23
25	k	102	BCR	C10-C11-C12	-2.90	114.79	123.20
23	C	511	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
23	C	513	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
35	c	520	DGD	O1G-C1A-C2A	2.90	120.67	111.83
23	B	609	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
23	b	603	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
23	B	612	CLA	C3B-C4B-NB	2.90	113.12	110.53
23	d	403	CLA	C3C-C4C-NC	2.90	114.14	110.43
23	b	614	CLA	CBC-CAC-C3C	-2.90	104.57	112.42
23	D	403	CLA	C1D-CHD-C4C	-2.89	119.87	126.02
23	C	506	CLA	CMB-C2B-C1B	2.89	129.82	125.42
23	B	606	CLA	CAC-C3C-C4C	2.89	128.55	124.79
23	c	510	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
23	C	505	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
23	c	511	CLA	CMC-C2C-C1C	2.89	129.55	125.03
33	B	629	LMT	C1-O1'-C1'	-2.89	108.75	113.68
23	c	507	CLA	O2A-CGA-CBA	2.89	120.64	111.83
31	d	406	LHG	O8-C23-C24	2.89	120.64	111.83
23	c	513	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
23	A	407	CLA	CMC-C2C-C1C	2.89	129.54	125.03
23	A	405	CLA	CMA-C3A-C2A	-2.89	102.82	113.98
23	B	605	CLA	O2A-CGA-CBA	2.89	120.63	111.83
25	b	619	BCR	C34-C9-C10	-2.88	118.14	122.82
23	B	610	CLA	CAA-CBA-CGA	-2.88	105.02	113.21
25	h	102	BCR	C24-C23-C22	-2.88	121.97	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	406	PL9	C37-C38-C39	-2.88	121.03	127.62
23	b	615	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
38	E	102	HEM	CHA-C4D-ND	2.88	127.93	124.37
23	C	514	CLA	O2A-CGA-CBA	2.88	120.61	111.83
29	D	406	PL9	C25-C24-C26	2.88	120.22	115.23
23	d	402	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
23	b	614	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
24	a	406	PHO	C1-C2-C3	-2.87	121.49	126.20
23	D	404	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
23	C	508	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
23	c	513	CLA	O2A-CGA-CBA	2.87	120.59	111.83
23	b	610	CLA	CBC-CAC-C3C	-2.87	104.64	112.42
32	b	624	HTG	C1'-S1-C1	2.87	106.65	100.45
25	T	101	BCR	C12-C13-C14	-2.87	114.50	119.01
23	b	602	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
23	c	509	CLA	O1D-CGD-CBD	-2.87	118.86	124.52
23	c	503	CLA	O2A-CGA-CBA	2.87	120.58	111.83
29	D	406	PL9	C53-C6-C1	2.87	121.15	115.28
23	c	509	CLA	CAC-C3C-C4C	2.87	128.52	124.79
25	H	101	BCR	C16-C17-C18	-2.87	123.26	127.28
23	c	504	CLA	C3B-C4B-NB	2.87	113.09	110.53
23	B	607	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
23	B	602	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	a	403	CLA	C1-C2-C3	-2.86	121.51	126.20
23	C	512	CLA	O2A-CGA-CBA	2.86	120.56	111.83
23	C	507	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	c	515	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
23	d	402	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
23	c	514	CLA	CMC-C2C-C1C	2.86	129.50	125.03
23	C	508	CLA	CMC-C2C-C1C	2.86	129.50	125.03
23	b	614	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
23	A	405	CLA	C1D-CHD-C4C	-2.85	119.95	126.02
23	C	512	CLA	CBC-CAC-C3C	-2.85	104.68	112.42
23	B	610	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
32	B	624	HTG	C3-C4-C5	2.85	115.40	110.23
31	d	407	LHG	O8-C23-C24	2.85	120.53	111.83
23	C	515	CLA	CMB-C2B-C1B	2.85	129.76	125.42
23	C	508	CLA	CMB-C2B-C1B	2.85	129.76	125.42
25	B	618	BCR	C16-C17-C18	-2.85	123.28	127.28
23	b	611	CLA	CHD-C4C-NC	2.85	128.65	124.23
23	a	407	CLA	CMA-C3A-C2A	-2.84	102.98	113.98
23	B	603	CLA	O2A-CGA-O1A	-2.84	116.51	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	SQD	O5-C5-C4	2.84	114.82	109.70
23	B	608	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
29	a	414[B]	PL9	C17-C18-C19	-2.84	121.12	127.62
23	a	407	CLA	C4-C3-C5	2.84	120.16	115.23
23	B	610	CLA	C3B-C4B-NB	2.84	113.06	110.53
23	b	614	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
23	a	403	CLA	CMA-C3A-C4A	-2.84	104.14	111.77
29	a	414[B]	PL9	C45-C44-C46	2.84	120.15	115.23
34	D	412	LMG	O8-C28-C29	2.84	120.48	111.83
25	D	405	BCR	C33-C5-C6	-2.84	121.39	124.48
29	d	405	PL9	C22-C23-C24	-2.83	121.14	127.62
23	C	513	CLA	CMC-C2C-C1C	2.83	129.46	125.03
23	C	506	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	b	607	CLA	CBC-CAC-C3C	-2.83	104.75	112.42
23	C	505	CLA	CMC-C2C-C1C	2.83	129.46	125.03
23	a	407	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
23	b	616	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
23	B	616	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
23	c	503	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
23	B	603	CLA	C4-C3-C5	2.83	120.13	115.23
23	C	515	CLA	CMC-C2C-C1C	2.83	129.45	125.03
23	c	513	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
23	b	610	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
23	C	509	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
23	c	510	CLA	OBD-CAD-C3D	-2.82	121.82	128.42
23	C	503	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
23	B	612	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
23	B	608	CLA	CHB-C4A-NA	2.82	128.47	124.40
23	B	614	CLA	CHC-C1C-C2C	-2.82	118.95	126.95
38	e	102	HEM	CHB-C1B-NB	2.81	127.85	124.37
23	B	603	CLA	CHD-C4C-NC	2.81	128.60	124.23
23	B	604	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
23	C	507	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
23	a	404	CLA	C2A-C1A-CHA	-2.81	118.98	123.87
23	B	611	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
23	C	503	CLA	CAC-C3C-C4C	2.81	128.45	124.79
29	a	414[B]	PL9	C53-C6-C1	2.81	121.04	115.28
25	k	101	BCR	C16-C17-C18	-2.81	123.34	127.28
25	D	405	BCR	C21-C20-C19	-2.81	115.06	123.20
23	b	609	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	b	611	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	A	405	CLA	CHC-C1C-C2C	-2.81	118.96	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	CMC-C2C-C1C	2.81	129.42	125.03
23	d	403	CLA	CMC-C2C-C1C	2.81	129.42	125.03
38	e	102	HEM	CBD-CAD-C3D	-2.81	104.77	112.53
23	b	605	CLA	CED-O2D-CGD	2.81	122.28	115.92
25	k	101	BCR	C36-C18-C19	2.81	122.38	118.09
23	b	602	CLA	C4C-C3C-C2C	-2.81	102.81	106.89
23	b	607	CLA	CHD-C4C-NC	2.81	128.58	124.23
25	d	404	BCR	C16-C17-C18	-2.81	123.34	127.28
23	A	407	CLA	CMB-C2B-C1B	2.80	129.69	125.42
23	d	403	CLA	CMB-C2B-C1B	2.80	129.69	125.42
23	b	603	CLA	C2A-C1A-CHA	-2.80	119.00	123.87
23	a	407	CLA	CHD-C4C-NC	2.80	128.58	124.23
23	b	611	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
23	C	513	CLA	C4-C3-C5	2.80	120.09	115.23
23	b	606	CLA	C1-O2A-CGA	2.80	123.43	116.65
25	B	619	BCR	C2-C3-C4	-2.80	105.13	111.28
23	C	514	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	A	407	CLA	C4-C3-C5	2.80	120.08	115.23
32	b	624	HTG	O5-C5-C4	2.80	114.74	109.70
29	D	406	PL9	C45-C44-C46	2.79	120.07	115.23
23	c	503	CLA	CAC-C3C-C4C	2.79	128.42	124.79
38	e	102	HEM	CHD-C1D-ND	2.79	127.43	124.42
26	f	101	SQD	O48-C23-C24	2.79	120.34	111.83
25	Y	101	BCR	C34-C9-C8	2.79	122.35	118.09
23	b	616	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
23	B	607	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
25	B	618	BCR	C2-C1-C6	2.78	114.48	110.44
31	A	416	LHG	C5-O7-C7	-2.78	111.13	117.80
23	c	508	CLA	CHC-C1C-C2C	-2.78	119.04	126.95
25	a	408	BCR	C39-C30-C25	-2.78	105.88	110.24
29	D	406	PL9	C10-C9-C11	2.78	120.06	115.23
26	D	413	SQD	O48-C23-C24	2.78	120.31	111.83
23	B	603	CLA	O2A-CGA-CBA	2.78	120.30	111.83
23	C	508	CLA	CBC-CAC-C3C	-2.78	104.89	112.42
23	B	605	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
23	c	515	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
25	k	102	BCR	C21-C20-C19	-2.78	115.16	123.20
29	A	413[B]	PL9	C53-C6-C1	2.77	120.96	115.28
23	b	606	CLA	CBC-CAC-C3C	-2.77	104.90	112.42
34	Z	101	LMG	C4-C3-C2	2.77	115.70	110.83
23	a	404	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
23	a	404	CLA	C3B-C4B-NB	2.77	113.00	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
23	B	616	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
34	c	521	LMG	O1-C7-C8	-2.77	104.09	110.82
23	b	604	CLA	CMB-C2B-C1B	2.77	129.63	125.42
23	c	506	CLA	C1-O2A-CGA	2.77	123.35	116.65
26	L	102	SQD	O48-C23-C24	2.77	120.27	111.83
23	d	403	CLA	C4C-C3C-C2C	-2.77	102.87	106.89
23	D	404	CLA	CHD-C4C-NC	2.77	128.52	124.23
23	B	611	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
29	a	414[A]	PL9	C10-C9-C11	2.76	120.02	115.23
23	b	614	CLA	CHD-C4C-NC	2.76	128.51	124.23
23	c	504	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
23	C	505	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	A	403	CLA	CMC-C2C-C1C	2.76	129.35	125.03
23	B	610	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
40	v	202	HEC	CBD-CAD-C3D	-2.76	104.90	112.53
31	d	406	LHG	C5-O7-C7	-2.76	111.19	117.80
23	C	503	CLA	CBC-CAC-C3C	-2.76	104.95	112.42
23	B	610	CLA	C1-C2-C3	-2.75	121.68	126.20
29	a	414[A]	PL9	C20-C19-C21	2.75	120.01	115.23
35	c	520	DGD	C2G-O2G-C1B	-2.75	111.21	117.80
23	A	403	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
24	a	406	PHO	C1A-C2A-C3A	-2.75	100.22	102.84
23	b	601	CLA	O2A-CGA-CBA	2.75	120.23	111.83
23	B	602	CLA	C2A-C1A-CHA	-2.75	119.09	123.87
25	d	404	BCR	C21-C20-C19	-2.75	115.23	123.20
23	C	506	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
23	c	505	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
23	c	513	CLA	CMC-C2C-C1C	2.75	129.33	125.03
25	d	404	BCR	C10-C11-C12	-2.75	115.24	123.20
23	C	509	CLA	C1-C2-C3	-2.75	121.69	126.20
23	B	602	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
23	c	508	CLA	CMC-C2C-C1C	2.75	129.33	125.03
23	C	505	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
29	a	414[A]	PL9	C17-C18-C19	-2.74	121.34	127.62
23	B	604	CLA	C6-C7-C8	-2.74	106.84	115.97
23	a	404	CLA	CMC-C2C-C1C	2.74	129.32	125.03
23	B	607	CLA	C1-O2A-CGA	2.74	123.29	116.65
23	b	604	CLA	CHD-C4C-NC	2.74	128.49	124.23
23	b	605	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
25	B	631	BCR	C2-C1-C6	2.74	114.42	110.44
29	D	406	PL9	C51-C49-C50	2.74	120.90	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	515	CLA	O2A-CGA-CBA	2.74	120.19	111.83
23	A	404	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
23	A	403	CLA	CAA-C2A-C1A	-2.74	103.01	111.97
25	C	517	BCR	C15-C16-C17	-2.74	117.92	123.52
23	b	611	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
23	b	605	CLA	CMB-C2B-C1B	2.73	129.58	125.42
23	C	512	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
23	c	510	CLA	CAA-C2A-C3A	-2.73	105.61	113.00
23	B	607	CLA	CHD-C4C-NC	2.73	128.47	124.23
24	A	415	PHO	CMA-C3A-C4A	-2.73	108.72	114.61
23	C	509	CLA	C3B-C4B-NB	2.73	112.97	110.53
31	L	101	LHG	O8-C23-C24	2.73	120.17	111.83
23	A	407	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
25	B	631	BCR	C21-C20-C19	-2.73	115.29	123.20
34	c	522	LMG	C3-C4-C5	2.73	115.18	110.23
25	C	516	BCR	C23-C24-C25	-2.73	119.71	127.00
23	b	603	CLA	C4-C3-C5	2.73	119.96	115.23
23	c	510	CLA	O2A-CGA-CBA	2.73	120.15	111.83
23	b	602	CLA	C11-C12-C13	-2.73	106.90	115.97
23	D	403	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
23	C	508	CLA	O2A-CGA-CBA	2.73	120.15	111.83
23	B	605	CLA	CAC-C3C-C4C	2.72	128.33	124.79
25	A	408	BCR	C31-C1-C6	-2.72	105.98	110.24
33	a	412	LMT	O5B-C5B-C4B	2.72	114.60	109.70
25	C	516	BCR	C38-C26-C25	-2.72	121.52	124.48
23	B	604	CLA	O2A-CGA-CBA	2.71	120.11	111.83
26	a	411	SQD	O48-C23-O10	-2.71	116.84	123.63
23	b	603	CLA	CHD-C4C-NC	2.71	128.44	124.23
23	c	506	CLA	CMB-C2B-C1B	2.71	129.55	125.42
23	D	403	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
23	a	407	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
23	c	514	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
23	b	612	CLA	CMC-C2C-C1C	2.71	129.27	125.03
25	H	101	BCR	C10-C11-C12	-2.71	115.36	123.20
23	c	513	CLA	C4-C3-C5	2.70	119.92	115.23
23	B	606	CLA	CBC-CAC-C3C	-2.70	105.09	112.42
25	b	618	BCR	C3-C4-C5	-2.70	109.24	114.06
23	C	506	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
23	b	606	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
29	d	405	PL9	C10-C9-C11	2.70	119.91	115.23
23	B	606	CLA	CHD-C4C-NC	2.70	128.41	124.23
23	C	512	CLA	CHC-C1C-C2C	-2.70	119.28	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	C4A-NA-C1A	-2.70	105.45	106.68
35	H	102	DGD	C3G-O3G-C1D	-2.70	108.02	113.80
29	A	413[B]	PL9	C45-C44-C46	2.70	119.91	115.23
25	b	618	BCR	C8-C7-C6	-2.70	119.80	127.00
23	B	616	CLA	CMC-C2C-C1C	2.69	129.25	125.03
23	c	506	CLA	CHD-C4C-NC	2.69	128.41	124.23
23	B	613	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
23	B	609	CLA	C2A-C1A-CHA	-2.69	119.19	123.87
23	b	601	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
23	c	504	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
25	b	619	BCR	C7-C8-C9	-2.69	122.26	126.23
23	B	607	CLA	C2A-C1A-CHA	-2.68	119.21	123.87
23	b	612	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
23	c	512	CLA	CMC-C2C-C1C	2.68	129.23	125.03
23	b	612	CLA	C2A-C1A-CHA	-2.68	119.21	123.87
23	c	514	CLA	CHD-C4C-NC	2.68	128.39	124.23
23	a	405	CLA	CAC-C3C-C4C	2.68	128.28	124.79
23	D	404	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
23	B	607	CLA	C3B-C4B-NB	2.68	112.92	110.53
23	B	601	CLA	CMC-C2C-C1C	2.68	129.22	125.03
25	B	618	BCR	C37-C22-C21	-2.68	118.48	122.82
23	C	511	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
23	A	407	CLA	CHD-C4C-NC	2.68	128.38	124.23
23	B	616	CLA	C3B-C4B-NB	2.68	112.92	110.53
23	D	404	CLA	C1-O2A-CGA	2.67	123.12	116.65
26	A	411	SQD	O5-C5-C4	2.67	114.51	109.70
23	a	403	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	A	407	CLA	O2A-CGA-CBA	2.67	119.97	111.83
25	Y	101	BCR	C40-C30-C25	-2.67	106.06	110.24
23	B	601	CLA	C3B-C4B-NB	2.67	112.91	110.53
23	C	509	CLA	O2A-CGA-CBA	2.67	119.97	111.83
35	c	519	DGD	C2G-O2G-C1B	-2.67	111.41	117.80
25	D	405	BCR	C10-C11-C12	-2.66	115.48	123.20
26	L	102	SQD	C44-O6-C1	-2.66	108.08	113.80
34	C	521	LMG	O8-C28-O10	-2.66	116.97	123.63
24	a	406	PHO	O2A-CGA-O1A	-2.66	116.97	123.63
23	b	608	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
23	c	503	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
25	B	617	BCR	C33-C5-C6	-2.66	121.58	124.48
29	D	406	PL9	O2-C1-C6	-2.66	116.25	120.48
29	A	413[A]	PL9	C40-C39-C41	2.66	119.84	115.23
26	D	413	SQD	O8-S-C6	2.66	111.10	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
23	b	610	CLA	CMC-C2C-C1C	2.66	129.19	125.03
38	E	102	HEM	CBA-CAA-C2A	-2.66	105.19	112.53
23	B	606	CLA	O2A-CGA-CBA	2.66	119.93	111.83
23	c	508	CLA	O2A-CGA-CBA	2.66	119.93	111.83
23	A	403	CLA	CHC-C1C-C2C	-2.65	119.40	126.95
23	C	513	CLA	CHD-C4C-NC	2.65	128.35	124.23
23	C	505	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
23	C	513	CLA	O2A-CGA-CBA	2.65	119.92	111.83
23	b	608	CLA	CHD-C4C-NC	2.65	128.34	124.23
23	B	607	CLA	CMC-C2C-C1C	2.65	129.18	125.03
23	C	509	CLA	CHD-C4C-NC	2.65	128.34	124.23
23	C	513	CLA	C1-C2-C3	-2.65	121.85	126.20
23	c	508	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
23	B	603	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
23	C	508	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
23	C	506	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
23	a	404	CLA	C1-O2A-CGA	2.65	123.06	116.65
23	c	503	CLA	CMC-C2C-C1C	2.65	129.17	125.03
29	A	413[A]	PL9	C30-C29-C31	2.65	119.82	115.23
23	c	504	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
23	C	503	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
25	k	102	BCR	C29-C28-C27	-2.65	105.46	111.28
23	C	508	CLA	C4C-C3C-C2C	-2.65	103.04	106.89
23	c	506	CLA	CED-O2D-CGD	2.65	121.92	115.92
25	D	405	BCR	C3-C4-C5	-2.64	109.34	114.06
23	c	506	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
23	B	608	CLA	O2A-CGA-CBA	2.64	119.89	111.83
25	B	618	BCR	C37-C22-C23	2.64	122.12	118.09
23	c	515	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
25	T	101	BCR	C21-C20-C19	-2.64	115.55	123.20
23	C	506	CLA	CBC-CAC-C3C	-2.64	105.26	112.42
35	H	102	DGD	O1G-C1A-C2A	2.64	119.88	111.83
31	d	408	LHG	O8-C23-O10	-2.64	117.03	123.63
23	B	615	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
23	C	510	CLA	CHD-C4C-NC	2.64	128.32	124.23
23	C	506	CLA	CMC-C2C-C1C	2.64	129.15	125.03
23	d	403	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	b	602	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
26	A	409	SQD	O47-C7-O49	-2.63	117.55	123.70
25	T	101	BCR	C10-C11-C12	-2.63	115.57	123.20
23	c	515	CLA	CAA-C2A-C3A	-2.63	105.89	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C11-C12-C13	-2.63	107.22	115.97
23	c	504	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
24	A	406	PHO	CMB-C2B-C3B	2.63	129.94	124.68
23	C	515	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	b	614	CLA	CAC-C3C-C4C	2.63	128.21	124.79
25	B	619	BCR	C10-C11-C12	-2.63	115.58	123.20
23	B	604	CLA	CHD-C1D-ND	-2.63	121.10	124.80
23	B	611	CLA	CED-O2D-CGD	2.63	121.88	115.92
23	B	615	CLA	C11-C10-C8	-2.63	107.23	115.97
23	b	608	CLA	C2A-C1A-CHA	-2.63	119.31	123.87
31	d	406	LHG	O7-C7-O9	-2.63	117.56	123.70
23	d	403	CLA	CAC-C3C-C4C	2.63	128.21	124.79
25	c	517	BCR	C21-C20-C19	-2.63	115.59	123.20
23	C	510	CLA	C1-C2-C3	-2.63	121.89	126.20
23	C	511	CLA	O2A-CGA-CBA	2.63	119.84	111.83
23	c	510	CLA	C4-C3-C5	2.63	119.79	115.23
24	A	406	PHO	O2D-CGD-O1D	-2.63	118.74	123.85
23	a	403	CLA	CHB-C4A-NA	2.62	128.19	124.40
24	A	415	PHO	C4A-C3A-C2A	-2.62	100.34	102.84
23	c	503	CLA	C4-C3-C5	2.62	119.78	115.23
23	b	604	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
23	C	504	CLA	O2A-CGA-CBA	2.62	119.83	111.83
25	T	101	BCR	C16-C17-C18	-2.62	123.60	127.28
23	b	608	CLA	O2A-CGA-CBA	2.62	119.83	111.83
23	A	405	CLA	CHD-C4C-NC	2.62	128.29	124.23
23	b	615	CLA	O2A-CGA-CBA	2.62	119.82	111.83
26	B	620	SQD	O48-C23-C24	2.62	119.82	111.83
25	A	408	BCR	C38-C26-C25	-2.62	121.63	124.48
23	A	407	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
25	h	102	BCR	C10-C11-C12	-2.62	115.61	123.20
34	a	417	LMG	C30-C29-C28	-2.62	104.10	113.69
25	b	618	BCR	C39-C30-C25	-2.62	106.14	110.24
23	b	602	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
25	b	618	BCR	C15-C16-C17	-2.62	118.16	123.52
23	B	603	CLA	CMA-C3A-C2A	-2.61	103.87	113.98
25	c	516	BCR	C33-C5-C6	-2.61	121.63	124.48
31	D	407	LHG	O8-C23-C24	2.61	119.80	111.83
23	b	614	CLA	C2A-C1A-CHA	-2.61	119.33	123.87
23	C	506	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
33	F	101	LMT	O5B-C1B-C2B	2.61	115.73	110.37
25	K	101	BCR	C10-C11-C12	-2.61	115.64	123.20
23	b	603	CLA	O2D-CGD-O1D	-2.61	118.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	CHD-C4C-NC	2.61	128.28	124.23
23	C	505	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
23	b	609	CLA	O2A-CGA-CBA	2.61	119.78	111.83
23	b	604	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
23	c	513	CLA	CMB-C2B-C1B	2.61	129.39	125.42
29	A	413[A]	PL9	C45-C44-C46	2.61	119.75	115.23
25	b	618	BCR	C38-C26-C25	-2.60	121.64	124.48
35	H	102	DGD	O1G-C1A-O1A	-2.60	117.11	123.63
23	C	510	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
23	c	503	CLA	CHD-C4C-NC	2.60	128.27	124.23
25	B	619	BCR	C21-C20-C19	-2.60	115.66	123.20
23	b	604	CLA	O2A-CGA-CBA	2.60	119.77	111.83
26	L	102	SQD	O7-S-C6	2.60	110.64	106.76
25	K	101	BCR	C3-C4-C5	-2.60	109.42	114.06
29	A	413[B]	PL9	C35-C34-C36	2.60	119.74	115.23
23	a	404	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
29	A	413[B]	PL9	C30-C29-C31	2.60	119.73	115.23
23	a	405	CLA	CBC-CAC-C3C	-2.59	105.39	112.42
23	C	511	CLA	CHD-C4C-NC	2.59	128.25	124.23
23	B	612	CLA	C2A-C1A-CHA	-2.59	119.37	123.87
29	A	413[B]	PL9	C40-C39-C41	2.59	119.73	115.23
23	b	602	CLA	CMB-C2B-C1B	2.59	129.37	125.42
23	c	514	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
23	A	404	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
23	c	512	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
23	c	505	CLA	O2A-CGA-CBA	2.59	119.73	111.83
29	D	406	PL9	C40-C39-C41	2.59	119.72	115.23
23	a	405	CLA	C3B-C4B-NB	2.59	112.84	110.53
23	B	603	CLA	CMC-C2C-C1C	2.59	129.08	125.03
23	B	609	CLA	CHD-C4C-NC	2.59	128.24	124.23
23	b	601	CLA	CBC-CAC-C3C	-2.59	105.41	112.42
23	C	509	CLA	O2A-CGA-O1A	-2.58	117.16	123.63
23	d	402	CLA	CMC-C2C-C1C	2.58	129.07	125.03
25	C	517	BCR	C11-C10-C9	-2.58	123.65	127.28
40	V	201	HEC	C2A-C1A-NA	-2.58	107.83	110.32
23	B	605	CLA	CMC-C2C-C1C	2.58	129.07	125.03
29	d	405	PL9	C53-C6-C1	2.58	120.57	115.28
23	C	507	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
25	a	408	BCR	C29-C30-C25	2.58	114.19	110.44
23	d	402	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
23	b	613	CLA	CMC-C2C-C1C	2.58	129.06	125.03
23	B	601	CLA	CAA-C2A-C3A	-2.58	106.03	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
31	a	419	LHG	O8-C23-C24	2.58	119.69	111.83
23	C	514	CLA	C4-C3-C5	2.58	119.70	115.23
23	b	608	CLA	C11-C10-C8	-2.58	107.40	115.97
23	b	604	CLA	C11-C12-C13	-2.58	107.40	115.97
23	B	611	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
23	B	611	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
23	b	611	CLA	CAC-C3C-C4C	2.57	128.14	124.79
23	c	503	CLA	C7-C6-C5	-2.57	106.41	113.26
23	b	606	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
25	B	631	BCR	C7-C8-C9	-2.57	122.43	126.23
25	T	101	BCR	C29-C28-C27	-2.57	105.62	111.28
23	B	608	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
23	C	508	CLA	CAA-C2A-C3A	-2.57	106.06	113.00
25	d	404	BCR	C29-C30-C25	2.57	114.17	110.44
23	A	404	CLA	CHB-C4A-NA	2.57	128.11	124.40
23	b	601	CLA	C2A-C1A-CHA	-2.57	119.41	123.87
23	B	601	CLA	CMB-C2B-C1B	2.57	129.33	125.42
23	D	403	CLA	C4C-C3C-C2C	-2.57	103.16	106.89
23	c	505	CLA	C4-C3-C5	2.56	119.68	115.23
23	c	505	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
23	B	611	CLA	OBD-CAD-C3D	-2.56	122.43	128.42
23	b	615	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
23	B	601	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
23	c	508	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
23	c	504	CLA	O2A-CGA-CBA	2.56	119.64	111.83
29	a	414[B]	PL9	C12-C13-C14	-2.56	121.77	127.62
23	C	507	CLA	C1-C2-C3	-2.56	122.01	126.20
29	D	406	PL9	C17-C18-C19	-2.56	121.78	127.62
23	c	515	CLA	CMC-C2C-C1C	2.56	129.03	125.03
34	d	411	LMG	O7-C10-C11	2.55	117.01	111.48
23	B	605	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
23	C	511	CLA	CMC-C2C-C1C	2.55	129.02	125.03
40	V	201	HEC	CMD-C2D-C1D	2.55	129.30	125.42
25	C	517	BCR	C29-C30-C25	2.55	114.14	110.44
26	f	101	SQD	O7-S-C6	2.55	110.56	106.76
24	A	415	PHO	C6-C5-C3	-2.55	107.26	113.47
29	a	414[A]	PL9	C53-C6-C1	2.55	120.50	115.28
23	A	404	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
23	b	608	CLA	C4-C3-C5	2.55	119.65	115.23
23	C	503	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
25	T	101	BCR	C7-C8-C9	-2.54	122.47	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	405	PL9	C35-C34-C36	2.54	119.64	115.23
23	c	507	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
33	C	526	LMT	O5'-C5'-C4'	2.54	114.98	109.72
25	B	617	BCR	C7-C8-C9	-2.54	122.47	126.23
23	C	508	CLA	C4-C3-C5	2.54	119.64	115.23
25	B	631	BCR	C1-C6-C7	2.54	122.54	115.65
23	c	508	CLA	C4-C3-C5	2.54	119.64	115.23
25	b	619	BCR	C21-C20-C19	-2.54	115.84	123.20
23	c	506	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
23	A	407	CLA	C4C-C3C-C2C	-2.54	103.20	106.89
23	A	405	CLA	C3B-C4B-NB	2.54	112.80	110.53
23	d	403	CLA	C3B-C4B-NB	2.54	112.80	110.53
24	a	406	PHO	O2D-CGD-O1D	-2.54	118.91	123.85
23	b	610	CLA	CHC-C1C-C2C	-2.54	119.74	126.95
23	D	403	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
23	D	403	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
23	a	407	CLA	CMB-C2B-C1B	2.53	129.28	125.42
29	d	405	PL9	C20-C19-C21	2.53	119.63	115.23
23	b	608	CLA	C4C-C3C-C2C	-2.53	103.20	106.89
23	D	403	CLA	C4B-C3B-C2B	-2.53	104.15	107.30
23	b	610	CLA	C3B-C4B-NB	2.53	112.79	110.53
29	a	414[A]	PL9	C45-C44-C46	2.53	119.62	115.23
23	B	601	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
25	C	517	BCR	C36-C18-C19	2.53	121.96	118.09
35	c	519	DGD	O1G-C1A-C2A	2.53	119.56	111.83
23	b	603	CLA	CAC-C3C-C4C	2.53	128.08	124.79
29	A	413[A]	PL9	C7-C8-C9	-2.53	122.47	126.83
23	A	403	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
34	a	417	LMG	C7-O1-C1	-2.53	108.37	113.80
23	B	615	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
23	b	602	CLA	C4-C3-C5	2.53	119.61	115.23
23	C	503	CLA	O2A-CGA-CBA	2.52	119.53	111.83
31	d	407	LHG	O8-C23-O10	-2.52	117.31	123.63
23	b	614	CLA	C4-C3-C5	2.52	119.61	115.23
26	L	102	SQD	O8-S-C6	2.52	110.84	105.97
23	b	614	CLA	CMB-C2B-C1B	2.52	129.26	125.42
25	a	408	BCR	C38-C26-C25	-2.52	121.73	124.48
23	c	505	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
23	C	512	CLA	C4-C3-C5	2.52	119.60	115.23
29	d	405	PL9	C36-C34-C33	-2.52	115.52	121.17
38	e	102	HEM	C4D-ND-C1D	2.51	108.18	105.21
23	b	615	CLA	O2A-CGA-O1A	-2.51	117.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	CAC-C3C-C4C	2.51	128.06	124.79
23	C	515	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
23	b	609	CLA	C4-C3-C5	2.51	119.58	115.23
23	D	403	CLA	CMB-C2B-C1B	2.51	129.24	125.42
33	B	627	LMT	C1-O1'-C1'	-2.51	109.40	113.68
25	B	631	BCR	C11-C10-C9	-2.51	123.76	127.28
40	v	202	HEC	CBA-CAA-C2A	-2.51	105.61	112.53
25	A	408	BCR	C15-C14-C13	-2.50	123.77	127.28
34	a	417	LMG	O6-C5-C4	2.50	114.21	109.70
23	b	603	CLA	CMA-C3A-C2A	-2.50	104.30	113.98
23	C	513	CLA	CED-O2D-CGD	2.50	121.59	115.92
23	C	515	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
23	C	509	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
23	b	612	CLA	CHD-C4C-NC	2.50	128.11	124.23
23	c	503	CLA	CMB-C2B-C1B	2.50	129.23	125.42
26	B	620	SQD	O7-S-C6	2.50	110.49	106.76
23	B	614	CLA	OBD-CAD-C3D	-2.50	122.57	128.42
35	H	102	DGD	O4D-C4D-C5D	-2.50	103.18	109.32
23	b	616	CLA	C3B-C4B-NB	2.49	112.76	110.53
23	c	506	CLA	CMC-C2C-C1C	2.49	128.93	125.03
23	c	506	CLA	C4-C3-C5	2.49	119.55	115.23
38	E	102	HEM	CMD-C2D-C1D	2.49	128.92	125.03
23	a	403	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
23	A	404	CLA	C1-C2-C3	-2.49	122.12	126.20
23	c	512	CLA	C11-C10-C8	-2.48	107.71	115.97
23	A	404	CLA	OBD-CAD-C3D	-2.48	122.61	128.42
23	b	602	CLA	C1-O2A-CGA	2.48	122.66	116.65
23	c	508	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
25	c	516	BCR	C8-C7-C6	-2.48	120.38	127.00
23	B	603	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
23	C	512	CLA	C4C-C3C-C2C	-2.48	103.28	106.89
23	A	404	CLA	C2A-C1A-CHA	-2.48	119.57	123.87
25	h	102	BCR	C34-C9-C8	2.48	121.87	118.09
25	B	619	BCR	C3-C4-C5	-2.48	109.64	114.06
23	B	614	CLA	CMB-C2B-C1B	2.48	129.19	125.42
24	a	416	PHO	CMA-C3A-C4A	-2.47	109.28	114.61
35	H	102	DGD	O2G-C1B-C2B	2.47	116.83	111.48
23	d	402	CLA	CAC-C3C-C4C	2.47	128.01	124.79
23	d	403	CLA	C4-C3-C5	2.47	119.52	115.23
29	A	413[B]	PL9	C16-C14-C13	-2.47	115.62	121.17
23	C	513	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
31	A	416	LHG	O7-C7-O9	-2.47	117.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
23	b	606	CLA	C4C-C3C-C2C	-2.47	103.30	106.89
23	B	612	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
25	C	516	BCR	C11-C10-C9	-2.47	123.82	127.28
23	c	514	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
23	C	506	CLA	O2A-CGA-CBA	2.46	119.34	111.83
23	C	515	CLA	C4-C3-C5	2.46	119.50	115.23
33	b	626	LMT	O1'-C1'-C2'	2.46	112.01	108.27
35	c	518	DGD	O6D-C1D-O3G	-2.46	104.23	110.04
23	b	615	CLA	CHD-C4C-NC	2.46	128.05	124.23
23	C	515	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
23	D	403	CLA	CMC-C2C-C1C	2.46	128.88	125.03
23	B	602	CLA	CED-O2D-CGD	2.46	121.50	115.92
29	d	405	PL9	C27-C28-C29	-2.46	121.99	127.62
23	b	607	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
23	c	515	CLA	CHD-C4C-NC	2.46	128.04	124.23
23	C	506	CLA	C4-C3-C5	2.46	119.50	115.23
25	D	405	BCR	C16-C17-C18	-2.46	123.83	127.28
23	c	510	CLA	CMB-C2B-C1B	2.46	129.16	125.42
25	K	101	BCR	C36-C18-C19	2.46	121.84	118.09
23	d	402	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
25	D	405	BCR	C37-C22-C21	-2.46	118.84	122.82
25	h	102	BCR	C38-C26-C25	-2.46	121.81	124.48
23	c	511	CLA	CAA-C2A-C3A	-2.45	106.36	113.00
25	c	517	BCR	C37-C22-C23	2.45	121.84	118.09
23	B	606	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
23	b	609	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
25	B	617	BCR	C29-C30-C25	2.45	114.00	110.44
40	v	202	HEC	C2A-C1A-NA	-2.45	107.96	110.32
23	A	403	CLA	CMA-C3A-C2A	-2.45	104.51	113.98
23	a	404	CLA	CAA-CBA-CGA	2.45	120.17	113.21
38	E	102	HEM	CHD-C1D-ND	2.45	127.06	124.42
23	D	404	CLA	CMC-C2C-C1C	2.45	128.86	125.03
25	C	516	BCR	C20-C21-C22	-2.45	123.85	127.28
25	C	516	BCR	C37-C22-C23	2.45	121.82	118.09
34	z	101	LMG	C8-O7-C10	-2.44	111.94	117.80
26	a	409	SQD	O9-S-C6	2.44	110.40	106.76
23	c	512	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
23	b	601	CLA	CMB-C2B-C1B	2.44	129.14	125.42
34	Z	101	LMG	C1-O6-C5	2.44	118.49	113.72
33	F	101	LMT	C4B-C3B-C2B	-2.44	106.55	110.83
23	C	515	CLA	CAC-C3C-C4C	2.44	127.96	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
23	b	613	CLA	CMB-C2B-C1B	2.44	129.13	125.42
23	A	407	CLA	CAC-C3C-C4C	2.44	127.96	124.79
23	C	505	CLA	CAC-C3C-C4C	2.44	127.96	124.79
35	c	518	DGD	C2G-O2G-C1B	-2.43	111.97	117.80
23	a	405	CLA	C2A-C1A-CHA	-2.43	119.64	123.87
23	a	405	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
35	h	103	DGD	O1G-C1A-O1A	-2.43	117.54	123.63
34	Z	101	LMG	C9-C8-C7	-2.43	106.11	111.78
23	C	506	CLA	OBD-CAD-C3D	-2.43	122.73	128.42
23	b	613	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	C	507	CLA	CHD-C4C-NC	2.43	128.00	124.23
23	b	601	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
25	B	617	BCR	C16-C17-C18	-2.43	123.88	127.28
33	B	627	LMT	O1B-C4'-C3'	2.43	113.40	107.23
23	B	611	CLA	C4-C3-C5	2.43	119.44	115.23
23	B	602	CLA	CHB-C1B-C2B	-2.43	120.39	127.43
31	d	407	LHG	O7-C7-C8	2.42	116.72	111.48
23	b	602	CLA	CMA-C3A-C2A	-2.42	104.61	113.98
23	C	504	CLA	CBC-CAC-C3C	-2.42	105.85	112.42
38	E	102	HEM	CBD-CAD-C3D	-2.42	105.84	112.53
23	a	407	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
23	c	509	CLA	C4C-C3C-C2C	-2.42	103.37	106.89
23	b	601	CLA	C1-O2A-CGA	2.42	122.50	116.65
23	c	506	CLA	O1D-CGD-CBD	-2.41	119.75	124.52
23	a	405	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
23	c	514	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
25	B	619	BCR	C38-C26-C25	-2.41	121.85	124.48
32	b	621	HTG	C1'-S1-C1	2.41	105.66	100.45
23	a	407	CLA	CAC-C3C-C4C	2.41	127.93	124.79
23	B	610	CLA	CMA-C3A-C4A	-2.41	105.29	111.77
23	C	508	CLA	CHD-C4C-NC	2.41	127.97	124.23
23	B	606	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
31	D	407	LHG	O8-C23-O10	-2.41	117.60	123.63
23	C	508	CLA	CGD-CBD-CAD	-2.41	103.05	110.85
29	D	406	PL9	C15-C14-C16	2.41	119.41	115.23
23	b	605	CLA	C3B-C4B-NB	2.41	112.68	110.53
25	a	408	BCR	C10-C11-C12	-2.41	116.23	123.20
23	b	607	CLA	C4-C3-C5	2.41	119.41	115.23
29	a	414[B]	PL9	C30-C29-C31	2.41	119.41	115.23
25	B	631	BCR	C36-C18-C19	2.40	121.76	118.09
23	b	616	CLA	CMB-C2B-C1B	2.40	129.08	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
31	D	408	LHG	O8-C23-O10	-2.40	117.62	123.63
24	A	406	PHO	O2A-CGA-CBA	2.40	119.15	111.83
23	b	604	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
23	c	509	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
23	c	511	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
23	B	602	CLA	C1-C2-C3	-2.39	122.28	126.20
31	d	408	LHG	C5-O7-C7	-2.39	112.08	117.80
23	a	404	CLA	C4C-C3C-C2C	-2.39	103.41	106.89
25	T	101	BCR	C16-C15-C14	2.39	128.41	123.52
29	d	405	PL9	C51-C49-C50	2.39	120.08	114.59
23	B	616	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
23	B	605	CLA	C4B-C3B-C2B	-2.39	104.34	107.30
23	b	603	CLA	CMC-C2C-C1C	2.39	128.76	125.03
23	B	606	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
33	M	103	LMT	O1B-C1B-C2B	2.38	113.95	108.09
23	A	404	CLA	C4A-NA-C1A	-2.38	105.59	106.68
29	D	406	PL9	C20-C19-C21	2.38	119.36	115.23
23	B	616	CLA	CHC-C1C-C2C	-2.38	120.18	126.95
31	L	101	LHG	O4-P-O5	2.38	123.52	112.44
23	B	610	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
25	H	101	BCR	C29-C30-C25	2.38	113.89	110.44
23	a	405	CLA	C4-C3-C5	2.38	119.36	115.23
23	B	605	CLA	C7-C6-C5	-2.38	106.93	113.26
23	C	509	CLA	C11-C12-C13	-2.37	108.07	115.97
25	c	517	BCR	C36-C18-C19	2.37	121.72	118.09
23	c	507	CLA	CAC-C3C-C4C	2.37	127.88	124.79
23	b	606	CLA	CMB-C2B-C1B	2.37	129.03	125.42
23	d	402	CLA	CHD-C4C-NC	2.37	127.91	124.23
23	c	509	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
23	c	514	CLA	CHB-C4A-NA	2.37	127.82	124.40
31	D	407	LHG	O7-C7-C8	2.37	116.60	111.48
23	c	507	CLA	C4-C3-C5	2.37	119.33	115.23
23	c	513	CLA	C1-O2A-CGA	2.36	122.37	116.65
32	B	621	HTG	C1-O5-C5	2.36	116.80	112.56
23	C	512	CLA	CAC-C3C-C4C	2.36	127.86	124.79
23	b	613	CLA	CHD-C4C-NC	2.36	127.89	124.23
25	T	101	BCR	C1-C6-C7	2.36	122.06	115.65
25	k	102	BCR	C16-C17-C18	-2.36	123.97	127.28
25	Y	101	BCR	C10-C11-C12	-2.36	116.36	123.20
23	C	510	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
23	d	403	CLA	CHB-C1B-C2B	-2.36	120.58	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	O2A-CGA-CBA	2.36	119.03	111.83
23	c	506	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
23	C	504	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
25	b	619	BCR	C8-C9-C10	2.36	122.72	119.01
23	c	507	CLA	C3B-C4B-NB	2.36	112.63	110.53
23	b	608	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
23	C	509	CLA	CAC-C3C-C4C	2.36	127.86	124.79
25	K	101	BCR	C33-C5-C6	-2.35	121.92	124.48
23	C	507	CLA	O2A-CGA-CBA	2.35	119.01	111.83
38	E	102	HEM	CHA-C1A-NA	2.35	128.13	123.86
34	c	521	LMG	O8-C28-O10	-2.35	117.74	123.63
34	c	522	LMG	O8-C28-O10	-2.35	117.75	123.63
23	C	504	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
33	m	103	LMT	O5B-C5B-C6B	2.35	112.26	106.44
23	c	505	CLA	CHD-C4C-NC	2.35	127.87	124.23
23	b	609	CLA	CAC-C3C-C4C	2.35	127.85	124.79
23	c	507	CLA	C1-C2-C3	-2.35	122.35	126.20
25	k	102	BCR	C7-C8-C9	-2.35	122.76	126.23
34	a	417	LMG	C8-O7-C10	-2.35	112.18	117.80
23	A	403	CLA	CHB-C4A-NA	2.35	127.79	124.40
23	c	512	CLA	CMB-C2B-C1B	2.35	128.99	125.42
25	d	404	BCR	C16-C15-C14	-2.34	118.72	123.52
23	C	506	CLA	CED-O2D-CGD	2.34	121.23	115.92
23	C	509	CLA	CMB-C2B-C1B	2.34	128.99	125.42
25	k	101	BCR	C7-C8-C9	-2.34	122.77	126.23
33	b	626	LMT	O5'-C5'-C4'	2.34	114.56	109.72
23	c	507	CLA	CHD-C4C-NC	2.34	127.86	124.23
35	C	518	DGD	C2G-O2G-C1B	-2.34	112.20	117.80
23	b	603	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
29	A	413[A]	PL9	C47-C48-C49	-2.34	119.86	127.64
23	C	514	CLA	CAC-C3C-C4C	2.33	127.83	124.79
23	c	515	CLA	CMB-C2B-C1B	2.33	128.97	125.42
25	b	619	BCR	C16-C17-C18	-2.33	124.01	127.28
23	C	514	CLA	CBC-CAC-C3C	-2.33	106.10	112.42
37	d	401[A]	BCT	O2-C-O1	2.33	125.64	119.68
25	k	101	BCR	C10-C11-C12	-2.33	116.45	123.20
24	a	416	PHO	CMB-C2B-C3B	2.33	129.34	124.68
23	c	503	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
26	a	409	SQD	C45-O47-C7	-2.33	112.23	117.80
23	C	510	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	D	405	BCR	C11-C10-C9	-2.32	124.02	127.28
23	c	504	CLA	O2A-CGA-O1A	-2.32	117.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
26	f	101	SQD	O47-C7-O49	-2.32	118.28	123.70
23	B	615	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	b	608	CLA	CMA-C3A-C4A	-2.32	105.53	111.77
23	a	405	CLA	CHC-C1C-C2C	-2.32	120.35	126.95
23	b	608	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
23	C	514	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	c	514	CLA	C3B-C4B-NB	2.32	112.60	110.53
23	B	616	CLA	CAC-C3C-C4C	2.32	127.81	124.79
23	b	602	CLA	CHD-C4C-NC	2.32	127.83	124.23
35	C	519	DGD	C1E-O6E-C5E	-2.32	109.19	113.72
23	B	608	CLA	C1-C2-C3	-2.32	122.40	126.20
23	A	403	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
26	A	409	SQD	O9-S-O7	-2.32	106.29	113.82
23	B	616	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	c	503	CLA	C1-C2-C3	-2.32	122.40	126.20
23	b	609	CLA	CMC-C2C-C1C	2.31	128.65	125.03
29	a	414[A]	PL9	C30-C29-C31	2.31	119.24	115.23
23	A	403	CLA	C1-C2-C3	-2.31	122.41	126.20
29	d	405	PL9	C47-C48-C49	-2.31	119.94	127.64
23	C	514	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
25	b	618	BCR	C2-C1-C6	2.31	113.79	110.44
32	B	621	HTG	O2-C2-C3	-2.31	104.93	110.38
29	D	406	PL9	C25-C24-C23	-2.31	117.70	123.63
24	A	406	PHO	CMC-C2C-C1C	2.31	128.89	124.73
38	E	102	HEM	C4C-NC-C1C	2.31	109.58	105.82
23	D	404	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
23	C	507	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
23	b	616	CLA	C4-C3-C5	2.30	119.23	115.23
23	a	403	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
33	m	103	LMT	O6'-C6'-C5'	-2.30	103.50	111.33
33	e	101	LMT	O1'-C1'-C2'	2.30	111.77	108.27
25	Y	101	BCR	C28-C27-C26	-2.30	109.96	114.06
23	B	609	CLA	C4-C3-C5	2.30	119.22	115.23
35	c	518	DGD	O1G-C1A-C2A	2.30	118.84	111.83
23	B	610	CLA	CHD-C4C-NC	2.30	127.79	124.23
23	c	514	CLA	C4B-C3B-C2B	-2.30	104.45	107.30
38	e	102	HEM	C4C-NC-C1C	2.29	109.56	105.82
25	B	618	BCR	C10-C11-C12	-2.29	116.55	123.20
23	c	508	CLA	CAC-C3C-C4C	2.29	127.77	124.79
25	T	101	BCR	C34-C9-C8	2.29	121.59	118.09
31	b	628	LHG	O8-C23-O10	-2.29	117.90	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C4-C3-C5	2.29	119.20	115.23
23	c	505	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
23	C	504	CLA	C3B-C4B-NB	2.29	112.57	110.53
23	c	504	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
32	b	624	HTG	C4-C3-C2	-2.29	106.81	110.83
35	c	520	DGD	O2G-C1B-O1B	-2.29	118.36	123.70
23	C	511	CLA	C11-C12-C13	-2.29	108.37	115.97
23	B	605	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
31	L	101	LHG	O8-C23-O10	-2.28	117.92	123.63
23	c	506	CLA	O2A-CGA-CBA	2.28	118.80	111.83
23	b	616	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
32	h	101	HTG	C6-C5-C4	-2.28	107.42	113.02
25	B	618	BCR	C7-C8-C9	-2.28	122.86	126.23
33	B	629	LMT	C3'-C4'-C5'	-2.28	105.88	110.93
29	D	406	PL9	C42-C41-C39	-2.28	105.63	113.19
23	B	610	CLA	CMA-C3A-C2A	-2.28	105.17	113.98
23	c	509	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
23	B	608	CLA	C2A-C1A-CHA	-2.28	119.92	123.87
23	c	507	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
33	a	418	LMT	O5B-C5B-C4B	2.28	113.80	109.70
23	D	404	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
26	A	411	SQD	O6-C1-C2	2.28	111.73	108.27
26	B	620	SQD	C1-C2-C3	-2.28	105.22	110.01
29	a	414[A]	PL9	C47-C48-C49	-2.28	120.06	127.64
26	a	409	SQD	O6-C44-C45	-2.27	105.29	110.82
23	c	512	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
24	a	416	PHO	CBA-CAA-C2A	-2.27	107.08	113.78
23	B	614	CLA	CBC-CAC-C3C	-2.27	106.26	112.42
23	B	607	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
23	C	511	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
23	b	604	CLA	CAC-C3C-C4C	2.27	127.74	124.79
25	B	618	BCR	C15-C16-C17	-2.27	118.88	123.52
25	a	408	BCR	C8-C7-C6	-2.27	120.94	127.00
34	M	101	LMG	C9-C8-C7	-2.27	106.50	111.78
23	d	402	CLA	C6-C5-C3	2.27	118.99	113.47
23	c	515	CLA	C4-C3-C5	2.26	119.16	115.23
23	A	404	CLA	CMC-C2C-C1C	2.26	128.57	125.03
34	m	101	LMG	O8-C28-O10	-2.26	117.97	123.63
23	C	503	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
25	a	408	BCR	C15-C16-C17	-2.26	118.89	123.52
34	C	502	LMG	O8-C28-C29	2.26	118.73	111.83
23	a	405	CLA	O2A-CGA-CBA	2.26	118.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	413	SQD	O48-C23-O10	-2.26	117.98	123.63
25	T	101	BCR	C7-C6-C5	-2.26	116.36	121.56
25	A	408	BCR	C34-C9-C8	2.26	121.53	118.09
25	D	405	BCR	C30-C25-C24	2.26	121.77	115.65
23	b	602	CLA	O2A-CGA-CBA	2.26	118.71	111.83
23	b	606	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
38	E	102	HEM	O2D-CGD-CBD	2.25	121.11	114.00
25	B	617	BCR	C38-C26-C25	-2.25	122.03	124.48
23	b	612	CLA	CMB-C2B-C3B	2.25	131.84	126.55
26	D	413	SQD	O47-C7-O49	-2.25	118.45	123.70
23	B	615	CLA	CAC-C3C-C4C	2.24	127.71	124.79
23	c	506	CLA	C1-C2-C3	-2.24	122.52	126.20
26	D	413	SQD	O7-S-C6	2.24	110.10	106.76
23	b	611	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
26	a	411	SQD	O5-C5-C4	2.24	113.74	109.70
35	C	518	DGD	O6E-C5E-C4E	2.24	113.73	109.70
23	b	615	CLA	C11-C12-C13	-2.24	108.52	115.97
24	a	416	PHO	CMC-C2C-C1C	2.24	128.76	124.73
32	h	101	HTG	C1-C2-C3	-2.24	106.17	110.55
23	C	513	CLA	C1-O2A-CGA	2.24	122.07	116.65
23	B	607	CLA	O2A-CGA-CBA	2.24	118.66	111.83
23	b	605	CLA	O2A-CGA-CBA	2.24	118.65	111.83
29	a	414[A]	PL9	C47-C46-C44	-2.24	105.78	113.19
29	D	406	PL9	C27-C28-C29	-2.24	122.51	127.62
25	C	517	BCR	C21-C20-C19	-2.23	116.73	123.20
29	d	405	PL9	C15-C14-C16	2.23	119.11	115.23
23	C	504	CLA	CED-O2D-CGD	2.23	120.98	115.92
23	b	609	CLA	CHB-C1B-C2B	-2.23	120.94	127.43
23	B	613	CLA	CHD-C4C-NC	2.23	127.69	124.23
23	B	608	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	B	620	SQD	O47-C7-O49	-2.23	118.49	123.70
23	A	404	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
23	c	513	CLA	C11-C12-C13	-2.23	108.55	115.97
26	A	411	SQD	O48-C23-O10	-2.23	118.05	123.63
23	C	504	CLA	CMC-C2C-C1C	2.23	128.52	125.03
23	c	512	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
23	c	504	CLA	CAC-C3C-C4C	2.23	127.69	124.79
31	L	101	LHG	O7-C7-O9	-2.23	118.50	123.70
23	b	609	CLA	C3B-C4B-NB	2.23	112.52	110.53
24	A	415	PHO	CMB-C2B-C3B	2.23	129.13	124.68
25	Y	101	BCR	C15-C16-C17	-2.23	118.97	123.52
29	D	406	PL9	C32-C33-C34	-2.22	122.53	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
23	C	514	CLA	CMC-C2C-C1C	2.22	128.51	125.03
33	B	627	LMT	O1B-C4'-C5'	-2.22	103.64	109.48
33	B	630	LMT	C3'-C4'-C5'	-2.22	106.00	110.93
35	H	102	DGD	O6E-C5E-C6E	2.22	111.94	106.44
23	b	610	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
35	H	102	DGD	C3E-C4E-C5E	-2.22	106.21	110.23
24	A	406	PHO	C4-C3-C5	2.22	119.08	115.23
23	d	403	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
34	c	522	LMG	C1-O6-C5	2.22	118.05	113.72
25	d	404	BCR	C23-C24-C25	-2.22	121.07	127.00
25	C	517	BCR	C39-C30-C25	-2.22	106.77	110.24
35	h	103	DGD	O3G-C1D-C2D	2.22	111.64	108.27
34	a	417	LMG	O7-C10-O9	-2.22	118.52	123.70
23	c	504	CLA	C4-C3-C5	2.21	119.07	115.23
23	A	403	CLA	CHD-C4C-NC	2.21	127.67	124.23
23	c	515	CLA	CED-O2D-CGD	2.21	120.93	115.92
23	B	601	CLA	C1-O2A-CGA	2.21	122.00	116.65
23	C	512	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
40	V	201	HEC	CAD-CBD-CGD	-2.21	107.80	113.67
23	c	506	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
23	B	611	CLA	C1-O2A-CGA	2.21	122.00	116.65
23	C	506	CLA	C1-O2A-CGA	2.21	122.00	116.65
23	D	404	CLA	C1-C2-C3	-2.21	122.58	126.20
25	b	617	BCR	C24-C23-C22	-2.21	122.97	126.23
23	c	515	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
23	a	403	CLA	CBC-CAC-C3C	-2.21	106.44	112.42
38	E	102	HEM	C4B-C3B-C2B	-2.20	105.25	107.28
23	C	506	CLA	CHD-C4C-NC	2.20	127.65	124.23
26	f	101	SQD	O48-C23-O10	-2.20	118.12	123.63
33	a	412	LMT	O1B-C1B-C2B	2.20	113.51	108.09
29	A	413[A]	PL9	C16-C14-C13	-2.20	116.22	121.17
31	d	408	LHG	O7-C7-O9	-2.20	118.56	123.70
23	d	402	CLA	CMB-C2B-C1B	2.20	128.77	125.42
23	b	605	CLA	CMC-C2C-C1C	2.20	128.47	125.03
29	A	413[B]	PL9	C37-C36-C34	-2.20	105.90	113.19
23	D	403	CLA	C4-C3-C5	2.20	119.04	115.23
23	B	608	CLA	C11-C12-C13	-2.20	108.66	115.97
34	C	522	LMG	O8-C28-O10	-2.20	118.14	123.63
31	D	408	LHG	C6-C5-C4	-2.20	106.67	111.78
33	m	103	LMT	C1-O1'-C1'	-2.19	109.93	113.68
23	B	614	CLA	C4B-C3B-C2B	-2.19	104.57	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	603	CLA	C1-C2-C3	-2.19	122.60	126.20
23	b	610	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
23	b	609	CLA	C16-C15-C13	-2.19	108.68	115.97
23	B	601	CLA	CMA-C3A-C2A	-2.19	105.51	113.98
25	B	631	BCR	C7-C6-C5	-2.19	116.51	121.56
33	F	101	LMT	O5'-C5'-C4'	2.19	114.25	109.72
34	C	522	LMG	C9-C8-C7	-2.19	106.69	111.78
35	c	519	DGD	O1G-C1A-O1A	-2.19	118.16	123.63
23	d	402	CLA	CMA-C3A-C2A	-2.19	105.53	113.98
23	c	505	CLA	OBD-CAD-C3D	-2.19	123.31	128.42
23	b	613	CLA	CED-O2D-CGD	2.19	120.87	115.92
23	B	610	CLA	CMC-C2C-C1C	2.18	128.45	125.03
23	b	607	CLA	C1-C2-C3	-2.18	122.62	126.20
23	B	615	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
23	D	403	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	C	508	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
23	B	616	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
34	c	521	LMG	C8-O7-C10	-2.18	112.58	117.80
29	A	413[B]	PL9	C51-C49-C50	2.18	119.60	114.59
23	C	507	CLA	CHA-C1A-NA	-2.18	121.46	126.39
23	c	508	CLA	C2A-C1A-CHA	-2.18	120.09	123.87
23	A	404	CLA	CAA-CBA-CGA	2.18	119.38	113.21
23	c	514	CLA	CHA-C1A-NA	-2.17	121.47	126.39
33	a	418	LMT	C1B-O1B-C4'	-2.17	112.83	117.98
25	B	631	BCR	C35-C13-C12	2.17	121.40	118.09
23	b	614	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
25	b	619	BCR	C29-C30-C25	2.17	113.59	110.44
23	b	605	CLA	C6-C7-C8	-2.17	108.75	115.97
23	b	615	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
34	D	412	LMG	C7-O1-C1	-2.17	109.15	113.80
25	B	631	BCR	C29-C30-C25	2.17	113.58	110.44
25	b	617	BCR	C39-C30-C25	-2.16	106.85	110.24
29	d	405	PL9	C25-C24-C26	2.16	118.98	115.23
25	c	517	BCR	C28-C27-C26	-2.16	110.20	114.06
23	b	611	CLA	C2A-C1A-CHA	-2.16	120.11	123.87
25	C	516	BCR	C3-C4-C5	-2.16	110.20	114.06
32	b	624	HTG	C6-C5-C4	-2.16	107.71	113.02
23	a	403	CLA	CMA-C3A-C2A	-2.16	105.62	113.98
23	D	403	CLA	CHD-C4C-NC	2.16	127.58	124.23
23	C	510	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
34	M	101	LMG	C9-O8-C28	2.16	125.02	117.12
23	b	607	CLA	CAA-CBA-CGA	2.16	119.34	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
23	b	613	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
25	H	101	BCR	C16-C15-C14	-2.16	119.10	123.52
25	k	102	BCR	C40-C30-C25	-2.16	106.86	110.24
38	e	102	HEM	O2D-CGD-CBD	2.16	120.82	114.00
25	Y	101	BCR	C21-C20-C19	-2.16	116.95	123.20
25	c	517	BCR	C29-C30-C25	2.16	113.57	110.44
23	B	614	CLA	CHB-C4A-NA	2.16	127.51	124.40
23	b	609	CLA	C2A-C1A-CHA	-2.16	120.13	123.87
23	B	605	CLA	C3B-C4B-NB	2.15	112.45	110.53
25	Y	101	BCR	C16-C15-C14	-2.15	119.11	123.52
23	c	513	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
29	A	413[A]	PL9	C35-C34-C36	2.15	118.96	115.23
23	B	602	CLA	C4-C3-C5	2.15	118.96	115.23
33	M	102	LMT	O5B-C5B-C6B	2.15	111.77	106.44
38	E	102	HEM	O2A-CGA-CBA	2.15	120.79	114.00
25	c	517	BCR	C16-C17-C18	-2.15	124.27	127.28
23	d	402	CLA	C4-C3-C2	-2.15	118.11	123.63
32	b	621	HTG	O2-C2-C3	-2.15	105.32	110.38
23	a	403	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
27	C	524	GOL	C3-C2-C1	-2.15	103.93	111.80
29	a	414[B]	PL9	C51-C49-C50	2.14	119.52	114.59
23	c	511	CLA	CHD-C4C-NC	2.14	127.56	124.23
23	B	610	CLA	CHB-C4A-NA	2.14	127.49	124.40
34	a	417	LMG	C3-C4-C5	2.14	114.12	110.23
23	b	607	CLA	CAC-C3C-C4C	2.14	127.58	124.79
23	b	610	CLA	CAC-C3C-C4C	2.14	127.58	124.79
25	B	618	BCR	C30-C25-C26	-2.14	119.71	122.64
25	k	101	BCR	C20-C21-C22	-2.14	124.28	127.28
23	B	604	CLA	C11-C10-C8	-2.14	108.85	115.97
23	c	510	CLA	CAC-C3C-C2C	2.14	131.49	127.56
23	B	615	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
23	b	606	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
23	C	509	CLA	OBD-CAD-C3D	-2.14	123.42	128.42
23	C	503	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
29	a	414[B]	PL9	C47-C48-C49	-2.14	120.52	127.64
23	c	505	CLA	C11-C12-C13	-2.13	108.87	115.97
29	A	413[A]	PL9	C51-C49-C50	2.13	119.50	114.59
23	c	505	CLA	C1-C2-C3	-2.13	122.70	126.20
23	b	609	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
32	h	101	HTG	C3-C4-C5	2.13	114.09	110.23
35	c	520	DGD	O3G-C1D-C2D	-2.13	105.04	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C3B-C4B-NB	2.13	112.43	110.53
23	b	616	CLA	CHA-C1A-NA	-2.13	121.57	126.39
23	a	404	CLA	C4-C3-C5	2.13	118.92	115.23
29	a	414[B]	PL9	C40-C39-C41	2.13	118.92	115.23
23	B	609	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
23	B	606	CLA	C2A-C1A-CHA	-2.12	120.18	123.87
23	B	613	CLA	CED-O2D-CGD	2.12	120.73	115.92
23	b	601	CLA	CAC-C3C-C2C	2.12	131.46	127.56
23	A	407	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
29	D	406	PL9	C2-C1-C6	2.12	121.52	119.00
35	C	520	DGD	O2G-C1B-O1B	-2.12	118.75	123.70
25	h	102	BCR	C29-C30-C25	2.12	113.52	110.44
23	a	405	CLA	C1-O2A-CGA	2.12	121.78	116.65
25	Y	101	BCR	C11-C10-C9	-2.12	124.31	127.28
25	D	405	BCR	C40-C30-C25	-2.12	106.92	110.24
33	B	627	LMT	C3B-C4B-C5B	2.12	114.07	110.23
35	c	520	DGD	O3G-C3G-C2G	-2.12	105.67	110.82
24	a	406	PHO	CBA-CAA-C2A	-2.12	107.54	113.78
23	A	404	CLA	CMA-C3A-C4A	-2.12	106.09	111.77
25	b	617	BCR	C36-C18-C19	2.12	121.32	118.09
33	M	102	LMT	O1B-C1B-C2B	2.11	113.29	108.09
23	C	509	CLA	C6-C7-C8	-2.11	108.94	115.97
34	D	412	LMG	O7-C10-O9	-2.11	118.77	123.70
23	C	507	CLA	C4-C3-C5	2.11	118.89	115.23
24	A	415	PHO	OBD-CAD-C3D	-2.11	124.60	127.89
23	b	606	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
34	C	522	LMG	O6-C1-C2	-2.11	106.04	110.37
25	A	408	BCR	C33-C5-C6	-2.11	122.19	124.48
23	b	605	CLA	C1-C2-C3	-2.11	122.75	126.20
26	a	409	SQD	O48-C23-O10	-2.10	118.36	123.63
23	C	508	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
23	B	602	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
23	C	513	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	k	101	BCR	C16-C15-C14	-2.10	119.22	123.52
23	B	604	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
23	D	403	CLA	CMA-C3A-C2A	-2.10	105.87	113.98
23	B	612	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
23	b	607	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
29	d	405	PL9	C7-C8-C9	-2.10	123.22	126.83
23	C	504	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
26	a	411	SQD	C1-O5-C5	2.09	117.81	113.72
23	D	404	CLA	C4-C3-C5	2.09	118.86	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	CHA-C1A-NA	-2.09	121.65	126.39
29	A	413[B]	PL9	C47-C48-C49	-2.09	120.67	127.64
23	c	515	CLA	C1-O2A-CGA	2.09	121.71	116.65
25	h	102	BCR	C36-C18-C17	-2.09	119.43	122.82
23	b	616	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
23	D	404	CLA	CMA-C3A-C2A	-2.09	105.90	113.98
23	D	404	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
23	B	608	CLA	CAC-C3C-C4C	2.09	127.51	124.79
25	c	517	BCR	C24-C23-C22	-2.09	123.15	126.23
29	a	414[A]	PL9	C40-C39-C41	2.09	118.85	115.23
23	a	404	CLA	O2A-CGA-CBA	2.09	118.20	111.83
23	b	615	CLA	C2A-C1A-CHA	-2.09	120.25	123.87
23	b	602	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
25	Y	101	BCR	C1-C6-C7	2.08	121.30	115.65
23	B	613	CLA	C2A-C1A-CHA	-2.08	120.25	123.87
25	A	408	BCR	C10-C11-C12	-2.08	117.17	123.20
23	b	611	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
32	b	621	HTG	O2-C2-C1	2.08	113.99	110.30
23	B	606	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
35	C	520	DGD	O1G-C1A-O1A	-2.08	118.43	123.63
23	B	609	CLA	CAC-C3C-C4C	2.08	127.49	124.79
23	b	607	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
23	B	616	CLA	C4-C3-C5	2.08	118.83	115.23
23	b	613	CLA	C2A-C1A-CHA	-2.07	120.27	123.87
23	b	605	CLA	C5-C3-C2	-2.07	116.51	121.17
23	C	503	CLA	C7-C6-C5	-2.07	107.73	113.26
25	B	618	BCR	C31-C1-C6	-2.07	106.99	110.24
23	c	507	CLA	CMC-C2C-C1C	2.07	128.27	125.03
23	b	601	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
25	H	101	BCR	C7-C6-C5	2.07	126.33	121.56
23	A	403	CLA	CAA-CBA-CGA	-2.07	107.33	113.21
27	a	410	GOL	C3-C2-C1	-2.07	104.20	111.80
25	T	101	BCR	C2-C1-C6	2.07	113.44	110.44
23	b	603	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
23	c	514	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
23	b	616	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
24	A	406	PHO	CBA-CAA-C2A	-2.07	107.69	113.78
23	A	403	CLA	CMB-C2B-C3B	2.07	131.41	126.55
23	C	506	CLA	CAC-C3C-C4C	2.07	127.48	124.79
24	a	416	PHO	O2A-CGA-CBA	2.07	118.13	111.83
23	B	611	CLA	CHB-C4A-NA	2.07	127.38	124.40
33	M	102	LMT	O1'-C1'-C2'	2.07	111.41	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C6-C7-C8	-2.07	109.10	115.97
35	C	519	DGD	O3G-C1D-C2D	2.06	111.41	108.27
23	b	604	CLA	C6-C7-C8	-2.06	109.11	115.97
26	a	409	SQD	O47-C7-O49	-2.06	118.88	123.70
33	a	412	LMT	C2'-C3'-C4'	2.06	114.36	109.68
23	C	508	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
23	C	511	CLA	CMB-C2B-C1B	2.06	128.56	125.42
32	b	622	HTG	C1-O5-C5	2.06	116.26	112.56
29	A	413[A]	PL9	C37-C36-C34	-2.06	106.35	113.19
27	b	623	GOL	C3-C2-C1	-2.06	104.24	111.80
25	D	405	BCR	C15-C14-C13	-2.06	124.39	127.28
25	h	102	BCR	C20-C21-C22	-2.06	124.39	127.28
23	B	615	CLA	O2A-CGA-CBA	2.06	118.12	111.83
25	b	618	BCR	C11-C10-C9	-2.06	124.39	127.28
23	b	616	CLA	CAC-C3C-C4C	2.06	127.47	124.79
23	c	510	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	c	514	CLA	CBA-CAA-C2A	-2.06	107.67	113.79
23	C	514	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	b	608	CLA	C11-C12-C13	-2.06	109.13	115.97
32	b	624	HTG	C1-O5-C5	2.06	116.25	112.56
23	a	404	CLA	CHB-C4A-NA	2.05	127.36	124.40
23	b	605	CLA	CAC-C3C-C4C	2.05	127.46	124.79
33	B	630	LMT	O1'-C1'-C2'	2.05	111.39	108.27
35	c	518	DGD	O3G-C3G-C2G	-2.05	105.82	110.82
27	c	527	GOL	C3-C2-C1	-2.05	104.27	111.80
25	k	102	BCR	C1-C6-C7	2.05	121.22	115.65
23	A	405	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
26	B	620	SQD	O9-S-C6	2.05	109.82	106.76
24	A	415	PHO	O2A-CGA-O1A	-2.05	118.50	123.63
38	E	102	HEM	C4D-ND-C1D	2.05	107.64	105.21
33	e	101	LMT	C1B-C2B-C3B	2.05	114.32	110.01
25	T	101	BCR	C29-C30-C25	2.05	113.41	110.44
26	L	102	SQD	O47-C7-O49	-2.05	118.92	123.70
35	c	520	DGD	O1G-C1A-O1A	-2.05	118.51	123.63
23	B	607	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
25	b	618	BCR	C21-C20-C19	-2.05	117.27	123.20
23	b	606	CLA	CAC-C3C-C4C	2.05	127.45	124.79
23	b	604	CLA	C4-C3-C5	2.04	118.78	115.23
33	e	101	LMT	C4B-C3B-C2B	2.04	114.42	110.83
23	B	602	CLA	CMA-C3A-C2A	-2.04	106.09	113.98
23	B	616	CLA	C1-O2A-CGA	2.04	121.59	116.65
23	C	506	CLA	C2A-C1A-CHA	-2.04	120.32	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	619	BCR	C33-C5-C6	-2.04	122.26	124.48
25	a	408	BCR	C7-C8-C9	-2.04	123.22	126.23
23	C	514	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
23	c	512	CLA	CHB-C4A-NA	2.04	127.34	124.40
33	F	101	LMT	O5B-C5B-C4B	2.04	113.37	109.70
23	B	603	CLA	CMB-C2B-C1B	2.03	128.52	125.42
23	B	606	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
23	B	602	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
23	b	608	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	d	402	CLA	C2A-C1A-CHA	-2.03	120.35	123.87
23	C	506	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	c	509	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
23	B	615	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
38	E	102	HEM	C4C-CHD-C1D	-2.03	121.71	126.02
23	B	616	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
23	A	405	CLA	CMA-C3A-C4A	-2.02	106.33	111.77
23	b	610	CLA	C4-C3-C2	-2.02	118.43	123.63
25	k	102	BCR	C28-C27-C26	-2.02	110.45	114.06
26	A	411	SQD	O8-S-C6	2.02	109.88	105.97
25	b	617	BCR	C20-C21-C22	-2.02	124.44	127.28
27	B	623	GOL	C3-C2-C1	-2.02	104.39	111.80
23	c	511	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
23	c	507	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
23	c	510	CLA	CHB-C4A-NA	2.02	127.31	124.40
27	b	627	GOL	C3-C2-C1	-2.02	104.40	111.80
23	a	407	CLA	C1-O2A-CGA	2.02	121.53	116.65
25	d	404	BCR	C30-C25-C24	2.02	121.12	115.65
23	C	510	CLA	CAC-C3C-C2C	2.02	131.26	127.56
23	c	503	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
23	C	507	CLA	C2A-C1A-CHA	-2.01	120.37	123.87
32	C	523	HTG	O5-C5-C6	2.01	111.43	106.44
26	A	411	SQD	O7-S-C6	2.01	109.76	106.76
23	B	602	CLA	C4B-C3B-C2B	-2.01	104.80	107.30
40	v	202	HEC	CHB-C4A-NA	2.01	126.64	124.45
23	c	509	CLA	CHA-C1A-NA	-2.01	121.84	126.39
23	d	403	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
23	b	612	CLA	C11-C10-C8	-2.00	109.30	115.97
25	B	618	BCR	C36-C18-C19	2.00	121.15	118.09
23	B	602	CLA	C11-C12-C13	-2.00	109.32	115.97

