



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 13, 2017 – 09:09 AM EDT

PDB ID : 5XNO
EMDB ID: : EMD-6744
Title : Structure of M-LHCII and CP24 complexes in the unstacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : unknown
Resolution : 3.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

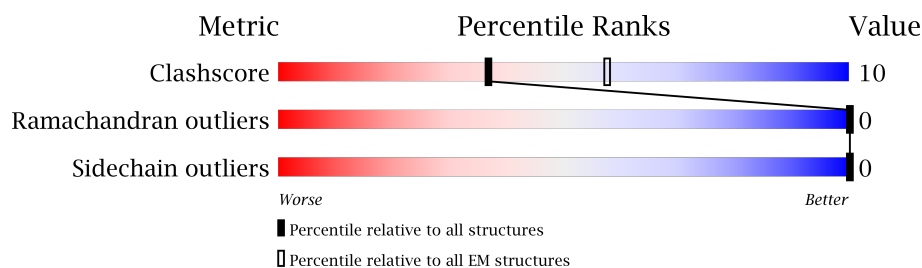
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	232	78% 16% 6%
1	2	232	77% 17% 6%
2	3	243	75% 16% 9%
3	4	210	78% 16% 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
5	CLA	1	602	X	-	-	-
5	CLA	1	603	X	-	-	-
5	CLA	1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	1	610	X	-	-	-
5	CLA	1	611	X	-	-	-
5	CLA	1	612	X	-	-	-
5	CLA	1	613	X	-	-	-
5	CLA	1	614	X	-	-	-
5	CLA	2	602	X	-	-	-
5	CLA	2	603	X	-	-	-
5	CLA	2	604	X	-	-	-
5	CLA	2	610	X	-	-	-
5	CLA	2	611	X	-	-	-
5	CLA	2	612	X	-	-	-
5	CLA	2	613	X	-	-	-
5	CLA	2	614	X	-	-	-
5	CLA	3	602	X	-	-	-
5	CLA	3	603	X	-	-	-
5	CLA	3	604	X	-	-	-
5	CLA	3	610	X	-	-	-
5	CLA	3	611	X	-	-	-
5	CLA	3	612	X	-	-	-
5	CLA	3	613	X	-	-	-
5	CLA	3	614	X	-	-	-
5	CLA	4	602	X	-	-	-
5	CLA	4	603	X	-	-	-
5	CLA	4	604	X	-	-	-
5	CLA	4	610	X	-	-	-
5	CLA	4	611	X	-	-	-
5	CLA	4	612	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		

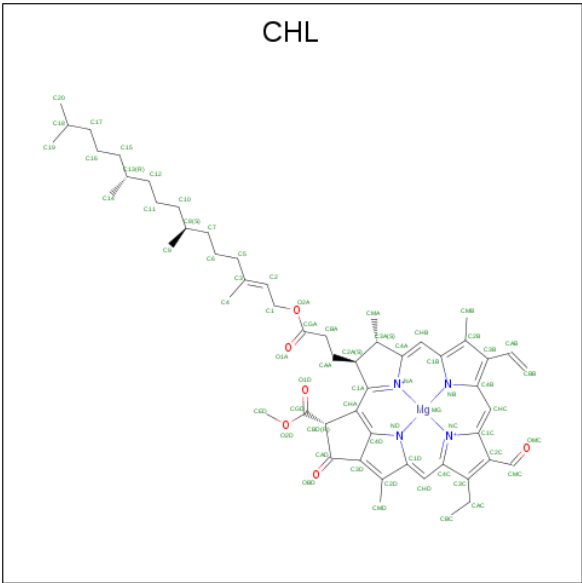
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



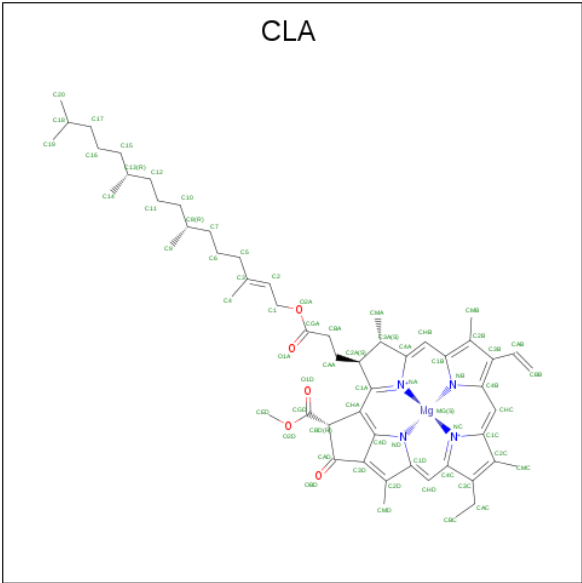
Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	

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Mol	Chain	Residues	Atoms					AltConf
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	

- Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



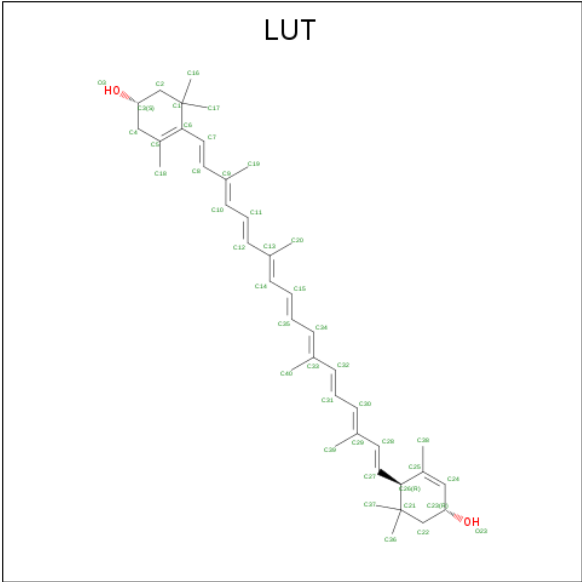
Mol	Chain	Residues	Atoms					AltConf
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	

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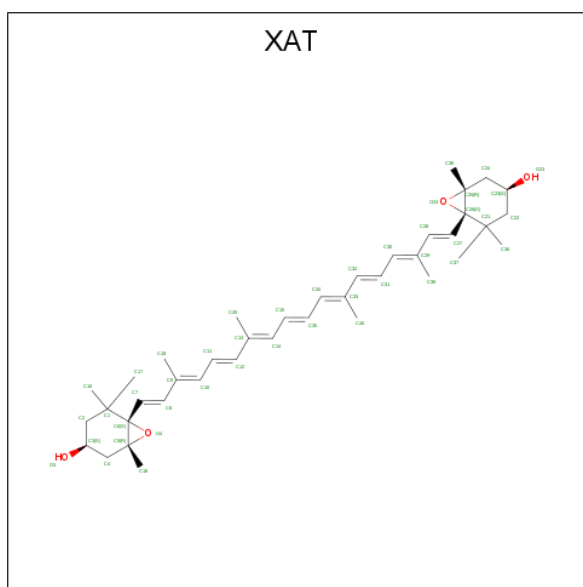
Mol	Chain	Residues	Atoms					AltConf
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



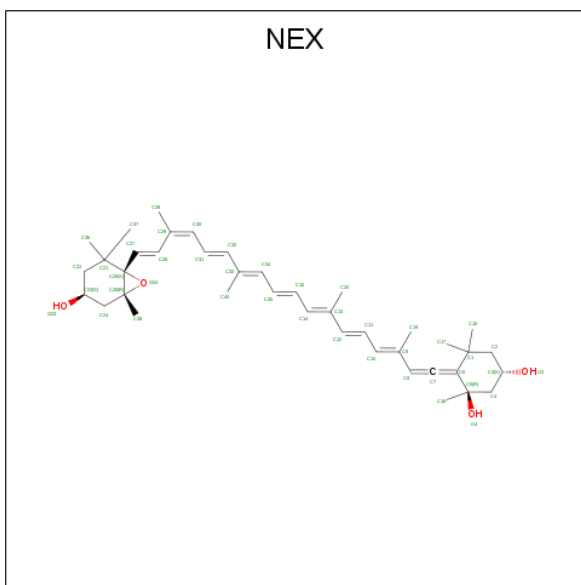
Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			84	80	4	
6	1	1	Total	C	O	0
			84	80	4	
6	2	1	Total	C	O	0
			84	80	4	
6	2	1	Total	C	O	0
			84	80	4	
6	3	1	Total	C	O	0
			84	80	4	
6	3	1	Total	C	O	0
			84	80	4	
6	4	1	Total	C	O	0
			42	40	2	

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



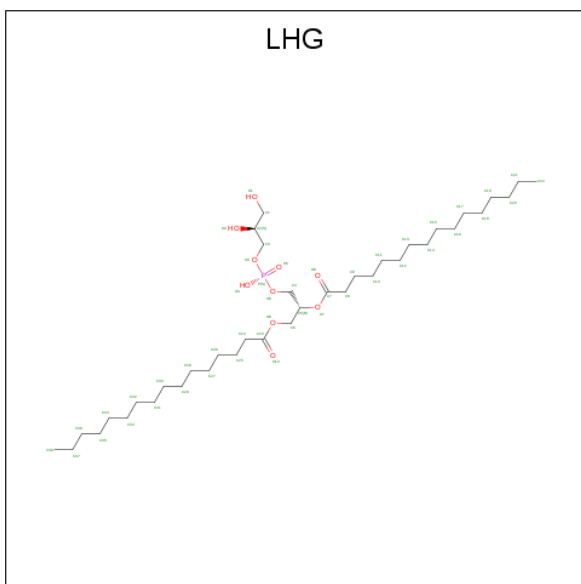
Mol	Chain	Residues	Atoms			AltConf
7	1	1	Total	C	O	0
			44	40	4	
7	2	1	Total	C	O	0
			44	40	4	
7	3	1	Total	C	O	0
			44	40	4	
7	4	1	Total	C	O	0
			44	40	4	

- Molecule 8 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



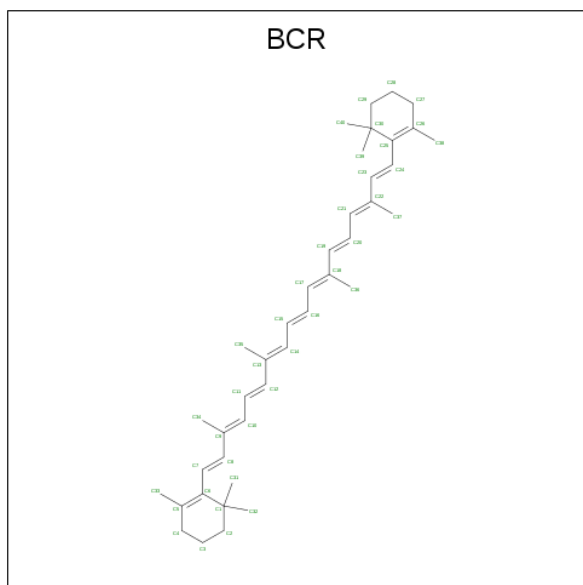
Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total 44	C 40	O 4	0
8	2	1	Total 44	C 40	O 4	0
8	3	1	Total 44	C 40	O 4	0

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
9	1	1	Total	C	O	P	0
			41	30	10	1	
9	2	1	Total	C	O	P	0
			37	26	10	1	
9	3	1	Total	C	O	P	0
			47	36	10	1	
9	4	1	Total	C	O	P	0
			21	10	10	1	

- Molecule 10 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

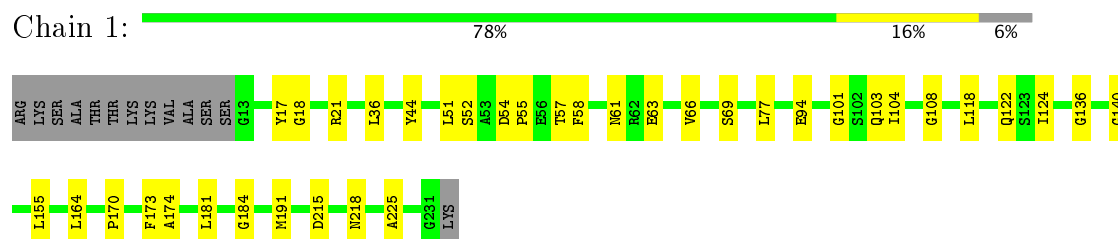


Mol	Chain	Residues	Atoms		AltConf
10	4	1	Total	C	0
			40	40	

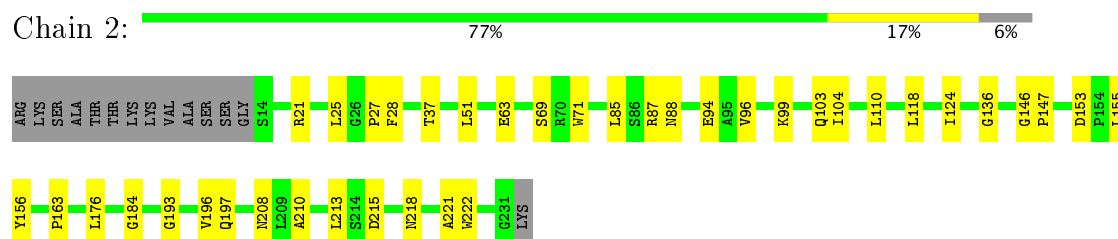
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

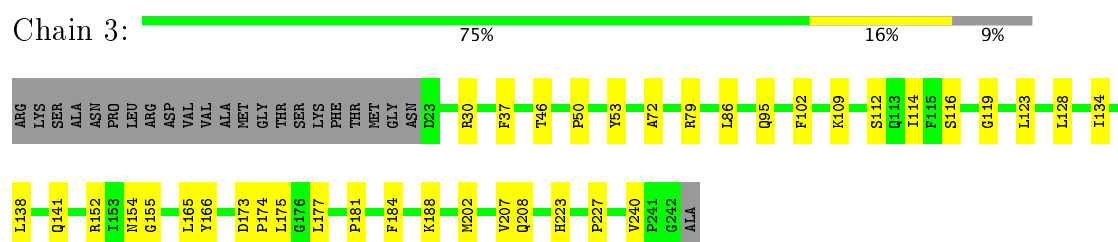
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



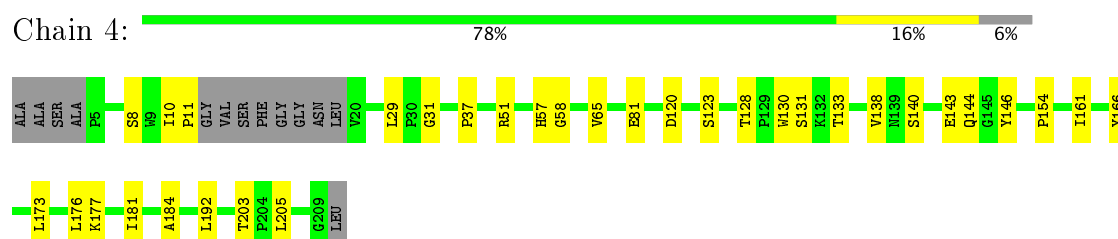
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LUT, CHL, XAT, CLA, NEX, BCR