All (66) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	503	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	C	515	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	ND
23	a	403	CLA	ND
23	a	404	CLA	ND
23	a	407	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	c	515	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (1336) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C6-C7-C8-C9
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	C	504	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C14-C13-C15-C16
23	C	507	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C6-C7-C8-C9
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
25	D	405	BCR	C21-C22-C23-C24
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C21-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	k	102	BCR	C1-C6-C7-C8
25	k	102	BCR	C5-C6-C7-C8
26	A	411	SQD	O6-C44-C45-O47
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	L	102	SQD	O49-C7-O47-C45
26	L	102	SQD	C8-C7-O47-C45
26	a	411	SQD	C5-C6-S-O7
26	a	411	SQD	C5-C6-S-O8
26	a	411	SQD	C5-C6-S-O9
26	f	101	SQD	C2-C1-O6-C44
26	f	101	SQD	O5-C1-O6-C44
26	f	101	SQD	C8-C7-O47-C45
27	B	623	GOL	C1-C2-C3-O3
27	a	410	GOL	O1-C1-C2-C3
27	b	623	GOL	C1-C2-C3-O3
27	v	201	GOL	O1-C1-C2-C3
29	A	413[A]	PL9	C25-C24-C26-C27
29	A	413[B]	PL9	C15-C14-C16-C17
29	A	413[B]	PL9	C35-C34-C36-C37
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C3-O3-P-O6
31	D	407	LHG	C4-O6-P-O3
31	D	407	LHG	C4-O6-P-O4
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	C3-O3-P-O6
31	L	101	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C4-O6-P-O5
31	a	419	LHG	C3-O3-P-O4
31	a	419	LHG	C3-O3-P-O5
31	a	419	LHG	C3-O3-P-O6
31	a	419	LHG	O10-C23-O8-C6
31	a	419	LHG	C24-C23-O8-C6
31	b	628	LHG	C4-O6-P-O3
31	b	628	LHG	C4-O6-P-O4
31	b	628	LHG	C4-O6-P-O5
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C3-O3-P-O5
31	d	406	LHG	C3-O3-P-O6
31	d	406	LHG	C4-O6-P-O5
31	d	407	LHG	O2-C2-C3-O3
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O6
31	d	407	LHG	C4-O6-P-O3
31	d	407	LHG	C4-O6-P-O4
33	B	630	LMT	O5'-C1'-O1'-C1
33	B	630	LMT	C2-C1-O1'-C1'
33	C	526	LMT	C3'-C4'-O1B-C1B
33	C	526	LMT	C2'-C1'-O1'-C1
33	C	526	LMT	O5'-C1'-O1'-C1
33	F	101	LMT	C2'-C1'-O1'-C1
33	F	101	LMT	O5'-C1'-O1'-C1
33	a	412	LMT	O5'-C1'-O1'-C1
33	b	620	LMT	O5'-C1'-O1'-C1
33	b	626	LMT	C2'-C1'-O1'-C1
33	b	626	LMT	O5'-C1'-O1'-C1
33	b	626	LMT	C2-C1-O1'-C1'
33	e	101	LMT	C2'-C1'-O1'-C1
34	C	522	LMG	C11-C10-O7-C8
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	a	417	LMG	O9-C10-O7-C8
34	a	417	LMG	C11-C10-O7-C8
34	c	522	LMG	C11-C10-O7-C8
34	z	101	LMG	O6-C1-O1-C7
34	z	101	LMG	C11-C10-O7-C8
38	E	102	HEM	C2C-C3C-CAC-CBC
38	E	102	HEM	C4C-C3C-CAC-CBC
38	e	102	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	e	102	HEM	C4C-C3C-CAC-CBC
40	V	201	HEC	C2B-C3B-CAB-CBB
40	V	201	HEC	C4B-C3B-CAB-CBB
40	V	201	HEC	C2C-C3C-CAC-CBC
40	V	201	HEC	C4C-C3C-CAC-CBC
40	v	202	HEC	C2B-C3B-CAB-CBB
40	v	202	HEC	C4B-C3B-CAB-CBB
40	v	202	HEC	C2C-C3C-CAC-CBC
40	v	202	HEC	C4C-C3C-CAC-CBC
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
26	B	620	SQD	O49-C7-O47-C45
26	f	101	SQD	O49-C7-O47-C45
34	c	522	LMG	O9-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	a	407	CLA	C3-C5-C6-C7
23	c	508	CLA	C3-C5-C6-C7
23	c	514	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
23	b	615	CLA	C13-C15-C16-C17
23	C	505	CLA	CBD-CGD-O2D-CED
23	A	407	CLA	C4-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	D	404	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	c	509	CLA	C4-C3-C5-C6
23	c	515	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	a	414[A]	PL9	C15-C14-C16-C17
29	a	414[B]	PL9	C25-C24-C26-C27
23	A	407	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	C	509	CLA	C2-C3-C5-C6
23	D	404	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	c	509	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	515	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
29	A	413[A]	PL9	C23-C24-C26-C27
29	A	413[B]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C13-C14-C16-C17
26	f	101	SQD	C24-C23-O48-C46
34	C	502	LMG	O6-C5-C6-O5
34	C	522	LMG	O9-C10-O7-C8
23	A	407	CLA	C3-C5-C6-C7
23	B	604	CLA	C3-C5-C6-C7
23	C	508	CLA	C3-C5-C6-C7
23	C	514	CLA	C3-C5-C6-C7
23	D	404	CLA	C3-C5-C6-C7
31	D	407	LHG	O2-C2-C3-O3
23	b	604	CLA	CBD-CGD-O2D-CED
32	c	523	HTG	O5-C5-C6-O6
33	F	101	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C3-C5-C6-C7
23	C	503	CLA	CBD-CGD-O2D-CED
32	B	624	HTG	O5-C5-C6-O6
33	M	103	LMT	O5'-C5'-C6'-O6'
34	a	417	LMG	O6-C5-C6-O5
23	B	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	a	414[A]	PL9	C25-C24-C26-C27
23	B	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	A	413[A]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C23-C24-C26-C27
29	a	414[B]	PL9	C23-C24-C26-C27
26	f	101	SQD	O10-C23-O48-C46
29	A	413[A]	PL9	C19-C21-C22-C23
29	A	413[B]	PL9	C14-C16-C17-C18
29	A	413[B]	PL9	C19-C21-C22-C23
29	A	413[B]	PL9	C24-C26-C27-C28
29	D	406	PL9	C39-C41-C42-C43
29	a	414[A]	PL9	C19-C21-C22-C23
29	a	414[A]	PL9	C24-C26-C27-C28
29	a	414[A]	PL9	C29-C31-C32-C33
29	a	414[B]	PL9	C9-C11-C12-C13
29	d	405	PL9	C39-C41-C42-C43
32	c	523	HTG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	CBD-CGD-O2D-CED
33	B	627	LMT	O5B-C5B-C6B-O6B
33	e	101	LMT	O5'-C5'-C6'-O6'
34	c	522	LMG	O6-C5-C6-O5
33	B	627	LMT	C3'-C4'-O1B-C1B
26	B	620	SQD	O5-C1-O6-C44
33	D	402	LMT	O5'-C1'-O1'-C1
33	M	103	LMT	O5'-C1'-O1'-C1
33	a	418	LMT	O5'-C1'-O1'-C1
34	c	522	LMG	O6-C1-O1-C7
34	C	502	LMG	C4-C5-C6-O5
23	b	601	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBA-CGA-O2A-C1
33	C	526	LMT	O5B-C5B-C6B-O6B
23	B	616	CLA	C4-C3-C5-C6
29	A	413[A]	PL9	C15-C14-C16-C17
29	A	413[B]	PL9	C30-C29-C31-C32
23	B	616	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
29	A	413[B]	PL9	C28-C29-C31-C32
23	B	602	CLA	C6-C7-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	C	515	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
23	b	615	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	C	505	CLA	O1D-CGD-O2D-CED
33	D	402	LMT	C2'-C1'-O1'-C1
33	M	103	LMT	C2'-C1'-O1'-C1
33	a	412	LMT	C2'-C1'-O1'-C1
33	a	418	LMT	C2'-C1'-O1'-C1
33	b	620	LMT	C2'-C1'-O1'-C1
25	D	405	BCR	C7-C8-C9-C34
25	D	405	BCR	C37-C22-C23-C24
25	Y	101	BCR	C37-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C34
33	M	103	LMT	C4'-C5'-C6'-O6'
31	b	628	LHG	C7-C8-C9-C10
23	c	511	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	C2-C1-O2A-CGA
33	B	627	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8
23	c	514	CLA	C15-C16-C17-C18
34	C	522	LMG	O6-C5-C6-O5
27	A	410	GOL	O2-C2-C3-O3
27	v	201	GOL	O1-C1-C2-O2
34	Z	101	LMG	C10-C11-C12-C13
29	A	413[A]	PL9	C12-C11-C9-C10
26	f	101	SQD	C23-C24-C25-C26
25	T	101	BCR	C13-C14-C15-C16
29	a	414[B]	PL9	C14-C16-C17-C18
29	a	414[B]	PL9	C24-C26-C27-C28
29	a	414[B]	PL9	C39-C41-C42-C43
29	d	405	PL9	C34-C36-C37-C38
33	C	526	LMT	O1'-C1-C2-C3
23	c	508	CLA	C15-C16-C17-C18
33	e	101	LMT	C4'-C5'-C6'-O6'
26	D	413	SQD	C7-C8-C9-C10
35	c	519	DGD	C1B-C2B-C3B-C4B
23	C	515	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
33	B	627	LMT	C5'-C4'-O1B-C1B
23	B	602	CLA	C15-C16-C17-C18
23	B	614	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	b	616	CLA	C13-C15-C16-C17
33	b	626	LMT	C11-C10-C9-C8
33	M	102	LMT	O5'-C1'-O1'-C1
33	e	101	LMT	O5'-C1'-O1'-C1
35	C	519	DGD	O6E-C1E-O5D-C6D
35	C	519	DGD	C5A-C6A-C7A-C8A
23	A	404	CLA	C15-C16-C17-C18
23	A	407	CLA	C5-C6-C7-C8
23	B	606	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13
34	c	522	LMG	C4-C5-C6-O5
31	d	406	LHG	C23-C24-C25-C26
23	C	507	CLA	C8-C10-C11-C12
23	C	507	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C13-C15-C16-C17
23	C	514	CLA	C15-C16-C17-C18
26	A	409	SQD	C11-C10-C9-C8
23	B	615	CLA	C10-C11-C12-C13
23	a	405	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	C	514	CLA	C13-C15-C16-C17
23	D	403	CLA	C15-C16-C17-C18
23	b	604	CLA	C8-C10-C11-C12
23	c	509	CLA	C8-C10-C11-C12
23	B	601	CLA	CBA-CGA-O2A-C1
34	a	417	LMG	C4-C5-C6-O5
23	C	510	CLA	CBD-CGD-O2D-CED
26	A	409	SQD	C18-C19-C20-C21
31	E	101	LHG	C26-C27-C28-C29
32	b	624	HTG	S1-C1'-C2'-C3'
35	H	102	DGD	C4E-C5E-C6E-O5E
23	C	510	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
31	d	407	LHG	C1-C2-C3-O3
23	d	403	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
23	B	613	CLA	C15-C16-C17-C18
23	b	616	CLA	C10-C11-C12-C13
23	B	614	CLA	C5-C6-C7-C8
23	b	603	CLA	C13-C15-C16-C17
23	a	404	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	C13-C15-C16-C17
23	c	512	CLA	C10-C11-C12-C13
31	d	408	LHG	C24-C23-O8-C6
35	C	519	DGD	CBB-CCB-CDB-CEB
23	C	508	CLA	C8-C10-C11-C12
23	b	604	CLA	C3-C5-C6-C7
33	M	102	LMT	C2'-C1'-O1'-C1
34	C	502	LMG	C2-C1-O1-C7
34	M	101	LMG	C2-C1-O1-C7
35	C	519	DGD	C2E-C1E-O5D-C6D
23	A	405	CLA	C15-C16-C17-C18
23	B	603	CLA	C8-C10-C11-C12
31	A	416	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	A	413[A]	PL9	C24-C26-C27-C28
31	d	406	LHG	O2-C2-C3-O3
33	m	103	LMT	O5'-C5'-C6'-O6'
25	B	631	BCR	C11-C12-C13-C35
25	b	619	BCR	C37-C22-C23-C24
25	d	404	BCR	C7-C8-C9-C34
25	D	405	BCR	C7-C8-C9-C10
31	D	408	LHG	O10-C23-O8-C6
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C15-C16-C17-C18
27	A	410	GOL	O1-C1-C2-C3
27	A	410	GOL	C1-C2-C3-O3
27	B	626	GOL	C1-C2-C3-O3
27	O	302	GOL	O1-C1-C2-C3
27	O	302	GOL	C1-C2-C3-O3
27	a	410	GOL	C1-C2-C3-O3
31	A	416	LHG	O1-C1-C2-C3
31	D	408	LHG	O1-C1-C2-C3
31	d	406	LHG	O1-C1-C2-C3
31	a	419	LHG	C23-C24-C25-C26
26	B	620	SQD	C46-C45-O47-C7
23	a	407	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	d	403	CLA	O1A-CGA-O2A-C1
23	b	605	CLA	C13-C15-C16-C17
34	C	502	LMG	O6-C1-O1-C7
33	a	412	LMT	C1-C2-C3-C4
23	c	511	CLA	C15-C16-C17-C18
32	b	621	HTG	S1-C1'-C2'-C3'
23	C	503	CLA	O1D-CGD-O2D-CED
35	c	518	DGD	O6D-C5D-C6D-O5D
23	b	601	CLA	C2-C1-O2A-CGA
23	B	615	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C20
23	b	609	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
31	D	408	LHG	C33-C34-C35-C36
23	B	601	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C13-C15-C16-C17
23	c	503	CLA	O1D-CGD-O2D-CED
31	b	628	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	b	620	LMT	C5-C6-C7-C8
34	D	412	LMG	C19-C20-C21-C22
34	M	101	LMG	C36-C37-C38-C39
34	d	411	LMG	C21-C22-C23-C24
35	C	518	DGD	C4B-C5B-C6B-C7B
32	h	101	HTG	O5-C5-C6-O6
23	b	606	CLA	C15-C16-C17-C18
34	C	502	LMG	C18-C19-C20-C21
26	B	620	SQD	C10-C11-C12-C13
31	L	101	LHG	C25-C26-C27-C28
31	b	628	LHG	C14-C15-C16-C17
34	C	522	LMG	C36-C37-C38-C39
35	H	102	DGD	C7B-C8B-C9B-CAB
35	c	519	DGD	C9A-CAA-CBA-CCA
34	M	101	LMG	O9-C10-O7-C8
27	O	302	GOL	O1-C1-C2-O2
27	O	302	GOL	O2-C2-C3-O3
27	b	623	GOL	O2-C2-C3-O3
26	A	409	SQD	C9-C10-C11-C12
35	c	519	DGD	C7A-C8A-C9A-CAA
23	b	604	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	C15-C16-C17-C18
23	C	506	CLA	C4B-C3B-CAB-CBB
23	C	515	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB
23	c	515	CLA	C4B-C3B-CAB-CBB
32	B	622	HTG	C1'-C2'-C3'-C4'
31	d	408	LHG	C29-C30-C31-C32
34	Z	101	LMG	O6-C5-C6-O5
23	B	615	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
31	D	408	LHG	C28-C29-C30-C31
34	C	502	LMG	C34-C35-C36-C37
23	A	407	CLA	C15-C16-C17-C18
23	D	403	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
26	A	409	SQD	C8-C7-O47-C45
34	M	101	LMG	C11-C10-O7-C8
33	B	627	LMT	C4'-C5'-C6'-O6'
23	a	407	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
34	m	101	LMG	C14-C15-C16-C17
23	B	601	CLA	C5-C6-C7-C8
26	a	411	SQD	C16-C17-C18-C19
31	D	408	LHG	C32-C33-C34-C35
35	c	518	DGD	C4D-C5D-C6D-O5D
23	C	508	CLA	C3A-C2A-CAA-CBA
26	A	411	SQD	C27-C28-C29-C30
34	C	521	LMG	C37-C38-C39-C40
23	B	604	CLA	C8-C10-C11-C12
33	M	103	LMT	O1'-C1-C2-C3
33	m	103	LMT	O1'-C1-C2-C3
35	h	103	DGD	CCB-CDB-CEB-CFB
33	B	629	LMT	C11-C10-C9-C8
23	c	513	CLA	CBA-CGA-O2A-C1
23	c	514	CLA	CBA-CGA-O2A-C1
26	L	102	SQD	C24-C23-O48-C46
26	a	409	SQD	C30-C31-C32-C33
26	a	411	SQD	C25-C26-C27-C28
31	d	407	LHG	C33-C34-C35-C36
31	d	408	LHG	C28-C29-C30-C31
31	E	101	LHG	C10-C11-C12-C13
31	L	101	LHG	C17-C18-C19-C20
33	D	402	LMT	C5-C6-C7-C8
34	C	521	LMG	C21-C22-C23-C24
34	M	101	LMG	C29-C30-C31-C32
35	C	519	DGD	C8A-C9A-CAA-CBA
35	c	518	DGD	C8B-C9B-CAB-CBB
31	d	408	LHG	O10-C23-O8-C6
33	B	627	LMT	O5'-C5'-C6'-O6'
32	B	624	HTG	C4-C5-C6-O6
33	D	402	LMT	C4'-C5'-C6'-O6'
35	h	103	DGD	CAB-CBB-CCB-CDB
23	a	405	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
23	c	515	CLA	C2B-C3B-CAB-CBB
34	c	522	LMG	C30-C31-C32-C33
34	C	502	LMG	C11-C10-O7-C8
26	A	411	SQD	C26-C27-C28-C29
34	C	502	LMG	C14-C15-C16-C17
26	B	620	SQD	C7-C8-C9-C10
23	C	512	CLA	C8-C10-C11-C12
31	b	628	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	B	622	HTG	C2'-C3'-C4'-C5'
32	B	624	HTG	C2'-C3'-C4'-C5'
35	C	518	DGD	C3A-C4A-C5A-C6A
23	c	513	CLA	O1A-CGA-O2A-C1
29	a	414[A]	PL9	C4-C3-C7-C8
26	A	411	SQD	C17-C18-C19-C20
33	e	101	LMT	C5-C6-C7-C8
26	A	409	SQD	O49-C7-O47-C45
29	A	413[B]	PL9	C33-C34-C36-C37
34	c	521	LMG	C36-C37-C38-C39
34	d	411	LMG	C38-C39-C40-C41
35	c	519	DGD	C7B-C8B-C9B-CAB
33	F	101	LMT	C4'-C5'-C6'-O6'
35	c	518	DGD	C2A-C1A-O1G-C1G
31	D	408	LHG	C12-C13-C14-C15
34	C	502	LMG	C12-C13-C14-C15
23	A	403	CLA	C13-C15-C16-C17
33	D	402	LMT	C7-C8-C9-C10
34	C	521	LMG	C17-C18-C19-C20
33	m	103	LMT	O5'-C1'-O1'-C1
34	M	101	LMG	O6-C1-O1-C7
31	D	407	LHG	C12-C13-C14-C15
34	C	522	LMG	C17-C18-C19-C20
26	D	413	SQD	C2-C1-O6-C44
33	B	630	LMT	C2'-C1'-O1'-C1
26	A	409	SQD	C15-C16-C17-C18
34	C	521	LMG	C30-C31-C32-C33
23	b	609	CLA	C16-C17-C18-C19
34	C	502	LMG	C37-C38-C39-C40
31	E	101	LHG	C23-C24-C25-C26
34	d	411	LMG	C28-C29-C30-C31
25	k	101	BCR	C7-C8-C9-C10
23	b	610	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	C	507	CLA	C4-C3-C5-C6
23	C	512	CLA	C4-C3-C5-C6
29	d	405	PL9	C15-C14-C16-C17
23	C	507	CLA	C2-C3-C5-C6
34	C	502	LMG	C17-C18-C19-C20
34	C	522	LMG	C18-C19-C20-C21
34	D	412	LMG	C35-C36-C37-C38
23	b	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	B	629	LMT	O1'-C1-C2-C3
34	C	502	LMG	C16-C17-C18-C19
23	C	506	CLA	C8-C10-C11-C12
23	b	605	CLA	C8-C10-C11-C12
23	c	510	CLA	C8-C10-C11-C12
26	L	102	SQD	C13-C14-C15-C16
29	A	413[A]	PL9	C14-C16-C17-C18
23	a	404	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C20
31	A	416	LHG	C26-C27-C28-C29
31	D	408	LHG	C29-C30-C31-C32
33	D	402	LMT	C3-C4-C5-C6
34	C	521	LMG	C13-C14-C15-C16
23	A	407	CLA	C13-C15-C16-C17
31	E	101	LHG	C11-C10-C9-C8
31	d	406	LHG	C34-C35-C36-C37
35	H	102	DGD	C9A-CAA-CBA-CCA
32	b	622	HTG	O5-C5-C6-O6
23	B	601	CLA	CBD-CGD-O2D-CED
26	A	409	SQD	O6-C44-C45-O47
26	a	411	SQD	O6-C44-C45-O47
26	f	101	SQD	O47-C45-C46-O48
32	C	523	HTG	C4-C5-C6-O6
31	A	416	LHG	C18-C19-C20-C21
31	d	407	LHG	C32-C33-C34-C35
34	a	417	LMG	C36-C37-C38-C39
33	b	626	LMT	C3-C4-C5-C6
34	Z	101	LMG	C16-C17-C18-C19
35	h	103	DGD	C5B-C6B-C7B-C8B
26	L	102	SQD	C27-C28-C29-C30
34	D	412	LMG	C30-C31-C32-C33
33	b	626	LMT	C5-C6-C7-C8
23	B	604	CLA	C4-C3-C5-C6
23	C	512	CLA	C2-C3-C5-C6
29	D	406	PL9	C28-C29-C31-C32
29	d	405	PL9	C13-C14-C16-C17
34	C	502	LMG	O9-C10-O7-C8
31	d	407	LHG	C34-C35-C36-C37
32	b	621	HTG	C2'-C3'-C4'-C5'
31	E	101	LHG	C24-C25-C26-C27
26	A	411	SQD	C24-C25-C26-C27
35	c	518	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
27	B	623	GOL	O2-C2-C3-O3
27	B	626	GOL	O2-C2-C3-O3
27	a	410	GOL	O1-C1-C2-O2
31	d	406	LHG	O1-C1-C2-O2
23	c	514	CLA	O1A-CGA-O2A-C1
26	L	102	SQD	O10-C23-O48-C46
23	b	601	CLA	C3-C5-C6-C7
23	C	503	CLA	C1A-C2A-CAA-CBA
34	d	411	LMG	C10-C11-C12-C13
34	C	522	LMG	C33-C34-C35-C36
31	a	419	LHG	C13-C14-C15-C16
34	a	417	LMG	C14-C15-C16-C17
35	H	102	DGD	C5B-C6B-C7B-C8B
31	a	419	LHG	C18-C19-C20-C21
23	B	602	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	b	610	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	512	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
32	c	523	HTG	S1-C1'-C2'-C3'
35	c	518	DGD	O1A-C1A-O1G-C1G
35	C	518	DGD	O6D-C5D-C6D-O5D
23	C	504	CLA	C15-C16-C17-C18
34	m	101	LMG	C39-C40-C41-C42
24	a	406	PHO	C4-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
24	a	406	PHO	C2-C3-C5-C6
34	D	412	LMG	O6-C5-C6-O5
23	c	511	CLA	C10-C11-C12-C13
34	m	101	LMG	C11-C10-O7-C8
23	a	403	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C11-C12-C13-C14
23	C	515	CLA	C11-C10-C8-C9
23	a	405	CLA	C14-C13-C15-C16
23	b	610	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	c	506	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	515	CLA	C6-C7-C8-C9
23	d	402	CLA	C11-C12-C13-C14
35	C	519	DGD	C8B-C9B-CAB-CBB
34	C	521	LMG	C29-C30-C31-C32
23	C	513	CLA	CBA-CGA-O2A-C1
26	D	413	SQD	C30-C31-C32-C33
34	d	411	LMG	O6-C5-C6-O5
26	B	620	SQD	C44-C45-C46-O48
26	a	409	SQD	O6-C44-C45-C46
29	A	413[A]	PL9	C9-C11-C12-C13
34	C	522	LMG	C7-C8-C9-O8
33	M	103	LMT	C2B-C1B-O1B-C4'
34	M	101	LMG	C32-C33-C34-C35
26	A	409	SQD	C12-C13-C14-C15
26	D	413	SQD	C28-C29-C30-C31
35	c	519	DGD	CCA-CDA-CEA-CFA
23	C	514	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
23	a	404	CLA	C16-C17-C18-C19
23	D	404	CLA	C10-C11-C12-C13
34	a	417	LMG	C30-C31-C32-C33
34	a	417	LMG	C32-C33-C34-C35
35	c	519	DGD	C6A-C7A-C8A-C9A
35	C	518	DGD	O6E-C5E-C6E-O5E
25	b	619	BCR	C21-C22-C23-C24
23	C	513	CLA	O1A-CGA-O2A-C1
31	L	101	LHG	C24-C25-C26-C27
33	B	627	LMT	C6-C7-C8-C9
35	H	102	DGD	CBA-CCA-CDA-CEA
26	a	409	SQD	C9-C10-C11-C12
23	C	512	CLA	CBA-CGA-O2A-C1
34	D	412	LMG	C38-C39-C40-C41
34	c	522	LMG	C29-C30-C31-C32
23	b	616	CLA	C15-C16-C17-C18
35	C	520	DGD	C6B-C7B-C8B-C9B
23	b	614	CLA	C3-C5-C6-C7
32	B	621	HTG	C3'-C4'-C5'-C6'
35	c	518	DGD	C3A-C4A-C5A-C6A
31	D	407	LHG	C1-C2-C3-O3
34	z	101	LMG	C4-C5-C6-O5
33	b	620	LMT	C3'-C4'-O1B-C1B
31	d	406	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
35	C	520	DGD	C9A-CAA-CBA-CCA
23	c	506	CLA	C4-C3-C5-C6
32	b	624	HTG	C4'-C5'-C6'-C7'
35	C	518	DGD	C6B-C7B-C8B-C9B
23	c	511	CLA	C16-C17-C18-C20
26	a	411	SQD	C26-C27-C28-C29
31	d	407	LHG	C30-C31-C32-C33
32	B	624	HTG	C4'-C5'-C6'-C7'
34	c	521	LMG	C40-C41-C42-C43
31	A	416	LHG	C32-C33-C34-C35
26	a	409	SQD	O6-C44-C45-O47
31	E	101	LHG	O7-C5-C6-O8
34	M	101	LMG	C28-C29-C30-C31
34	c	521	LMG	C32-C33-C34-C35
31	d	407	LHG	C13-C14-C15-C16
23	B	616	CLA	C2-C1-O2A-CGA
34	D	412	LMG	C12-C13-C14-C15
35	H	102	DGD	CCA-CDA-CEA-CFA
29	a	414[A]	PL9	C39-C41-C42-C43
31	E	101	LHG	C7-C8-C9-C10
34	M	101	LMG	C29-C28-O8-C9
34	M	101	LMG	C17-C18-C19-C20
23	A	407	CLA	C8-C10-C11-C12
26	L	102	SQD	C14-C15-C16-C17
35	C	519	DGD	CDA-CEA-CFA-CGA
23	C	514	CLA	C10-C11-C12-C13
33	b	626	LMT	C1-C2-C3-C4
23	A	405	CLA	C16-C17-C18-C20
23	b	601	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
29	D	406	PL9	C15-C14-C16-C17
29	a	414[B]	PL9	C30-C29-C31-C32
29	D	406	PL9	C13-C14-C16-C17
23	B	610	CLA	C15-C16-C17-C18
35	c	518	DGD	C1A-C2A-C3A-C4A
31	d	408	LHG	C11-C10-C9-C8
33	b	620	LMT	C3-C4-C5-C6
34	C	502	LMG	C35-C36-C37-C38
31	A	416	LHG	O1-C1-C2-O2
23	B	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	512	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	515	CLA	C6-C7-C8-C9
23	D	404	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
35	c	520	DGD	O6E-C5E-C6E-O5E
23	a	405	CLA	C4B-C3B-CAB-CBB
23	b	602	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
32	B	621	HTG	C2'-C3'-C4'-C5'
33	C	526	LMT	C4-C5-C6-C7
33	D	402	LMT	C4-C5-C6-C7
23	a	405	CLA	C10-C11-C12-C13
23	b	604	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
31	d	408	LHG	C9-C10-C11-C12
23	a	405	CLA	O1D-CGD-O2D-CED
33	m	103	LMT	C2'-C1'-O1'-C1
31	a	419	LHG	O6-C4-C5-C6
34	m	101	LMG	C32-C33-C34-C35
33	e	101	LMT	C2B-C1B-O1B-C4'
23	B	602	CLA	C6-C7-C8-C10
23	B	605	CLA	C6-C7-C8-C10
23	C	515	CLA	C11-C10-C8-C7
23	D	404	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	508	CLA	C6-C7-C8-C10
23	d	402	CLA	C11-C12-C13-C15
23	B	615	CLA	C8-C10-C11-C12
35	c	520	DGD	CDB-CEB-CFB-CGB
23	b	603	CLA	C16-C17-C18-C20
26	A	411	SQD	C30-C31-C32-C33
23	C	512	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
32	V	202	HTG	O5-C5-C6-O6
23	b	609	CLA	C3A-C2A-CAA-CBA
29	a	414[A]	PL9	C30-C29-C31-C32
23	B	606	CLA	C8-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
23	C	514	CLA	O1A-CGA-O2A-C1
23	b	602	CLA	C10-C11-C12-C13
35	h	103	DGD	CDB-CEB-CFB-CGB
34	C	521	LMG	C31-C32-C33-C34
26	a	411	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
34	a	417	LMG	C20-C21-C22-C23
34	m	101	LMG	C38-C39-C40-C41
35	H	102	DGD	O6E-C5E-C6E-O5E
35	C	518	DGD	C3B-C4B-C5B-C6B
33	B	630	LMT	C4-C5-C6-C7
26	a	411	SQD	C24-C23-O48-C46
26	A	409	SQD	C14-C15-C16-C17
35	C	519	DGD	CAB-CBB-CCB-CDB
26	A	409	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
31	E	101	LHG	C4-C5-C6-O8
31	a	419	LHG	C4-C5-C6-O8
34	Z	101	LMG	C7-C8-C9-O8
31	b	628	LHG	C10-C11-C12-C13
31	b	628	LHG	C34-C35-C36-C37
32	B	622	HTG	C4'-C5'-C6'-C7'
23	a	403	CLA	C16-C17-C18-C19
23	c	513	CLA	C8-C10-C11-C12
33	B	630	LMT	C3-C4-C5-C6
34	a	417	LMG	C40-C41-C42-C43
23	C	505	CLA	C10-C11-C12-C13
35	C	518	DGD	C5A-C6A-C7A-C8A
26	A	411	SQD	C7-C8-C9-C10
23	B	608	CLA	C16-C17-C18-C20
31	a	419	LHG	O6-C4-C5-O7
25	D	405	BCR	C23-C24-C25-C30
25	d	404	BCR	C23-C24-C25-C30
34	M	101	LMG	C34-C35-C36-C37
23	a	404	CLA	C13-C15-C16-C17
35	C	519	DGD	C2A-C3A-C4A-C5A
35	C	518	DGD	C4D-C5D-C6D-O5D
26	a	411	SQD	C31-C32-C33-C34
23	c	514	CLA	C10-C11-C12-C13
26	a	409	SQD	C26-C27-C28-C29
31	a	419	LHG	O7-C5-C6-O8
34	C	522	LMG	O7-C8-C9-O8
29	A	413[A]	PL9	C4-C3-C7-C8
29	A	413[B]	PL9	C4-C3-C7-C8
29	a	414[B]	PL9	C4-C3-C7-C8
23	c	512	CLA	C4-C3-C5-C6
29	D	406	PL9	C30-C29-C31-C32
34	C	522	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C8-C10-C11-C12
23	b	601	CLA	C2-C3-C5-C6
23	c	512	CLA	C2-C3-C5-C6
29	a	414[B]	PL9	C28-C29-C31-C32
29	a	414[B]	PL9	C2-C3-C7-C8
34	c	521	LMG	C30-C31-C32-C33
33	M	102	LMT	C4B-C5B-C6B-O6B
23	C	508	CLA	C13-C15-C16-C17
26	B	620	SQD	C9-C10-C11-C12
23	B	611	CLA	C11-C12-C13-C14
23	a	404	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C13-C15-C16-C17
26	a	409	SQD	C33-C34-C35-C36
33	C	526	LMT	C3-C4-C5-C6
34	C	521	LMG	C12-C13-C14-C15
35	H	102	DGD	CBB-CCB-CDB-CEB
35	c	518	DGD	C2B-C3B-C4B-C5B
35	c	518	DGD	O6E-C1E-O5D-C6D
23	c	510	CLA	C5-C6-C7-C8
23	C	515	CLA	O1D-CGD-O2D-CED
29	A	413[B]	PL9	C39-C41-C42-C43
34	C	502	LMG	C32-C33-C34-C35
23	C	507	CLA	C5-C6-C7-C8
27	a	410	GOL	O2-C2-C3-O3
31	d	407	LHG	C24-C23-O8-C6
29	a	414[A]	PL9	C28-C29-C31-C32
23	c	511	CLA	C16-C17-C18-C19
35	C	519	DGD	C6A-C7A-C8A-C9A
35	c	520	DGD	CBA-CCA-CDA-CEA
34	M	101	LMG	O10-C28-O8-C9
23	a	407	CLA	CBA-CGA-O2A-C1
31	d	406	LHG	C24-C23-O8-C6
31	b	628	LHG	O6-C4-C5-C6
23	A	405	CLA	C16-C17-C18-C19
23	b	603	CLA	C16-C17-C18-C19
24	a	416	PHO	C2C-C3C-CAC-CBC
23	a	404	CLA	C15-C16-C17-C18
33	C	526	LMT	C4B-C5B-C6B-O6B
23	A	405	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	609	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C11-C12-C13-C15
23	c	508	CLA	C11-C10-C8-C7
25	B	631	BCR	C11-C12-C13-C14
25	d	404	BCR	C7-C8-C9-C10
25	d	404	BCR	C21-C22-C23-C24
26	A	411	SQD	C24-C23-O48-C46
35	c	520	DGD	C2A-C1A-O1G-C1G
26	L	102	SQD	C15-C16-C17-C18
23	c	512	CLA	O1A-CGA-O2A-C1
26	a	411	SQD	O10-C23-O48-C46
35	c	519	DGD	C2G-C3G-O3G-C1D
35	c	519	DGD	C5D-C6D-O5D-C1E
33	b	626	LMT	C4-C5-C6-C7
34	m	101	LMG	O9-C10-O7-C8
35	h	103	DGD	O2G-C1B-C2B-C3B
23	a	407	CLA	O1A-CGA-O2A-C1
38	e	102	HEM	C2B-C3B-CAB-CBB
23	b	607	CLA	C3-C5-C6-C7
26	L	102	SQD	C46-C45-O47-C7
31	d	407	LHG	O10-C23-O8-C6
35	C	519	DGD	C9B-CAB-CBB-CCB
23	a	403	CLA	C16-C17-C18-C20
31	d	406	LHG	C29-C30-C31-C32
35	c	518	DGD	C2A-C3A-C4A-C5A
31	b	628	LHG	O6-C4-C5-O7
31	d	406	LHG	C16-C17-C18-C19
26	a	411	SQD	O5-C1-O6-C44
29	a	414[A]	PL9	C9-C11-C12-C13
26	a	411	SQD	C30-C31-C32-C33
29	A	413[B]	PL9	C2-C3-C7-C8
33	m	103	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C3-C5-C6-C7
31	d	407	LHG	C29-C30-C31-C32
26	B	620	SQD	O47-C45-C46-O48
26	L	102	SQD	O47-C45-C46-O48
32	b	621	HTG	C4'-C5'-C6'-C7'
23	b	616	CLA	C6-C7-C8-C9
23	c	504	CLA	C14-C13-C15-C16
26	B	620	SQD	C29-C30-C31-C32
26	f	101	SQD	C33-C34-C35-C36
31	A	416	LHG	C11-C10-C9-C8
33	F	101	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	a	417	LMG	C18-C19-C20-C21
23	B	606	CLA	C13-C15-C16-C17
33	M	103	LMT	O5B-C1B-O1B-C4'
26	D	413	SQD	C34-C35-C36-C37
31	D	407	LHG	C18-C19-C20-C21
23	B	610	CLA	C13-C15-C16-C17
31	d	406	LHG	O10-C23-O8-C6
35	c	518	DGD	C2E-C1E-O5D-C6D
29	a	414[B]	PL9	C35-C34-C36-C37
26	a	411	SQD	C18-C19-C20-C21
26	a	411	SQD	C24-C25-C26-C27
31	a	419	LHG	C16-C17-C18-C19
31	d	407	LHG	C9-C10-C11-C12
32	C	523	HTG	O5-C5-C6-O6
23	B	606	CLA	C16-C17-C18-C20
35	c	518	DGD	CAA-CBA-CCA-CDA
31	D	407	LHG	C11-C12-C13-C14
31	d	407	LHG	C25-C26-C27-C28
35	H	102	DGD	CAA-CBA-CCA-CDA
34	c	522	LMG	C29-C28-O8-C9
31	L	101	LHG	C27-C28-C29-C30
23	B	601	CLA	O1D-CGD-O2D-CED
33	e	101	LMT	O5B-C1B-O1B-C4'
29	A	413[A]	PL9	C44-C46-C47-C48
33	D	402	LMT	C6-C7-C8-C9
23	D	404	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
29	a	414[A]	PL9	C12-C11-C9-C10
33	a	412	LMT	C4-C5-C6-C7
23	c	506	CLA	C2-C3-C5-C6
23	a	403	CLA	C15-C16-C17-C18
35	C	518	DGD	CCB-CDB-CEB-CFB
26	A	411	SQD	O10-C23-O48-C46
35	c	520	DGD	O1A-C1A-O1G-C1G
23	B	612	CLA	C10-C11-C12-C13
26	A	411	SQD	O49-C7-O47-C45
33	b	620	LMT	C6-C7-C8-C9
34	C	521	LMG	C15-C16-C17-C18
35	h	103	DGD	CAA-CBA-CCA-CDA
23	B	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	C	515	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	b	615	CLA	C6-C7-C8-C10
23	c	503	CLA	C11-C12-C13-C15
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
26	a	411	SQD	C27-C28-C29-C30
23	A	407	CLA	C16-C17-C18-C19
23	B	608	CLA	C16-C17-C18-C19
23	C	510	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	CBA-CGA-O2A-C1
31	A	416	LHG	C29-C30-C31-C32
24	a	406	PHO	C2C-C3C-CAC-CBC
29	a	414[B]	PL9	C43-C44-C46-C47
23	a	407	CLA	C5-C6-C7-C8
31	L	101	LHG	C23-C24-C25-C26
33	B	627	LMT	C4-C5-C6-C7
23	A	405	CLA	C14-C13-C15-C16
23	b	609	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C14
35	H	102	DGD	O2G-C1B-C2B-C3B
26	B	620	SQD	C33-C34-C35-C36
34	M	101	LMG	C20-C21-C22-C23
31	a	419	LHG	C25-C26-C27-C28
34	C	502	LMG	C38-C39-C40-C41
35	C	520	DGD	C9B-CAB-CBB-CCB
34	Z	101	LMG	O7-C8-C9-O8
23	C	505	CLA	C15-C16-C17-C18
26	A	411	SQD	O6-C44-C45-C46
26	L	102	SQD	C44-C45-C46-O48
26	f	101	SQD	C44-C45-C46-O48
34	C	502	LMG	O1-C7-C8-C9
34	c	522	LMG	O10-C28-O8-C9
29	A	413[A]	PL9	C12-C11-C9-C8
31	E	101	LHG	C17-C18-C19-C20
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
26	L	102	SQD	C28-C29-C30-C31
31	A	416	LHG	C9-C10-C11-C12
26	L	102	SQD	O5-C1-O6-C44
23	C	507	CLA	C10-C11-C12-C13
23	C	514	CLA	C16-C17-C18-C19
26	L	102	SQD	C12-C13-C14-C15
33	M	102	LMT	C9-C10-C11-C12
33	D	402	LMT	O5'-C5'-C6'-O6'
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D
31	D	407	LHG	C4-O6-P-O5
31	E	101	LHG	C4-O6-P-O5
31	L	101	LHG	C3-O3-P-O6
31	d	407	LHG	C4-O6-P-O5
23	C	514	CLA	C16-C17-C18-C20
31	d	407	LHG	C28-C29-C30-C31
35	C	518	DGD	C2B-C3B-C4B-C5B
23	B	603	CLA	C4-C3-C5-C6
23	C	515	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
23	a	407	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C2B-C3B-CAB-CBB
35	h	103	DGD	CBA-CCA-CDA-CEA
25	b	617	BCR	C36-C18-C19-C20
31	D	408	LHG	C2-C3-O3-P
31	d	408	LHG	C2-C3-O3-P
23	b	606	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	C	502	LMG	C13-C14-C15-C16
31	A	416	LHG	C19-C20-C21-C22
35	C	519	DGD	C9A-CAA-CBA-CCA
35	H	102	DGD	C6B-C7B-C8B-C9B
32	b	622	HTG	C3'-C4'-C5'-C6'
23	B	613	CLA	C13-C15-C16-C17
33	a	418	LMT	C2-C3-C4-C5
34	C	522	LMG	C12-C13-C14-C15
23	b	610	CLA	C13-C15-C16-C17
26	A	409	SQD	C33-C34-C35-C36
23	B	616	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C9
35	c	518	DGD	CDA-CEA-CFA-CGA
23	B	615	CLA	C11-C12-C13-C15
23	B	606	CLA	C16-C17-C18-C19
34	M	101	LMG	C33-C34-C35-C36
26	B	620	SQD	C34-C35-C36-C37
35	c	518	DGD	C6B-C7B-C8B-C9B
26	B	620	SQD	C24-C23-O48-C46
26	B	620	SQD	C11-C10-C9-C8
34	C	502	LMG	O1-C7-C8-O7
26	B	620	SQD	C19-C20-C21-C22
25	H	101	BCR	C9-C10-C11-C12
23	b	601	CLA	CAA-CBA-CGA-O2A
23	c	509	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C5-C6-C7-C8
31	d	407	LHG	C11-C10-C9-C8
31	d	408	LHG	C10-C11-C12-C13
34	C	502	LMG	C21-C22-C23-C24
34	M	101	LMG	C15-C16-C17-C18
29	A	413[B]	PL9	C9-C11-C12-C13
29	a	414[B]	PL9	C34-C36-C37-C38
23	B	612	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	CAA-CBA-CGA-O2A
35	C	518	DGD	C5B-C6B-C7B-C8B
32	B	622	HTG	C2'-C1'-S1-C1
32	b	621	HTG	C2'-C1'-S1-C1
25	b	617	BCR	C17-C18-C19-C20
25	k	102	BCR	C21-C22-C23-C24
31	A	416	LHG	C34-C35-C36-C37
32	D	411	HTG	C4-C5-C6-O6
23	a	407	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C2A-CAA-CBA-CGA
26	B	620	SQD	C30-C31-C32-C33
31	D	407	LHG	C16-C17-C18-C19
29	a	414[B]	PL9	C45-C44-C46-C47
35	H	102	DGD	CDB-CEB-CFB-CGB
23	B	609	CLA	C2-C3-C5-C6
29	a	414[A]	PL9	C43-C44-C46-C47
23	b	612	CLA	C8-C10-C11-C12
29	A	413[A]	PL9	C2-C3-C7-C8
23	b	601	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C12-C13-C14
26	D	413	SQD	C24-C23-O48-C46
26	L	102	SQD	C19-C20-C21-C22
24	a	416	PHO	CBD-CGD-O2D-CED
33	M	102	LMT	C7-C8-C9-C10
33	a	418	LMT	C4-C5-C6-C7
33	B	630	LMT	O1'-C1-C2-C3
23	B	612	CLA	O1A-CGA-O2A-C1
26	B	620	SQD	O10-C23-O48-C46
29	D	406	PL9	C35-C34-C36-C37
31	D	407	LHG	C28-C29-C30-C31
38	e	102	HEM	C4B-C3B-CAB-CBB
31	D	408	LHG	C30-C31-C32-C33
23	B	613	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
26	f	101	SQD	C29-C30-C31-C32
31	D	408	LHG	C9-C10-C11-C12
31	d	407	LHG	C31-C32-C33-C34
23	B	603	CLA	C13-C15-C16-C17
23	B	604	CLA	C13-C15-C16-C17
23	c	515	CLA	O1A-CGA-O2A-C1
26	D	413	SQD	O10-C23-O48-C46
23	c	504	CLA	C3-C5-C6-C7
23	B	609	CLA	C4-C3-C5-C6
23	b	616	CLA	C4-C3-C5-C6
31	L	101	LHG	C12-C13-C14-C15
34	z	101	LMG	C18-C19-C20-C21
34	Z	101	LMG	C14-C15-C16-C17
23	b	604	CLA	C2C-C3C-CAC-CBC
35	C	519	DGD	CCA-CDA-CEA-CFA
23	B	613	CLA	C10-C11-C12-C13
26	A	409	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	d	406	LHG	C27-C28-C29-C30
34	C	521	LMG	C36-C37-C38-C39
23	C	504	CLA	C3-C5-C6-C7
35	c	520	DGD	C4A-C5A-C6A-C7A
26	a	409	SQD	C34-C35-C36-C37
35	c	519	DGD	CDA-CEA-CFA-CGA
23	C	508	CLA	C4-C3-C5-C6
38	e	102	HEM	C2A-CAA-CBA-CGA
31	A	416	LHG	C10-C11-C12-C13
26	L	102	SQD	C18-C19-C20-C21
35	C	519	DGD	C6B-C7B-C8B-C9B
29	a	414[B]	PL9	C29-C31-C32-C33
29	d	405	PL9	C9-C11-C12-C13
31	d	407	LHG	C4-C5-C6-O8
23	A	404	CLA	C2C-C3C-CAC-CBC
23	B	613	CLA	C11-C12-C13-C14
23	a	407	CLA	C11-C10-C8-C9
23	b	601	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	c	513	CLA	C11-C10-C8-C9
24	A	415	PHO	C6-C7-C8-C9
23	C	514	CLA	CBD-CGD-O2D-CED
33	B	630	LMT	C5-C6-C7-C8
23	B	602	CLA	O2A-C1-C2-C3
34	M	101	LMG	C7-C8-O7-C10
40	v	202	HEC	CAD-CBD-CGD-O1D
29	a	414[A]	PL9	C45-C44-C46-C47
35	c	519	DGD	C6B-C7B-C8B-C9B
23	C	508	CLA	C2-C3-C5-C6
29	A	413[A]	PL9	C43-C44-C46-C47
38	E	102	HEM	CAD-CBD-CGD-O1D
26	B	620	SQD	C14-C15-C16-C17
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C1A-C2A-CAA-CBA
32	B	624	HTG	C3'-C4'-C5'-C6'
23	C	506	CLA	C2B-C3B-CAB-CBB
23	b	602	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C2B-C3B-CAB-CBB
23	c	509	CLA	C2B-C3B-CAB-CBB
25	C	517	BCR	C1-C6-C7-C8
25	D	405	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	D	405	BCR	C23-C24-C25-C26
25	Y	101	BCR	C23-C24-C25-C30
25	b	617	BCR	C1-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
26	A	411	SQD	C8-C7-O47-C45
35	C	520	DGD	C5B-C6B-C7B-C8B
23	c	515	CLA	CBA-CGA-O2A-C1
35	C	520	DGD	C4B-C5B-C6B-C7B
31	L	101	LHG	C35-C36-C37-C38
35	c	519	DGD	CBA-CCA-CDA-CEA
33	a	412	LMT	C9-C10-C11-C12
23	B	606	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
34	C	521	LMG	C34-C35-C36-C37
26	f	101	SQD	C28-C29-C30-C31
40	V	201	HEC	CAD-CBD-CGD-O2D
23	B	613	CLA	C12-C13-C15-C16
23	C	514	CLA	C12-C13-C15-C16
23	b	604	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C15
23	c	515	CLA	C12-C13-C15-C16
26	a	409	SQD	C27-C28-C29-C30
32	B	622	HTG	C3'-C4'-C5'-C6'
33	e	101	LMT	C4-C5-C6-C7
33	B	629	LMT	C3-C4-C5-C6
33	a	412	LMT	C6-C7-C8-C9
34	a	417	LMG	O8-C28-C29-C30
35	c	520	DGD	C2B-C3B-C4B-C5B
29	A	413[B]	PL9	C40-C39-C41-C42
34	C	502	LMG	O8-C28-C29-C30
23	B	605	CLA	C13-C15-C16-C17
24	a	416	PHO	C8-C10-C11-C12
23	B	604	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
29	a	414[A]	PL9	C12-C11-C9-C8
35	c	520	DGD	O6D-C5D-C6D-O5D
23	C	514	CLA	C2-C1-O2A-CGA
29	a	414[A]	PL9	C2-C3-C7-C8
26	D	413	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
40	V	201	HEC	CAD-CBD-CGD-O1D
40	v	202	HEC	CAD-CBD-CGD-O2D
24	a	416	PHO	O1D-CGD-O2D-CED
23	b	615	CLA	C15-C16-C17-C18
33	B	629	LMT	C4-C5-C6-C7
35	c	519	DGD	C2A-C3A-C4A-C5A
31	d	406	LHG	C26-C27-C28-C29
29	D	406	PL9	C45-C44-C46-C47
29	d	405	PL9	C45-C44-C46-C47
23	C	510	CLA	C13-C15-C16-C17
33	m	103	LMT	C3-C4-C5-C6
23	B	606	CLA	C2-C3-C5-C6
34	d	411	LMG	C29-C30-C31-C32
35	C	518	DGD	C7A-C8A-C9A-CAA
35	C	518	DGD	CBB-CCB-CDB-CEB
34	c	521	LMG	C31-C32-C33-C34
35	C	519	DGD	C5B-C6B-C7B-C8B
27	B	626	GOL	O1-C1-C2-O2
33	e	101	LMT	C2-C1-O1'-C1'
23	c	508	CLA	C4-C3-C5-C6
35	C	520	DGD	C8A-C9A-CAA-CBA
35	h	103	DGD	C8B-C9B-CAB-CBB
23	C	509	CLA	C4B-C3B-CAB-CBB
24	a	416	PHO	CHA-CBD-CGD-O1D
26	A	411	SQD	C16-C17-C18-C19
33	b	626	LMT	C7-C8-C9-C10
26	a	409	SQD	C25-C26-C27-C28
31	a	419	LHG	C17-C18-C19-C20
29	A	413[A]	PL9	C45-C44-C46-C47
31	d	407	LHG	O7-C5-C6-O8
32	B	621	HTG	C1'-C2'-C3'-C4'
26	D	413	SQD	O5-C1-O6-C44
35	c	519	DGD	O6E-C1E-O5D-C6D
35	C	520	DGD	C7A-C8A-C9A-CAA
23	a	404	CLA	C6-C7-C8-C10
31	L	101	LHG	C9-C10-C11-C12
23	D	404	CLA	C11-C10-C8-C9
23	a	405	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C12-C13-C14
34	M	101	LMG	C8-C7-O1-C1
35	c	518	DGD	C5D-C6D-O5D-C1E
35	c	519	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
23	A	403	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
23	B	612	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
34	C	521	LMG	C32-C33-C34-C35
34	D	412	LMG	C18-C19-C20-C21
23	B	604	CLA	C4C-C3C-CAC-CBC
38	E	102	HEM	CAD-CBD-CGD-O2D
35	h	103	DGD	C9A-CAA-CBA-CCA
35	c	519	DGD	C2E-C1E-O5D-C6D
26	a	409	SQD	C35-C36-C37-C38
23	C	512	CLA	C10-C11-C12-C13
23	c	510	CLA	C13-C15-C16-C17
32	D	411	HTG	C1'-C2'-C3'-C4'
23	B	603	CLA	C2-C3-C5-C6
29	A	413[B]	PL9	C43-C44-C46-C47
26	A	411	SQD	C31-C32-C33-C34
23	c	515	CLA	C10-C11-C12-C13
34	z	101	LMG	O6-C5-C6-O5
31	D	407	LHG	C26-C27-C28-C29
31	d	406	LHG	C11-C10-C9-C8
32	h	101	HTG	C4-C5-C6-O6
23	B	613	CLA	CAA-CBA-CGA-O2A
31	d	407	LHG	C23-C24-C25-C26
26	a	409	SQD	C31-C32-C33-C34
31	L	101	LHG	C15-C16-C17-C18
23	B	605	CLA	C14-C13-C15-C16
23	B	610	CLA	C14-C13-C15-C16
23	C	508	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	b	606	CLA	C6-C7-C8-C9
31	b	628	LHG	O7-C7-C8-C9
35	c	519	DGD	CBB-CCB-CDB-CEB
25	k	101	BCR	C17-C18-C19-C20
34	d	411	LMG	C19-C20-C21-C22
23	D	403	CLA	C2C-C3C-CAC-CBC
23	C	514	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
31	D	407	LHG	C15-C16-C17-C18
23	a	404	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	C2B-C3B-CAB-CBB
23	b	601	CLA	C2B-C3B-CAB-CBB
23	b	603	CLA	C2B-C3B-CAB-CBB
25	B	631	BCR	C1-C6-C7-C8
25	B	631	BCR	C5-C6-C7-C8
25	C	517	BCR	C5-C6-C7-C8
25	D	405	BCR	C5-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	k	102	BCR	C23-C24-C25-C26
25	k	102	BCR	C23-C24-C25-C30
35	C	518	DGD	CDB-CEB-CFB-CGB
23	B	612	CLA	CAA-CBA-CGA-O2A
23	C	514	CLA	CAA-CBA-CGA-O2A
35	c	520	DGD	CAB-CBB-CCB-CDB
23	B	613	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
23	c	515	CLA	C2-C1-O2A-CGA
34	m	101	LMG	C33-C34-C35-C36
29	a	414[A]	PL9	C14-C16-C17-C18
26	f	101	SQD	O48-C23-C24-C25
32	c	523	HTG	C1'-C2'-C3'-C4'
23	B	602	CLA	C3-C5-C6-C7
34	D	412	LMG	O7-C10-C11-C12
34	Z	101	LMG	O7-C10-C11-C12
31	d	408	LHG	C31-C32-C33-C34
32	B	621	HTG	C2'-C1'-S1-C1
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	612	CLA	CAA-CBA-CGA-O2A
23	A	403	CLA	C16-C17-C18-C19
23	B	604	CLA	C2C-C3C-CAC-CBC
23	c	512	CLA	CAA-CBA-CGA-O2A
34	C	502	LMG	O7-C10-C11-C12
34	m	101	LMG	C13-C14-C15-C16
33	D	402	LMT	C4B-C5B-C6B-O6B
35	H	102	DGD	C5A-C6A-C7A-C8A
32	b	621	HTG	C3'-C4'-C5'-C6'
38	e	102	HEM	CAD-CBD-CGD-O1D
23	b	611	CLA	C14-C13-C15-C16
23	c	515	CLA	C14-C13-C15-C16
26	a	409	SQD	C13-C14-C15-C16
25	k	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	M	101	LMG	O1-C7-C8-C9
23	b	601	CLA	C4B-C3B-CAB-CBB
38	e	102	HEM	CAA-CBA-CGA-O2A
33	B	627	LMT	O5'-C1'-O1'-C1
31	A	416	LHG	O8-C23-C24-C25
31	a	419	LHG	C28-C29-C30-C31
23	C	512	CLA	CAA-CBA-CGA-O2A
23	c	514	CLA	CAA-CBA-CGA-O2A
31	d	406	LHG	O8-C23-C24-C25
23	B	602	CLA	C2A-CAA-CBA-CGA
35	h	103	DGD	C2A-C3A-C4A-C5A
35	c	518	DGD	O2G-C1B-C2B-C3B
23	b	602	CLA	C8-C10-C11-C12
23	c	505	CLA	C15-C16-C17-C18
23	c	513	CLA	C2-C1-O2A-CGA
26	L	102	SQD	O48-C23-C24-C25
31	L	101	LHG	O7-C7-C8-C9
23	B	606	CLA	C12-C13-C15-C16
23	C	503	CLA	C11-C12-C13-C15
23	B	602	CLA	C16-C17-C18-C20
35	c	518	DGD	C7A-C8A-C9A-CAA
23	C	508	CLA	C5-C6-C7-C8
34	C	502	LMG	C15-C16-C17-C18
23	C	509	CLA	C5-C6-C7-C8
23	b	612	CLA	C10-C11-C12-C13
38	e	102	HEM	CAD-CBD-CGD-O2D
35	h	103	DGD	O1B-C1B-C2B-C3B
29	a	414[B]	PL9	C13-C14-C16-C17
24	a	406	PHO	C8-C10-C11-C12
23	c	512	CLA	CAA-CBA-CGA-O1A
31	d	406	LHG	C31-C32-C33-C34
33	B	630	LMT	C6-C7-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	a	403	CLA	C14-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C14
23	b	616	CLA	C14-C13-C15-C16
26	D	413	SQD	C31-C32-C33-C34
26	A	409	SQD	O47-C7-C8-C9
31	b	628	LHG	O9-C7-C8-C9
33	a	412	LMT	C2-C3-C4-C5
23	b	604	CLA	C4C-C3C-CAC-CBC
26	B	620	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C10-C11-C12-C13
31	L	101	LHG	O9-C7-C8-C9
38	e	102	HEM	CAA-CBA-CGA-O1A
23	B	612	CLA	CAA-CBA-CGA-O1A
23	c	514	CLA	CAA-CBA-CGA-O1A
26	f	101	SQD	O10-C23-C24-C25
31	A	416	LHG	O10-C23-C24-C25
35	c	518	DGD	O1B-C1B-C2B-C3B
29	d	405	PL9	C11-C12-C13-C14
23	B	612	CLA	C8-C10-C11-C12
33	M	103	LMT	C9-C10-C11-C12
31	A	416	LHG	O10-C23-O8-C6
25	C	517	BCR	C7-C8-C9-C10
23	C	514	CLA	CAA-CBA-CGA-O1A
31	d	406	LHG	O10-C23-C24-C25
34	D	412	LMG	O9-C10-C11-C12
35	H	102	DGD	O1B-C1B-C2B-C3B
35	C	518	DGD	C8A-C9A-CAA-CBA
35	C	518	DGD	C5D-C6D-O5D-C1E
35	h	103	DGD	C2G-C3G-O3G-C1D
34	M	101	LMG	O1-C7-C8-O7
23	B	613	CLA	CAA-CBA-CGA-O1A
23	b	612	CLA	CAA-CBA-CGA-O1A
31	a	419	LHG	O8-C23-C24-C25
35	c	520	DGD	C3B-C4B-C5B-C6B
34	C	502	LMG	O9-C10-C11-C12
34	Z	101	LMG	O9-C10-C11-C12
29	a	414[B]	PL9	C11-C12-C13-C14
35	C	519	DGD	C1B-C2B-C3B-C4B
34	m	101	LMG	C17-C18-C19-C20
23	C	513	CLA	C8-C10-C11-C12
23	b	609	CLA	C15-C16-C17-C18
23	c	503	CLA	C8-C10-C11-C12
23	c	511	CLA	C8-C10-C11-C12
23	c	513	CLA	C15-C16-C17-C18
23	b	613	CLA	CAA-CBA-CGA-O2A
34	z	101	LMG	O7-C10-C11-C12
38	E	102	HEM	C2B-C3B-CAB-CBB
33	M	102	LMT	O5B-C5B-C6B-O6B
23	B	603	CLA	C16-C17-C18-C20
23	C	508	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	A	415	PHO	CAD-CBD-CGD-O2D
35	H	102	DGD	C8A-C9A-CAA-CBA
34	c	521	LMG	O7-C10-C11-C12
35	c	519	DGD	C1A-C2A-C3A-C4A
35	C	520	DGD	O6D-C5D-C6D-O5D
23	b	614	CLA	C2-C1-O2A-CGA
31	E	101	LHG	C25-C26-C27-C28
29	A	413[A]	PL9	C46-C47-C48-C49
35	C	518	DGD	CAB-CBB-CCB-CDB
31	D	407	LHG	C33-C34-C35-C36
34	C	522	LMG	C35-C36-C37-C38
34	M	101	LMG	C37-C38-C39-C40
23	b	601	CLA	C8-C10-C11-C12
29	A	413[B]	PL9	C45-C44-C46-C47
31	A	416	LHG	C24-C23-O8-C6
34	C	521	LMG	O7-C10-C11-C12
31	a	419	LHG	O10-C23-C24-C25
34	d	411	LMG	O7-C10-C11-C12
34	M	101	LMG	C14-C15-C16-C17

There are no ring outliers.

154 monomers are involved in 364 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	406	LHG	3	0
23	c	509	CLA	3	0
23	C	505	CLA	4	0
23	b	603	CLA	3	0
23	C	510	CLA	4	0
26	D	413	SQD	3	0
23	A	404	CLA	4	0
23	b	610	CLA	2	0
40	v	202	HEC	1	0
31	E	101	LHG	5	0
24	A	406	PHO	1	0
27	B	626	GOL	1	0
25	Y	101	BCR	2	0
34	C	502	LMG	4	0
33	M	102	LMT	2	0
23	C	509	CLA	1	0
31	d	407	LHG	3	0
23	b	605	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	411	HTG	2	0
31	A	416	LHG	4	0
23	c	510	CLA	4	0
23	d	402	CLA	2	0
23	B	616	CLA	4	0
23	B	614	CLA	2	0
33	a	412	LMT	1	0
25	B	619	BCR	5	0
23	c	508	CLA	3	0
34	C	521	LMG	3	0
34	M	101	LMG	2	0
25	h	102	BCR	5	0
23	b	612	CLA	2	0
25	c	516	BCR	5	0
34	d	411	LMG	4	0
25	b	619	BCR	6	0
29	A	413[A]	PL9	5	0
27	b	627	GOL	1	0
25	C	517	BCR	3	0
23	d	403	CLA	3	0
31	D	408	LHG	3	0
35	c	519	DGD	1	0
23	B	606	CLA	2	0
23	C	513	CLA	1	0
32	c	523	HTG	1	0
25	k	102	BCR	2	0
33	M	103	LMT	1	0
23	a	405	CLA	2	0
34	C	522	LMG	3	0
26	L	102	SQD	1	0
38	e	102	HEM	4	0
23	c	512	CLA	5	0
34	z	101	LMG	2	0
23	A	403	CLA	3	0
23	C	515	CLA	1	0
23	B	601	CLA	4	0
33	b	626	LMT	1	0
25	a	408	BCR	1	0
29	A	413[B]	PL9	8	0
32	b	624	HTG	1	0
23	b	609	CLA	2	0
23	b	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	624	HTG	1	0
35	C	520	DGD	2	0
23	c	506	CLA	2	0
29	a	414[A]	PL9	3	0
25	C	516	BCR	2	0
25	B	631	BCR	5	0
25	H	101	BCR	3	0
26	a	409	SQD	3	0
35	c	518	DGD	2	0
23	B	604	CLA	3	0
35	C	518	DGD	5	0
33	B	629	LMT	1	0
34	Z	101	LMG	2	0
23	c	513	CLA	4	0
32	h	101	HTG	1	0
33	C	526	LMT	1	0
23	A	405	CLA	4	0
25	D	405	BCR	1	0
24	A	415	PHO	1	0
23	b	601	CLA	1	0
23	c	507	CLA	7	0
40	V	201	HEC	2	0
23	A	407	CLA	4	0
23	B	612	CLA	3	0
25	T	101	BCR	8	0
29	d	405	PL9	1	0
27	c	502	GOL	1	0
23	B	602	CLA	2	0
26	A	409	SQD	3	0
32	B	621	HTG	3	0
23	D	403	CLA	2	0
25	K	101	BCR	1	0
35	c	520	DGD	2	0
26	f	101	SQD	3	0
23	b	602	CLA	2	0
31	a	419	LHG	3	0
26	B	620	SQD	3	0
31	D	407	LHG	3	0
35	C	519	DGD	5	0
23	b	606	CLA	3	0
23	b	616	CLA	3	0
23	c	504	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	610	CLA	1	0
23	c	515	CLA	4	0
29	D	406	PL9	3	0
26	a	411	SQD	1	0
24	a	416	PHO	1	0
23	C	504	CLA	7	0
23	c	514	CLA	6	0
32	B	622	HTG	2	0
38	E	102	HEM	3	0
33	a	418	LMT	3	0
25	k	101	BCR	2	0
23	C	507	CLA	2	0
23	a	404	CLA	6	0
23	c	505	CLA	7	0
23	C	512	CLA	5	0
23	b	614	CLA	1	0
23	C	508	CLA	6	0
23	B	603	CLA	1	0
25	b	617	BCR	1	0
31	d	408	LHG	7	0
23	D	404	CLA	2	0
29	a	414[B]	PL9	9	0
25	B	617	BCR	1	0
23	B	607	CLA	3	0
25	A	408	BCR	2	0
23	B	613	CLA	4	0
23	B	615	CLA	2	0
23	C	514	CLA	1	0
25	c	517	BCR	2	0
23	b	604	CLA	7	0
24	a	406	PHO	1	0
23	a	407	CLA	3	0
27	a	410	GOL	1	0
25	B	618	BCR	4	0
32	b	621	HTG	1	0
23	a	403	CLA	2	0
23	b	615	CLA	2	0
35	H	102	DGD	1	0
23	C	506	CLA	3	0
33	D	402	LMT	2	0
23	c	503	CLA	3	0
23	B	605	CLA	4	0

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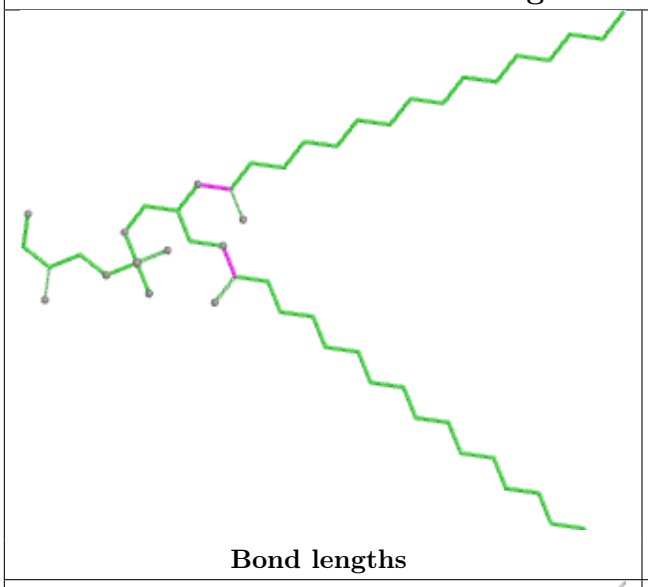
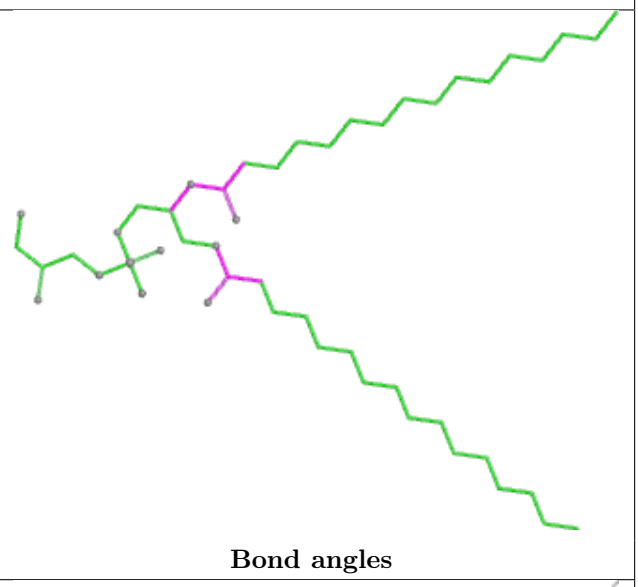
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	618	BCR	4	0
31	L	101	LHG	3	0
34	a	417	LMG	4	0
23	b	613	CLA	4	0
25	d	404	BCR	4	0
23	c	511	CLA	1	0
23	C	511	CLA	3	0
27	v	201	GOL	1	0
33	F	101	LMT	1	0
23	C	503	CLA	3	0

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

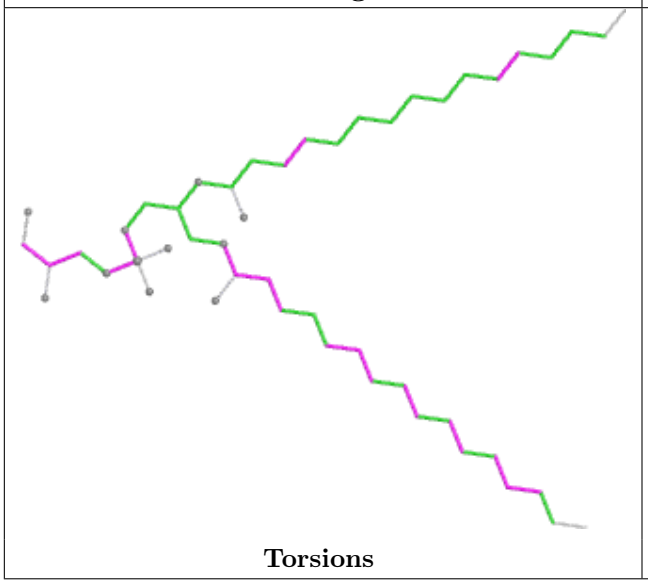
Ligand LHG d 406



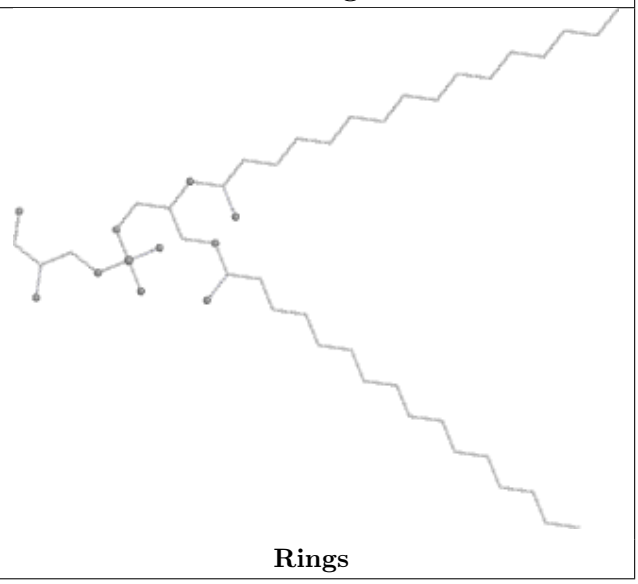
Bond lengths



Bond angles

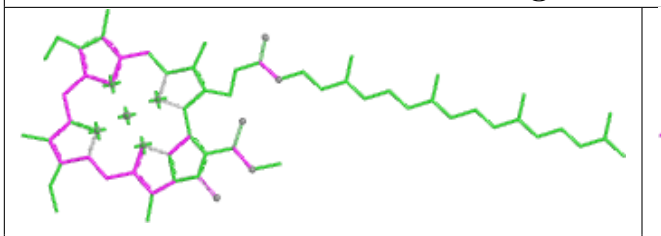


Torsions

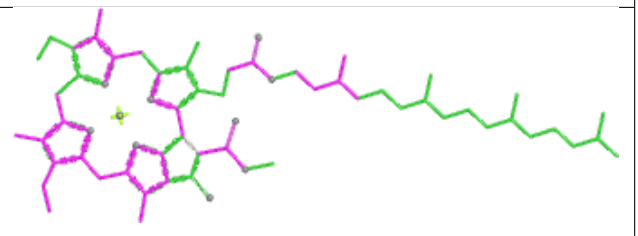


Rings

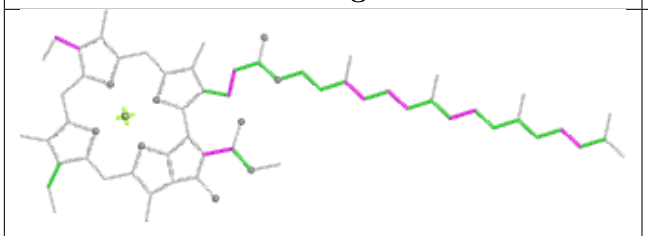
Ligand CLA c 509



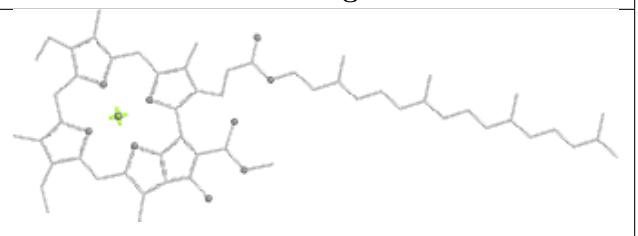
Bond lengths



Bond angles

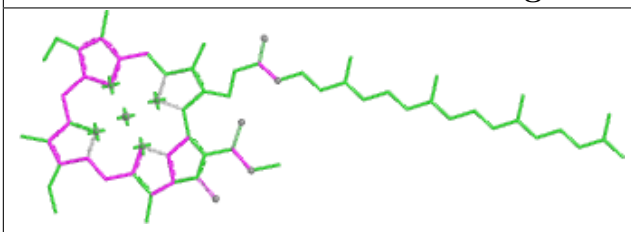


Torsions

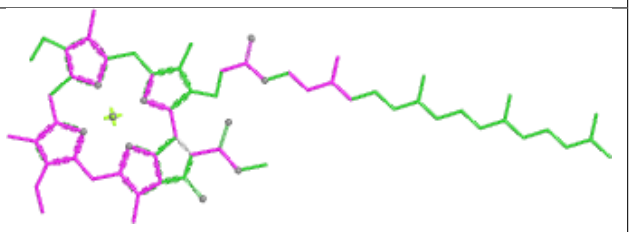


Rings

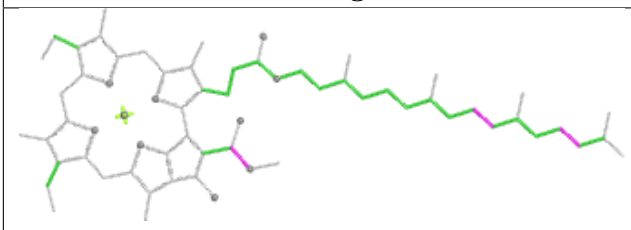
Ligand CLA C 505



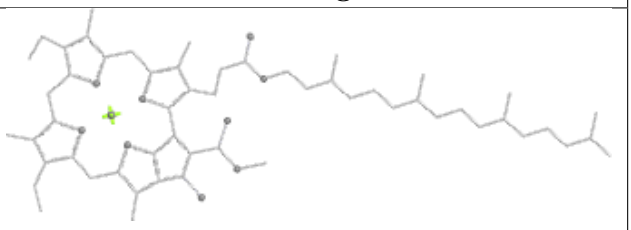
Bond lengths



Bond angles

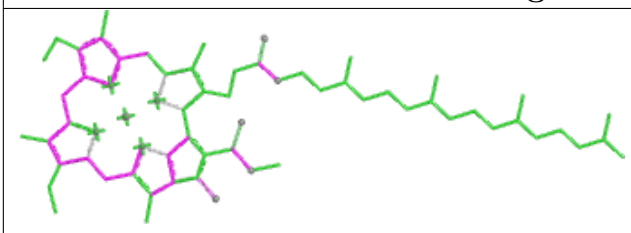


Torsions

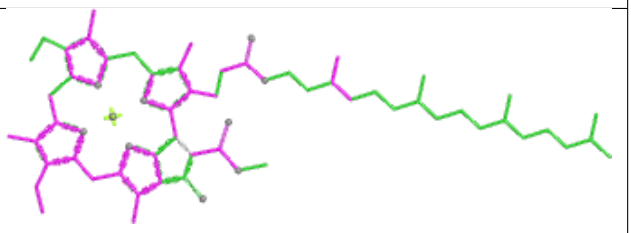


Rings

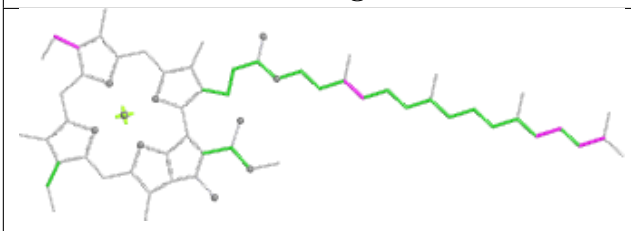
Ligand CLA b 603



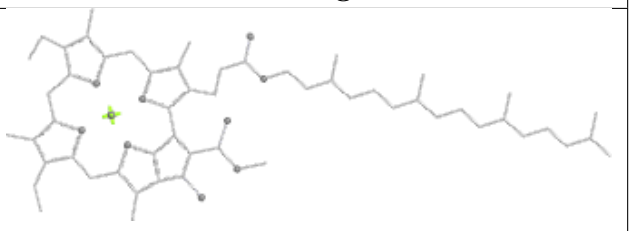
Bond lengths



Bond angles

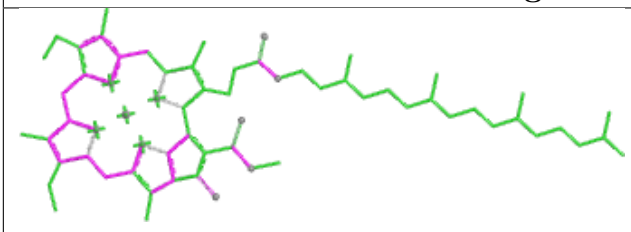


Torsions



Rings

Ligand CLA C 510



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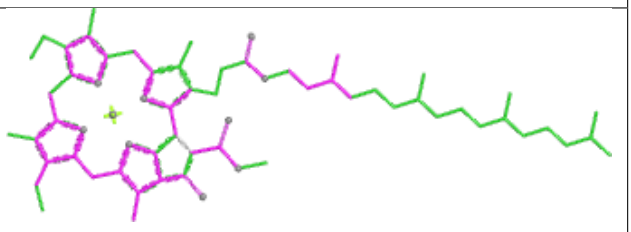
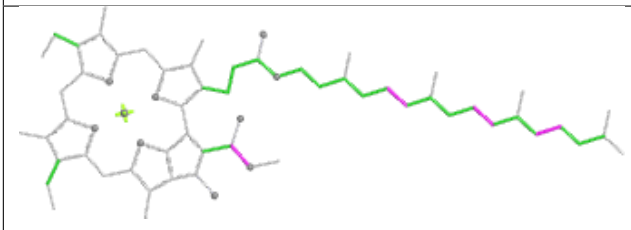


Bond angles



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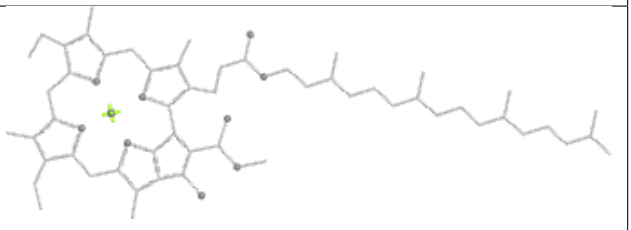
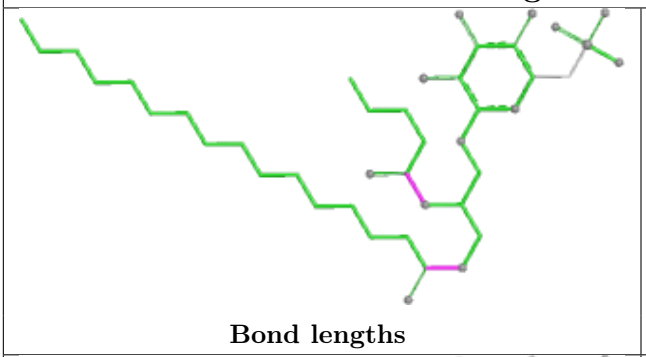


Rings

Ligand SQD D 413



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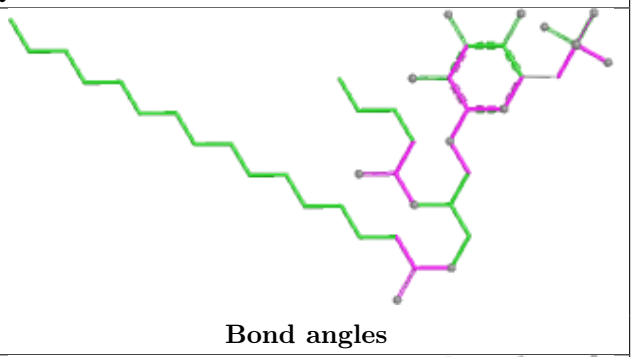

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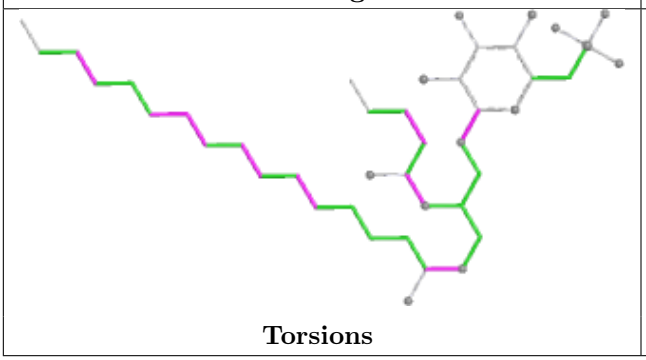

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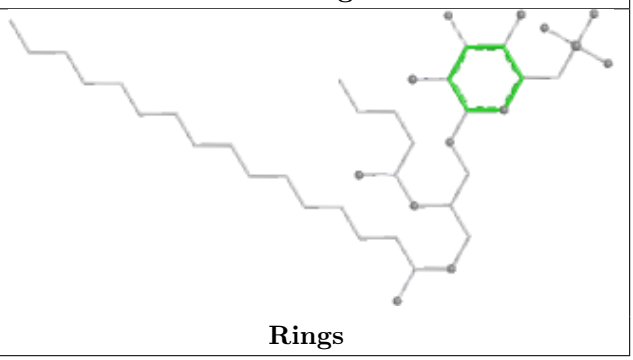
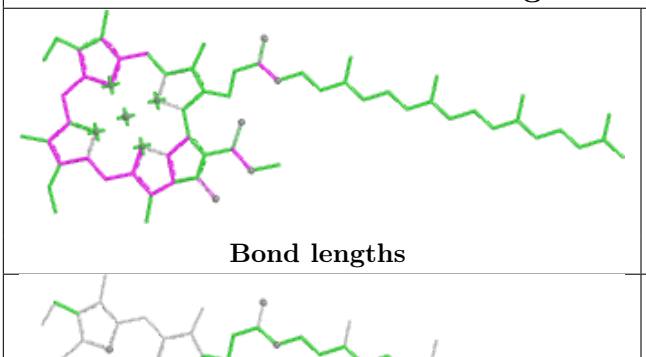


Rings

Ligand CLA A 404



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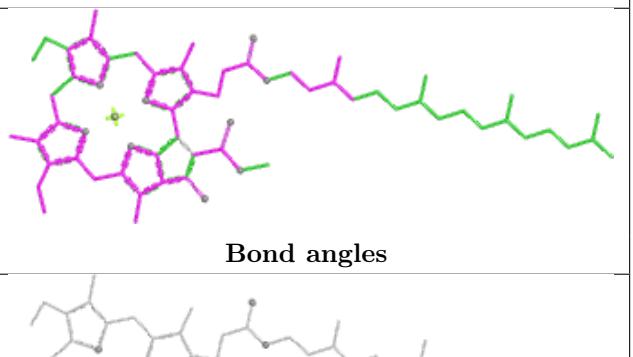

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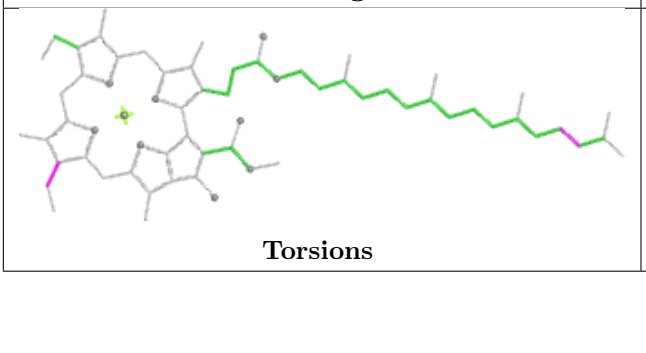

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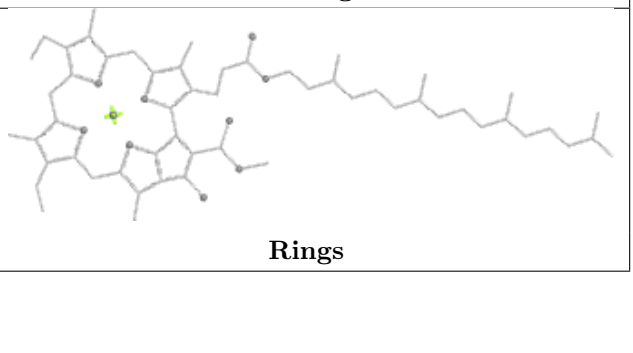
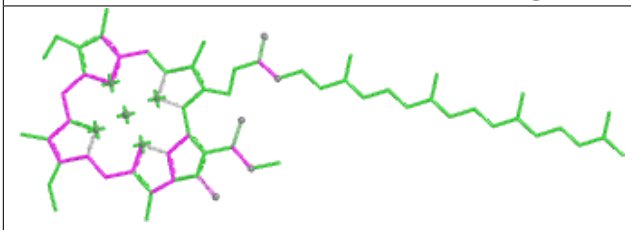


Rings

Ligand CLA b 610



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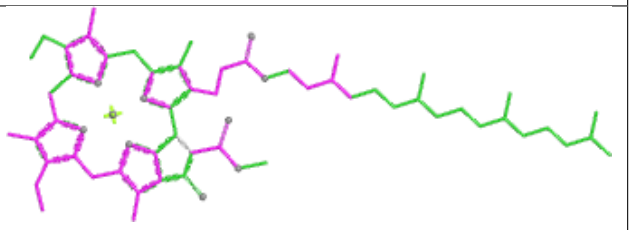

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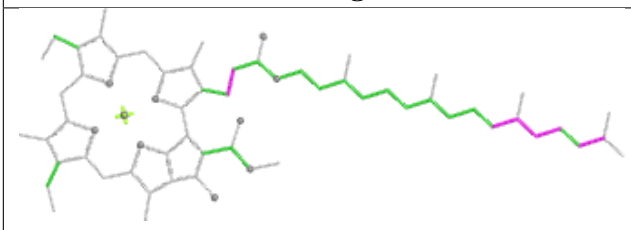

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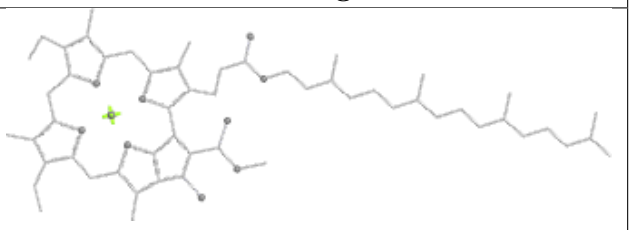

Rings

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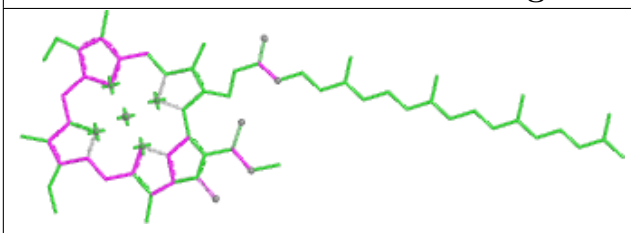

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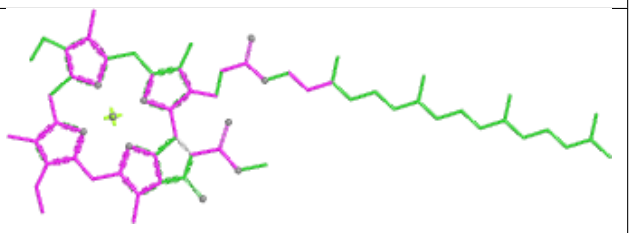

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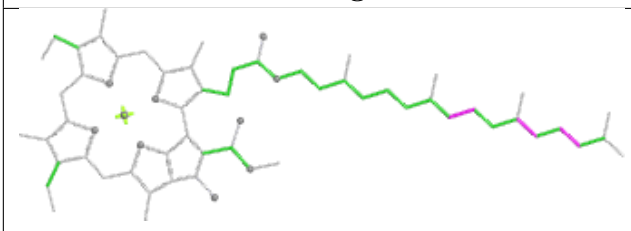

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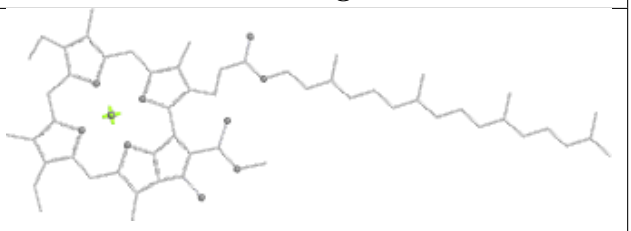
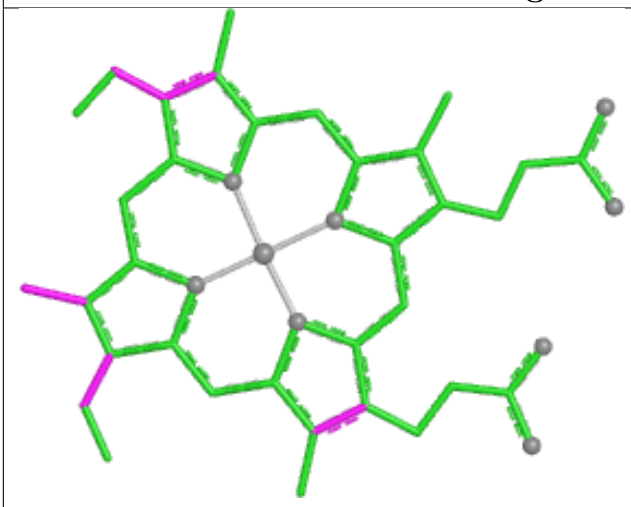


Rings

Ligand HEC v 202



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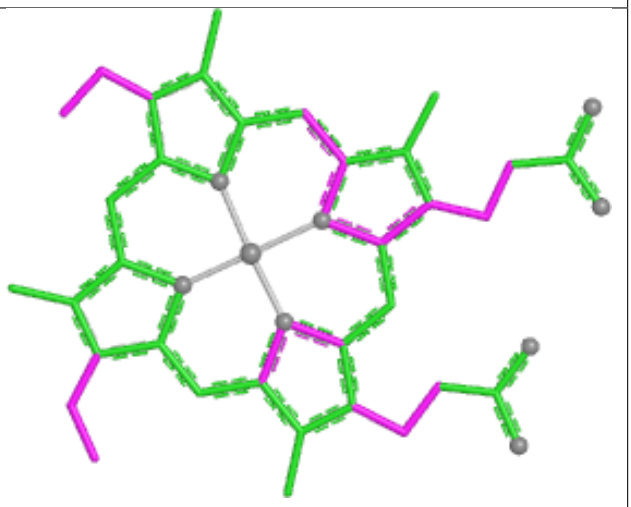

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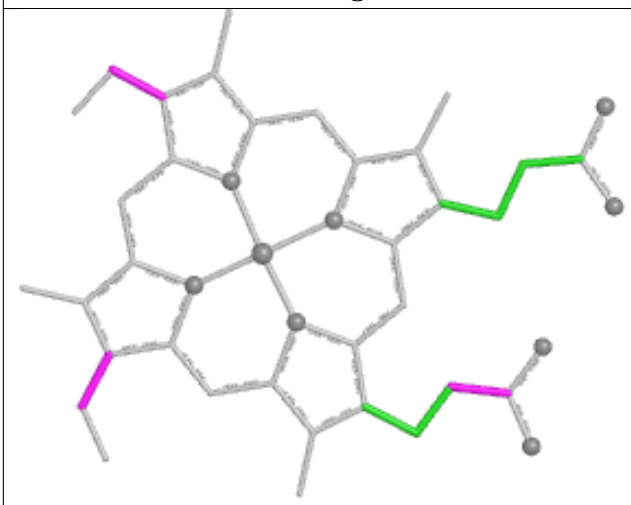

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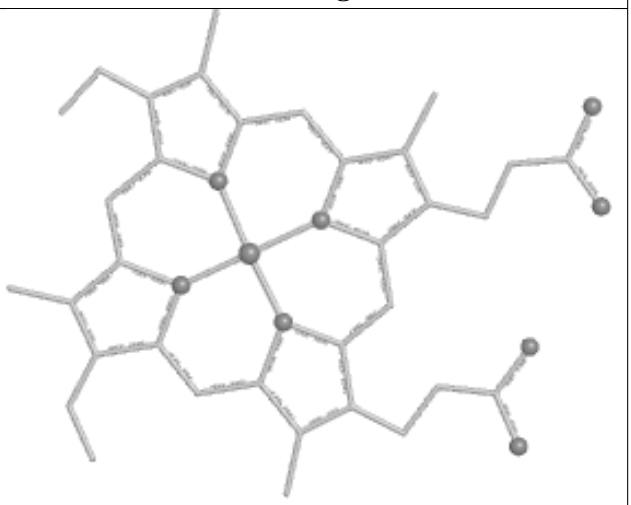
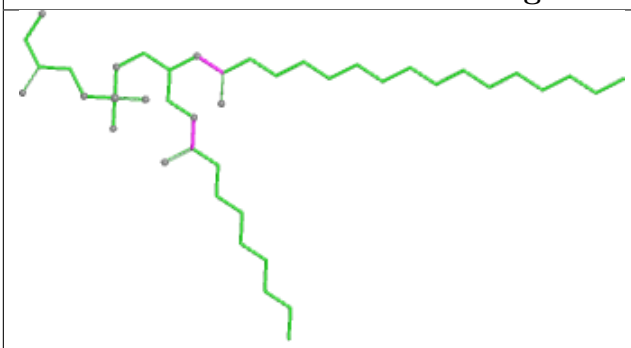


Rings

Ligand LHG E 101



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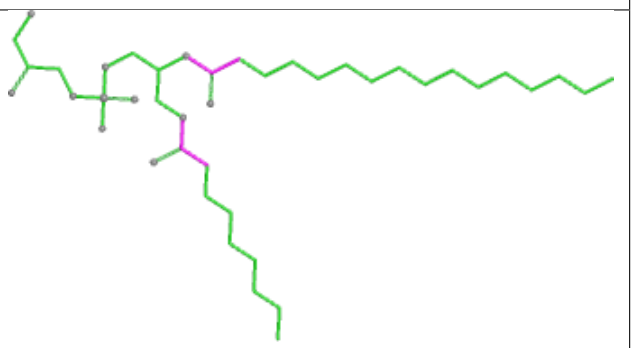

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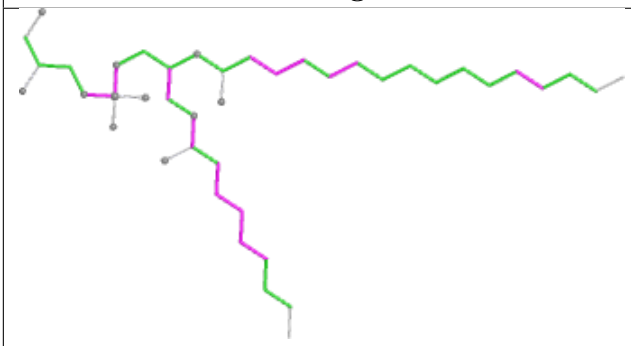
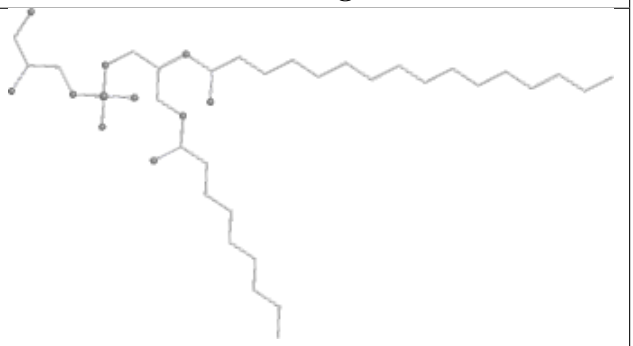
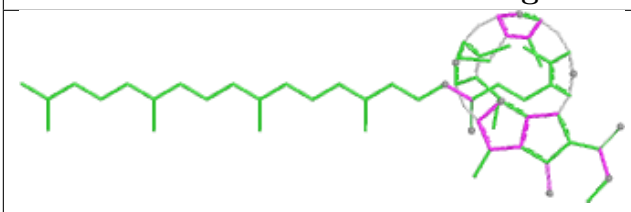


Torsions



Rings

Ligand PHO A 406



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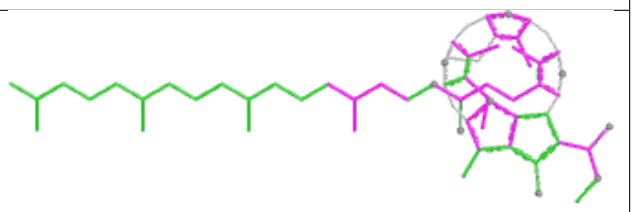
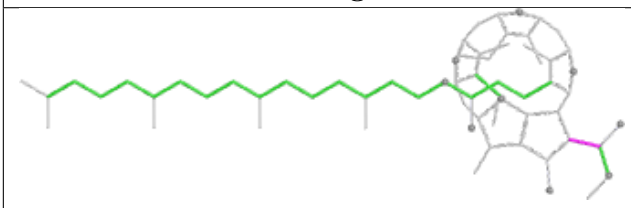


Bond angles



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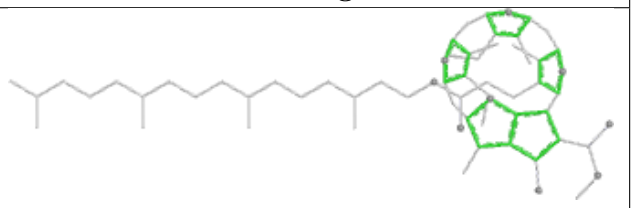
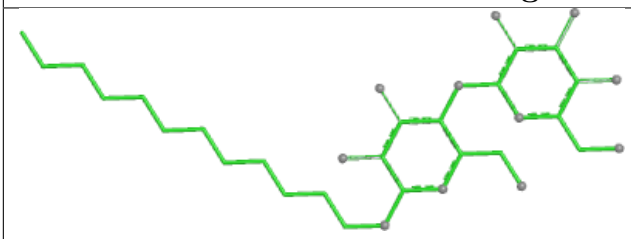


Rings

Ligand LMT B 627



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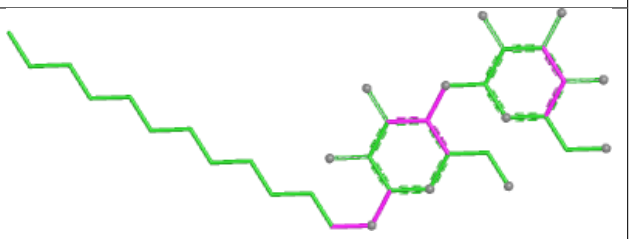
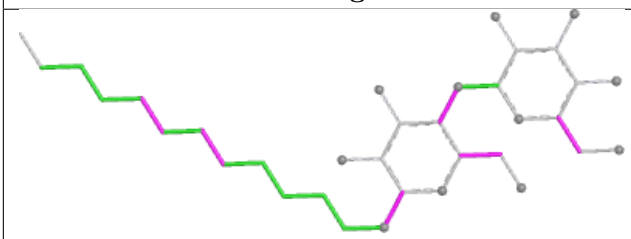


Bond angles



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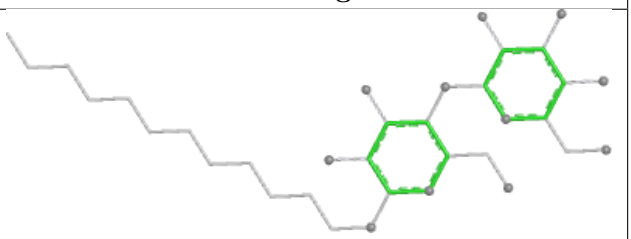
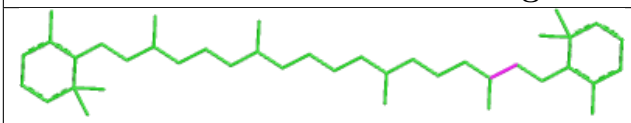


Rings

Ligand BCR Y 101



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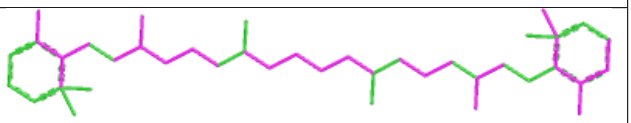
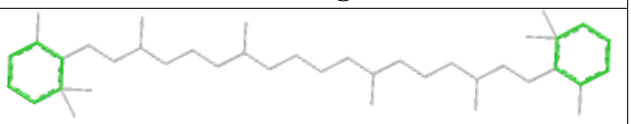


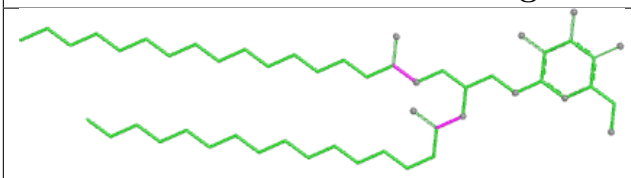
Bond angles

Torsions

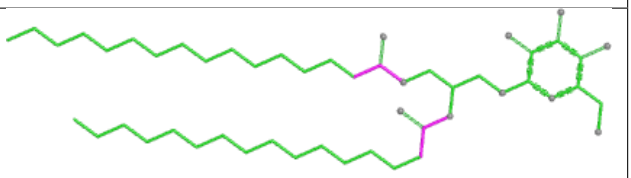


Rings

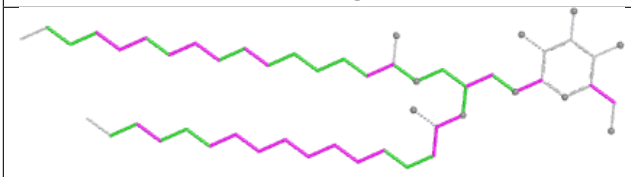
Ligand LMG C 502



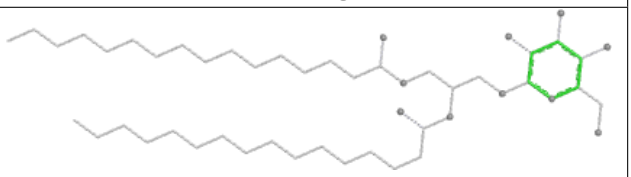
Bond lengths



Bond angles

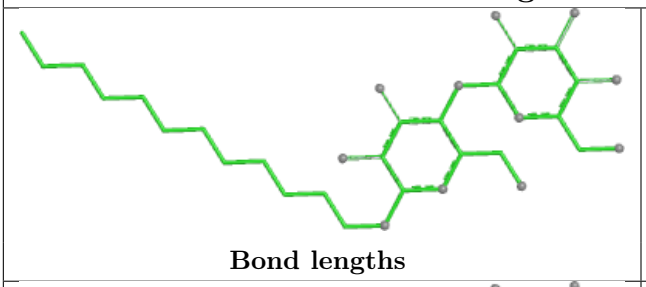


Torsions



Rings

Ligand LMT M 102



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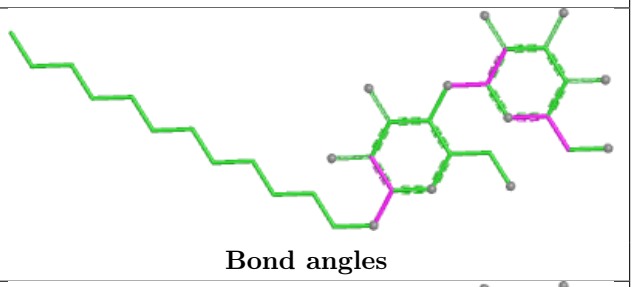
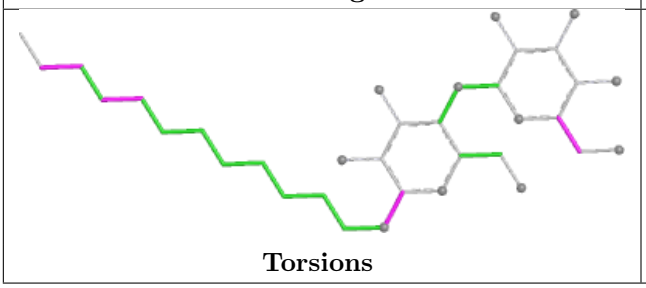


Bond angles



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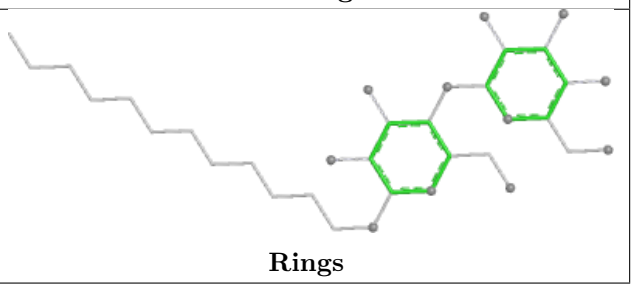
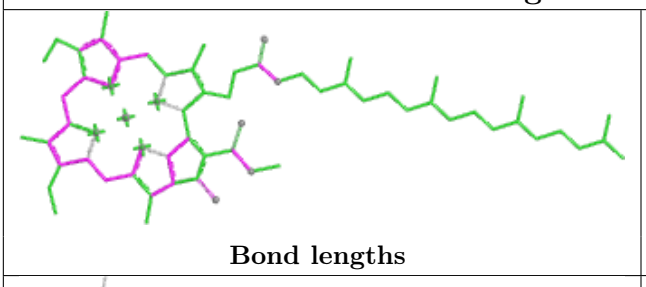


Rings

Ligand CLA C 509



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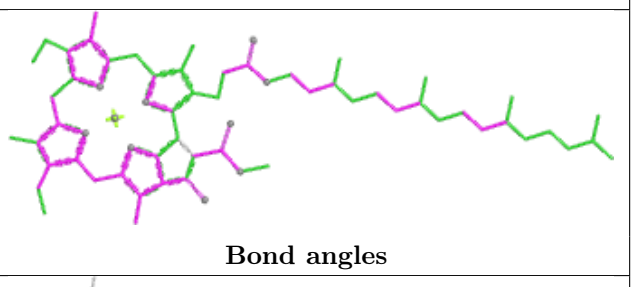
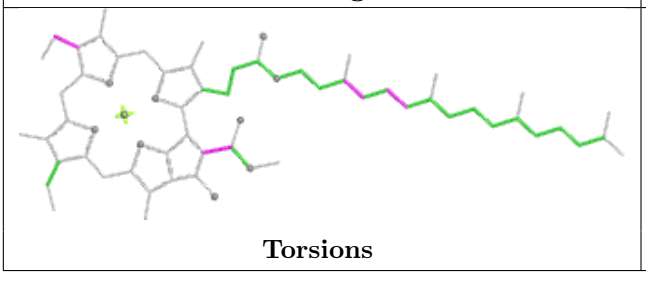
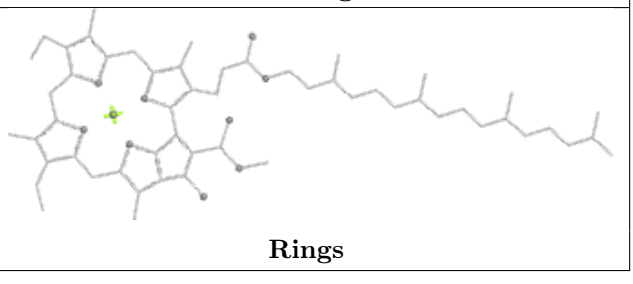


Bond angles

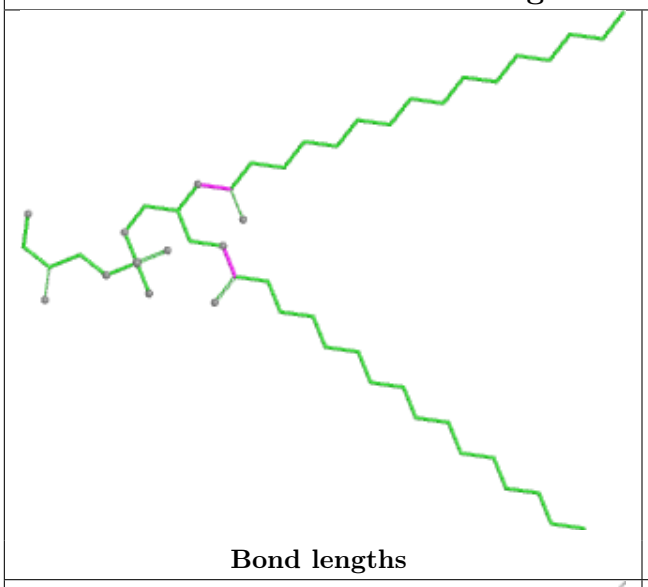


Torsions



Rings

Ligand LHG d 407



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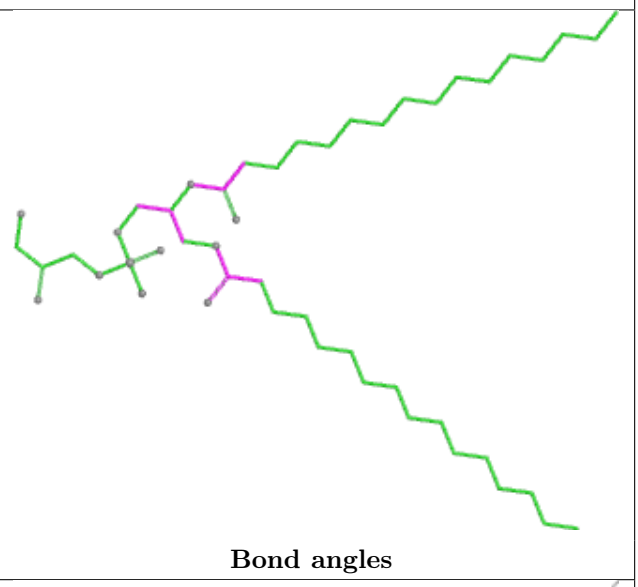
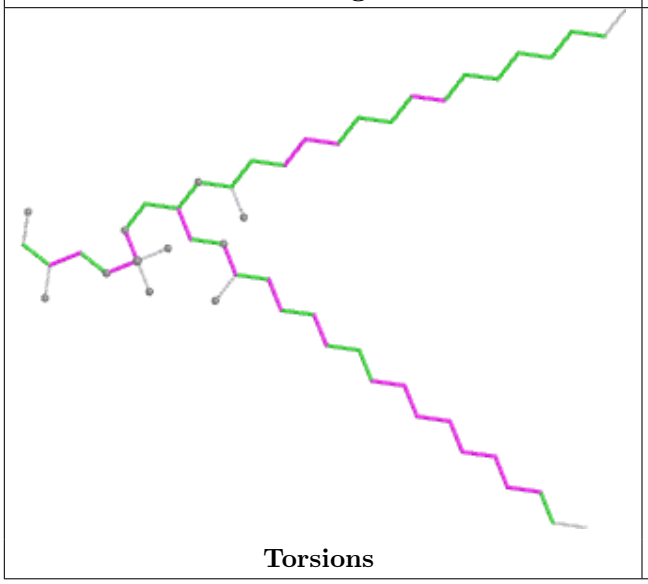
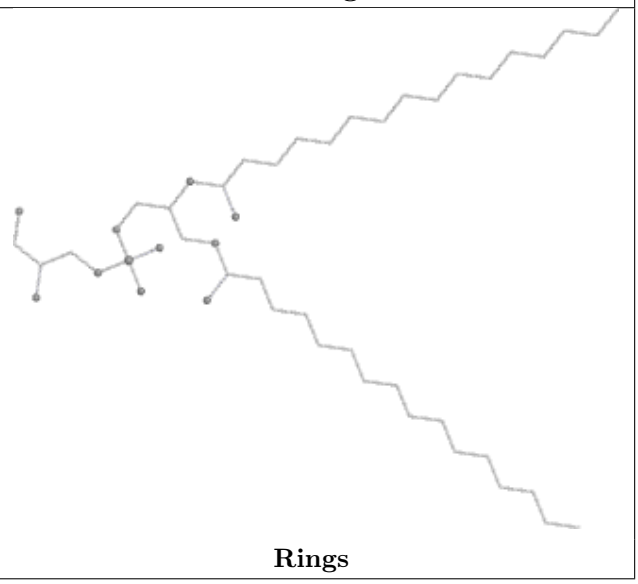


Bond angles

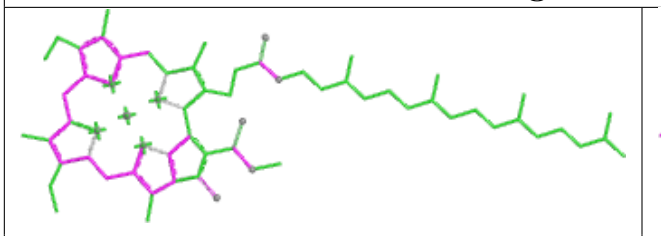


Torsions



Rings

Ligand CLA b 605



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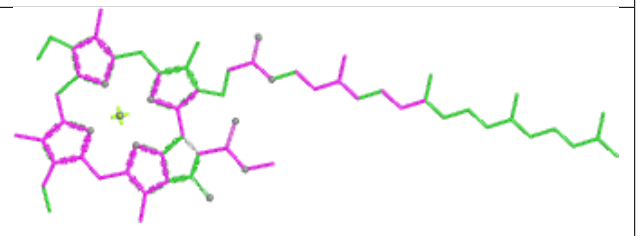
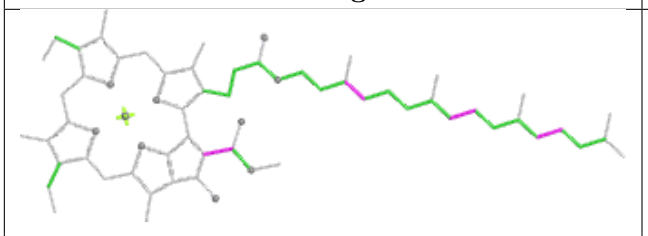


Bond angles



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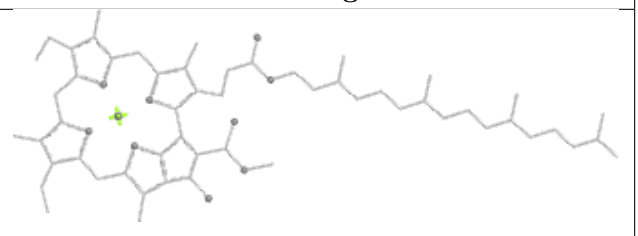
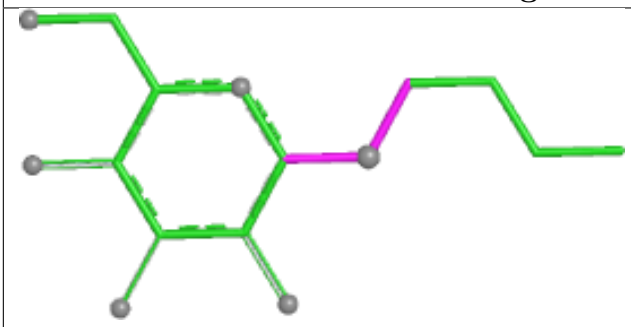


Rings

Ligand HTG D 411



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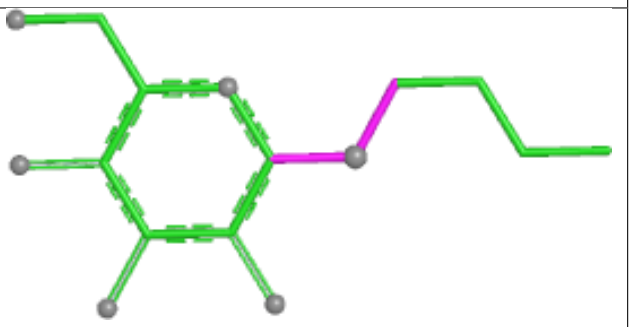
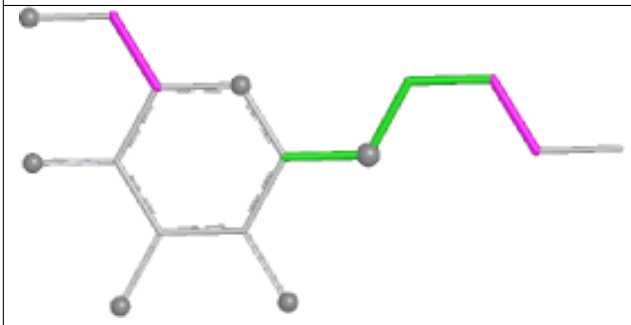


Bond angles



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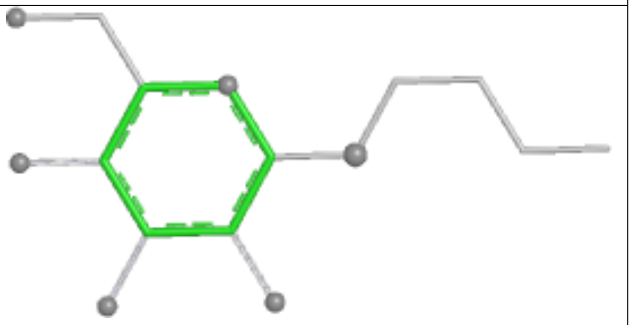
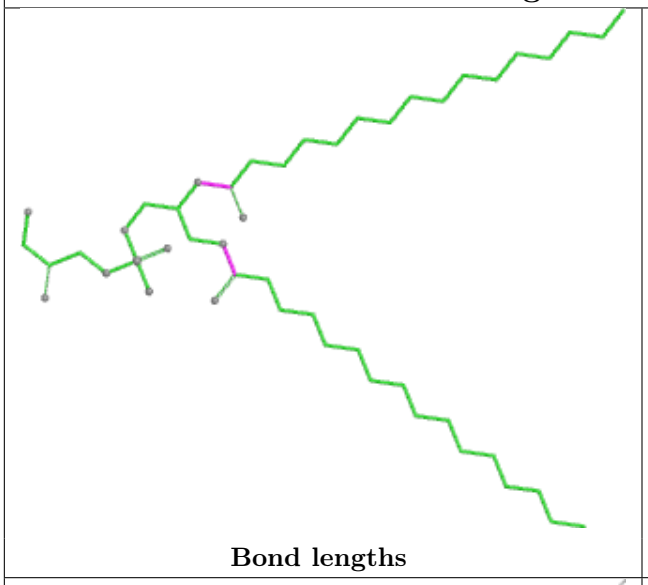


Rings

Ligand LHG A 416



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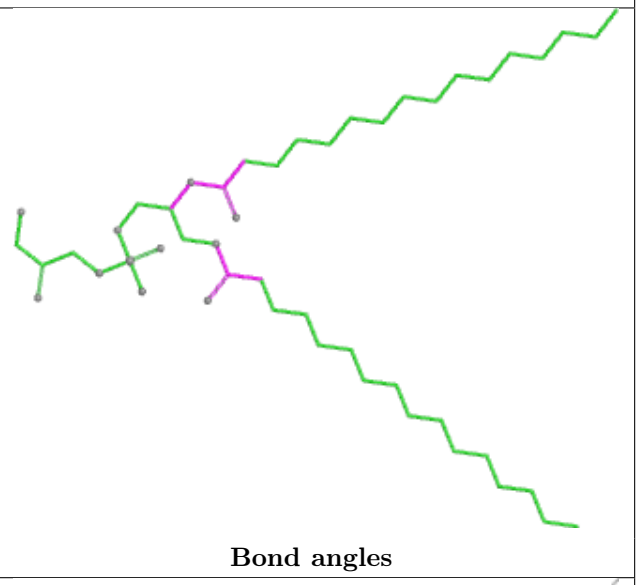
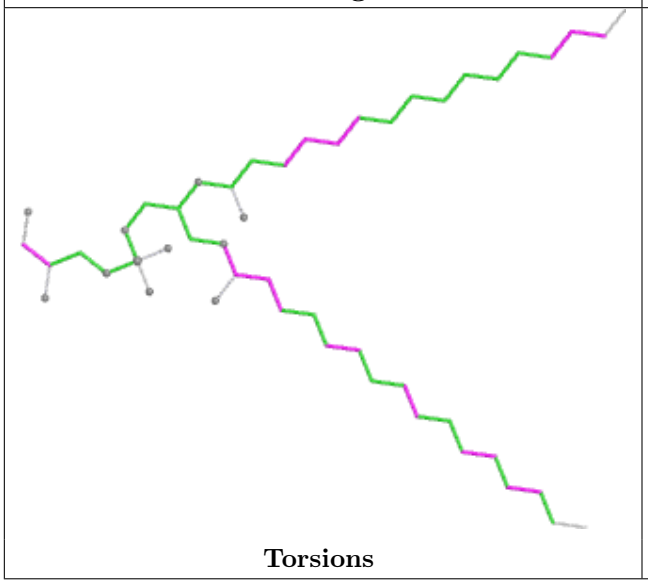


Bond angles



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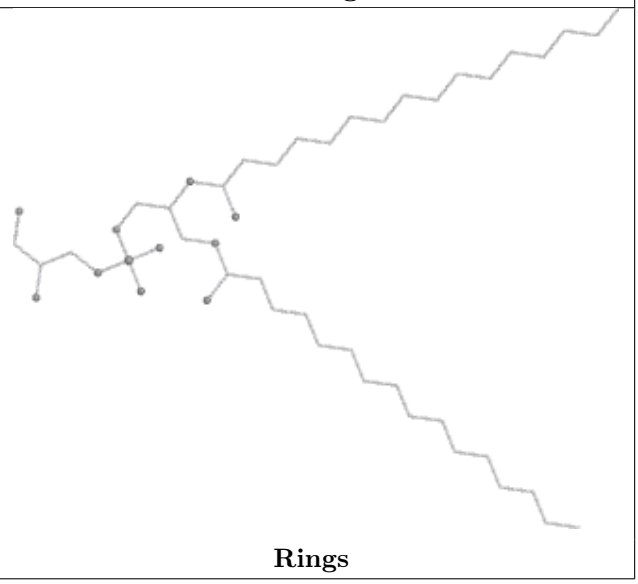
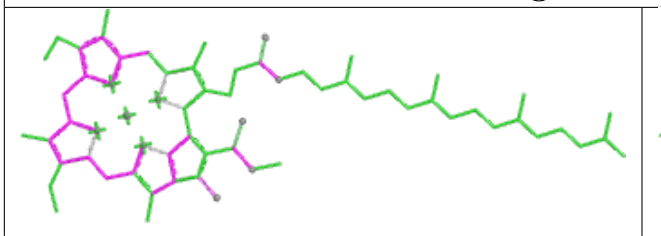


Rings

Ligand CLA c 510



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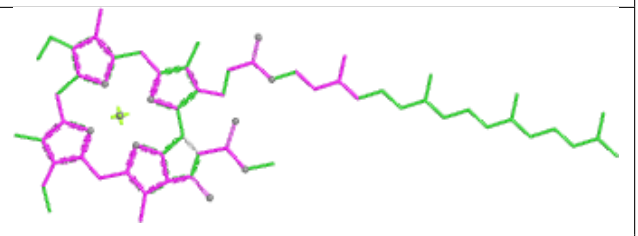
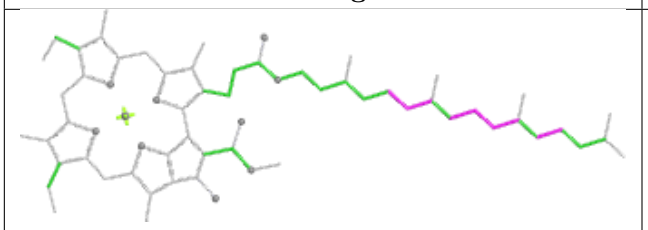


Bond angles



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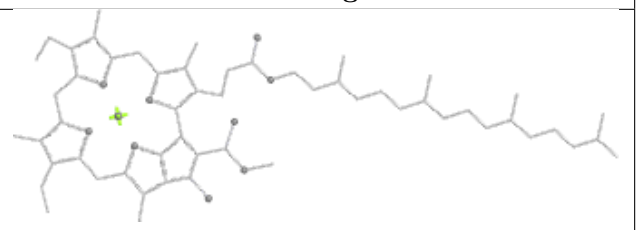
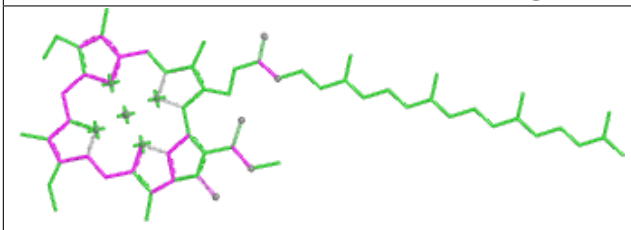