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.48	0/1720	0.55	0/2342
1	2	0.43	0/1716	0.54	0/2337
2	3	0.49	0/1759	0.59	1/2396 (0.0%)
3	4	0.42	0/1586	0.59	0/2158
All	All	0.46	0/6781	0.57	1/9233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	123	LEU	CA-CB-CG	6.24	129.65	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	26	0
1	2	1664	0	1593	29	0
2	3	1707	0	1659	31	0
3	4	1534	0	1486	23	0
4	1	309	0	244	10	0
4	2	306	0	238	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	316	0	254	18	0
4	4	229	0	152	4	0
5	1	412	0	348	14	0
5	2	391	0	314	15	0
5	3	426	0	373	20	0
5	4	270	0	198	4	0
6	1	84	0	112	9	0
6	2	84	0	112	7	0
6	3	84	0	112	11	0
6	4	42	0	56	4	0
7	1	44	0	56	4	0
7	2	44	0	56	6	0
7	3	44	0	56	5	0
7	4	44	0	56	3	0
8	1	44	0	56	2	0
8	2	44	0	56	1	0
8	3	44	0	56	3	0
9	1	41	0	55	0	0
9	2	37	0	44	2	0
9	3	47	0	67	5	0
9	4	21	0	12	1	0
10	4	40	0	56	3	0
All	All	10020	0	9473	186	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 10.