Rings

Ligand CLA d 402



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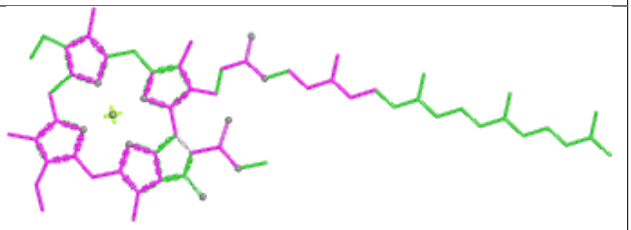
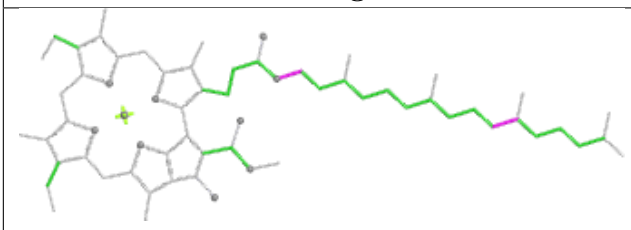


Bond angles



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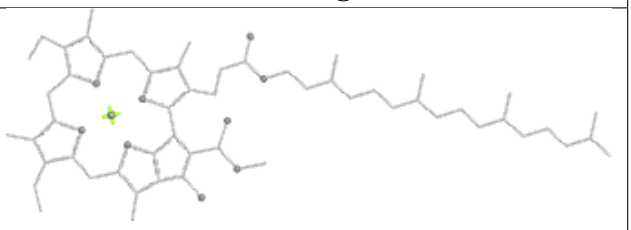
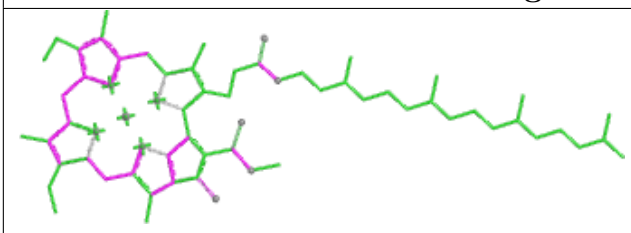


Rings

Ligand CLA B 616



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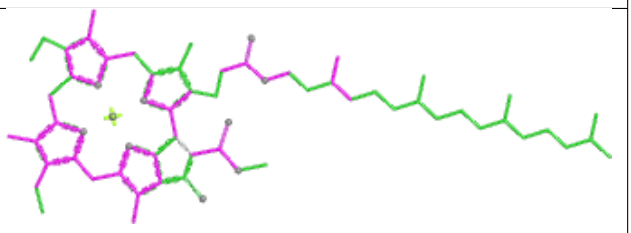
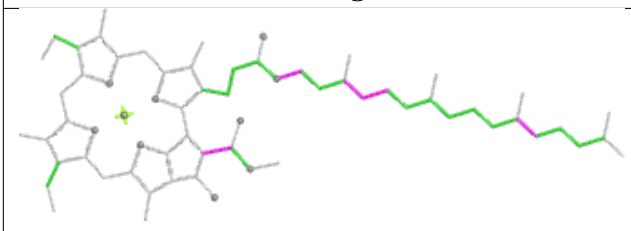
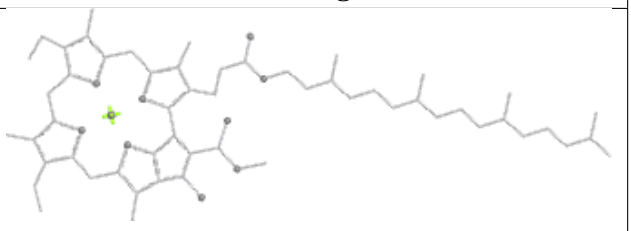


Bond angles



Torsions



Rings

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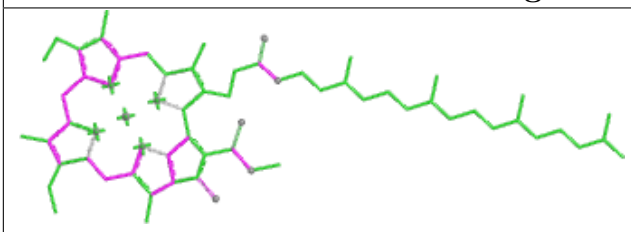

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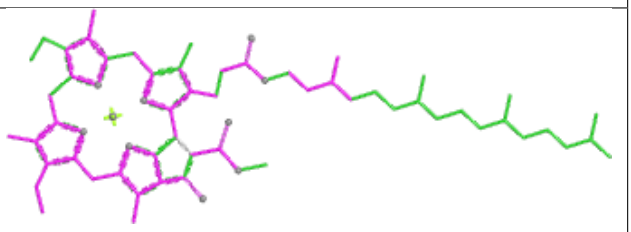
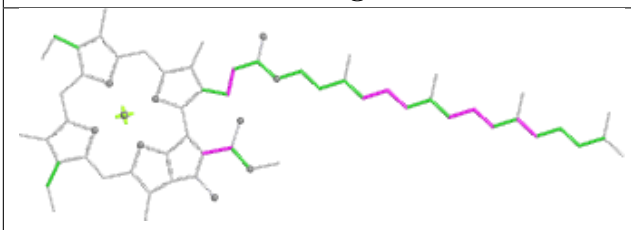


Bond angles



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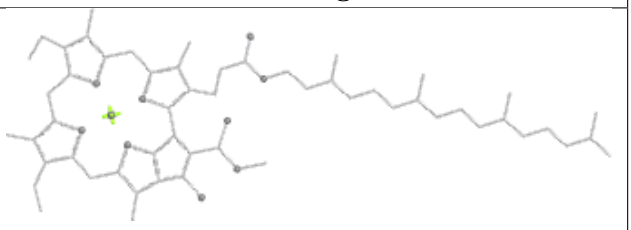
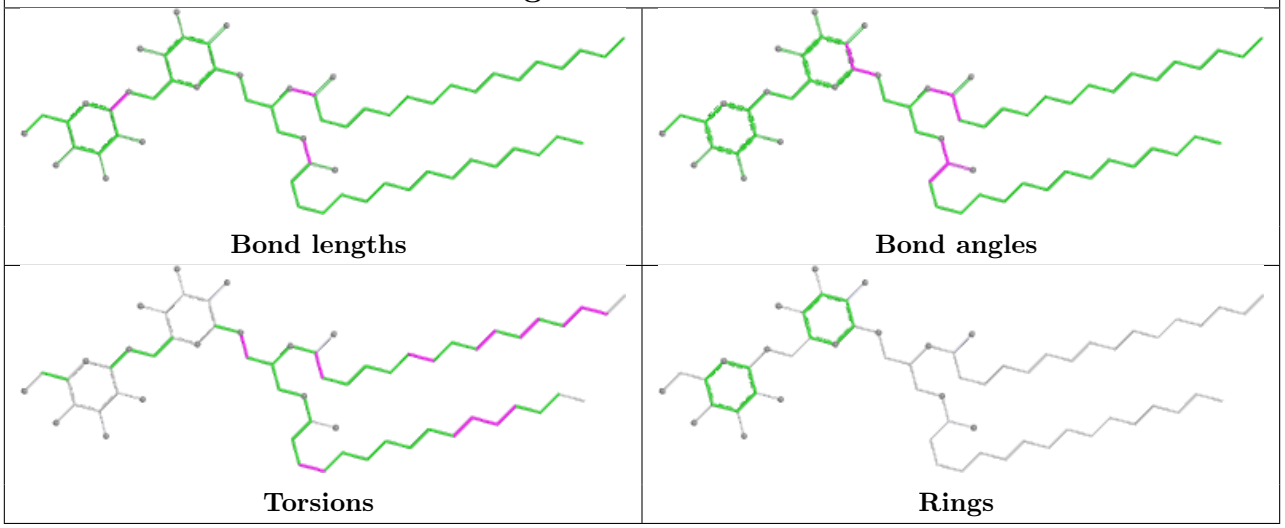
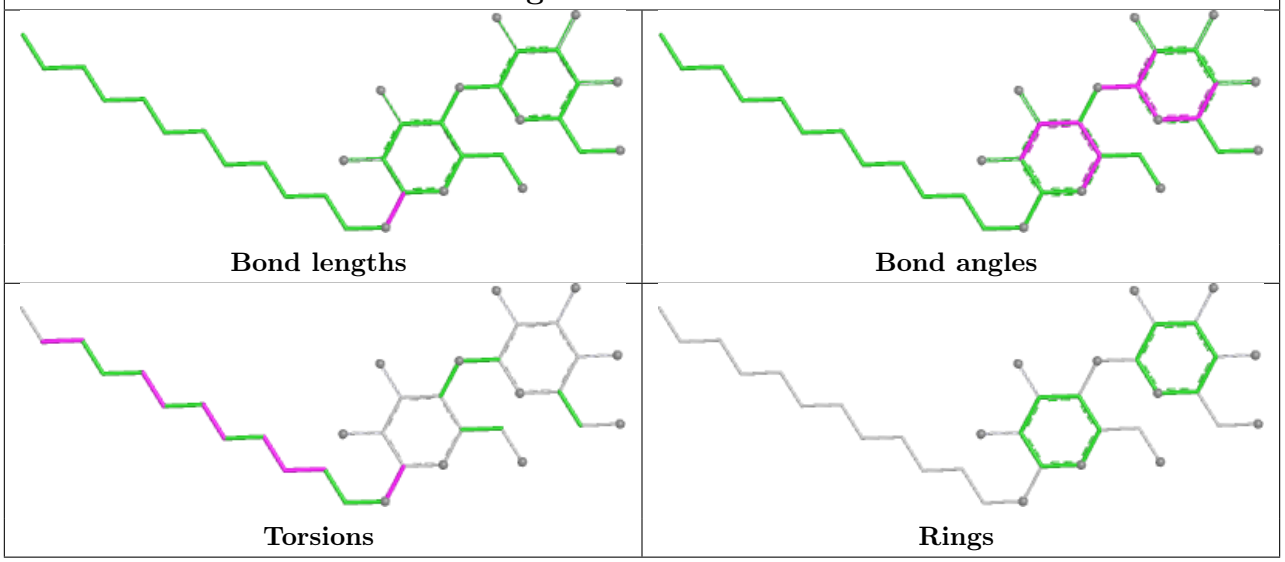


Rings

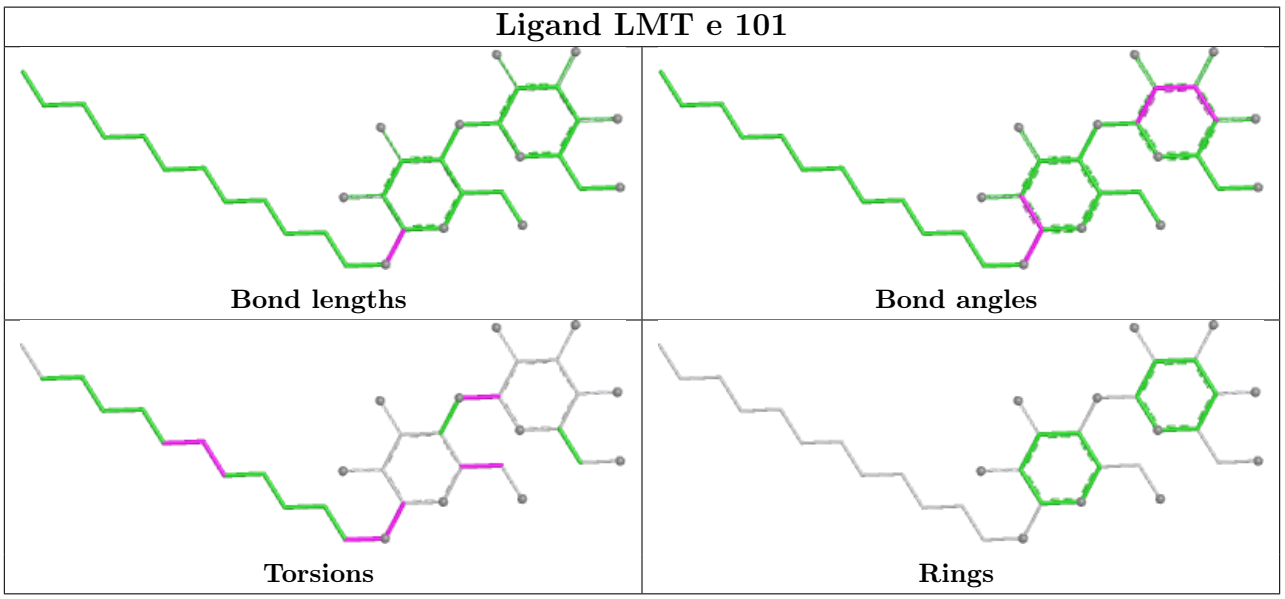
Ligand DGD h 103



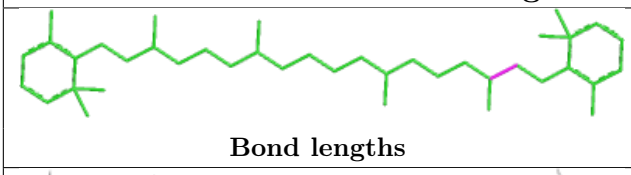
Ligand LMT a 412



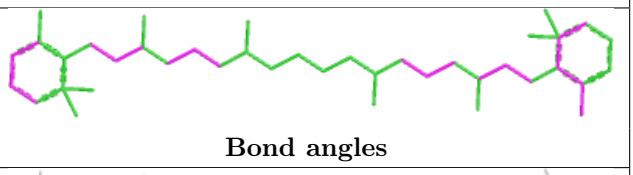
Ligand LMT e 101



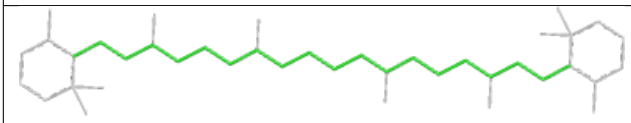
Ligand BCR B 619



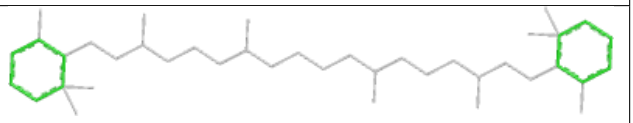
Bond lengths



Bond angles

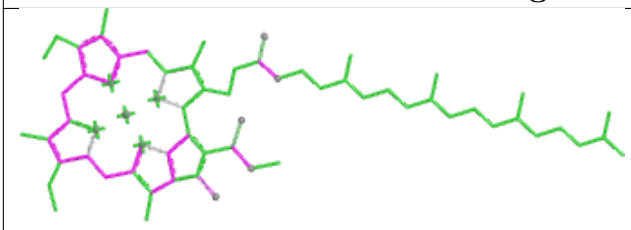


Torsions

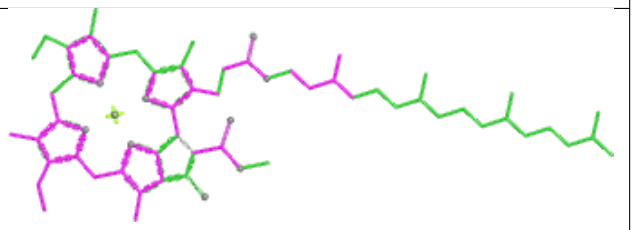


Rings

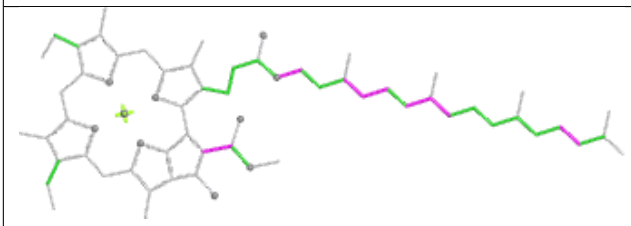
Ligand CLA c 508



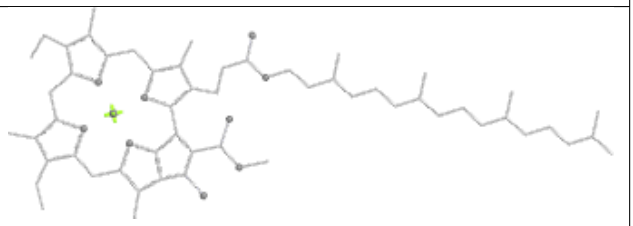
Bond lengths



Bond angles

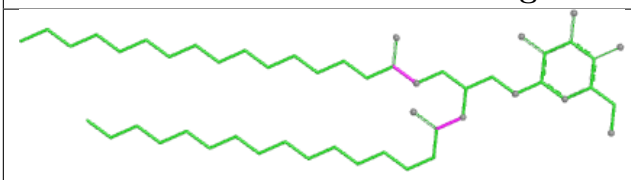


Torsions

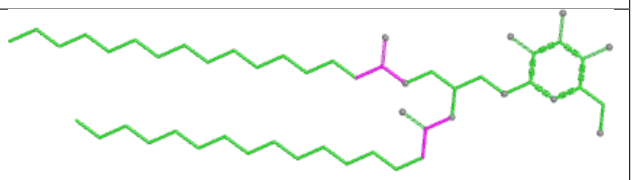


Rings

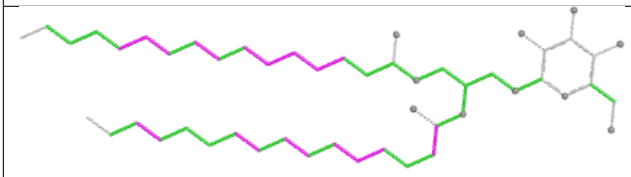
Ligand LMG C 521



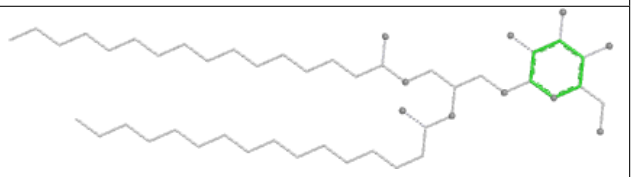
Bond lengths



Bond angles

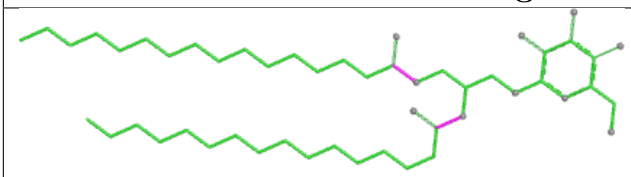


Torsions

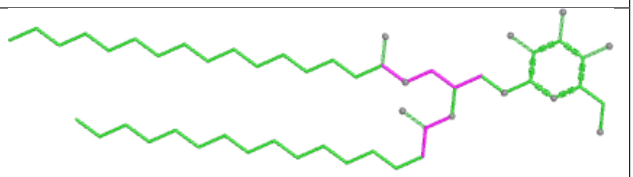


Rings

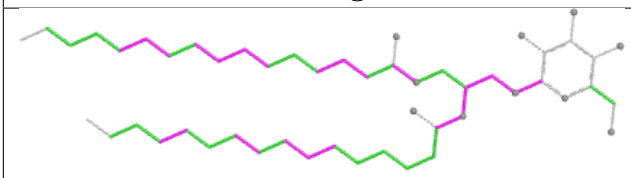
Ligand LMG M 101



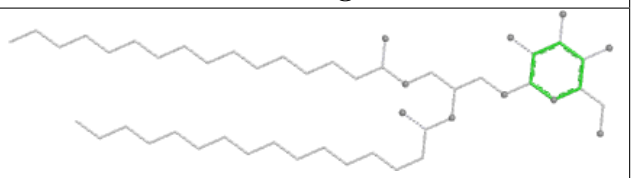
Bond lengths



Bond angles

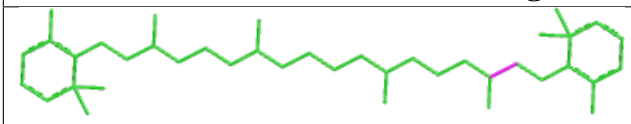


Torsions

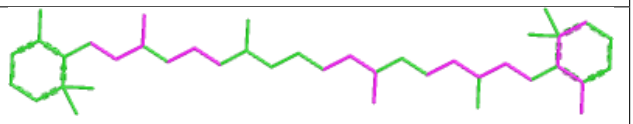


Rings

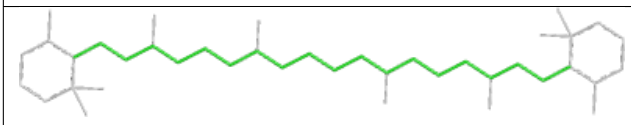
Ligand BCR h 102



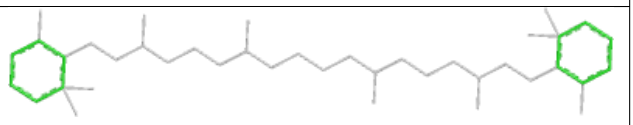
Bond lengths



Bond angles

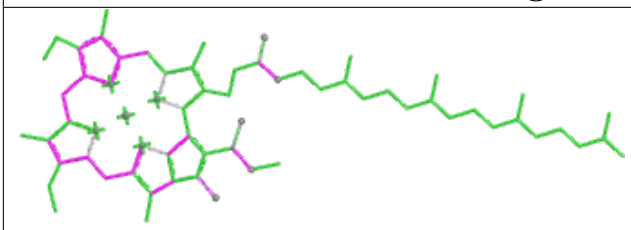


Torsions

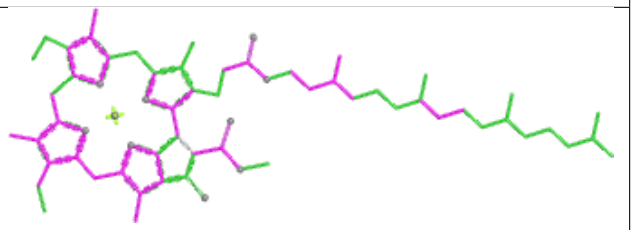


Rings

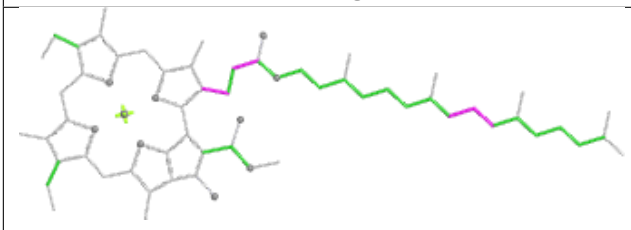
Ligand CLA b 612



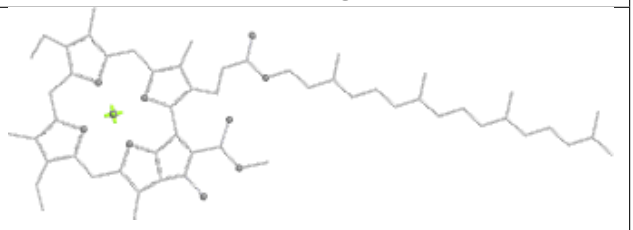
Bond lengths



Bond angles

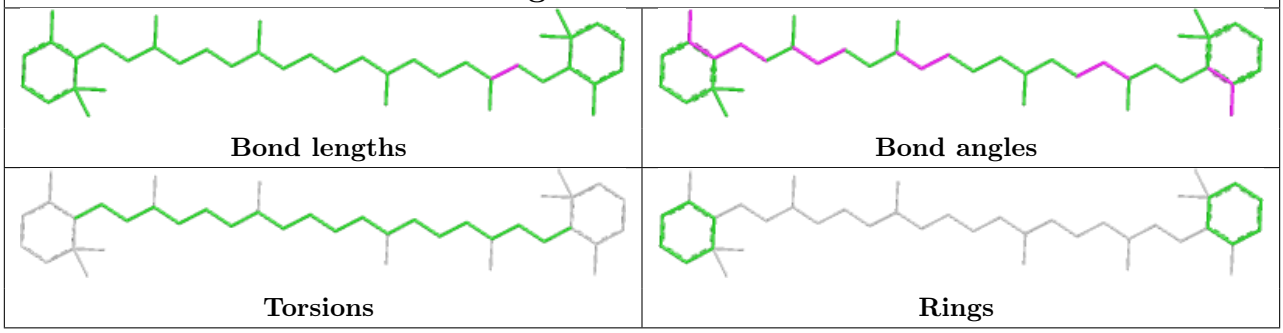


Torsions

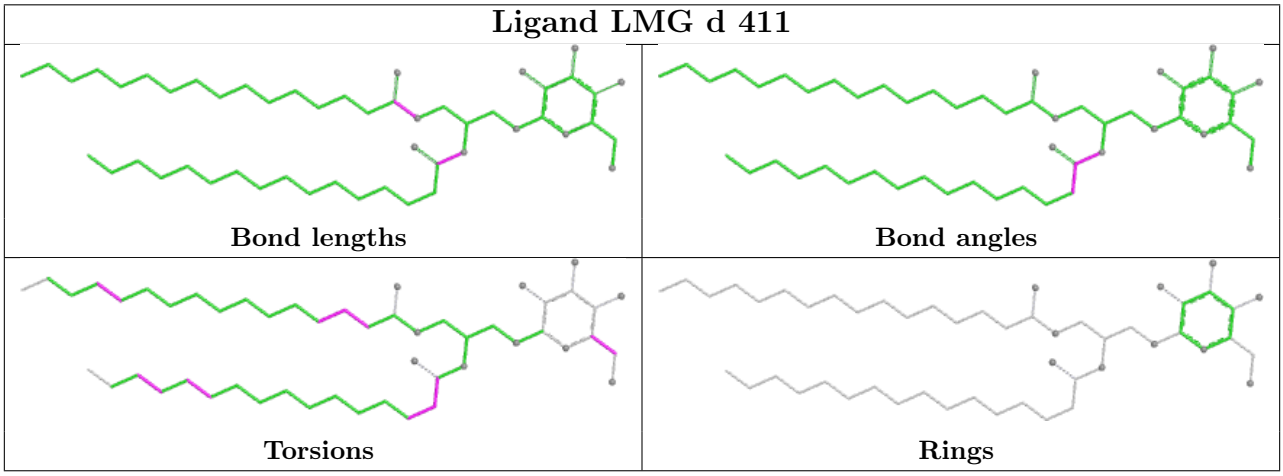


Rings

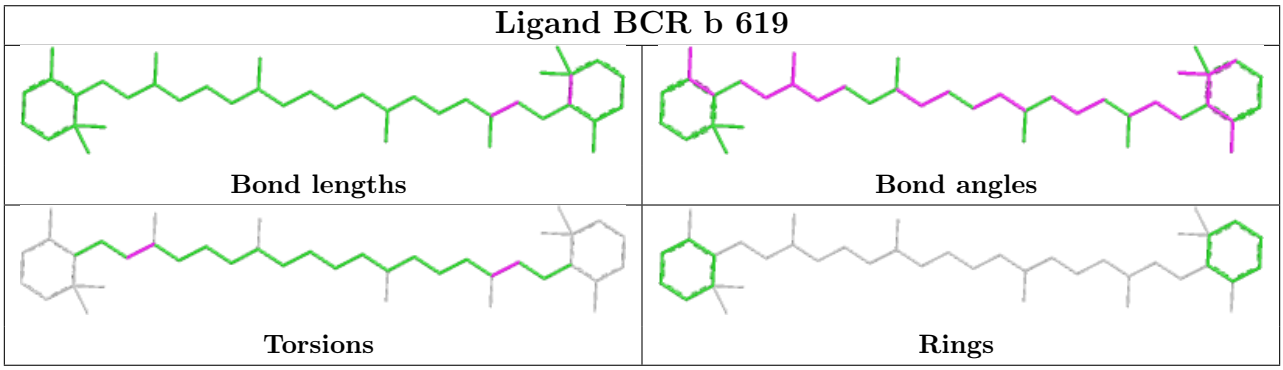
Ligand BCR c 516



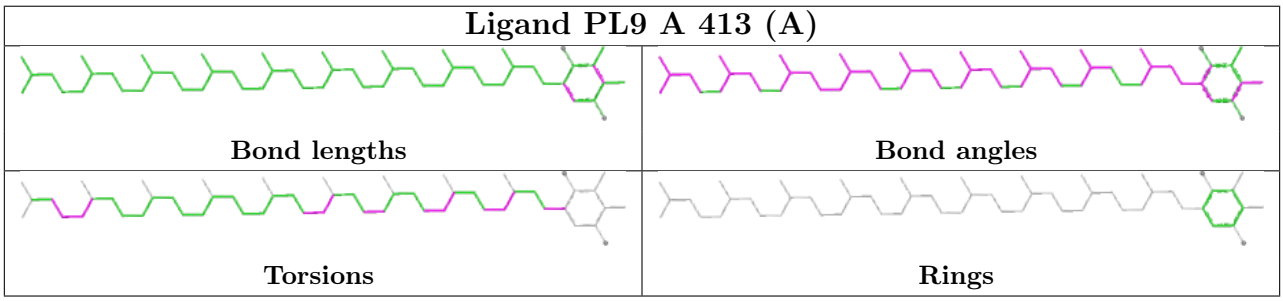
Ligand LMG d 411



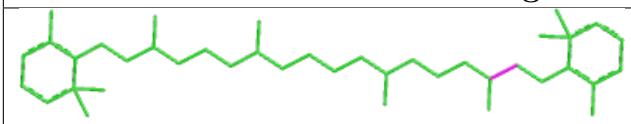
Ligand BCR b 619



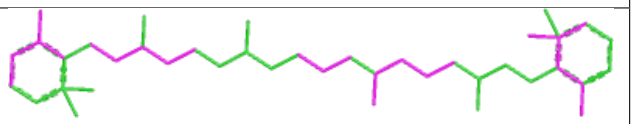
Ligand PL9 A 413 (A)



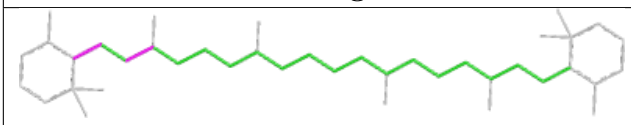
Ligand BCR C 517



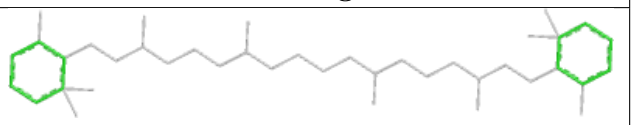
Bond lengths



Bond angles

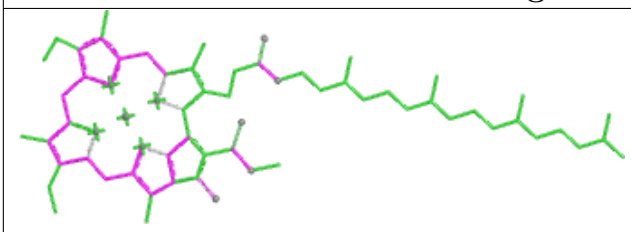


Torsions

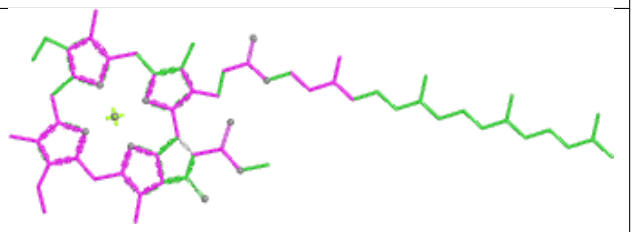


Rings

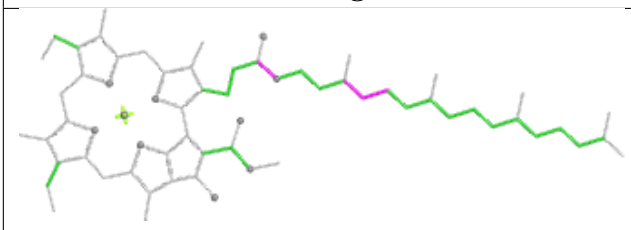
Ligand CLA d 403



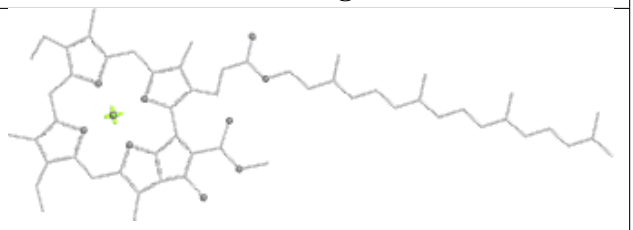
Bond lengths



Bond angles

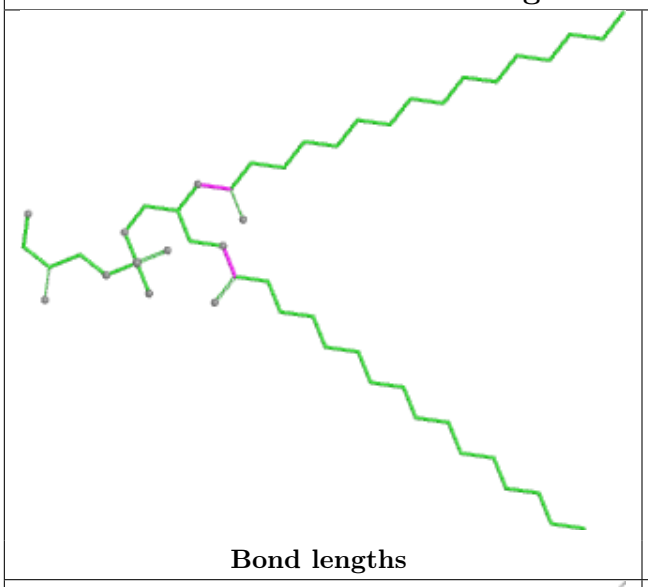


Torsions

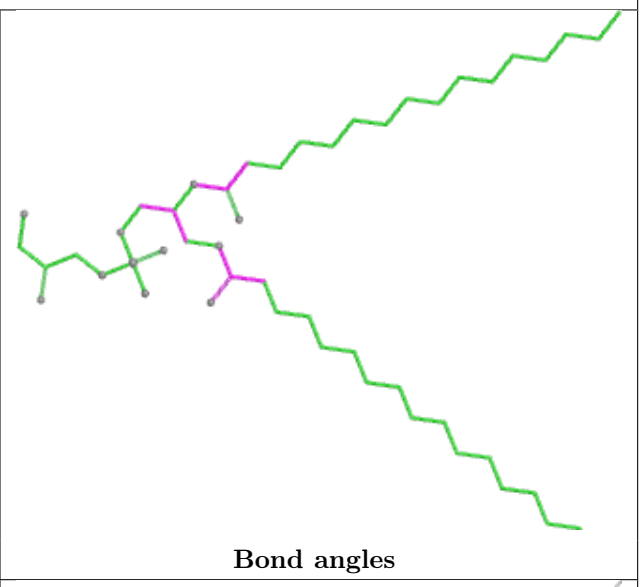


Rings

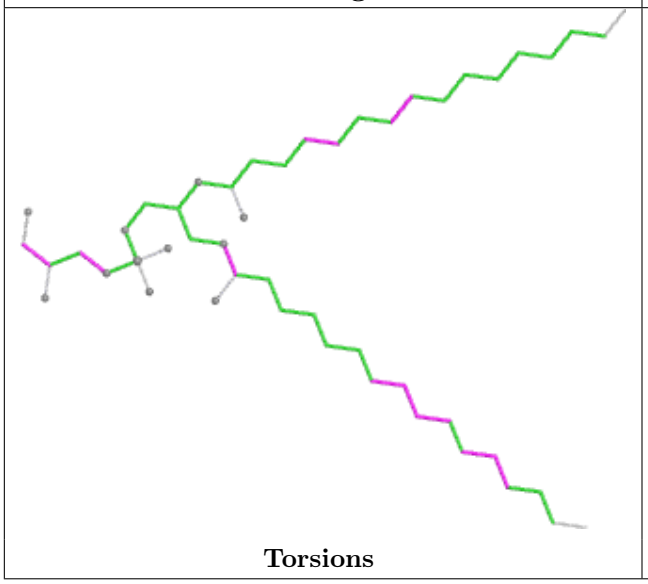
Ligand LHG D 408



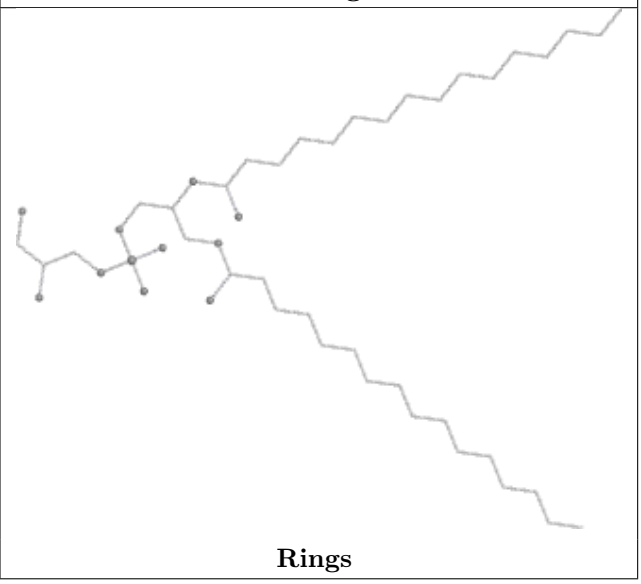
Bond lengths



Bond angles

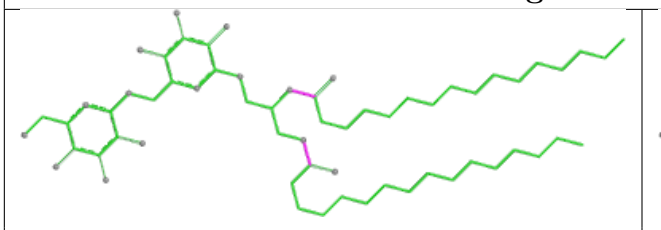


Torsions



Rings

Ligand DGD c 519



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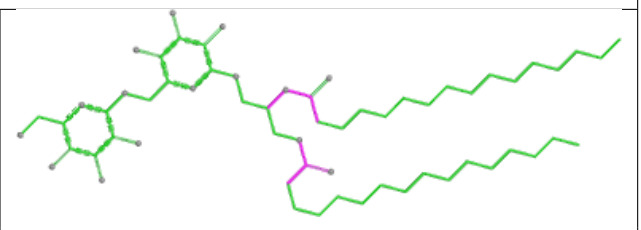
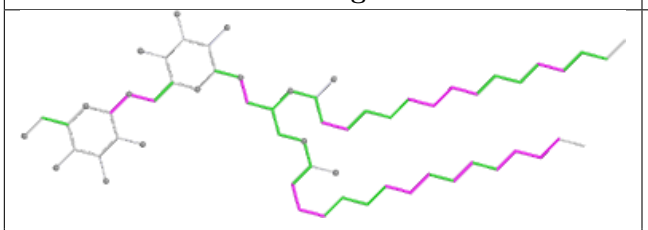
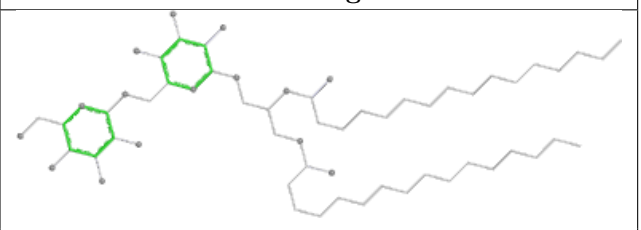


Bond angles

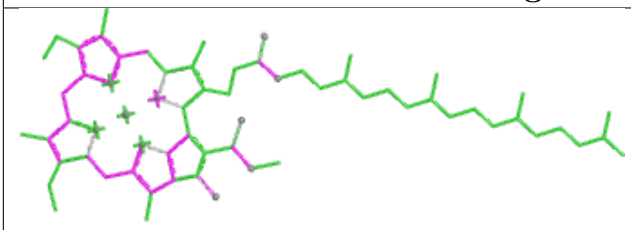


Torsions

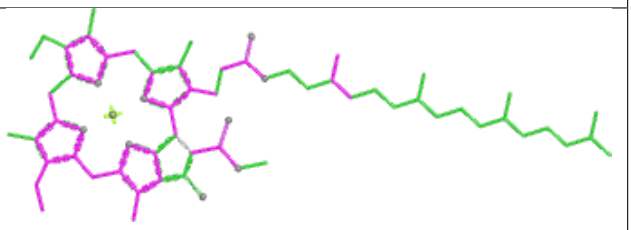


Rings

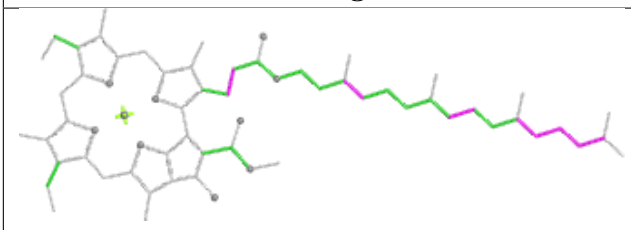
Ligand CLA B 606



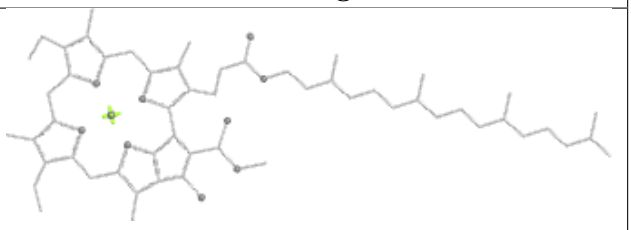
Bond lengths



Bond angles

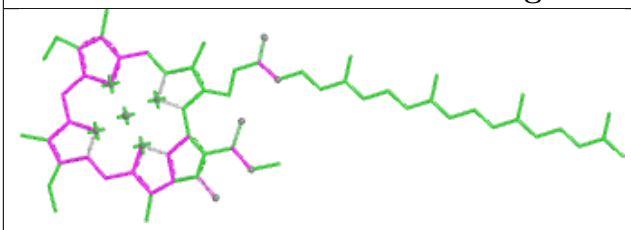


Torsions

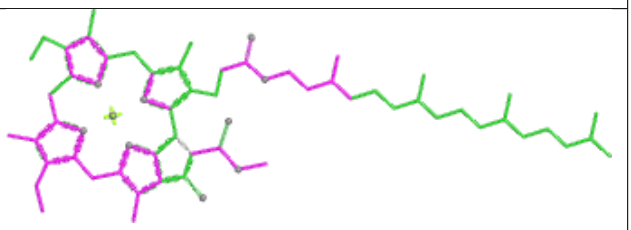


Rings

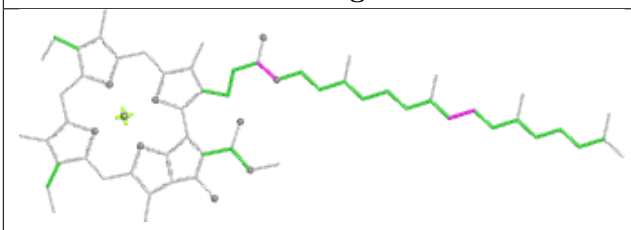
Ligand CLA C 513



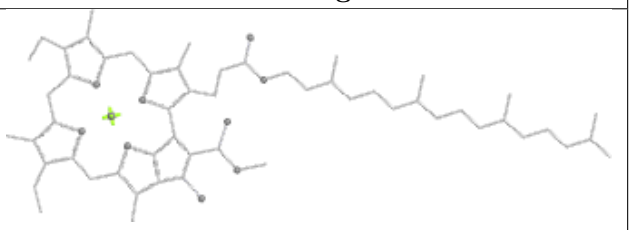
Bond lengths



Bond angles

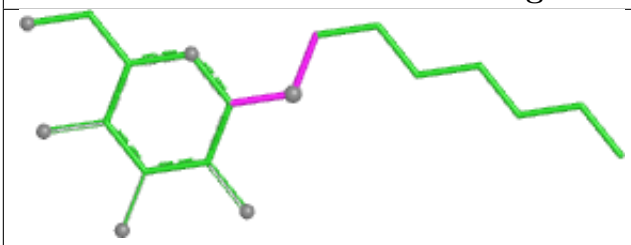


Torsions

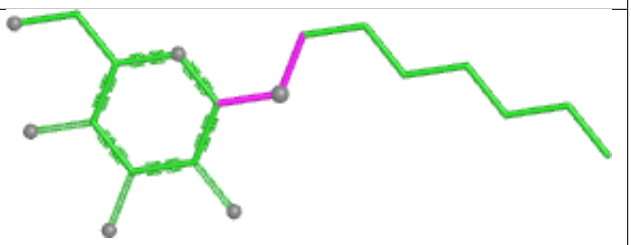


Rings

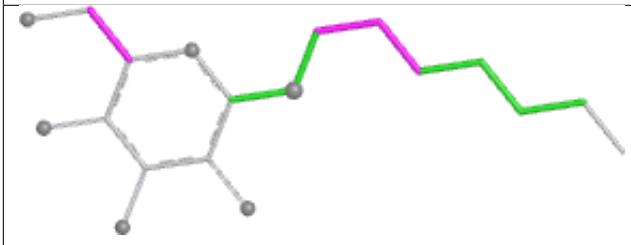
Ligand HTG c 523



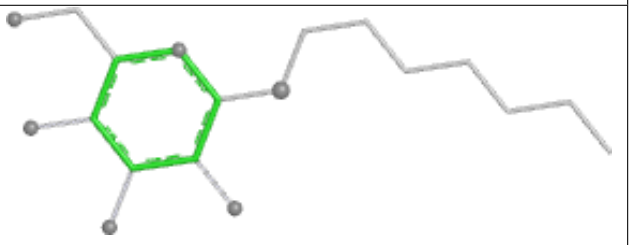
Bond lengths



Bond angles

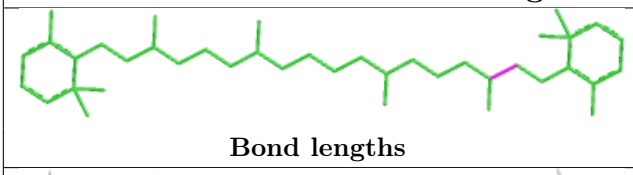


Torsions

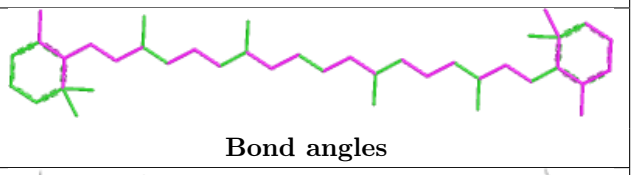


Rings

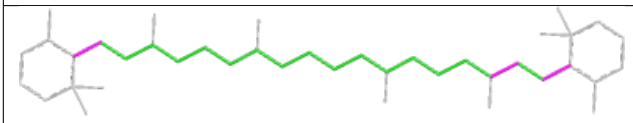
Ligand BCR k 102



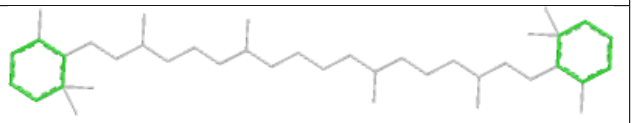
Bond lengths



Bond angles



Torsions

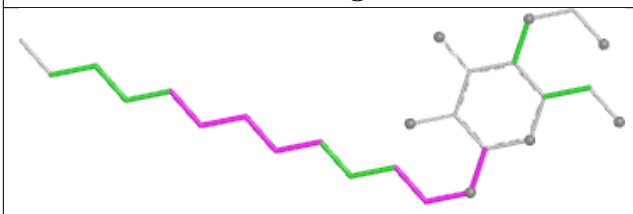


Rings

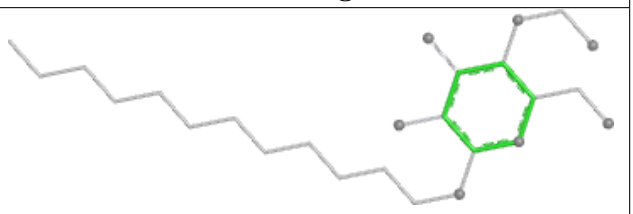
Ligand LMT B 630

Bond lengths

Bond angles

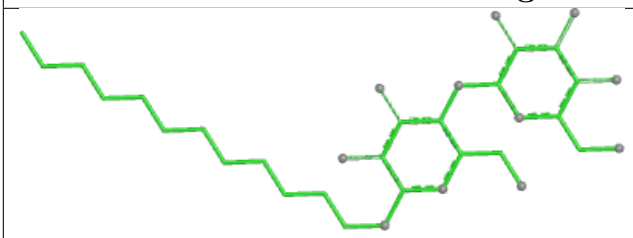


Torsions

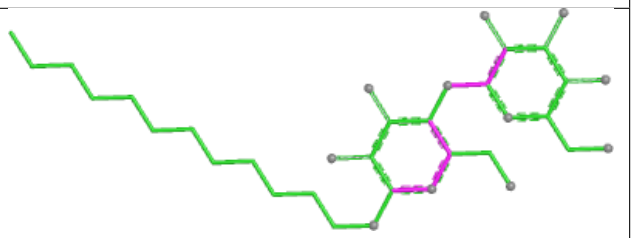


Rings

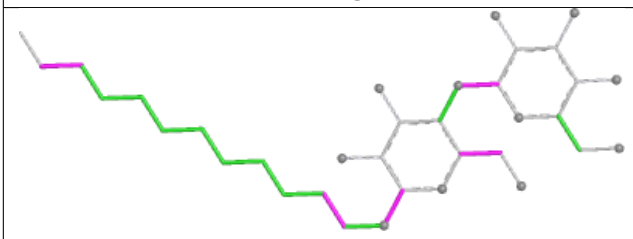
Ligand LMT M 103



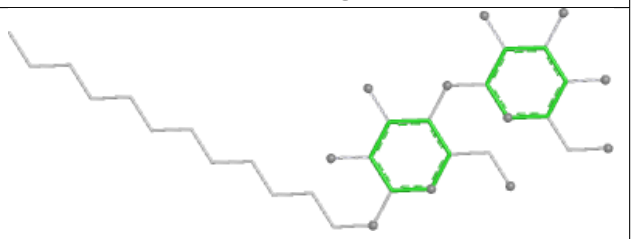
Bond lengths



Bond angles

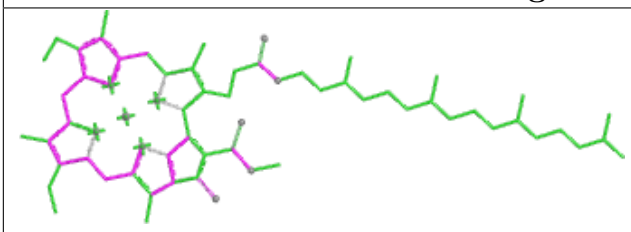


Torsions

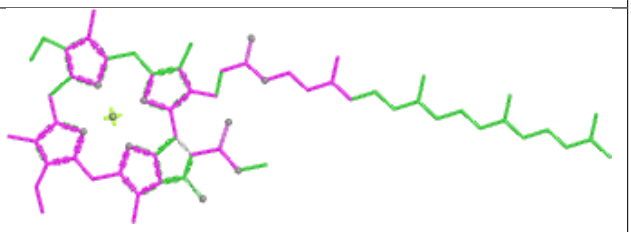


Rings

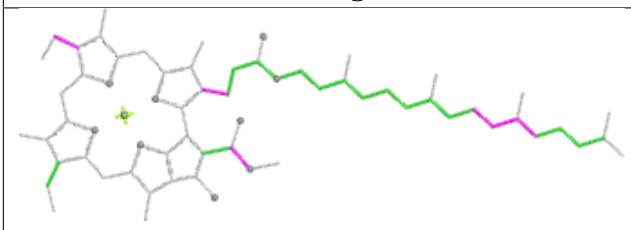
Ligand CLA a 405



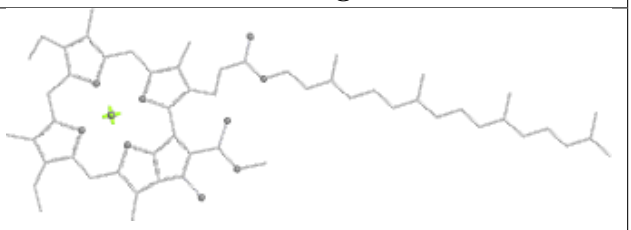
Bond lengths



Bond angles

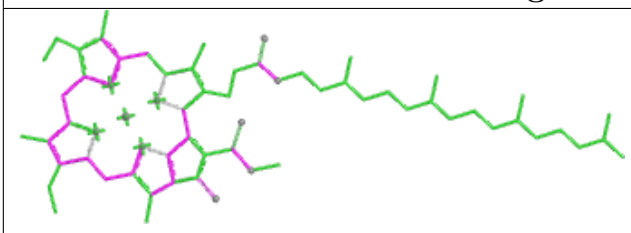


Torsions



Rings

Ligand CLA b 607



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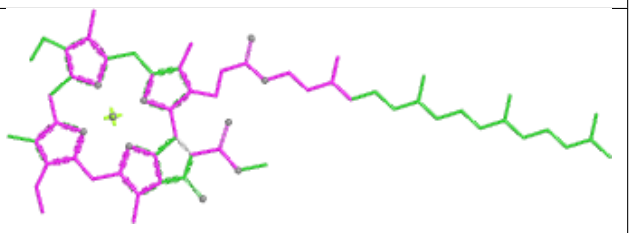
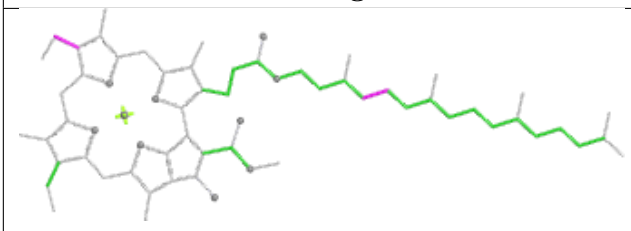
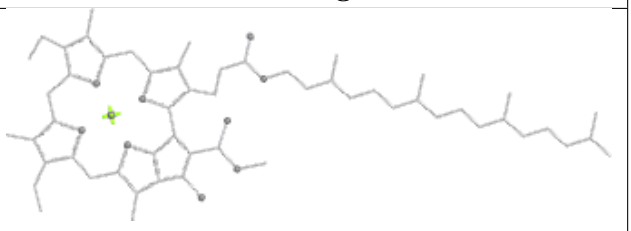


Bond angles

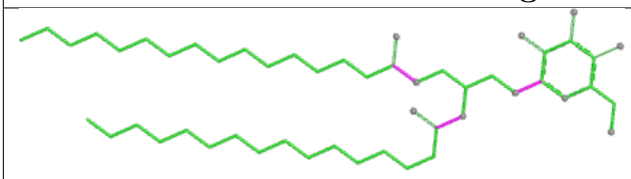


Torsions



Rings

Ligand LMG C 522



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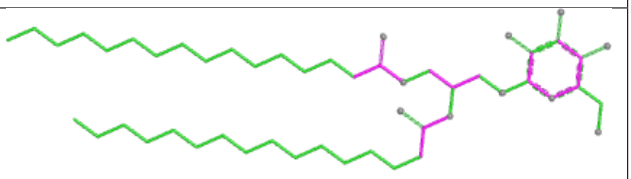
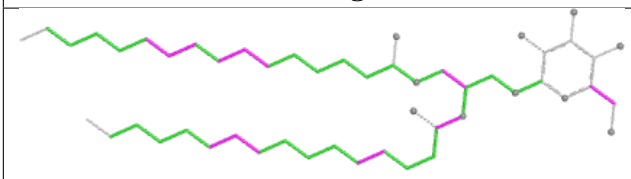
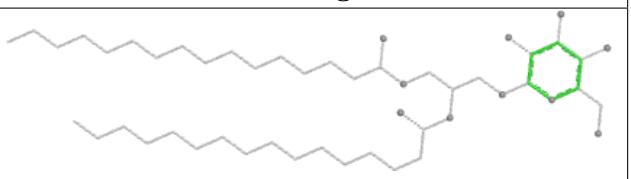


Bond angles

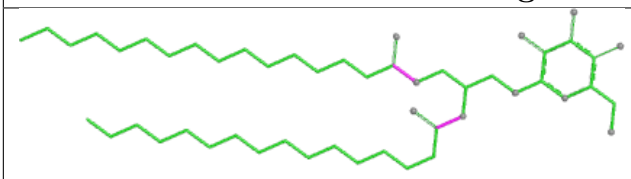


Torsions



Rings

Ligand LMG m 101



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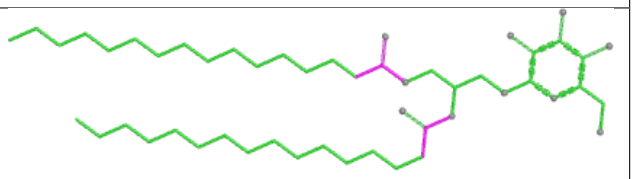
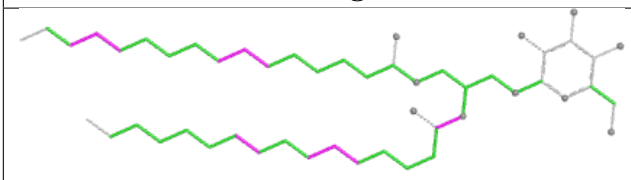


Bond angles



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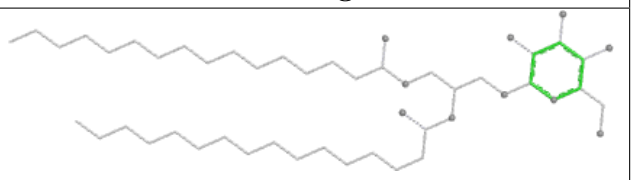
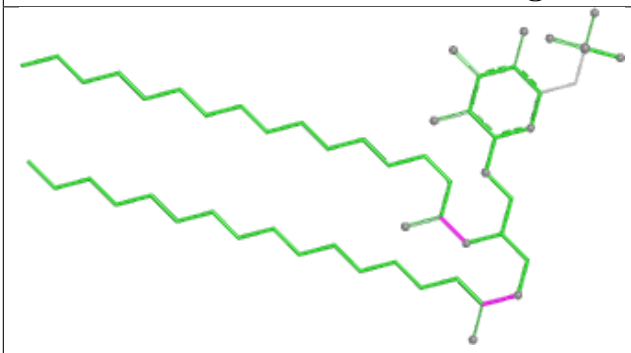
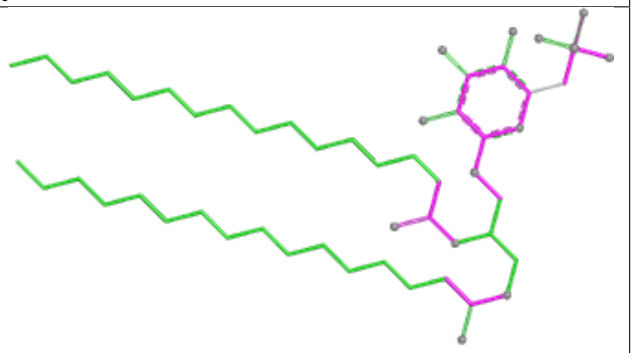


Rings

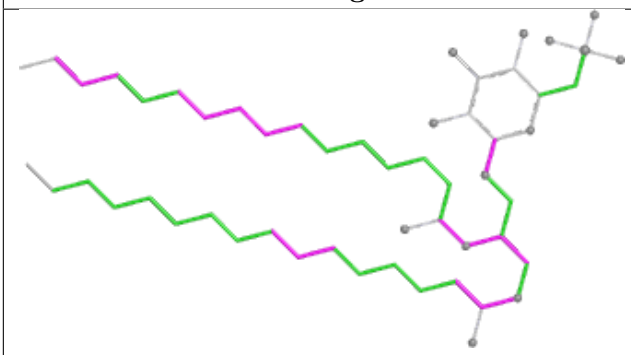
Ligand SQD L 102



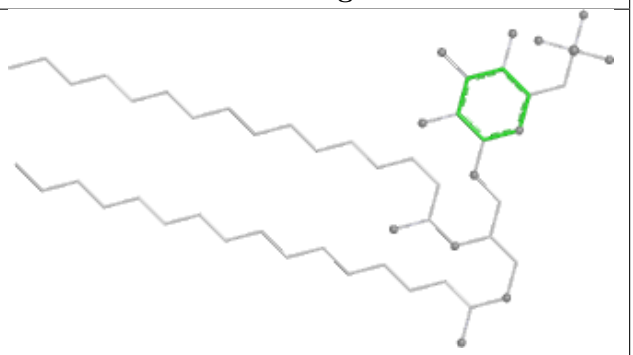
Bond lengths



Bond angles

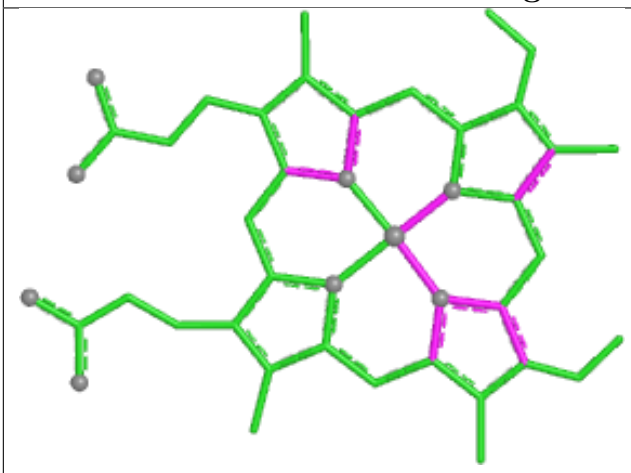


Torsions

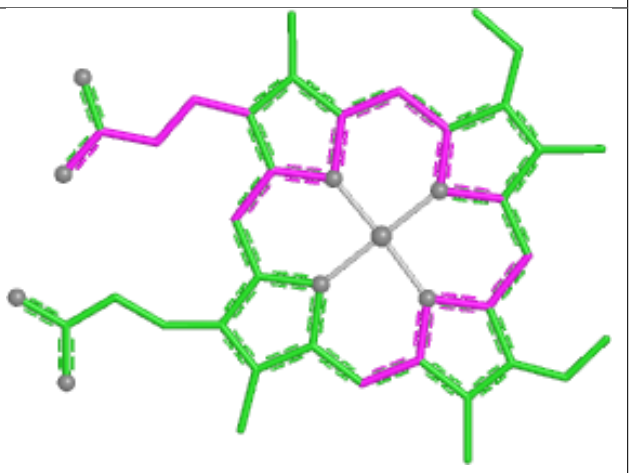


Rings

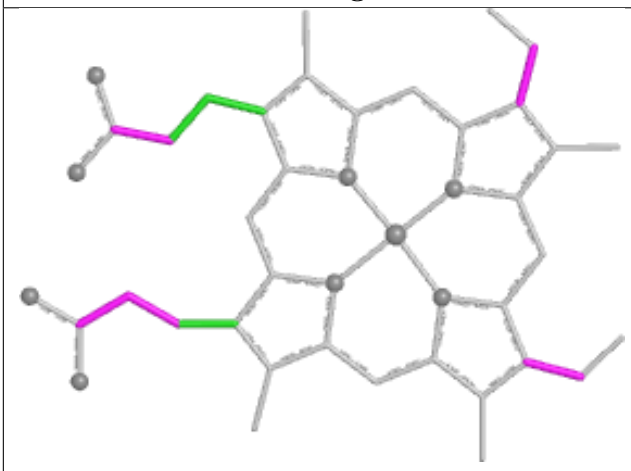
Ligand HEM e 102



Bond lengths



Bond angles



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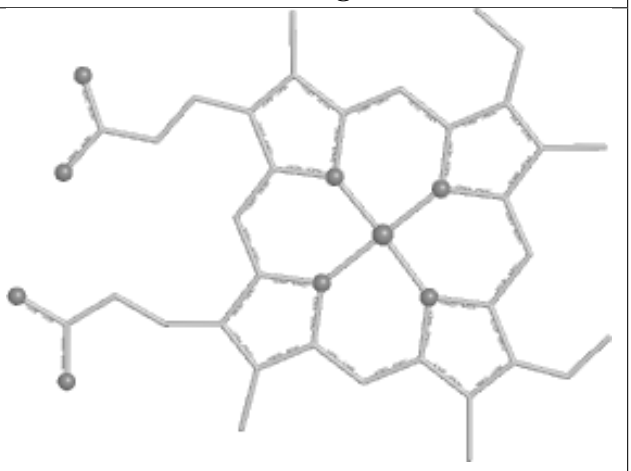
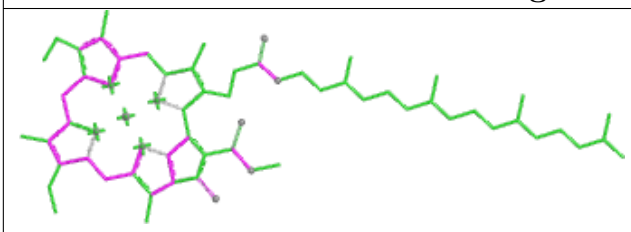
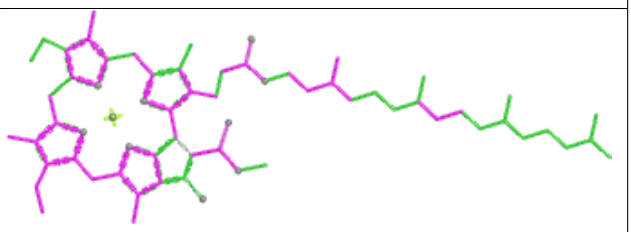


Rings

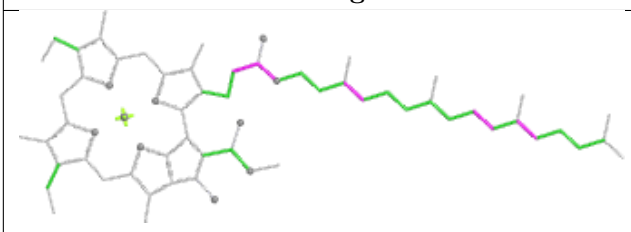
Ligand CLA c 512



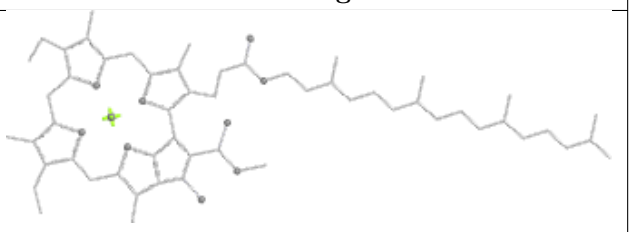
Bond lengths



Bond angles

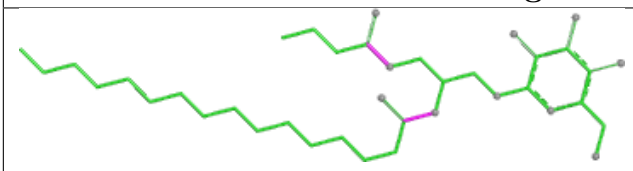


Torsions

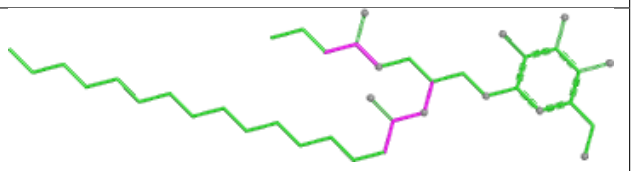


Rings

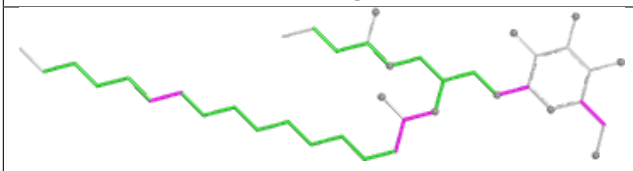
Ligand LMG z 101



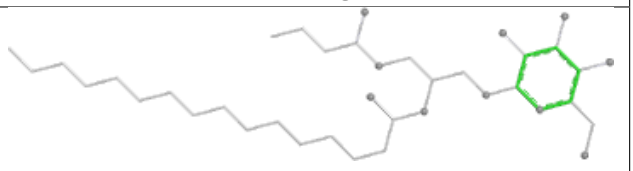
Bond lengths



Bond angles

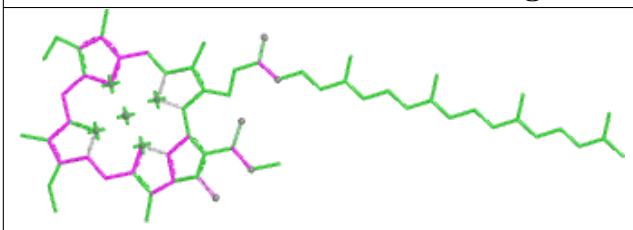


Torsions



Rings

Ligand CLA A 403



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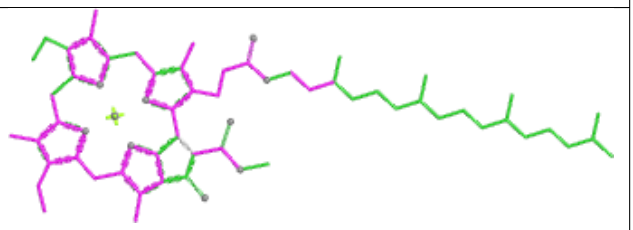
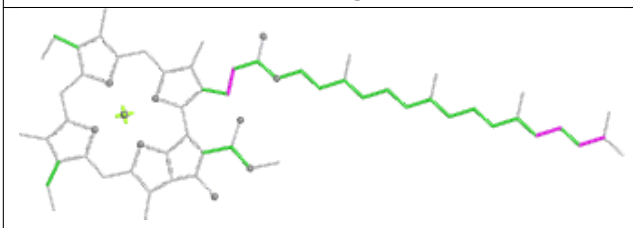


Bond angles



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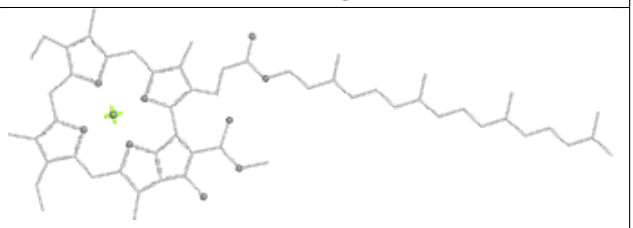
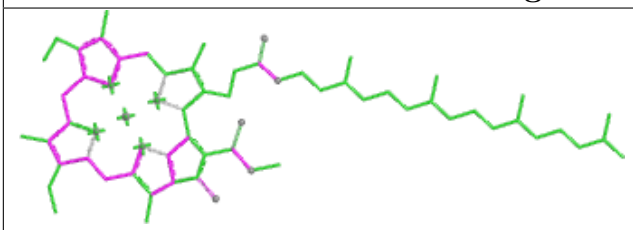


Rings

Ligand CLA C 515



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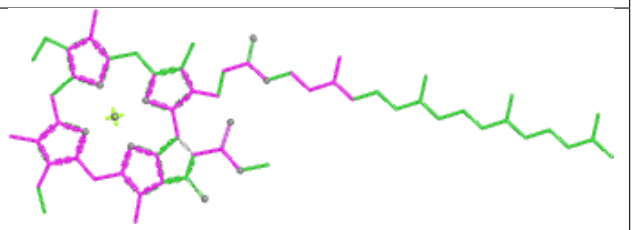
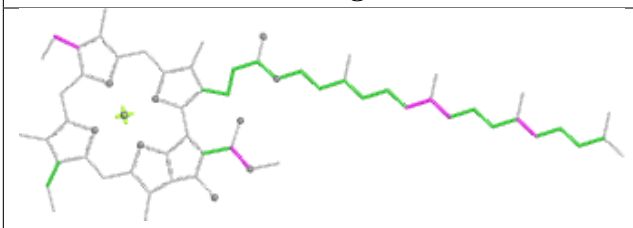
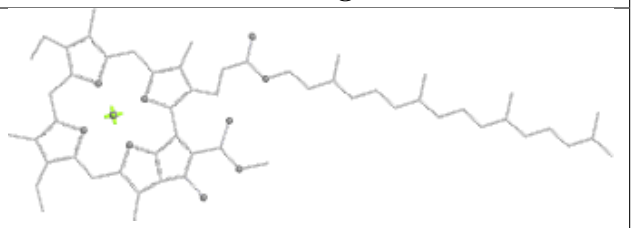


Bond angles

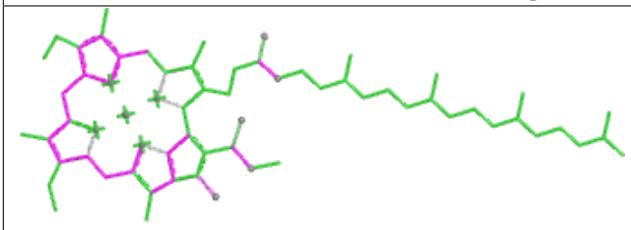


Torsions

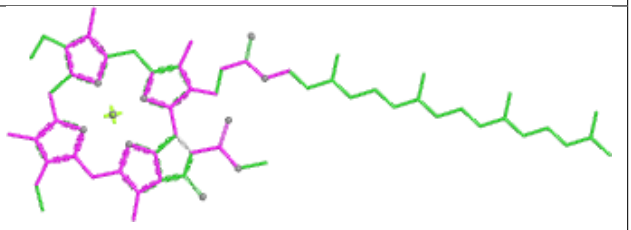


Rings

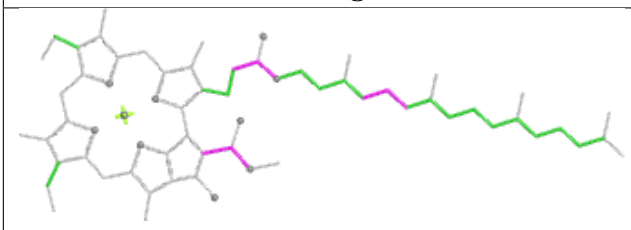
Ligand CLA B 601



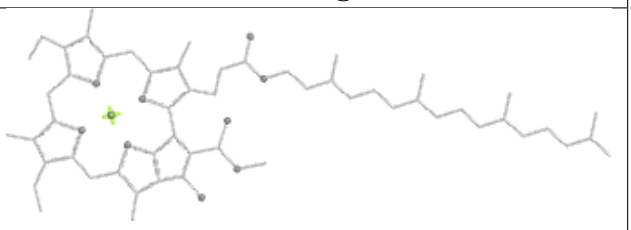
Bond lengths



Bond angles



Torsions

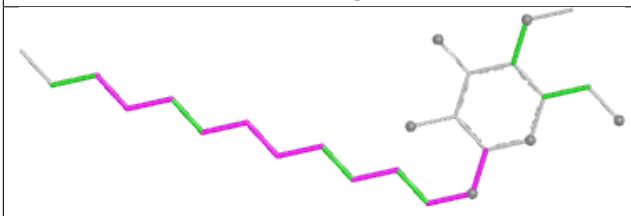


Rings

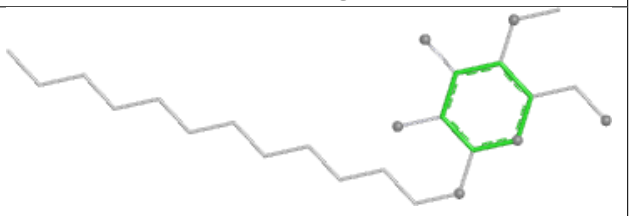
Ligand LMT b 626

Bond lengths

Bond angles

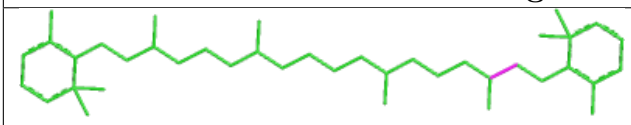


Torsions

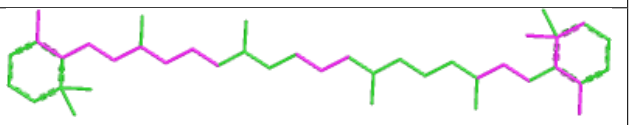


Rings

Ligand BCR a 408

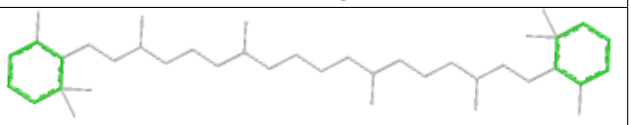


Bond lengths



Bond angles

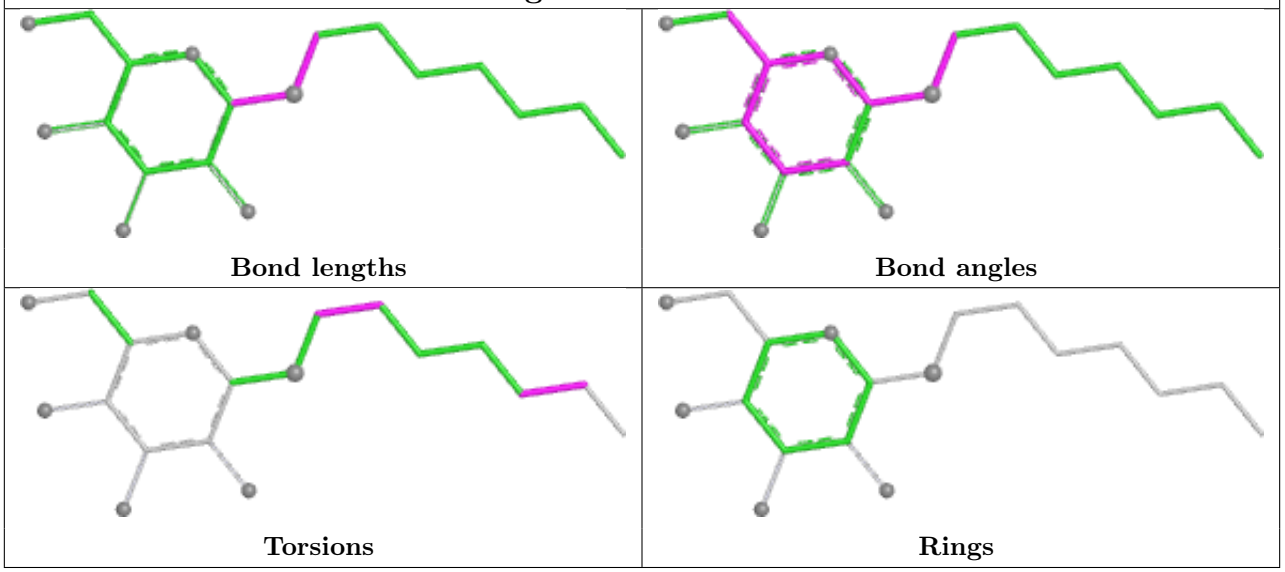
Torsions



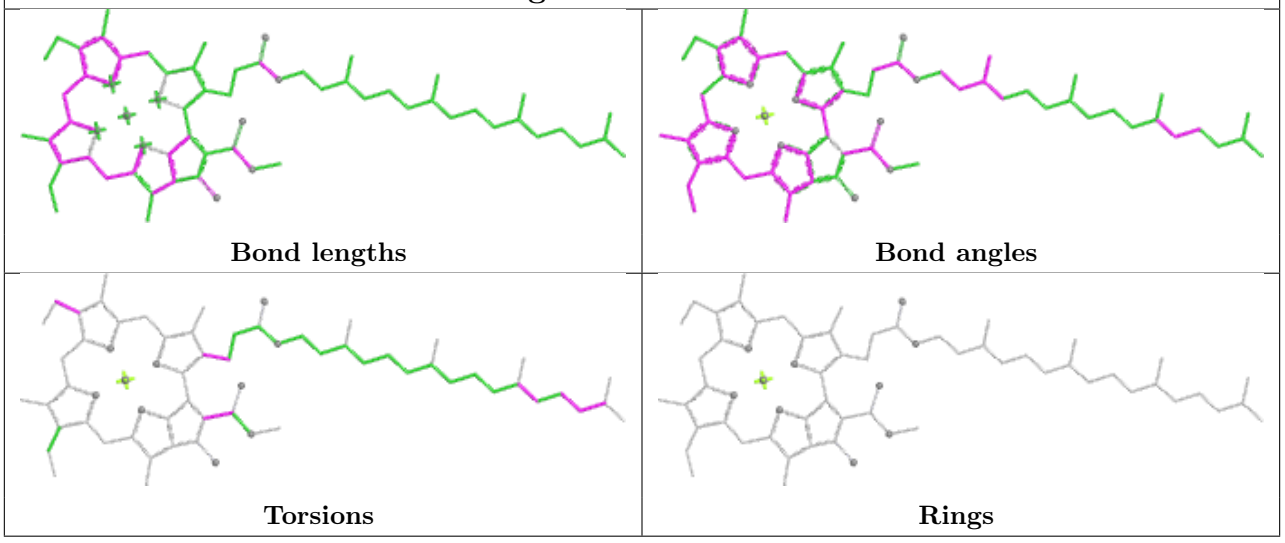
Rings

Ligand PL9 A 413 (B)

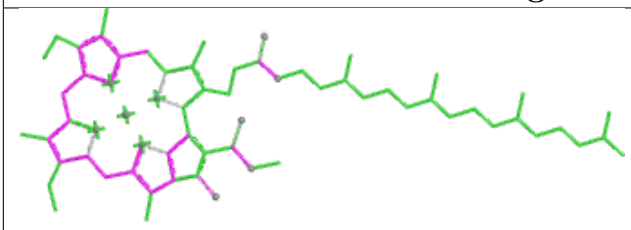
Ligand HTG b 624



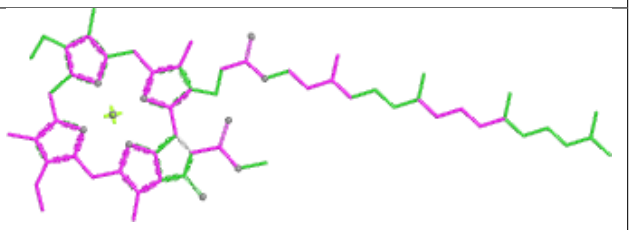
Ligand CLA b 609



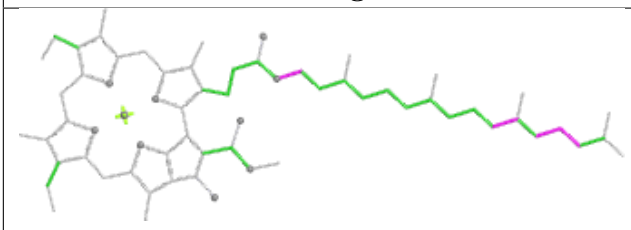
Ligand CLA b 608



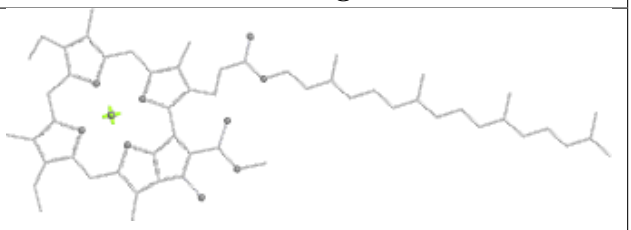
Bond lengths



Bond angles

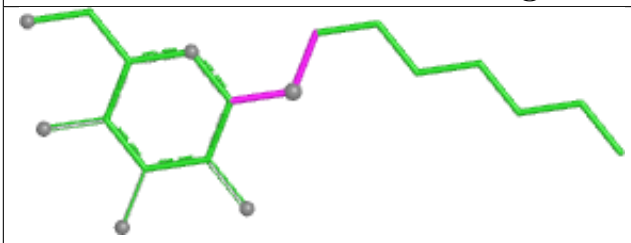


Torsions

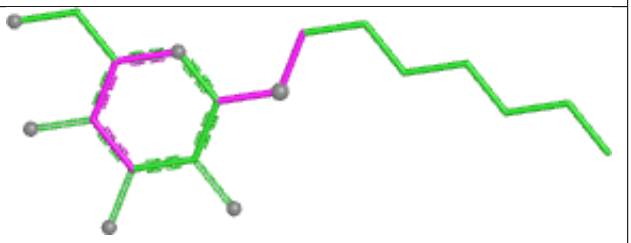


Rings

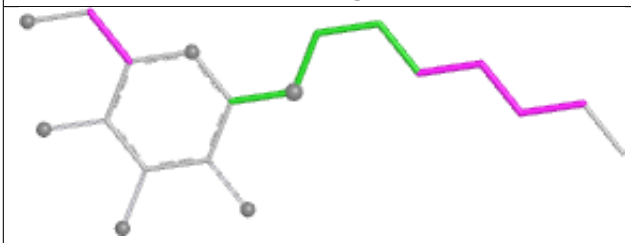
Ligand HTG B 624



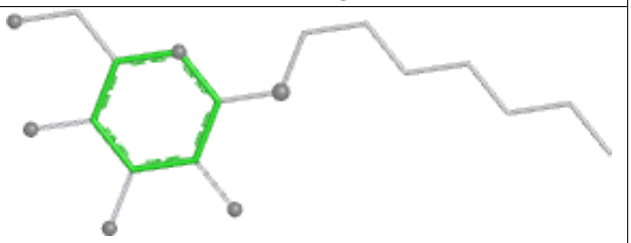
Bond lengths



Bond angles

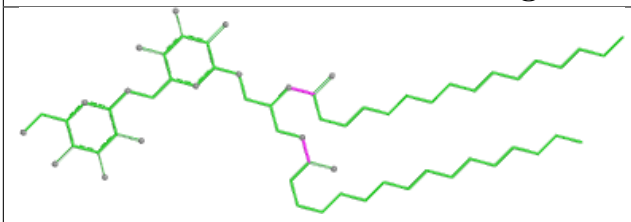


Torsions

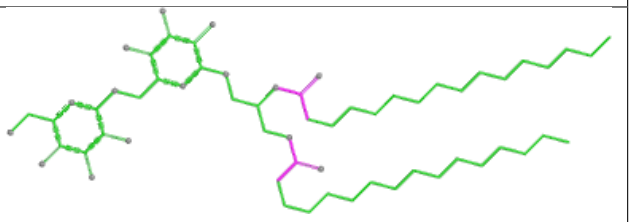


Rings

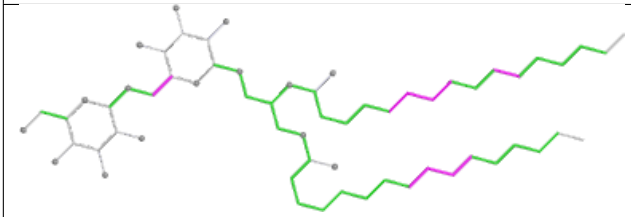
Ligand DGD C 520



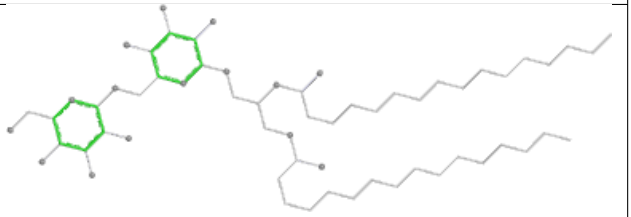
Bond lengths



Bond angles

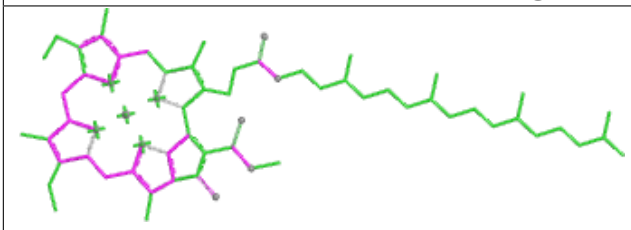


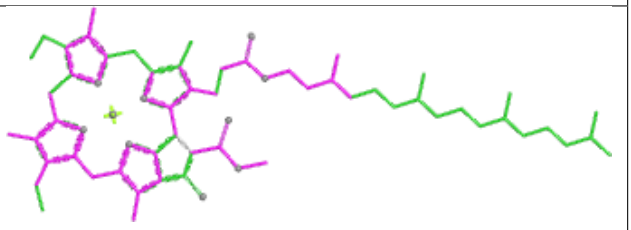
Torsions

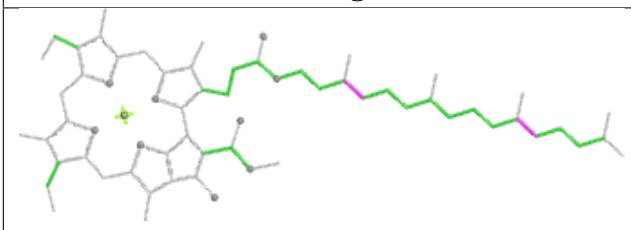


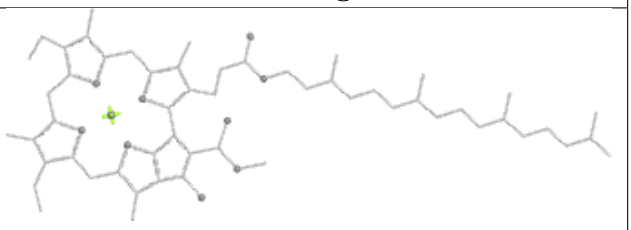
Rings

Ligand CLA c 506


Bond lengths

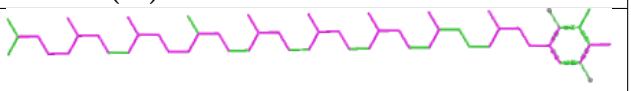

Bond angles

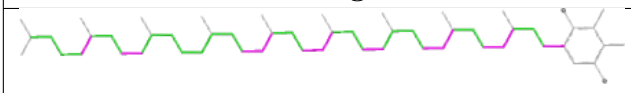

Torsions

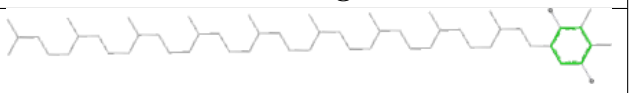

Rings

Ligand PL9 a 414 (A)