All (186) 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)
4:3:606:CHL:HBB2	4:3:607:CHL:HBB1	1.57	0.86
5:1:602:CLA:HAB	6:1:1621:LUT:H32	1.66	0.77
5:2:610:CLA:H2	6:2:1620:LUT:H28	1.72	0.72
2:3:95:GLN:HE22	2:3:102:PHE:H	1.39	0.70
2:3:208:GLN:HE22	6:3:1620:LUT:H41	1.63	0.64
3:4:138:VAL:HG22	3:4:140:SER:H	1.64	0.61
5:1:610:CLA:H2	6:1:1620:LUT:H28	1.81	0.61
5:1:602:CLA:HBA1	6:1:1621:LUT:H382	1.83	0.61
4:2:606:CHL:HMB1	4:2:609:CHL:HAC1	1.83	0.60
1:2:163:PRO:HD2	6:2:1620:LUT:H23	1.83	0.59
1:1:103:GLN:HE22	5:1:604:CLA:HED3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:104:ILE:HG21	1:2:124:ILE:HD13	1.83	0.59
7:3:1622:XAT:H12	9:3:2630:LHG:H191	1.83	0.59
2:3:50:PRO:HG3	2:3:188:LYS:HD3	1.83	0.59
1:2:21:ARG:NH1	1:2:37:THR:O	2.35	0.59
1:1:66:VAL:HG22	1:1:181:LEU:HD21	1.85	0.59
2:3:79:ARG:NH1	4:3:608:CHL:OBD	2.36	0.58
5:3:611:CLA:HAB	7:3:1622:XAT:H221	1.86	0.57
5:3:603:CLA:HMD1	4:3:609:CHL:HBA2	1.86	0.57
1:2:213:LEU:HD21	5:2:614:CLA:HMC3	1.86	0.57
5:4:611:CLA:HBA2	5:4:612:CLA:HMD1	1.87	0.56
2:3:141:GLN:HE22	4:3:607:CHL:HMC	1.69	0.56
2:3:109:LYS:HA	4:3:607:CHL:HED3	1.87	0.56
5:1:603:CLA:HMD1	4:1:609:CHL:HBA2	1.86	0.56
1:1:21:ARG:NH2	1:1:36:LEU:O	2.39	0.55
1:1:94:GLU:N	1:1:103:GLN:OE1	2.38	0.55
1:2:193:GLY:O	1:2:197:GLN:HG2	2.07	0.55
1:2:215:ASP:OD2	1:2:218:ASN:ND2	2.41	0.55
1:2:27:PRO:O	2:3:154:ASN:ND2	2.40	0.55
2:3:175:LEU:HD13	6:3:1620:LUT:H222	1.88	0.54
4:1:607:CHL:HBB1	4:3:601:CHL:H141	1.89	0.54
3:4:161:ILE:HA	3:4:166:TYR:HA	1.90	0.54
5:3:603:CLA:H2	5:3:603:CLA:HMA2	1.90	0.54
1:1:164:LEU:HD13	6:1:1620:LUT:H222	1.90	0.54
1:2:85:LEU:HD23	1:2:88:ASN:HD22	1.73	0.53
3:4:31:GLY:HA3	3:4:181:ILE:HG21	1.90	0.53
5:3:611:CLA:H3A	3:4:131:SER:HA	1.90	0.53
7:2:1622:XAT:H14	9:2:2630:LHG:H171	1.91	0.53
5:2:603:CLA:HED2	4:2:609:CHL:H93	1.90	0.53
2:3:174:PRO:HD2	6:3:1620:LUT:H23	1.91	0.52
4:1:608:CHL:HBB1	4:1:608:CHL:HHC	1.92	0.52
1:1:52:SER:OG	1:1:61:ASN:ND2	2.43	0.52
1:2:221:ALA:N	5:2:613:CLA:O1A	2.43	0.52
2:3:112:SER:HB3	4:3:607:CHL:HED2	1.90	0.52
1:2:63:GLU:HA	1:2:155:LEU:HD21	1.91	0.52
1:2:25:LEU:HB3	1:2:28:PHE:HB2	1.91	0.52
1:1:69:SER:HB3	1:1:184:GLY:HA3	1.92	0.52
3:4:65:VAL:HG21	6:4:620:LUT:H12	1.91	0.51
1:2:94:GLU:N	1:2:103:GLN:OE1	2.43	0.51
5:3:602:CLA:H72	6:3:1621:LUT:H30	1.93	0.51
3:4:120:ASP:O	3:4:123:SER:OG	2.28	0.51
2:3:114:ILE:HG21	2:3:134:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:51:LEU:HD13	5:1:602:CLA:H42	1.93	0.51
3:4:10:ILE:HG23	3:4:11:PRO:HD3	1.93	0.51
3:4:58:GLY:HA3	3:4:184:ALA:HB1	1.93	0.51
5:2:602:CLA:HBA1	6:2:1621:LUT:H382	1.93	0.50
1:1:77:LEU:HD13	5:1:612:CLA:HBB2	1.92	0.50
7:2:1622:XAT:H41	4:3:607:CHL:HAA2	1.93	0.50
2:3:175:LEU:HB3	2:3:177:LEU:HD13	1.93	0.50
3:4:57:HIS:HD2	7:4:622:XAT:H15	1.77	0.50
5:4:612:CLA:H2A	5:4:612:CLA:HED2	1.94	0.50
2:3:152:ARG:NH2	4:3:609:CHL:O1D	2.45	0.50
4:4:608:CHL:HHC	4:4:608:CHL:HBB1	1.93	0.50
3:4:154:PRO:HD2	6:4:620:LUT:H23	1.94	0.50
1:2:208:ASN:ND2	5:2:613:CLA:O1D	2.45	0.49
4:3:606:CHL:HMB1	4:3:609:CHL:HAC1	1.94	0.49
4:1:607:CHL:HAA2	7:3:1622:XAT:H41	1.95	0.49
1:2:222:TRP:HZ2	2:3:138:LEU:HD22	1.78	0.49
5:2:603:CLA:HMD1	4:2:609:CHL:HBA2	1.94	0.49
1:2:103:GLN:HG3	1:2:110:LEU:HD13	1.96	0.48
1:2:176:LEU:HB3	5:2:610:CLA:H3A	1.95	0.48
7:3:1622:XAT:H393	9:3:2630:LHG:H101	1.94	0.48
3:4:143:GLU:H	3:4:146:TYR:HB2	1.79	0.48
1:2:96:VAL:HG12	1:2:99:LYS:H	1.78	0.48
1:2:87:ARG:HH12	1:2:210:ALA:HB2	1.79	0.48
1:2:51:LEU:HD13	5:2:602:CLA:H42	1.95	0.48
9:4:2630:LHG:O3	9:4:2630:LHG:O1	2.24	0.48
7:1:1622:XAT:H41	4:2:607:CHL:HAA2	1.95	0.48
4:3:608:CHL:H2A	4:3:608:CHL:HED3	1.96	0.47
3:4:37:PRO:HD2	7:4:622:XAT:H242	1.95	0.47
1:2:118:LEU:HD23	4:2:605:CHL:HED2	1.96	0.47
2:3:116:SER:OG	2:3:119:GLY:O	2.33	0.47
2:3:30:ARG:NH1	2:3:46:THR:O	2.48	0.47
2:3:53:TYR:HB2	5:3:602:CLA:HMD1	1.96	0.47
5:1:613:CLA:H61	5:1:613:CLA:H2	1.60	0.47
5:2:610:CLA:H43	5:2:612:CLA:HBA1	1.97	0.47
1:2:69:SER:HB3	1:2:184:GLY:HA3	1.96	0.47
2:3:128:LEU:HD23	4:3:605:CHL:HED2	1.96	0.47
3:4:29:LEU:HD11	3:4:51:ARG:HD3	1.97	0.47
5:3:611:CLA:HMB2	3:4:130:TRP:HB2	1.95	0.46
1:1:191:MET:HE2	6:1:1621:LUT:H12	1.96	0.46
5:1:613:CLA:H2	5:1:614:CLA:HMD1	1.97	0.46
1:2:153:ASP:OD2	1:2:156:TYR:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:17:TYR:HE2	1:1:174:ALA:HB1	1.81	0.46
10:4:623:BCR:H15C	10:4:623:BCR:H351	1.76	0.46
7:1:1622:XAT:H31	7:1:1622:XAT:H391	1.74	0.46
8:1:1623:NEX:H191	8:1:1623:NEX:H11	1.78	0.46
7:2:1622:XAT:H391	7:2:1622:XAT:H31	1.71	0.46
5:3:602:CLA:HBA1	6:3:1621:LUT:H382	1.98	0.46
2:3:72:ALA:HA	2:3:165:LEU:HD11	1.96	0.46
1:1:108:GLY:O	1:1:122:GLN:NE2	2.39	0.46
1:2:147:PRO:HB2	4:2:608:CHL:HBB2	1.98	0.46
4:3:606:CHL:HBC2	4:3:607:CHL:HHD	1.97	0.46
4:3:609:CHL:H91	4:3:609:CHL:H112	1.83	0.46
8:2:1623:NEX:H15	8:2:1623:NEX:H201	1.71	0.46
4:3:606:CHL:HBB1	4:3:606:CHL:HHC	1.98	0.46
3:4:131:SER:O	3:4:133:THR:OG1	2.24	0.46
5:3:611:CLA:HMB3	9:3:2630:LHG:HC11	1.99	0.45
1:1:104:ILE:HG21	1:1:124:ILE:HD13	1.98	0.45
1:1:18:GLY:O	1:1:21:ARG:NH1	2.40	0.45
5:1:610:CLA:CBB	6:1:1620:LUT:H32	2.46	0.45
3:4:173:LEU:HG	3:4:177:LYS:HE3	1.98	0.45
8:3:1623:NEX:H201	8:3:1623:NEX:H15	1.67	0.45
2:3:207:VAL:HG11	5:3:613:CLA:HAC2	1.99	0.44
4:2:606:CHL:HBC2	4:2:607:CHL:HHD	1.98	0.44
4:3:601:CHL:HAC1	9:3:2630:LHG:HC2	1.99	0.44
5:3:611:CLA:HMC1	9:3:2630:LHG:H311	1.98	0.44
6:4:620:LUT:H201	6:4:620:LUT:H15	1.79	0.44
2:3:173:ASP:OD1	6:3:1620:LUT:O23	2.24	0.43
3:4:51:ARG:HH21	3:4:144:GLN:HB2	1.82	0.43
6:1:1620:LUT:H201	6:1:1620:LUT:H15	1.86	0.43
4:1:607:CHL:H91	4:1:607:CHL:H112	1.79	0.43
4:4:601:CHL:H3A	4:4:601:CHL:HBA1	1.76	0.43
1:2:136:GLY:HA2	4:2:609:CHL:HAB	2.00	0.43
1:2:146:GLY:HA3	1:2:147:PRO:HD3	1.85	0.43
4:4:606:CHL:HBA2	10:4:623:BCR:H19C	2.00	0.43
1:1:215:ASP:OD2	1:1:218:ASN:ND2	2.46	0.43
7:2:1622:XAT:H363	9:2:2630:LHG:HC41	2.01	0.43
2:3:227:PRO:HG2	5:3:614:CLA:HMB3	2.01	0.43
2:3:202:MET:HE2	6:3:1621:LUT:H10	2.00	0.43
5:2:603:CLA:HBA1	5:2:603:CLA:H3A	1.80	0.43
5:3:613:CLA:HMB3	6:3:1620:LUT:H162	2.01	0.43
6:1:1621:LUT:H15	6:1:1621:LUT:H201	1.80	0.43
2:3:166:TYR:HB3	5:3:610:CLA:HED2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:192:LEU:HD13	5:4:603:CLA:HBB2	2.01	0.43
7:2:1622:XAT:H401	7:2:1622:XAT:H35	1.88	0.42
1:2:71:TRP:CE2	4:2:608:CHL:HED2	2.54	0.42
1:2:96:VAL:HB	1:2:99:LYS:HB2	2.01	0.42
3:4:8:SER:HB2	3:4:11:PRO:HD2	2.01	0.42
1:1:225:ALA:HA	7:1:1622:XAT:H42	2.02	0.42
5:2:604:CLA:HBA1	4:2:606:CHL:C1D	2.49	0.42
10:4:623:BCR:H11C	10:4:623:BCR:H341	1.85	0.42
7:2:1622:XAT:H202	2:3:138:LEU:HD21	2.01	0.42
6:4:620:LUT:H401	6:4:620:LUT:H35	1.80	0.42
2:3:181:PRO:HA	2:3:184:PHE:HB3	2.02	0.42
1:1:63:GLU:HA	1:1:155:LEU:HD11	2.01	0.42
6:3:1620:LUT:H401	6:3:1620:LUT:H35	1.86	0.41
4:2:601:CHL:H3A	4:3:609:CHL:HMB2	2.01	0.41
1:1:170:PRO:HA	1:1:173:PHE:HB3	2.00	0.41
7:4:622:XAT:H15	7:4:622:XAT:H201	1.82	0.41
8:1:1623:NEX:H35	8:1:1623:NEX:H401	1.93	0.41
1:1:57:THR:HG22	1:1:61:ASN:HD21	1.85	0.41
5:2:612:CLA:HBB1	6:2:1620:LUT:C13	2.51	0.41
1:2:196:VAL:HG12	5:2:613:CLA:HMD3	2.02	0.41
1:1:54:ASP:HA	1:1:55:PRO:HD3	1.95	0.41
1:1:44:TYR:N	5:1:602:CLA:OBD	2.40	0.41
5:3:610:CLA:CBB	6:3:1620:LUT:H32	2.51	0.41
1:1:52:SER:HB3	1:1:58:PHE:HD1	1.85	0.41
5:1:602:CLA:H92	5:1:603:CLA:HMA1	2.02	0.41
5:2:602:CLA:CBB	6:2:1621:LUT:H32	2.50	0.41
8:3:1623:NEX:H191	8:3:1623:NEX:H11	1.80	0.41
8:3:1623:NEX:H35	8:3:1623:NEX:H401	1.87	0.41
5:3:613:CLA:H61	5:3:613:CLA:H2	1.81	0.41
5:1:612:CLA:HBB1	6:1:1620:LUT:H35	2.03	0.41
2:3:223:HIS:CG	5:3:613:CLA:HAA2	2.56	0.41
3:4:128:THR:OG1	3:4:133:THR:N	2.53	0.41
1:1:118:LEU:HA	1:1:118:LEU:HD23	1.86	0.41
5:1:603:CLA:HBA1	5:1:603:CLA:H3A	1.78	0.41
1:1:101:GLY:HA2	4:1:606:CHL:HAC2	2.03	0.41
6:2:1620:LUT:H15	6:2:1620:LUT:H201	1.85	0.41
4:1:607:CHL:HED1	2:3:240:VAL:HG13	2.02	0.41
3:4:176:LEU:HB3	5:4:610:CLA:H3A	2.02	0.41
4:1:601:CHL:HMB2	4:2:609:CHL:HMB1	2.03	0.41
1:2:155:LEU:HA	1:2:155:LEU:HD23	1.89	0.41
4:1:609:CHL:H42	5:3:602:CLA:H143	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:86:LEU:HD23	5:3:604:CLA:HMC1	2.03	0.41
3:4:203:THR:HG22	3:4:205:LEU:H	1.86	0.40
7:1:1622:XAT:H15	7:1:1622:XAT:H201	1.76	0.40
7:3:1622:XAT:H201	7:3:1622:XAT:H15	1.78	0.40
5:3:602:CLA:H111	5:3:602:CLA:H93	1.86	0.40
6:2:1621:LUT:H191	6:2:1621:LUT:H11	1.98	0.40
6:3:1620:LUT:H31	6:3:1620:LUT:H391	1.94	0.40
1:1:136:GLY:HA2	4:1:609:CHL:HAB	2.03	0.40
1:1:140:GLY:HA3	2:3:37:PHE:CD2	2.57	0.40
2:3:155:GLY:HA2	4:3:608:CHL:HAC1	2.04	0.40
3:4:81:GLU:HA	4:4:607:CHL:HED2	2.03	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 PDB entries followed by that with respect to all EM entries.