Bond lengths

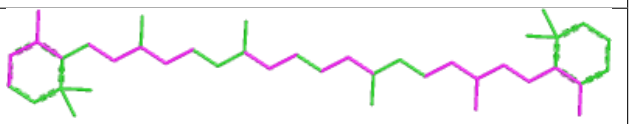

Bond angles

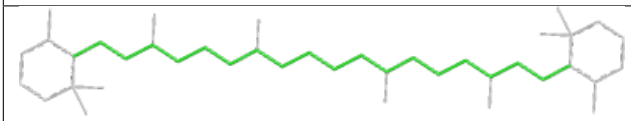

Torsions

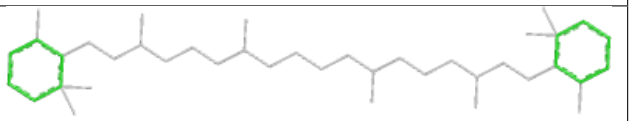

Rings

Ligand BCR C 516

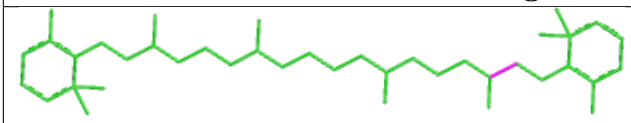
Bond lengths

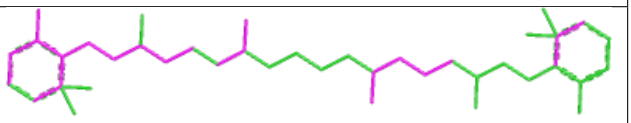

Bond angles


Torsions

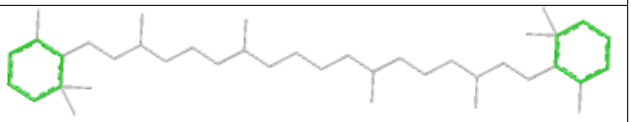

Rings

Ligand BCR B 631

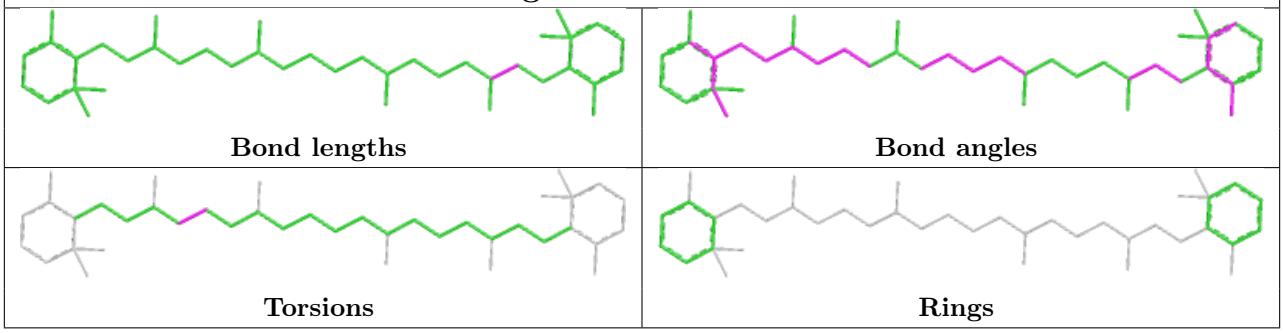

Bond lengths


Bond angles

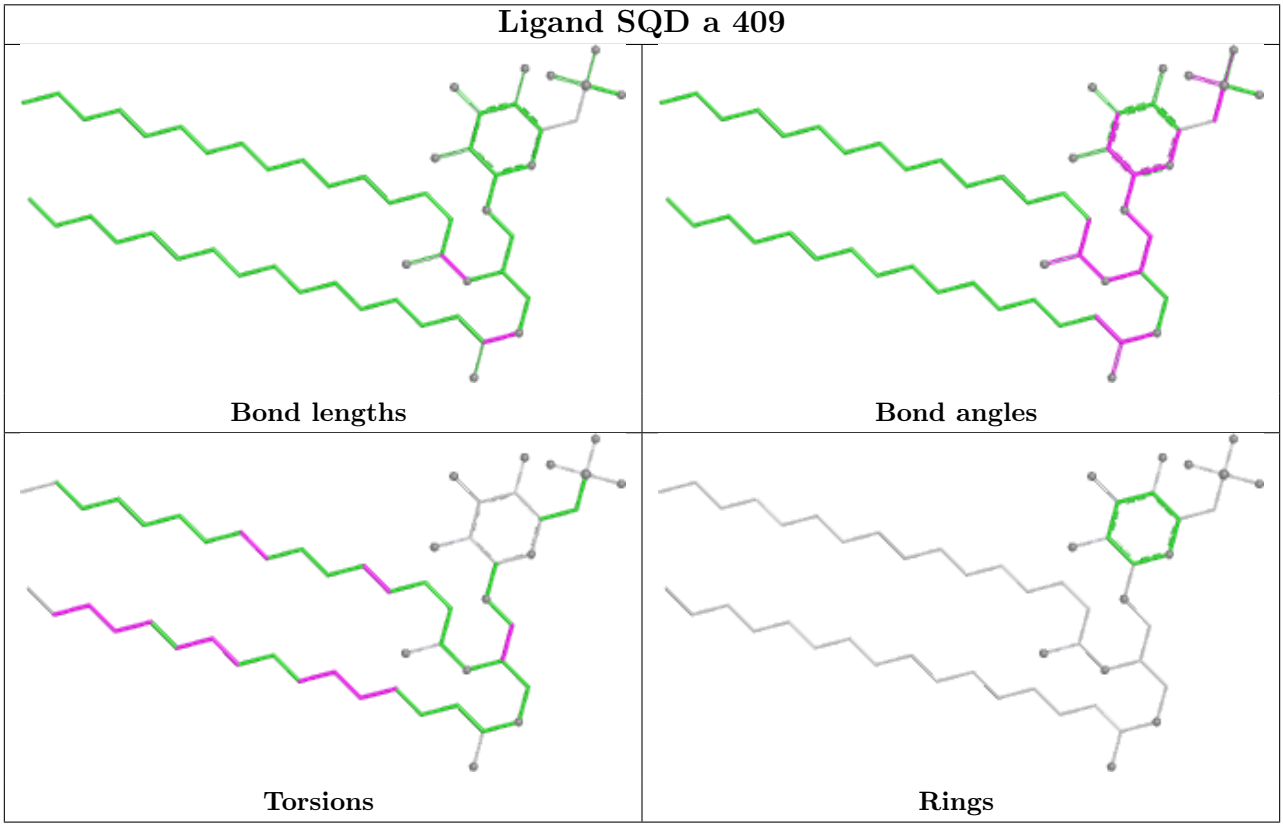
Torsions


Rings

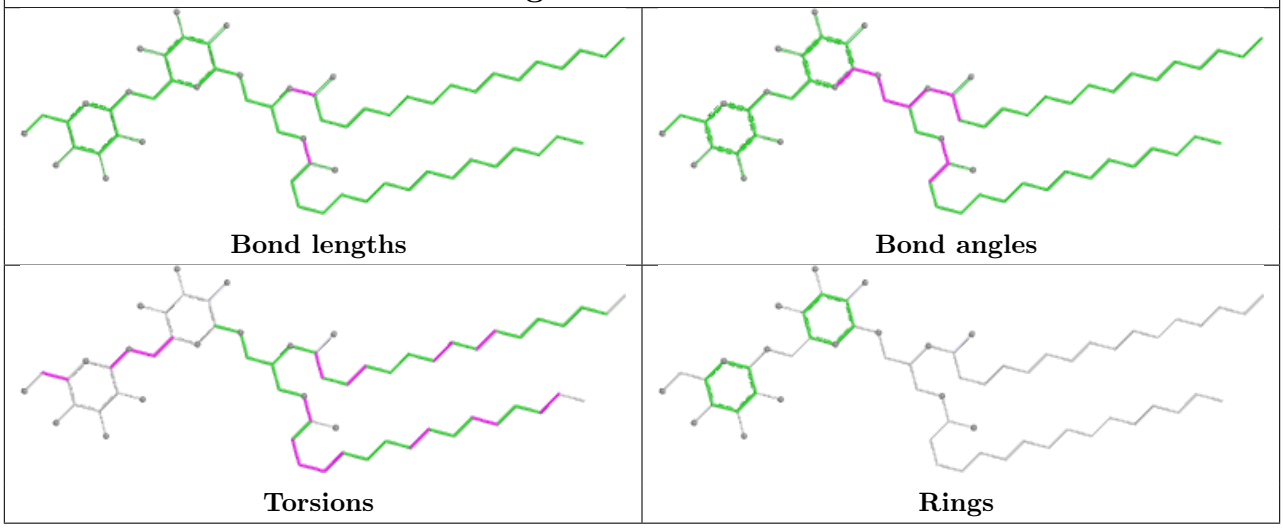
Ligand BCR H 101



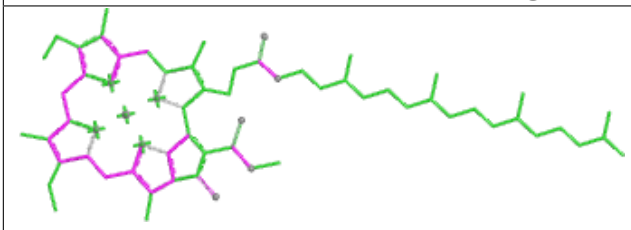
Ligand SQD a 409



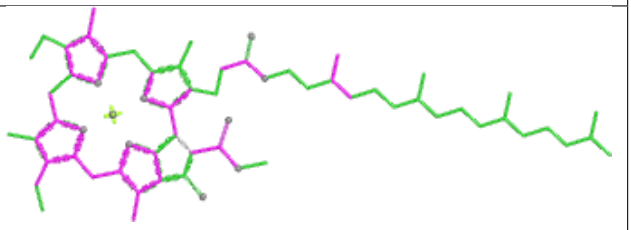
Ligand DGD c 518



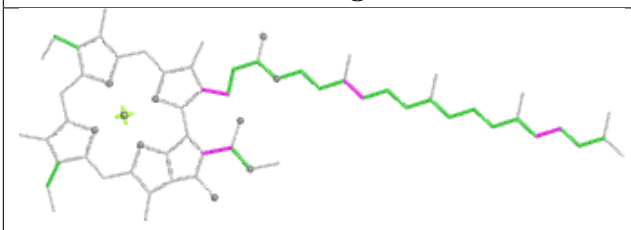
Ligand CLA B 609



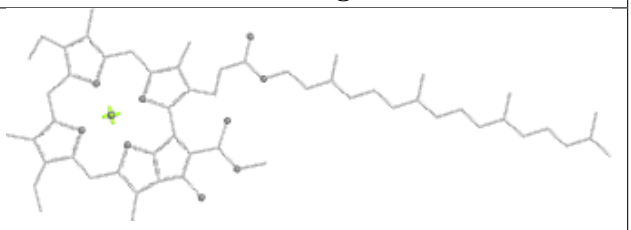
Bond lengths



Bond angles

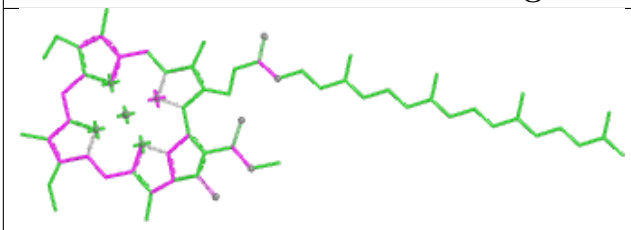


Torsions

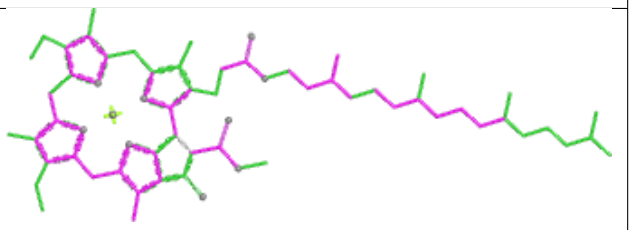


Rings

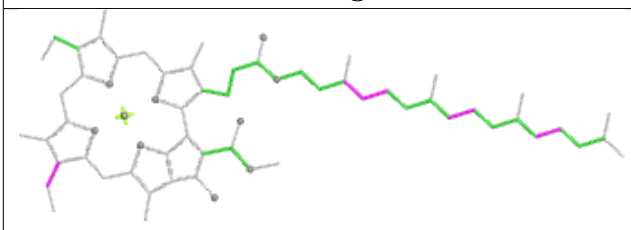
Ligand CLA B 604



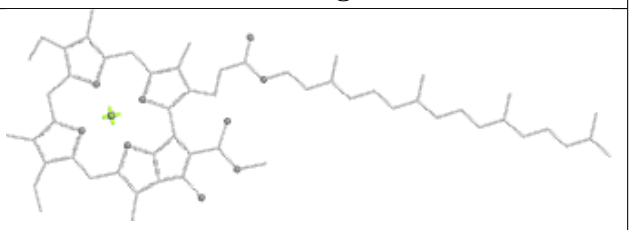
Bond lengths



Bond angles

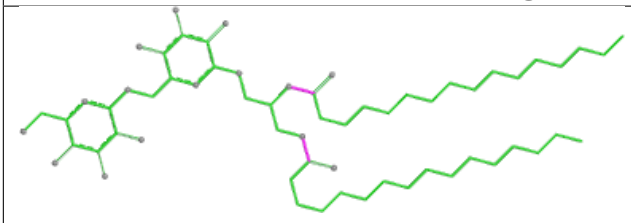


Torsions

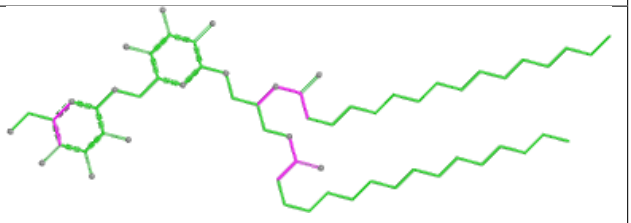


Rings

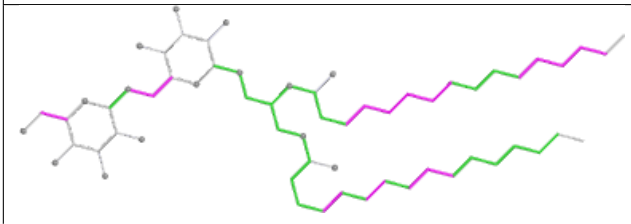
Ligand DGD C 518



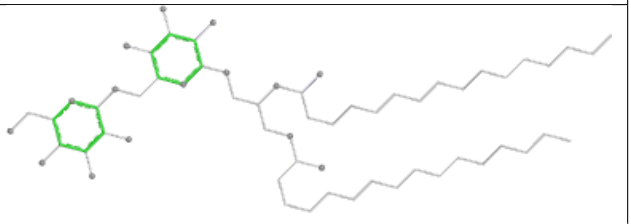
Bond lengths



Bond angles

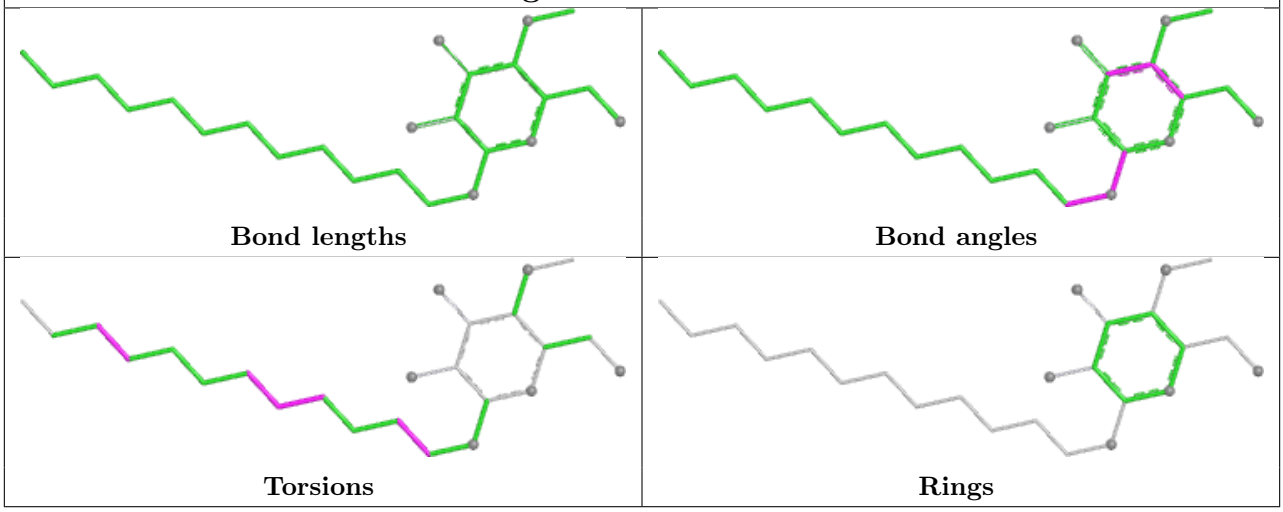


Torsions

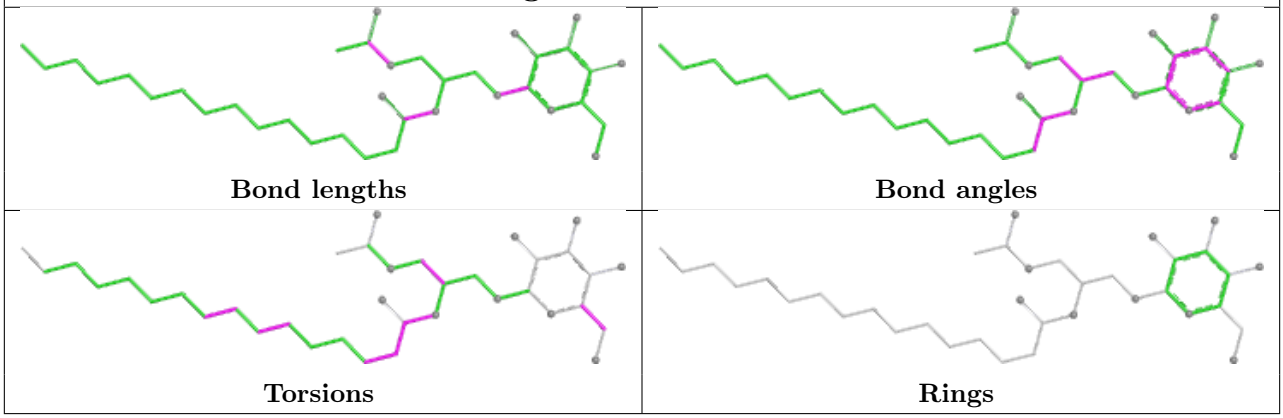


Rings

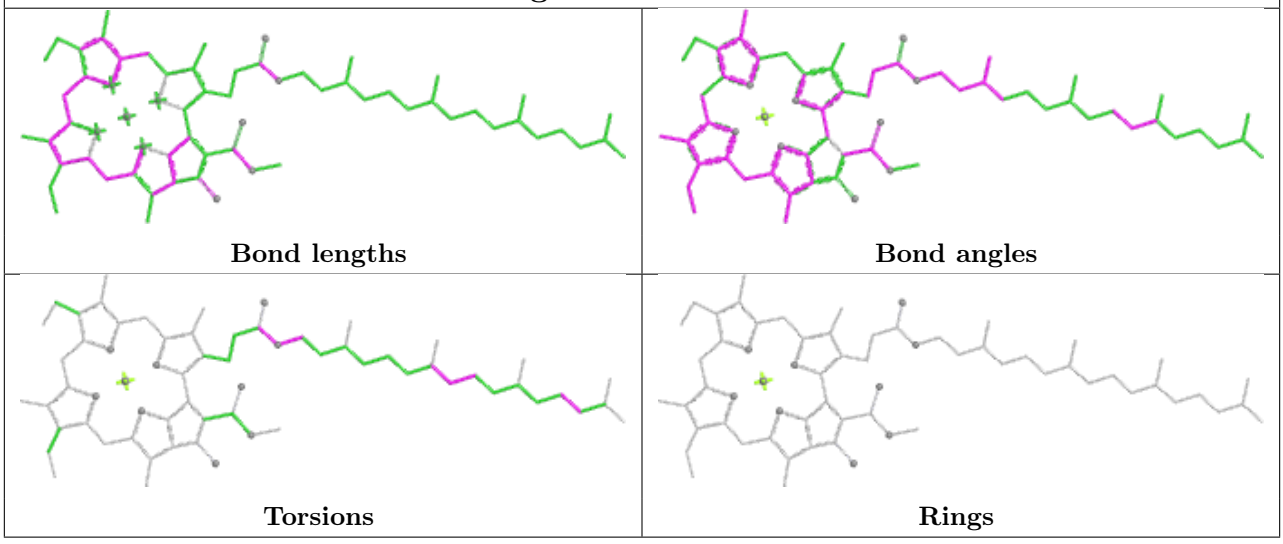
Ligand LMT B 629



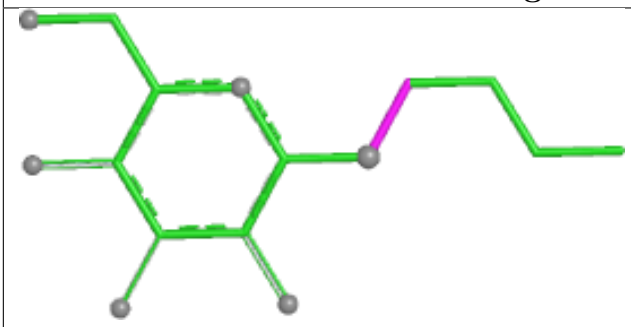
Ligand LMG Z 101



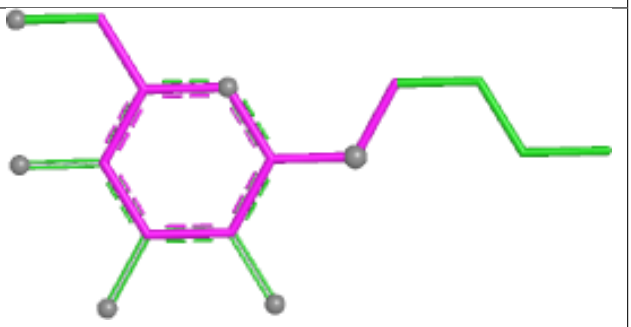
Ligand CLA c 513



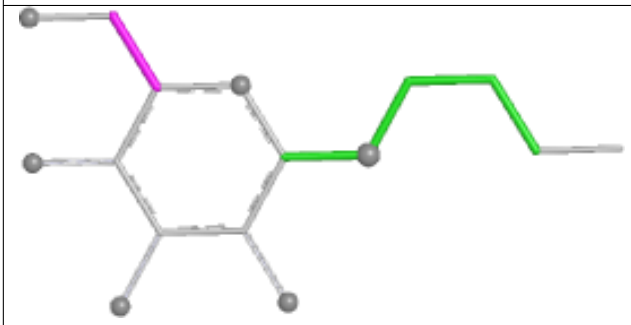
Ligand HTG h 101



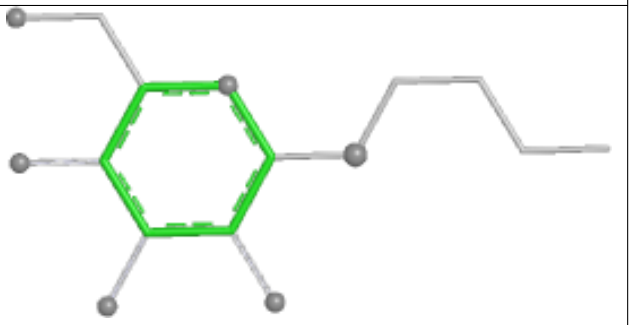
Bond lengths



Bond angles

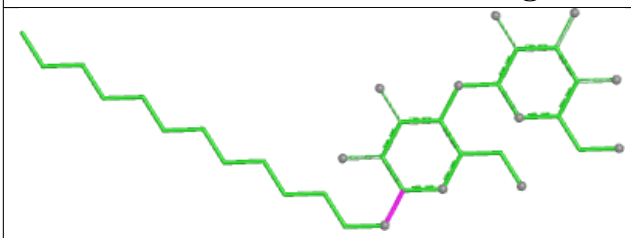


Torsions

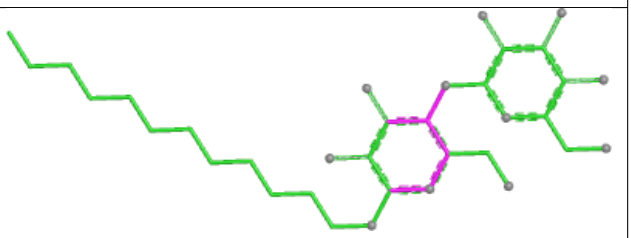


Rings

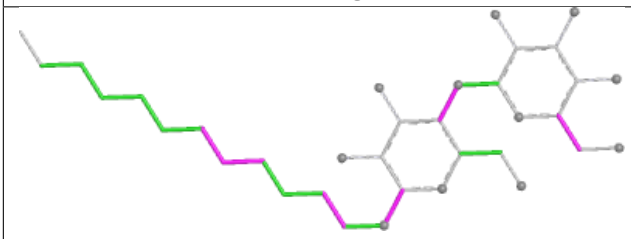
Ligand LMT C 526



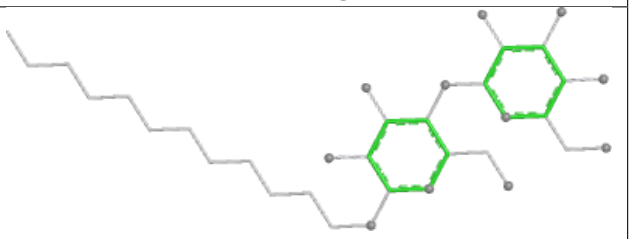
Bond lengths



Bond angles

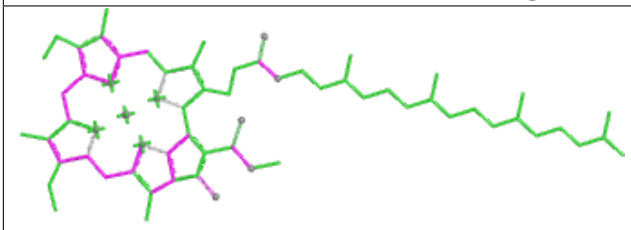


Torsions

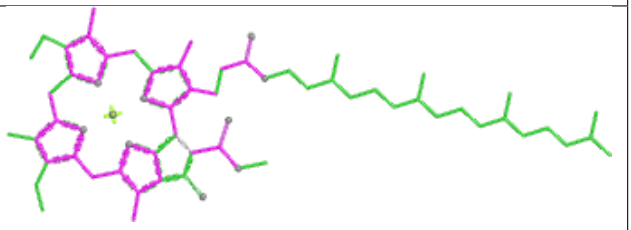


Rings

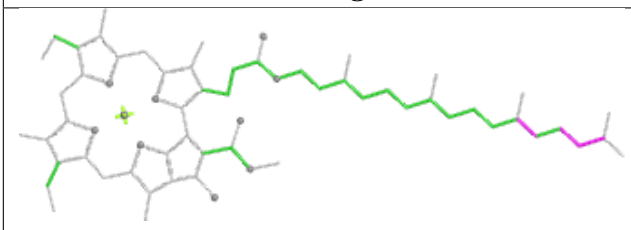
Ligand CLA A 405



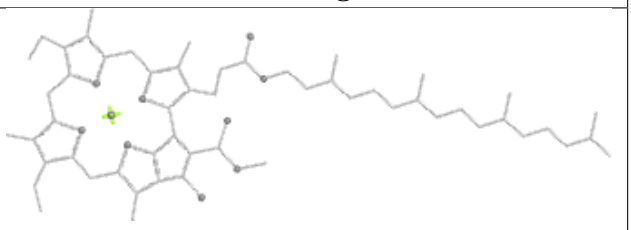
Bond lengths



Bond angles



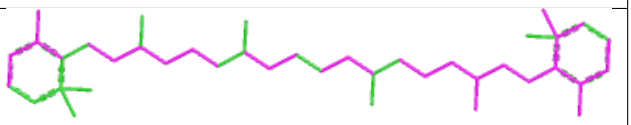
Torsions



Rings

Ligand BCR D 405

Bond lengths



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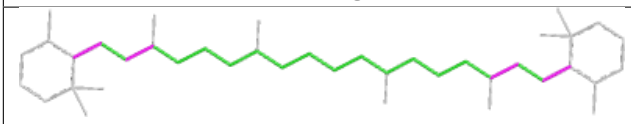

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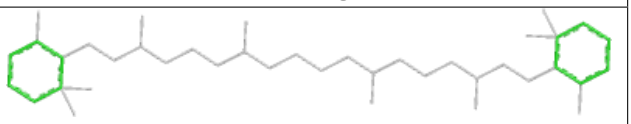
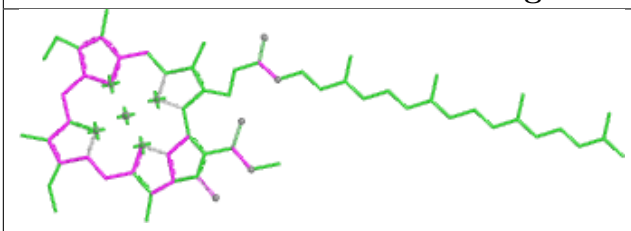


Rings

Ligand CLA B 608



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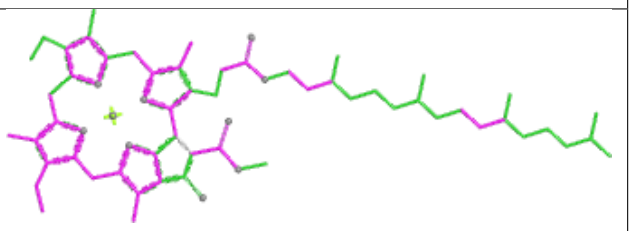
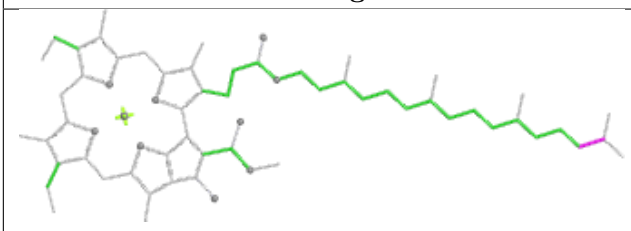


Bond angles



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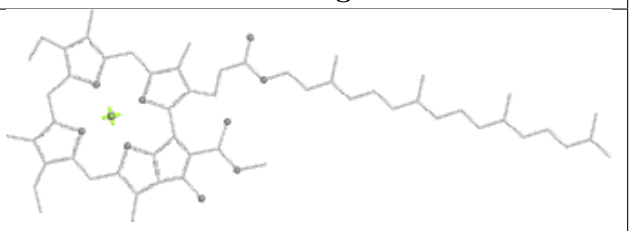
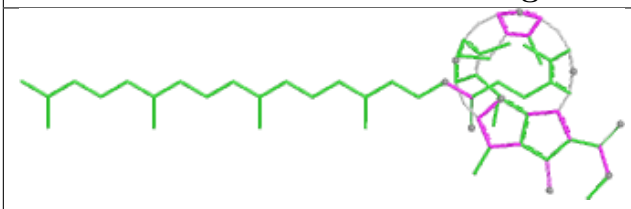


Rings

Ligand PHO A 415



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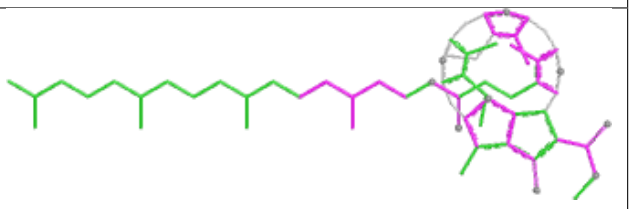
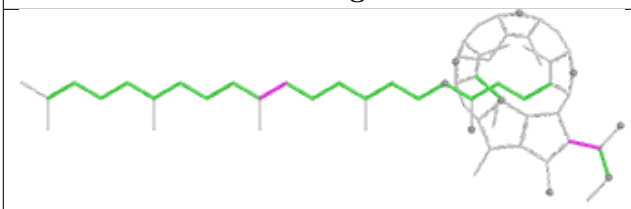


Bond angles



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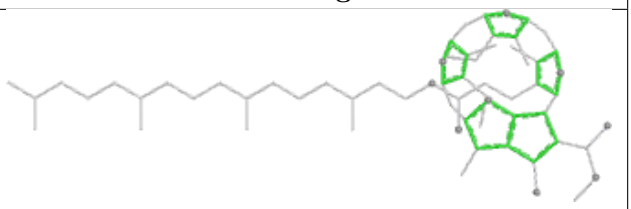
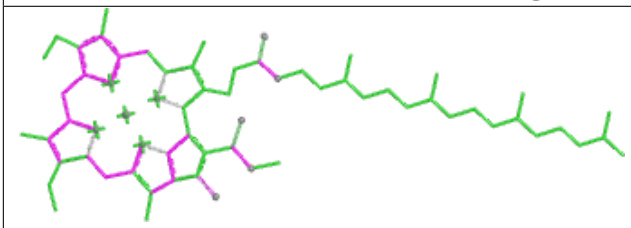
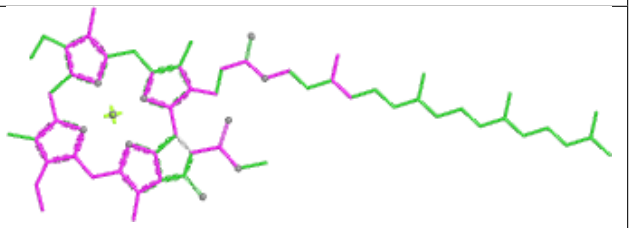


Rings

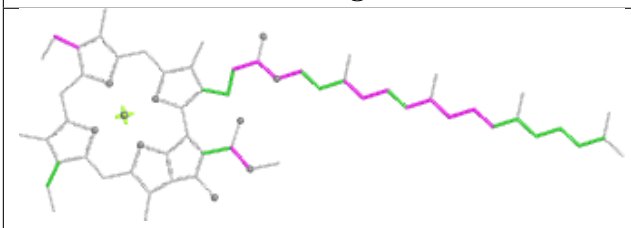
Ligand CLA b 601



Bond lengths



Bond angles



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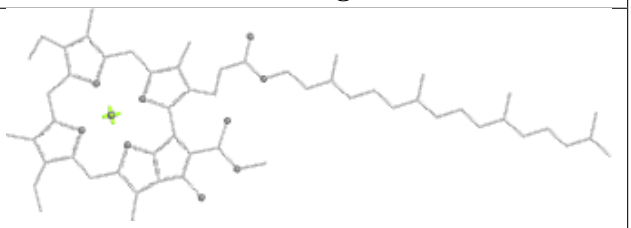
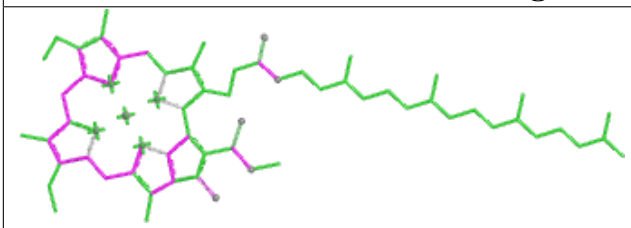


Rings

Ligand CLA c 507



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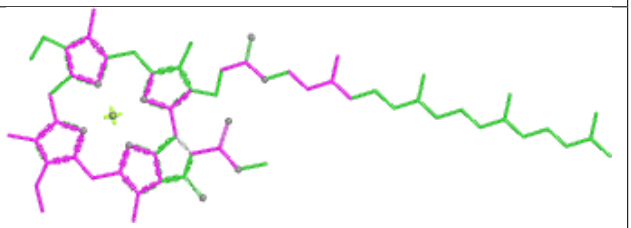
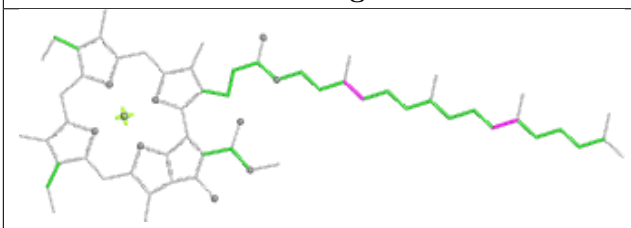


Bond angles



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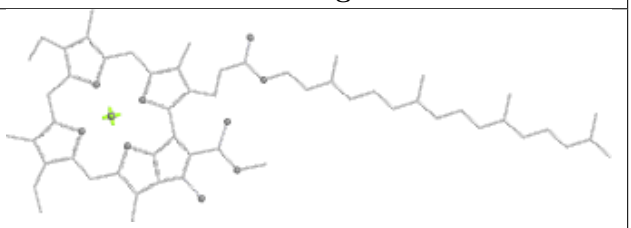
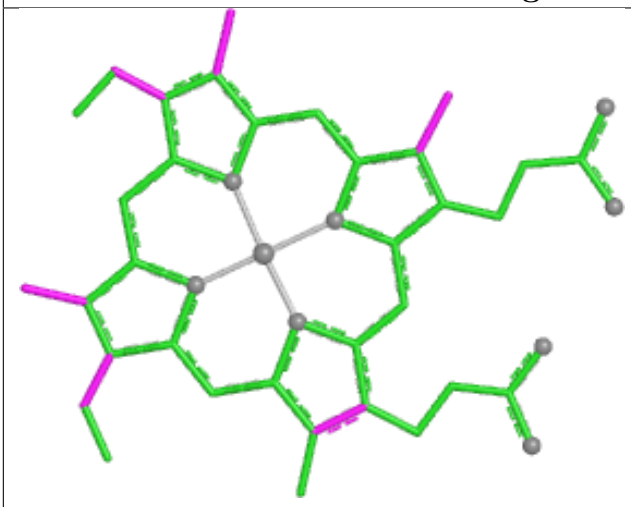


Rings

Ligand HEC V 201



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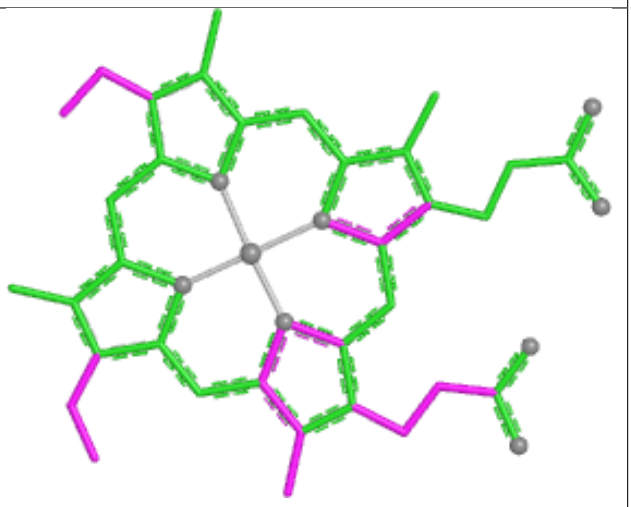
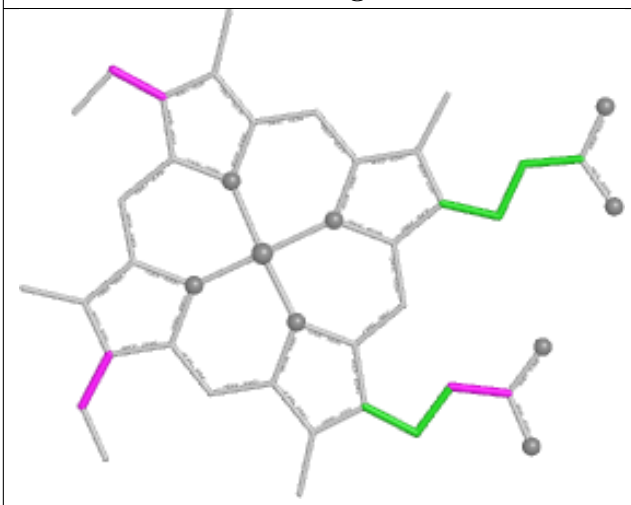


Bond angles



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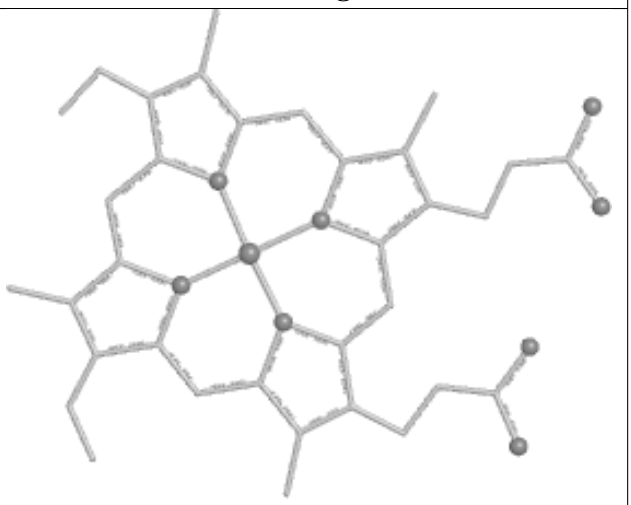
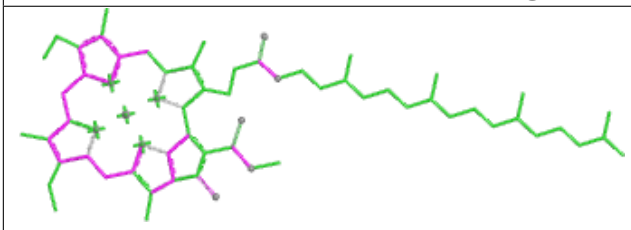


Rings

Ligand CLA A 407



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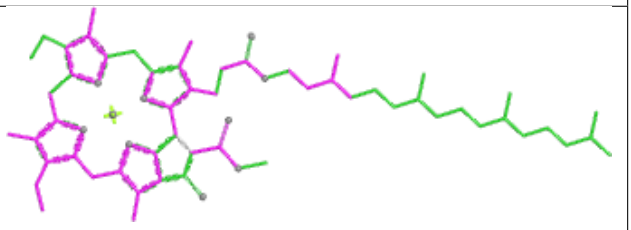
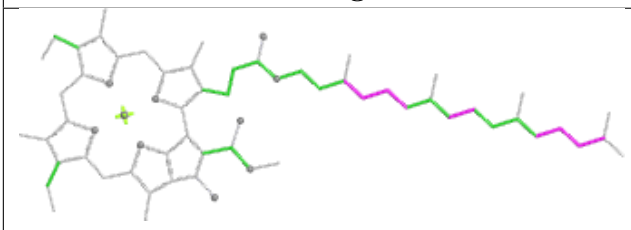


Bond angles



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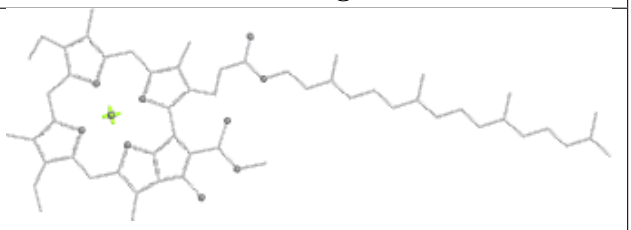
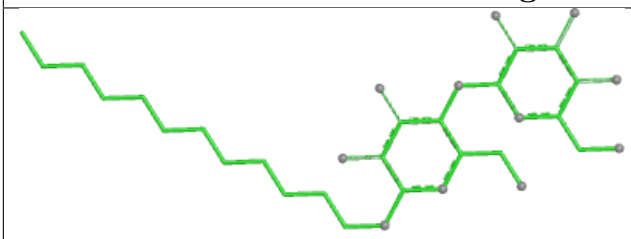
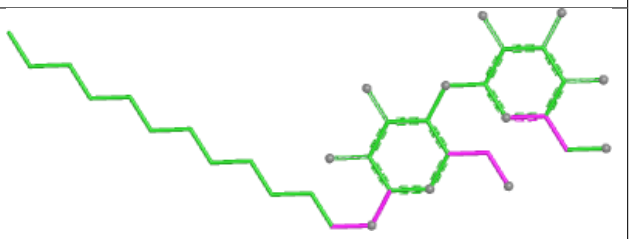


Rings

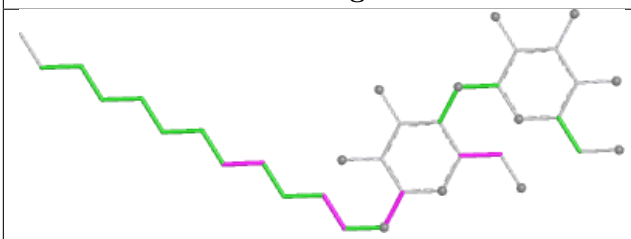
Ligand LMT m 103



Bond lengths



Bond angles



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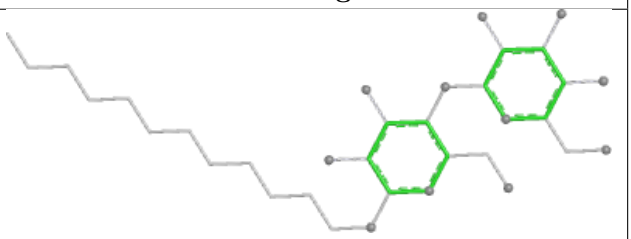
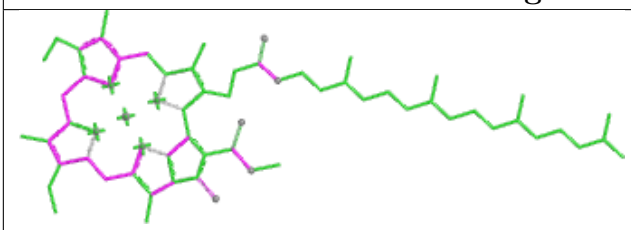
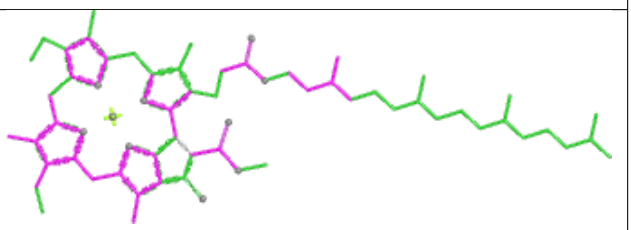


Rings

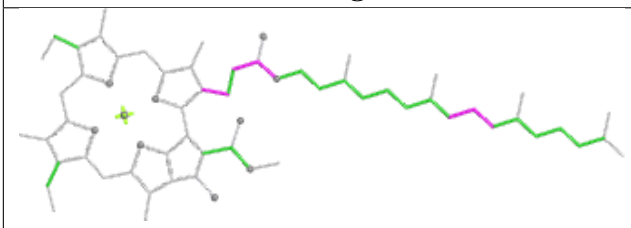
Ligand CLA B 612



Bond lengths



Bond angles



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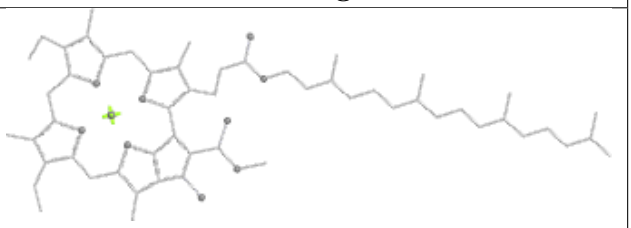
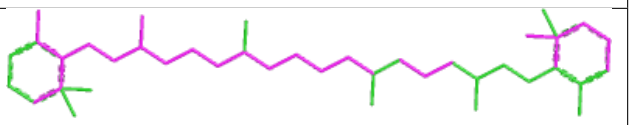


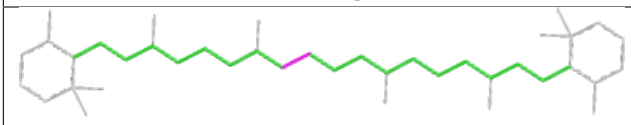
Rings

Ligand BCR T 101

Bond lengths



Bond angles



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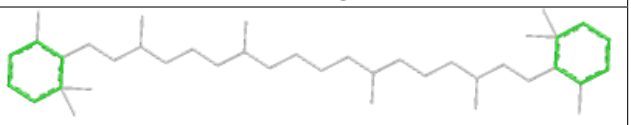
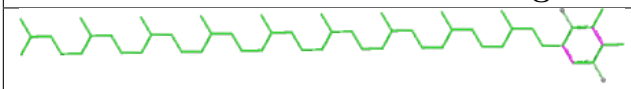


Rings

Ligand PL9 d 405



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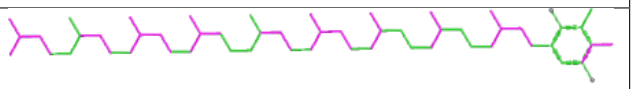
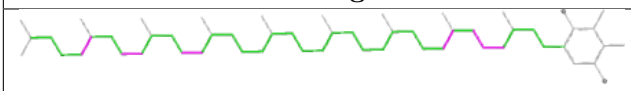
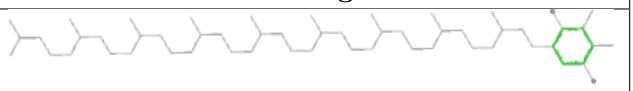


Bond angles

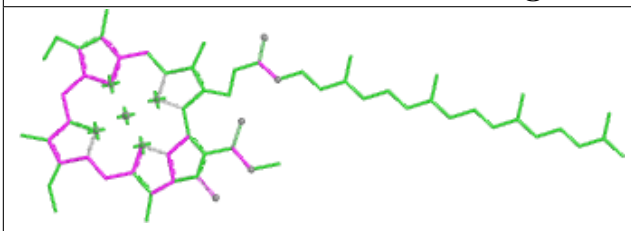


Torsions



Rings

Ligand CLA B 602



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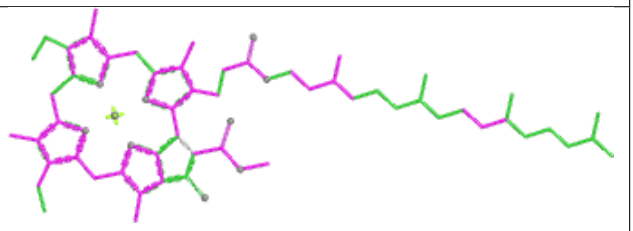
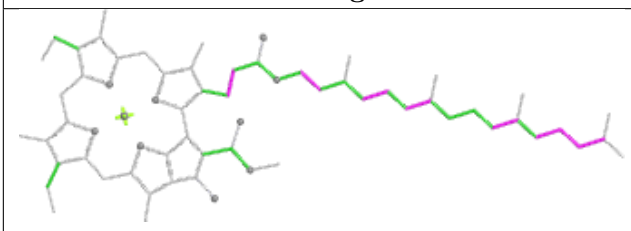
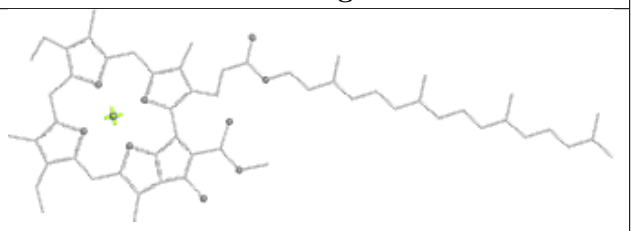


Bond angles

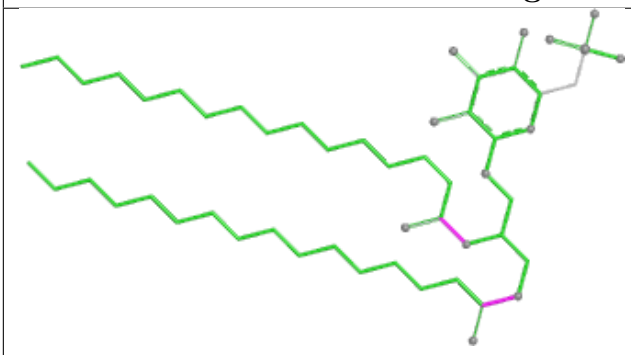


Torsions

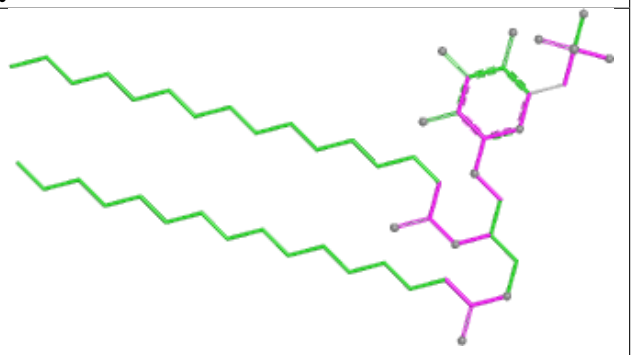


Rings

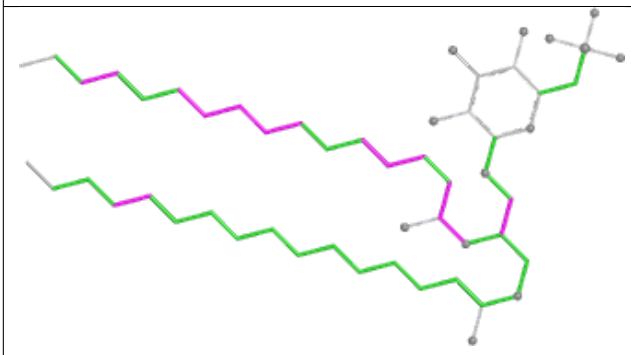
Ligand SQD A 409



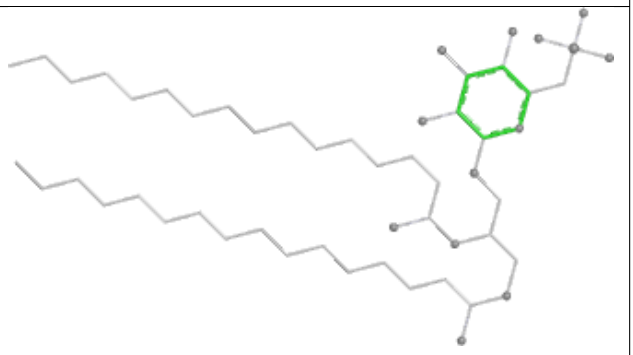
Bond lengths



Bond angles

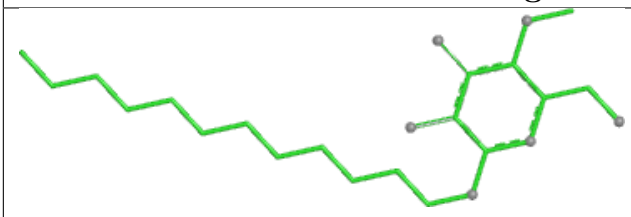


Torsions

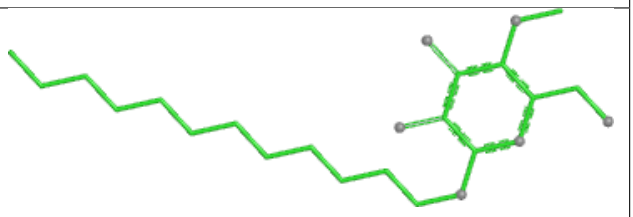


Rings

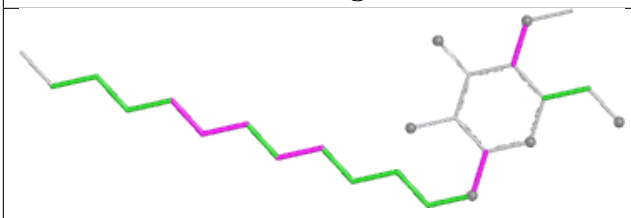
Ligand LMT b 620



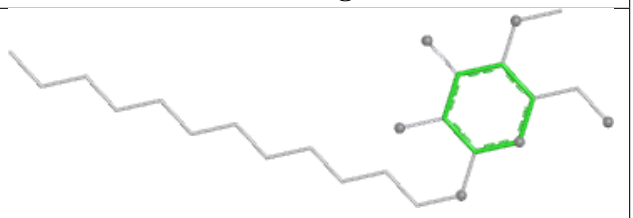
Bond lengths



Bond angles

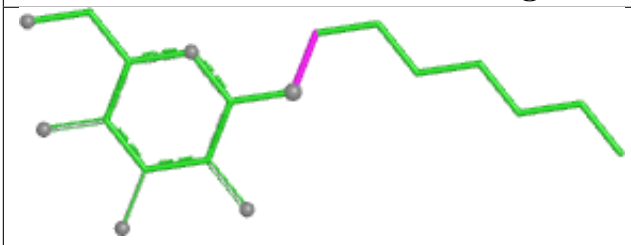


Torsions

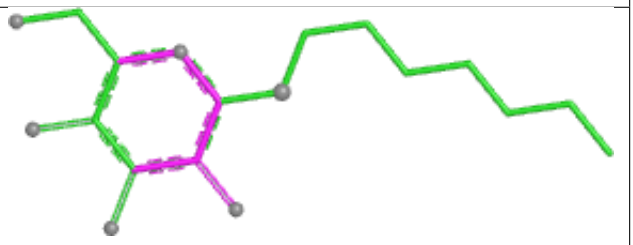


Rings

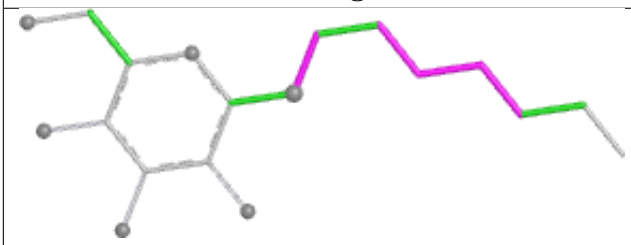
Ligand HTG B 621



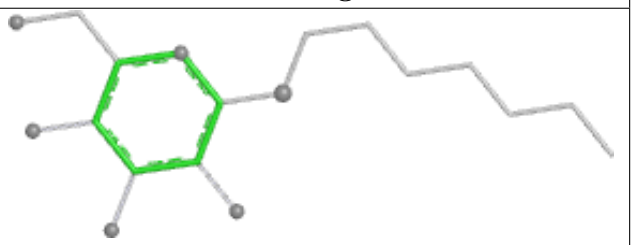
Bond lengths



Bond angles

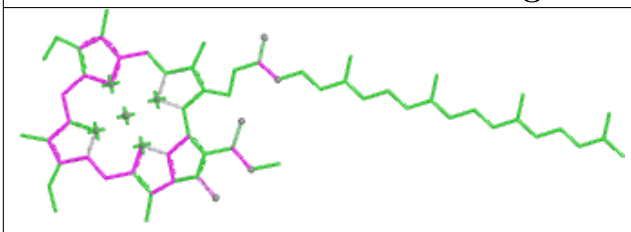


Torsions

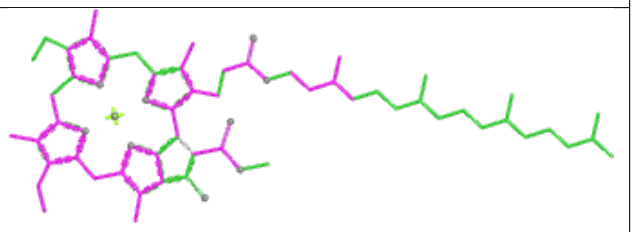


Rings

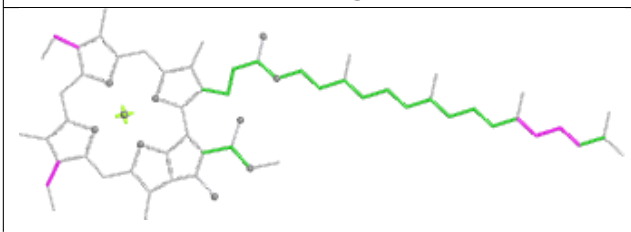
Ligand CLA D 403



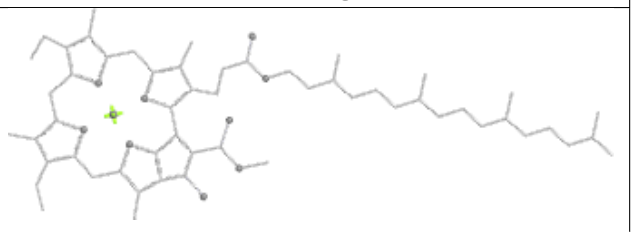
Bond lengths



Bond angles

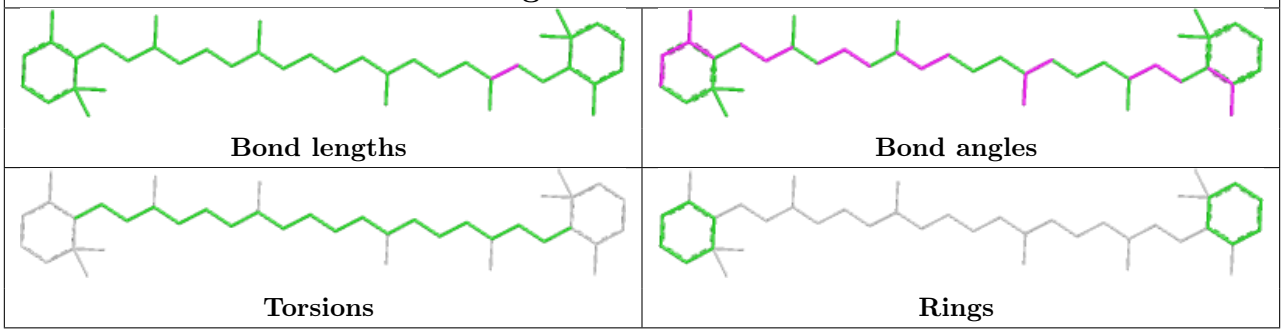


Torsions

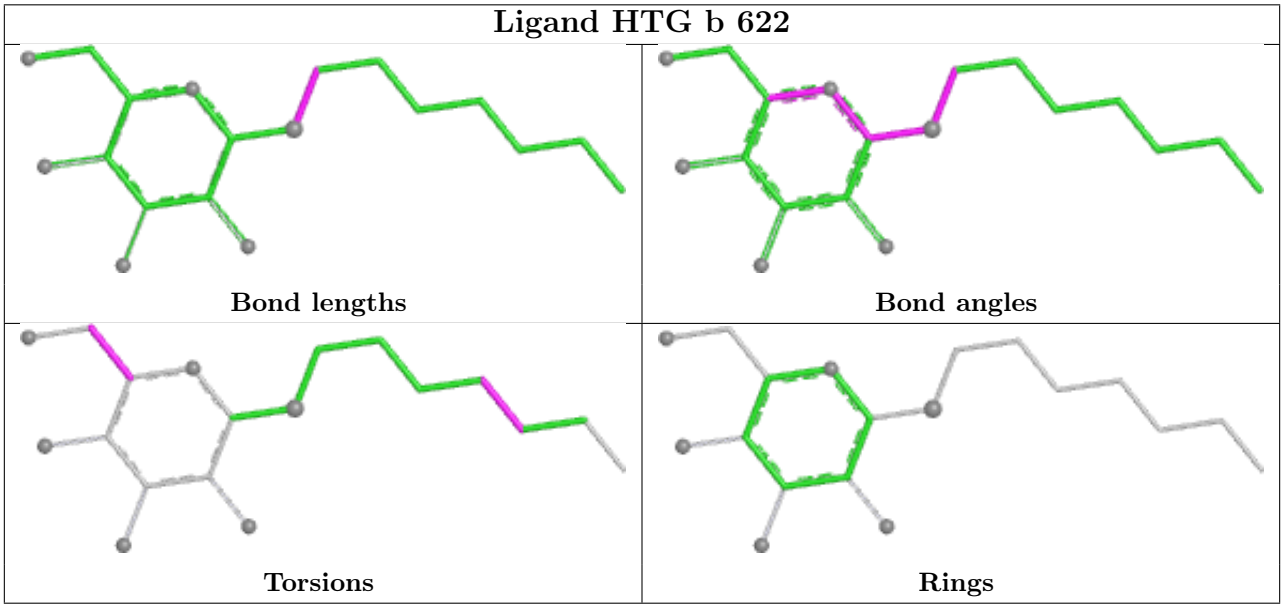


Rings

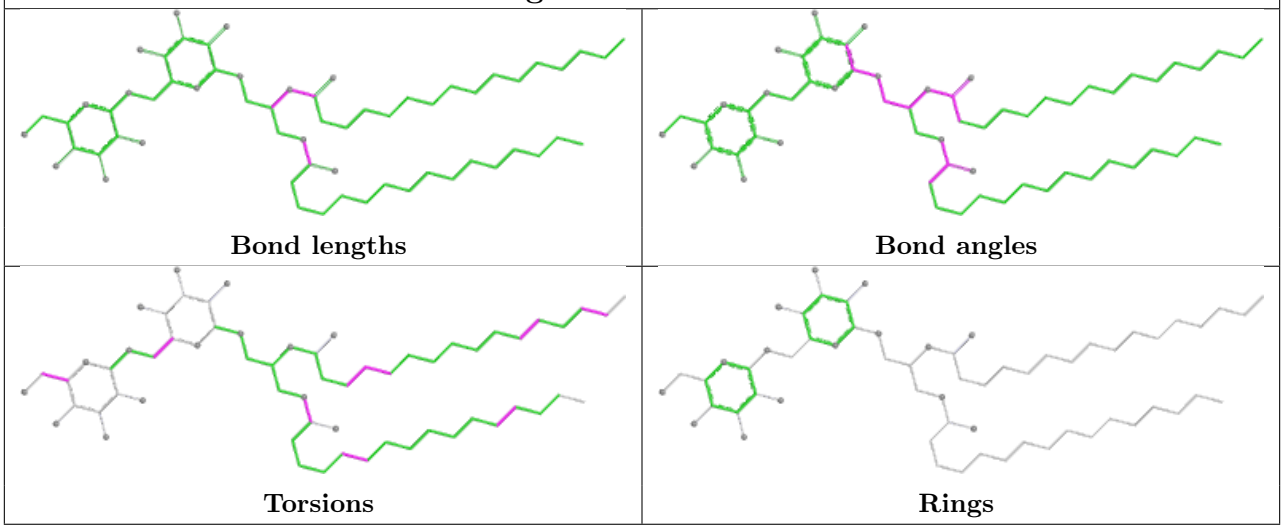
Ligand BCR K 101



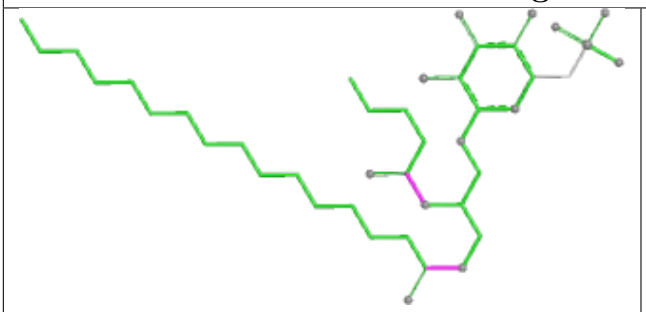
Ligand HTG b 622



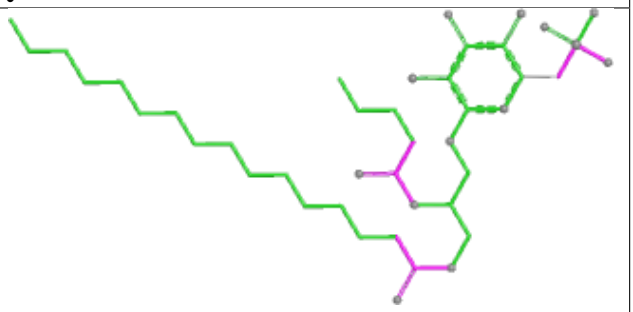
Ligand DGD c 520



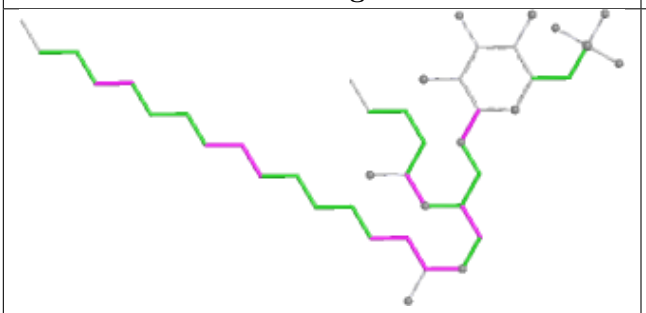
Ligand SQD f 101



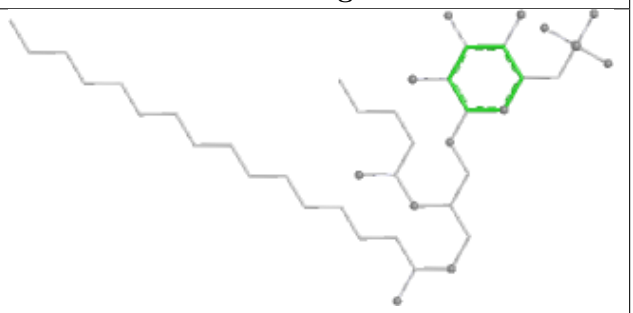
Bond lengths



Bond angles

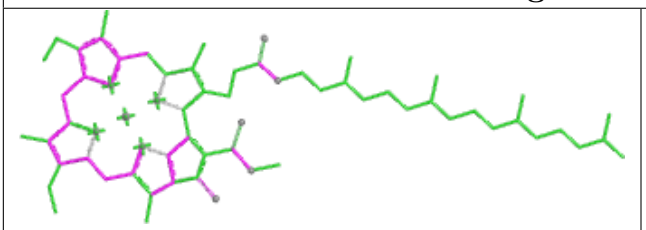


Torsions

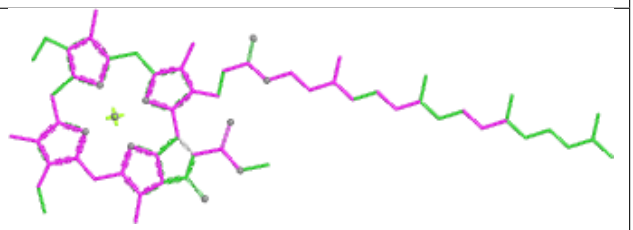


Rings

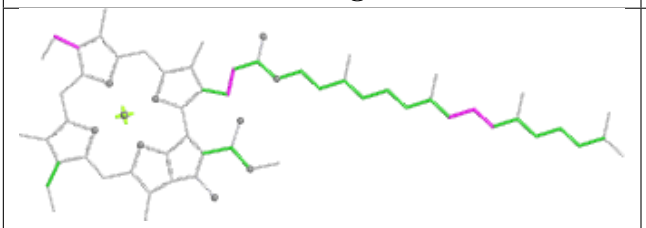
Ligand CLA b 602



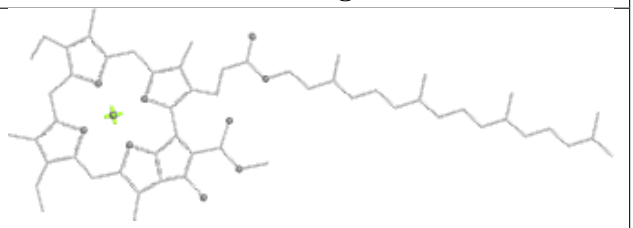
Bond lengths



Bond angles

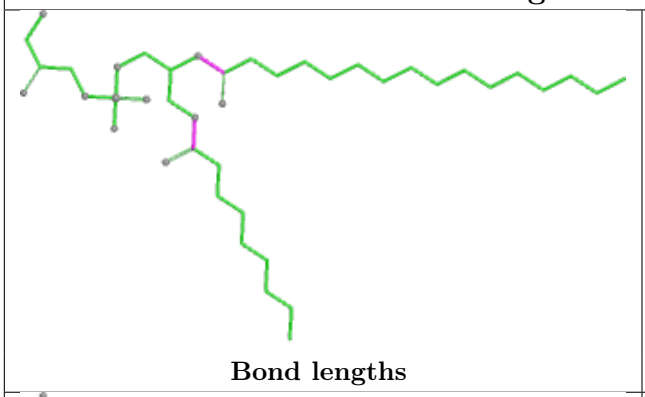


Torsions

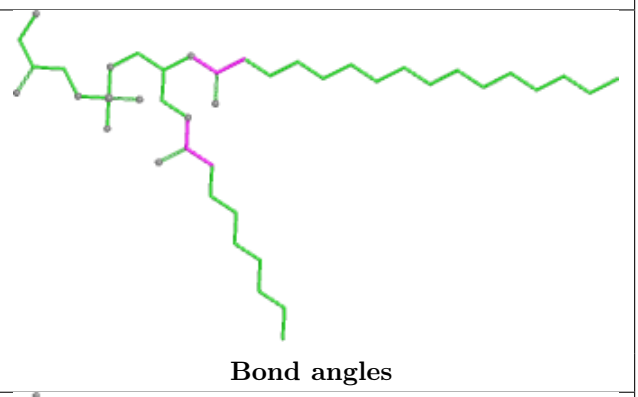


Rings

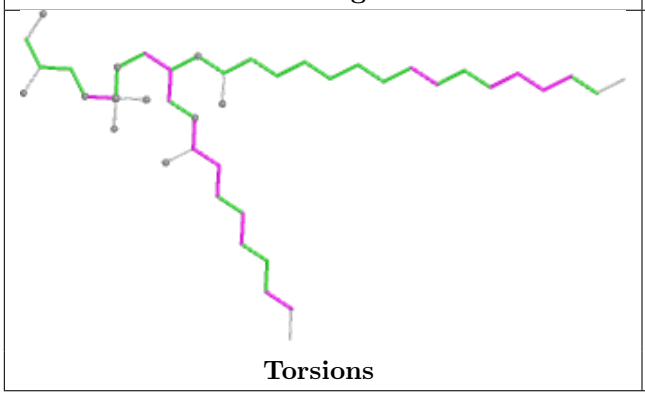
Ligand LHG a 419



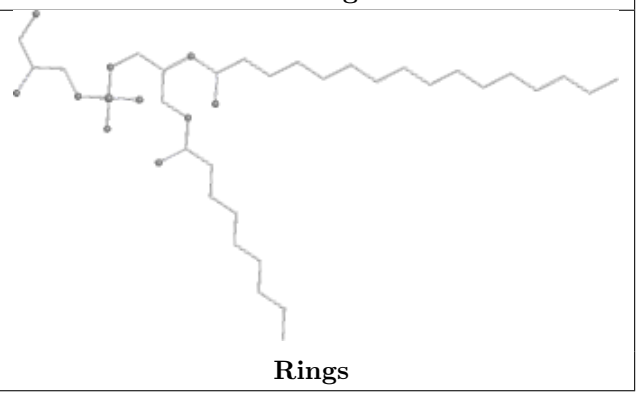
Bond lengths



Bond angles

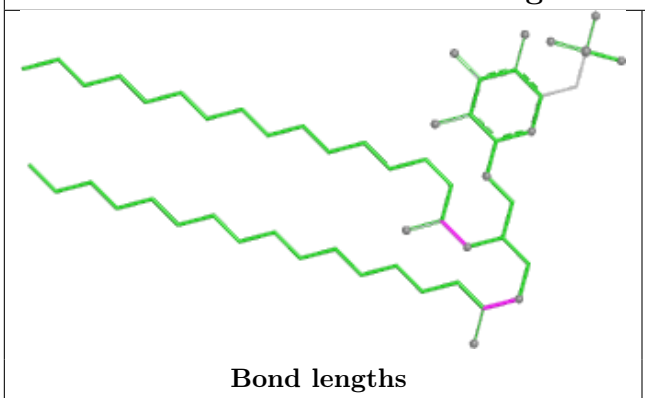


Torsions

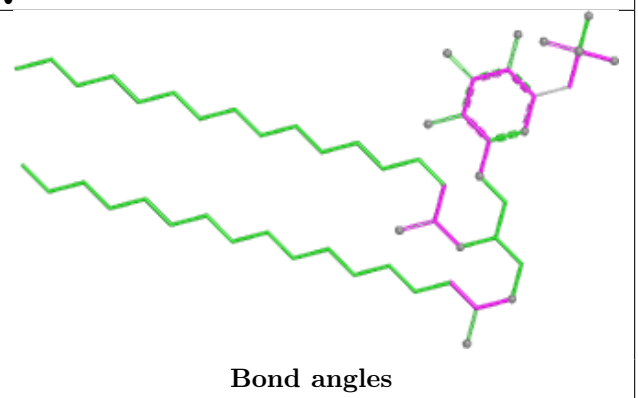


Rings

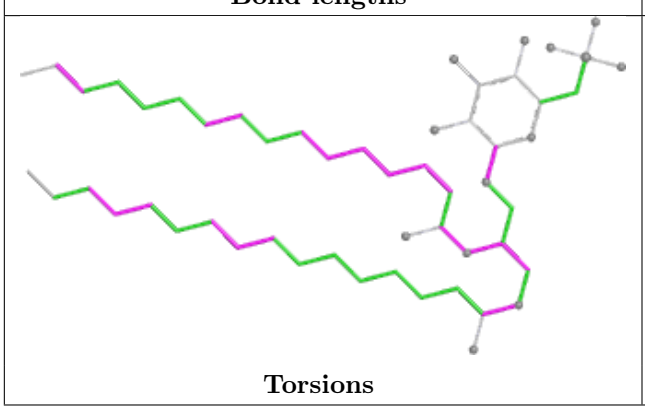
Ligand SQD B 620



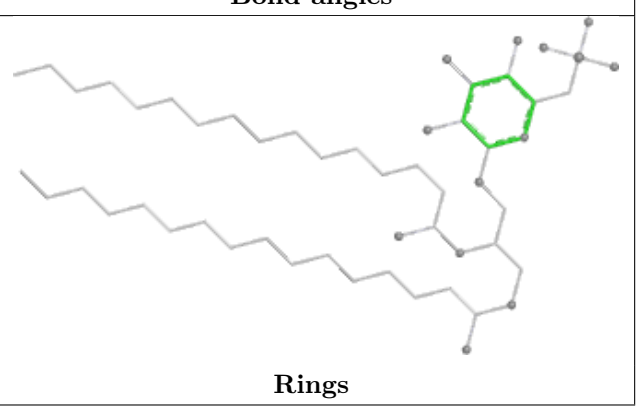
Bond lengths



Bond angles

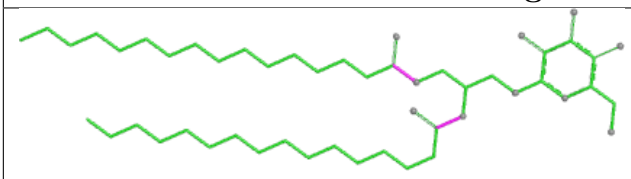


Torsions

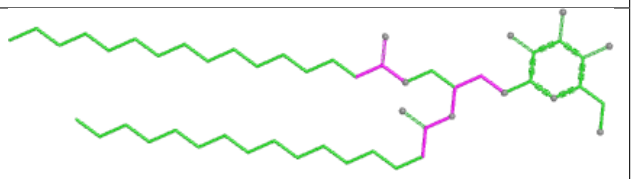


Rings

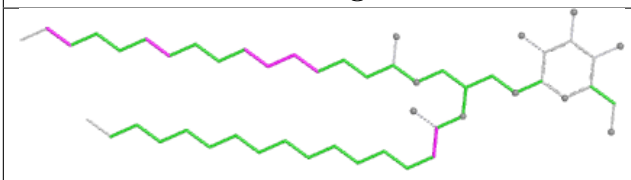
Ligand LMG c 521



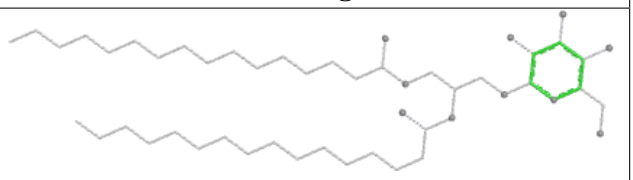
Bond lengths



Bond angles

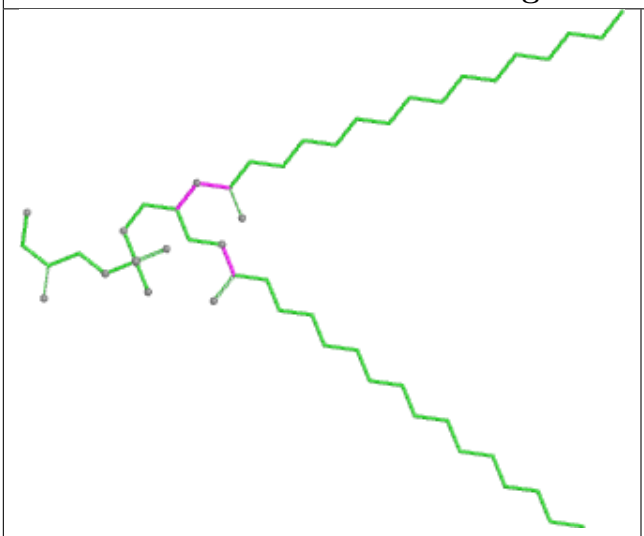


Torsions

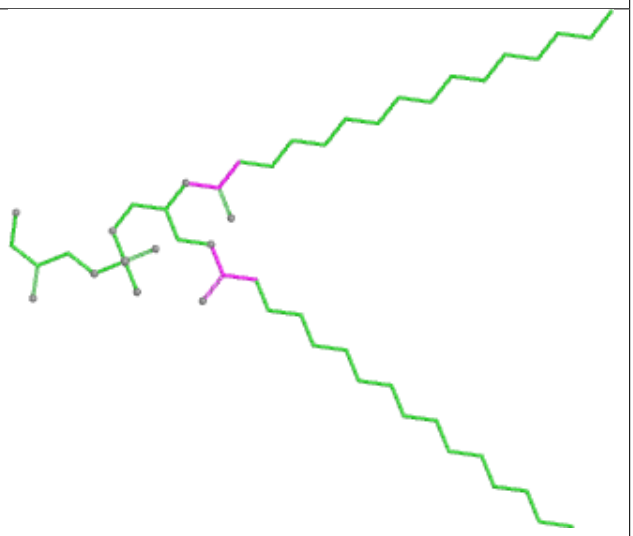


Rings

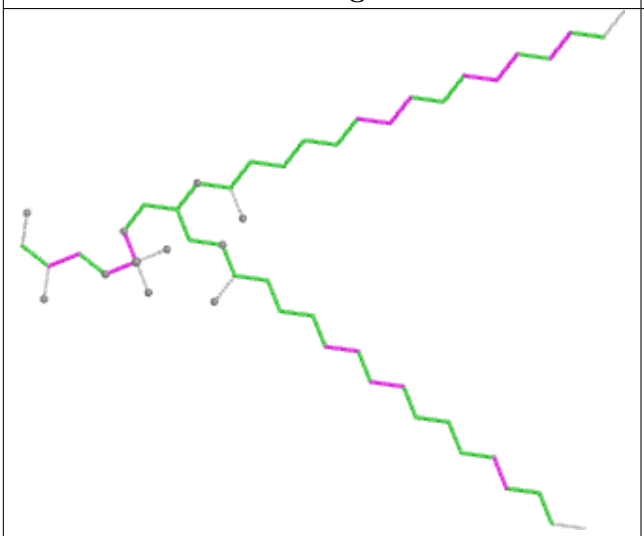
Ligand LHG D 407



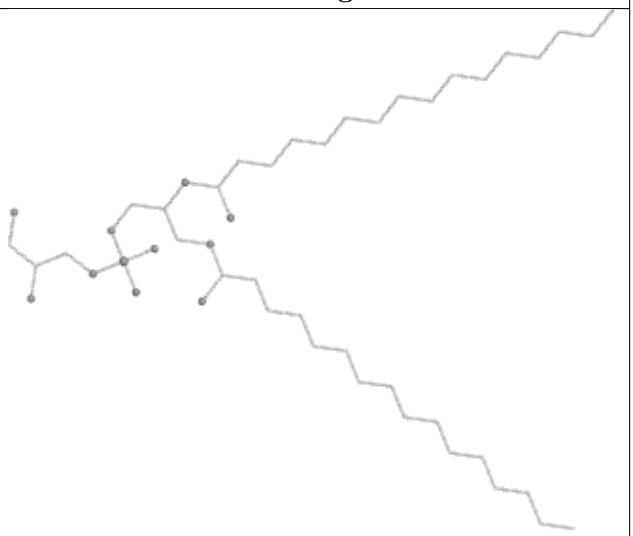
Bond lengths



Bond angles

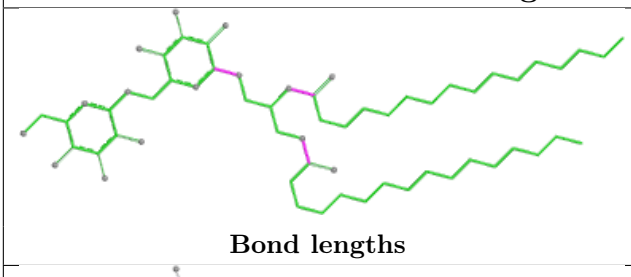


Torsions



Rings

Ligand DGD C 519



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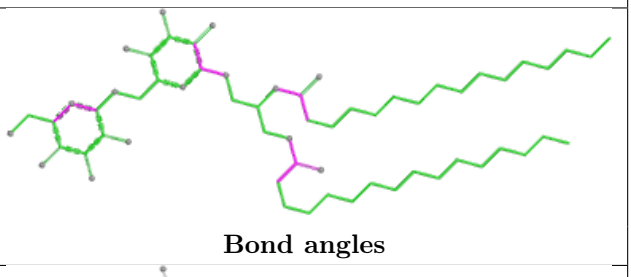
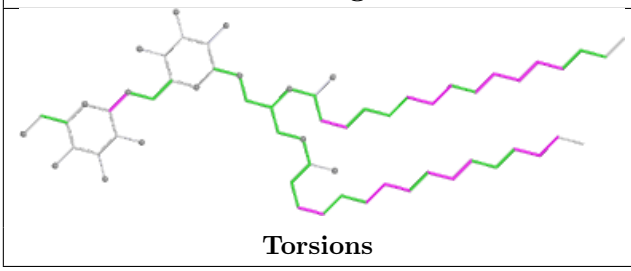


Bond angles



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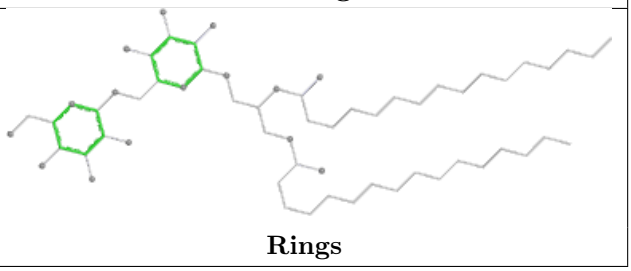
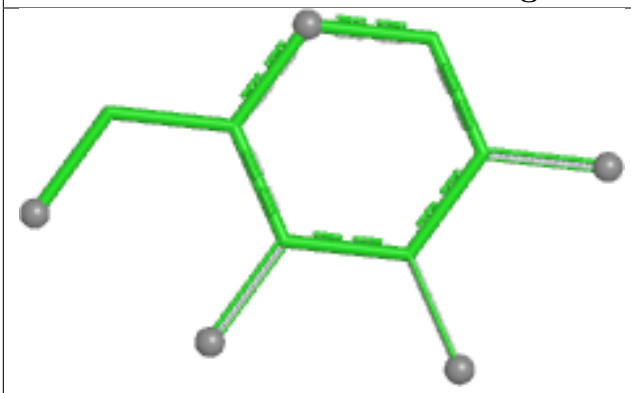


Rings

Ligand HTG V 202



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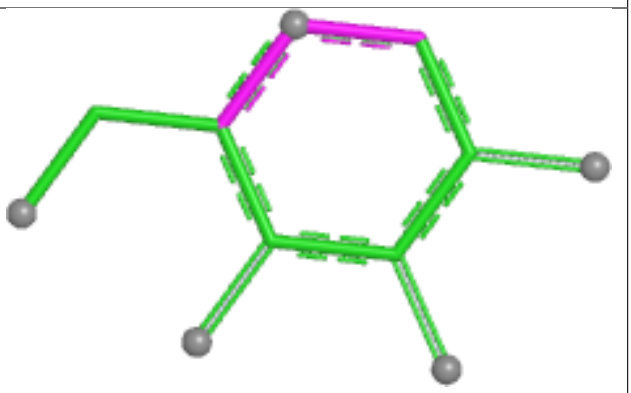
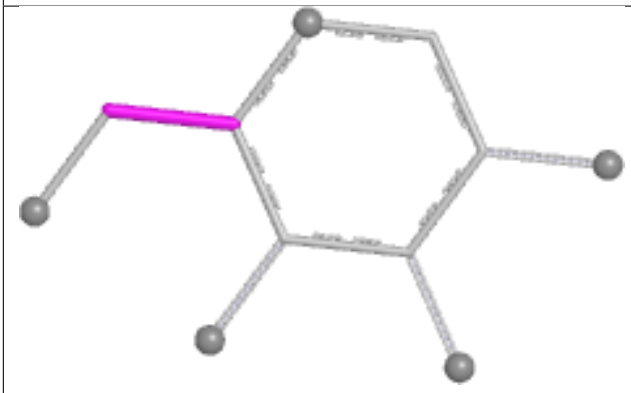
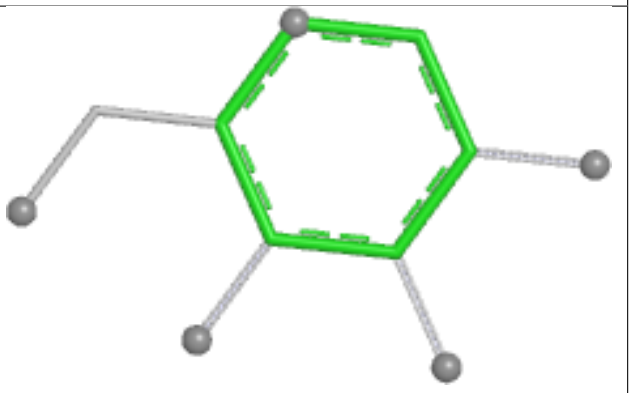


Bond angles

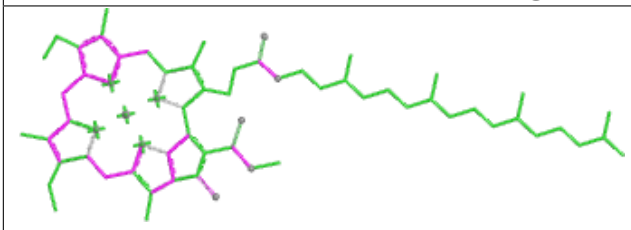


Torsions

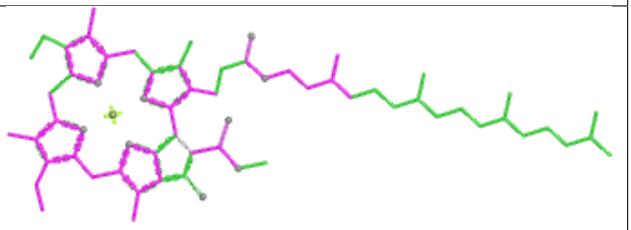


Rings

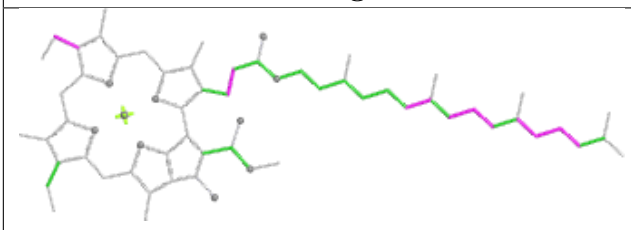
Ligand CLA b 606



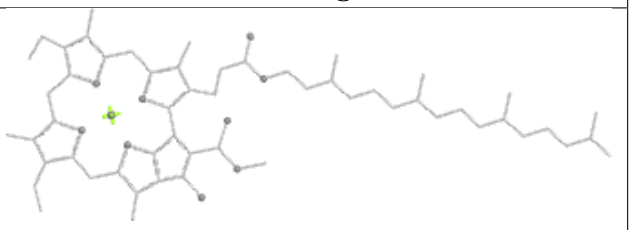
Bond lengths



Bond angles

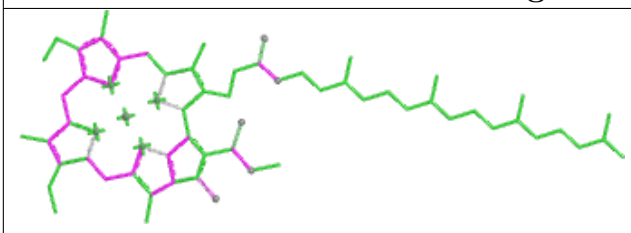


Torsions

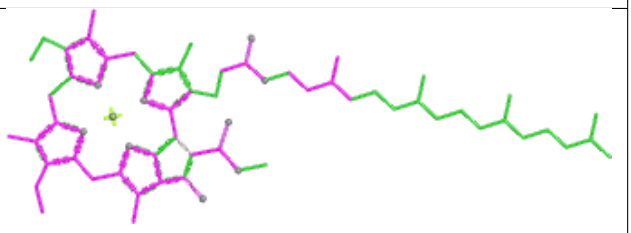


Rings

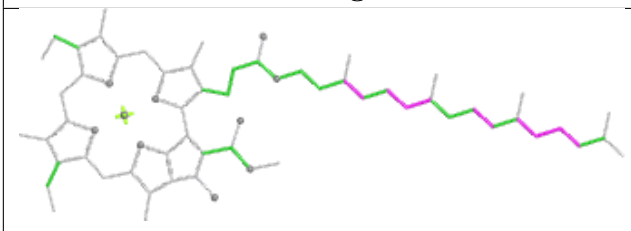
Ligand CLA b 616



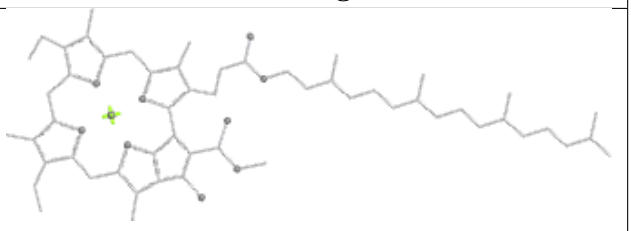
Bond lengths



Bond angles

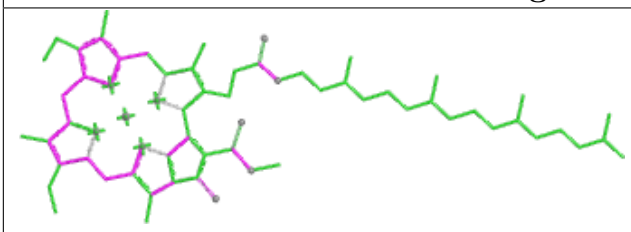


Torsions

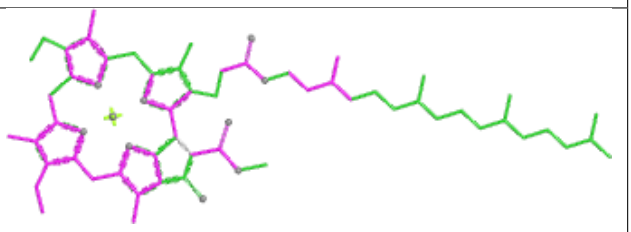


Rings

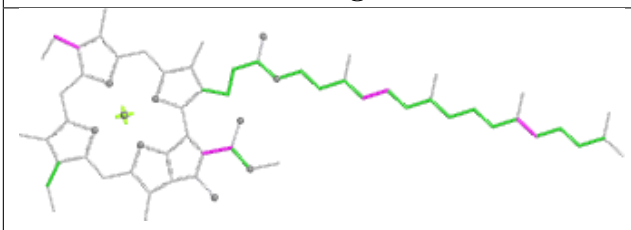
Ligand CLA c 504



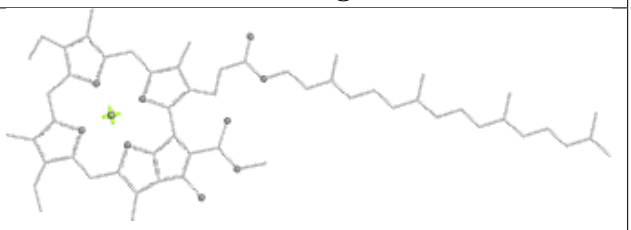
Bond lengths



Bond angles

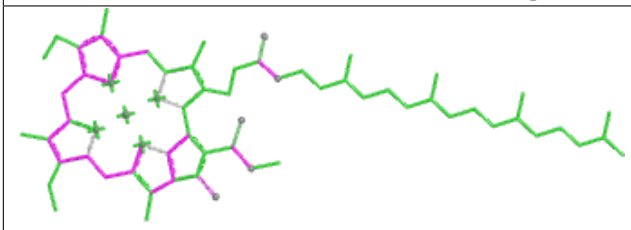


Torsions



Rings

Ligand CLA B 610



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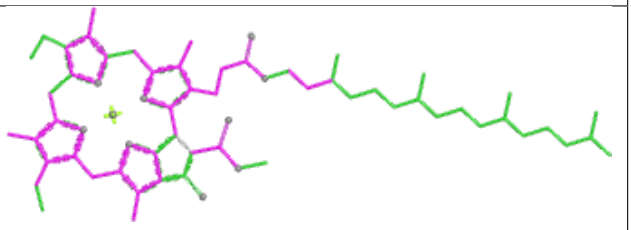
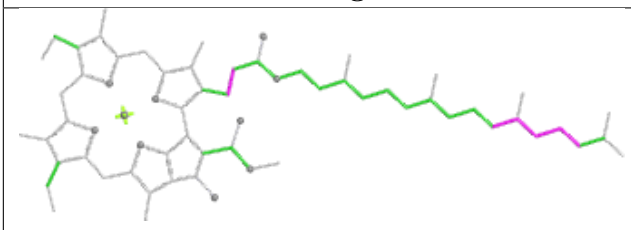
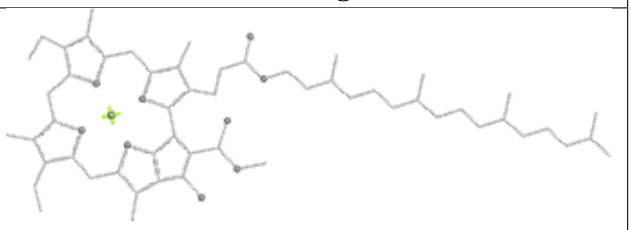


Bond angles

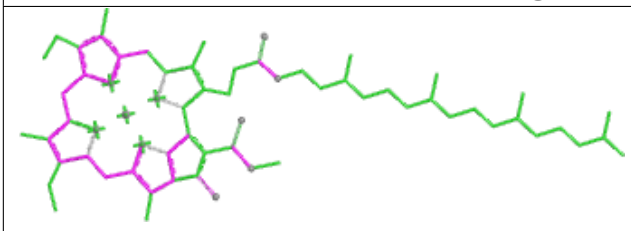


Torsions



Rings

Ligand CLA c 515



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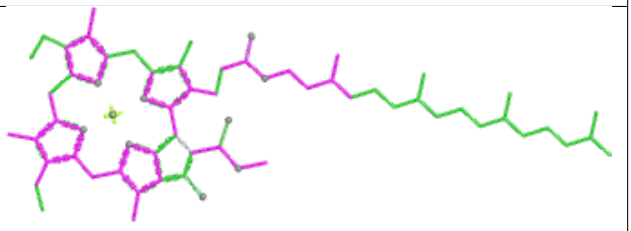
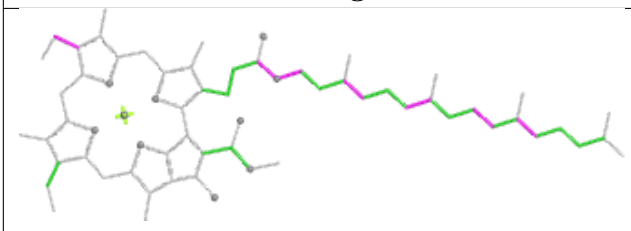


Bond angles



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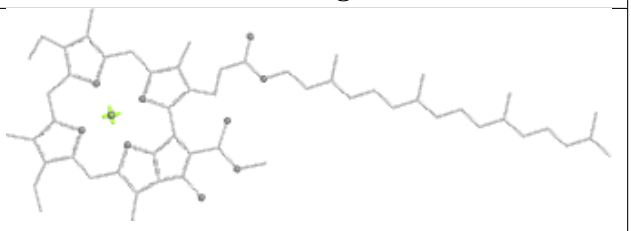
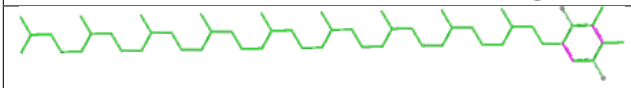
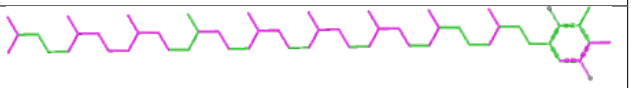


Rings

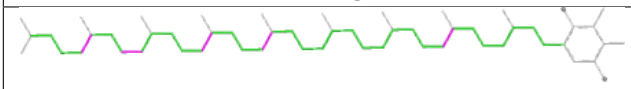
Ligand PL9 D 406



Bond lengths



Bond angles



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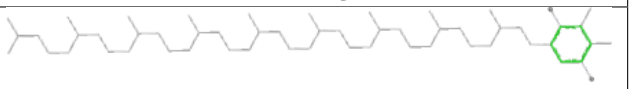
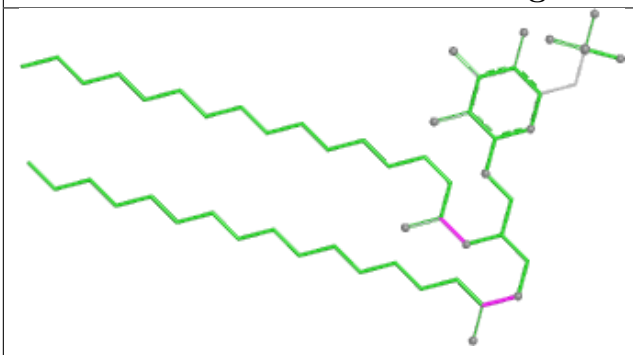
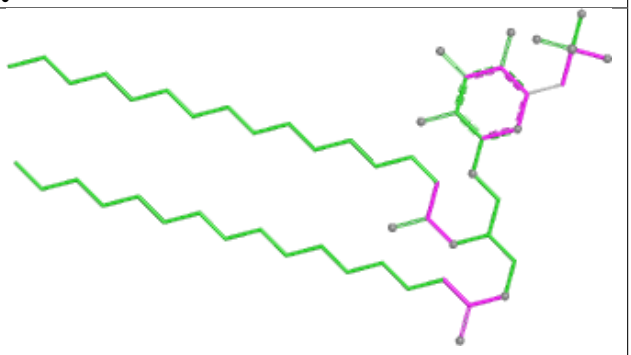


Rings

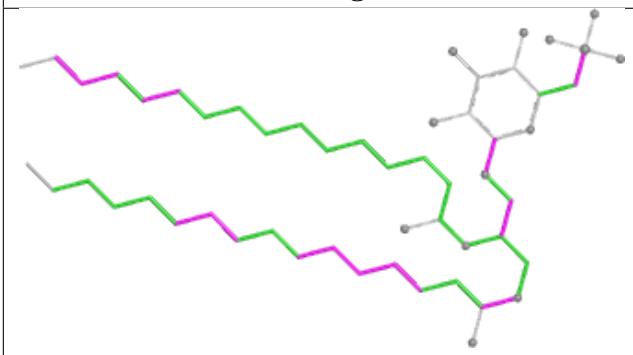
Ligand SQD a 411



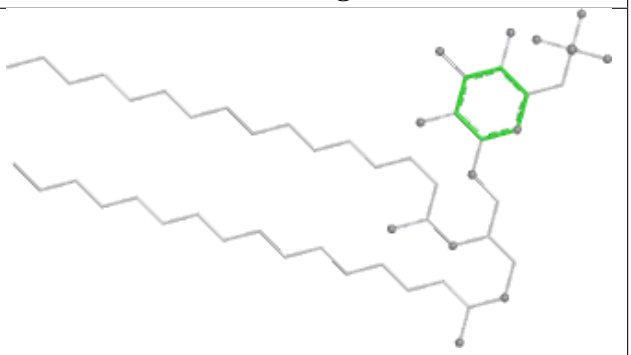
Bond lengths



Bond angles

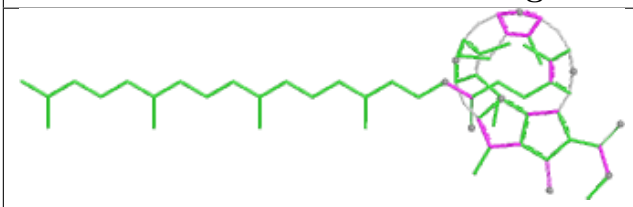


Torsions



Rings

Ligand PHO a 416



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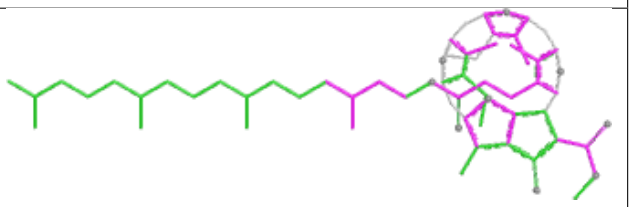
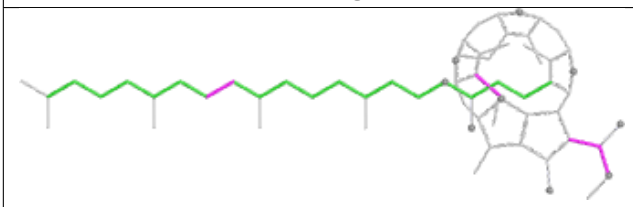


Bond angles



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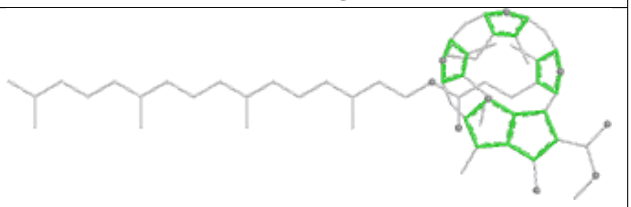
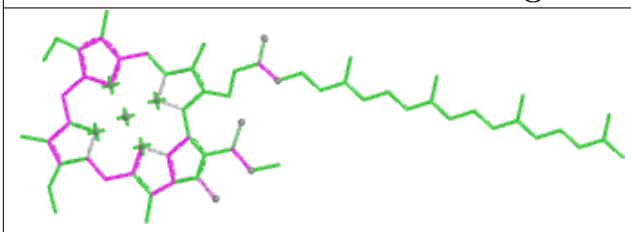


Rings

Ligand CLA C 504



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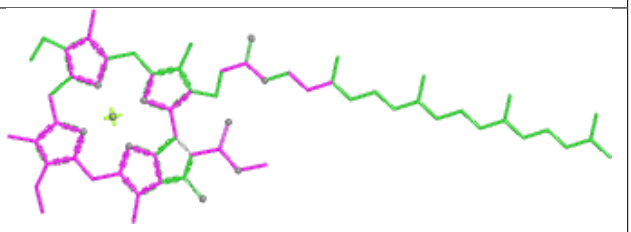
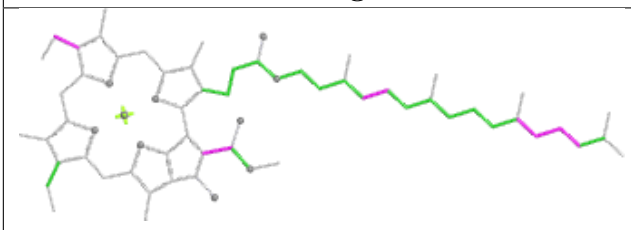


Bond angles



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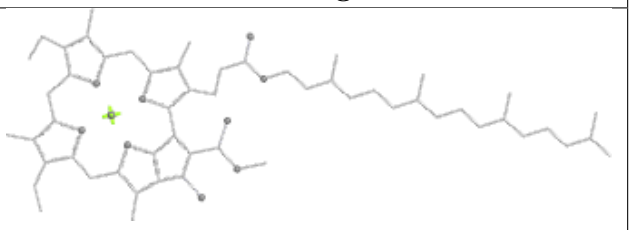
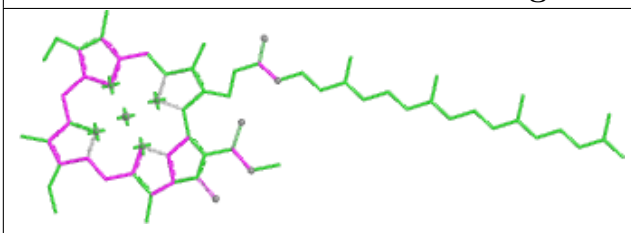