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	1	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
All	All	844/917 (92%)	809 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
All	All	671/719 (93%)	671 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	2	61	ASN
1	2	88	ASN
2	3	95	GLN
2	3	219	ASN
3	4	72	GLN
3	4	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

72 ligands 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$
6	LUT	1	1620	-	41,43,43	0.91	2 (4%)	50,60,60	2.03	15 (30%)
6	LUT	1	1621	-	41,43,43	1.02	3 (7%)	50,60,60	1.96	17 (34%)
7	XAT	1	1622	-	39,47,47	0.93	1 (2%)	54,74,74	2.89	21 (38%)
8	NEX	1	1623	-	38,46,46	1.11	4 (10%)	49,70,70	2.65	18 (36%)
9	LHG	1	2630	5	40,40,48	0.73	1 (2%)	41,46,54	1.36	6 (14%)
4	CHL	1	601	1	41,54,74	5.23	27 (65%)	24,90,114	3.44	14 (58%)
5	CLA	1	602	1	52,69,73	1.21	7 (13%)	60,108,113	1.39	9 (15%)
5	CLA	1	603	1	46,63,73	1.34	8 (17%)	53,101,113	1.52	11 (20%)
5	CLA	1	604	-	41,58,73	1.38	8 (19%)	47,95,113	1.53	9 (19%)
4	CHL	1	605	1	41,54,74	5.12	24 (58%)	24,90,114	3.45	15 (62%)
4	CHL	1	606	-	41,54,74	5.20	27 (65%)	24,90,114	3.37	14 (58%)
4	CHL	1	607	-	61,71,74	4.29	27 (44%)	46,110,114	2.69	16 (34%)
4	CHL	1	608	-	41,54,74	5.25	27 (65%)	24,90,114	3.41	14 (58%)
4	CHL	1	609	1	60,70,74	4.43	28 (46%)	46,109,114	2.76	17 (36%)
5	CLA	1	610	1	47,64,73	1.22	6 (12%)	54,102,113	1.47	8 (14%)
5	CLA	1	611	9	33,53,73	1.39	7 (21%)	37,89,113	1.52	7 (18%)
5	CLA	1	612	1	33,53,73	1.42	7 (21%)	37,89,113	1.67	10 (27%)
5	CLA	1	613	1	46,63,73	1.22	8 (17%)	53,101,113	1.40	7 (13%)
5	CLA	1	614	1	33,53,73	1.37	6 (18%)	37,89,113	1.50	5 (13%)
6	LUT	2	1620	-	41,43,43	0.79	0	50,60,60	1.84	16 (32%)
6	LUT	2	1621	-	41,43,43	0.85	1 (2%)	50,60,60	1.83	16 (32%)
7	XAT	2	1622	-	39,47,47	1.00	0	54,74,74	3.01	22 (40%)
8	NEX	2	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.45	13 (26%)
9	LHG	2	2630	5	36,36,48	0.72	1 (2%)	37,42,54	1.30	5 (13%)
4	CHL	2	601	1	41,54,74	5.10	26 (63%)	24,90,114	3.52	12 (50%)
5	CLA	2	602	1	52,69,73	1.16	5 (9%)	60,108,113	1.42	10 (16%)
5	CLA	2	603	1	46,63,73	1.23	7 (15%)	53,101,113	1.49	10 (18%)
5	CLA	2	604	-	33,53,73	1.35	8 (24%)	37,89,113	1.70	6 (16%)
4	CHL	2	605	1	41,54,74	4.99	24 (58%)	24,90,114	3.58	17 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	2	606	-	41,54,74	5.16	25 (60%)	24,90,114	3.47	14 (58%)
4	CHL	2	607	-	59,69,74	4.31	26 (44%)	45,108,114	2.76	18 (40%)
4	CHL	2	608	-	41,54,74	5.09	27 (65%)	24,90,114	3.31	12 (50%)
4	CHL	2	609	1	59,69,74	4.31	27 (45%)	45,108,114	2.82	20 (44%)
5	CLA	2	610	1	41,58,73	1.33	7 (17%)	47,95,113	1.32	7 (14%)
5	CLA	2	611	9	33,53,73	1.33	6 (18%)	37,89,113	1.61	8 (21%)
5	CLA	2	612	1	33,53,73	1.41	5 (15%)	37,89,113	1.68	10 (27%)
5	CLA	2	613	1	33,53,73	1.39	7 (21%)	37,89,113	1.51	6 (16%)
5	CLA	2	614	1	33,53,73	1.35	6 (18%)	37,89,113	1.55	6 (16%)
6	LUT	3	1620	-	41,43,43	0.97	3 (7%)	50,60,60	2.02	18 (36%)
6	LUT	3	1621	-	41,43,43	0.92	1 (2%)	50,60,60	1.68	12 (24%)
7	XAT	3	1622	-	39,47,47	1.16	4 (10%)	54,74,74	3.07	27 (50%)
8	NEX	3	1623	-	38,46,46	0.93	2 (5%)	49,70,70	2.51	16 (32%)
9	LHG	3	2630	5	46,46,48	0.77	1 (2%)	47,52,54	1.33	4 (8%)
4	CHL	3	601	2	62,72,74	4.36	27 (43%)	48,111,114	2.71	19 (39%)
5	CLA	3	602	2	51,68,73	1.18	7 (13%)	59,107,113	1.41	7 (11%)
5	CLA	3	603	2	46,63,73	1.26	9 (19%)	53,101,113	1.50	11 (20%)
5	CLA	3	604	-	33,53,73	1.43	7 (21%)	37,89,113	1.46	7 (18%)
4	CHL	3	605	2	41,54,74	5.04	25 (60%)	24,90,114	3.52	16 (66%)
4	CHL	3	606	-	41,54,74	5.22	26 (63%)	24,90,114	3.68	15 (62%)
4	CHL	3	607	-	51,61,74	4.57	27 (52%)	35,98,114	2.93	16 (45%)
4	CHL	3	608	-	41,54,74	5.19	27 (65%)	24,90,114	3.40	13 (54%)
4	CHL	3	609	2	59,69,74	4.31	27 (45%)	45,108,114	2.78	19 (42%)
5	CLA	3	610	2	51,68,73	1.21	7 (13%)	59,107,113	1.32	8 (13%)
5	CLA	3	611	9	46,63,73	1.38	6 (13%)	53,101,113	1.42	11 (20%)
5	CLA	3	612	2	33,53,73	1.48	8 (24%)	37,89,113	1.77	10 (27%)
5	CLA	3	613	2	49,66,73	1.22	7 (14%)	56,104,113	1.34	7 (12%)
5	CLA	3	614	2	39,56,73	1.25	5 (12%)	45,92,113	1.40	7 (15%)
9	LHG	4	2630	5	20,20,48	0.85	0	21,26,54	1.35	1 (4%)
4	CHL	4	601	3	36,53,74	5.08	21 (58%)	19,89,114	3.73	14 (73%)
5	CLA	4	602	3	33,53,73	1.31	6 (18%)	37,89,113	1.78	7 (18%)
5	CLA	4	603	3	33,53,73	1.39	6 (18%)	37,89,113	1.58	8 (21%)
5	CLA	4	604	-	33,53,73	1.44	7 (21%)	37,89,113	1.55	6 (16%)
4	CHL	4	606	-	41,54,74	5.06	26 (63%)	24,90,114	3.37	14 (58%)
4	CHL	4	607	-	41,54,74	5.02	25 (60%)	24,90,114	3.45	15 (62%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	4	608	-	41,54,74	5.10	25 (60%)	24,90,114	3.50	16 (66%)
4	CHL	4	609	3	41,54,74	5.11	25 (60%)	24,90,114	3.46	15 (62%)
5	CLA	4	610	3	33,53,73	1.43	7 (21%)	37,89,113	1.52	5 (13%)
5	CLA	4	611	9	33,53,73	1.41	6 (18%)	37,89,113	1.38	6 (16%)
5	CLA	4	612	3	33,53,73	1.32	5 (15%)	37,89,113	1.70	8 (21%)
6	LUT	4	620	-	41,43,43	0.95	3 (7%)	50,60,60	2.23	15 (30%)
7	XAT	4	622	-	39,47,47	0.95	1 (2%)	54,74,74	2.70	20 (37%)
10	BCR	4	623	-	41,41,41	0.76	0	56,56,56	2.18	14 (25%)