Rings

Ligand CLA c 514



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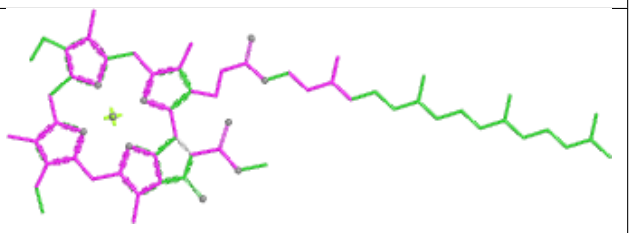
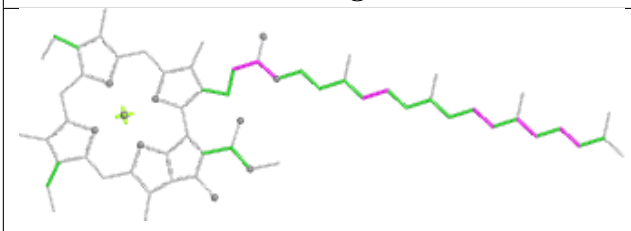


Bond angles



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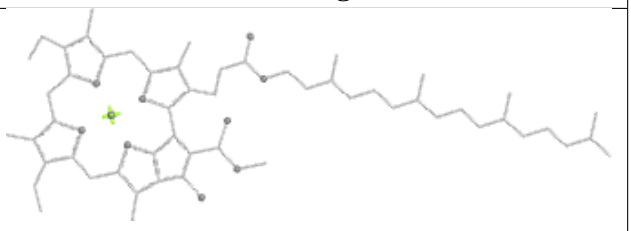
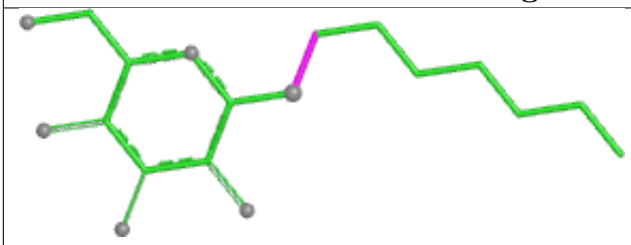
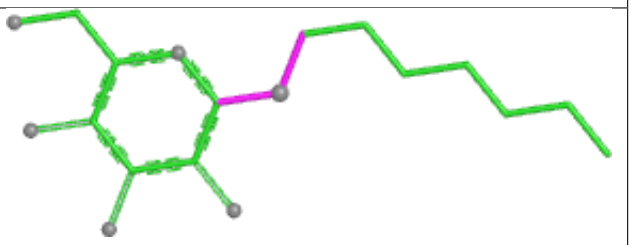


Rings

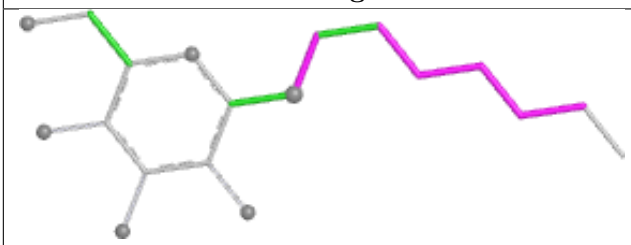
Ligand HTG B 622



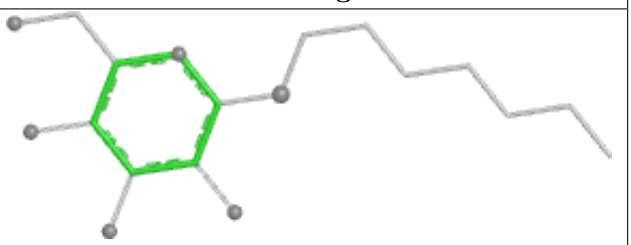
Bond lengths



Bond angles

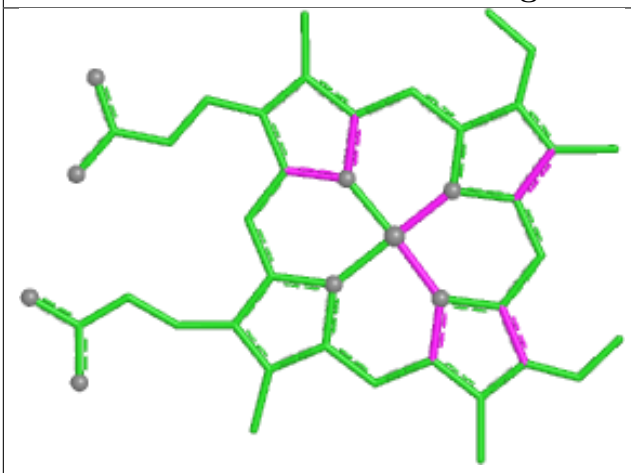


Torsions



Rings

Ligand HEM E 102



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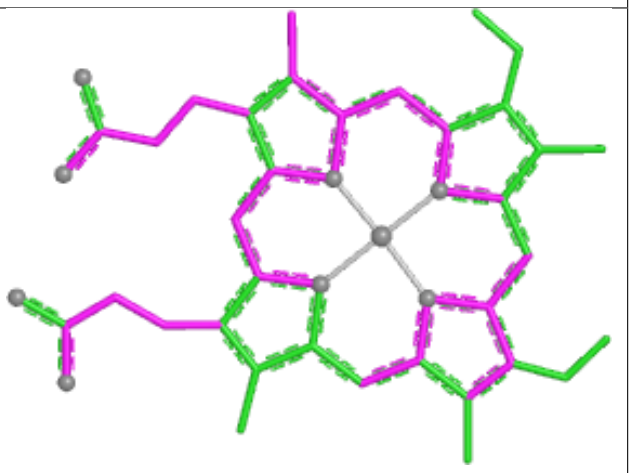
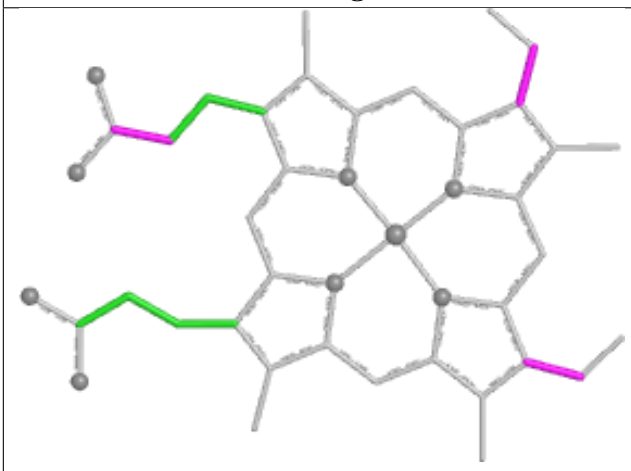


Bond angles



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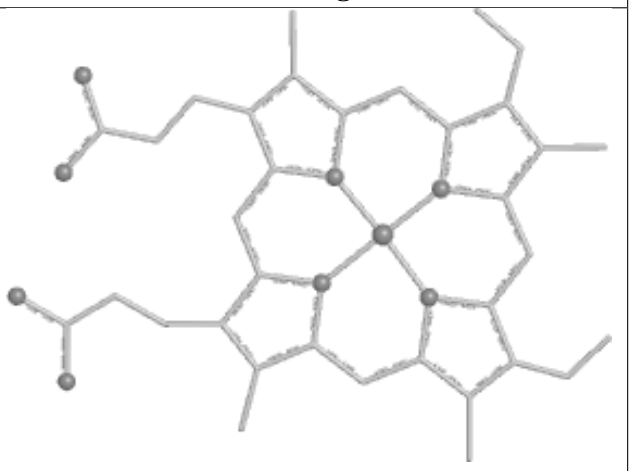
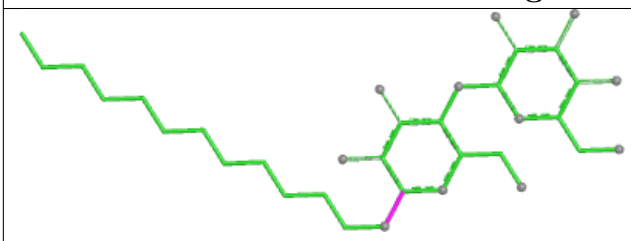


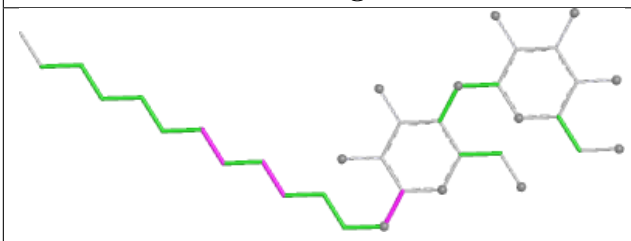
Rings

Ligand LMT a 418



Bond lengths

Bond angles



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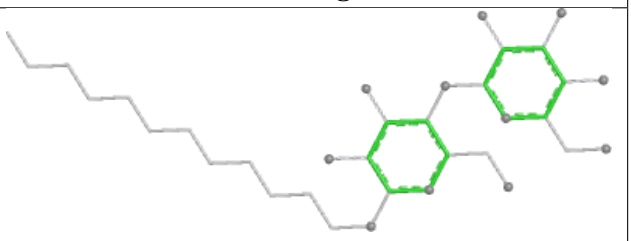
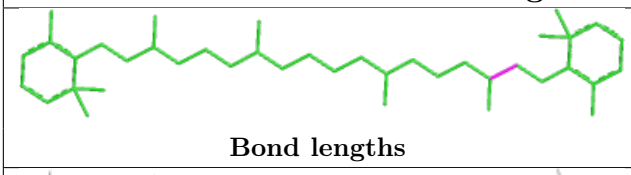


Rings

Ligand BCR k 101



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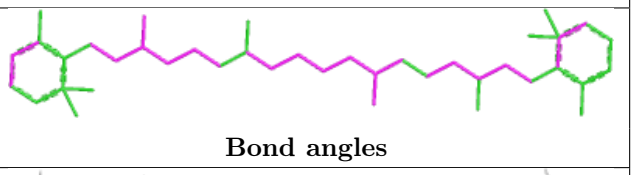
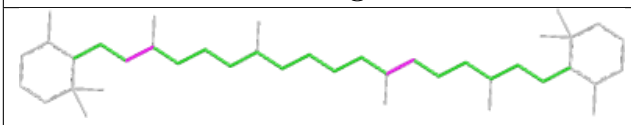
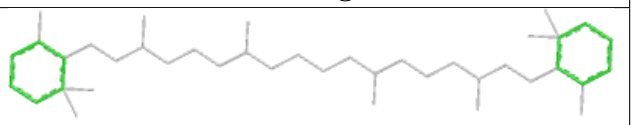


Bond angles

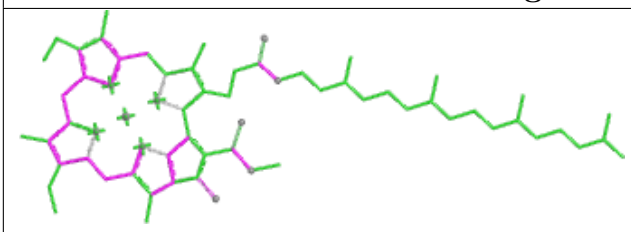


Torsions

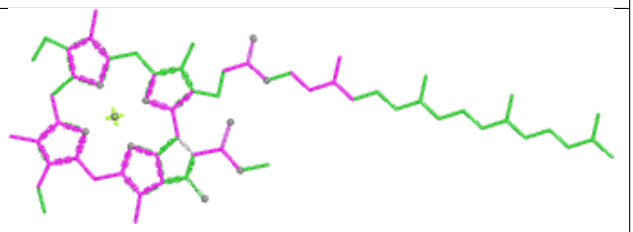


Rings

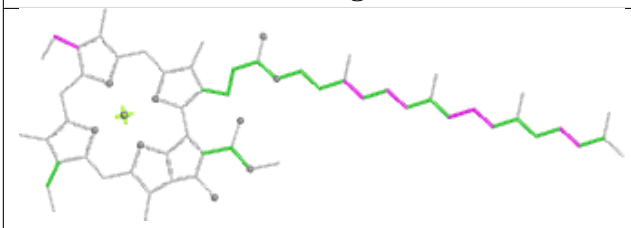
Ligand CLA C 507



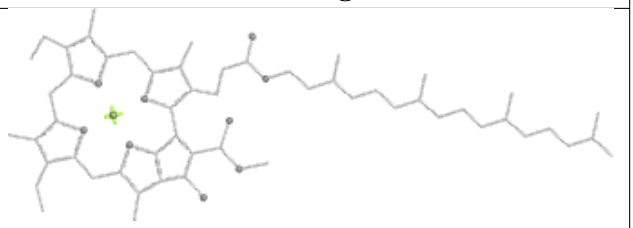
Bond lengths



Bond angles

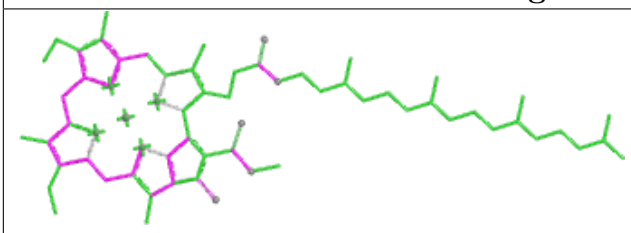


Torsions

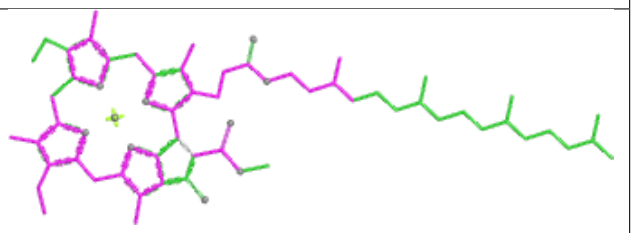


Rings

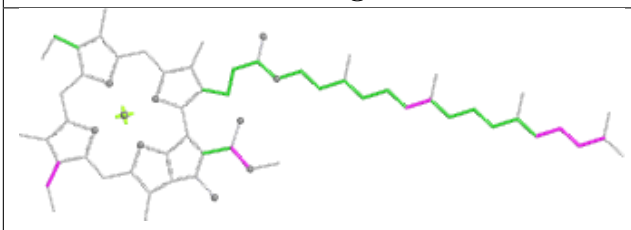
Ligand CLA a 404



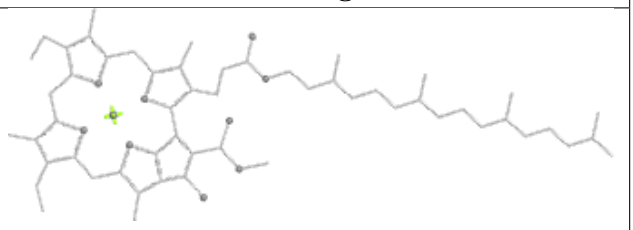
Bond lengths



Bond angles

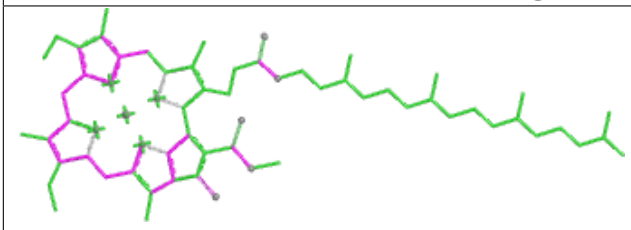


Torsions

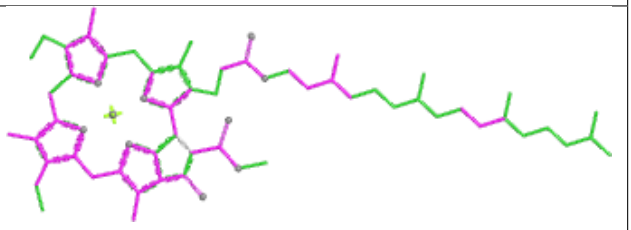


Rings

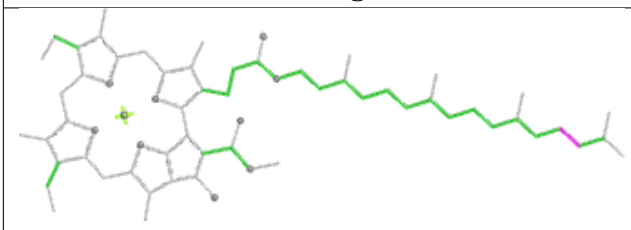
Ligand CLA c 505



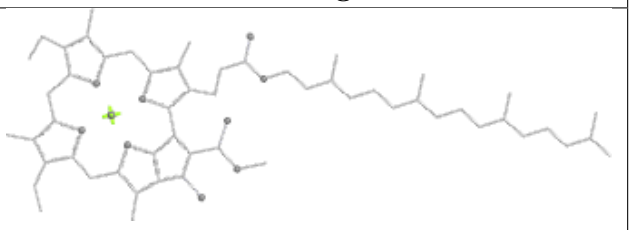
Bond lengths



Bond angles

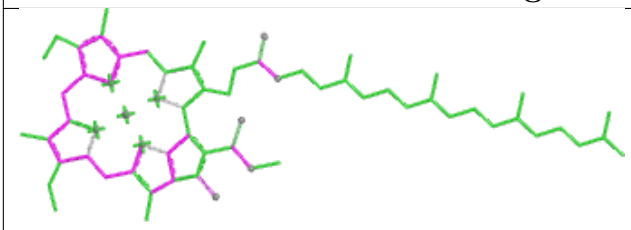


Torsions

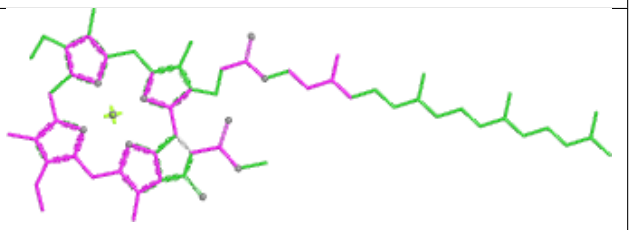


Rings

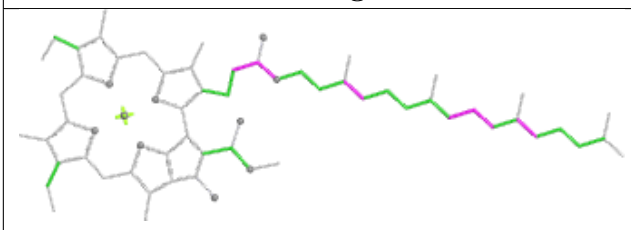
Ligand CLA C 512



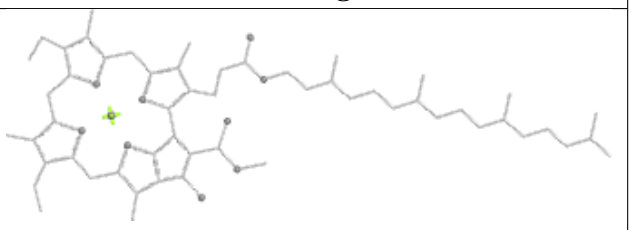
Bond lengths



Bond angles

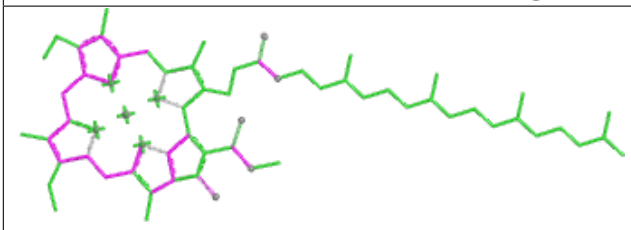


Torsions

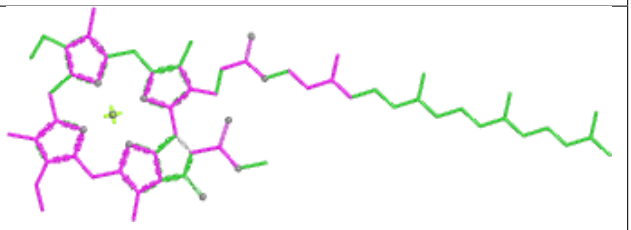


Rings

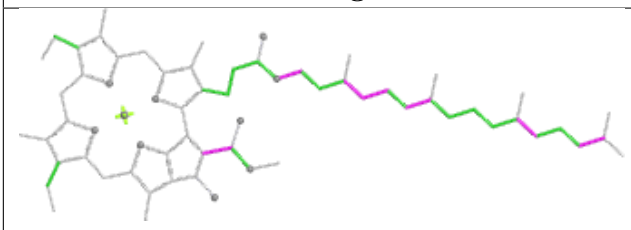
Ligand CLA b 614



Bond lengths



Bond angles



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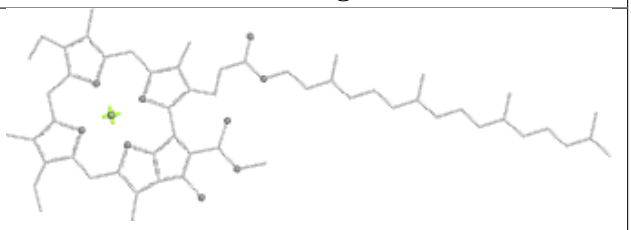
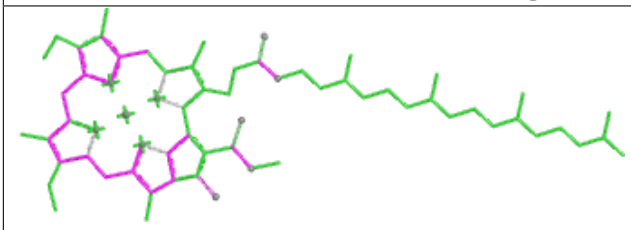


Rings

Ligand CLA C 508



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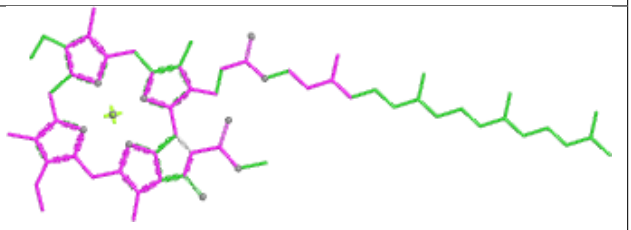
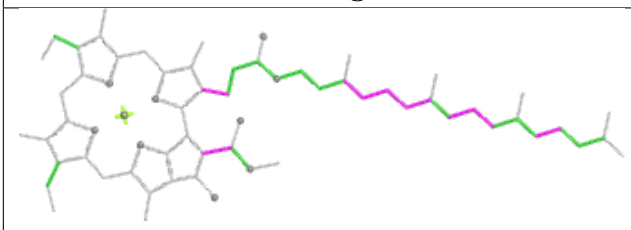
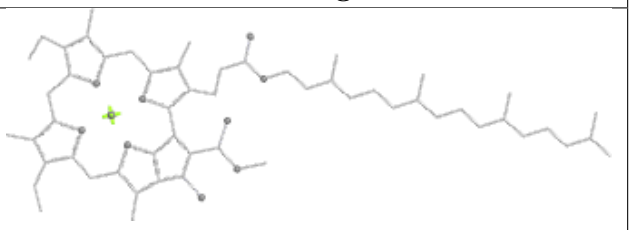


Bond angles

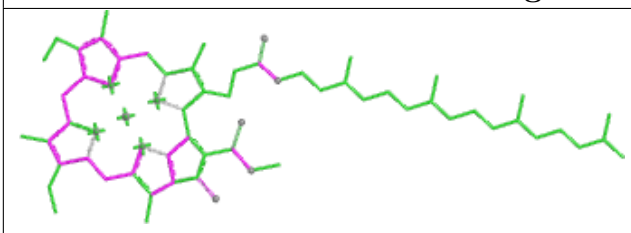


Torsions

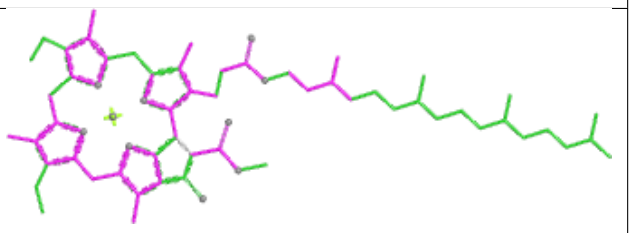


Rings

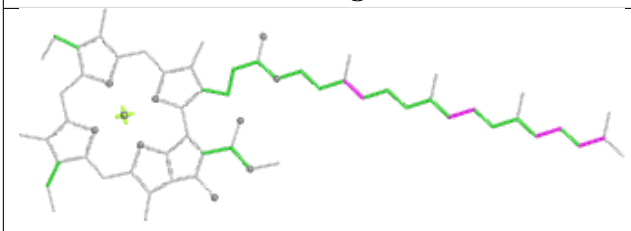
Ligand CLA B 603



Bond lengths



Bond angles



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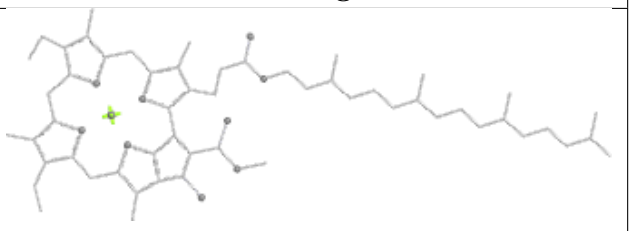
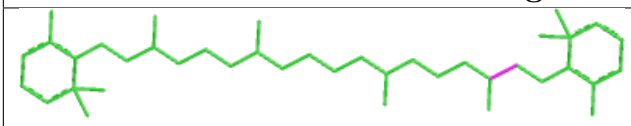
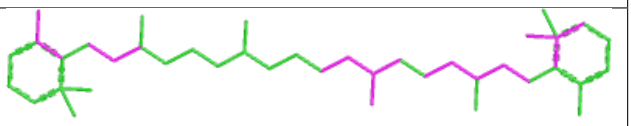


Rings

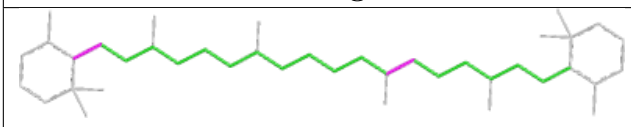
Ligand BCR b 617



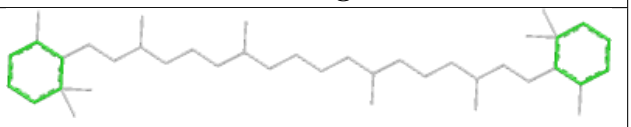
Bond lengths



Bond angles

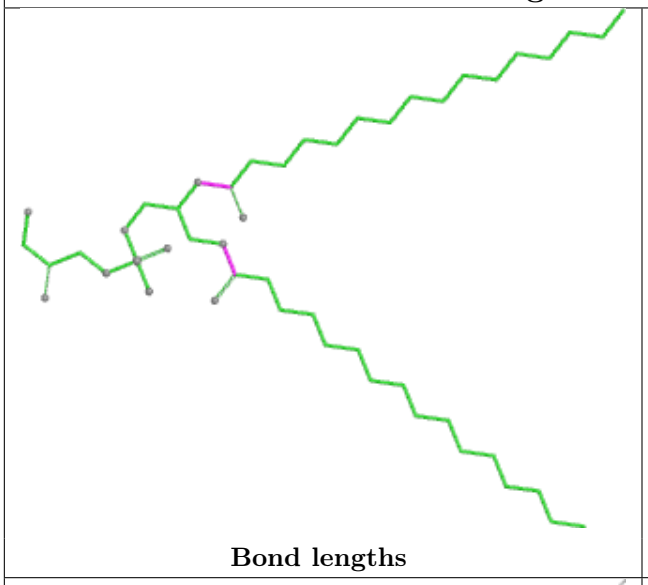


Torsions



Rings

Ligand LHG d 408



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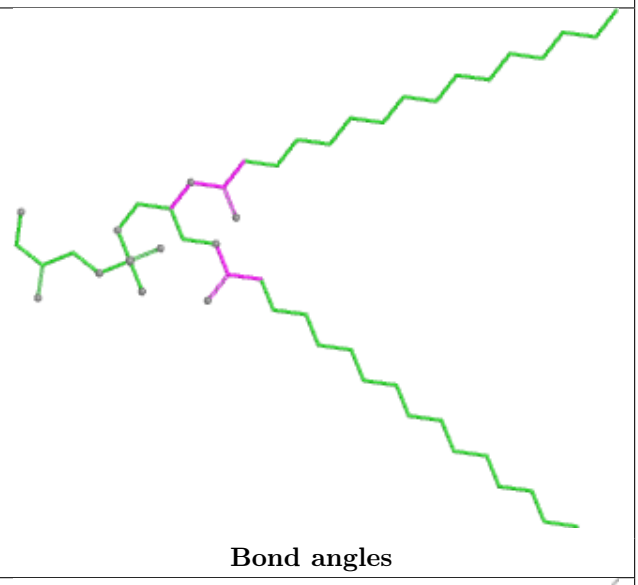
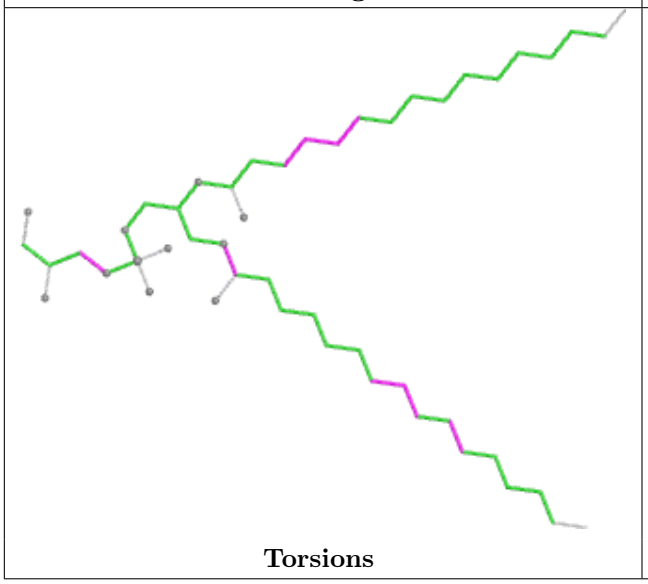
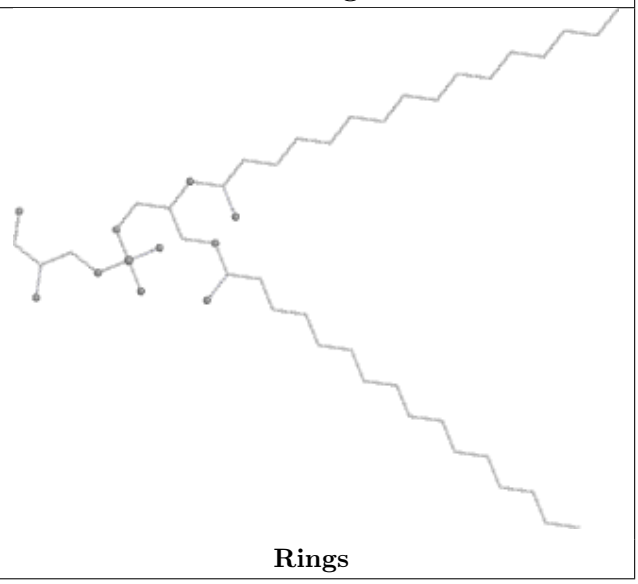


Bond angles

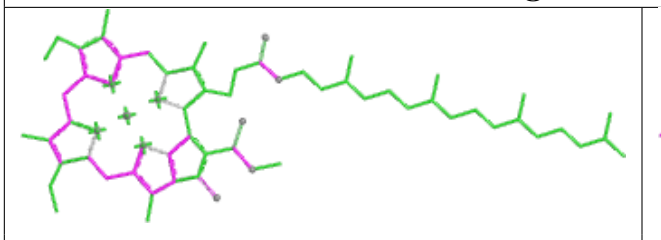


Torsions

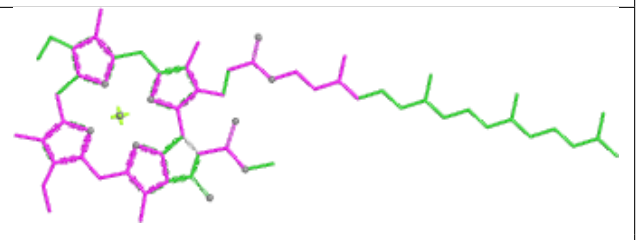


Rings

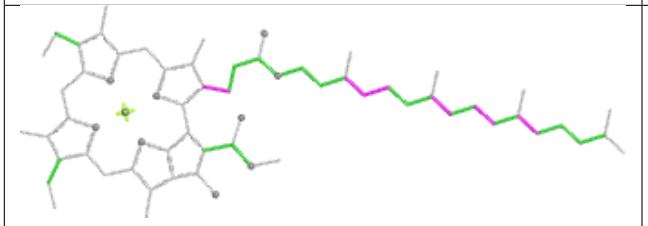
Ligand CLA D 404



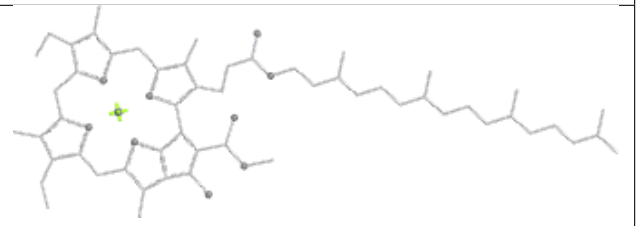
Bond lengths



Bond angles



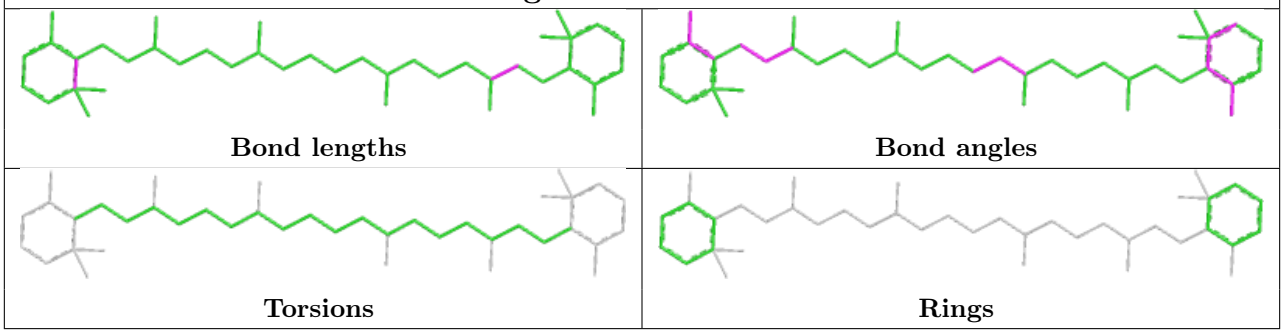
Torsions



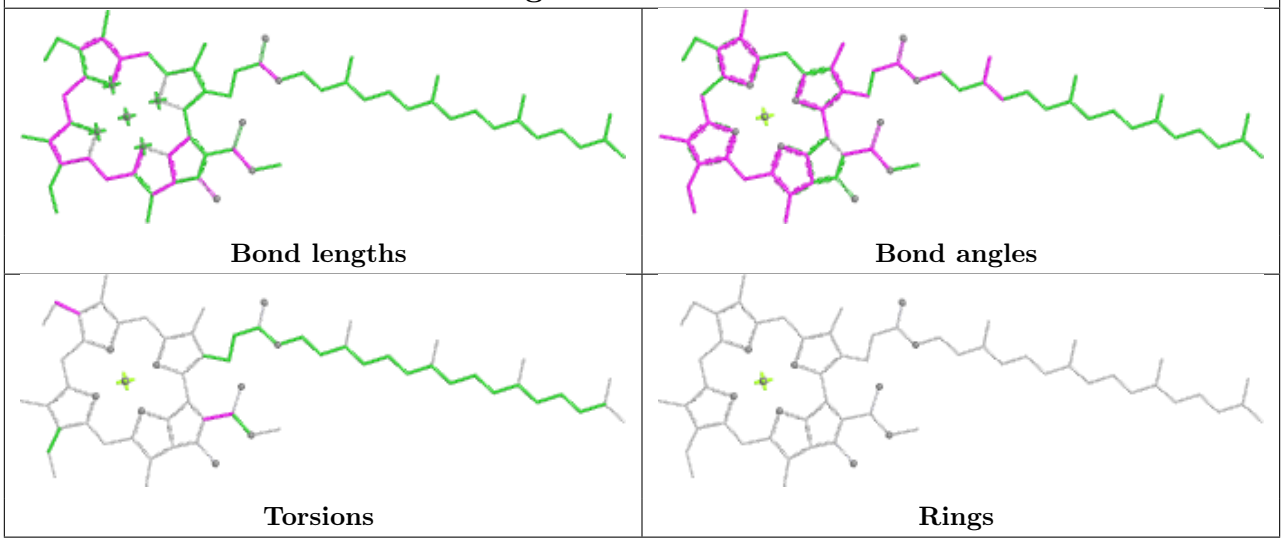
Rings

Ligand PL9 a 414 (B)

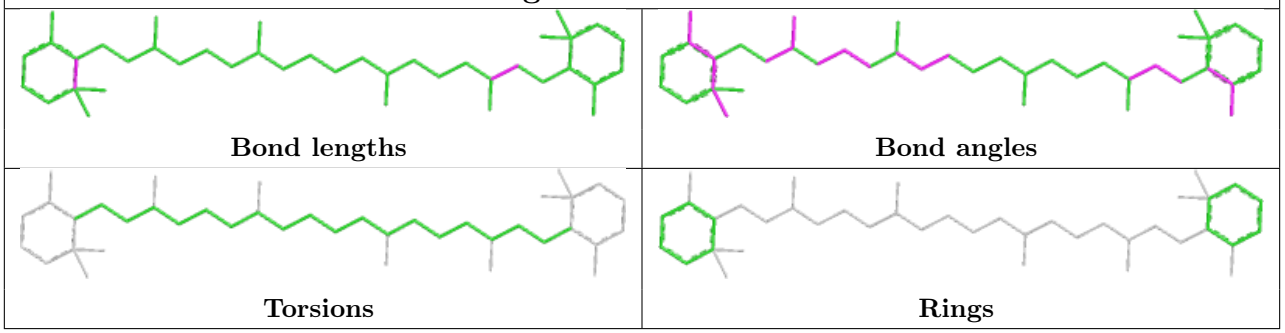
Ligand BCR B 617



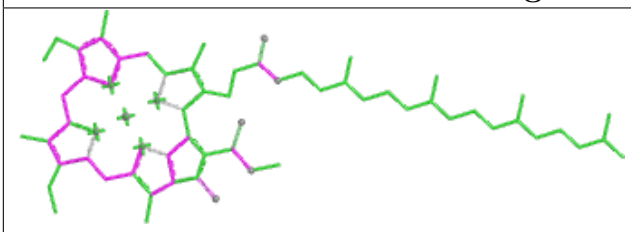
Ligand CLA B 607



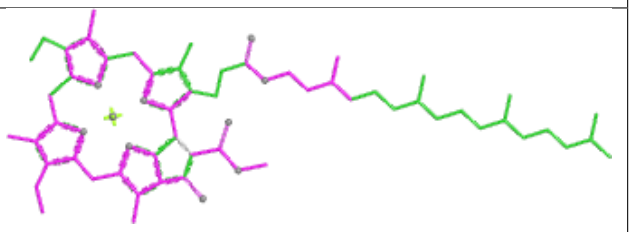
Ligand BCR A 408



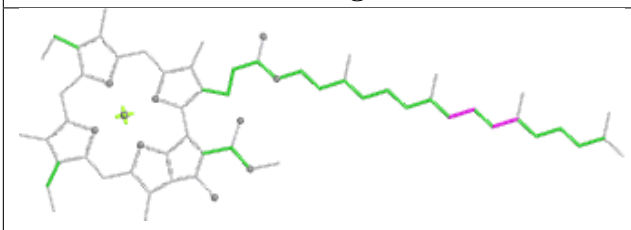
Ligand CLA B 611



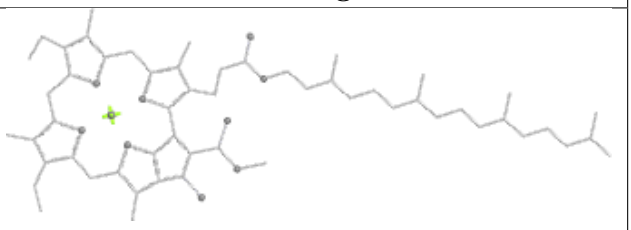
Bond lengths



Bond angles

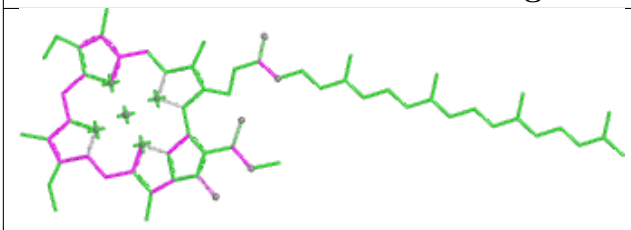


Torsions



Rings

Ligand CLA B 613



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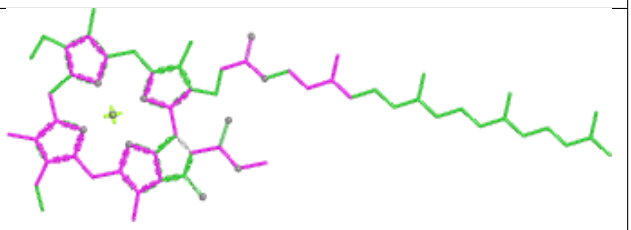
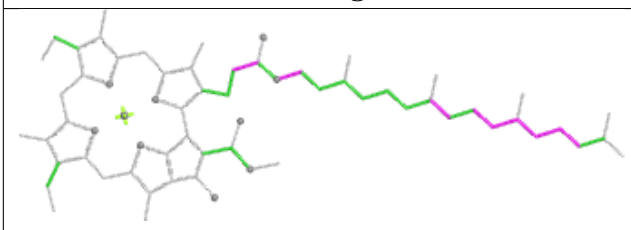
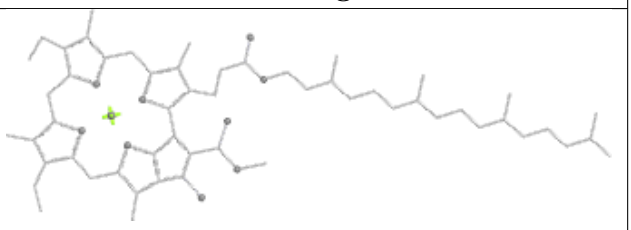


Bond angles

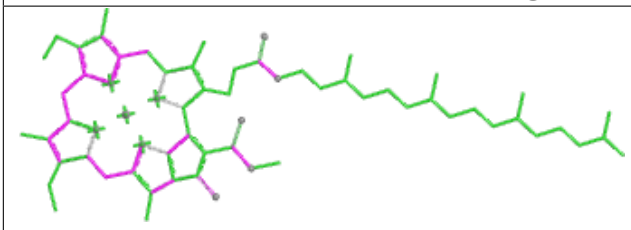


Torsions

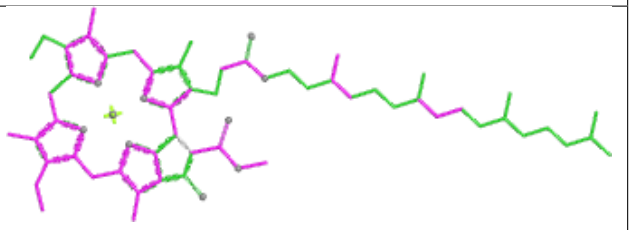


Rings

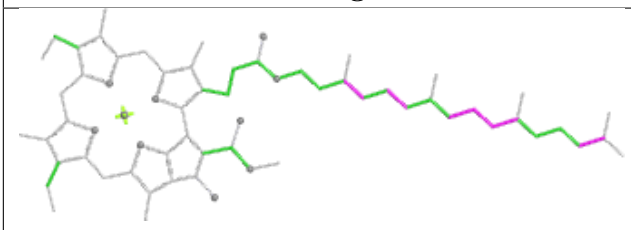
Ligand CLA B 615



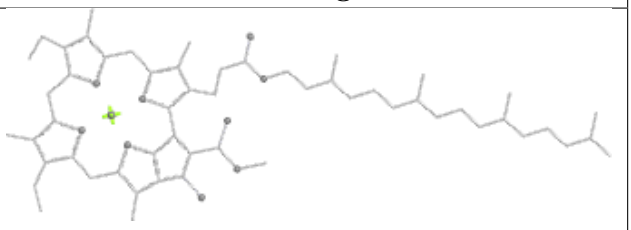
Bond lengths



Bond angles

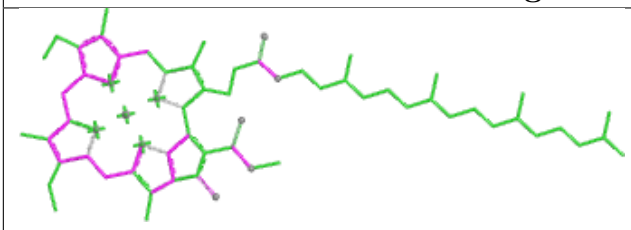


Torsions

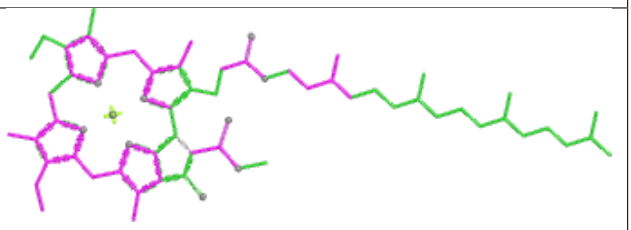


Rings

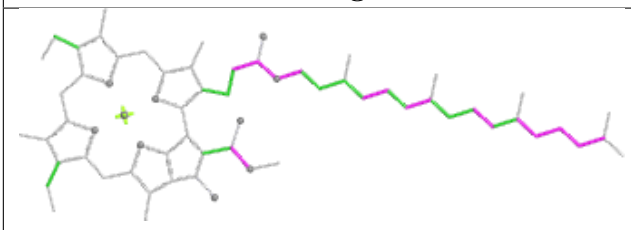
Ligand CLA C 514



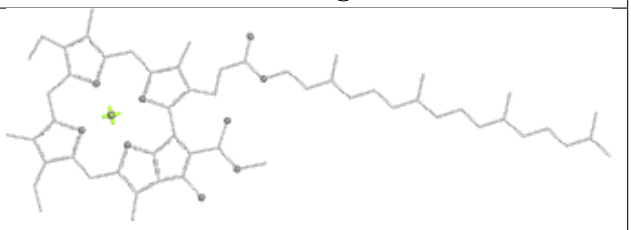
Bond lengths



Bond angles

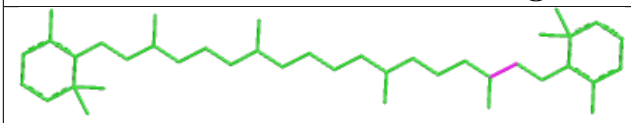


Torsions

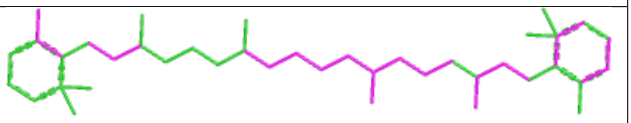


Rings

Ligand BCR c 517

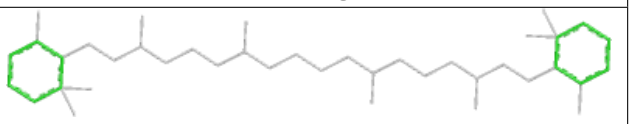


Bond lengths



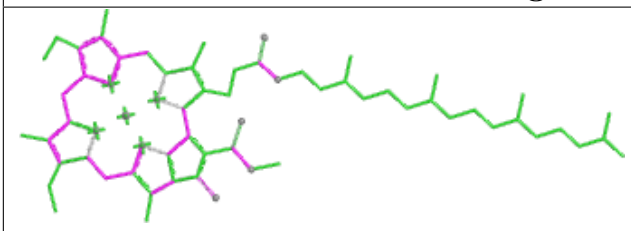
Bond angles

Torsions

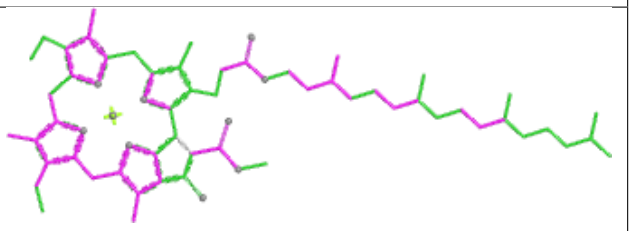


Rings

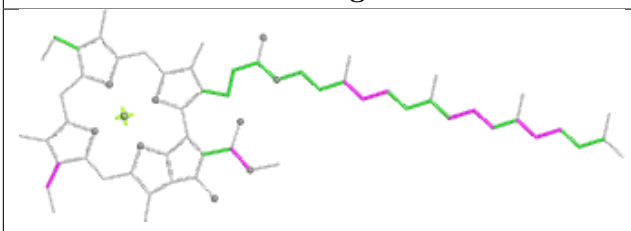
Ligand CLA b 604



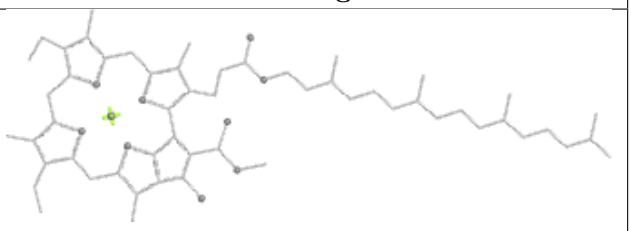
Bond lengths



Bond angles

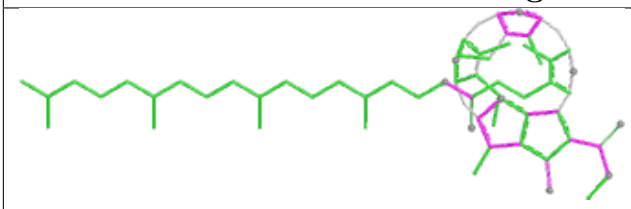


Torsions

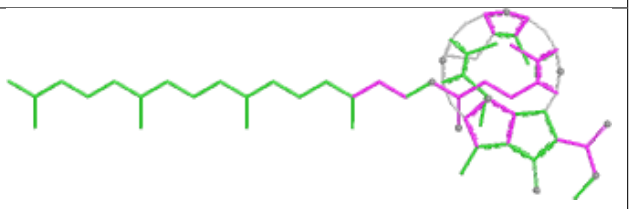


Rings

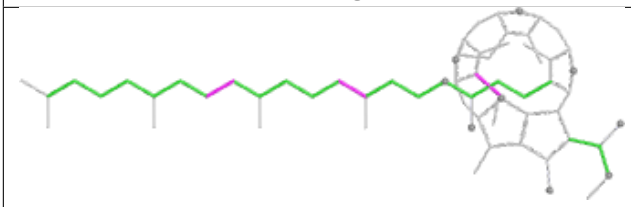
Ligand PHO a 406



Bond lengths



Bond angles



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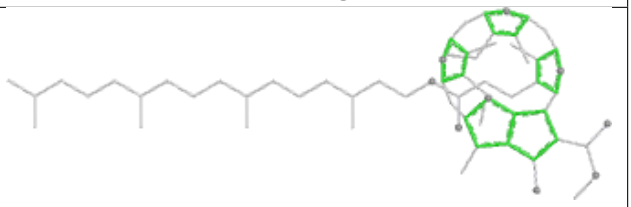
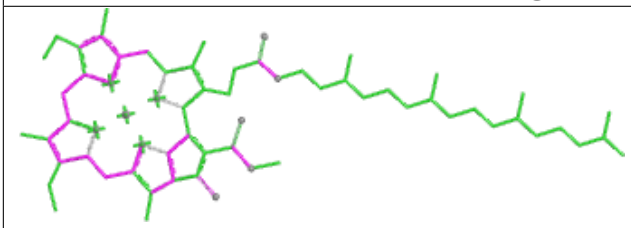
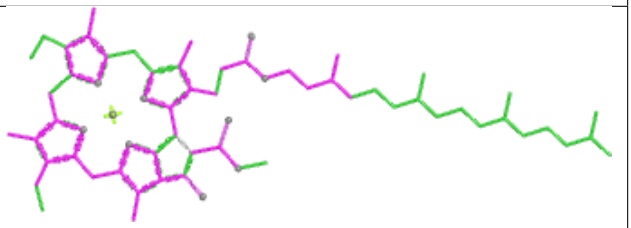


Rings

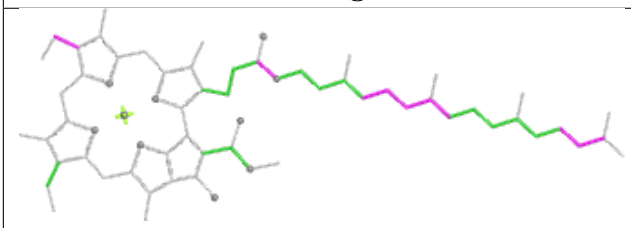
Ligand CLA a 407



Bond lengths



Bond angles



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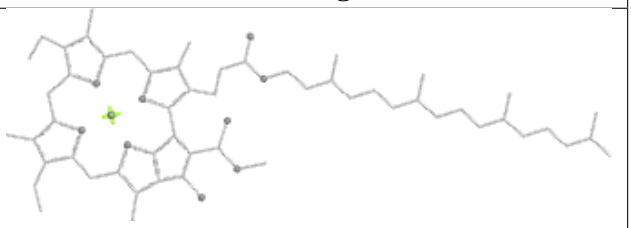
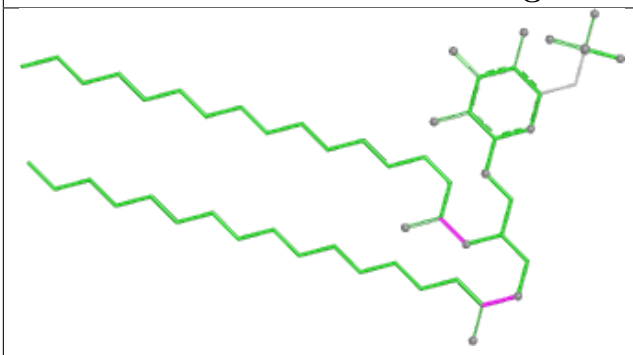
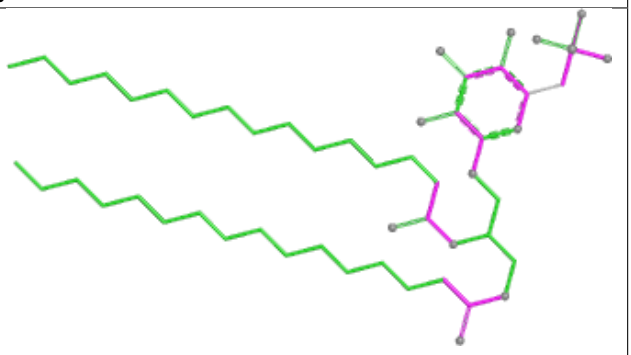


Rings

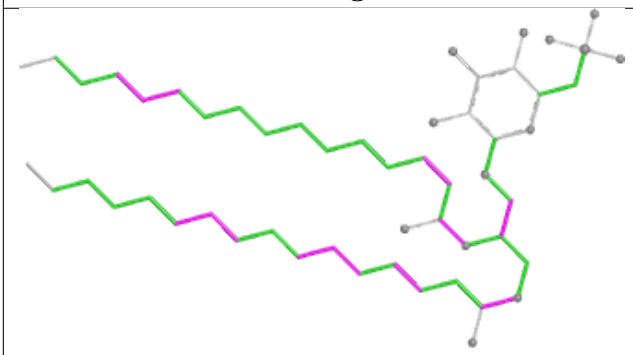
Ligand SQD A 411



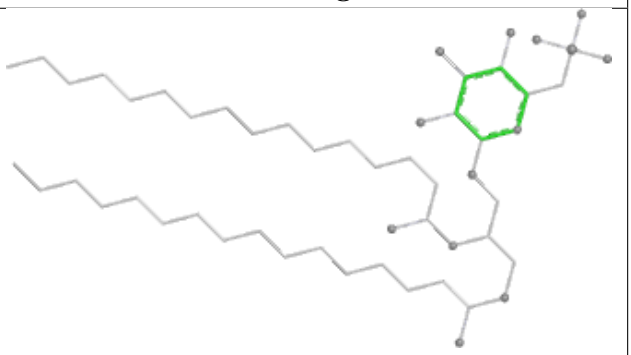
Bond lengths



Bond angles



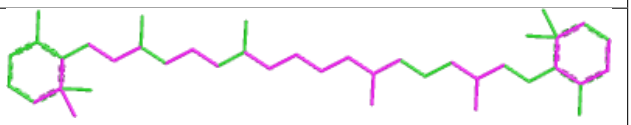
Torsions



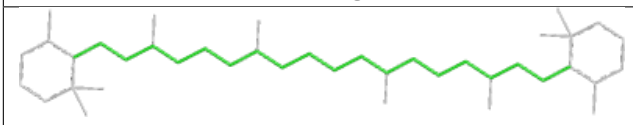
Rings

Ligand BCR B 618

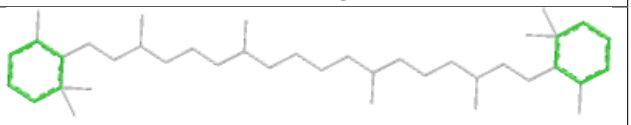
Bond lengths



Bond angles

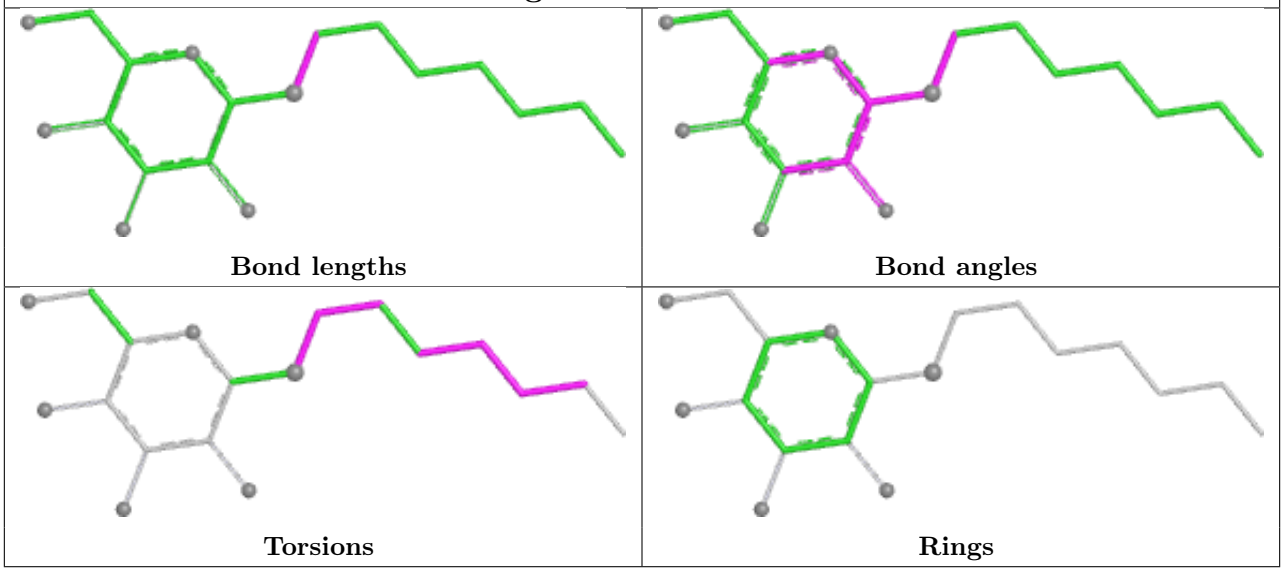


Torsions

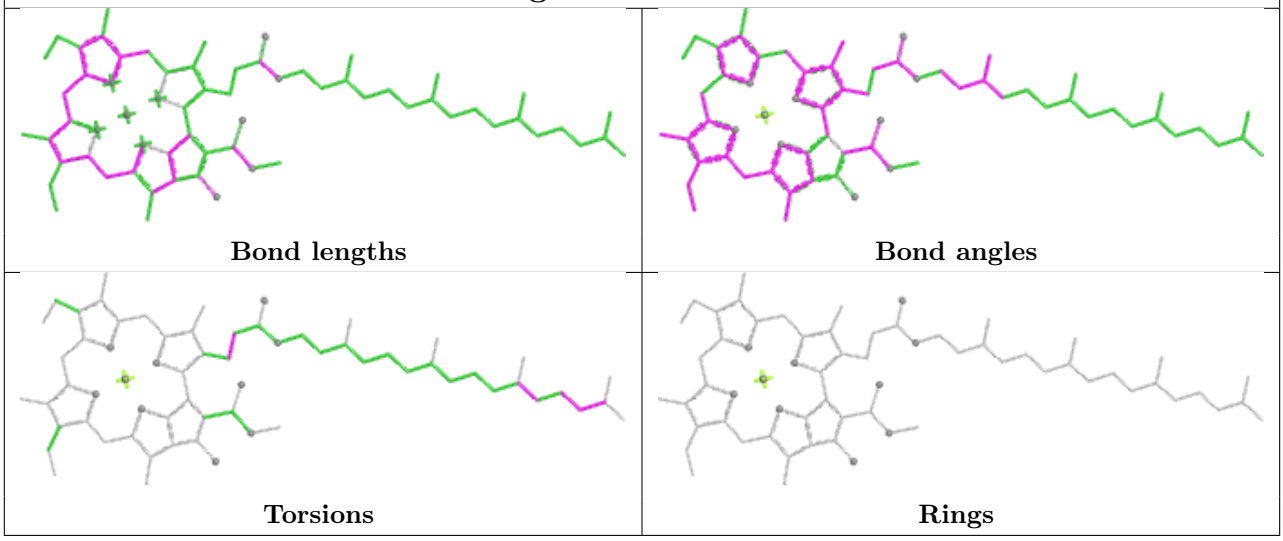


Rings

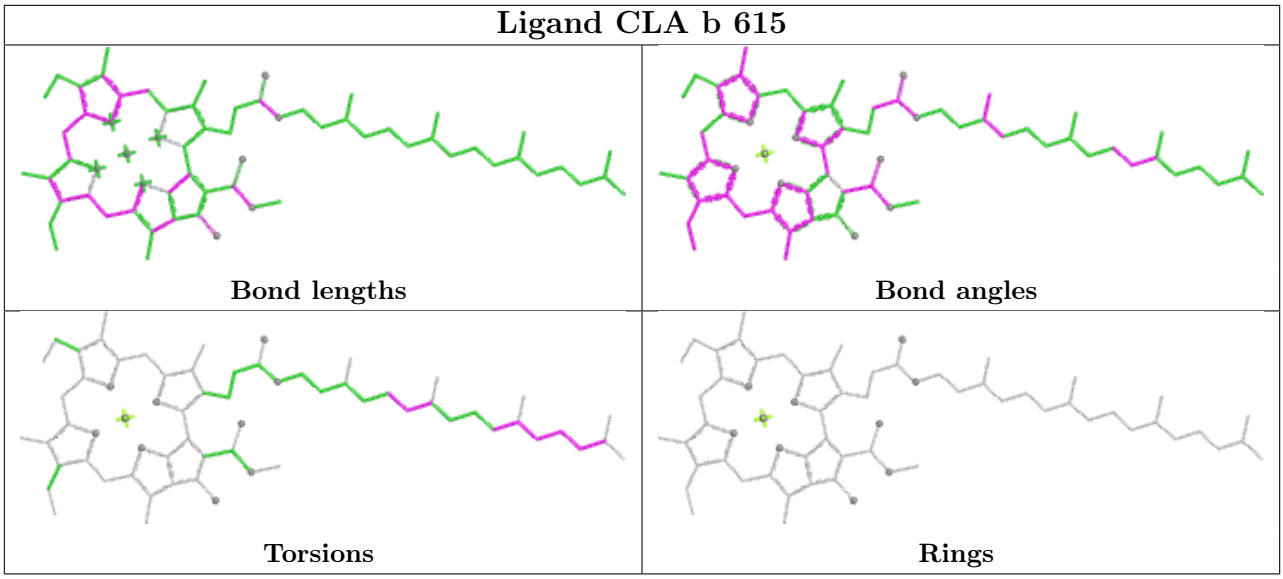
Ligand HTG b 621



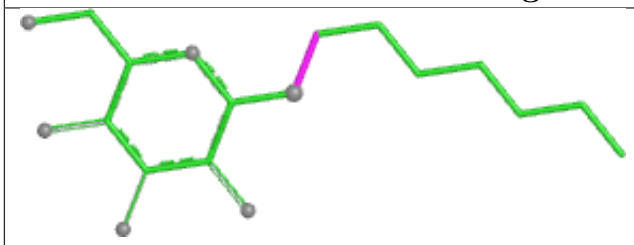
Ligand CLA a 403



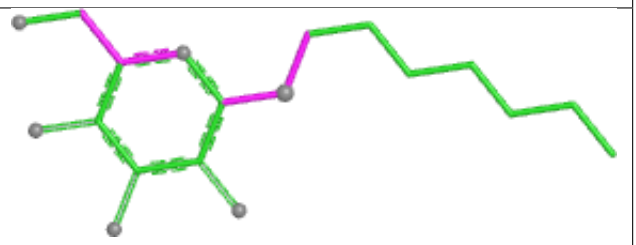
Ligand CLA b 615



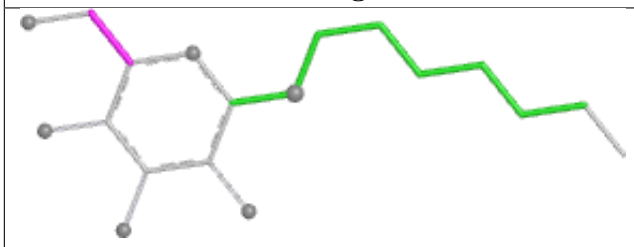
Ligand HTG C 523



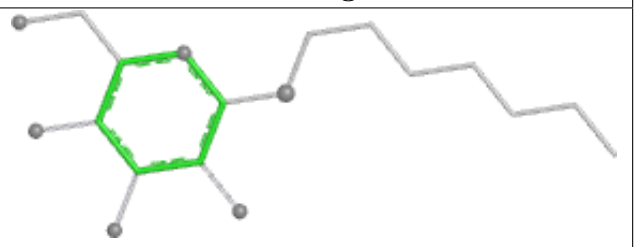
Bond lengths



Bond angles

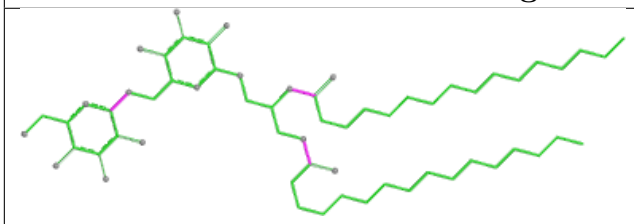


Torsions

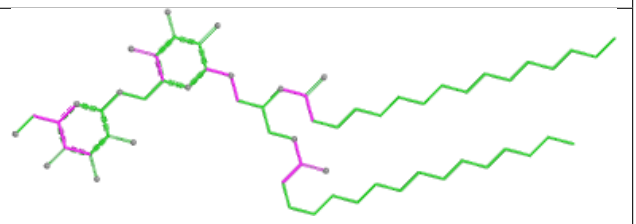


Rings

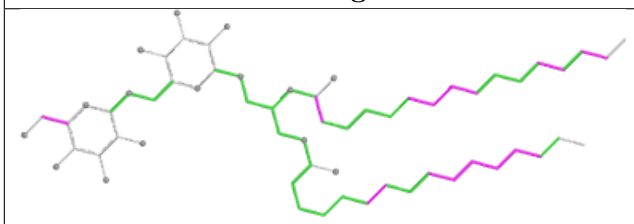
Ligand DGD H 102



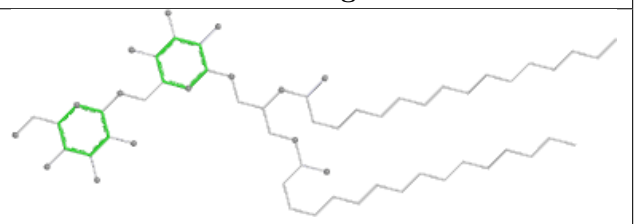
Bond lengths



Bond angles

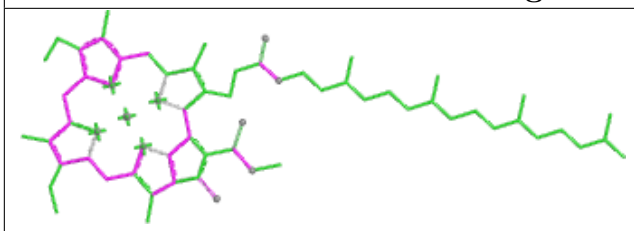


Torsions

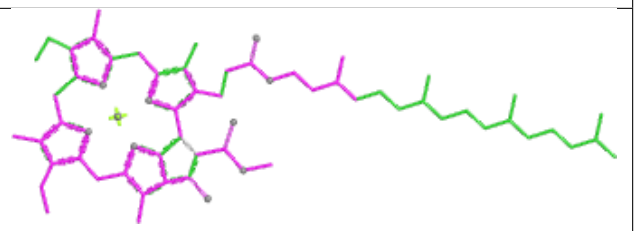


Rings

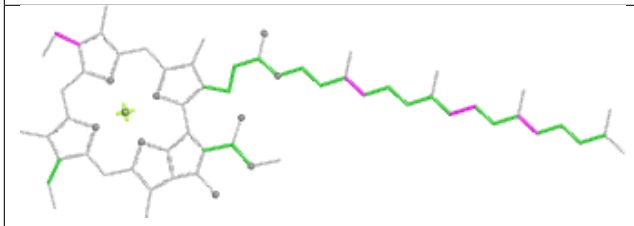
Ligand CLA C 506



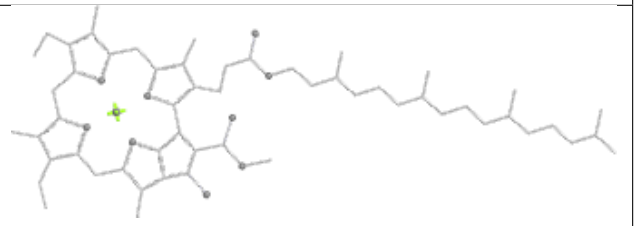
Bond lengths



Bond angles

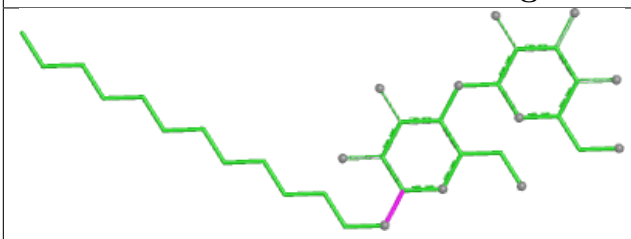


Torsions

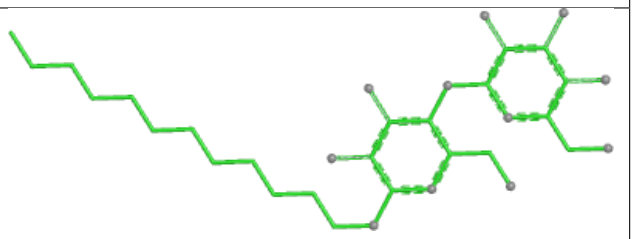


Rings

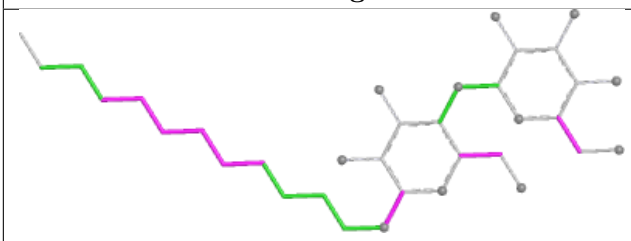
Ligand LMT D 402



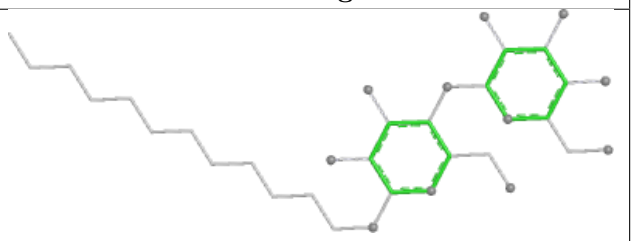
Bond lengths



Bond angles

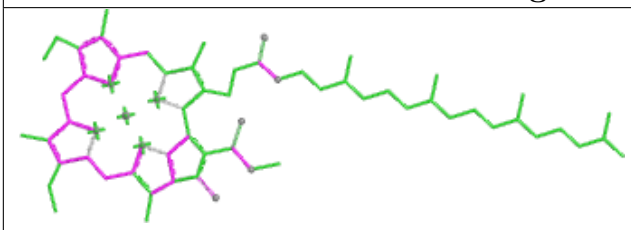


Torsions



Rings

Ligand CLA c 503



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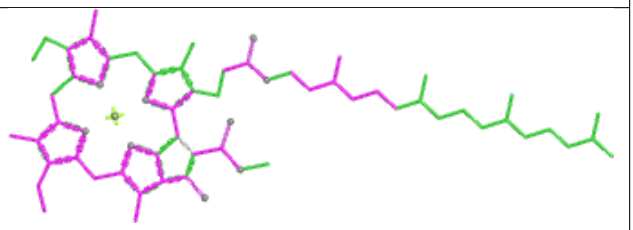
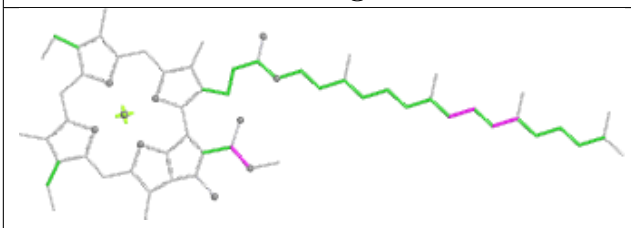


Bond angles



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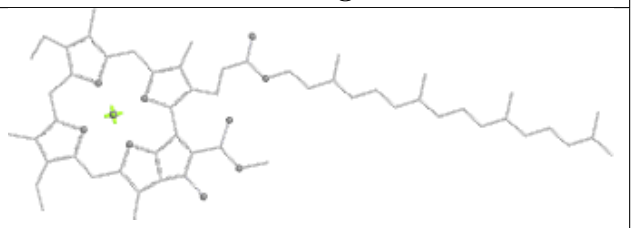
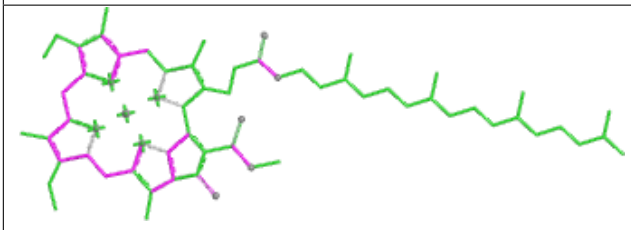
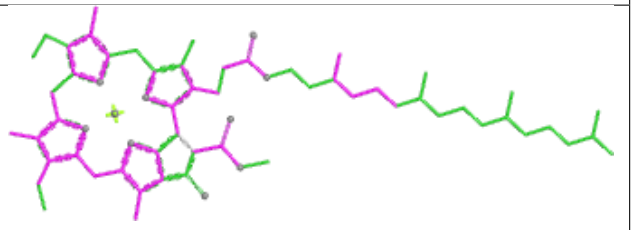