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
6	LUT	1	1620	-	-	0/29/67/67	0/2/2/2
6	LUT	1	1621	-	-	0/29/67/67	0/2/2/2
7	XAT	1	1622	-	-	0/31/93/93	0/2/4/4
8	NEX	1	1623	-	-	0/27/83/83	0/2/3/3
9	LHG	1	2630	5	-	0/45/45/53	0/0/0/0
4	CHL	1	601	1	-	0/15/153/177	0/0/9/9
5	CLA	1	602	1	3/3/19/25	0/33/131/135	0/0/9/9
5	CLA	1	603	1	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	1	604	-	3/3/17/25	0/19/117/135	0/0/9/9
4	CHL	1	605	1	-	0/15/153/177	0/0/9/9
4	CHL	1	606	-	-	0/15/153/177	0/0/9/9
4	CHL	1	607	-	-	0/38/174/177	0/0/9/9
4	CHL	1	608	-	-	0/15/153/177	0/0/9/9
4	CHL	1	609	1	-	0/37/173/177	0/0/9/9
5	CLA	1	610	1	3/3/18/25	0/27/125/135	0/0/9/9
5	CLA	1	611	9	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	1	612	1	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	1	613	1	2/2/18/25	0/25/123/135	0/0/9/9
5	CLA	1	614	1	3/3/16/25	0/11/111/135	0/0/9/9
6	LUT	2	1620	-	-	0/29/67/67	0/2/2/2
6	LUT	2	1621	-	-	0/29/67/67	0/2/2/2
7	XAT	2	1622	-	-	0/31/93/93	0/2/4/4
8	NEX	2	1623	-	-	0/27/83/83	0/2/3/3
9	LHG	2	2630	5	-	0/41/41/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	2	601	1	-	0/15/153/177	0/0/9/9
5	CLA	2	602	1	3/3/19/25	0/33/131/135	0/0/9/9
5	CLA	2	603	1	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	2	604	-	2/2/16/25	0/11/111/135	0/0/9/9
4	CHL	2	605	1	-	0/15/153/177	0/0/9/9
4	CHL	2	606	-	-	0/15/153/177	0/0/9/9
4	CHL	2	607	-	-	0/35/171/177	0/0/9/9
4	CHL	2	608	-	-	0/15/153/177	0/0/9/9
4	CHL	2	609	1	-	0/35/171/177	0/0/9/9
5	CLA	2	610	1	3/3/17/25	0/19/117/135	0/0/9/9
5	CLA	2	611	9	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	2	612	1	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	2	613	1	2/2/16/25	0/11/111/135	0/0/9/9
5	CLA	2	614	1	2/2/16/25	0/11/111/135	0/0/9/9
6	LUT	3	1620	-	-	0/29/67/67	0/2/2/2
6	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
7	XAT	3	1622	-	-	0/31/93/93	0/2/4/4
8	NEX	3	1623	-	-	0/27/83/83	0/2/3/3
9	LHG	3	2630	5	-	0/51/51/53	0/0/0/0
4	CHL	3	601	2	-	0/39/175/177	0/0/9/9
5	CLA	3	602	2	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	3	603	2	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	3	604	-	3/3/16/25	0/11/111/135	0/0/9/9
4	CHL	3	605	2	-	0/15/153/177	0/0/9/9
4	CHL	3	606	-	-	0/15/153/177	0/0/9/9
4	CHL	3	607	-	-	0/26/162/177	0/0/9/9
4	CHL	3	608	-	-	0/15/153/177	0/0/9/9
4	CHL	3	609	2	-	0/35/171/177	0/0/9/9
5	CLA	3	610	2	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	3	611	9	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	3	612	2	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	3	613	2	3/3/18/25	0/29/127/135	0/0/9/9
5	CLA	3	614	2	3/3/16/25	0/17/115/135	0/0/9/9
9	LHG	4	2630	5	-	0/23/23/53	0/0/0/0
4	CHL	4	601	3	-	0/9/151/177	0/0/9/9
5	CLA	4	602	3	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	603	3	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	604	-	2/2/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	4	606	-	-	0/15/153/177	0/0/9/9
4	CHL	4	607	-	-	0/15/153/177	0/0/9/9
4	CHL	4	608	-	-	0/15/153/177	0/0/9/9
4	CHL	4	609	3	-	0/15/153/177	0/0/9/9
5	CLA	4	610	3	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	611	9	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	612	3	3/3/16/25	0/11/111/135	0/0/9/9
6	LUT	4	620	-	-	0/29/67/67	0/2/2/2
7	XAT	4	622	-	-	0/31/93/93	0/2/4/4
10	BCR	4	623	-	-	0/29/63/63	0/2/2/2