Rings

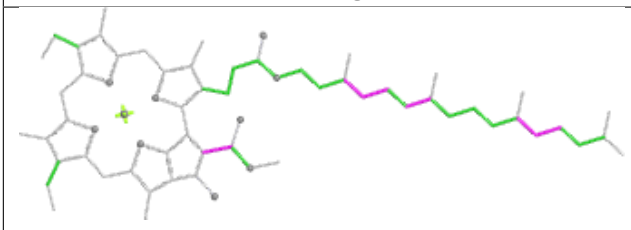
Ligand CLA B 605



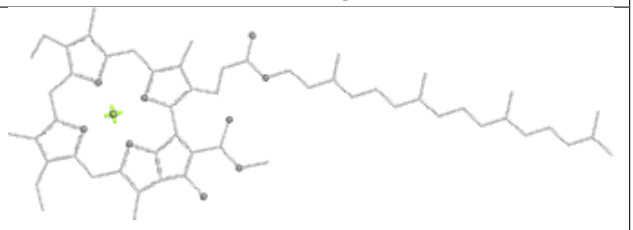
Bond lengths



Bond angles

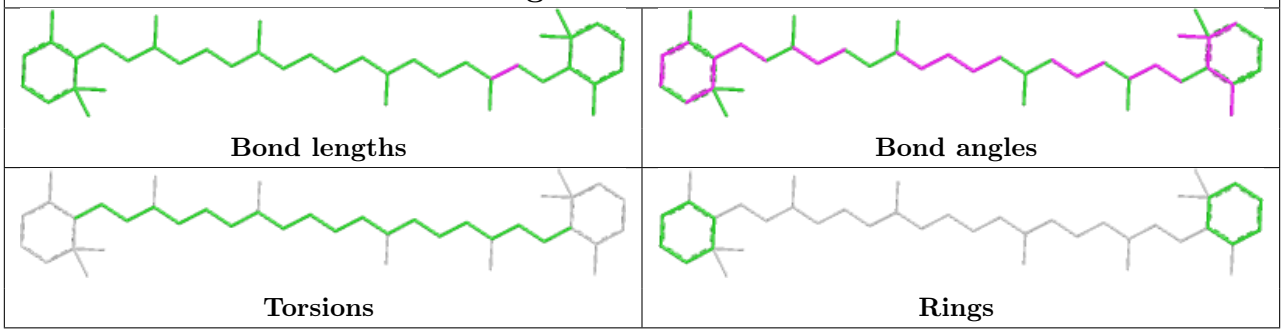


Torsions

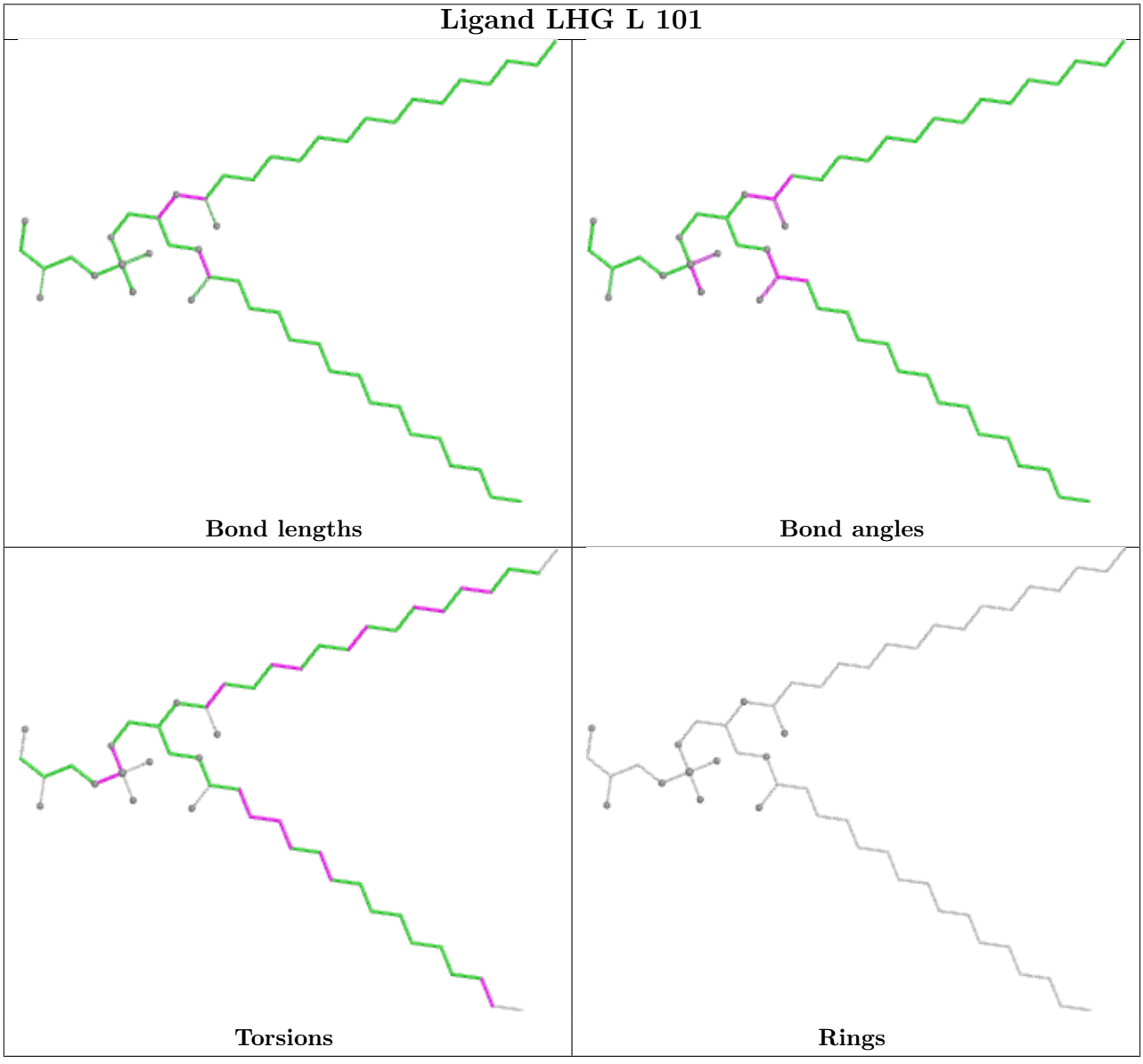


Rings

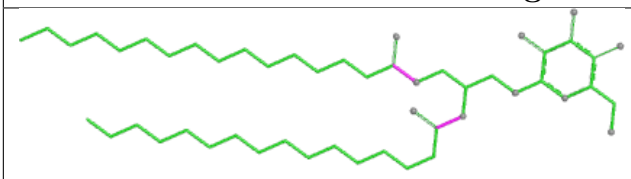
Ligand BCR b 618



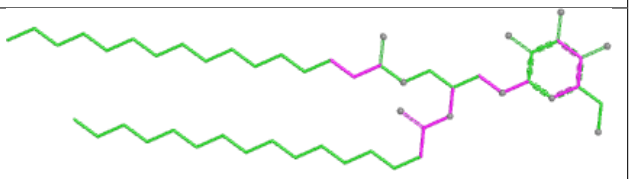
Ligand LHG L 101



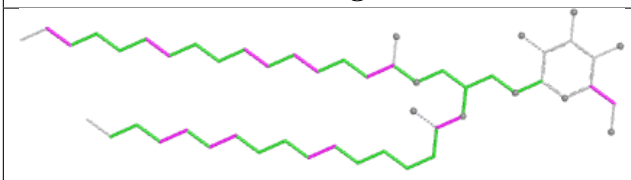
Ligand LMG a 417



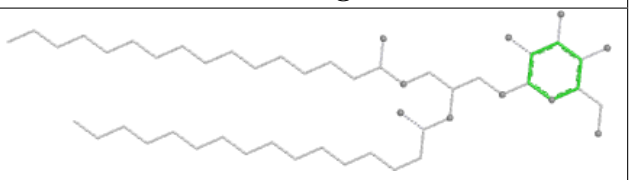
Bond lengths



Bond angles

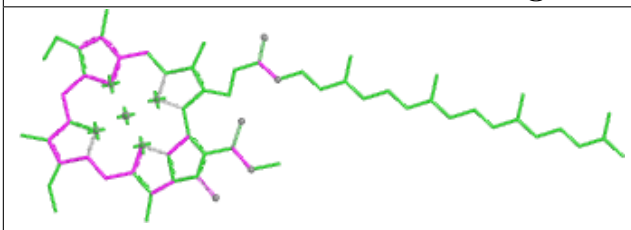


Torsions

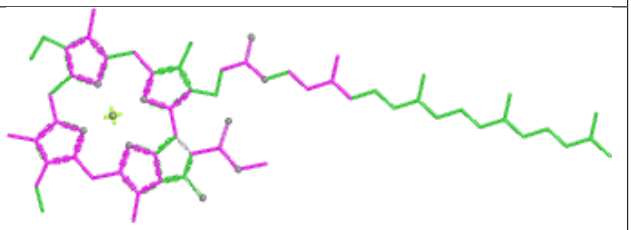


Rings

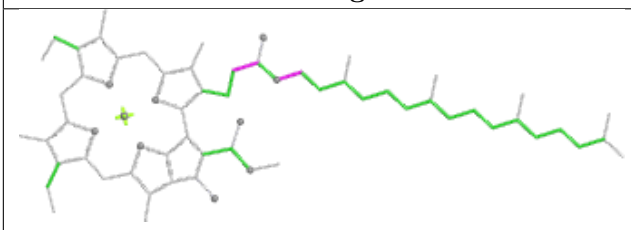
Ligand CLA b 613



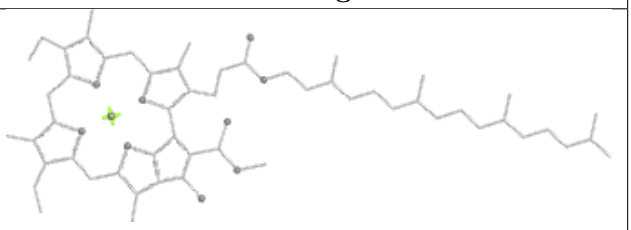
Bond lengths



Bond angles



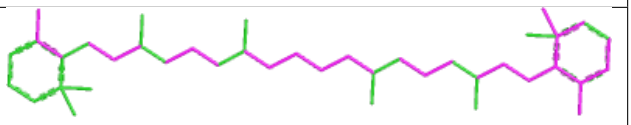
Torsions



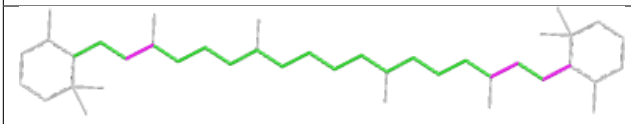
Rings

Ligand BCR d 404

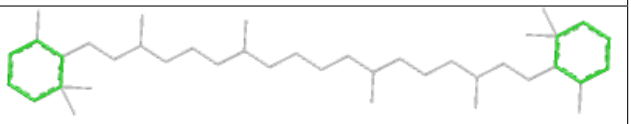
Bond lengths



Bond angles

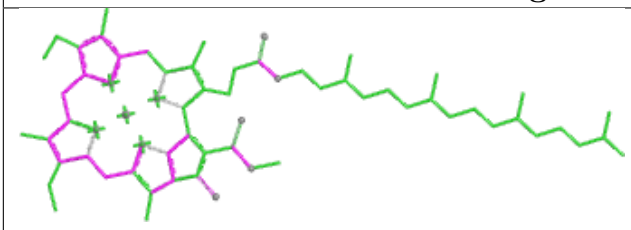


Torsions

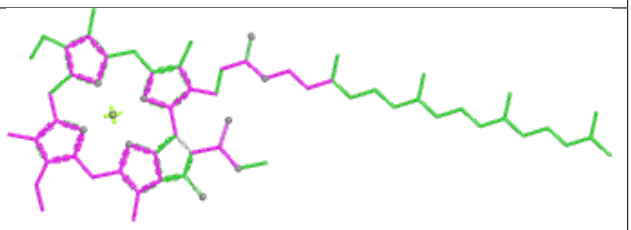


Rings

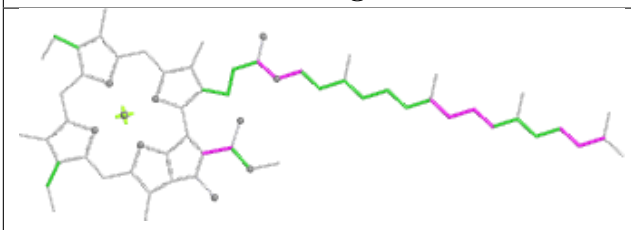
Ligand CLA c 511



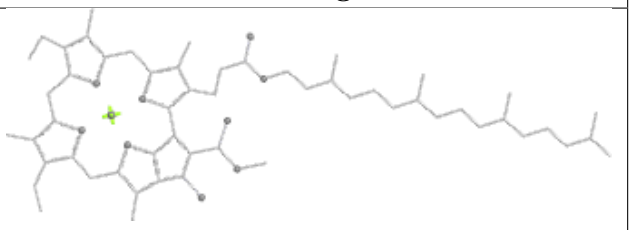
Bond lengths



Bond angles

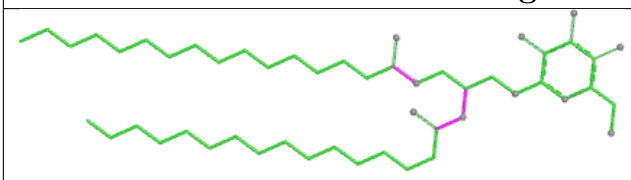


Torsions

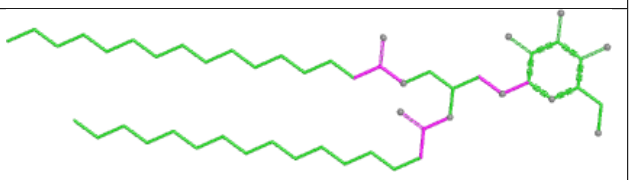


Rings

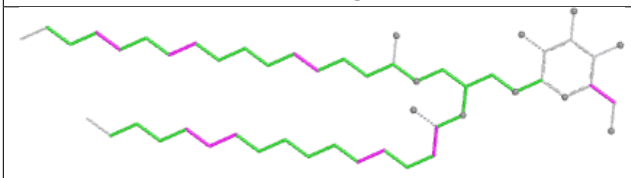
Ligand LMG D 412



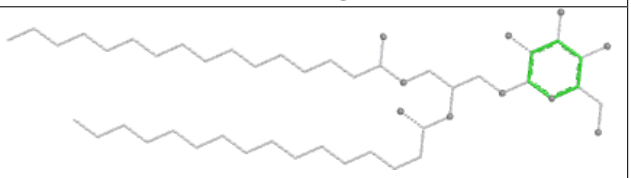
Bond lengths



Bond angles

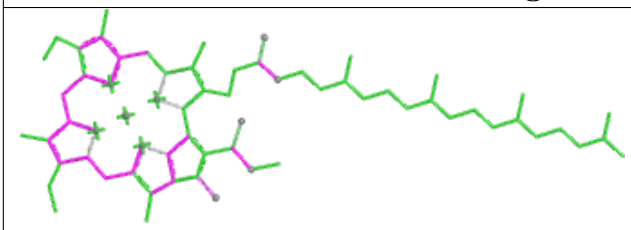


Torsions

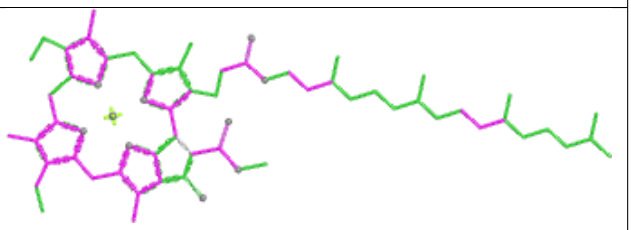


Rings

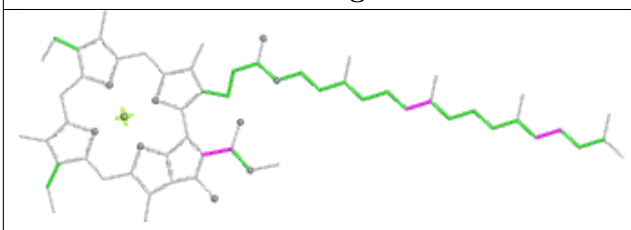
Ligand CLA C 511



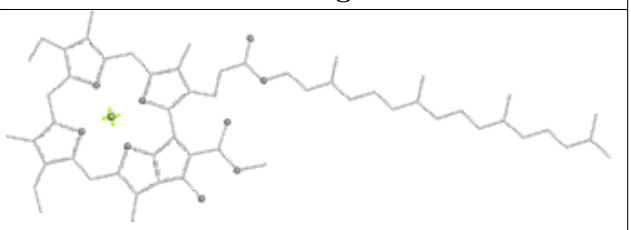
Bond lengths



Bond angles

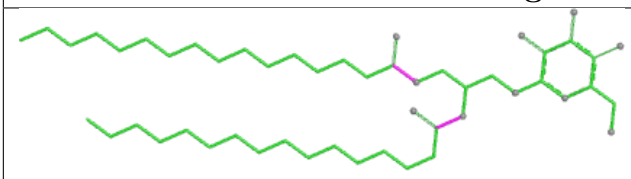


Torsions

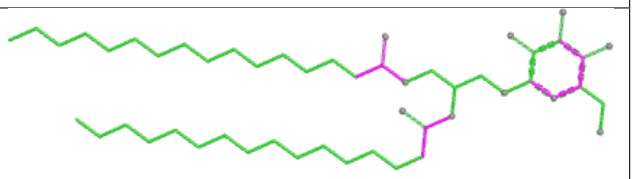


Rings

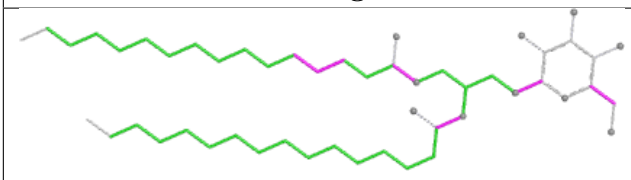
Ligand LMG c 522



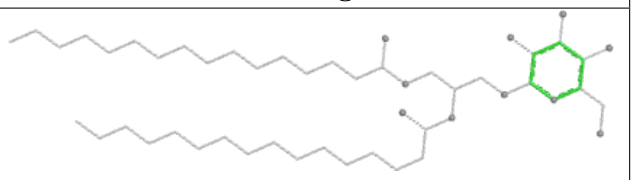
Bond lengths



Bond angles

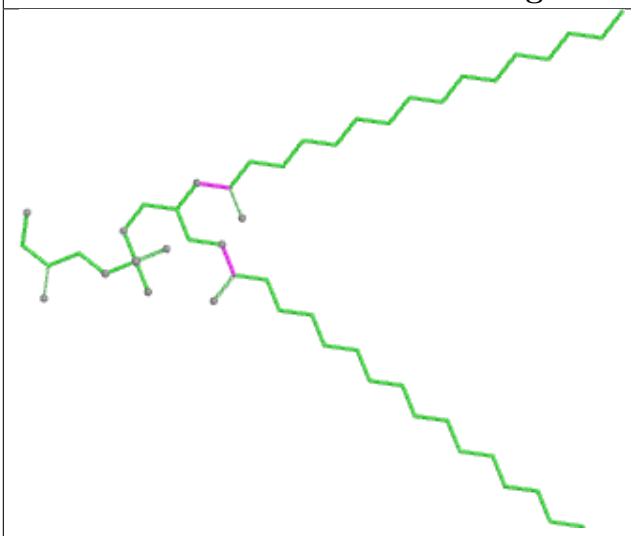


Torsions

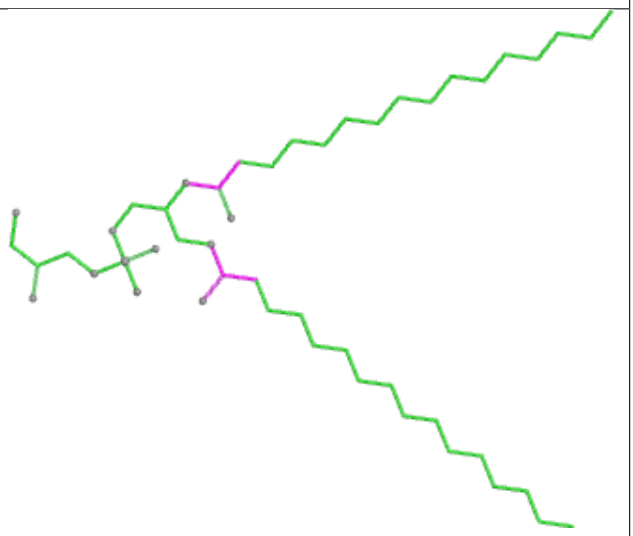


Rings

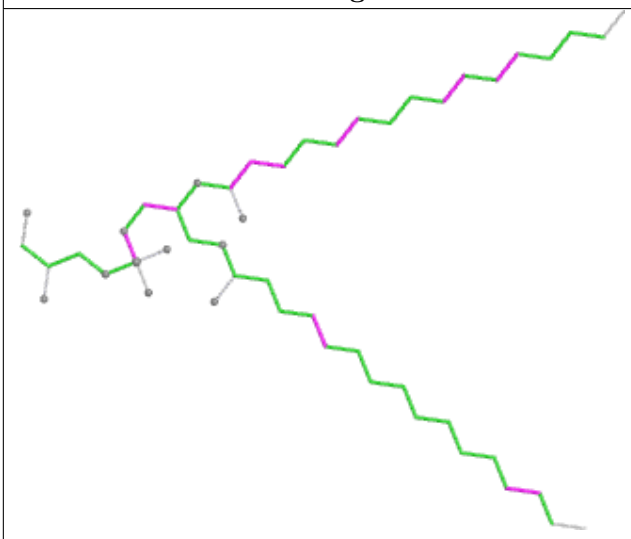
Ligand LHG b 628



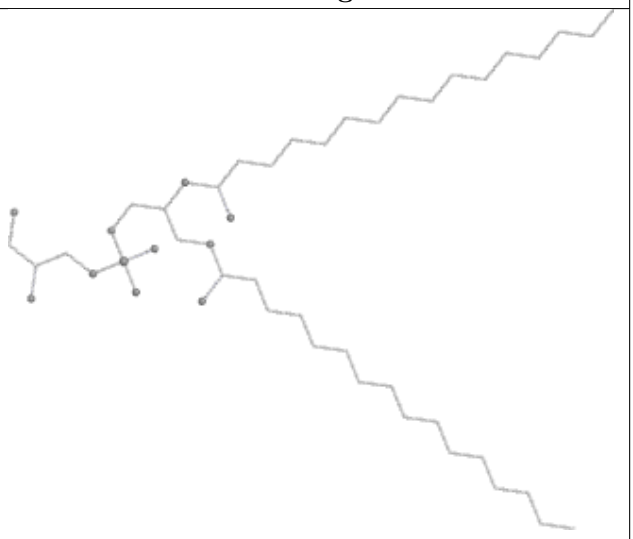
Bond lengths



Bond angles

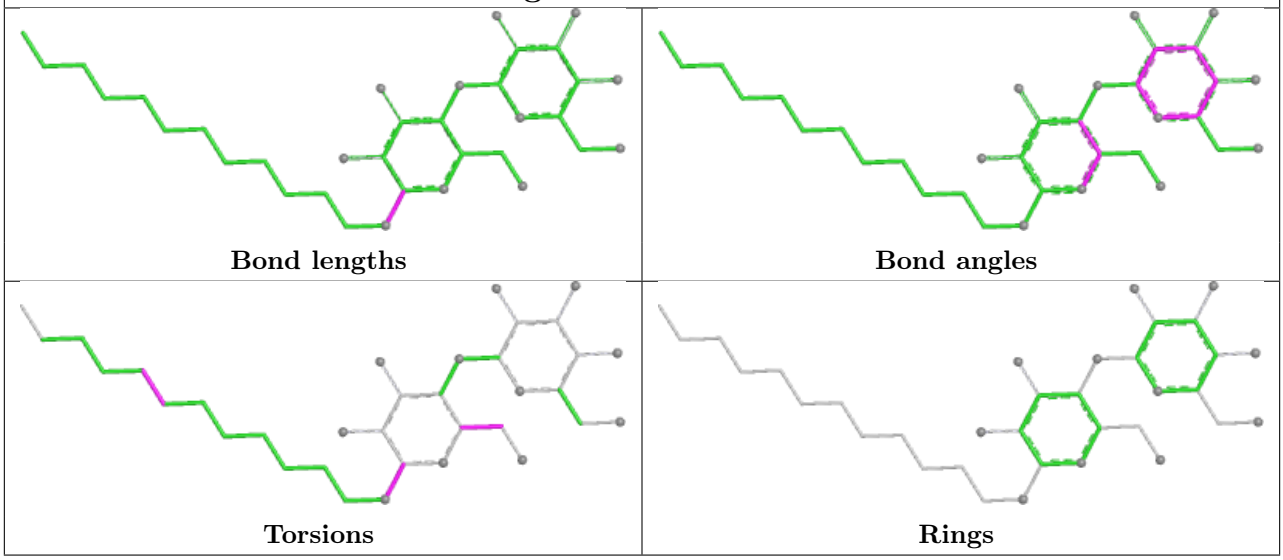


Torsions

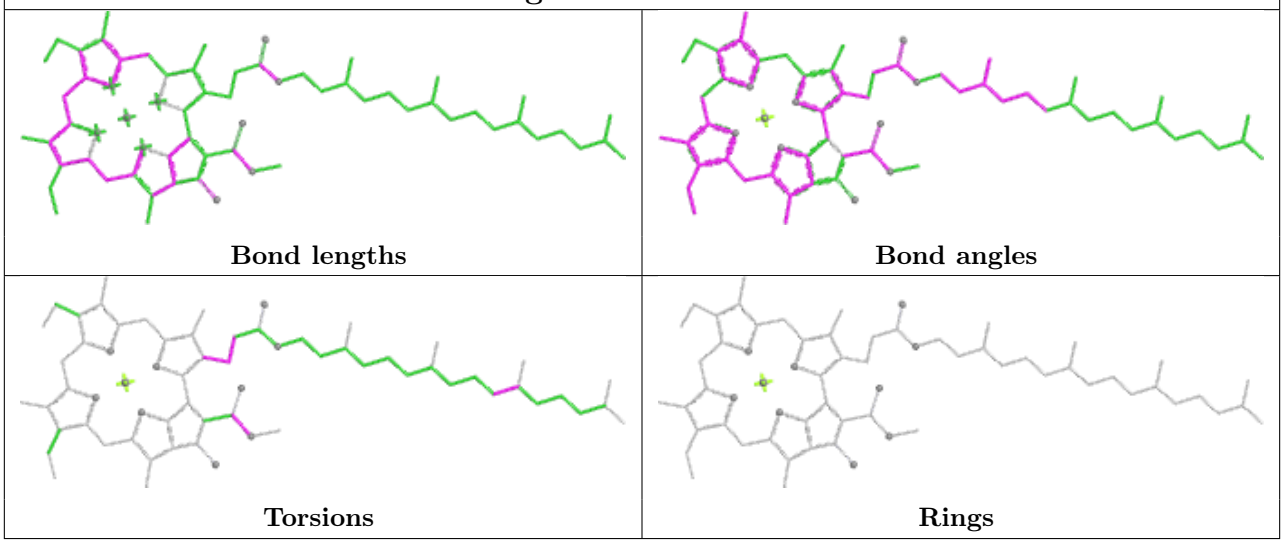


Rings

Ligand LMT F 101



Ligand CLA C 503



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.60	0 100 100	20, 43, 67, 128	18 (5%)
1	a	334/344 (97%)	-0.57	3 (0%) 81 78	21, 47, 75, 110	19 (5%)
2	B	504/505 (99%)	-0.52	0 100 100	21, 49, 81, 127	10 (1%)
2	b	504/505 (99%)	-0.39	4 (0%) 82 80	23, 52, 92, 158	4 (0%)
3	C	451/455 (99%)	-0.38	2 (0%) 88 86	21, 56, 81, 156	5 (1%)
3	c	455/455 (100%)	-0.38	1 (0%) 91 89	24, 64, 86, 133	3 (0%)
4	D	342/342 (100%)	-0.57	0 100 100	22, 45, 68, 139	4 (1%)
4	d	341/342 (99%)	-0.63	0 100 100	23, 50, 73, 129	4 (1%)
5	E	81/84 (96%)	-0.15	1 (1%) 76 73	34, 70, 96, 139	1 (1%)
5	e	79/84 (94%)	-0.10	1 (1%) 75 71	59, 74, 116, 157	0
6	F	34/44 (77%)	-0.09	1 (2%) 53 50	50, 62, 85, 108	0
6	f	31/44 (70%)	-0.12	1 (3%) 50 46	58, 67, 92, 144	0
7	H	64/65 (98%)	-0.06	2 (3%) 51 47	29, 59, 81, 133	1 (1%)
7	h	64/65 (98%)	-0.07	1 (1%) 70 66	52, 65, 91, 105	0
8	I	37/38 (97%)	-0.13	0 100 100	49, 60, 124, 148	0
8	i	37/38 (97%)	-0.21	0 100 100	52, 60, 114, 145	0
9	J	38/39 (97%)	-0.16	1 (2%) 57 53	50, 70, 131, 177	0
9	j	39/39 (100%)	0.05	1 (2%) 57 53	58, 73, 125, 165	0
10	K	37/37 (100%)	-0.33	0 100 100	58, 67, 89, 113	0
10	k	37/37 (100%)	-0.31	0 100 100	66, 73, 95, 113	0
11	L	36/37 (97%)	-0.28	1 (2%) 55 51	20, 41, 93, 140	1 (2%)
11	l	36/37 (97%)	-0.29	0 100 100	20, 42, 105, 134	1 (2%)
12	M	32/36 (88%)	-0.41	0 100 100	21, 44, 73, 146	1 (3%)
12	m	33/36 (91%)	-0.57	0 100 100	38, 44, 82, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.37	0 100 100	25, 60, 113, 178	3 (1%)
13	o	243/244 (99%)	-0.26	0 100 100	26, 61, 119, 171	2 (0%)
14	T	29/32 (90%)	-0.59	1 (3%) 48 44	38, 43, 83, 104	0
14	t	29/32 (90%)	-0.57	1 (3%) 48 44	38, 46, 74, 139	0
15	U	96/104 (92%)	-0.52	0 100 100	44, 56, 88, 92	0
15	u	97/104 (93%)	-0.52	0 100 100	48, 61, 80, 129	0
16	V	137/137 (100%)	-0.55	0 100 100	43, 55, 80, 112	0
16	v	137/137 (100%)	-0.39	0 100 100	50, 69, 103, 131	0
17	X	38/40 (95%)	-0.06	0 100 100	54, 69, 91, 110	0
17	x	38/40 (95%)	-0.03	0 100 100	60, 74, 124, 157	0
18	Y	29/30 (96%)	0.29	2 (6%) 23 19	67, 89, 136, 169	0
18	y	29/30 (96%)	0.14	0 100 100	75, 87, 113, 116	0
19	Z	62/62 (100%)	-0.08	0 100 100	69, 83, 138, 186	0
19	z	62/62 (100%)	0.31	2 (3%) 50 46	76, 95, 137, 185	0
20	R	34/34 (100%)	0.94	1 (2%) 53 50	91, 106, 138, 142	0
All	All	5283/5384 (98%)	-0.40	27 (0%) 87 85	20, 55, 99, 186	77 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.7
14	t	30	THR	3.7
7	h	65	LEU	3.2
1	a	264[A]	SER	3.2
3	C	23	ALA	3.1
1	a	263	ALA	2.8
14	T	30	THR	2.8
6	f	15	ILE	2.7
9	J	2	SER	2.6
7	H	64	ALA	2.6
19	z	30	PRO	2.5
2	b	495	PHE	2.4
2	b	491	VAL	2.4
5	e	6	GLY	2.2
1	a	11	ALA	2.2
3	C	155	ASN	2.2
9	j	5	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
18	Y	18	VAL	2.1
5	E	4	THR	2.1
2	b	505	ARG	2.1
19	z	5	PHE	2.1
2	b	488	PRO	2.1
20	R	3	TRP	2.1
6	F	28	VAL	2.0
3	c	143	TYR	2.0
11	L	10	VAL	2.0
18	Y	20	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.95	0.08	46,67,72,75	0
12	FME	M	1	10/11	0.96	0.10	31,59,83,93	0
14	FME	T	1	10/11	0.97	0.07	39,48,63,64	0
8	FME	i	1	10/11	0.97	0.05	52,62,75,81	0
12	FME	m	1	10/11	0.97	0.06	38,52,79,90	0
14	FME	t	1	10/11	0.97	0.07	35,44,61,70	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
33	LMT	F	101	35/35	0.65	0.20	105,152,164,167	0
33	LMT	C	526	35/35	0.66	0.17	93,147,159,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMT	e	101	35/35	0.67	0.18	121,173,177,179	0
30	UNL	A	414	28/-	0.73	0.19	88,103,120,121	0
30	UNL	j	101	10/-	0.73	0.27	81,90,102,103	0
32	HTG	D	411	16/19	0.73	0.14	82,116,129,129	0
32	HTG	b	622	19/19	0.74	0.15	86,138,148,150	0
33	LMT	a	418	35/35	0.75	0.16	113,144,152,153	0
33	LMT	a	412	35/35	0.75	0.19	63,131,144,146	0
30	UNL	J	101	10/-	0.78	0.27	69,84,88,90	0
33	LMT	D	402	35/35	0.78	0.20	75,130,140,142	0
32	HTG	c	523	19/19	0.78	0.14	119,131,139,141	0
30	UNL	m	102	10/-	0.79	0.20	59,67,88,90	0
30	UNL	C	527	34/-	0.79	0.18	83,110,123,129	0
26	SQD	f	101	43/54	0.80	0.16	111,129,159,160	0
30	UNL	i	101	40/-	0.81	0.19	72,97,151,154	0
30	UNL	a	415	30/-	0.81	0.15	100,110,133,140	0
34	LMG	C	522	51/55	0.81	0.18	76,125,159,161	0
30	UNL	I	101	40/-	0.82	0.20	74,108,148,149	0
30	UNL	c	526	32/-	0.83	0.18	91,111,125,129	0
32	HTG	B	622	19/19	0.83	0.17	79,89,99,100	0
32	HTG	C	523	19/19	0.83	0.15	108,122,132,133	0
33	LMT	m	103	35/35	0.83	0.14	59,97,109,113	0
33	LMT	M	103	35/35	0.83	0.15	75,140,160,163	0
34	LMG	c	522	51/55	0.83	0.17	80,125,151,152	0
30	UNL	b	625	33/-	0.84	0.17	65,94,146,147	0
33	LMT	B	627	35/35	0.84	0.14	68,112,127,131	0
34	LMG	Z	101	37/55	0.84	0.15	73,129,162,169	0
31	LHG	a	419	42/49	0.84	0.14	86,136,170,174	0
33	LMT	b	626	25/35	0.85	0.14	46,70,129,135	0
31	LHG	E	101	42/49	0.85	0.16	74,114,131,133	0
36	CA	F	102	1/1	0.85	0.10	103,103,103,103	0
32	HTG	h	101	16/19	0.86	0.12	99,134,140,142	0
30	UNL	B	625	33/-	0.87	0.15	56,105,148,152	0
30	UNL	d	410	36/-	0.87	0.16	72,92,117,120	0
32	HTG	b	621	19/19	0.87	0.15	61,78,111,112	0
33	LMT	b	620	25/35	0.87	0.16	90,129,147,148	0
27	GOL	B	626	6/6	0.87	0.20	82,99,100,103	0
30	UNL	D	410	40/-	0.87	0.17	52,87,126,132	0
30	UNL	l	101	10/-	0.87	0.17	63,74,83,85	0
27	GOL	B	628	6/6	0.87	0.16	90,102,105,109	0
27	GOL	O	302	6/6	0.87	0.10	78,84,85,85	0
27	GOL	c	527	6/6	0.87	0.19	105,109,114,116	0
26	SQD	a	411	54/54	0.87	0.12	63,89,126,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMT	B	630	26/35	0.88	0.15	78,117,140,143	0
32	HTG	V	202	11/19	0.88	0.12	109,114,122,124	0
26	SQD	D	413	43/54	0.88	0.14	70,105,125,136	0
23	CLA	b	601	65/65	0.88	0.12	58,80,119,128	0
33	LMT	B	629	25/35	0.88	0.14	56,79,132,133	0
26	SQD	B	620	54/54	0.89	0.13	60,89,121,127	0
23	CLA	B	601	65/65	0.89	0.12	54,73,118,127	0
33	LMT	M	102	35/35	0.89	0.11	54,105,130,138	0
29	PL9	A	413[A]	55/55	0.89	0.22	89,97,103,104	55
29	PL9	A	413[B]	55/55	0.89	0.22	88,97,104,104	55
26	SQD	A	411	54/54	0.89	0.13	60,84,125,128	0
34	LMG	z	101	39/55	0.89	0.16	81,136,147,148	0
32	HTG	B	621	19/19	0.89	0.15	72,87,118,120	0
36	CA	O	301	1/1	0.89	0.10	118,118,118,118	0
26	SQD	L	102	54/54	0.90	0.13	55,91,118,119	0
34	LMG	C	521	51/55	0.90	0.14	59,84,115,118	0
27	GOL	b	623	6/6	0.91	0.16	87,92,94,102	0
29	PL9	a	414[A]	55/55	0.91	0.24	93,104,111,112	55
29	PL9	a	414[B]	55/55	0.91	0.24	92,104,111,112	55
27	GOL	c	502	6/6	0.91	0.15	67,70,80,85	0
27	GOL	A	410	6/6	0.91	0.12	65,67,74,83	0
27	GOL	v	201	6/6	0.91	0.17	59,82,83,86	0
23	CLA	C	515	65/65	0.91	0.12	59,76,108,109	0
34	LMG	a	417	51/55	0.92	0.13	59,90,115,128	0
32	HTG	b	624	19/19	0.92	0.11	64,77,95,104	0
30	UNL	d	409	17/-	0.92	0.15	68,84,106,108	0
23	CLA	c	515	65/65	0.92	0.11	68,85,111,112	0
30	UNL	D	409	17/-	0.92	0.16	60,78,113,114	0
36	CA	o	301	1/1	0.92	0.07	104,104,104,104	0
25	BCR	D	405	40/40	0.93	0.11	48,57,94,99	0
34	LMG	C	502	51/55	0.93	0.12	58,89,113,120	0
25	BCR	d	404	40/40	0.93	0.11	52,64,87,93	0
25	BCR	h	102	40/40	0.93	0.10	50,66,74,75	0
34	LMG	D	412	51/55	0.93	0.12	46,69,108,116	0
31	LHG	A	416	49/49	0.93	0.13	41,61,78,84	0
25	BCR	k	102	40/40	0.93	0.10	58,72,89,92	0
34	LMG	c	521	51/55	0.93	0.13	66,93,123,128	0
23	CLA	C	508	65/65	0.93	0.12	51,69,117,126	0
23	CLA	c	509	65/65	0.93	0.11	55,65,78,87	0
35	DGD	C	519	62/66	0.93	0.11	45,64,116,121	0
30	UNL	d	412	18/-	0.93	0.13	72,81,121,124	0
32	HTG	B	624	19/19	0.93	0.09	63,79,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	506	65/65	0.93	0.11	43,53,92,102	0
25	BCR	c	516	40/40	0.94	0.10	68,85,89,95	0
27	GOL	B	623	6/6	0.94	0.12	79,89,96,98	0
23	CLA	B	616	65/65	0.94	0.11	45,56,134,137	0
23	CLA	c	514	65/65	0.94	0.11	62,80,117,125	0
23	CLA	C	514	65/65	0.94	0.12	55,69,119,122	0
26	SQD	A	409	54/54	0.94	0.11	57,74,105,111	0
34	LMG	M	101	51/55	0.94	0.10	48,69,87,101	0
31	LHG	b	628	49/49	0.94	0.10	42,54,68,80	0
27	GOL	b	627	6/6	0.94	0.16	91,93,95,97	0
25	BCR	B	619	40/40	0.94	0.09	43,55,74,76	0
25	BCR	B	631	40/40	0.94	0.08	36,57,68,70	0
34	LMG	m	101	51/55	0.94	0.11	53,69,98,101	0
25	BCR	C	516	40/40	0.94	0.11	64,80,88,91	0
23	CLA	b	616	65/65	0.94	0.11	41,58,112,116	0
35	DGD	C	520	62/66	0.94	0.10	43,57,92,104	0
26	SQD	a	409	54/54	0.94	0.11	62,81,108,113	0
25	BCR	H	101	40/40	0.94	0.09	47,59,77,80	0
25	BCR	T	101	40/40	0.94	0.07	35,51,63,63	0
23	CLA	c	507	65/65	0.95	0.09	44,57,80,84	0
23	CLA	c	508	65/65	0.95	0.10	56,69,122,127	0
23	CLA	C	510	65/65	0.95	0.10	44,55,118,130	0
23	CLA	c	510	65/65	0.95	0.09	48,59,116,123	0
30	UNL	X	101	18/-	0.95	0.11	57,74,95,98	0
23	CLA	C	512	65/65	0.95	0.08	47,57,77,83	0
23	CLA	C	513	65/65	0.95	0.09	51,65,83,84	0
23	CLA	d	403	65/65	0.95	0.09	49,60,108,119	0
24	PHO	A	415	64/64	0.95	0.07	36,46,53,54	0
25	BCR	B	618	40/40	0.95	0.08	39,53,64,68	0
23	CLA	C	503	65/65	0.95	0.09	47,56,66,81	0
23	CLA	C	505	65/65	0.95	0.08	48,58,73,76	0
23	CLA	D	404	65/65	0.95	0.10	43,55,120,122	0
23	CLA	B	614	65/65	0.95	0.09	34,44,96,103	0
27	GOL	a	410	6/6	0.95	0.11	60,70,83,86	0
23	CLA	b	606	65/65	0.95	0.09	40,52,114,120	0
31	LHG	D	408	49/49	0.95	0.12	43,60,115,123	0
25	BCR	K	101	40/40	0.95	0.10	57,69,78,81	0
31	LHG	L	101	49/49	0.95	0.10	41,52,63,88	0
23	CLA	b	612	65/65	0.95	0.08	38,47,59,75	0
25	BCR	Y	101	40/40	0.95	0.08	53,67,77,84	0
31	LHG	d	406	49/49	0.95	0.11	50,62,82,94	0
31	LHG	d	408	49/49	0.95	0.12	56,66,109,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	b	617	40/40	0.95	0.07	39,49,57,59	0
25	BCR	b	618	40/40	0.95	0.08	39,53,69,75	0
23	CLA	b	614	65/65	0.95	0.09	36,45,103,107	0
29	PL9	D	406	55/55	0.95	0.09	32,44,58,67	0
25	BCR	c	517	40/40	0.95	0.10	54,67,73,75	0
23	CLA	B	606	65/65	0.95	0.09	39,50,95,104	0
35	DGD	c	519	62/66	0.95	0.10	51,73,114,122	0
23	CLA	c	505	65/65	0.95	0.08	52,65,75,81	0
25	BCR	k	101	40/40	0.95	0.10	60,73,84,87	0
23	CLA	c	506	65/65	0.95	0.09	51,59,100,110	0
37	BCT	D	401[A]	4/4	0.95	0.08	57,57,60,62	4
37	BCT	D	401[B]	4/4	0.95	0.08	59,59,61,64	4
37	BCT	d	401[A]	4/4	0.95	0.08	55,59,59,60	4
37	BCT	d	401[B]	4/4	0.95	0.08	53,58,60,67	4
23	CLA	a	407	65/65	0.96	0.10	40,51,124,127	0
23	CLA	B	607	65/65	0.96	0.07	32,42,62,72	0
25	BCR	A	408	40/40	0.96	0.07	35,46,55,56	0
25	BCR	B	617	40/40	0.96	0.06	38,47,58,61	0
23	CLA	b	602	65/65	0.96	0.08	48,56,68,81	0
23	CLA	b	605	65/65	0.96	0.08	36,47,67,70	0
23	CLA	C	507	65/65	0.96	0.08	43,52,86,87	0
23	CLA	b	607	65/65	0.96	0.08	33,43,72,80	0
25	BCR	C	517	40/40	0.96	0.08	50,61,74,79	0
31	LHG	D	407	49/49	0.96	0.09	41,50,67,84	0
23	CLA	b	609	65/65	0.96	0.08	49,57,76,98	0
23	CLA	b	610	65/65	0.96	0.09	44,52,66,73	0
23	CLA	B	610	65/65	0.96	0.09	42,50,63,75	0
23	CLA	C	509	65/65	0.96	0.09	48,57,78,86	0
23	CLA	B	611	65/65	0.96	0.07	35,41,60,68	0
25	BCR	a	408	40/40	0.96	0.07	38,48,56,59	0
31	LHG	d	407	49/49	0.96	0.08	39,51,69,80	0
23	CLA	c	503	65/65	0.96	0.08	56,63,75,79	0
23	CLA	c	504	65/65	0.96	0.08	49,58,73,89	0
25	BCR	b	619	40/40	0.96	0.08	46,55,77,86	0
34	LMG	d	411	51/55	0.96	0.10	53,67,107,116	0
23	CLA	C	511	65/65	0.96	0.09	49,58,76,83	0
29	PL9	d	405	55/55	0.96	0.08	36,47,56,65	0
35	DGD	C	518	62/66	0.96	0.10	41,57,98,102	0
23	CLA	A	405	65/65	0.96	0.08	34,46,107,111	0
23	CLA	B	602	65/65	0.96	0.08	40,51,74,84	0
35	DGD	H	102	62/66	0.96	0.08	41,57,76,80	0
35	DGD	c	518	62/66	0.96	0.09	46,59,90,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	603	65/65	0.96	0.08	38,49,65,68	0
35	DGD	c	520	62/66	0.96	0.09	49,60,97,101	0
35	DGD	h	103	62/66	0.96	0.09	46,62,73,78	0
23	CLA	C	504	65/65	0.96	0.08	44,57,77,85	0
23	CLA	A	407	65/65	0.96	0.09	39,47,109,116	0
23	CLA	c	511	65/65	0.96	0.08	54,63,79,88	0
23	CLA	c	512	65/65	0.96	0.07	52,61,74,79	0
23	CLA	c	513	65/65	0.96	0.09	56,66,80,83	0
23	CLA	a	403	65/65	0.96	0.07	37,43,66,74	0
23	CLA	a	405	65/65	0.96	0.09	40,50,112,117	0
38	HEM	e	102	43/43	0.96	0.08	63,77,113,121	0
39	MG	J	102	1/1	0.96	0.10	56,56,56,56	0
23	CLA	D	403	65/65	0.97	0.07	33,40,57,69	0
23	CLA	B	612	65/65	0.97	0.07	36,44,58,67	0
23	CLA	b	611	65/65	0.97	0.07	38,47,70,82	0
23	CLA	B	613	65/65	0.97	0.07	36,43,86,93	0
27	GOL	C	524	6/6	0.97	0.16	49,58,63,63	0
23	CLA	b	613	65/65	0.97	0.07	34,45,80,86	0
24	PHO	A	406	64/64	0.97	0.06	33,41,49,58	0
23	CLA	a	404	65/65	0.97	0.06	35,43,52,58	0
24	PHO	a	416	64/64	0.97	0.06	40,48,55,63	0
23	CLA	b	615	65/65	0.97	0.07	41,52,73,79	0
23	CLA	A	404	65/65	0.97	0.06	32,40,51,56	0
36	CA	C	525	1/1	0.97	0.11	68,68,68,68	0
23	CLA	B	615	65/65	0.97	0.07	40,47,75,84	0
23	CLA	A	403	65/65	0.97	0.07	34,38,63,71	0
36	CA	a	420	1/1	0.97	0.09	108,108,108,108	0
36	CA	c	525	1/1	0.97	0.04	81,81,81,81	0
23	CLA	B	608	65/65	0.97	0.07	39,49,66,67	0
23	CLA	b	603	65/65	0.97	0.07	41,53,74,81	0
23	CLA	b	604	65/65	0.97	0.08	35,46,105,111	0
23	CLA	B	609	65/65	0.97	0.07	45,54,72,80	0
23	CLA	B	604	65/65	0.97	0.08	34,41,98,103	0
23	CLA	B	605	65/65	0.97	0.07	37,43,59,71	0
23	CLA	b	608	65/65	0.97	0.07	45,53,68,73	0
40	HEC	v	202	43/43	0.97	0.07	53,60,67,72	0
38	HEM	E	102	43/43	0.98	0.07	58,65,82,93	0
23	CLA	d	402	65/65	0.98	0.06	37,44,70,78	0
24	PHO	a	406	64/64	0.98	0.06	35,44,51,58	0
40	HEC	V	201	43/43	0.98	0.07	44,51,55,56	0
36	CA	c	524	1/1	0.98	0.07	75,75,75,75	0
22	CL	c	501	1/1	0.99	0.06	46,46,46,46	0

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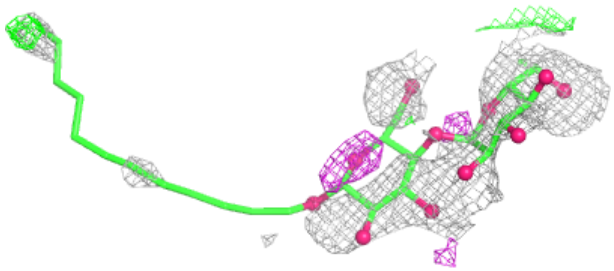
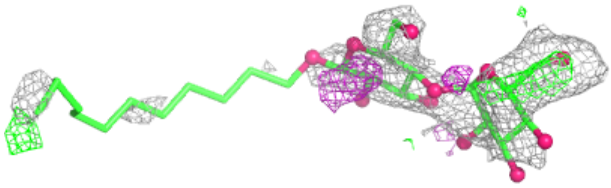
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CL	C	501	1/1	0.99	0.03	43,43,43,43	0
22	CL	a	402	1/1	0.99	0.05	46,46,46,46	0
39	MG	j	102	1/1	0.99	0.04	61,61,61,61	0
28	OEX	A	412[A]	10/10	0.99	0.04	42,45,49,49	10
28	OEX	A	412[B]	10/10	0.99	0.04	39,46,51,51	10
28	OEX	a	413[A]	10/10	1.00	0.03	46,48,52,56	10
28	OEX	a	413[B]	10/10	1.00	0.03	44,50,54,54	10
21	FE2	A	401[B]	1/1	1.00	0.04	57,57,57,57	1
21	FE2	a	401[A]	1/1	1.00	0.04	56,56,56,56	1
21	FE2	a	401[B]	1/1	1.00	0.04	63,63,63,63	1
22	CL	A	402	1/1	1.00	0.04	39,39,39,39	0
21	FE2	A	401[A]	1/1	1.00	0.04	54,54,54,54	1

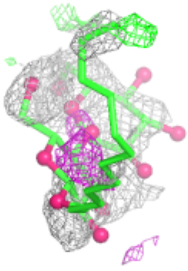
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT F 101:

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

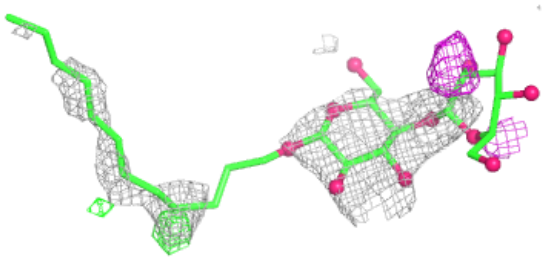


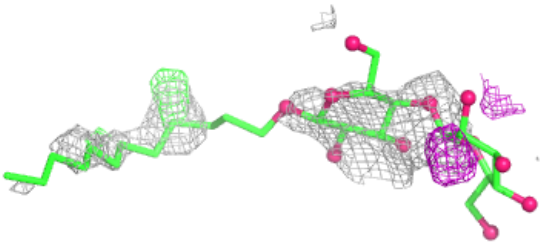


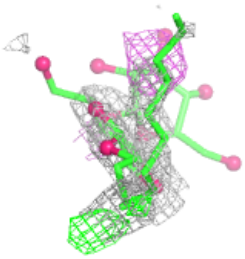


Electron density around LMT C 526:

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

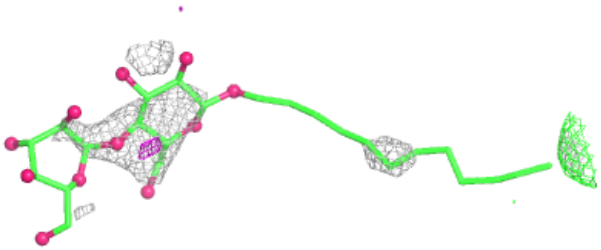


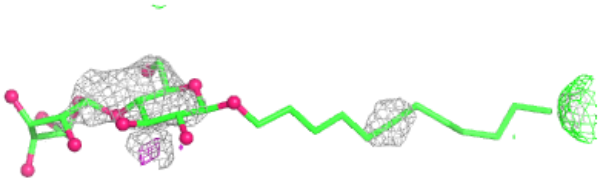


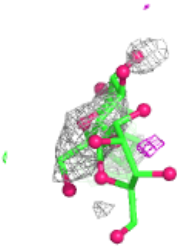


Electron density around LMT e 101:

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

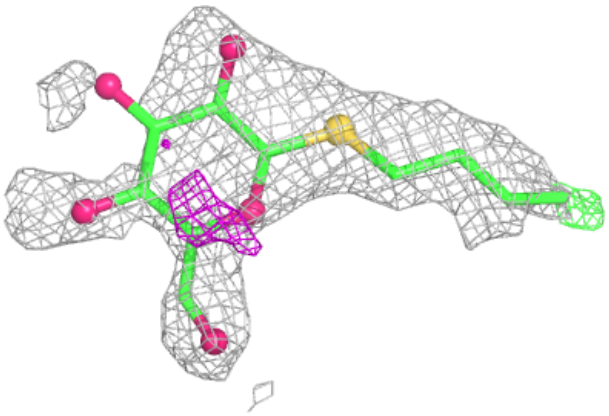


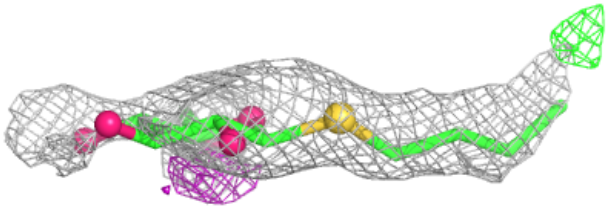


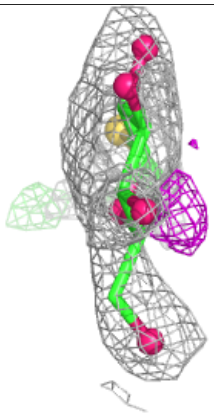


Electron density around HTG D 411:

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

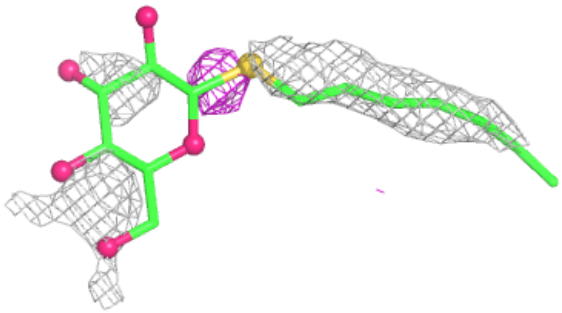


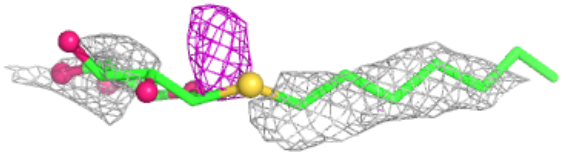


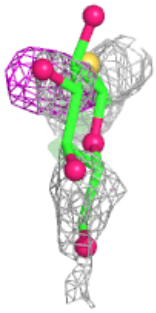


Electron density around HTG b 622:

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

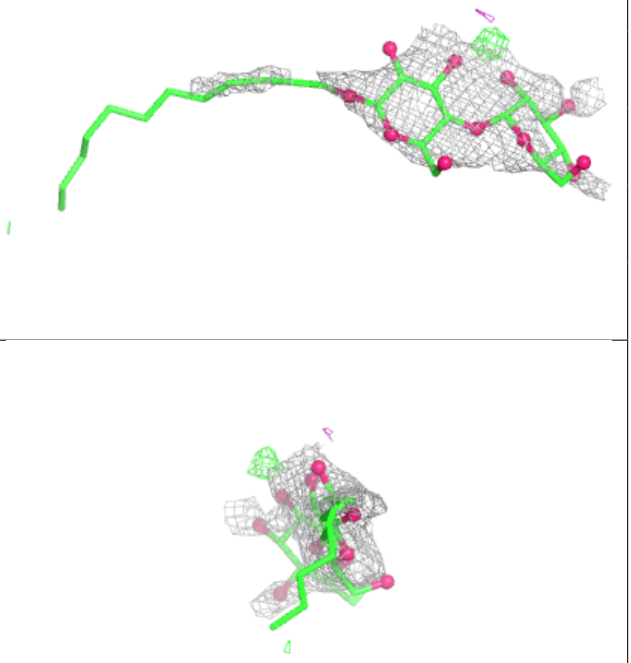


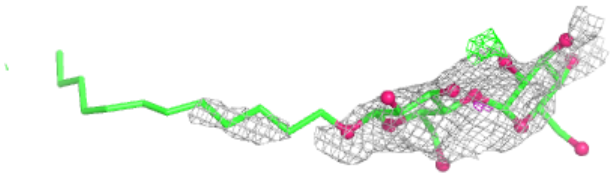




Electron density around LMT a 418:

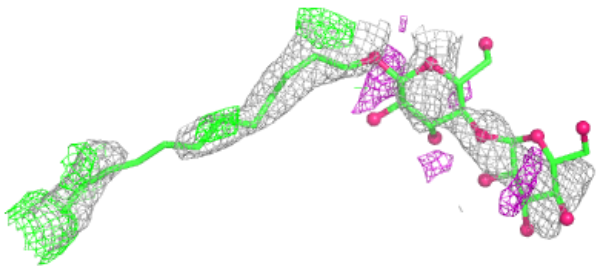
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

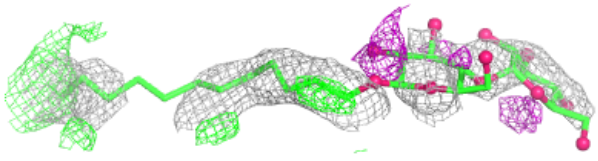


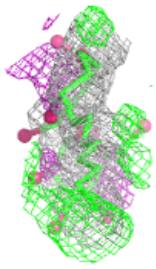


Electron density around LMT a 412:

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

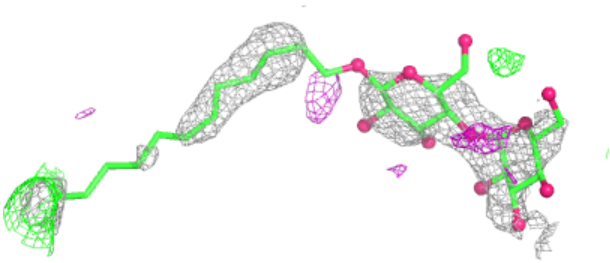


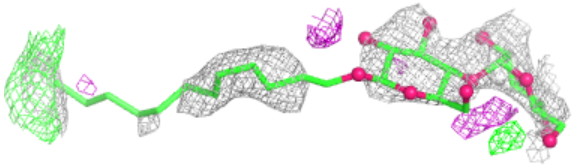


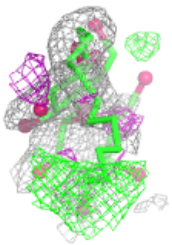


Electron density around LMT D 402:

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

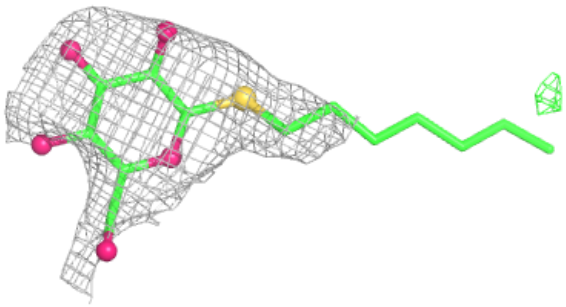


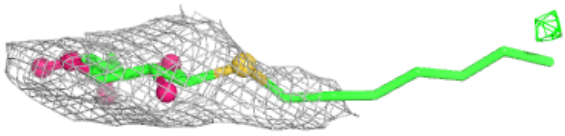


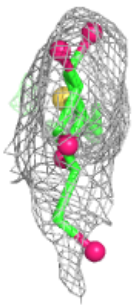


Electron density around HTG c 523:

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

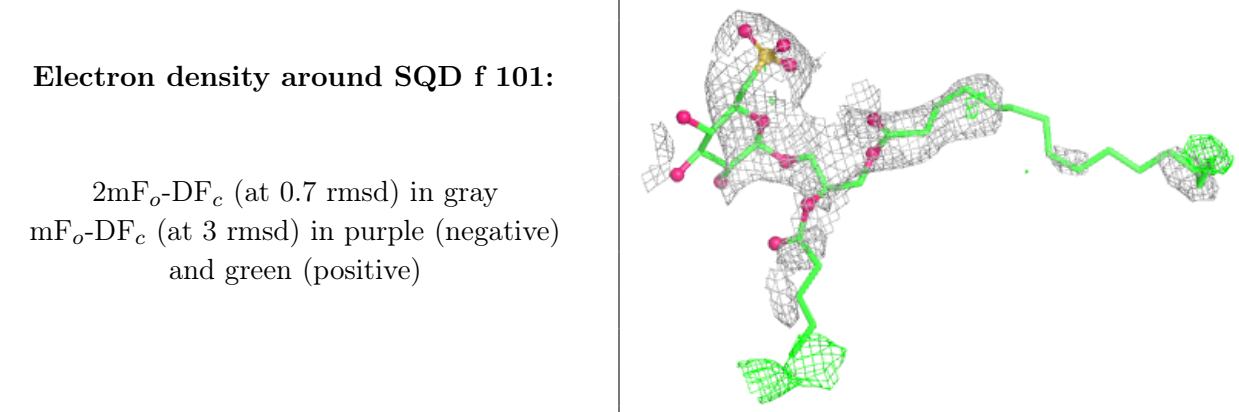


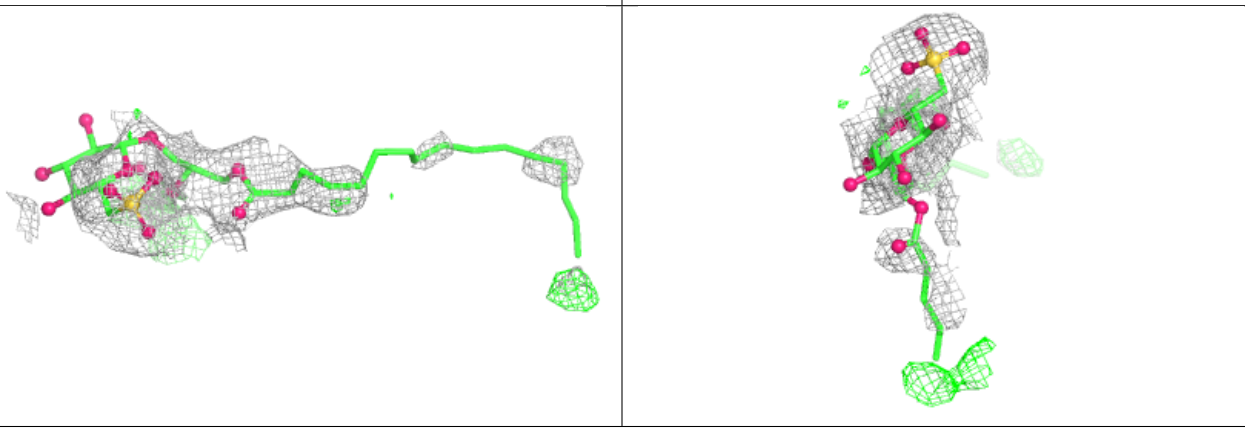




Electron density around SQD f 101:

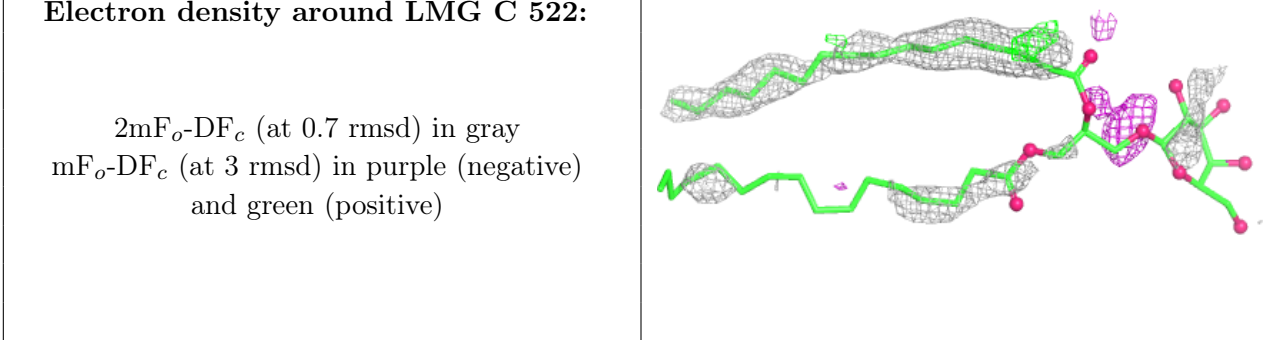
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

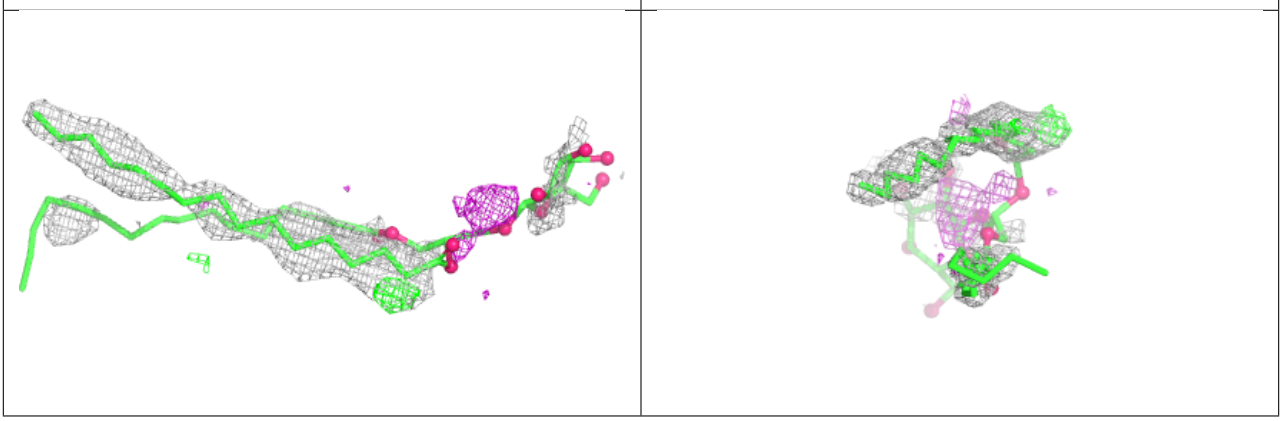




Electron density around LMG C 522:

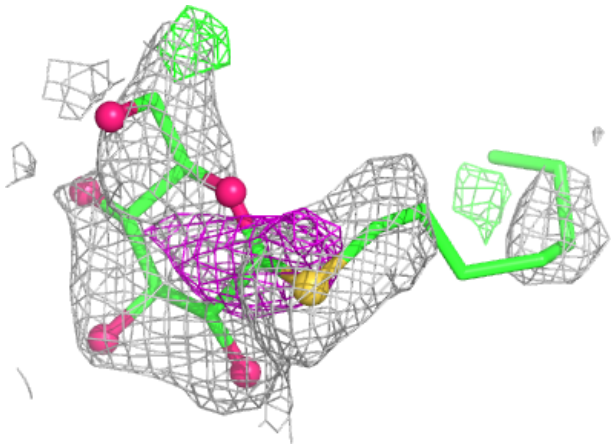
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

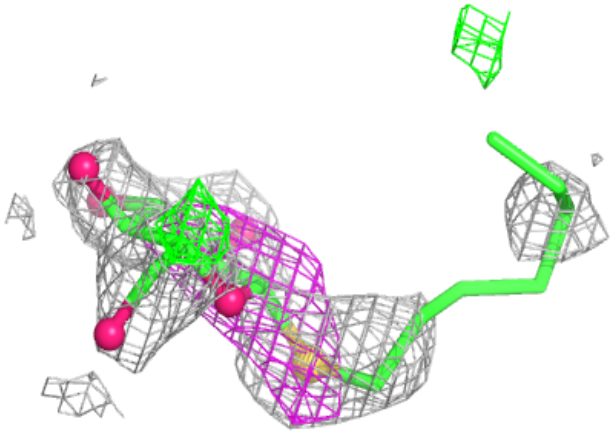


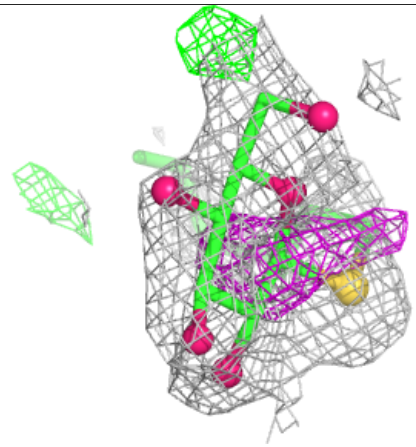


Electron density around HTG B 622:

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

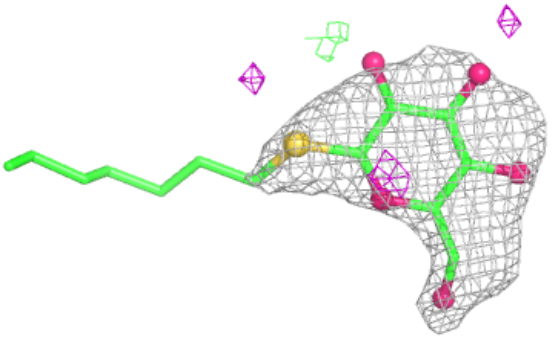


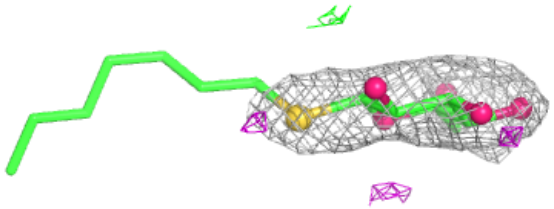


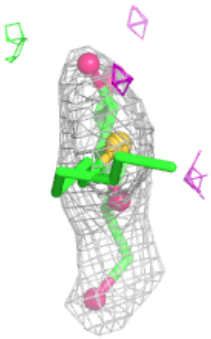


Electron density around HTG C 523:

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

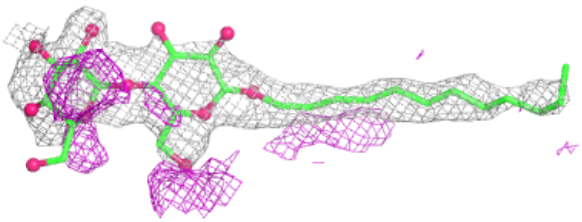


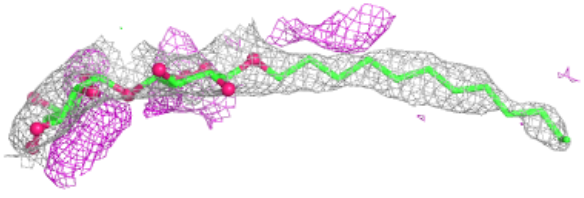


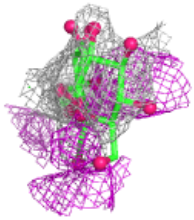


Electron density around LMT m 103:

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

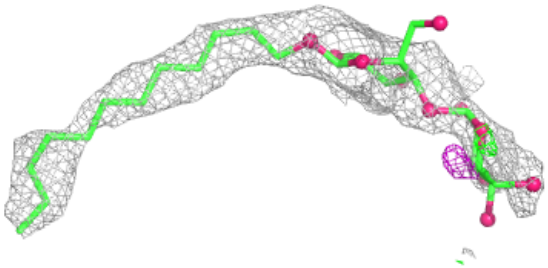


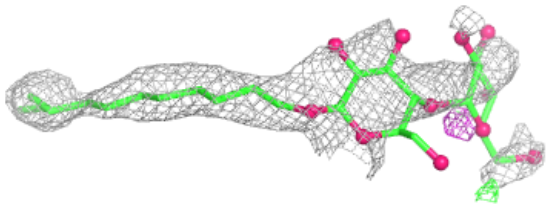


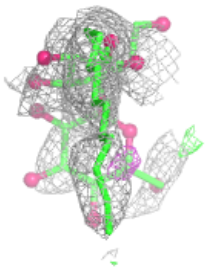


Electron density around LMT M 103:

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

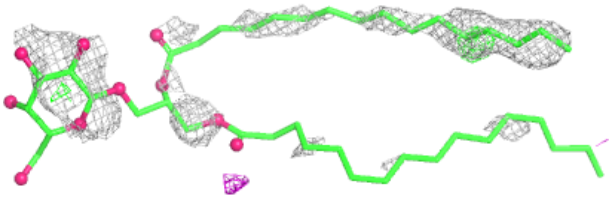


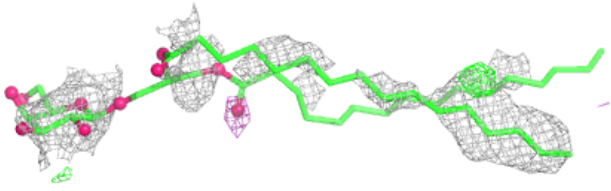


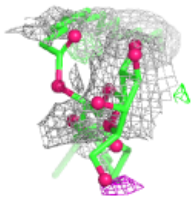


Electron density around LMG c 522:

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

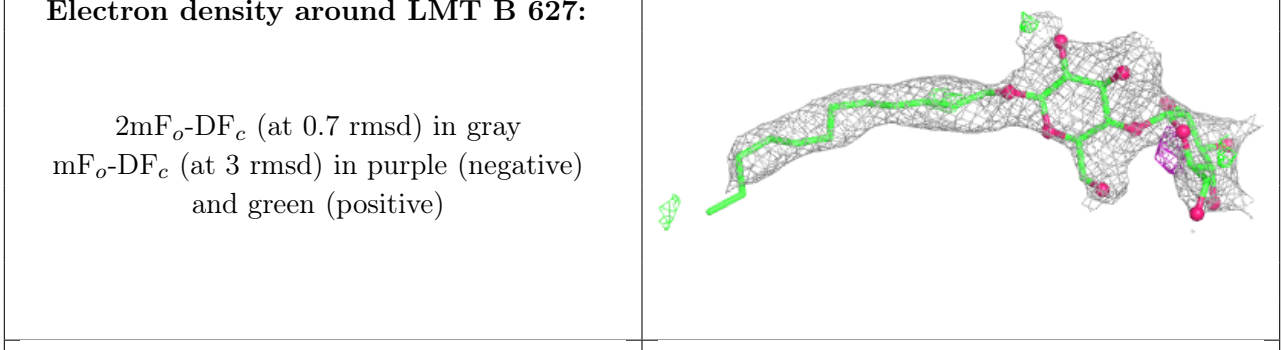






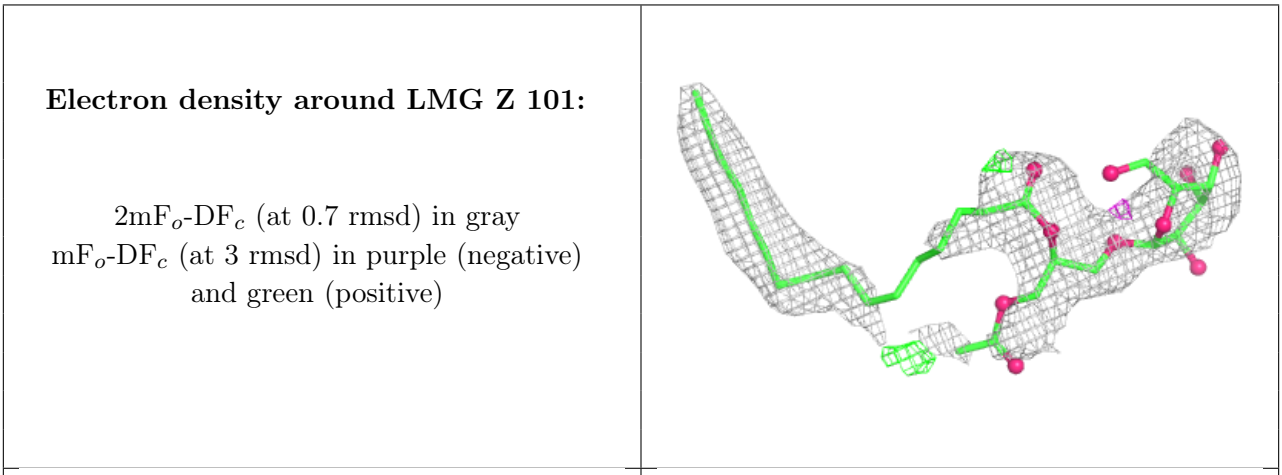
Electron density around LMT B 627:

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



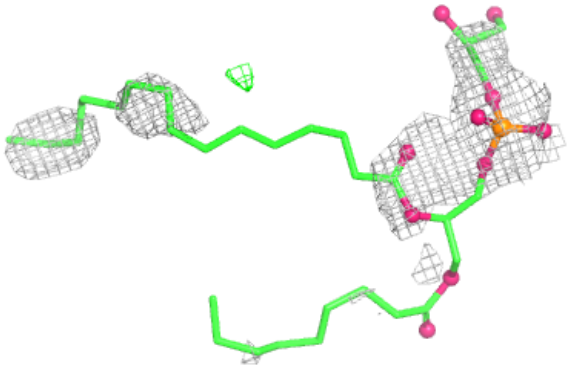
Electron density around LMG Z 101:

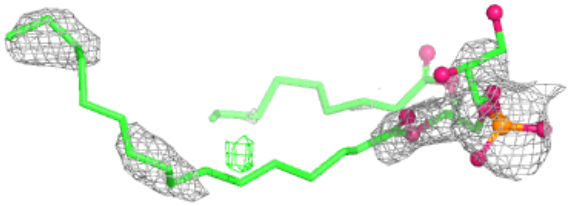
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

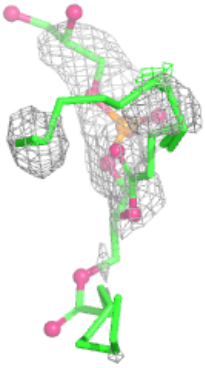


Electron density around LHG a 419:

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

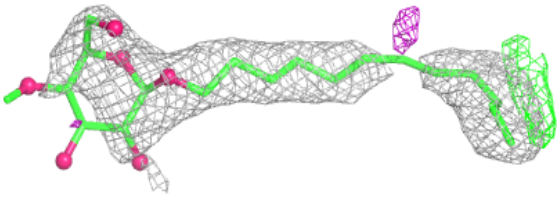


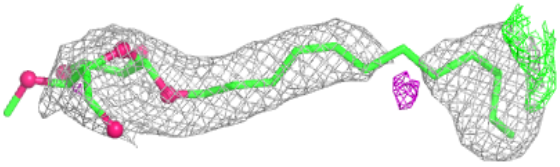


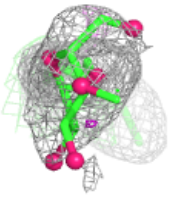


Electron density around LMT b 626:

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

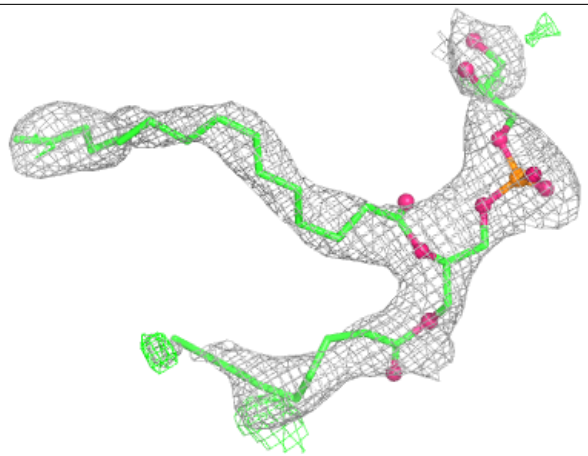


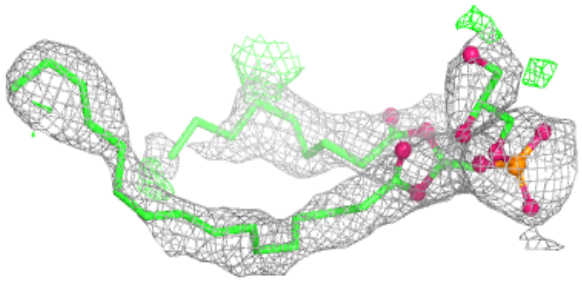


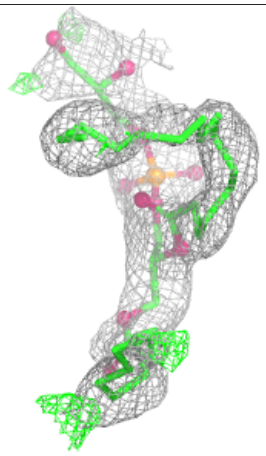


Electron density around LHG E 101:

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

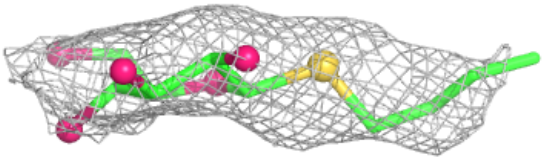


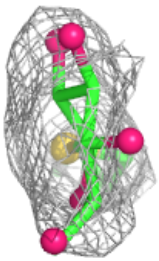




Electron density around HTG h 101:

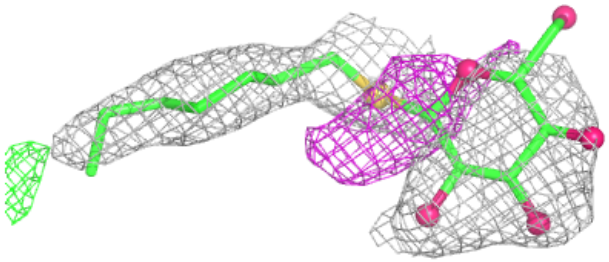
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

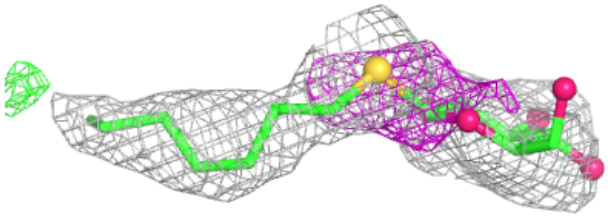


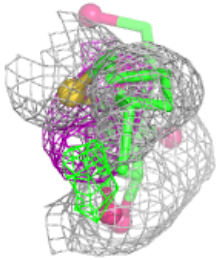


Electron density around HTG b 621:

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

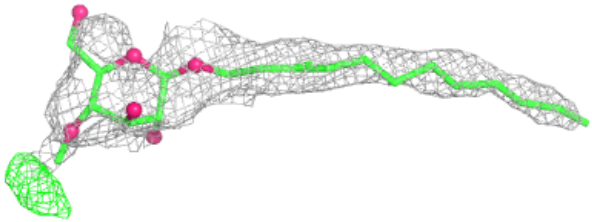


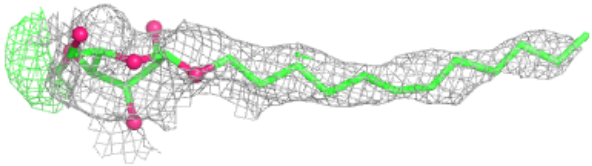


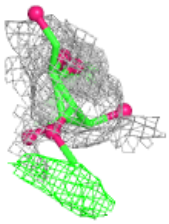


Electron density around LMT b 620:

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

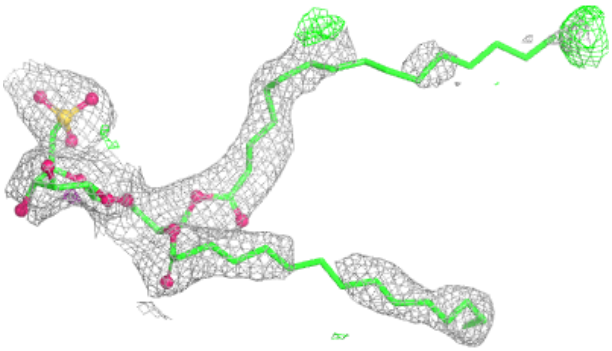


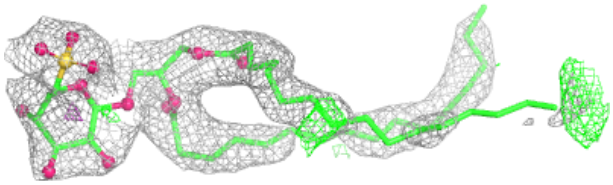


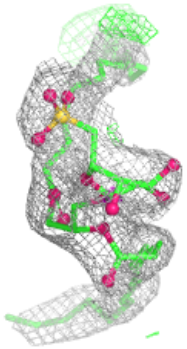


Electron density around SQD a 411:

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

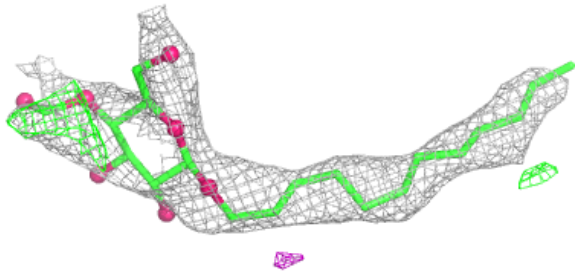


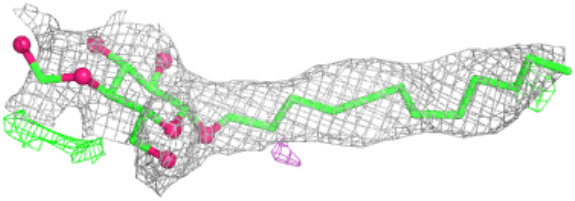


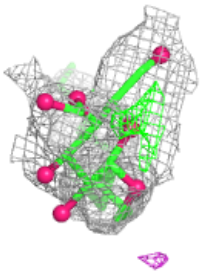


Electron density around LMT B 630:

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

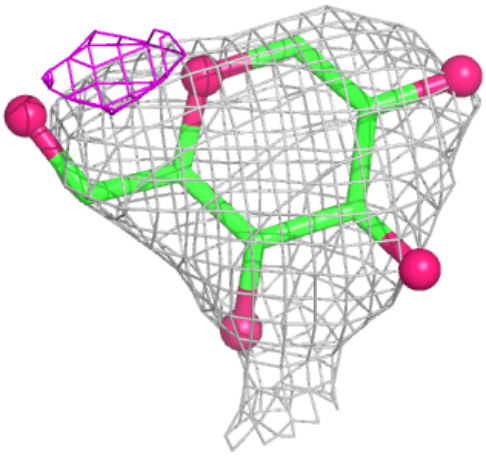


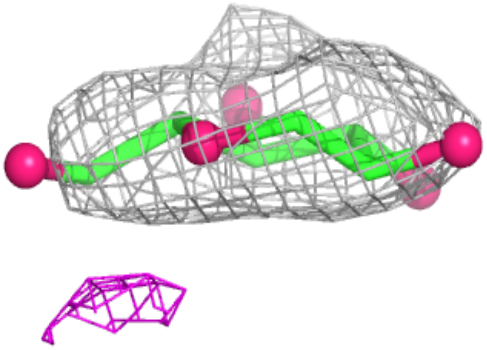


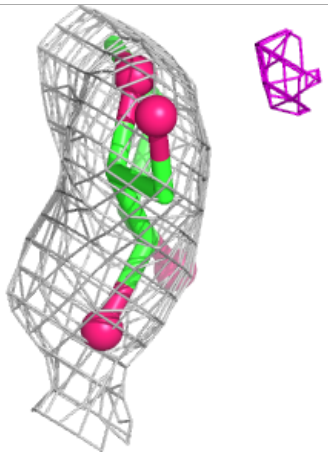


Electron density around HTG V 202:

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

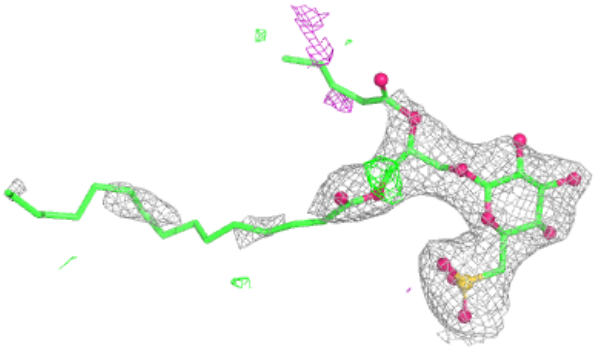


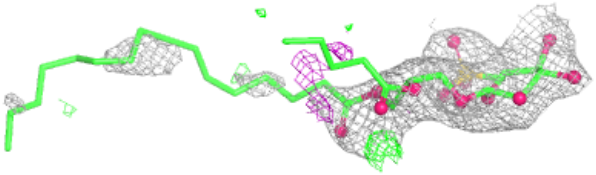


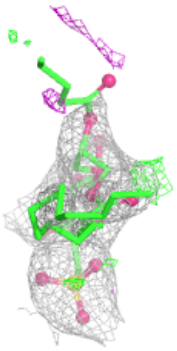


Electron density around SQD D 413:

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

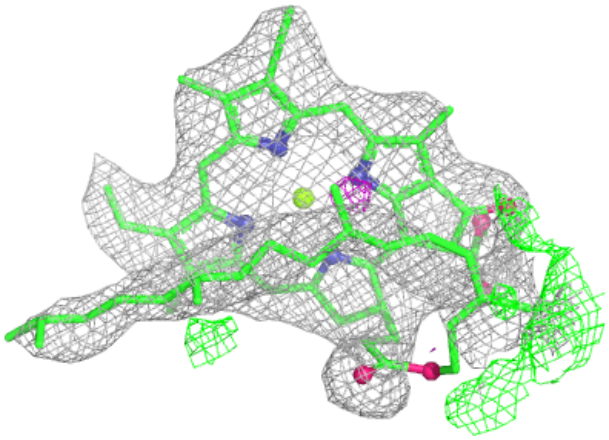


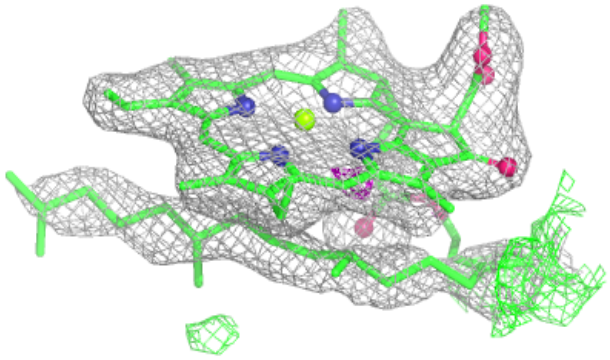


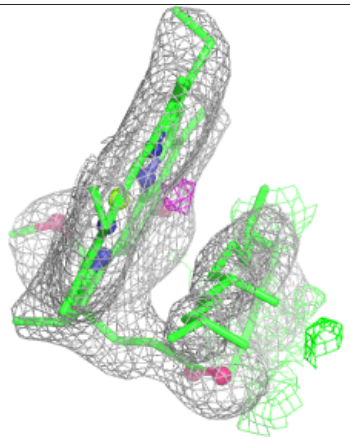


Electron density around CLA b 601:

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

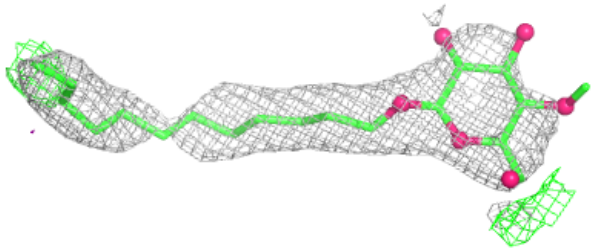


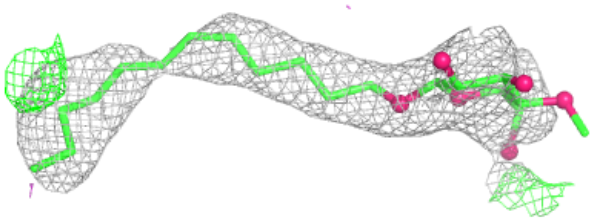


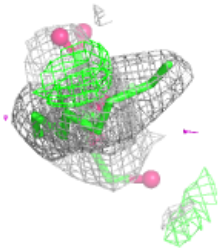


Electron density around LMT B 629:

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

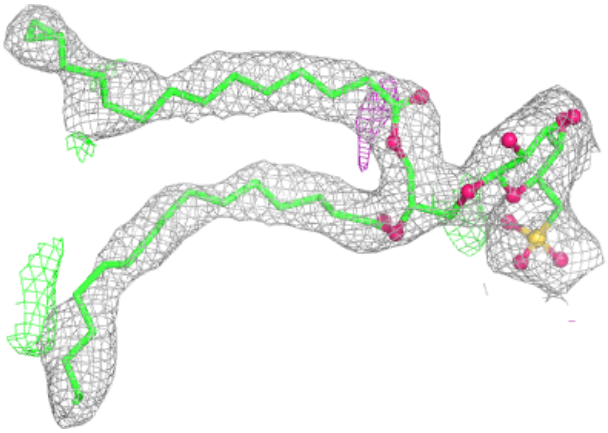


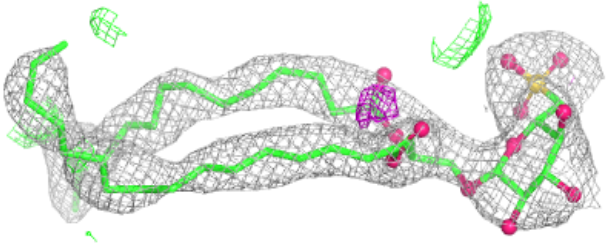


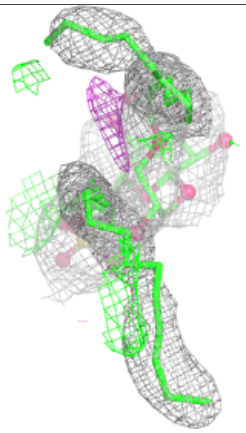


Electron density around SQD B 620:

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

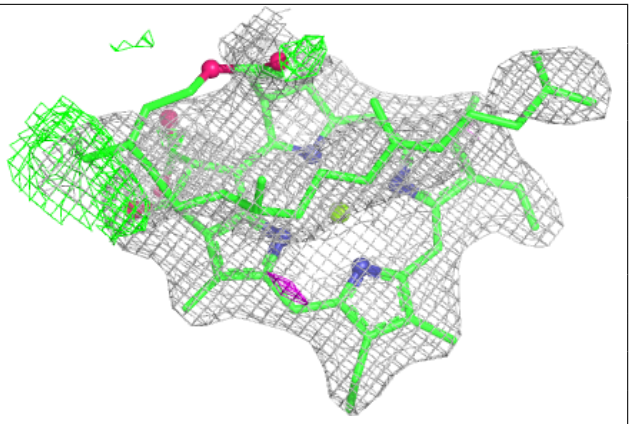


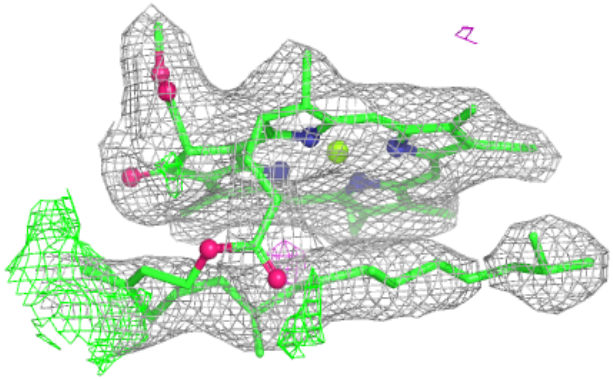


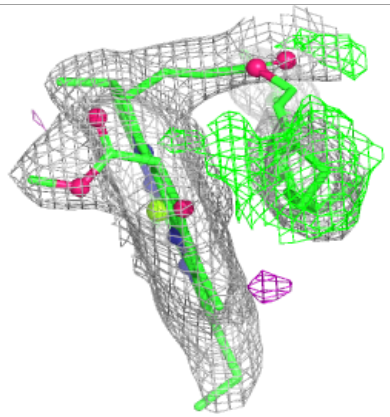


Electron density around CLA B 601:

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

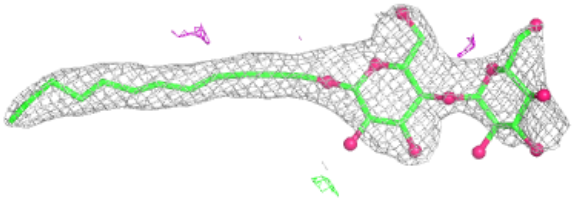


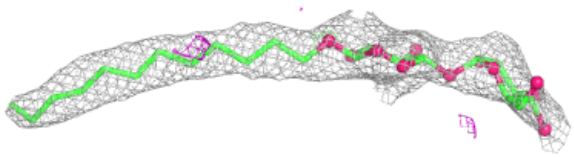


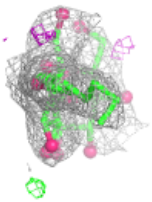


Electron density around LMT M 102:

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

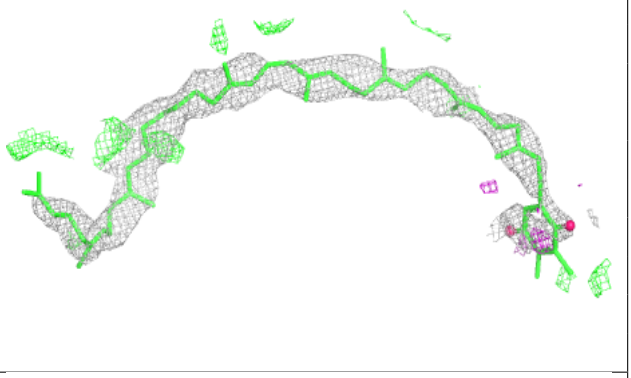


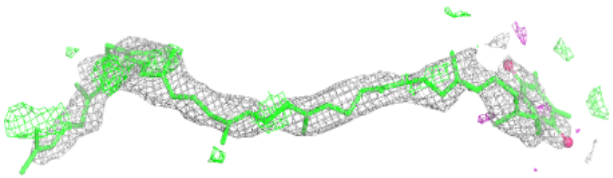


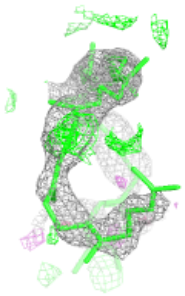


Electron density around PL9 A 413 (A):

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

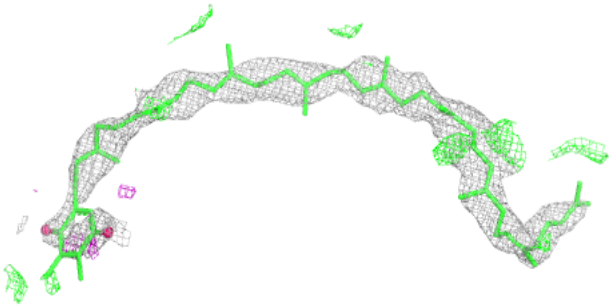


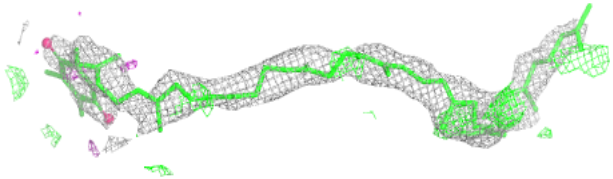


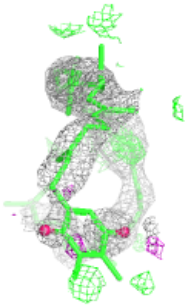


Electron density around PL9 A 413 (B):

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

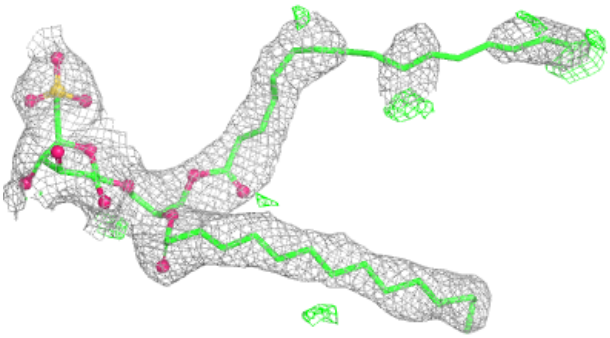


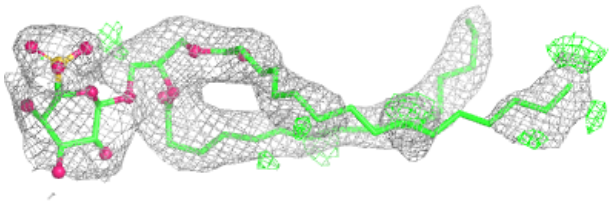


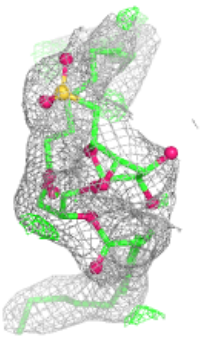


Electron density around SQD A 411:

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

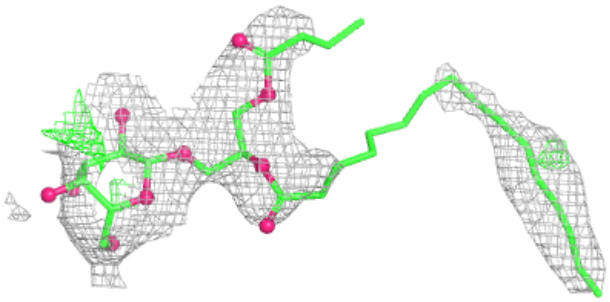


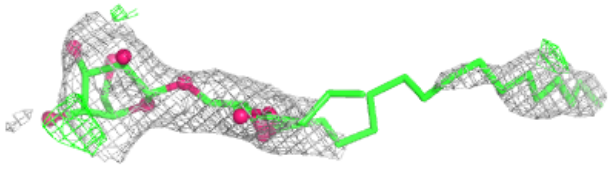


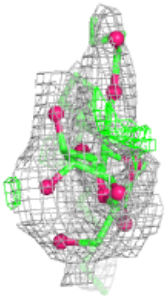


Electron density around LMG z 101:

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

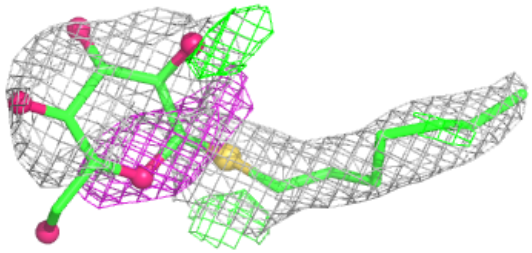


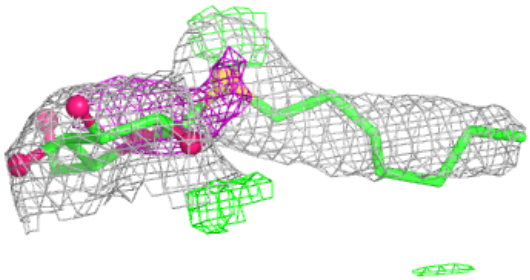


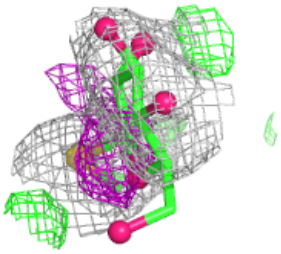


Electron density around HTG B 621:

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

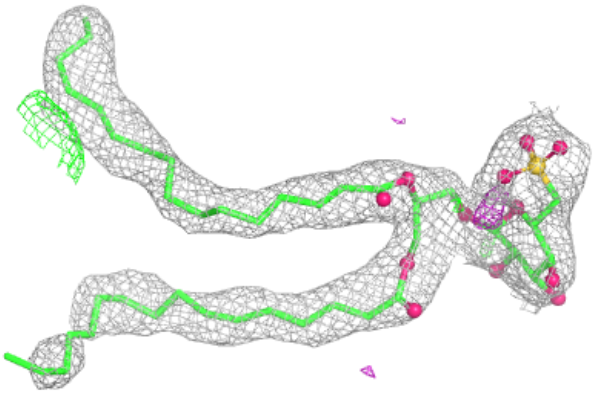


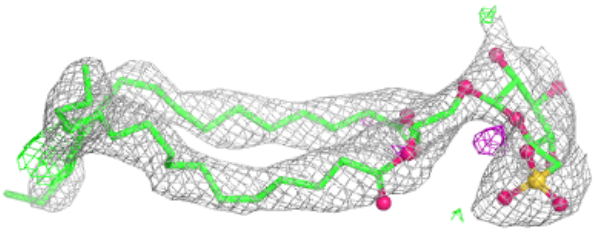


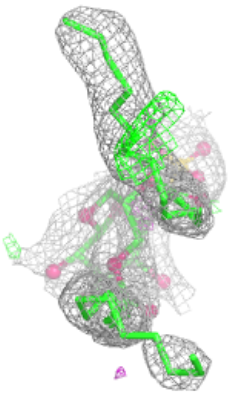


Electron density around SQD L 102:

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

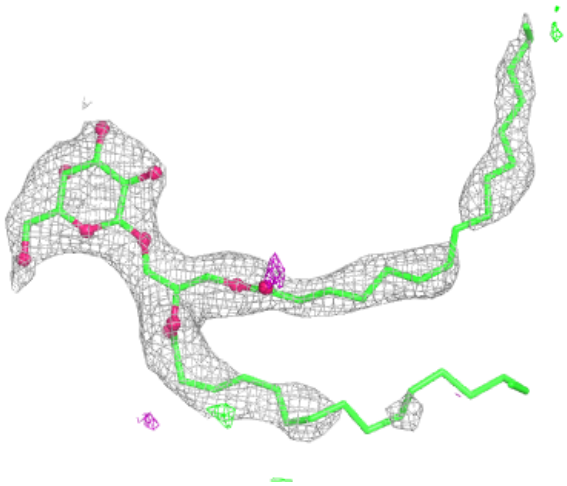


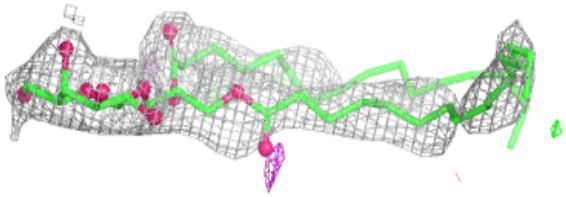


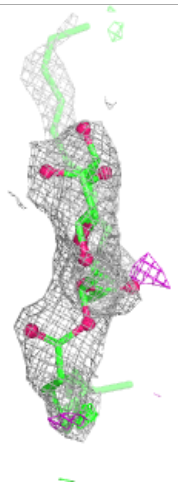


Electron density around LMG C 521:

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

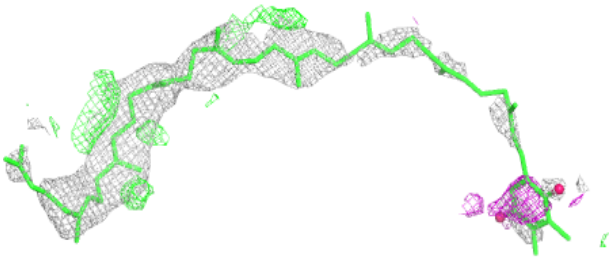


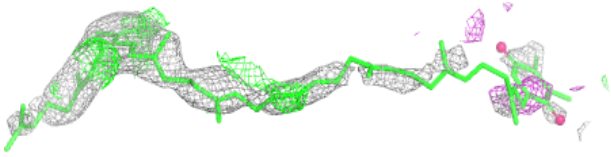


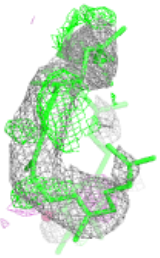


Electron density around PL9 a 414 (A):

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

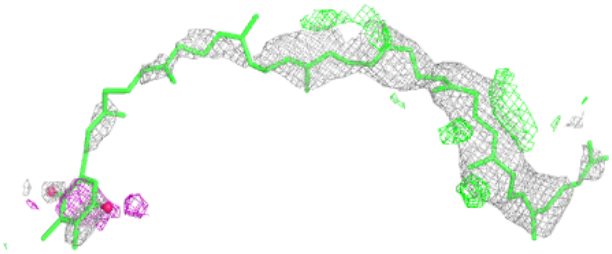


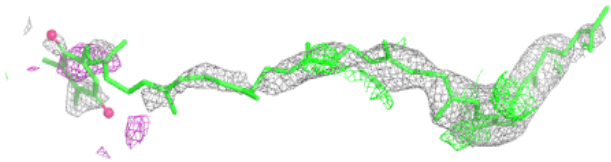


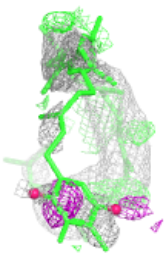


Electron density around PL9 a 414 (B):

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

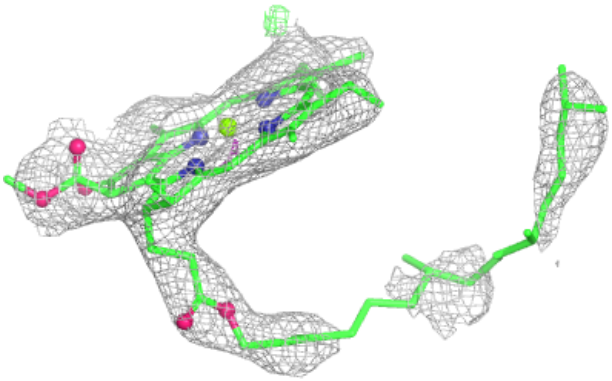


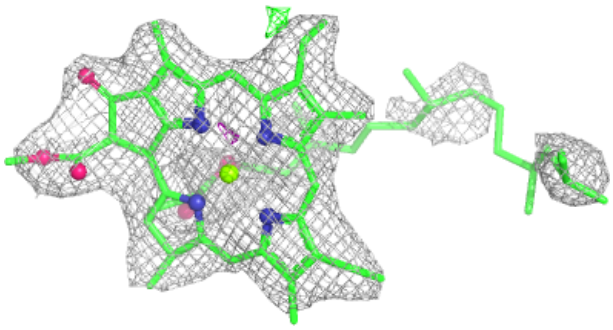


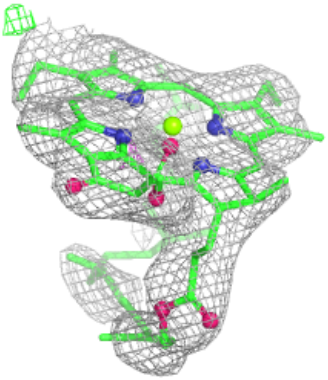


Electron density around CLA C 515:

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

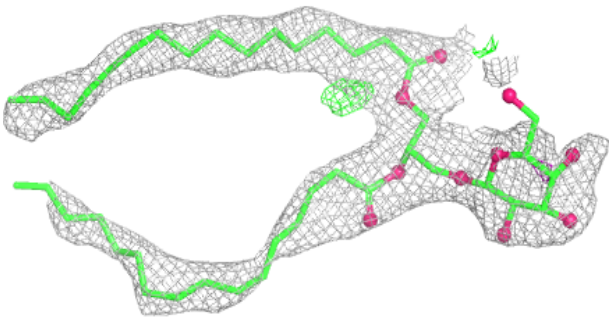


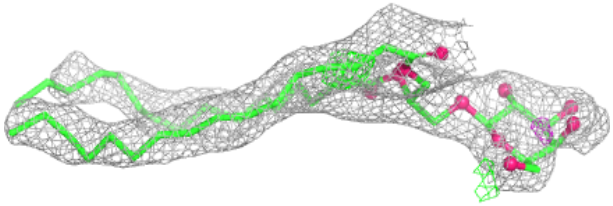


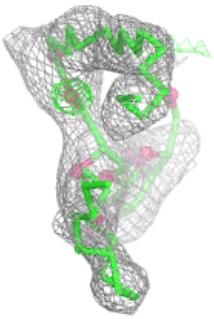


Electron density around LMG a 417:

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

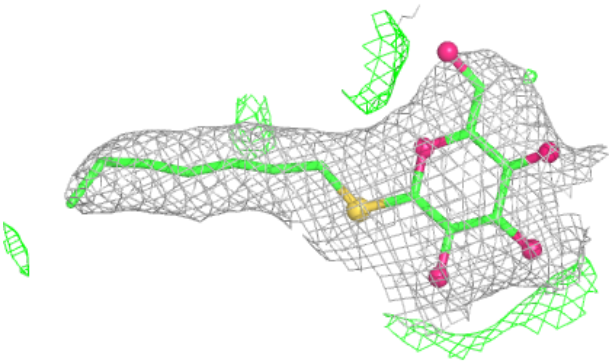


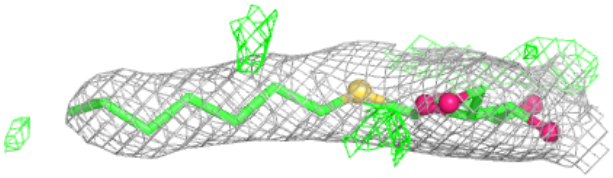


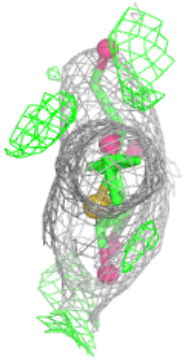


Electron density around HTG b 624:

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

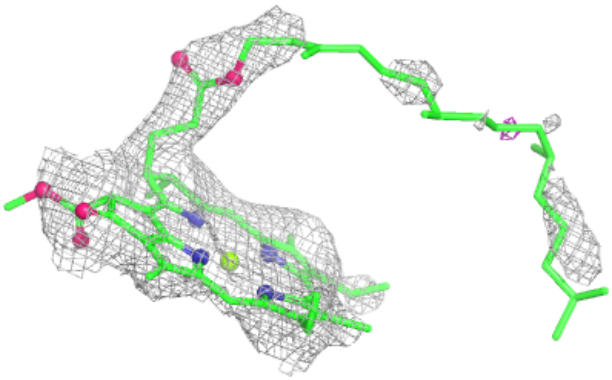


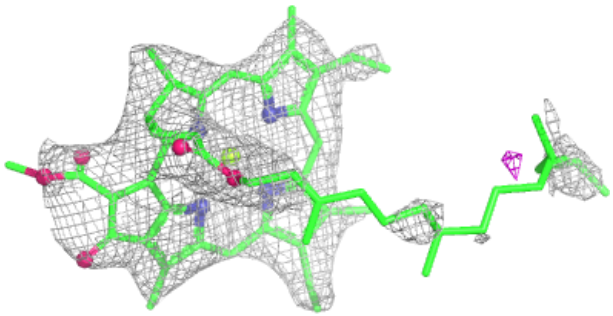


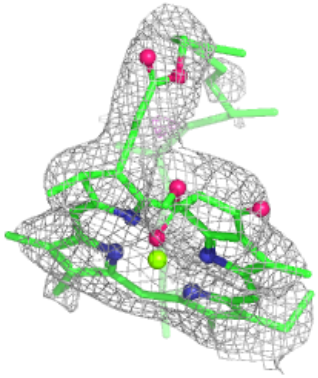


Electron density around CLA c 515:

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

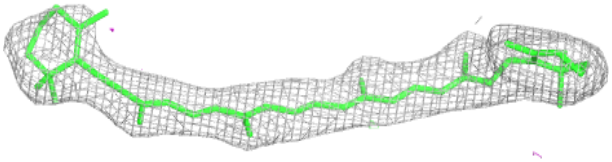


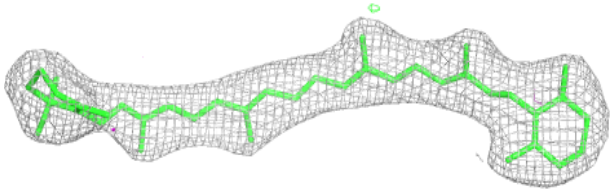


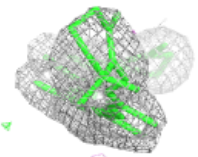


Electron density around BCR D 405:

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

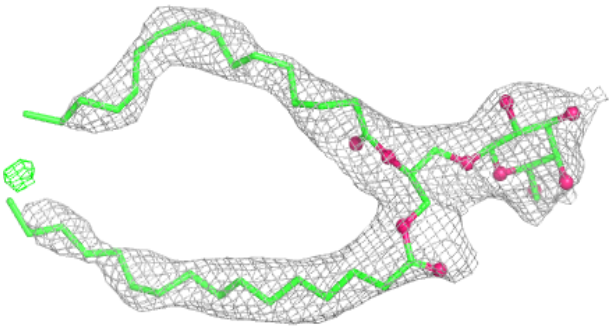


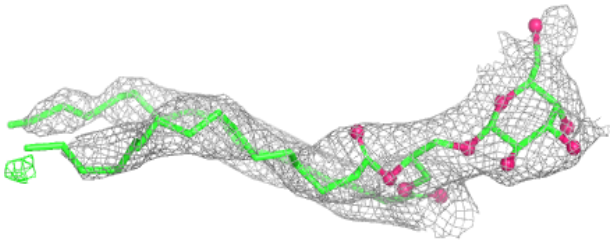


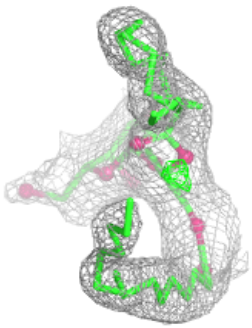


Electron density around LMG C 502:

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

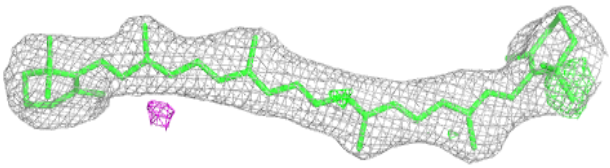


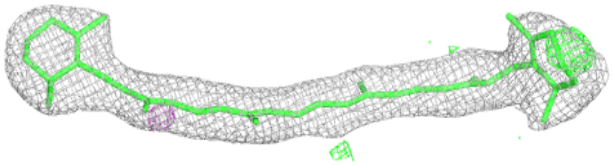


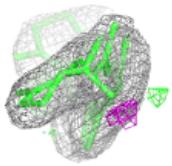


Electron density around BCR d 404:

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

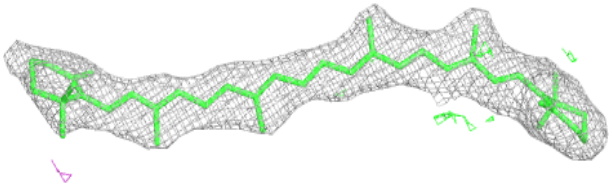


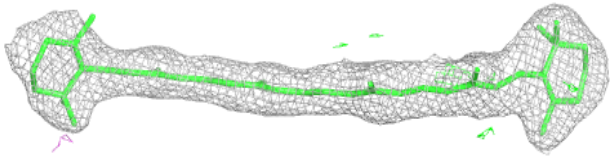


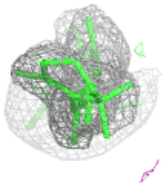


Electron density around BCR h 102:

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

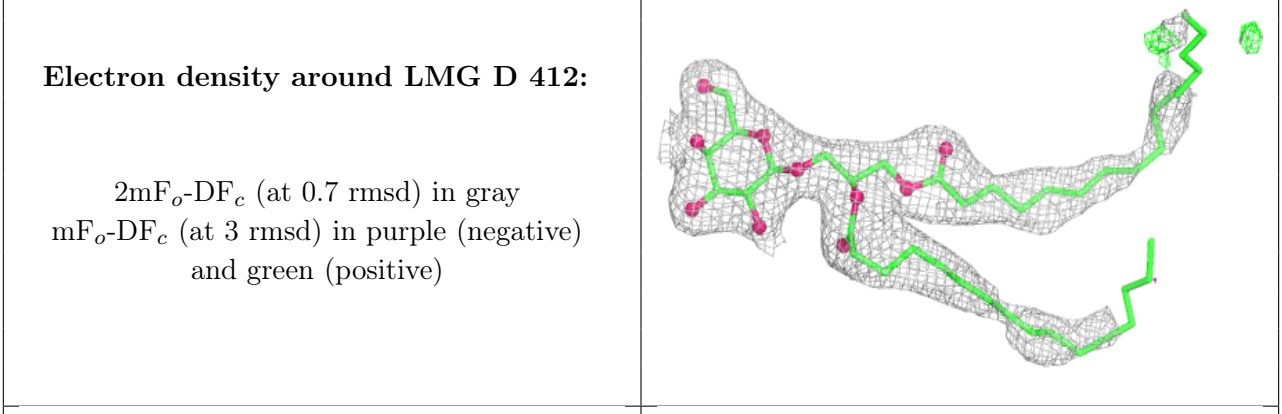






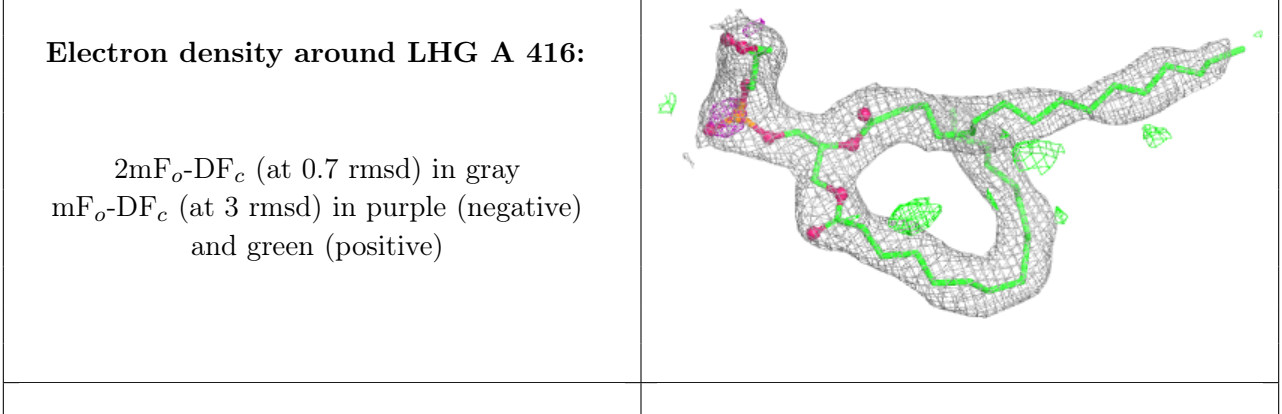
Electron density around LMG D 412:

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



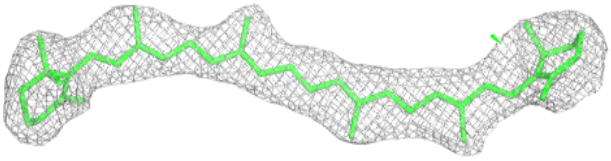
Electron density around LHG A 416:

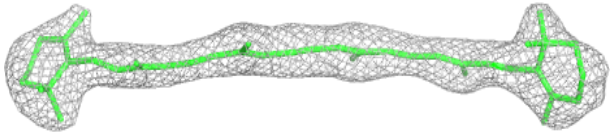
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

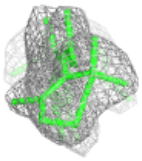


Electron density around BCR k 102:

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

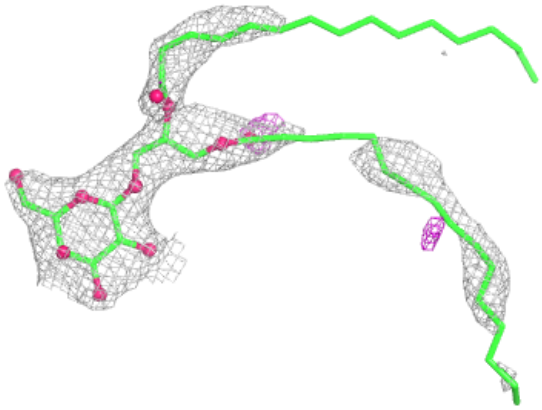


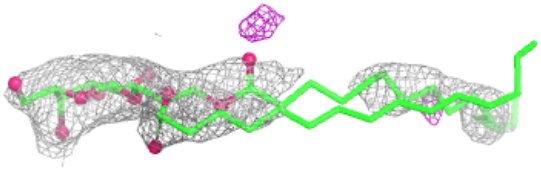


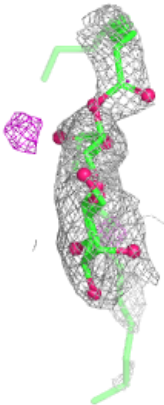


Electron density around LMG c 521:

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

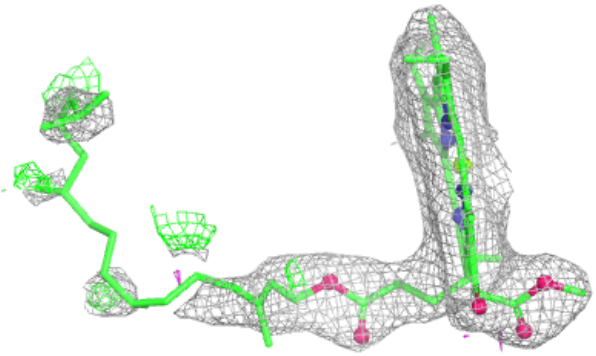


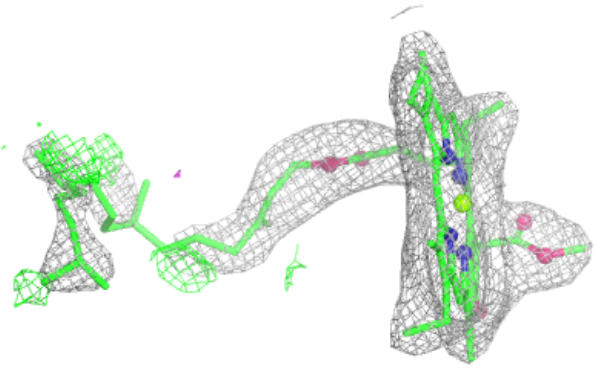


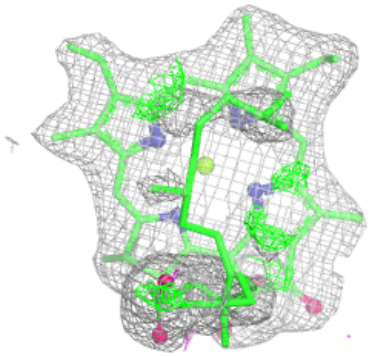


Electron density around CLA C 508:

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

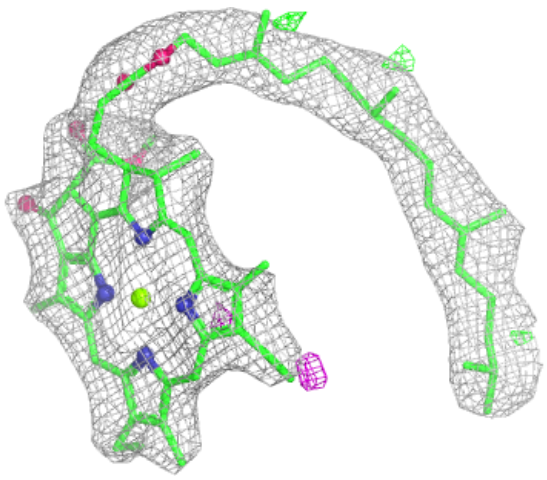


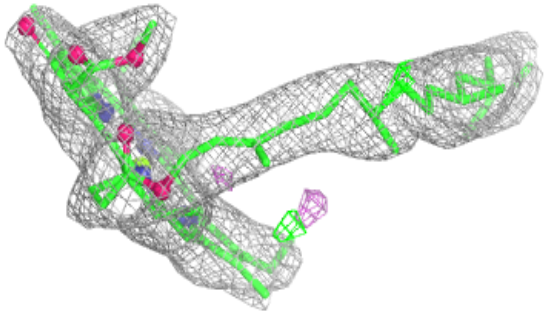


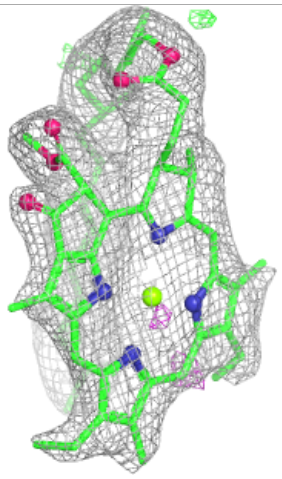


Electron density around CLA c 509:

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

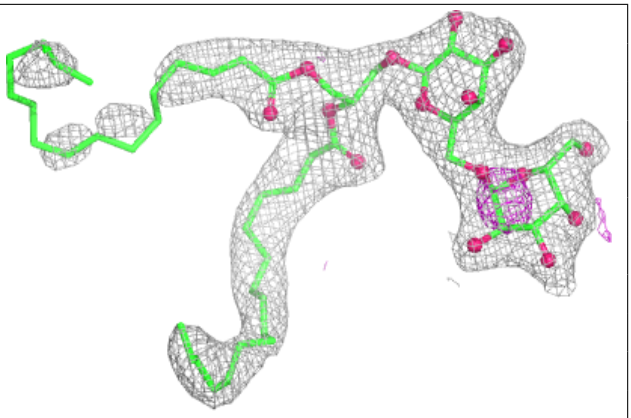


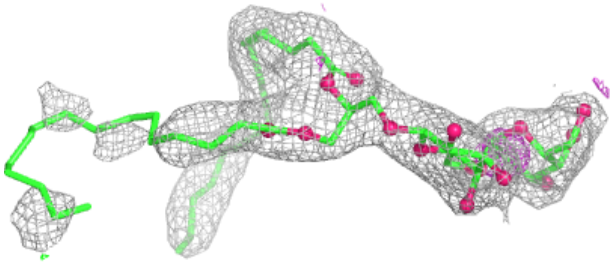


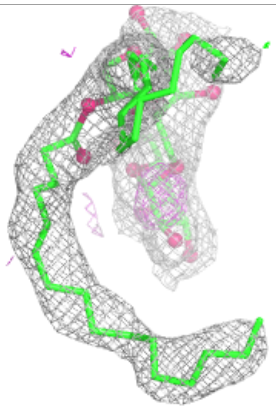


Electron density around DGD C 519:

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

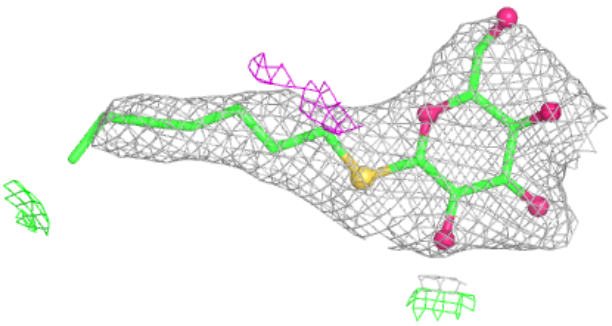


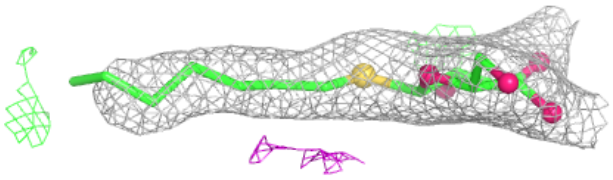


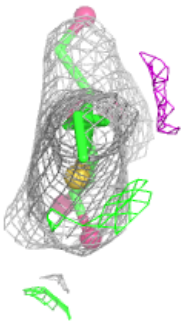


Electron density around HTG B 624:

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

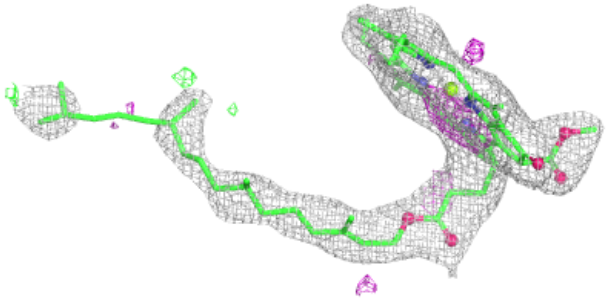


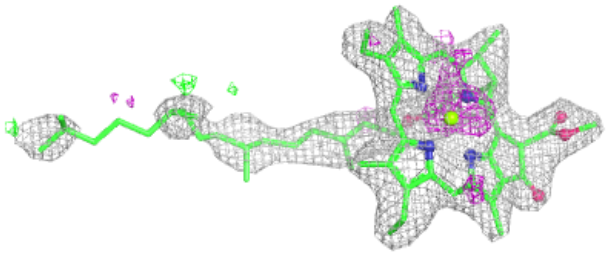


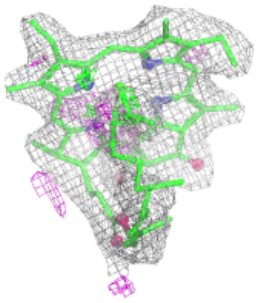


Electron density around CLA C 506:

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

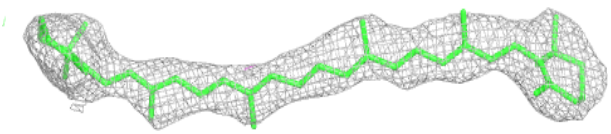


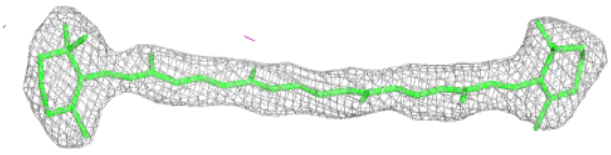


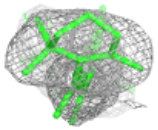


Electron density around BCR c 516:

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

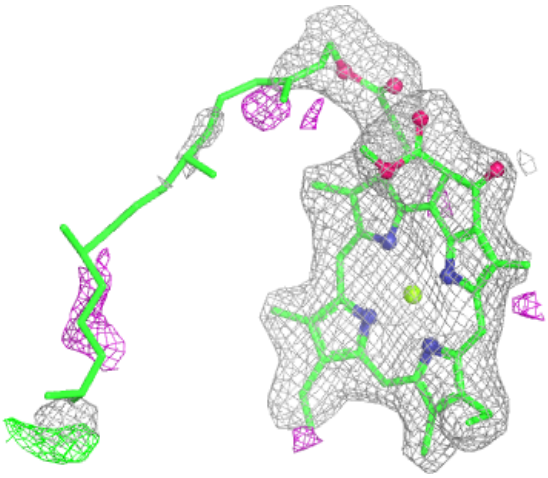


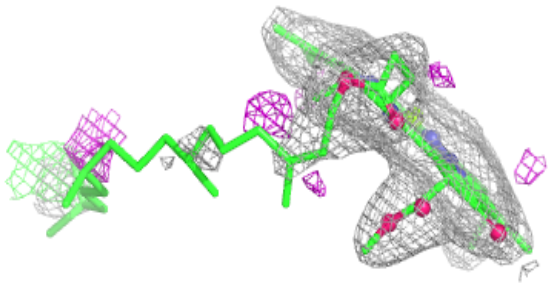


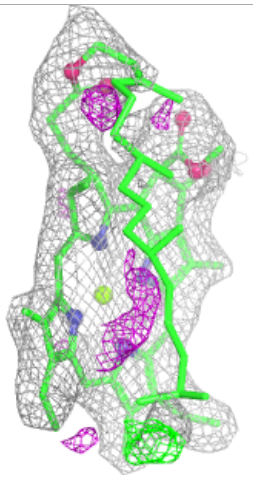


Electron density around CLA B 616:

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

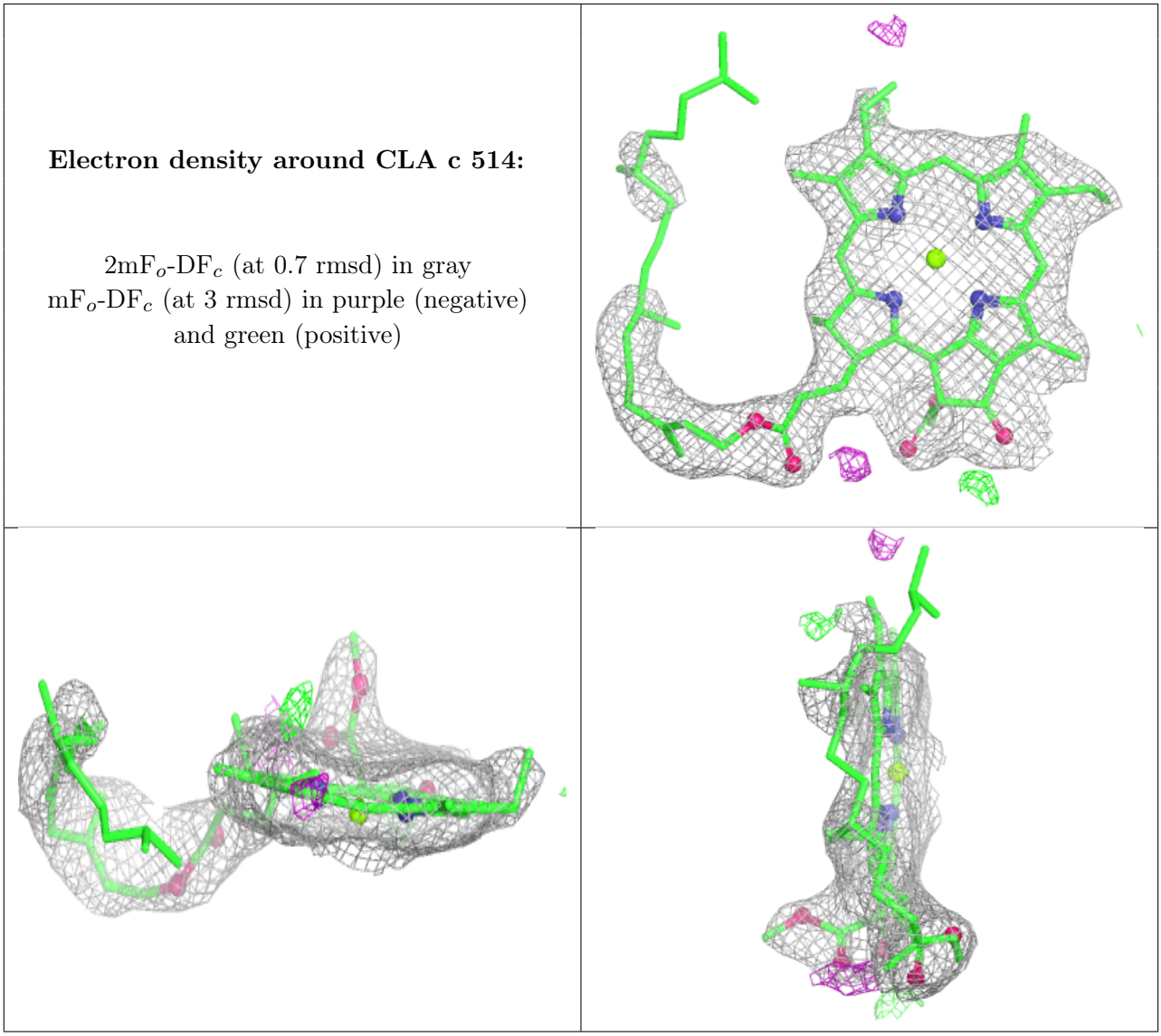






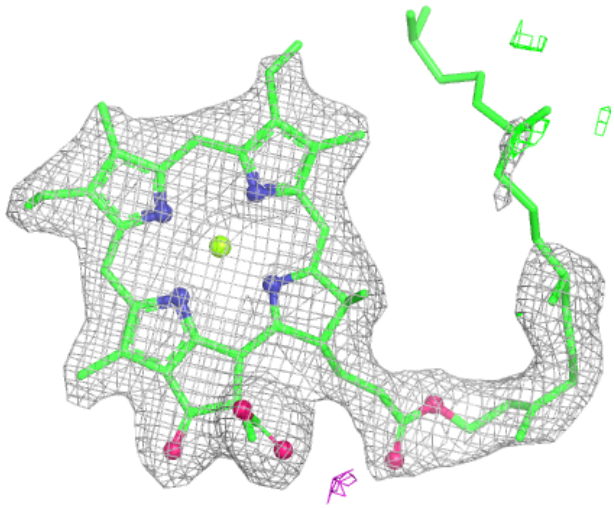
Electron density around CLA c 514:

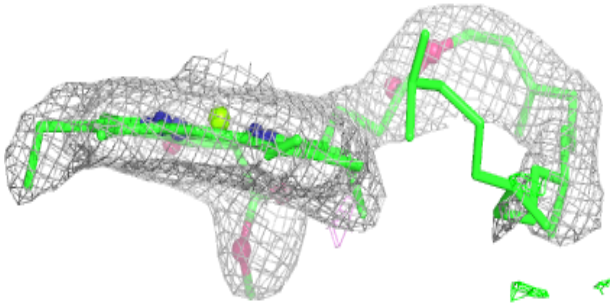
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

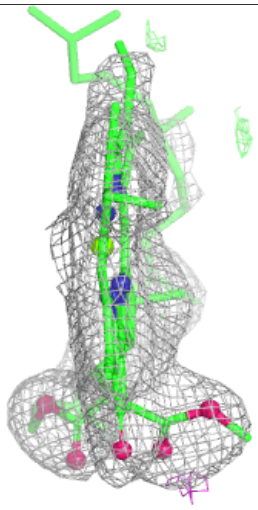


Electron density around CLA C 514:

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

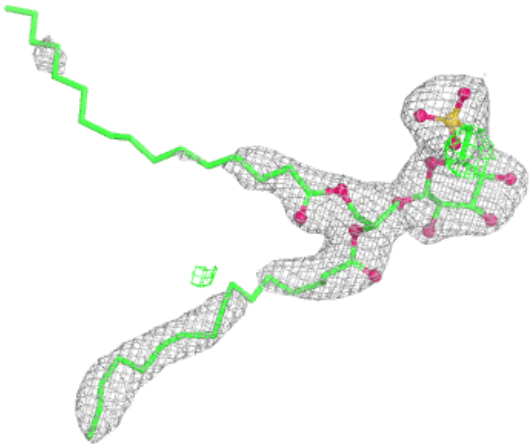


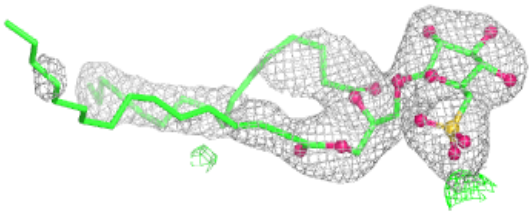


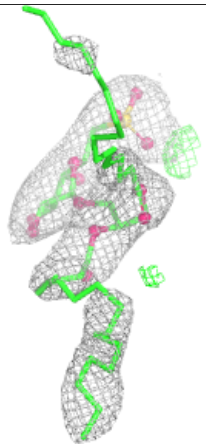


Electron density around SQD A 409:

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

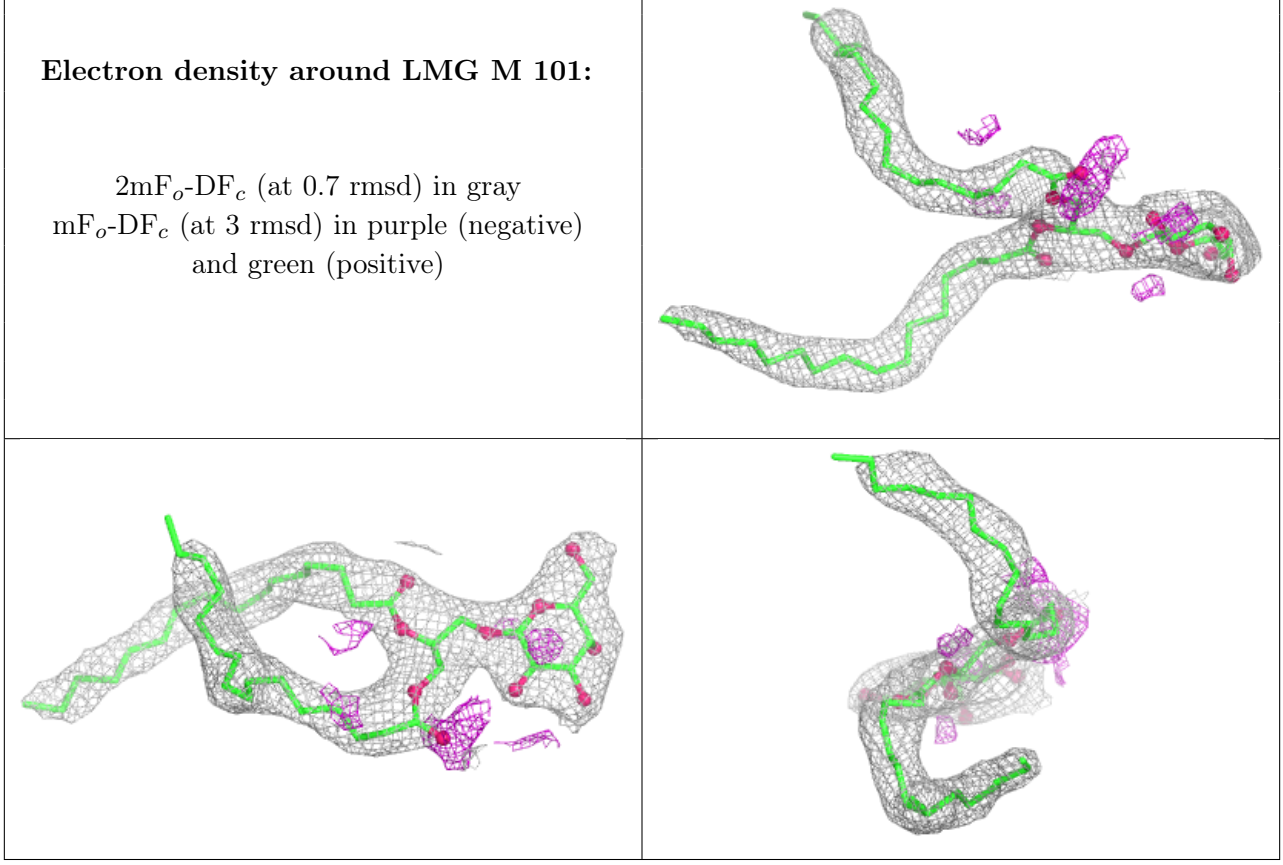






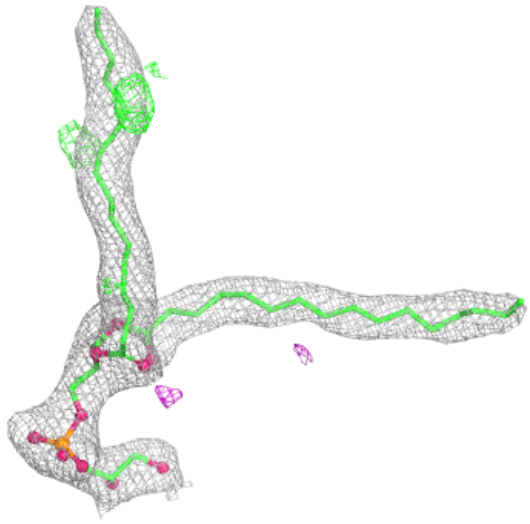
Electron density around LMG M 101:

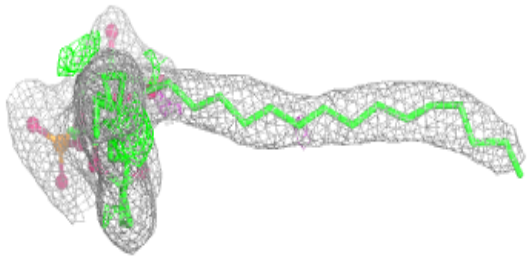
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

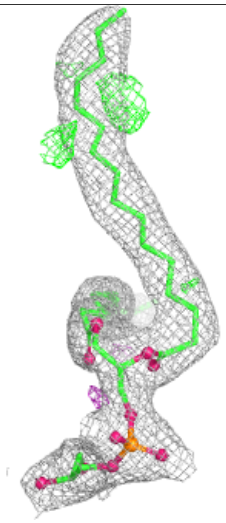


Electron density around LHG b 628:

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

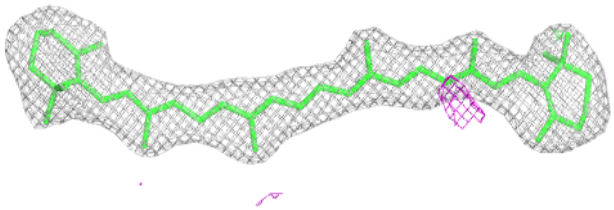


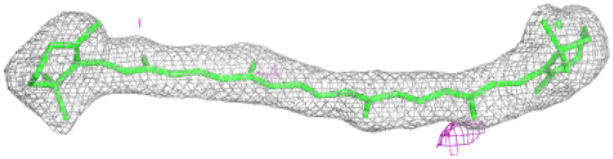


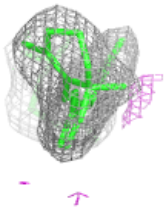


Electron density around BCR B 619:

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

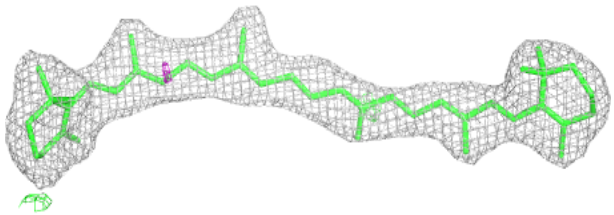


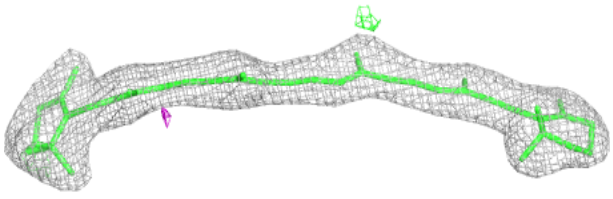


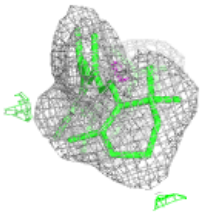


Electron density around BCR B 631:

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

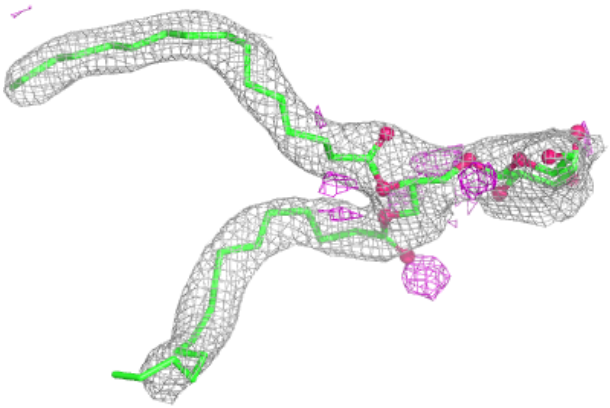


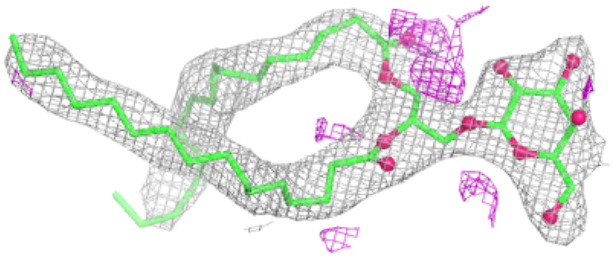


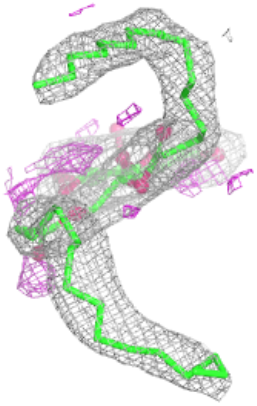


Electron density around LMG m 101:

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

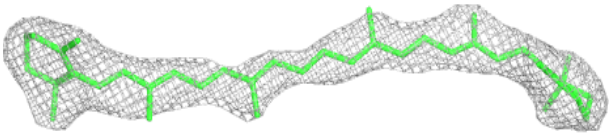


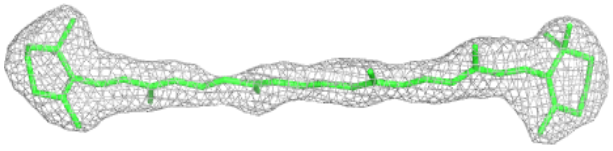


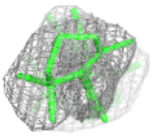


Electron density around BCR C 516:

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

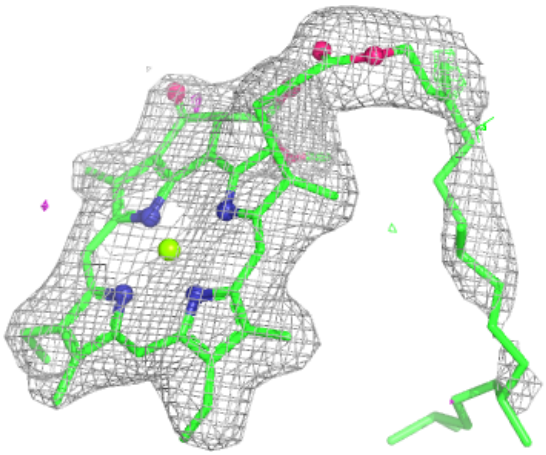


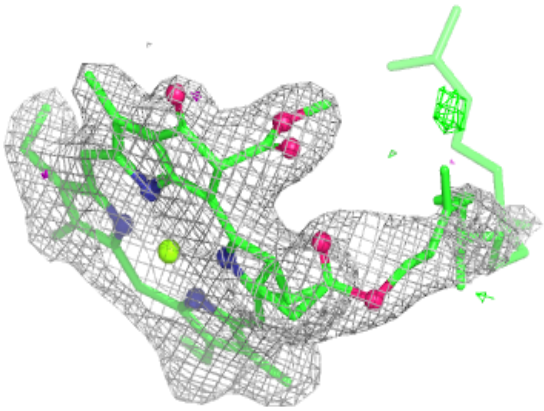


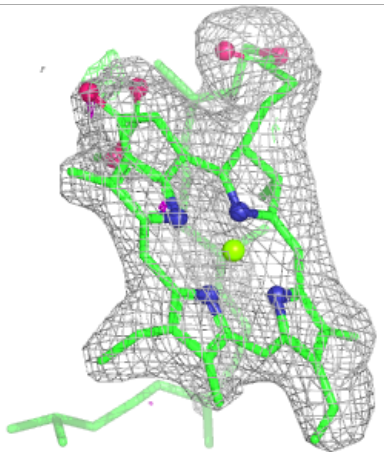


Electron density around CLA b 616:

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

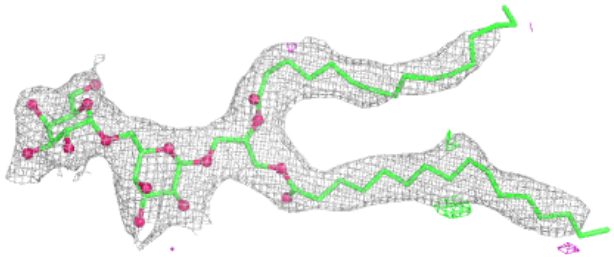


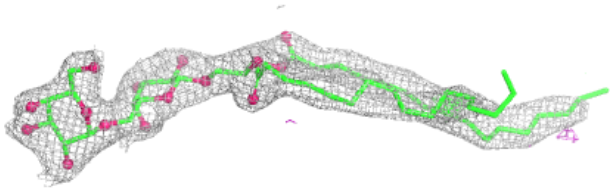


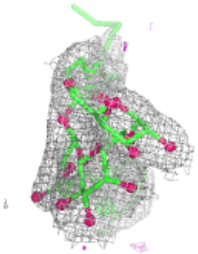


Electron density around DGD C 520:

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

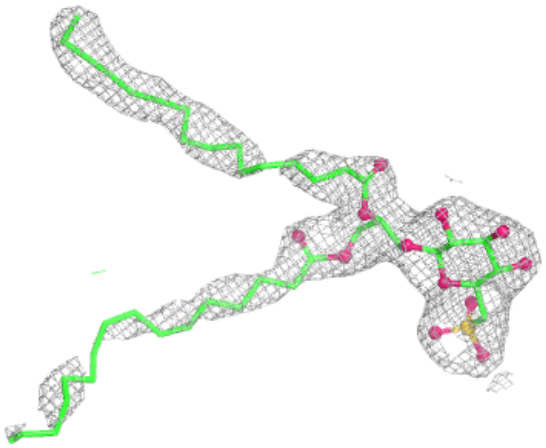


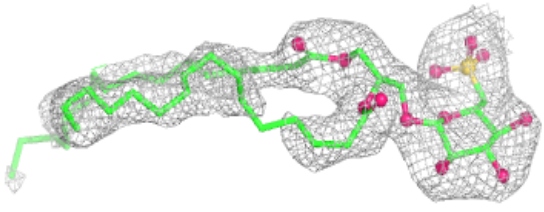


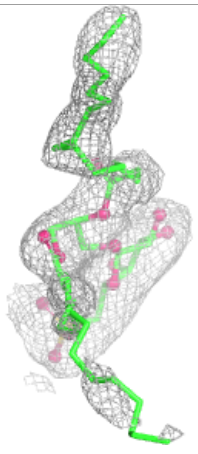


Electron density around SQD a 409:

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

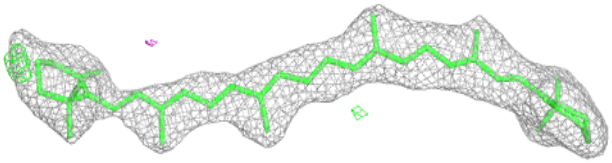


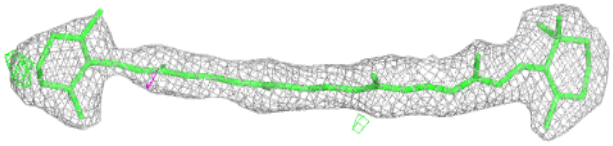


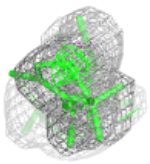


Electron density around BCR H 101:

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

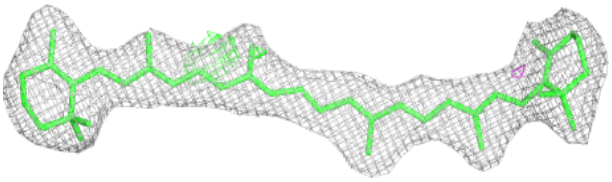


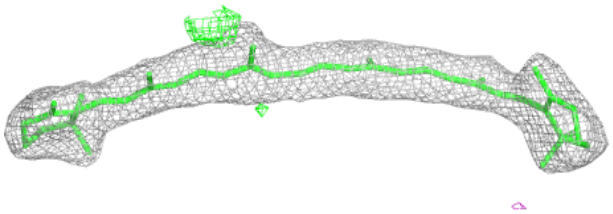


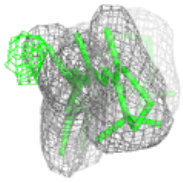


Electron density around BCR T 101:

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

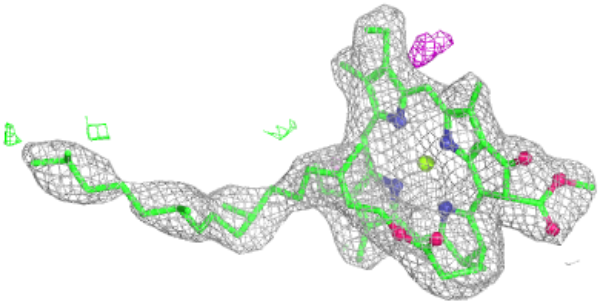


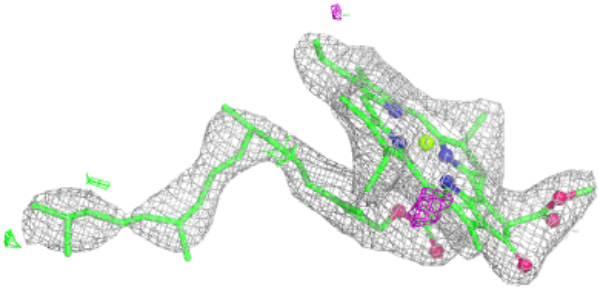


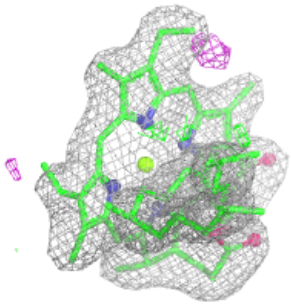


Electron density around CLA c 507:

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

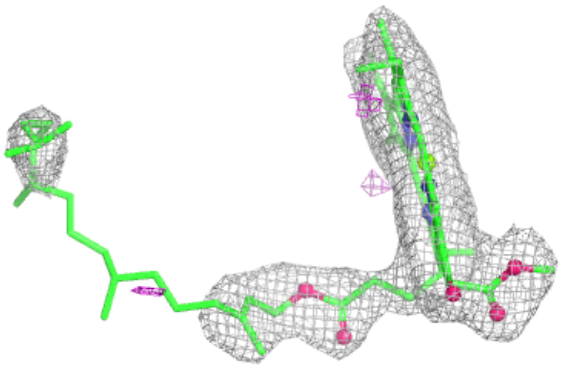


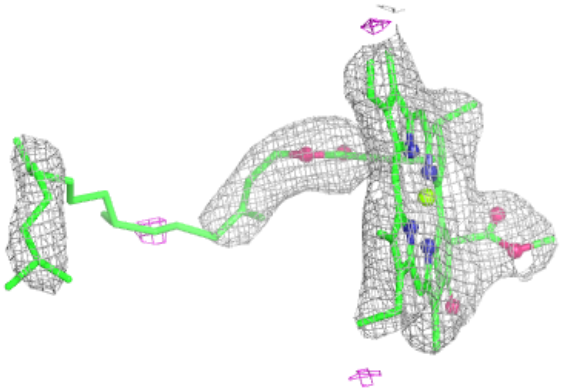


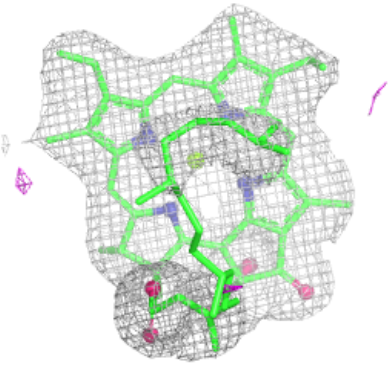


Electron density around CLA c 508:

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

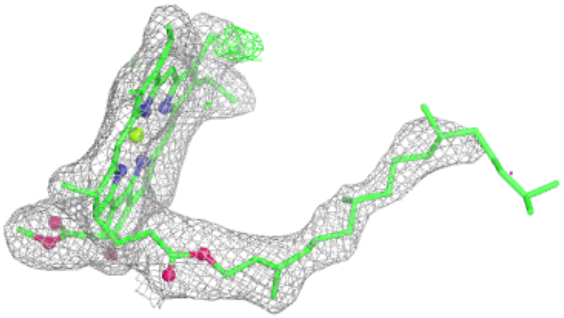


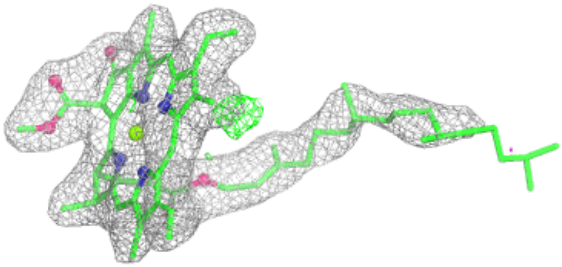


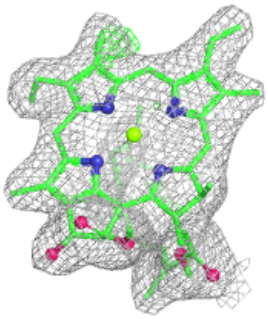


Electron density around CLA C 510:

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

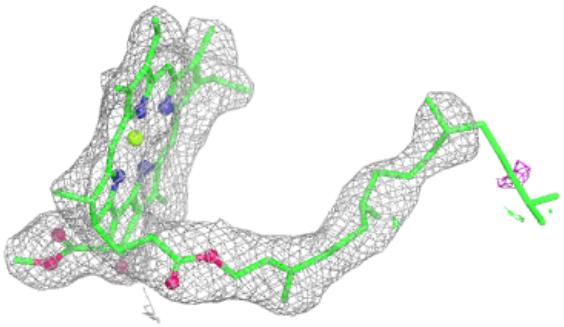


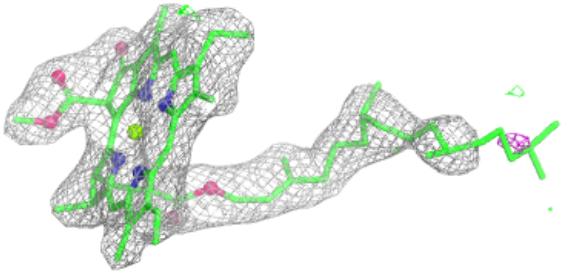


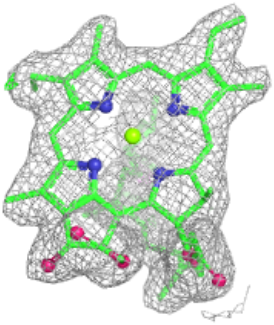


Electron density around CLA c 510:

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

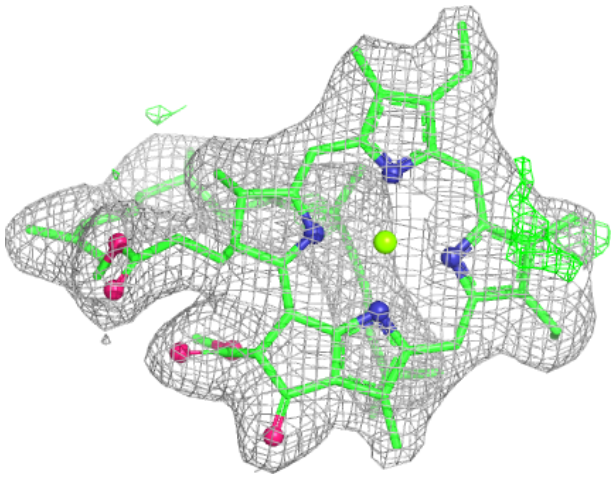


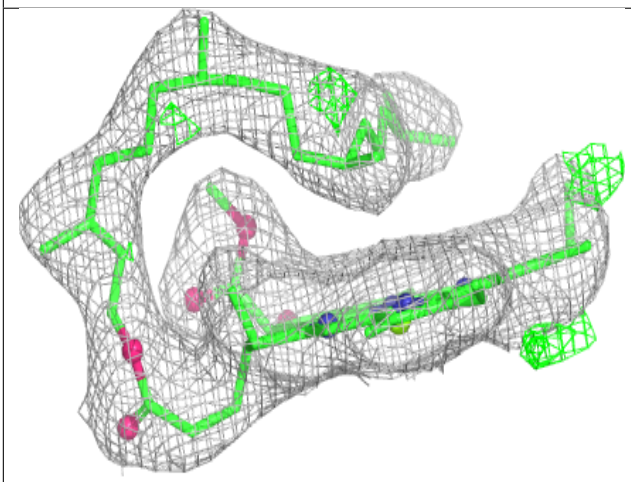


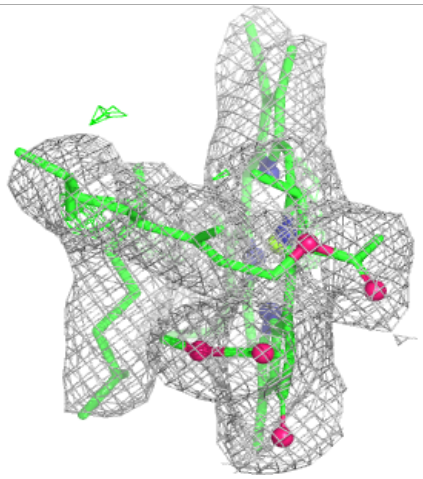


Electron density around CLA C 512:

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

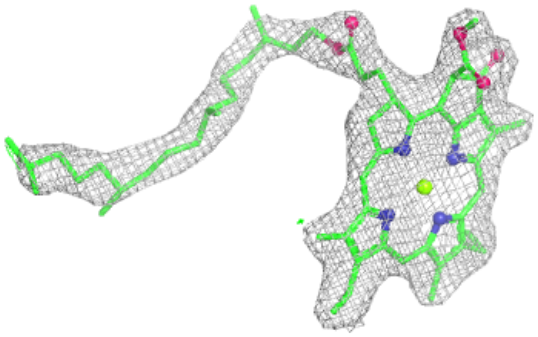


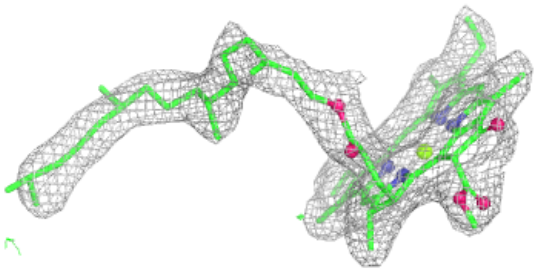


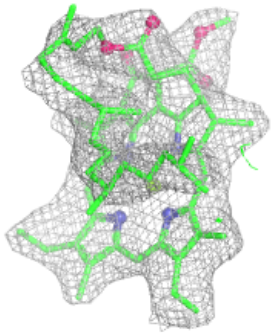


Electron density around CLA C 513:

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

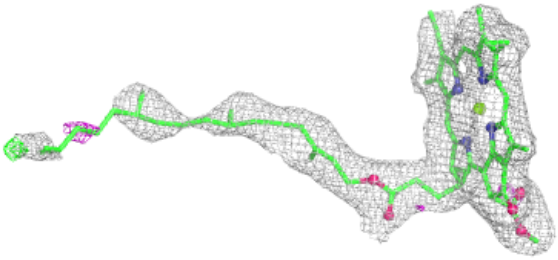


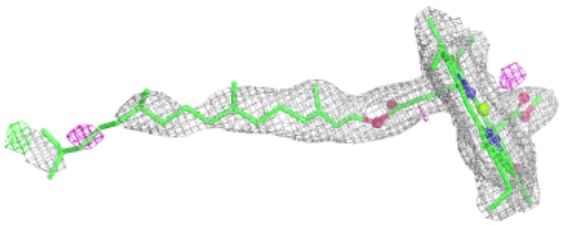


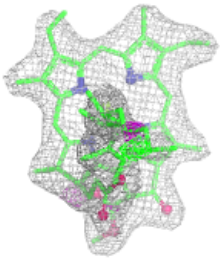


Electron density around CLA d 403:

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

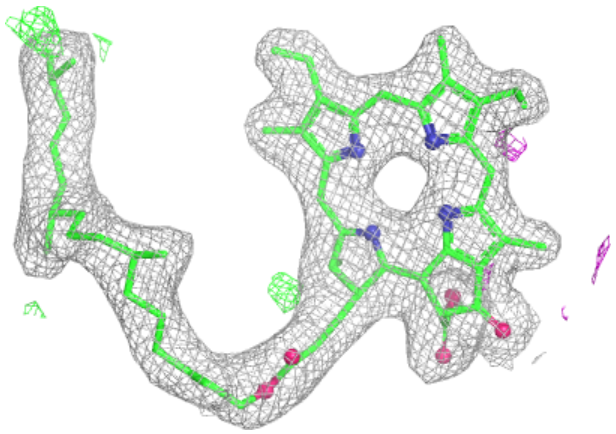


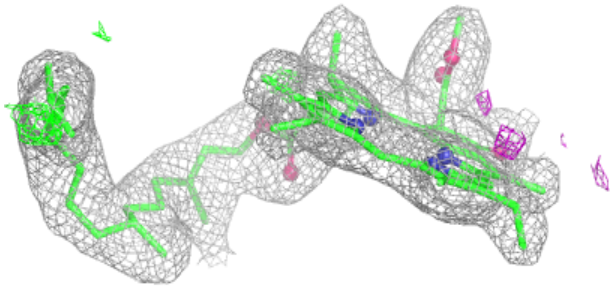


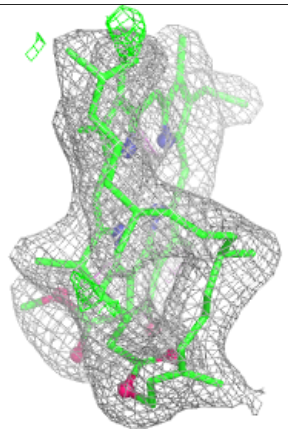


Electron density around PHO A 415:

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

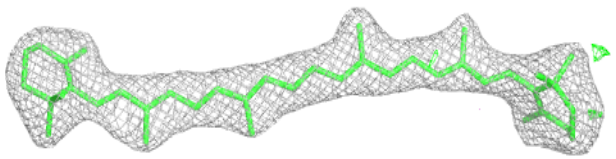


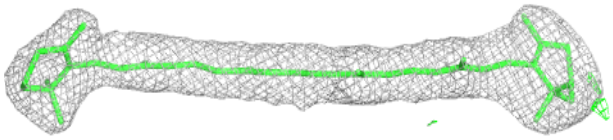


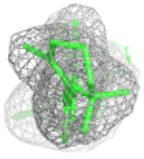


Electron density around BCR B 618:

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

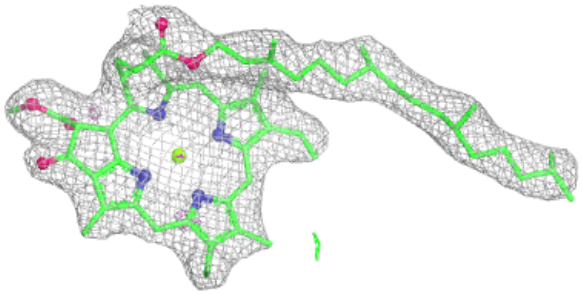


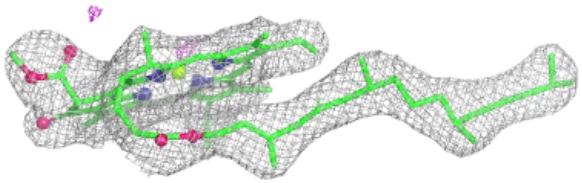


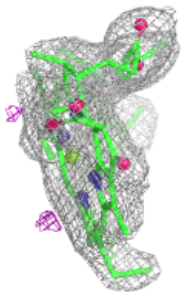


Electron density around CLA C 503:

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

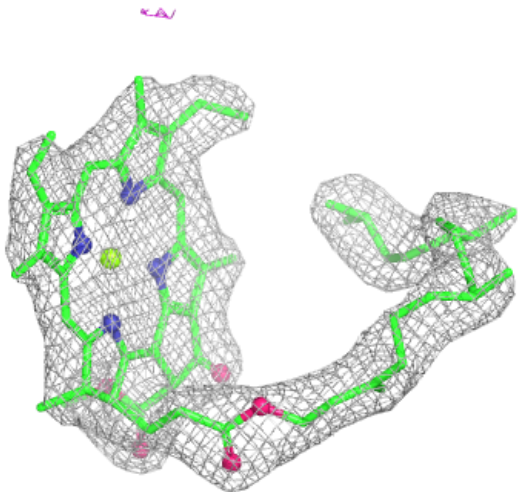


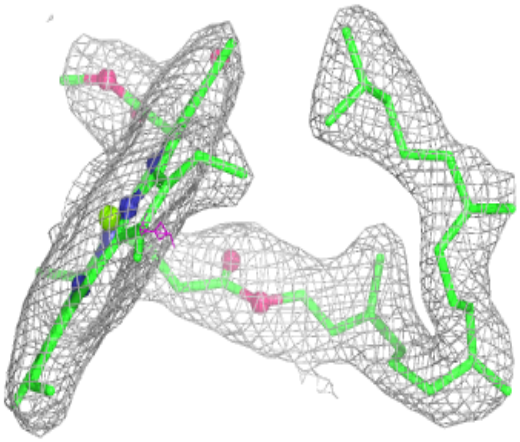


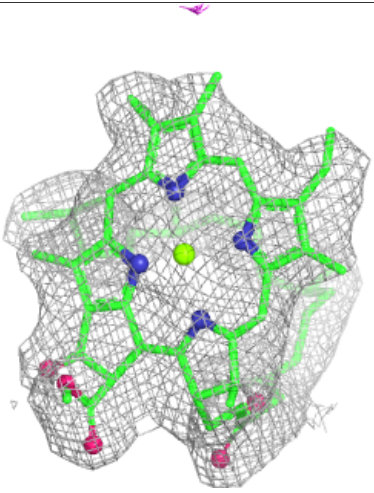


Electron density around CLA C 505:

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

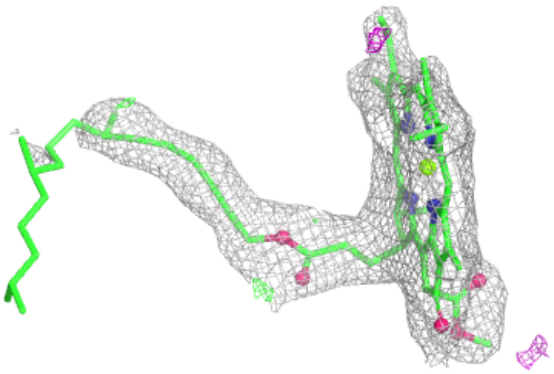


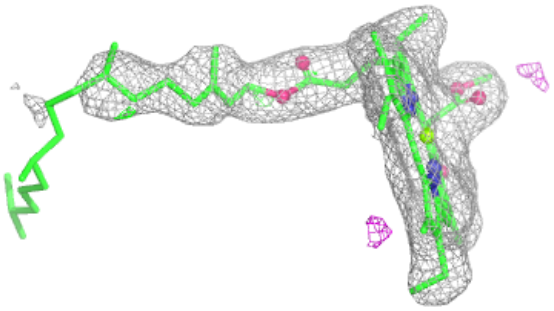


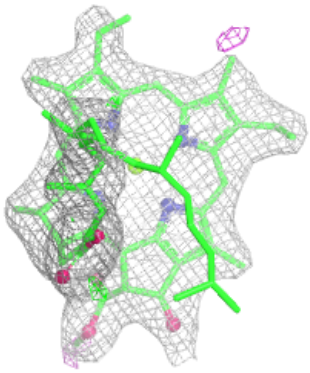


Electron density around CLA D 404:

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

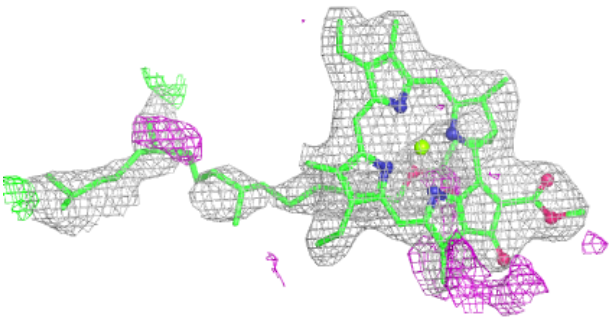


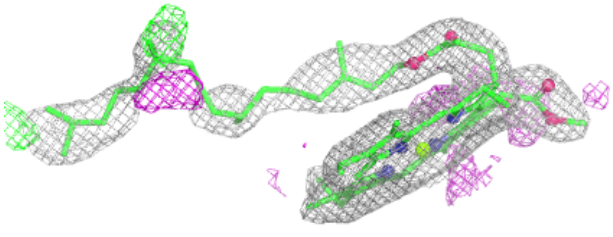


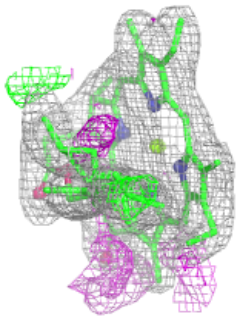


Electron density around CLA B 614:

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

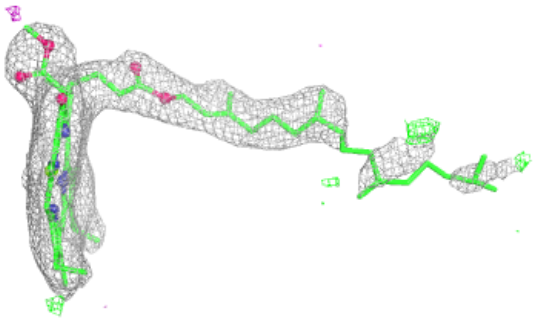


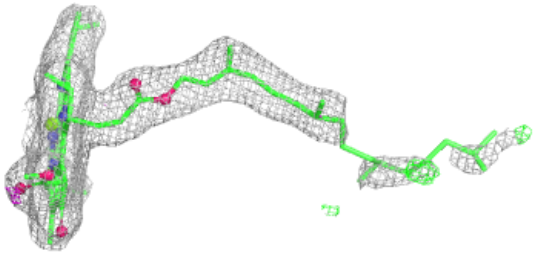


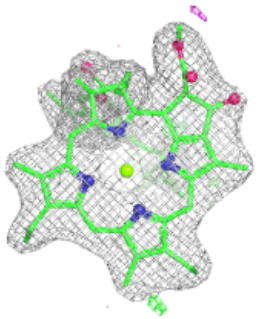


Electron density around CLA b 606:

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

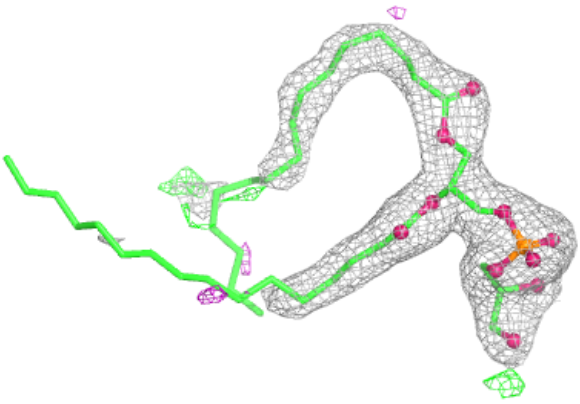


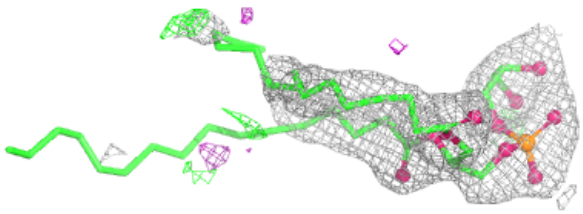




Electron density around LHG D 408:

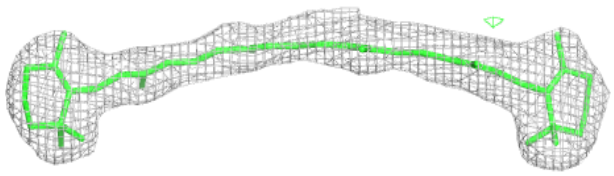
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

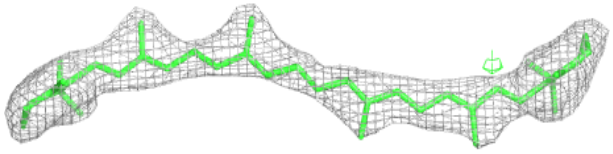


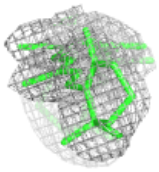


Electron density around BCR K 101:

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

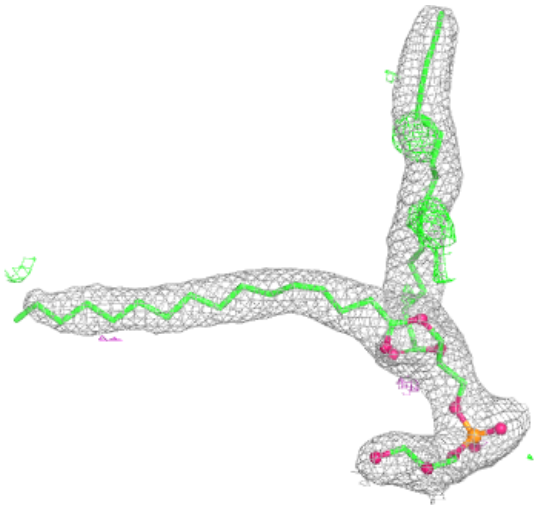


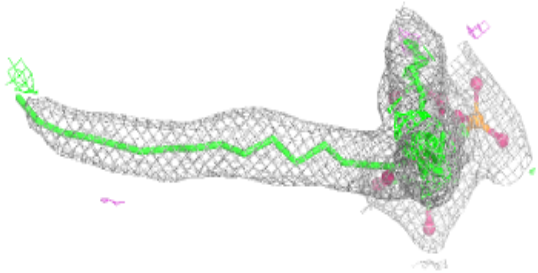


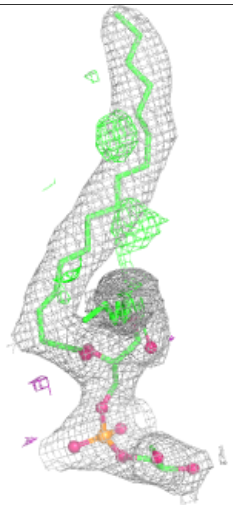


Electron density around LHG L 101:

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

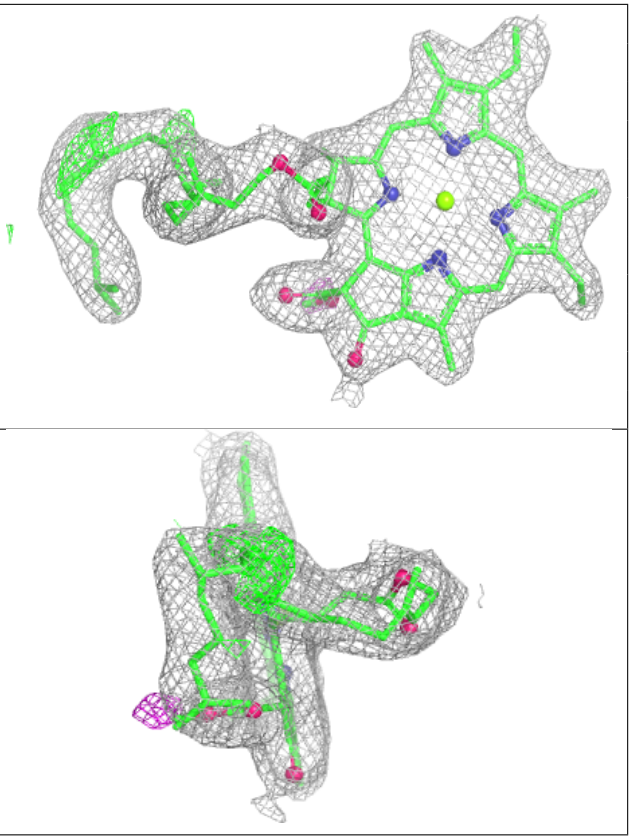






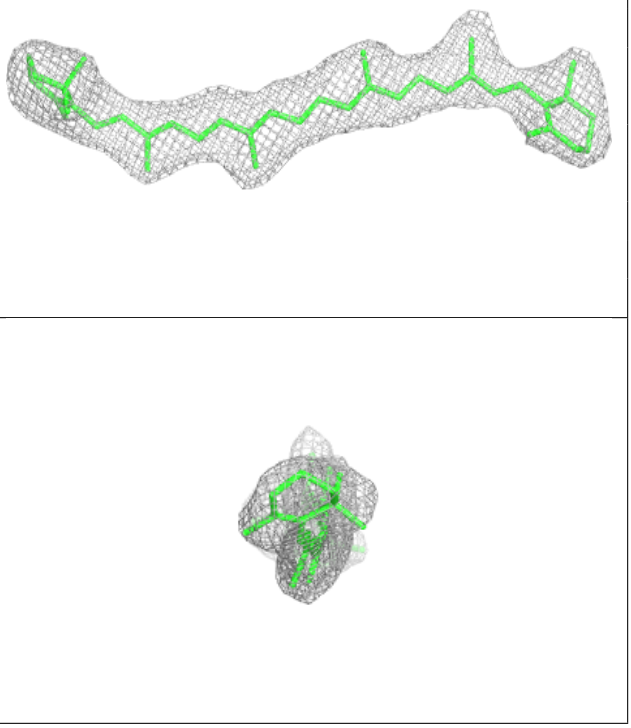
Electron density around CLA b 612:

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



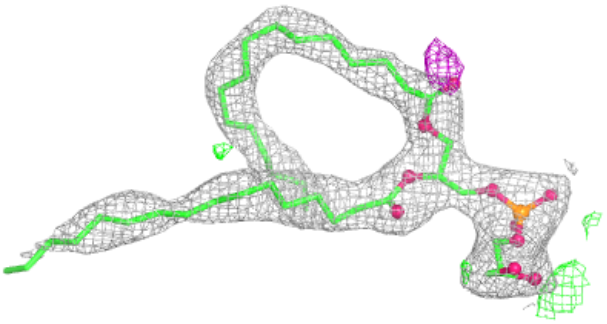
Electron density around BCR Y 101:

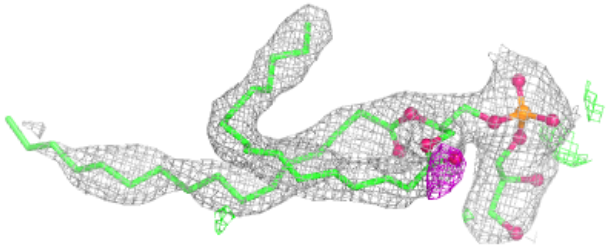
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

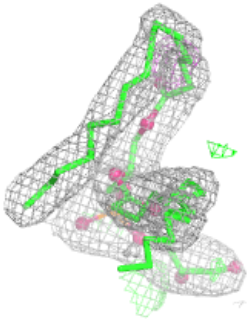


Electron density around LHG d 406:

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

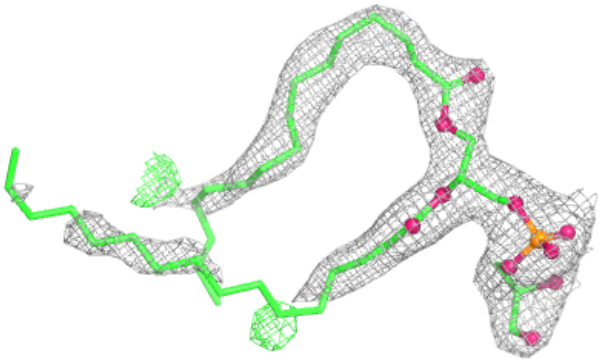


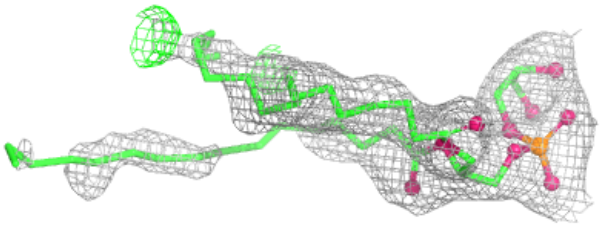


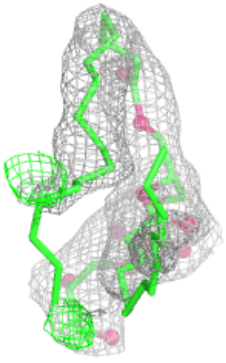


Electron density around LHG d 408:

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

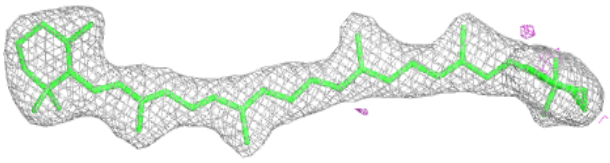


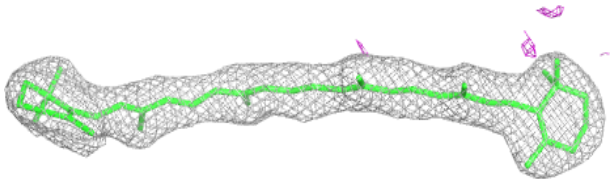


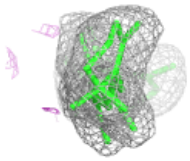


Electron density around BCR b 617:

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

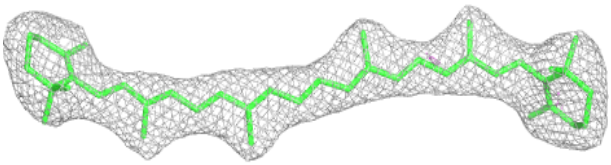


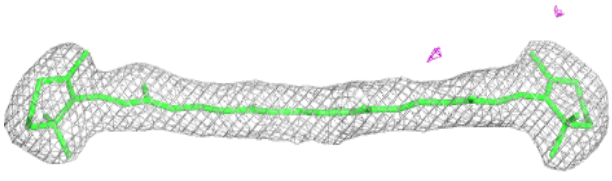


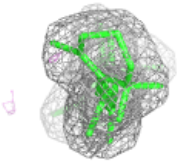


Electron density around BCR b 618:

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

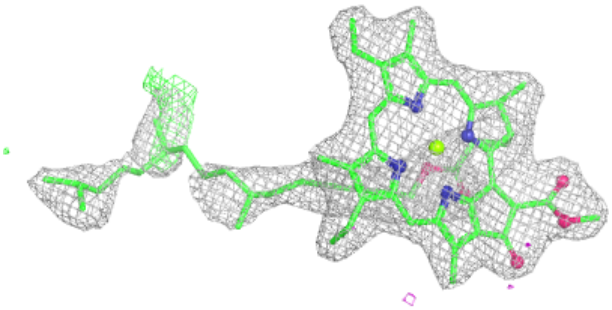


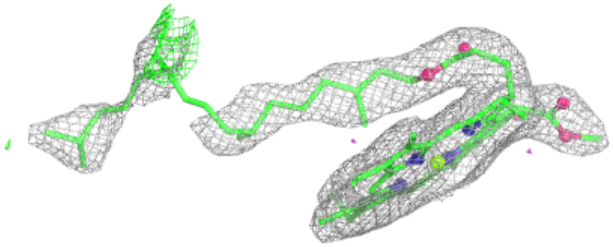


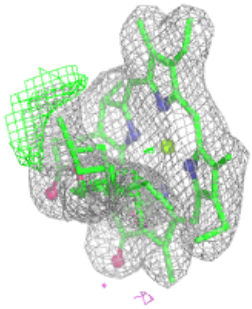


Electron density around CLA b 614:

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

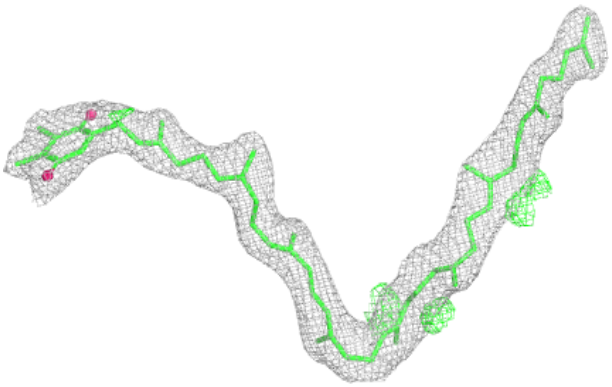


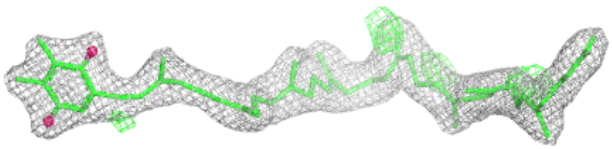


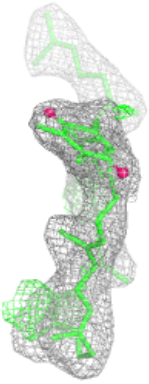


Electron density around PL9 D 406:

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

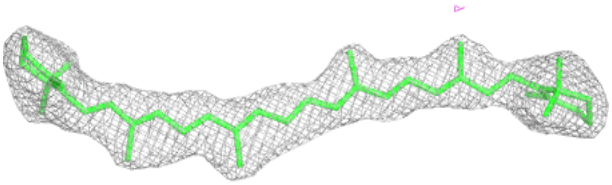


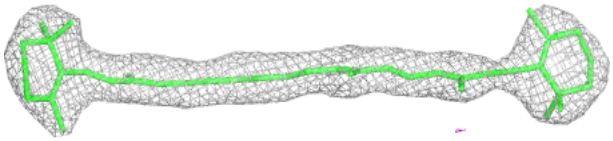


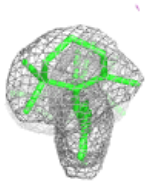


Electron density around BCR c 517:

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

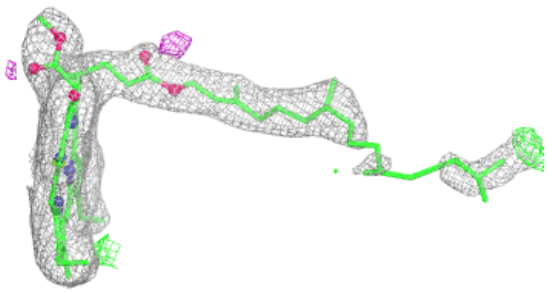


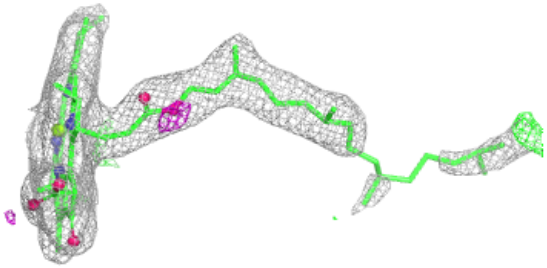


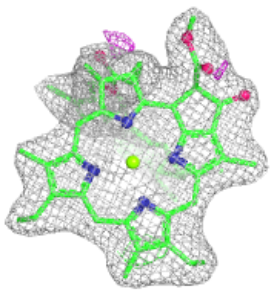


Electron density around CLA B 606:

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

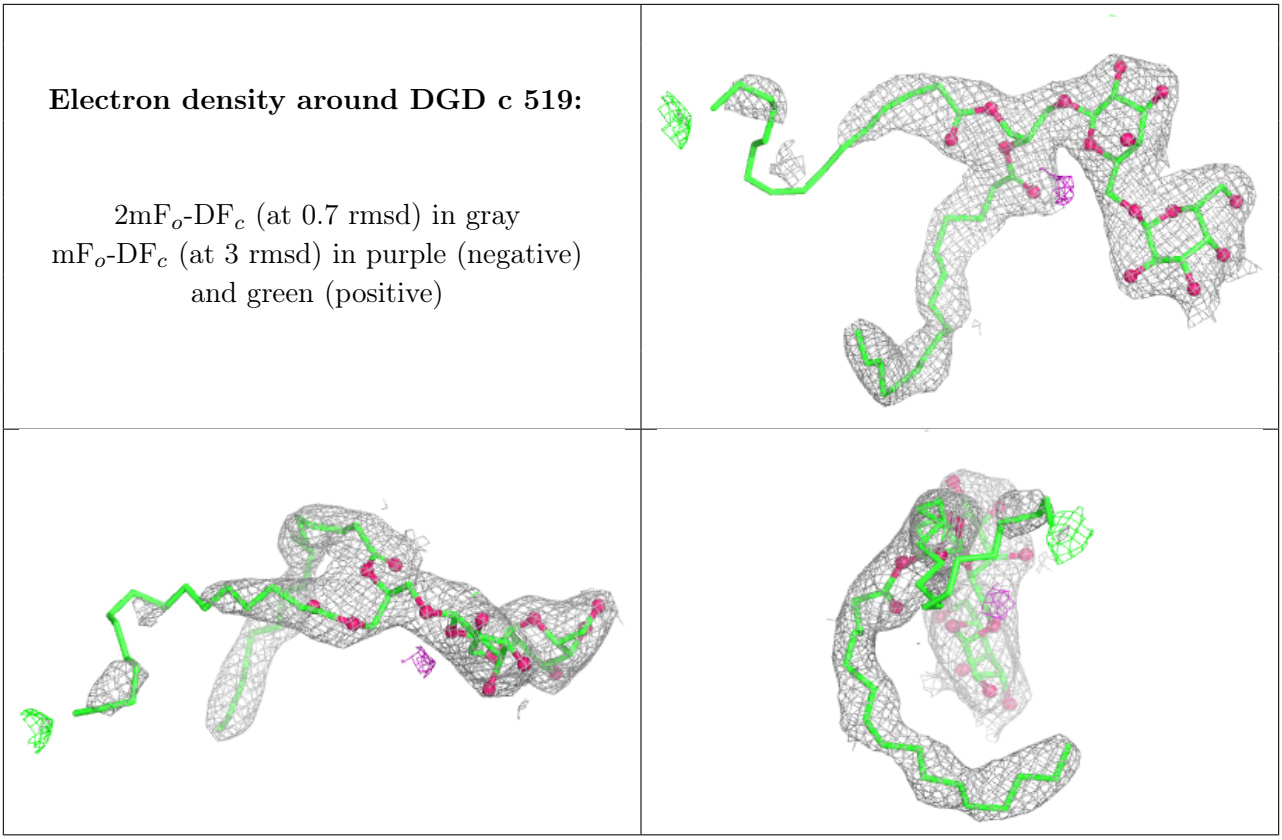






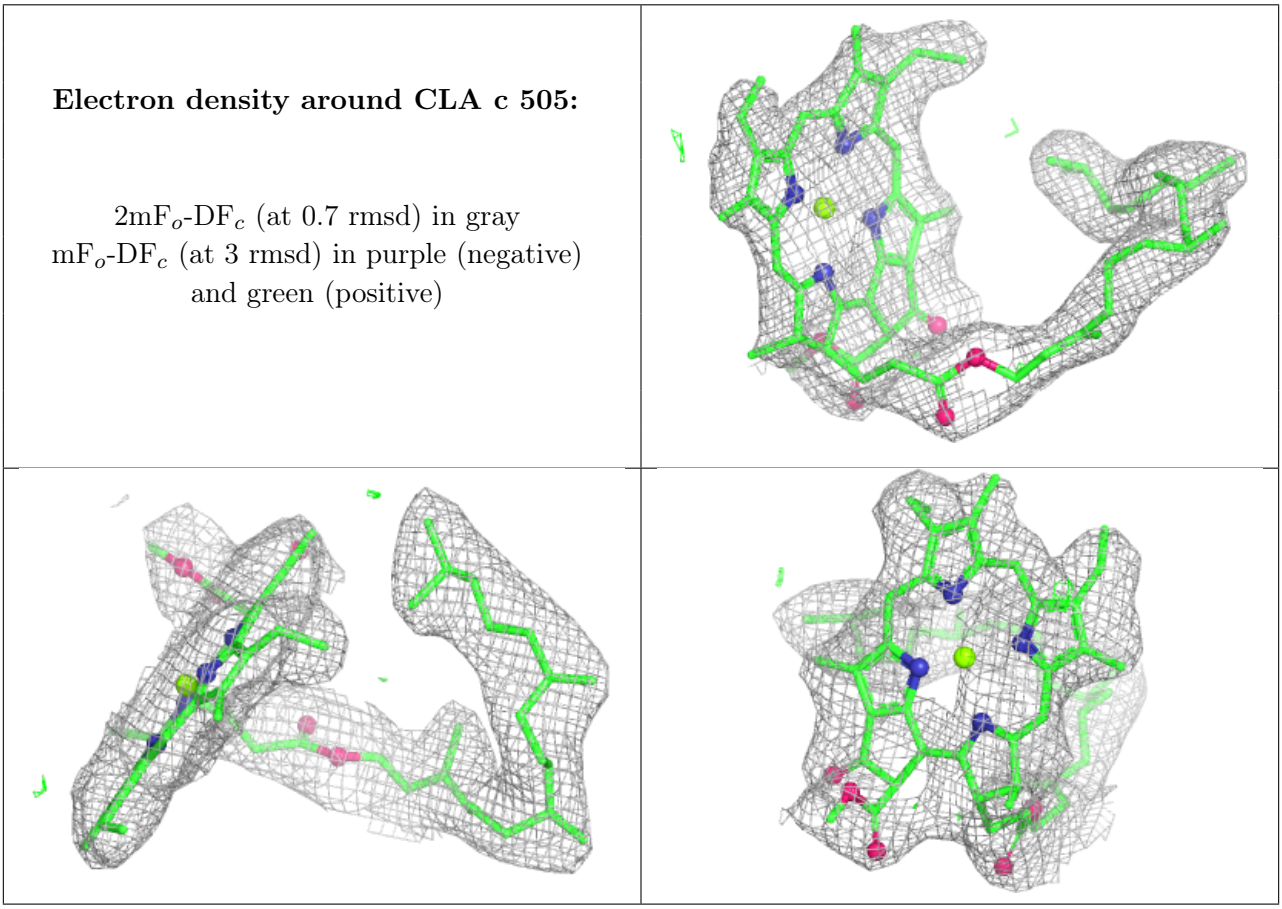
Electron density around DGD c 519:

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



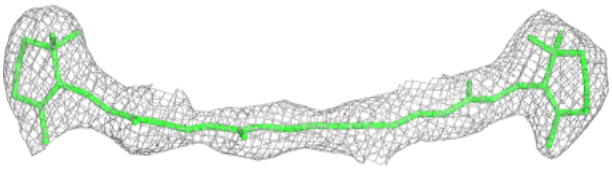
Electron density around CLA c 505:

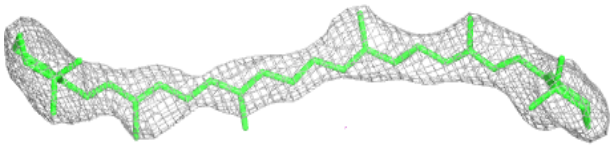
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

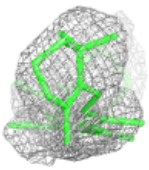


Electron density around BCR k 101:

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

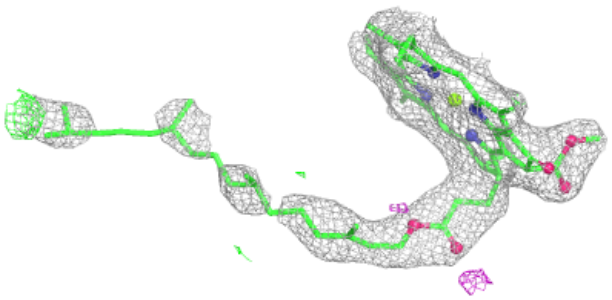


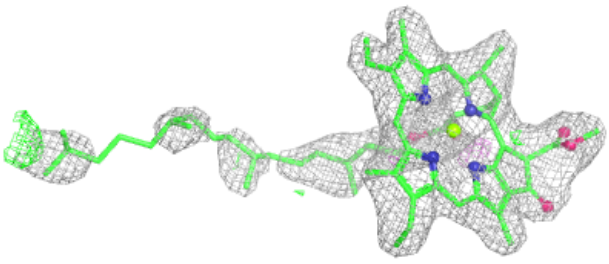


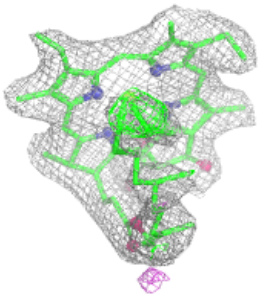


Electron density around CLA c 506:

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

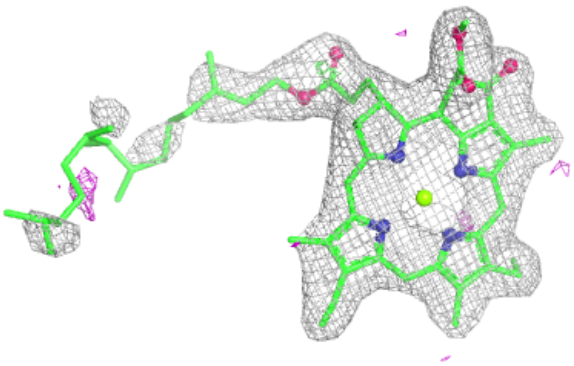


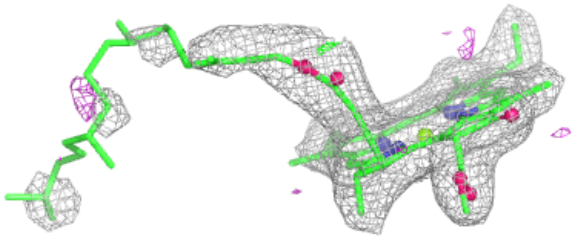


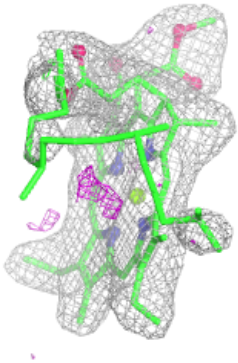


Electron density around CLA a 407:

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

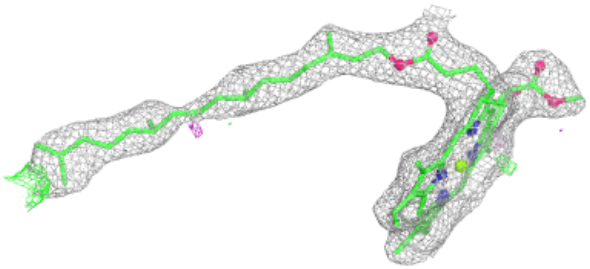


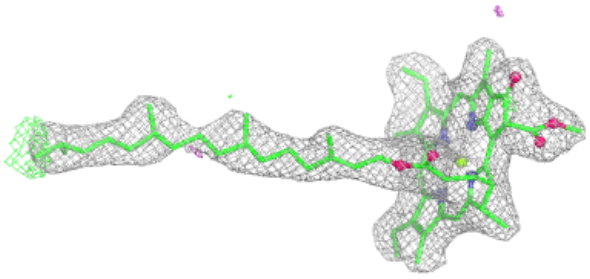


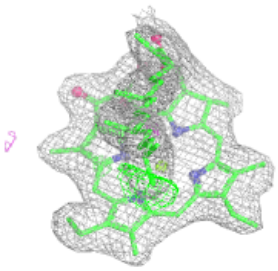


Electron density around CLA B 607:

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

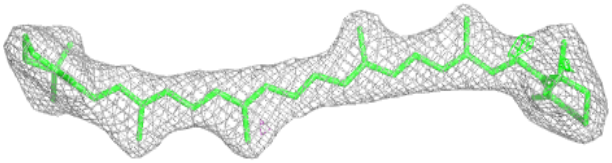


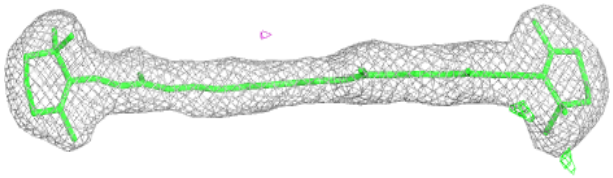


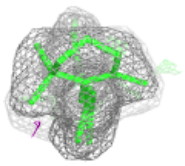


Electron density around BCR A 408:

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

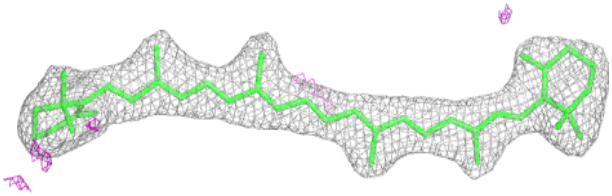


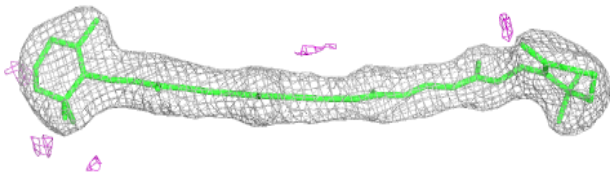


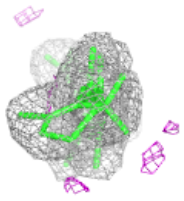


Electron density around BCR B 617:

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

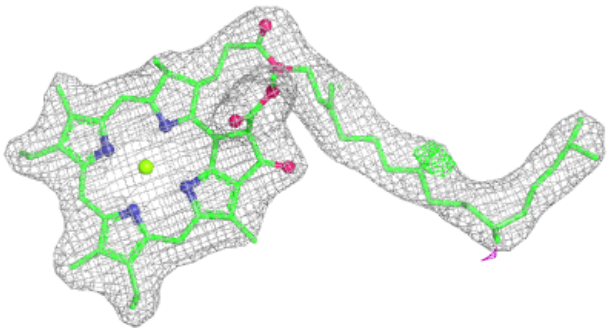


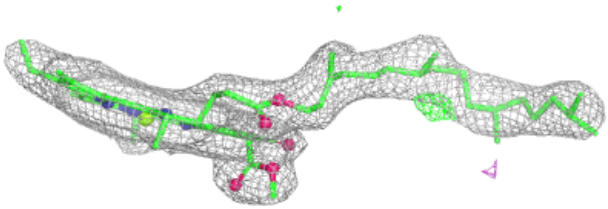




Electron density around CLA b 602:

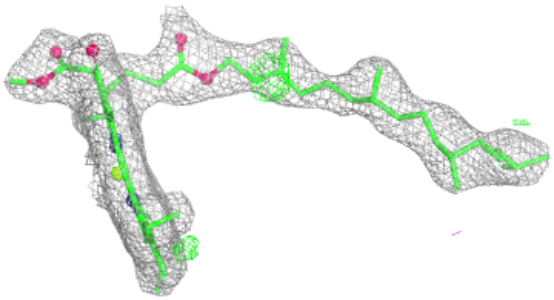
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

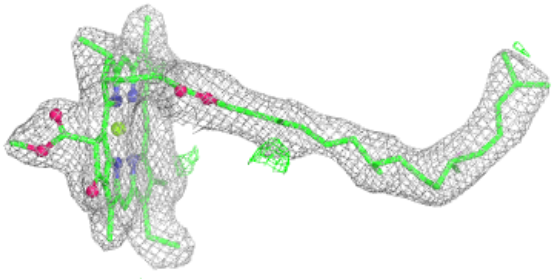


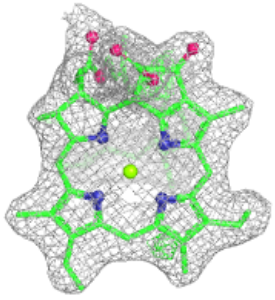


Electron density around CLA b 605:

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

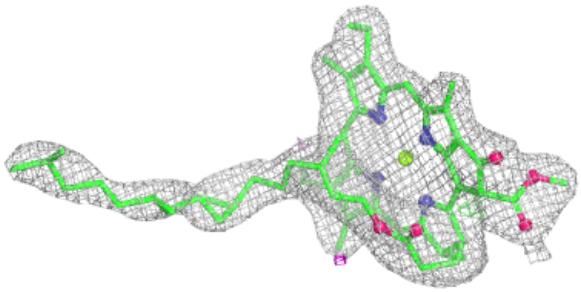


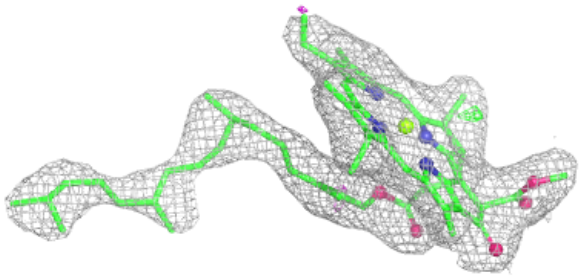


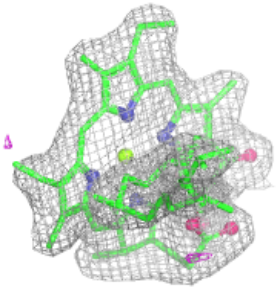


Electron density around CLA C 507:

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

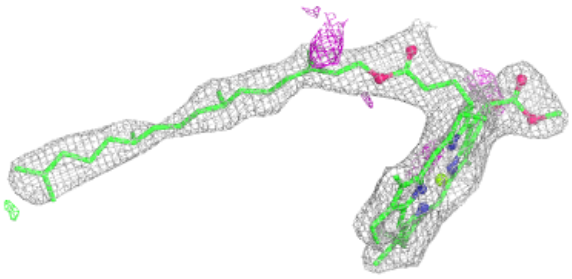


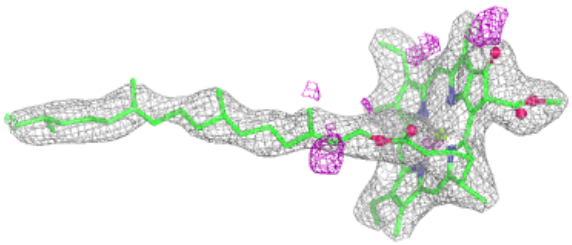


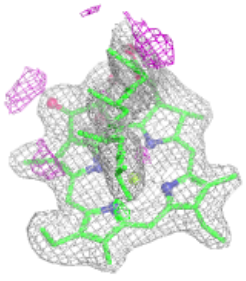


Electron density around CLA b 607:

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

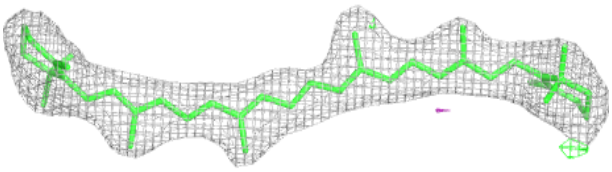


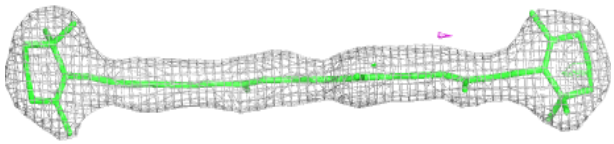


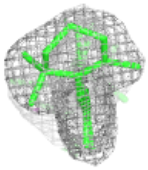


Electron density around BCR C 517:

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

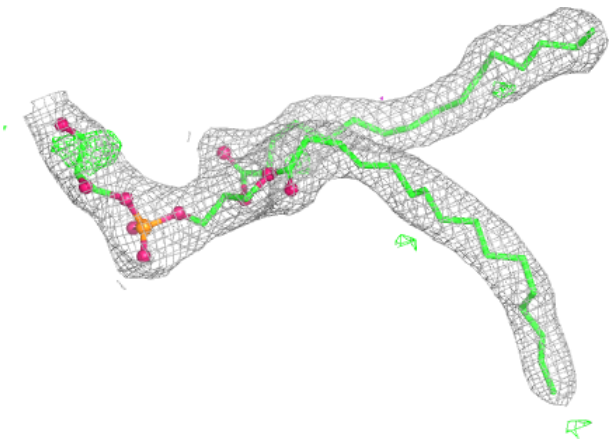


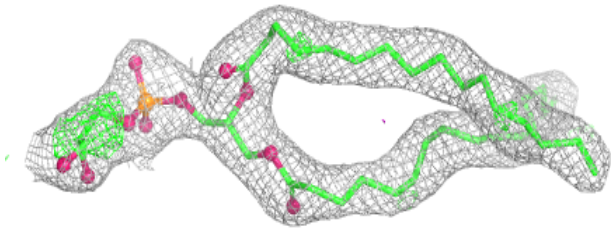


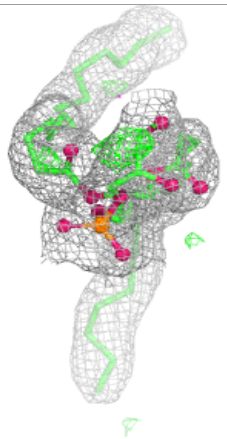


Electron density around LHG D 407:

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

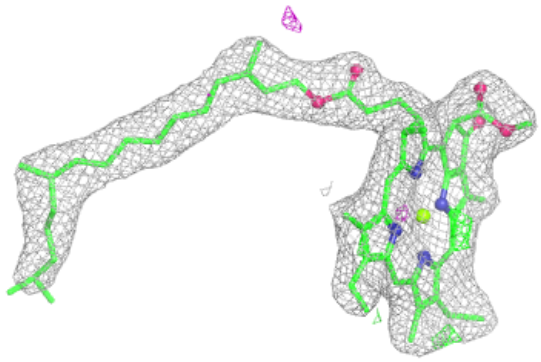


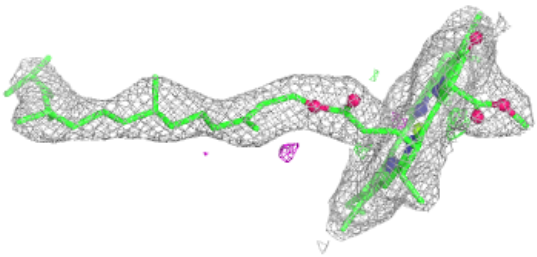


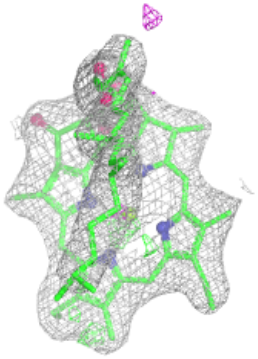


Electron density around CLA b 609:

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

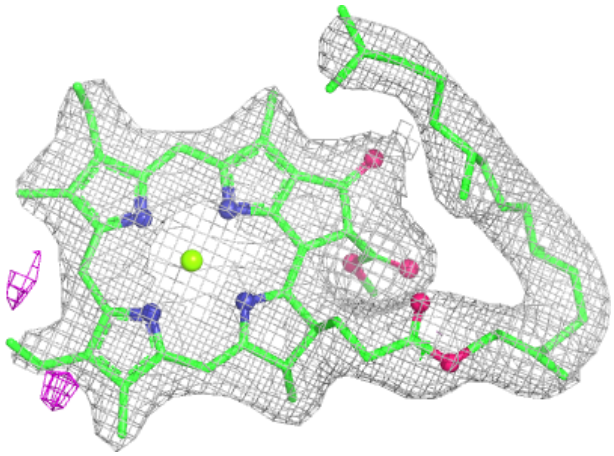


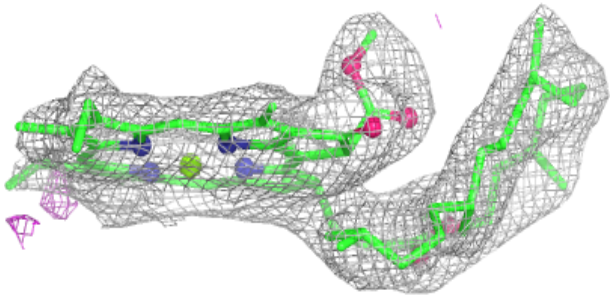


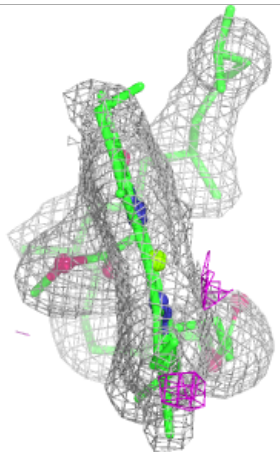


Electron density around CLA b 610:

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

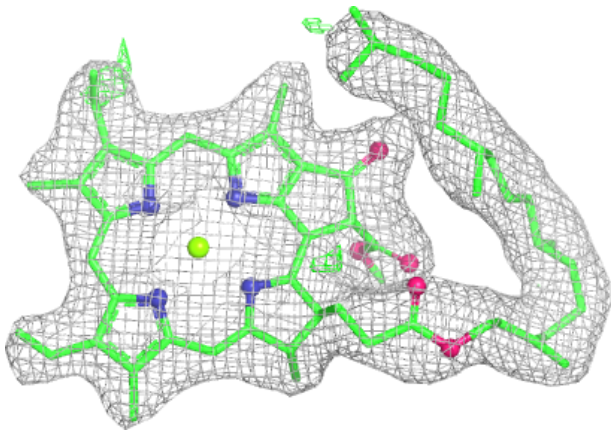


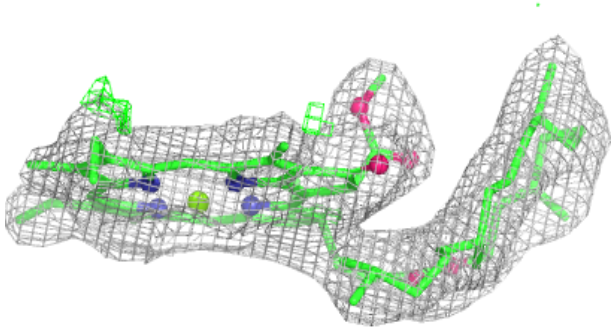


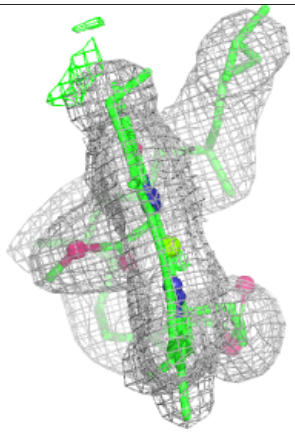


Electron density around CLA B 610:

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

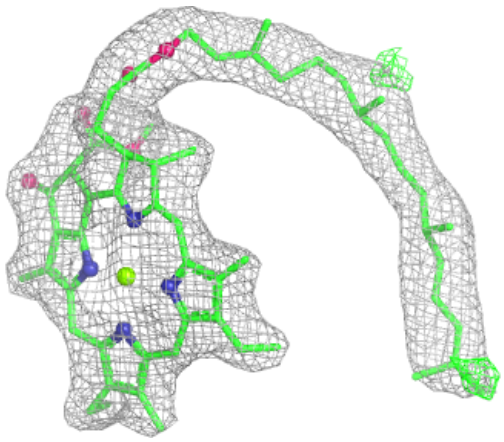


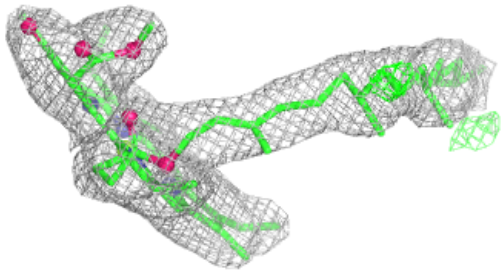


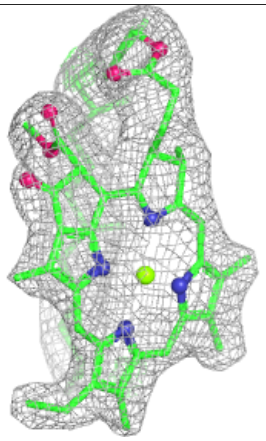


Electron density around CLA C 509:

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

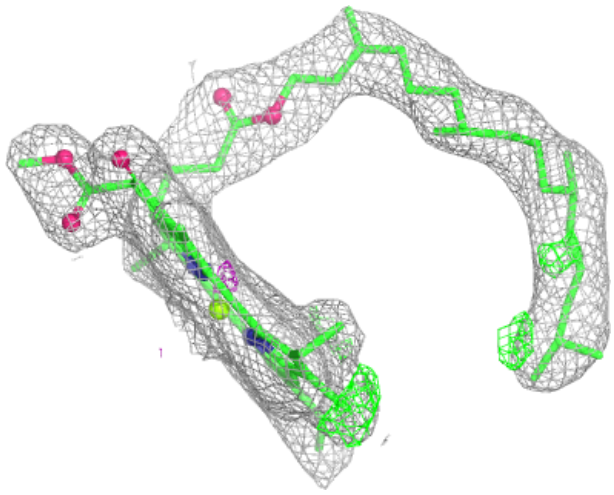


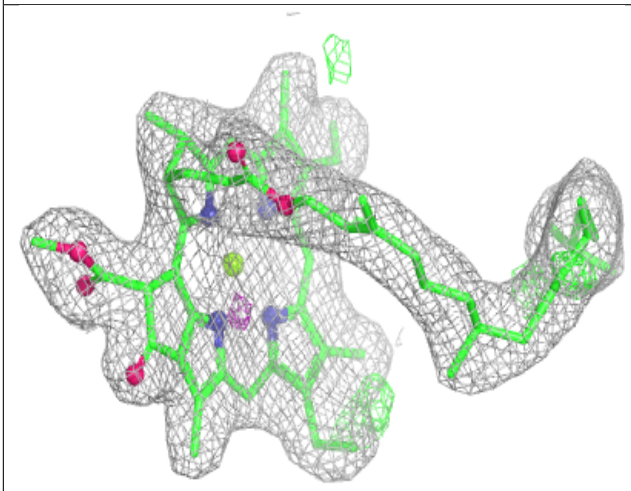


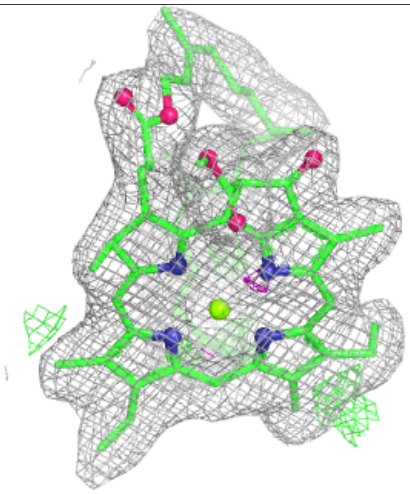


Electron density around CLA B 611:

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

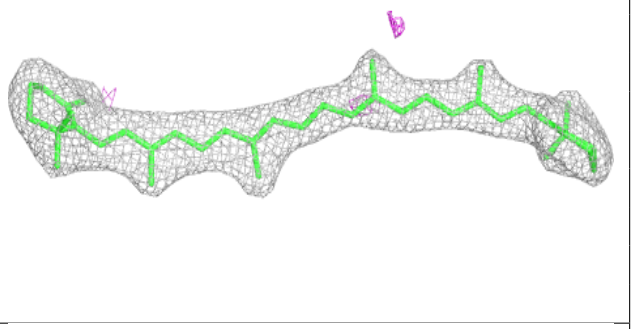


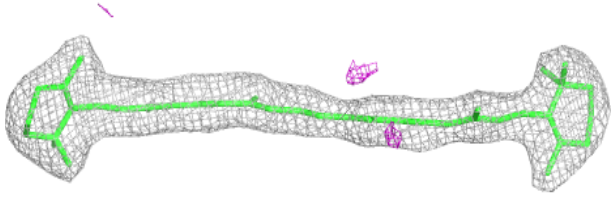


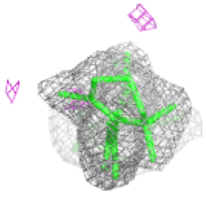


Electron density around BCR a 408:

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

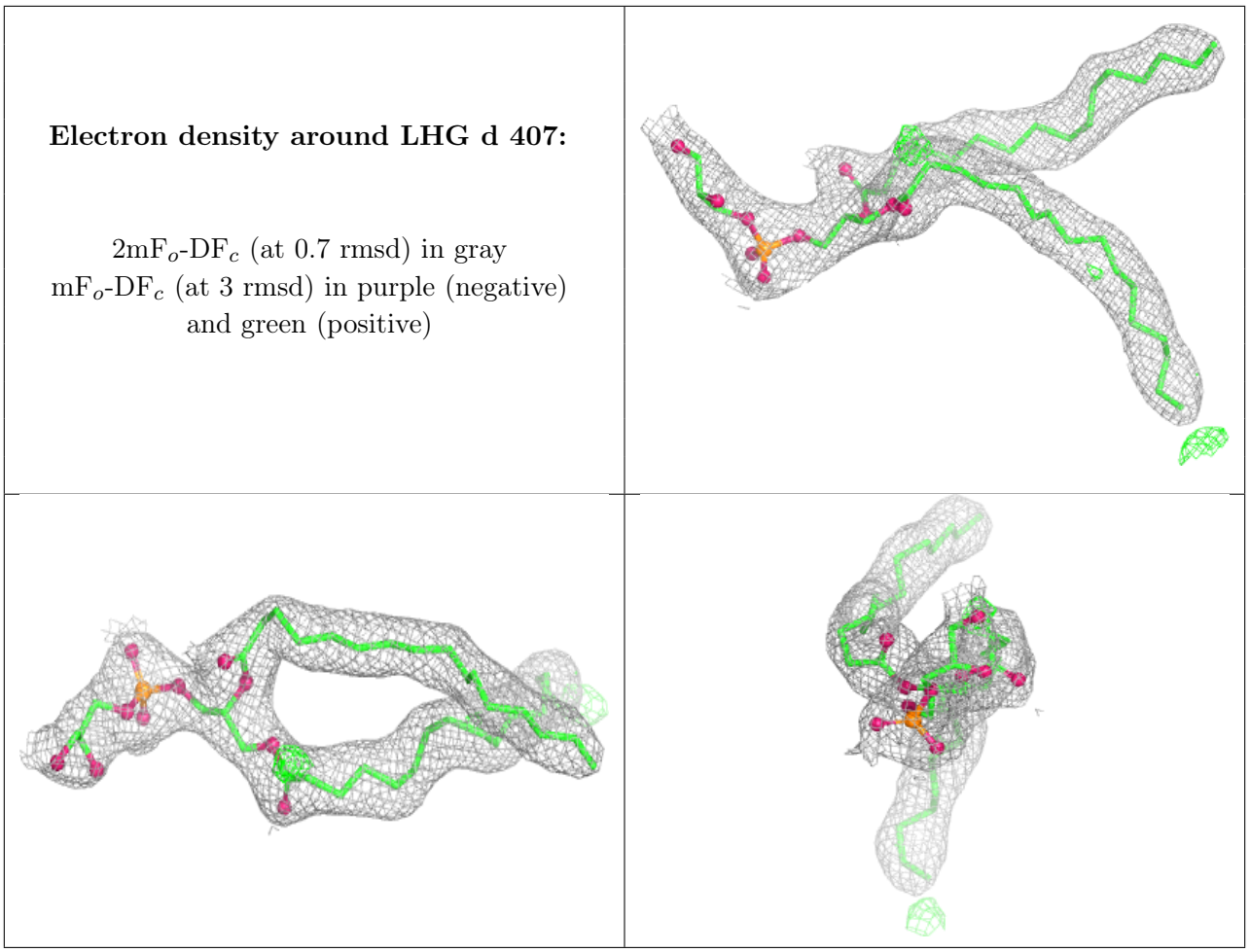






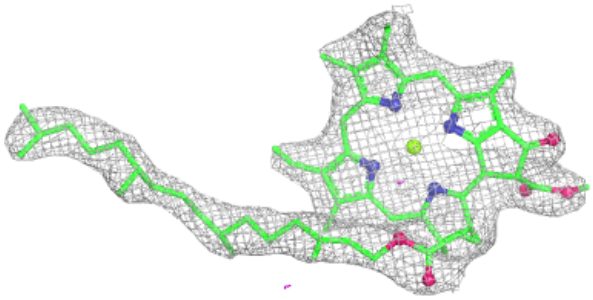
Electron density around LHG d 407:

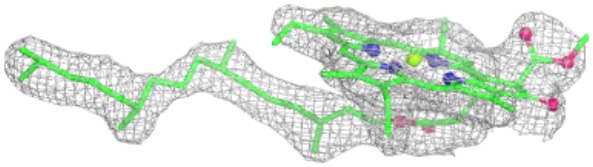
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

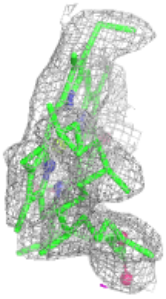


Electron density around CLA c 503:

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

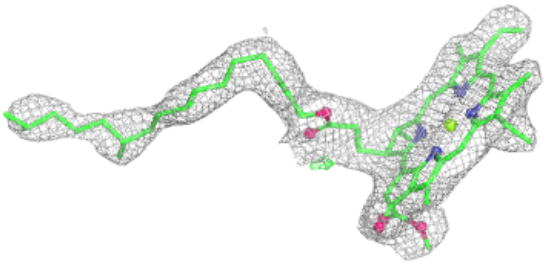


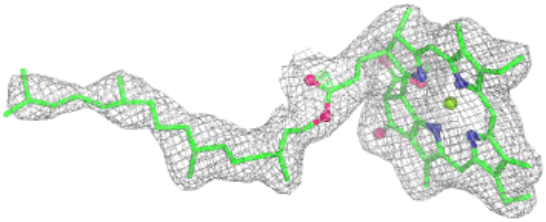


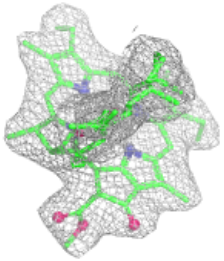


Electron density around CLA c 504:

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

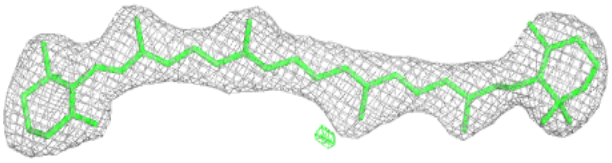


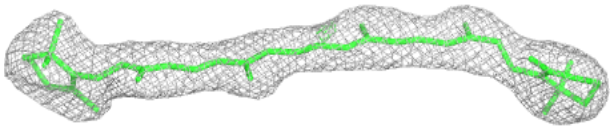


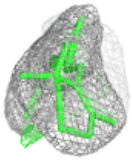


Electron density around BCR b 619:

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

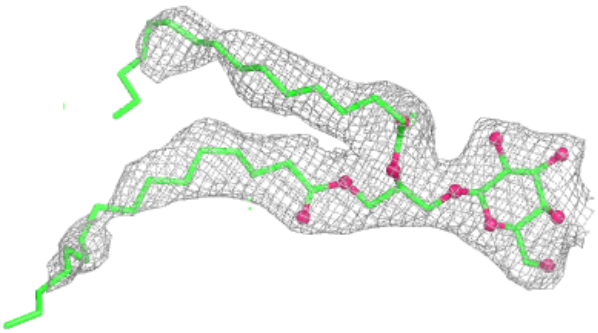


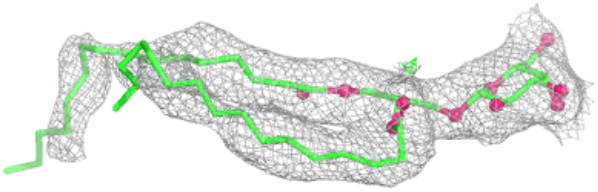


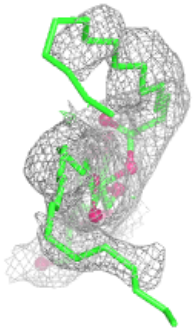


Electron density around LMG d 411:

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

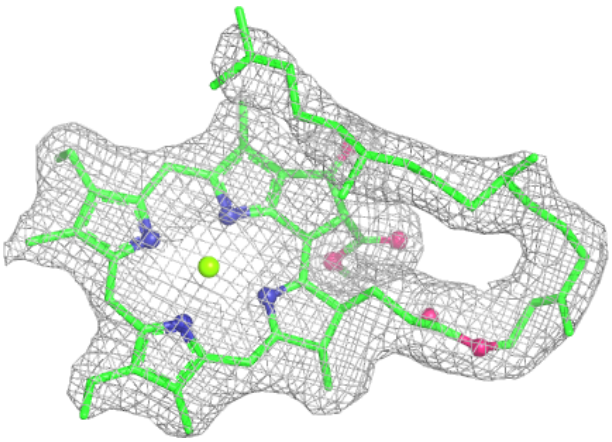


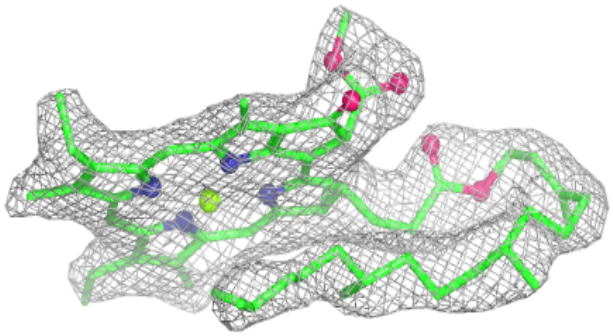


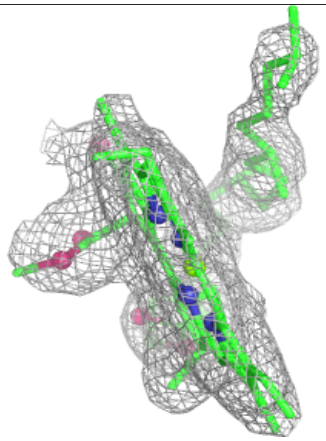


Electron density around CLA C 511:

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

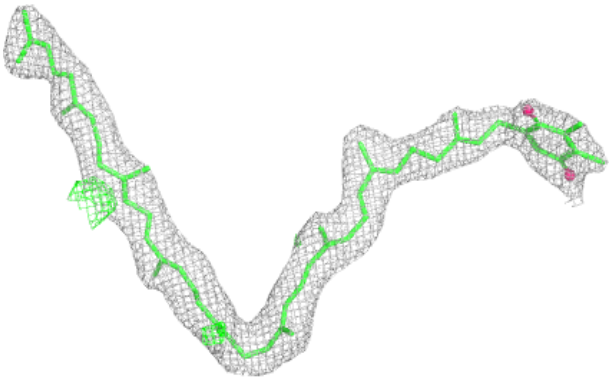


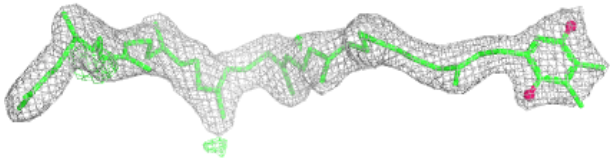


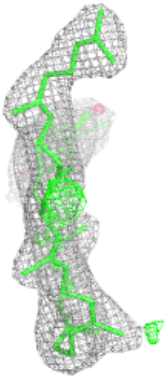


Electron density around PL9 d 405:

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

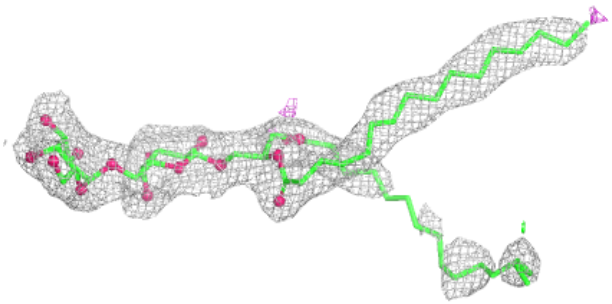


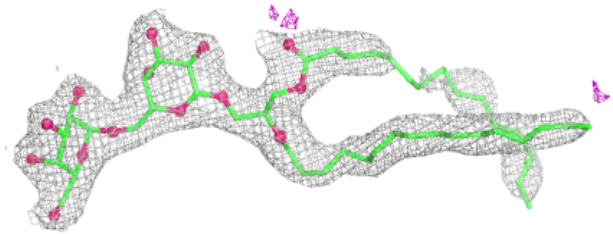


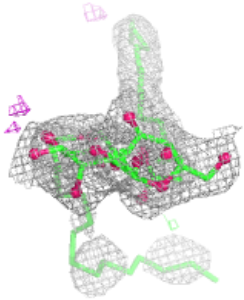


Electron density around DGD C 518:

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

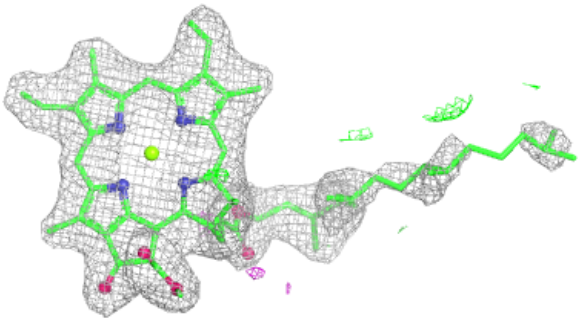


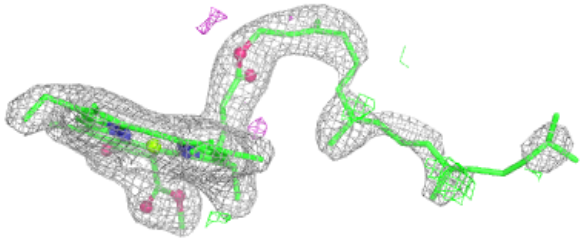




Electron density around CLA A 405:

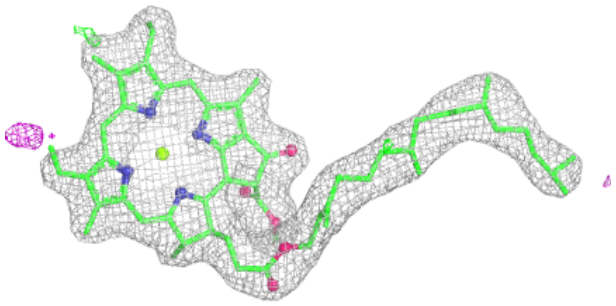
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

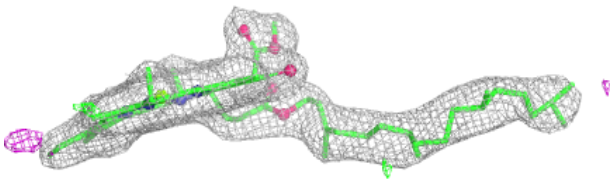


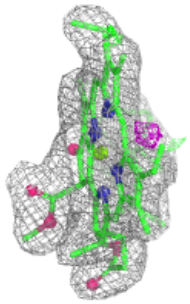


Electron density around CLA B 602:

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

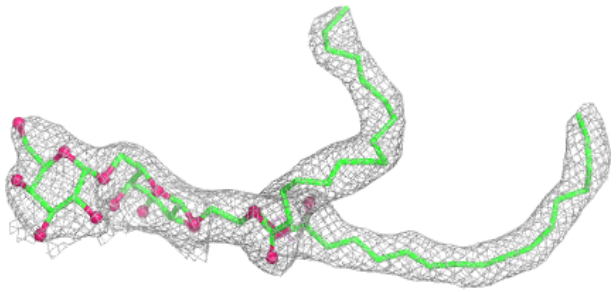


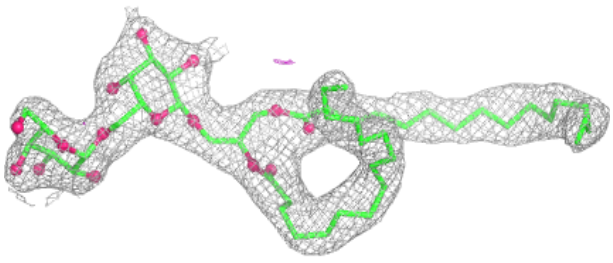


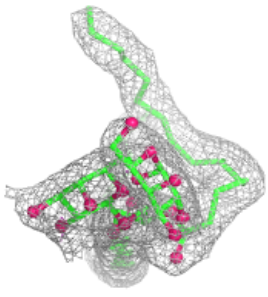


Electron density around DGD H 102:

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

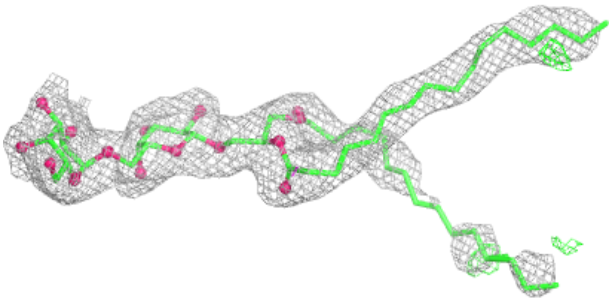


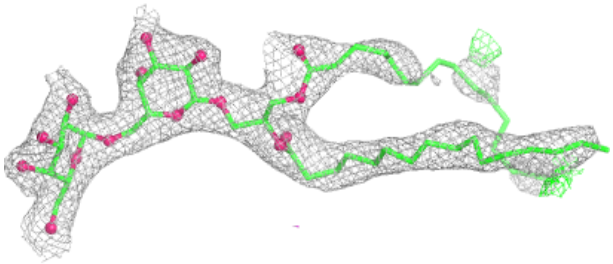


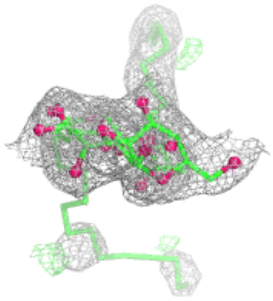


Electron density around DGD c 518:

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

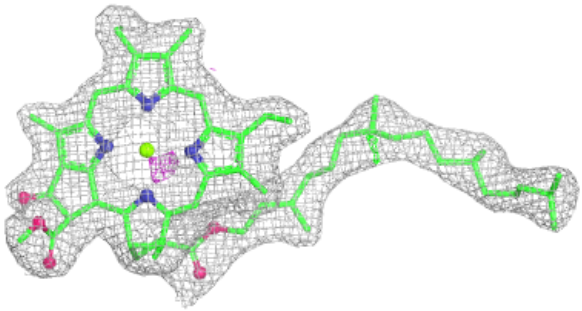


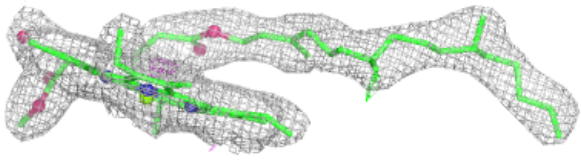


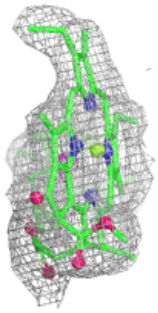


Electron density around CLA B 603:

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

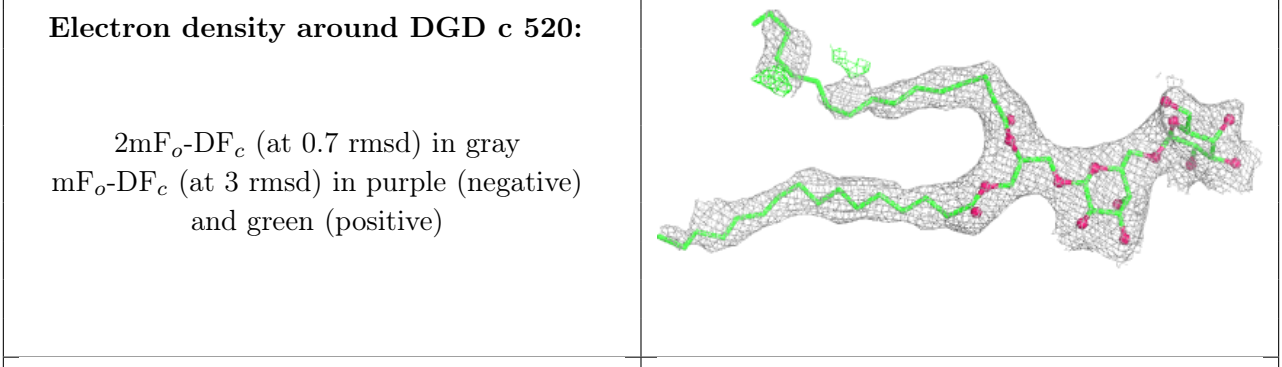


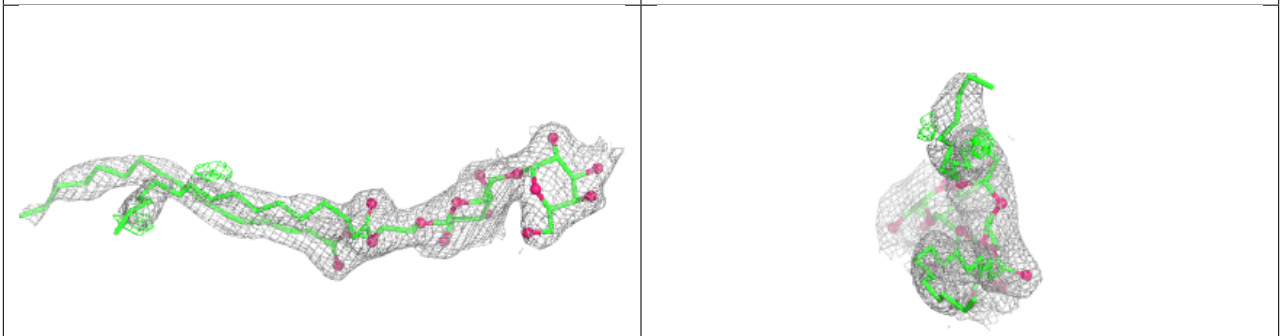




Electron density around DGD c 520:

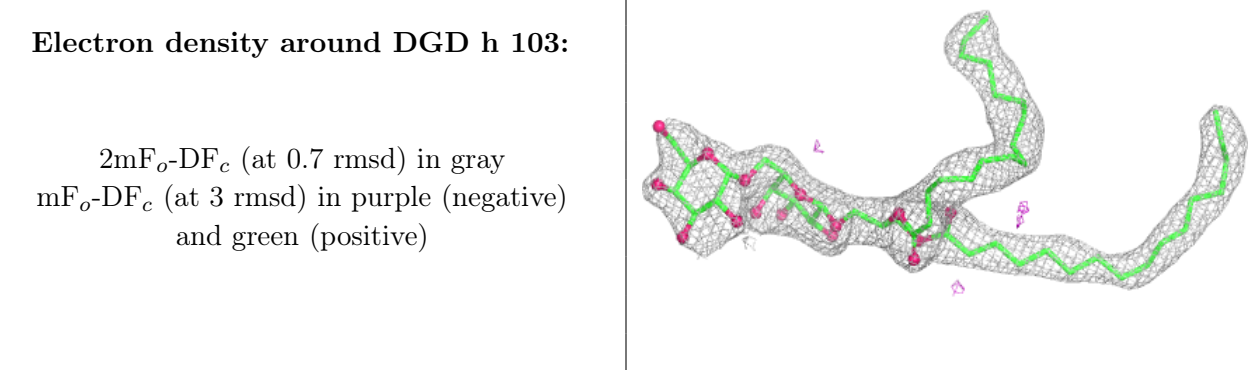
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

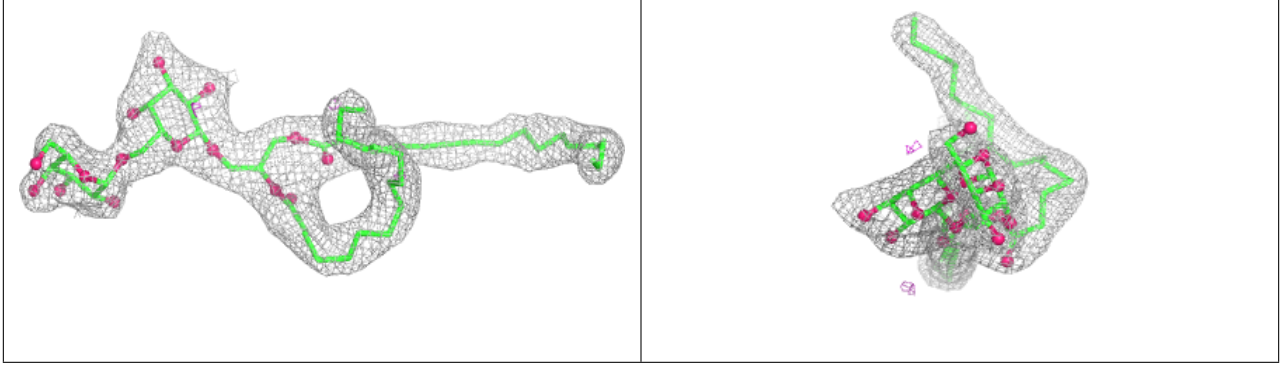




Electron density around DGD h 103:

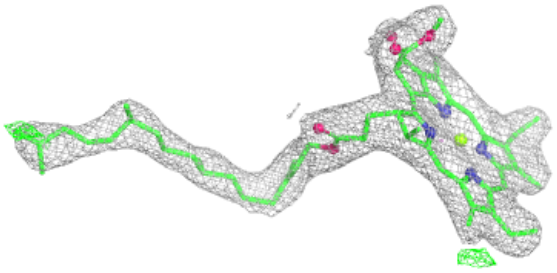
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

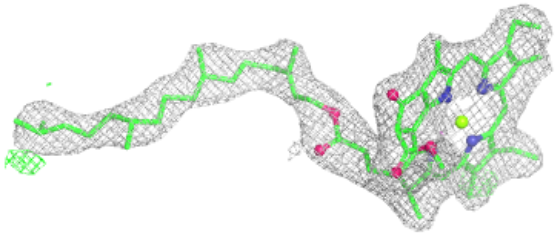


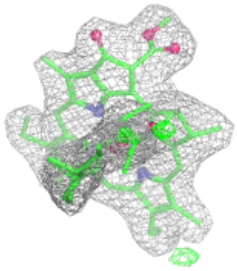


Electron density around CLA C 504:

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

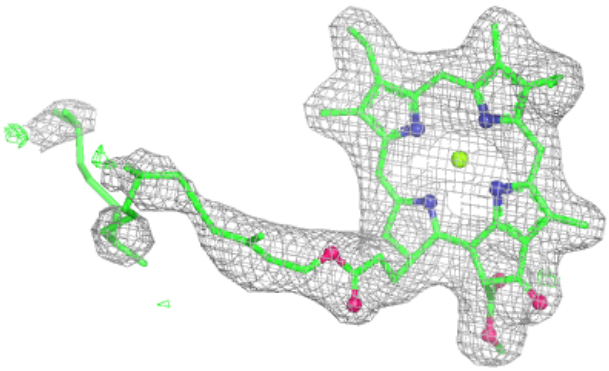


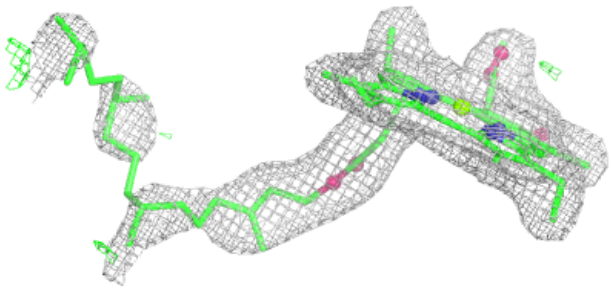


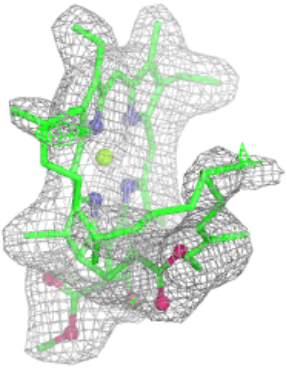


Electron density around CLA A 407:

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

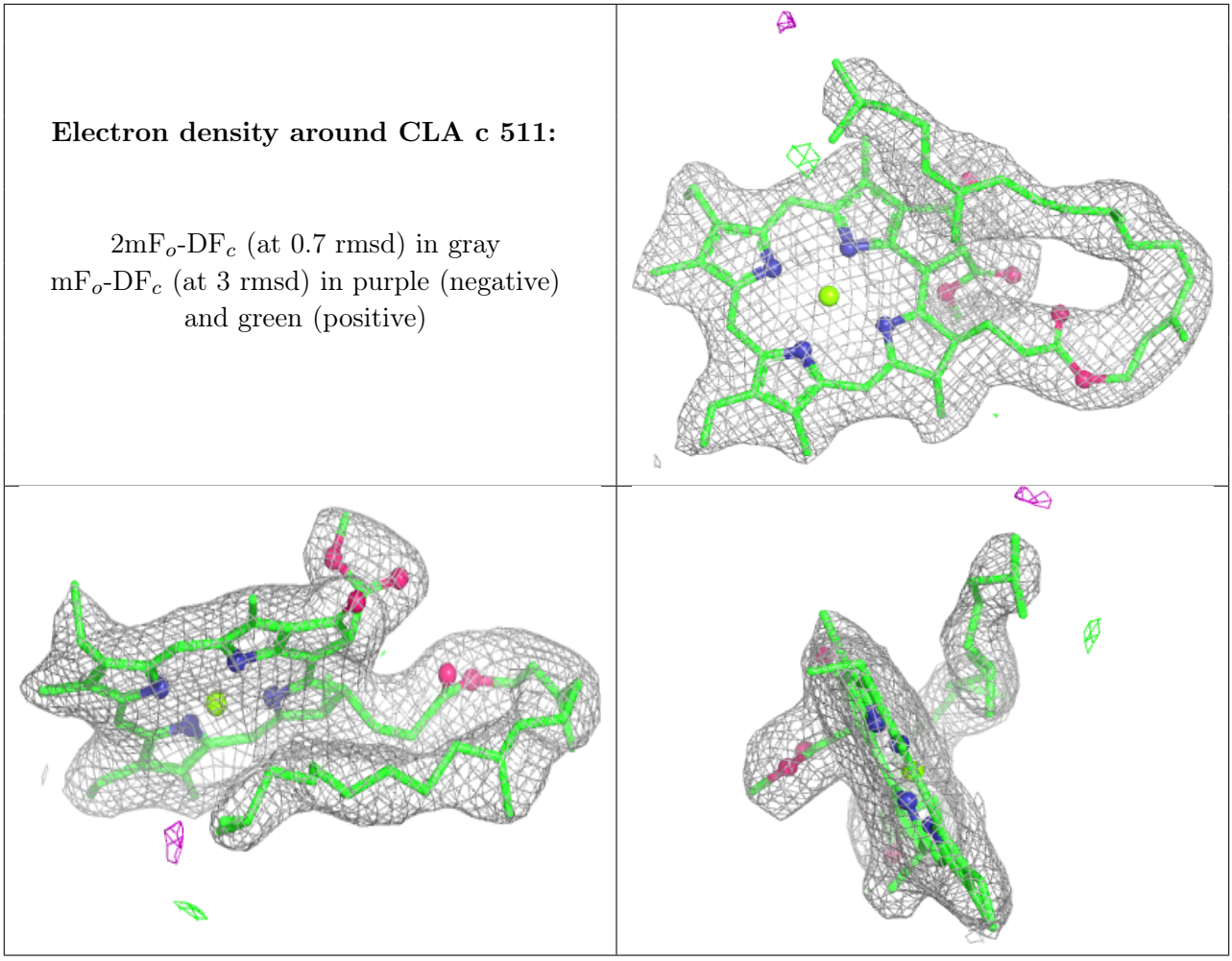






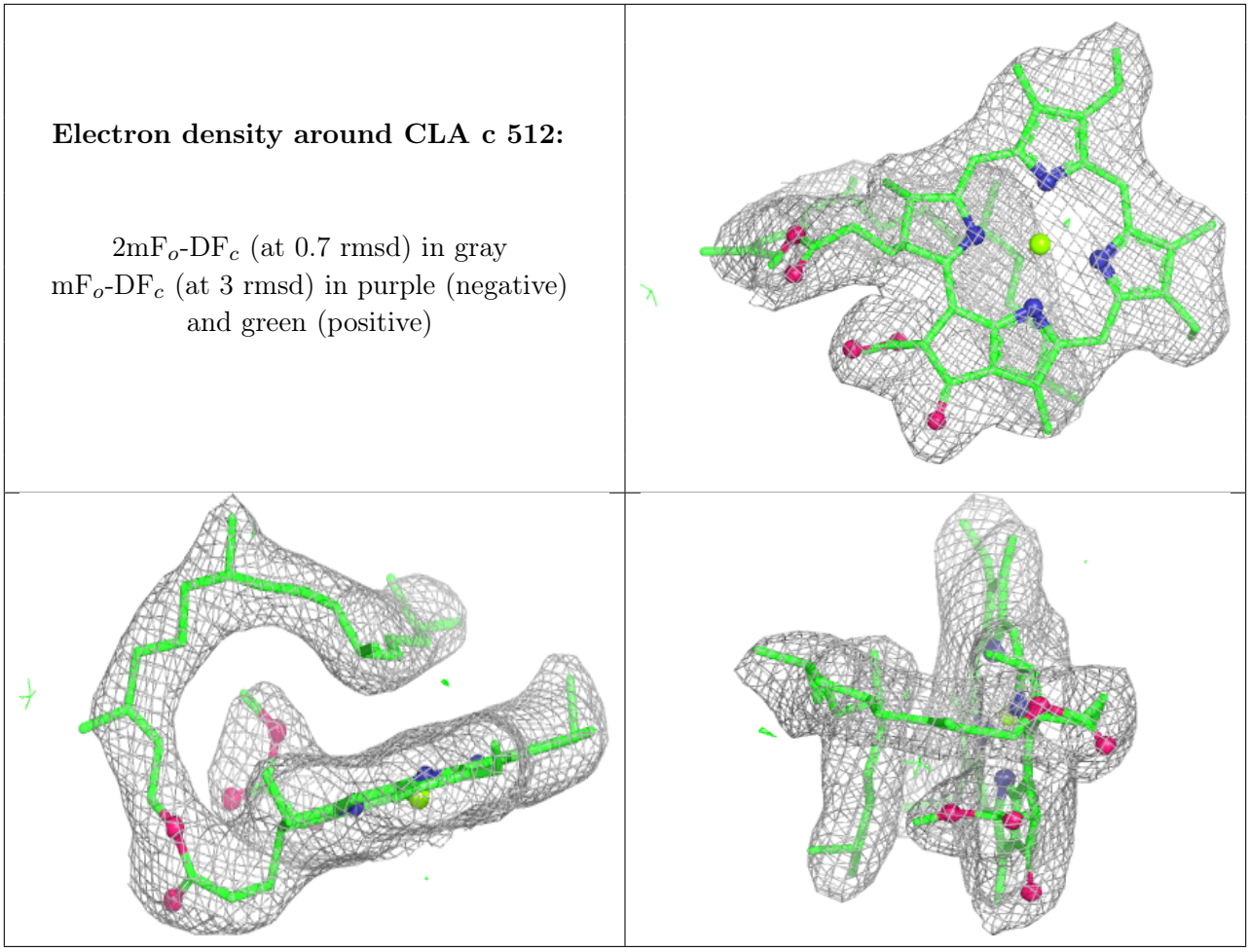
Electron density around CLA c 511:

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



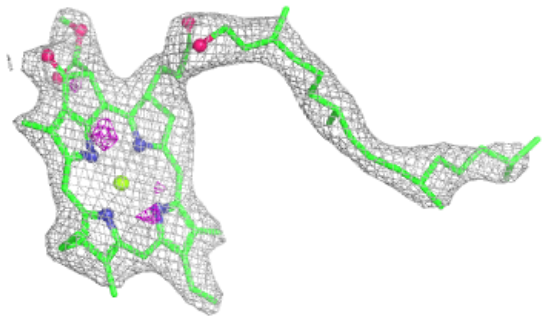
Electron density around CLA c 512:

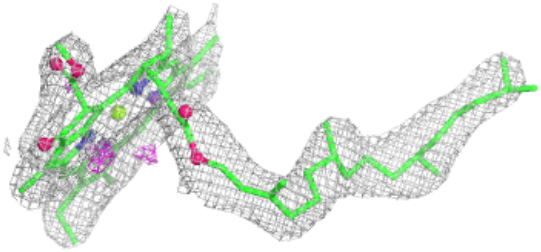
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

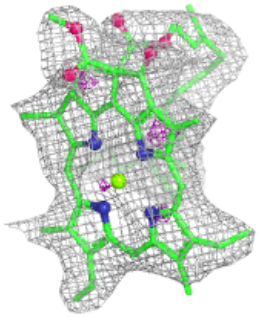


Electron density around CLA c 513:

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

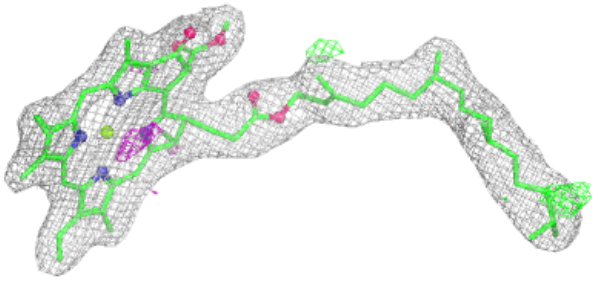


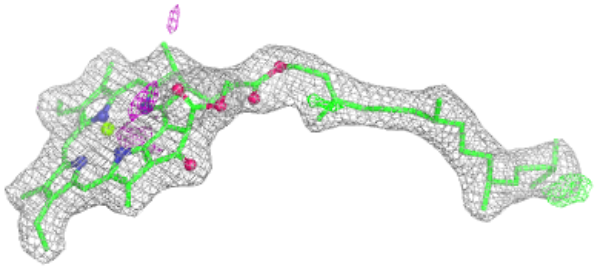


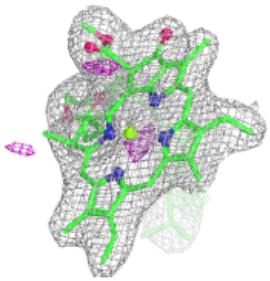


Electron density around CLA a 403:

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

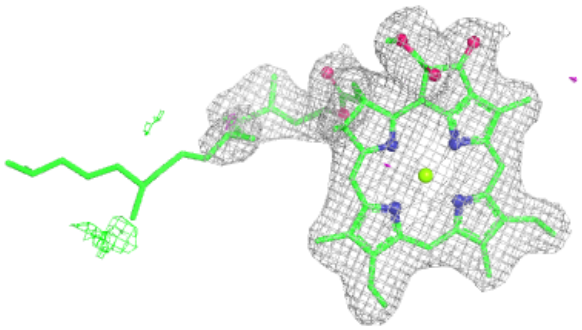


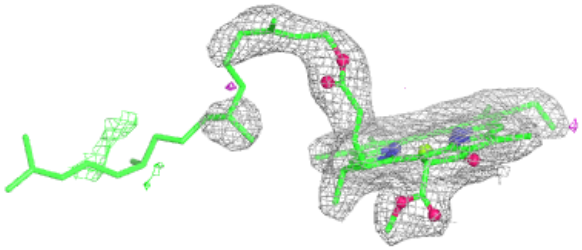


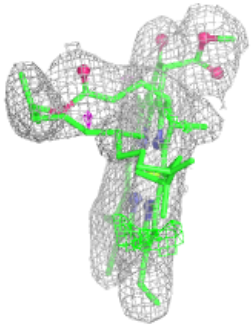


Electron density around CLA a 405:

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

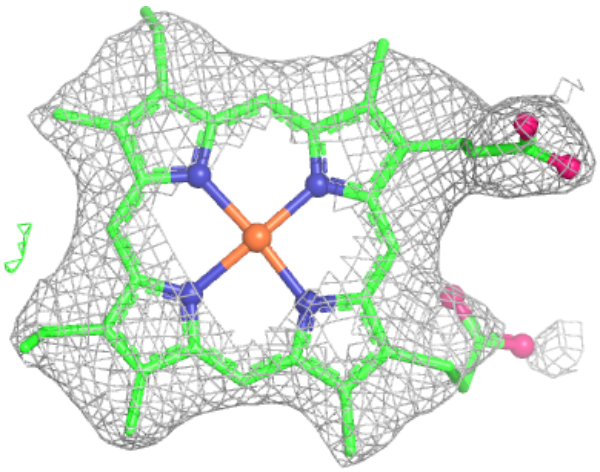


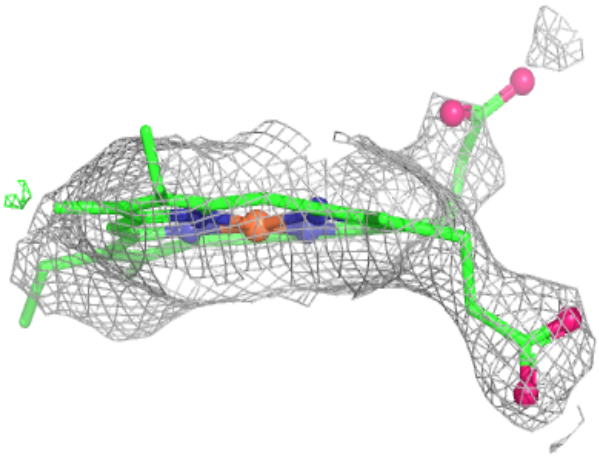


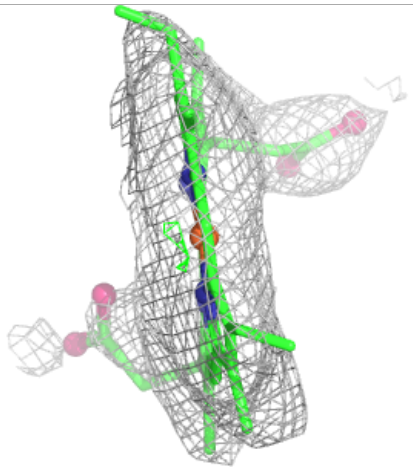


Electron density around HEM e 102:

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

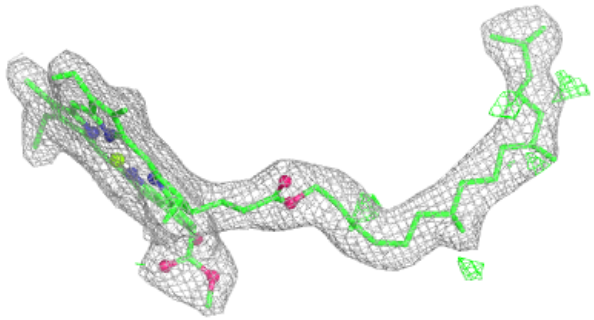


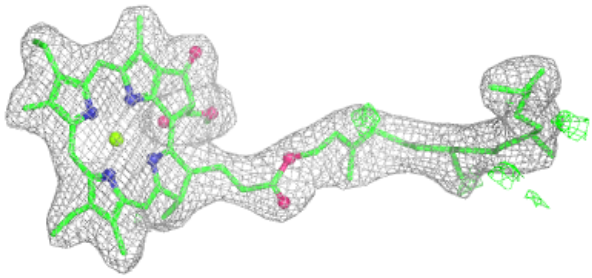


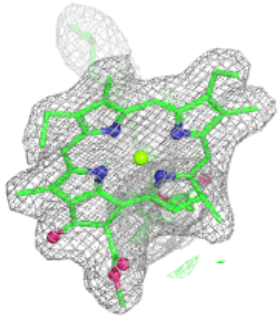


Electron density around CLA D 403:

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

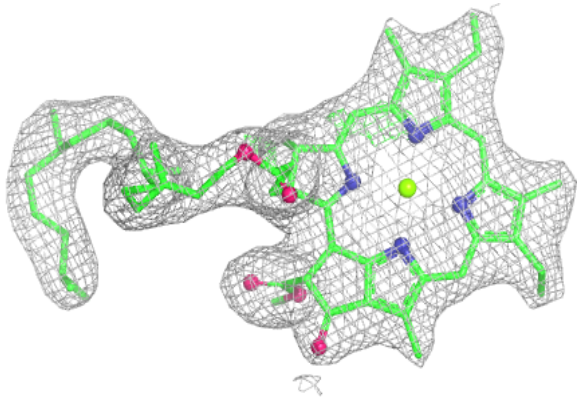


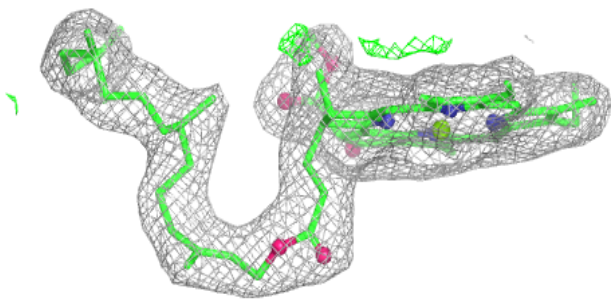


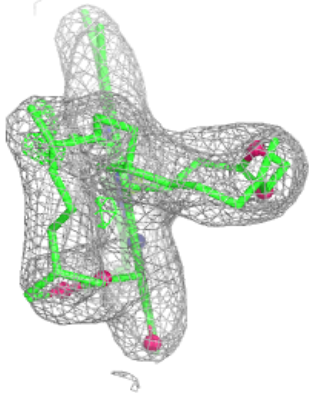


Electron density around CLA B 612:

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

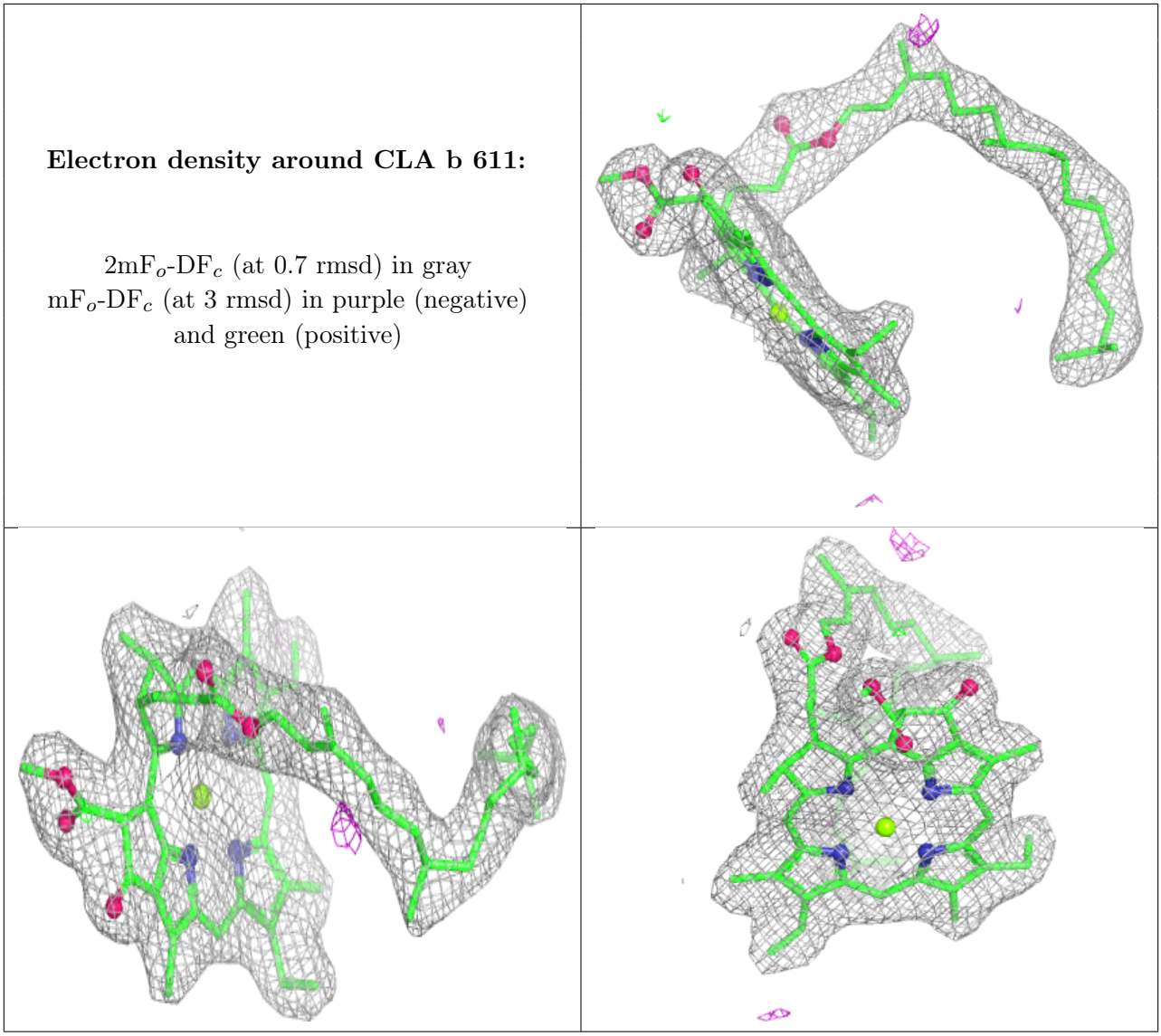






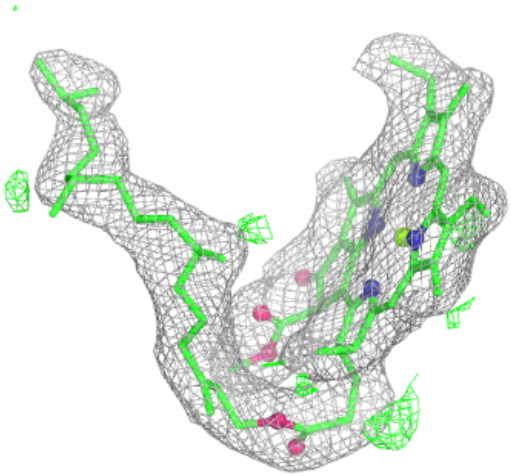
Electron density around CLA b 611:

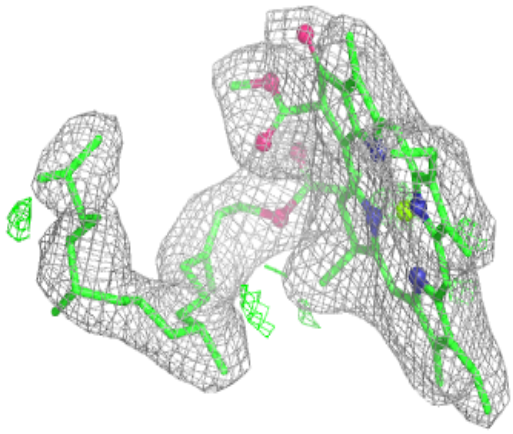
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

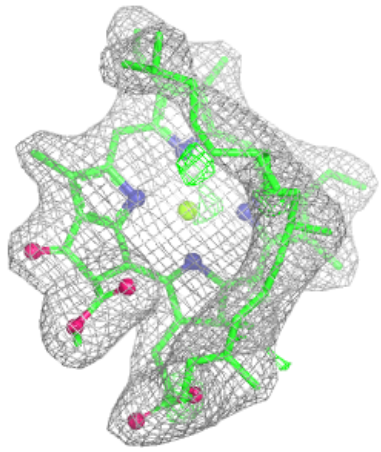


Electron density around CLA B 613:

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

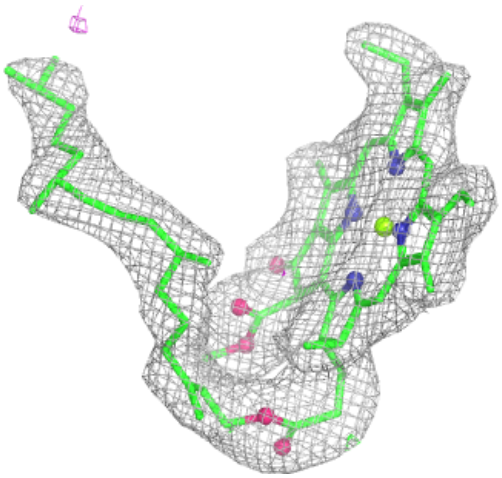


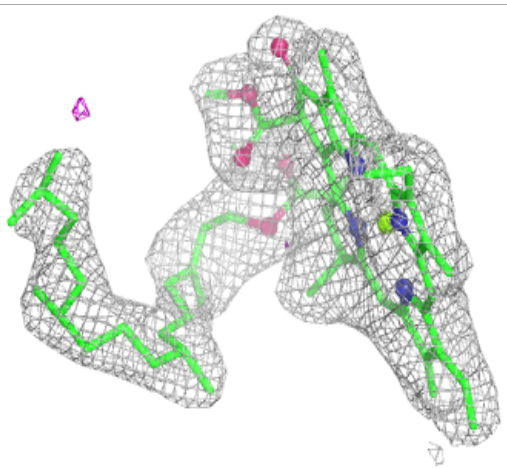


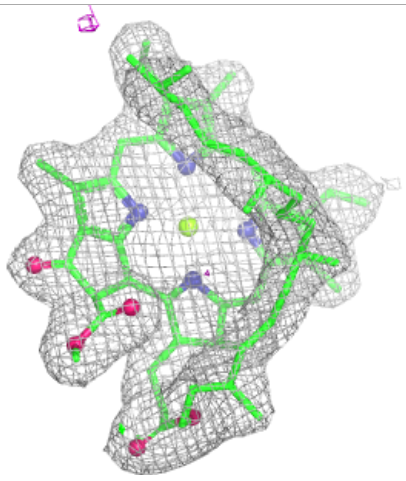


Electron density around CLA b 613:

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

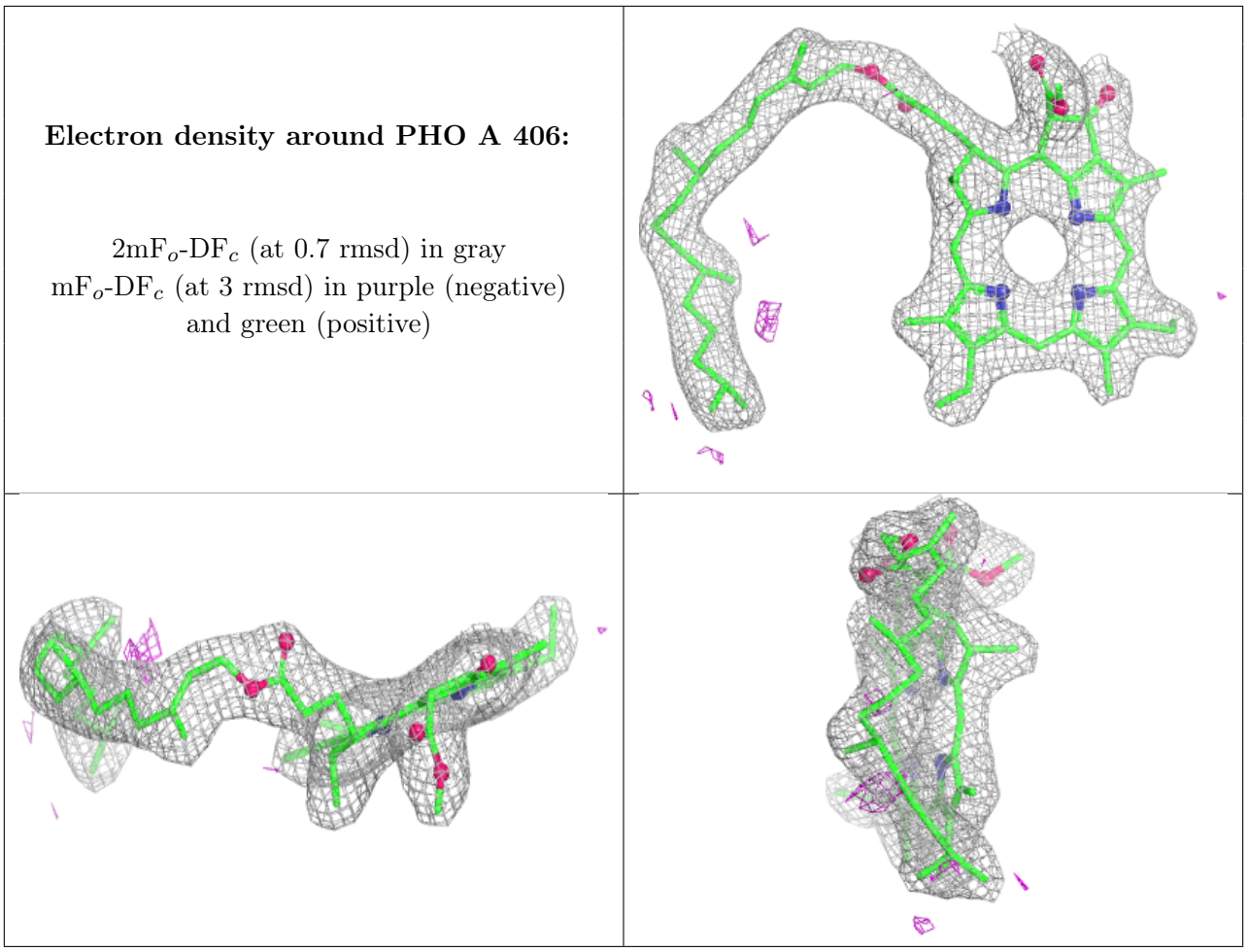






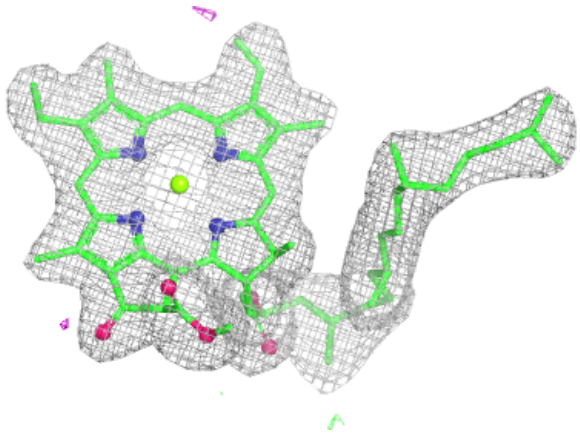
Electron density around PHO A 406:

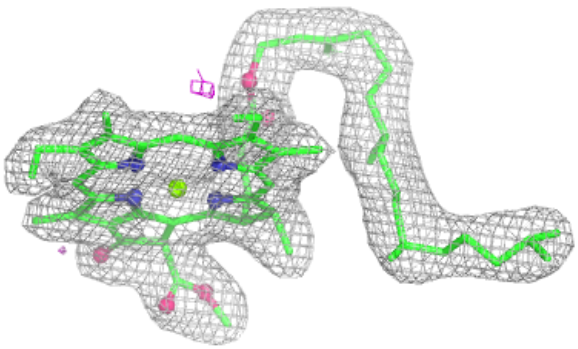
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

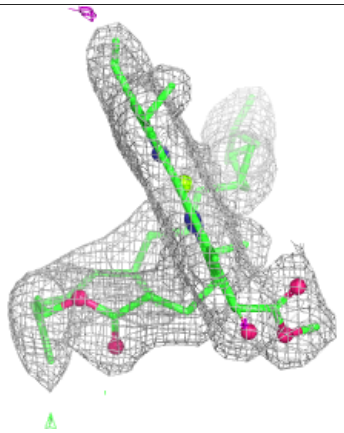


Electron density around CLA a 404:

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

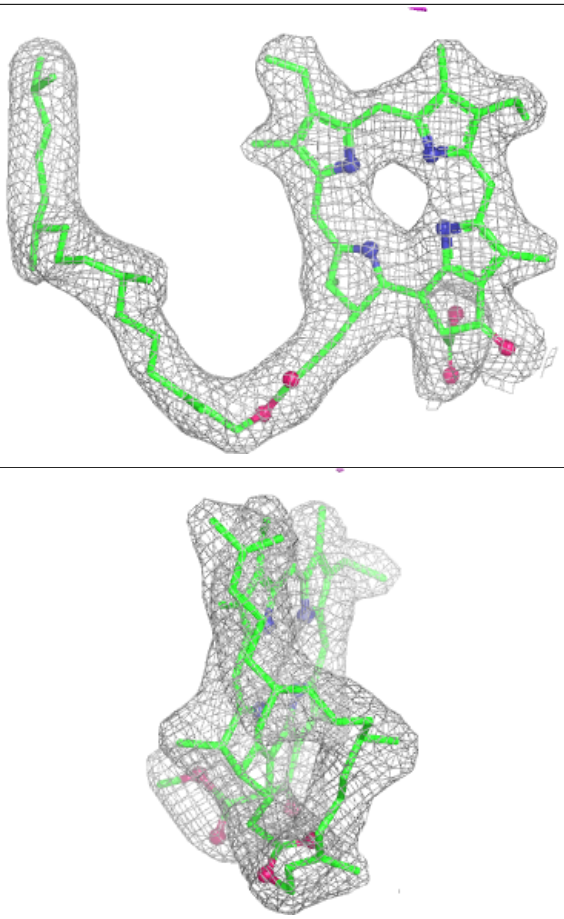


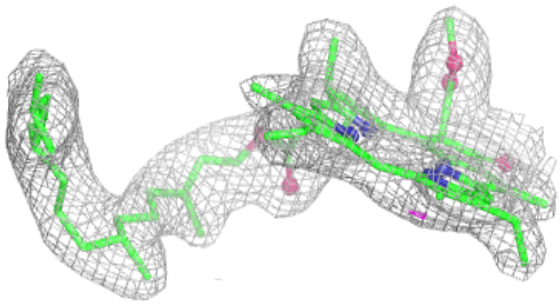




Electron density around PHO a 416:

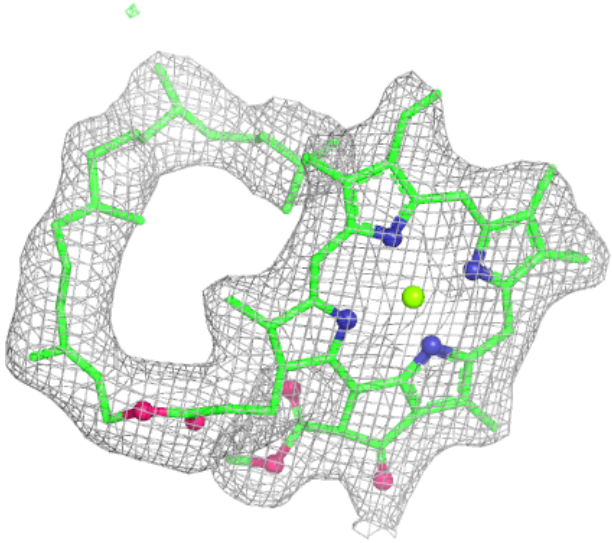
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

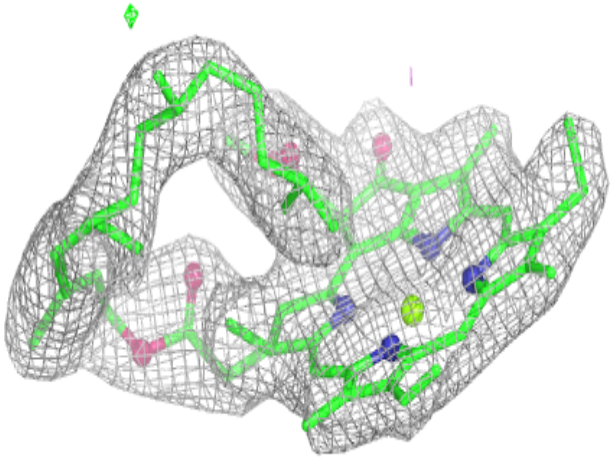


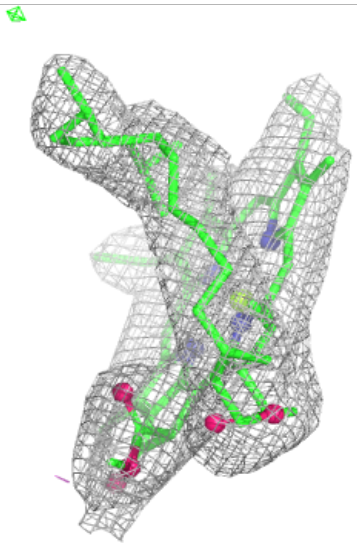


Electron density around CLA b 615:

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

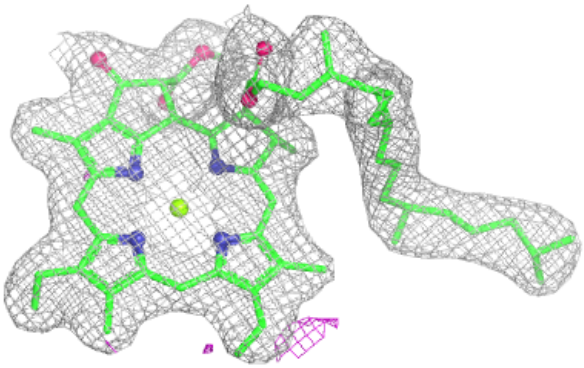


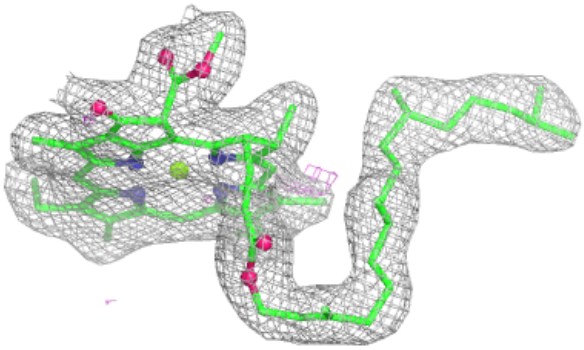


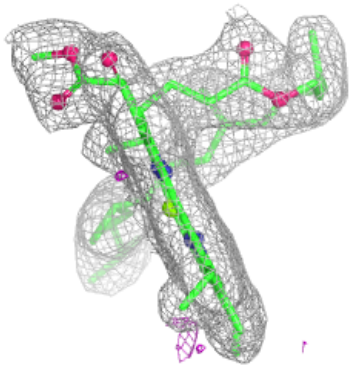


Electron density around CLA A 404:

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

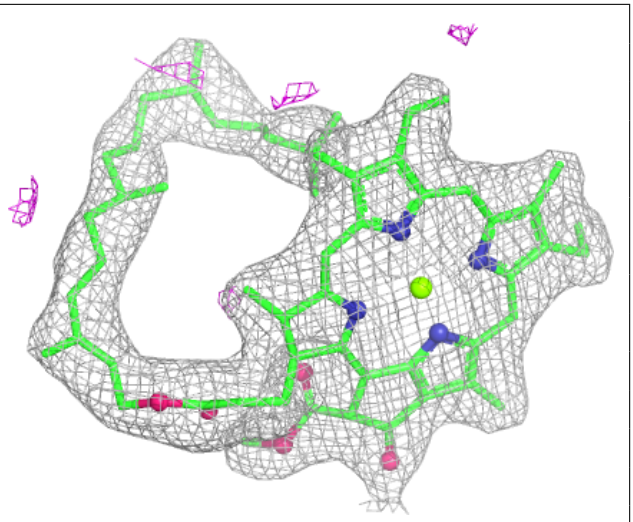


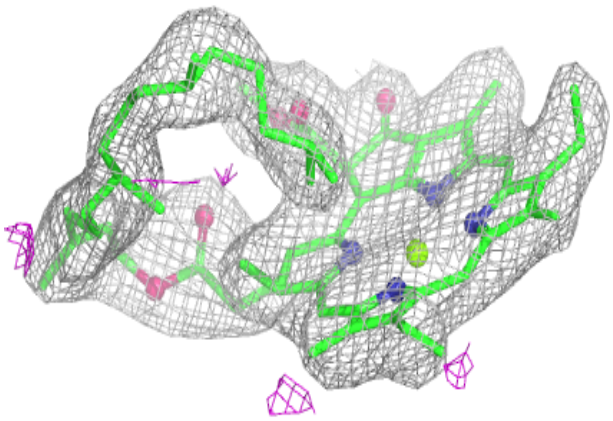




Electron density around CLA B 615:

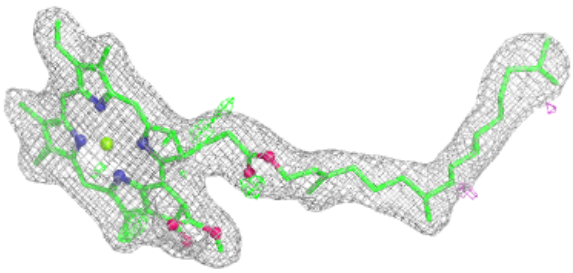
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

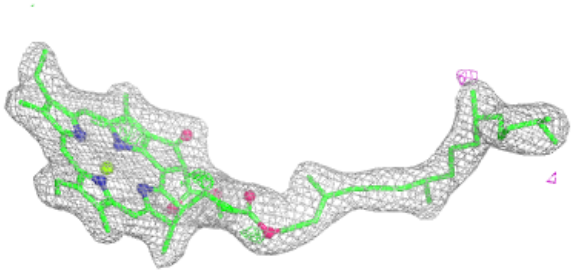


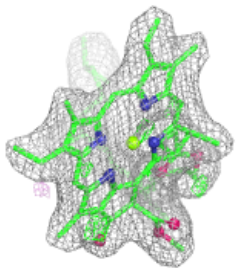


Electron density around CLA A 403:

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

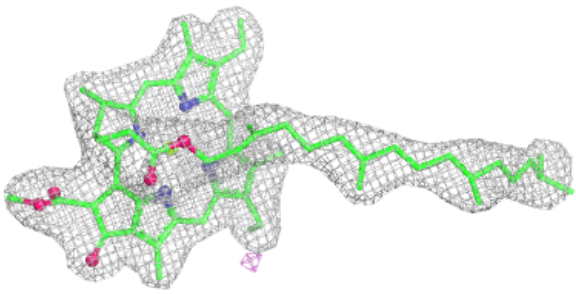


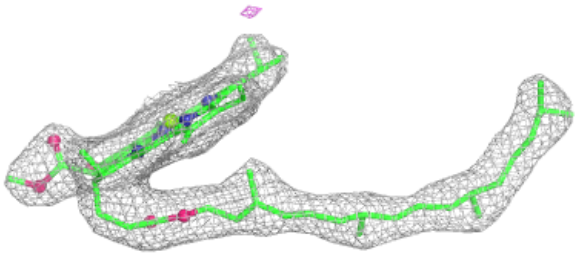


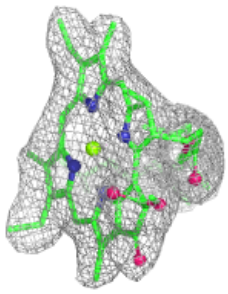


Electron density around CLA B 608:

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

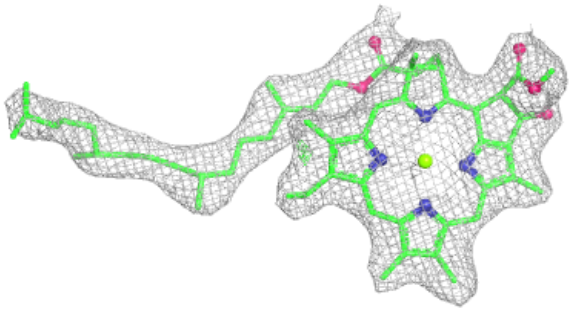


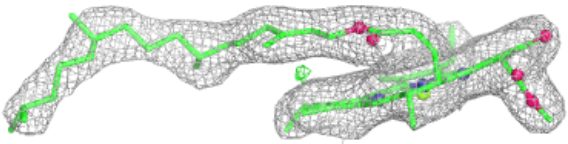




Electron density around CLA b 603:

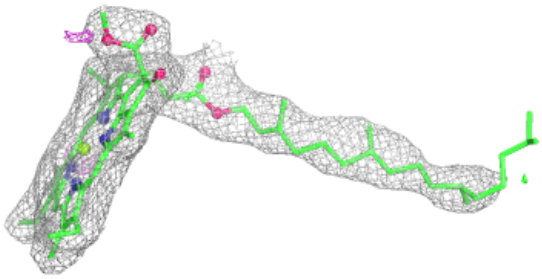
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

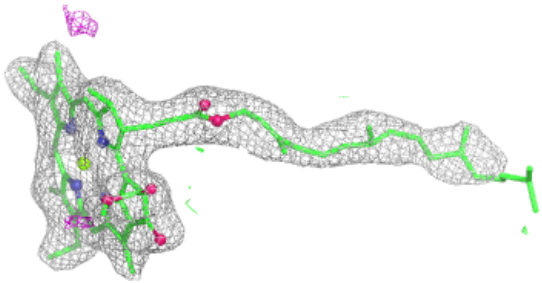


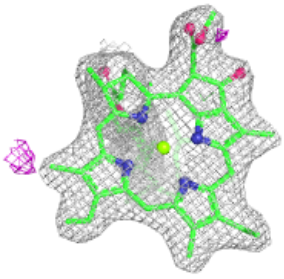


Electron density around CLA b 604:

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

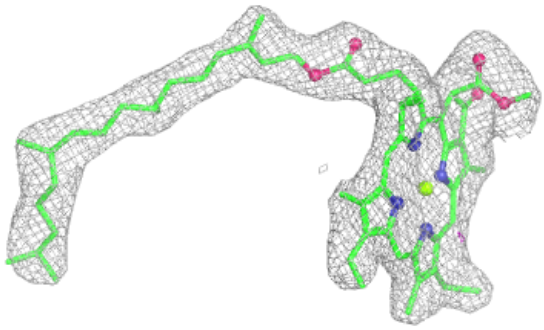


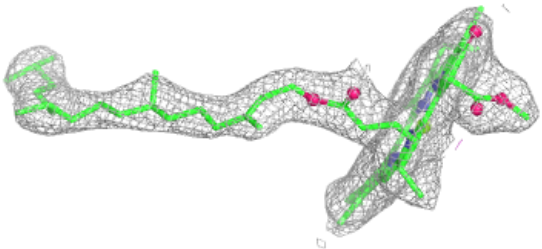




Electron density around CLA B 609:

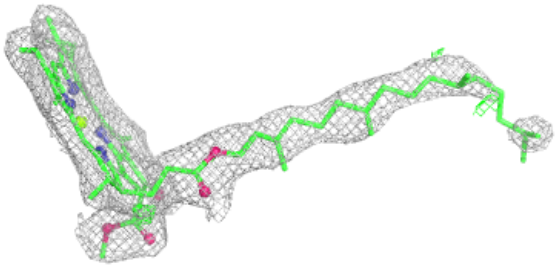
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

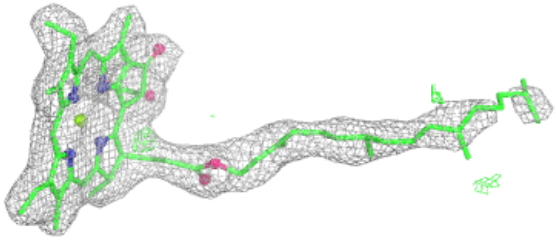


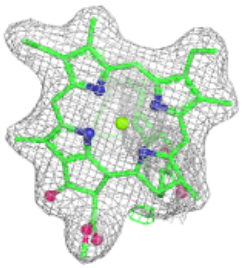


Electron density around CLA B 604:

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

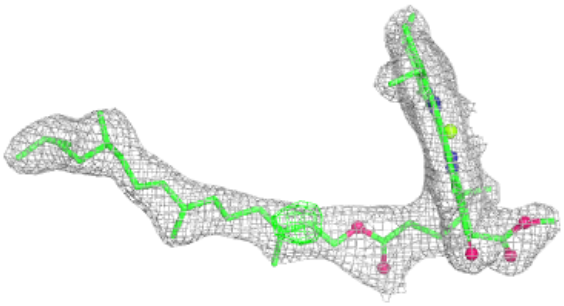


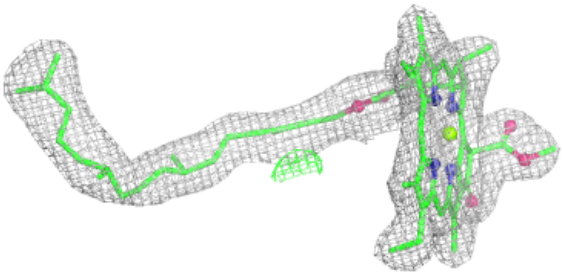


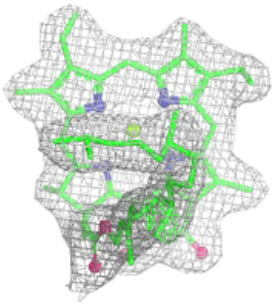


Electron density around CLA B 605:

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

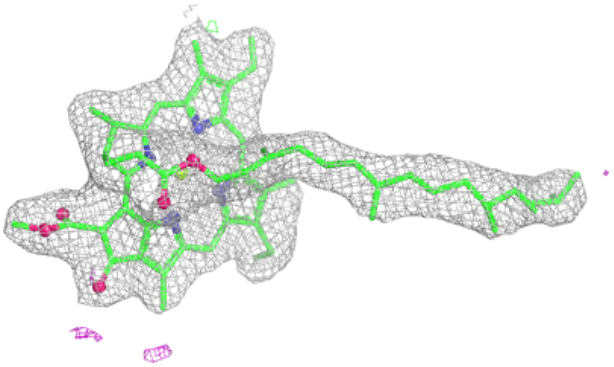


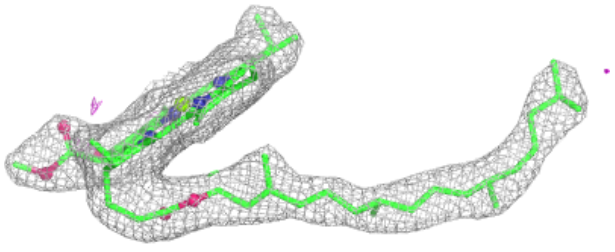


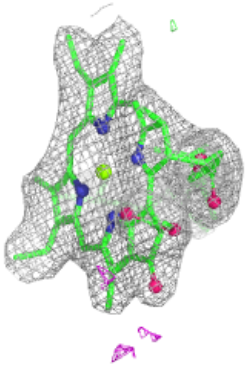


Electron density around CLA b 608:

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

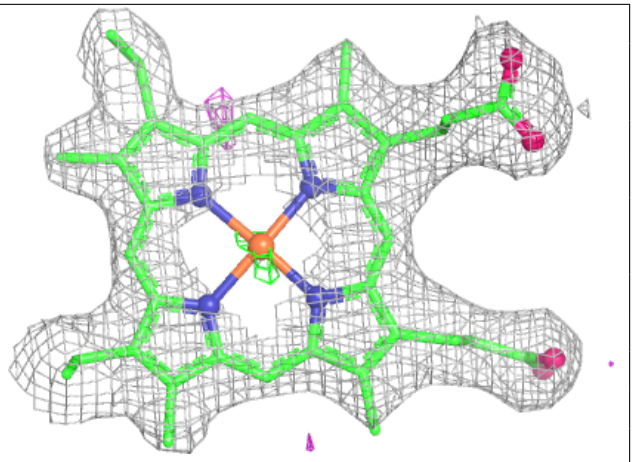


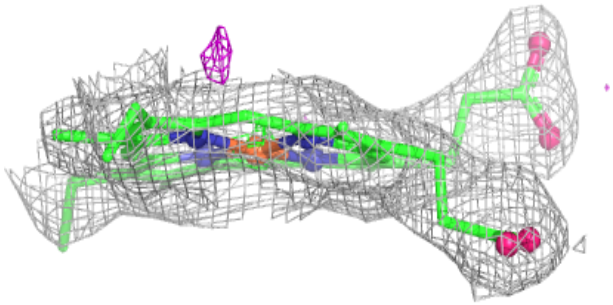


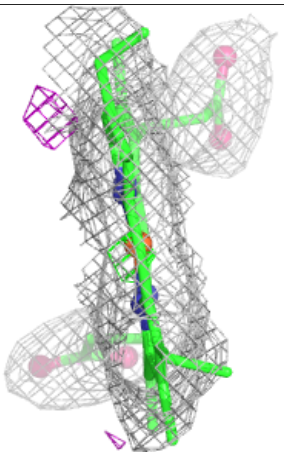


Electron density around HEC v 202:

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

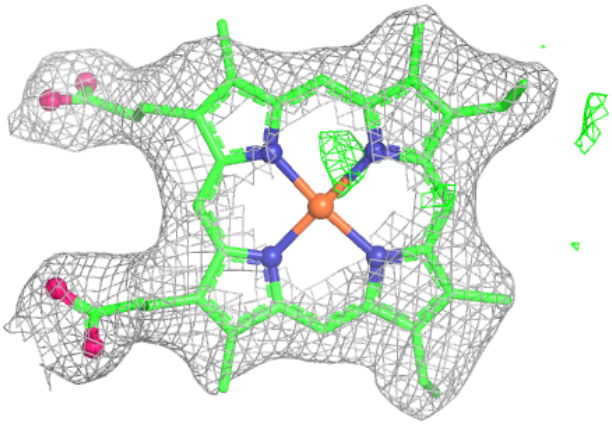


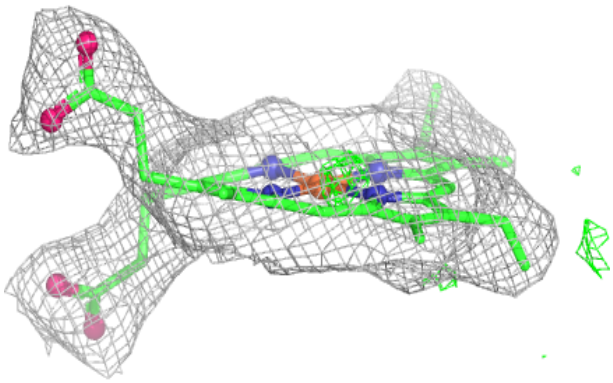


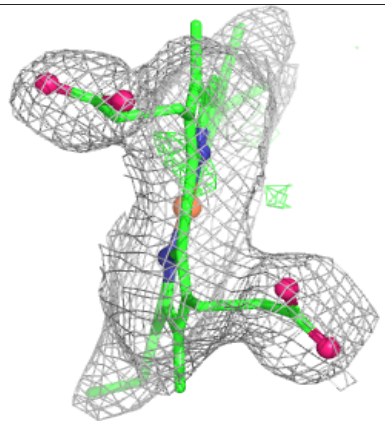


Electron density around HEM E 102:

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

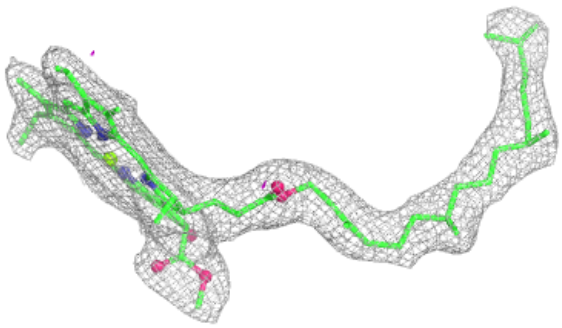


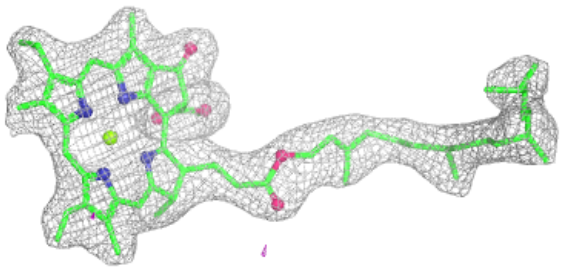


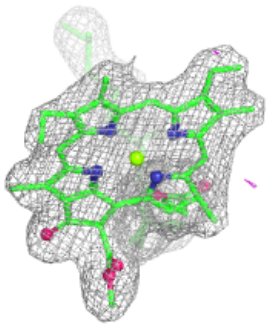


Electron density around CLA d 402:

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

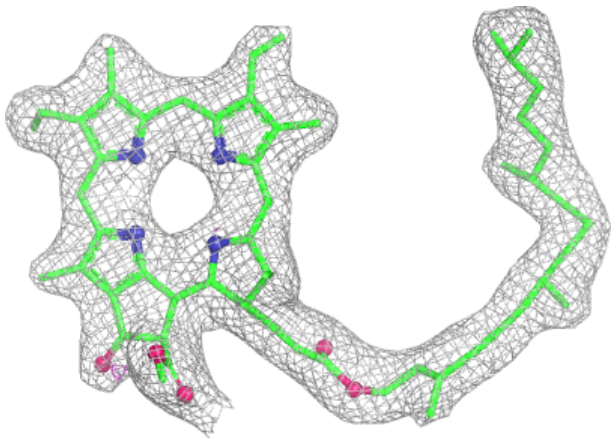


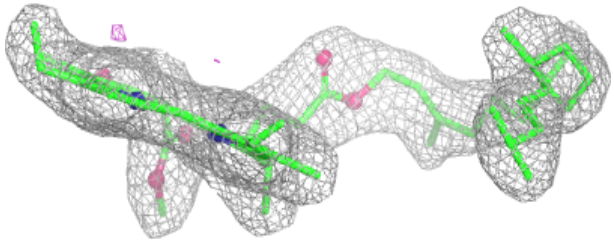


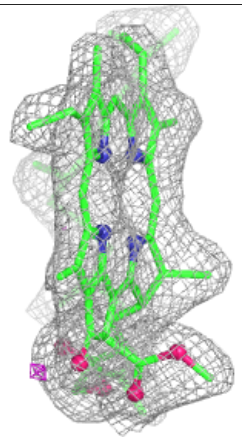


Electron density around PHO a 406:

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

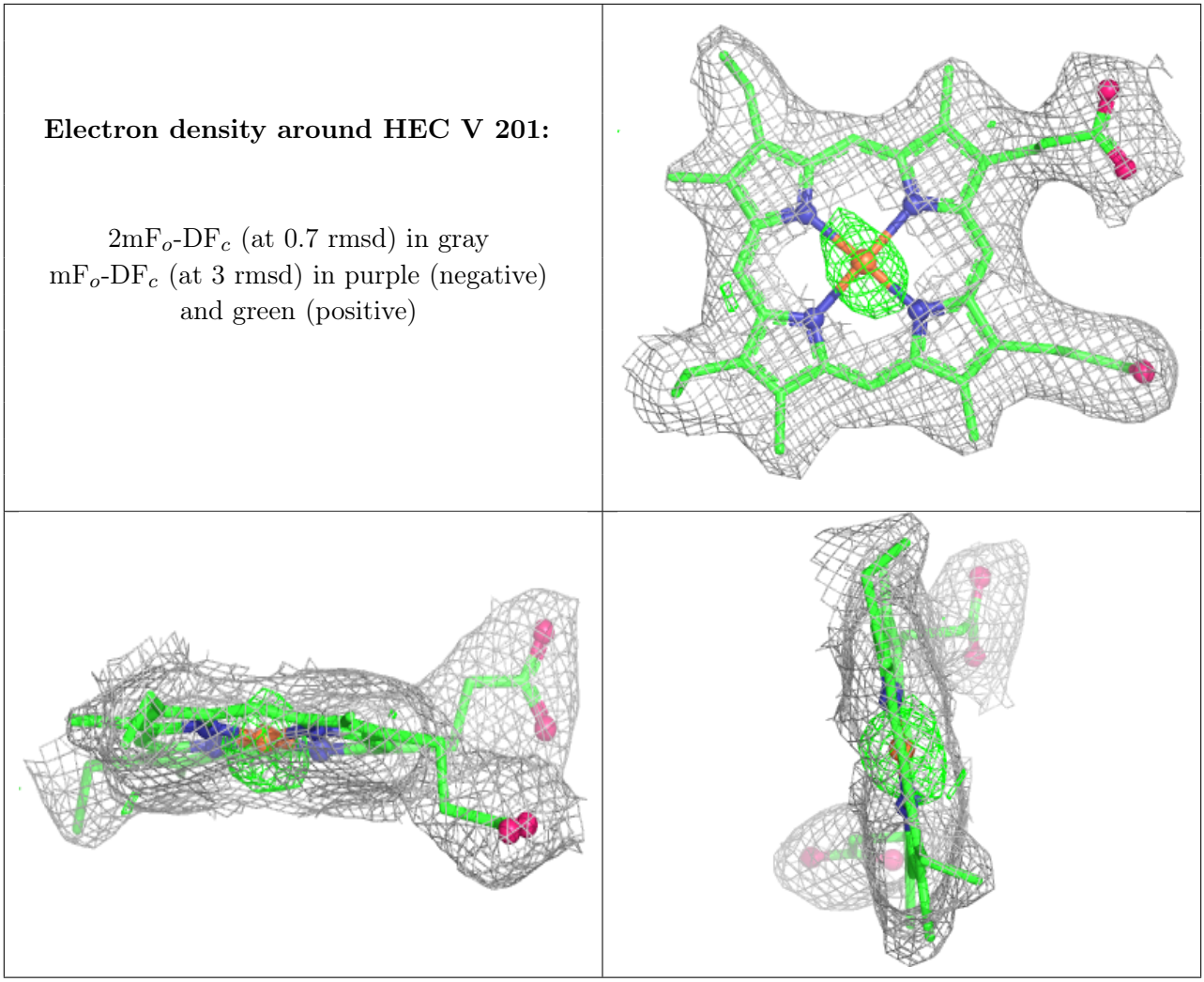






Electron density around HEC V 201:

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



6.5 Other polymers

There are no such residues in this entry.