All (826) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	606	CHL	C3D-C4D	-20.50	1.31	1.54
4	3	601	CHL	C3D-C4D	-20.47	1.31	1.54
4	1	601	CHL	C3D-C4D	-20.41	1.31	1.54
4	1	608	CHL	C3D-C4D	-20.35	1.31	1.54
4	1	609	CHL	C3D-C4D	-20.26	1.31	1.54
4	4	608	CHL	C3D-C4D	-20.15	1.31	1.54
4	2	601	CHL	C3D-C4D	-19.96	1.32	1.54
4	3	609	CHL	C3D-C4D	-19.90	1.32	1.54
4	1	606	CHL	C3D-C4D	-19.84	1.32	1.54
4	3	608	CHL	C3D-C4D	-19.81	1.32	1.54
4	2	609	CHL	C3D-C4D	-19.76	1.32	1.54
4	2	607	CHL	C3D-C4D	-19.74	1.32	1.54
4	1	605	CHL	C3D-C4D	-19.72	1.32	1.54
4	3	607	CHL	C3D-C4D	-19.61	1.32	1.54
4	1	607	CHL	C3D-C4D	-19.60	1.32	1.54
4	4	609	CHL	C3D-C4D	-19.58	1.32	1.54
4	2	606	CHL	C3D-C4D	-19.46	1.32	1.54
4	4	607	CHL	C3D-C4D	-19.42	1.32	1.54
4	4	606	CHL	C3D-C4D	-19.42	1.32	1.54
4	2	608	CHL	C3D-C4D	-19.38	1.32	1.54
4	3	605	CHL	C3D-C4D	-19.27	1.32	1.54
4	2	605	CHL	C3D-C4D	-19.14	1.32	1.54
4	4	601	CHL	C3D-C4D	-18.83	1.33	1.54
4	3	606	CHL	CHB-C4A	-8.78	1.31	1.52
4	1	609	CHL	CHB-C4A	-8.77	1.31	1.52
4	1	607	CHL	CHB-C4A	-8.65	1.32	1.52
4	3	601	CHL	CHB-C4A	-8.65	1.32	1.52
4	1	608	CHL	CHB-C4A	-8.64	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	606	CHL	CHB-C4A	-8.57	1.32	1.52
4	2	606	CHL	CHB-C4A	-8.53	1.32	1.52
4	1	608	CHL	C3B-C2B	-8.50	1.45	1.55
4	3	609	CHL	CHB-C4A	-8.50	1.32	1.52
4	4	609	CHL	CHB-C4A	-8.47	1.32	1.52
4	2	607	CHL	CHB-C4A	-8.45	1.32	1.52
4	2	609	CHL	CHB-C4A	-8.42	1.32	1.52
4	3	607	CHL	CHB-C4A	-8.42	1.32	1.52
4	3	608	CHL	CHB-C4A	-8.40	1.32	1.52
4	1	606	CHL	CHB-C4A	-8.39	1.32	1.52
4	2	605	CHL	CHB-C4A	-8.36	1.32	1.52
4	3	605	CHL	CHB-C4A	-8.36	1.32	1.52
4	4	607	CHL	CHB-C4A	-8.36	1.32	1.52
4	1	609	CHL	C1B-NB	-8.35	1.32	1.50
4	1	605	CHL	CHB-C4A	-8.34	1.32	1.52
4	4	608	CHL	CHB-C4A	-8.33	1.32	1.52
4	2	608	CHL	CHB-C4A	-8.32	1.32	1.52
4	2	601	CHL	CHB-C4A	-8.30	1.32	1.52
4	1	601	CHL	CHB-C4A	-8.27	1.32	1.52
4	1	607	CHL	C3B-C2B	-8.21	1.45	1.55
4	4	601	CHL	CHB-C4A	-8.15	1.33	1.52
4	2	606	CHL	C3B-C2B	-7.96	1.45	1.55
4	3	601	CHL	C3B-C2B	-7.96	1.45	1.55
4	4	609	CHL	C3B-C2B	-7.96	1.45	1.55
4	1	606	CHL	C1B-NB	-7.95	1.33	1.50
4	3	601	CHL	C1B-NB	-7.92	1.33	1.50
4	1	609	CHL	C4B-NB	-7.91	1.33	1.50
4	1	609	CHL	C3B-C2B	-7.91	1.45	1.55
4	3	609	CHL	C1B-NB	-7.88	1.33	1.50
4	3	608	CHL	C3B-C2B	-7.86	1.45	1.55
4	1	606	CHL	C3B-C2B	-7.83	1.45	1.55
4	2	609	CHL	C1B-NB	-7.82	1.33	1.50
4	3	607	CHL	C1B-NB	-7.82	1.33	1.50
4	2	607	CHL	C4B-NB	-7.80	1.33	1.50
4	1	601	CHL	C4B-NB	-7.78	1.33	1.50
4	3	609	CHL	C4B-NB	-7.75	1.33	1.50
4	1	608	CHL	C1B-NB	-7.74	1.33	1.50
4	3	601	CHL	C4B-NB	-7.73	1.33	1.50
4	3	606	CHL	C3B-C2B	-7.72	1.45	1.55
4	1	606	CHL	C4B-NB	-7.72	1.33	1.50
4	2	607	CHL	C1B-NB	-7.70	1.33	1.50
4	4	601	CHL	C4B-NB	-7.65	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	606	CHL	C1B-NB	-7.65	1.33	1.50
4	2	606	CHL	C4B-NB	-7.64	1.33	1.50
4	1	605	CHL	C4B-NB	-7.63	1.33	1.50
4	3	606	CHL	C1B-NB	-7.63	1.33	1.50
4	3	607	CHL	C3B-C2B	-7.63	1.46	1.55
4	2	608	CHL	C3B-C2B	-7.62	1.46	1.55
4	4	606	CHL	C1B-NB	-7.62	1.33	1.50
4	1	607	CHL	C1B-NB	-7.61	1.34	1.50
4	1	601	CHL	C3B-C2B	-7.61	1.46	1.55
4	3	606	CHL	C4B-NB	-7.60	1.34	1.50
4	4	608	CHL	C3B-C2B	-7.59	1.46	1.55
4	4	609	CHL	C4B-NB	-7.58	1.34	1.50
4	2	609	CHL	C4B-NB	-7.56	1.34	1.50
4	3	608	CHL	C4B-NB	-7.56	1.34	1.50
4	3	608	CHL	C1B-NB	-7.55	1.34	1.50
4	2	601	CHL	C1B-NB	-7.54	1.34	1.50
4	2	609	CHL	C3B-C2B	-7.54	1.46	1.55
4	3	605	CHL	C1B-NB	-7.53	1.34	1.50
4	1	607	CHL	C4B-NB	-7.51	1.34	1.50
4	4	609	CHL	C1B-NB	-7.51	1.34	1.50
4	4	608	CHL	C1B-NB	-7.50	1.34	1.50
4	4	607	CHL	C1B-NB	-7.49	1.34	1.50
4	3	605	CHL	C4B-NB	-7.48	1.34	1.50
4	1	605	CHL	C1B-NB	-7.48	1.34	1.50
4	2	601	CHL	C4B-NB	-7.48	1.34	1.50
4	4	601	CHL	C1B-NB	-7.47	1.34	1.50
4	1	601	CHL	C1B-NB	-7.46	1.34	1.50
4	4	607	CHL	C4B-NB	-7.46	1.34	1.50
4	4	606	CHL	C3B-C2B	-7.46	1.46	1.55
4	2	608	CHL	C1B-NB	-7.40	1.34	1.50
4	2	605	CHL	C4B-NB	-7.39	1.34	1.50
4	2	608	CHL	C4B-NB	-7.38	1.34	1.50
4	3	607	CHL	C4B-NB	-7.38	1.34	1.50
4	1	608	CHL	C4B-NB	-7.36	1.34	1.50
4	2	605	CHL	C1B-NB	-7.34	1.34	1.50
4	3	605	CHL	C3B-C2B	-7.30	1.46	1.55
4	1	605	CHL	C3B-C2B	-7.30	1.46	1.55
4	2	607	CHL	C3B-C2B	-7.28	1.46	1.55
4	4	608	CHL	C4B-NB	-7.25	1.34	1.50
4	2	601	CHL	C3B-C2B	-7.24	1.46	1.55
4	4	607	CHL	C3B-C2B	-7.22	1.46	1.55
4	4	606	CHL	C4B-NB	-7.16	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	605	CHL	C1D-ND	-7.15	1.34	1.50
4	2	607	CHL	C1D-ND	-7.13	1.35	1.50
4	3	601	CHL	C1D-ND	-7.12	1.35	1.50
4	2	605	CHL	C3B-C2B	-7.11	1.46	1.55
4	3	608	CHL	C1D-ND	-7.09	1.35	1.50
4	1	606	CHL	C1D-ND	-7.08	1.35	1.50
4	3	609	CHL	C3B-C2B	-7.07	1.46	1.55
4	3	607	CHL	C1D-ND	-7.04	1.35	1.50
4	1	608	CHL	C1D-ND	-7.03	1.35	1.50
4	1	601	CHL	C1D-ND	-6.96	1.35	1.50
4	3	606	CHL	C1D-ND	-6.94	1.35	1.50
4	1	609	CHL	C1D-ND	-6.94	1.35	1.50
4	4	607	CHL	C1D-ND	-6.93	1.35	1.50
4	2	606	CHL	C1D-ND	-6.91	1.35	1.50
4	4	606	CHL	C1D-ND	-6.87	1.35	1.50
4	3	605	CHL	C1D-ND	-6.86	1.35	1.50
4	2	609	CHL	C1D-ND	-6.85	1.35	1.50
4	2	608	CHL	C1D-ND	-6.83	1.35	1.50
4	3	609	CHL	C1D-ND	-6.78	1.35	1.50
4	2	601	CHL	C1D-ND	-6.78	1.35	1.50
4	4	608	CHL	C1D-ND	-6.78	1.35	1.50
4	1	608	CHL	C4D-ND	-6.75	1.35	1.50
4	2	605	CHL	C1D-ND	-6.74	1.35	1.50
4	1	609	CHL	C4D-ND	-6.73	1.35	1.50
4	1	601	CHL	C4D-ND	-6.73	1.35	1.50
4	4	601	CHL	C1D-ND	-6.69	1.35	1.50
4	4	608	CHL	C4D-ND	-6.68	1.35	1.50
4	3	608	CHL	C4D-ND	-6.67	1.36	1.50
4	1	605	CHL	C4D-ND	-6.66	1.36	1.50
4	1	607	CHL	C1D-ND	-6.66	1.36	1.50
4	3	609	CHL	C4D-ND	-6.58	1.36	1.50
4	4	609	CHL	C1D-ND	-6.54	1.36	1.50
4	2	608	CHL	C4D-ND	-6.51	1.36	1.50
4	2	609	CHL	C4D-ND	-6.48	1.36	1.50
4	4	601	CHL	C3B-C2B	-6.44	1.47	1.55
4	3	606	CHL	C4D-ND	-6.42	1.36	1.50
4	4	606	CHL	C4D-ND	-6.42	1.36	1.50
4	3	601	CHL	C4D-ND	-6.40	1.36	1.50
4	4	609	CHL	C4D-ND	-6.40	1.36	1.50
4	2	601	CHL	C4D-ND	-6.39	1.36	1.50
4	1	606	CHL	C4D-ND	-6.39	1.36	1.50
4	4	607	CHL	C4D-ND	-6.35	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	607	CHL	C4D-ND	-6.35	1.36	1.50
4	3	607	CHL	C4D-ND	-6.34	1.36	1.50
4	1	607	CHL	C4D-ND	-6.33	1.36	1.50
4	2	606	CHL	C4D-ND	-6.31	1.36	1.50
4	2	605	CHL	C4D-ND	-6.30	1.36	1.50
4	1	606	CHL	C3B-C4B	-6.25	1.47	1.54
4	1	609	CHL	C3B-C4B	-6.25	1.47	1.54
4	3	605	CHL	C4D-ND	-6.24	1.36	1.50
4	4	601	CHL	C4D-ND	-6.23	1.36	1.50
4	2	606	CHL	C3B-C4B	-6.23	1.47	1.54
4	4	609	CHL	C3B-C4B	-6.21	1.47	1.54
4	2	609	CHL	C3B-C4B	-6.18	1.47	1.54
4	1	601	CHL	C3B-C4B	-6.15	1.47	1.54
4	3	601	CHL	C3B-C4B	-6.11	1.47	1.54
4	2	608	CHL	C3B-C4B	-6.09	1.47	1.54
4	2	607	CHL	C3B-C4B	-6.08	1.47	1.54
4	3	608	CHL	C3B-C4B	-5.81	1.47	1.54
4	1	607	CHL	C4A-C3A	-5.81	1.46	1.53
4	1	605	CHL	C3B-C4B	-5.78	1.47	1.54
4	3	609	CHL	C3B-C4B	-5.54	1.48	1.54
4	2	605	CHL	C3B-C4B	-5.52	1.48	1.54
4	3	605	CHL	C3B-C4B	-5.51	1.48	1.54
4	3	608	CHL	CHD-C1D	-5.50	1.44	1.53
4	3	601	CHL	C4A-C3A	-5.49	1.47	1.53
4	4	607	CHL	C3B-C4B	-5.38	1.48	1.54
4	1	609	CHL	CHC-C4B	-5.29	1.45	1.53
4	4	608	CHL	CHD-C1D	-5.29	1.45	1.53
4	1	607	CHL	C3B-C4B	-5.26	1.48	1.54
4	3	601	CHL	CHD-C1D	-5.20	1.45	1.53
4	1	608	CHL	CHD-C1D	-5.18	1.45	1.53
4	1	606	CHL	CHD-C1D	-5.09	1.45	1.53
4	3	607	CHL	C4A-C3A	-5.07	1.47	1.53
4	1	609	CHL	C4A-C3A	-5.07	1.47	1.53
4	3	601	CHL	CHB-C1B	-5.05	1.45	1.53
4	4	608	CHL	C3B-C4B	-5.04	1.48	1.54
4	4	606	CHL	C3B-C4B	-5.02	1.48	1.54
4	2	601	CHL	C3B-C4B	-4.99	1.48	1.54
4	1	607	CHL	CHB-C1B	-4.98	1.45	1.53
4	4	601	CHL	C3B-C4B	-4.96	1.48	1.54
4	1	607	CHL	CHC-C4B	-4.94	1.45	1.53
4	1	608	CHL	C3B-C4B	-4.93	1.48	1.54
4	2	608	CHL	CHD-C1D	-4.93	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	607	CHL	C3B-C4B	-4.93	1.48	1.54
4	3	605	CHL	CHD-C1D	-4.86	1.45	1.53
4	2	601	CHL	CHD-C1D	-4.86	1.45	1.53
4	1	606	CHL	CHB-C1B	-4.85	1.45	1.53
4	4	609	CHL	CHD-C1D	-4.83	1.45	1.53
4	1	605	CHL	CHD-C1D	-4.83	1.45	1.53
4	2	606	CHL	C4A-C3A	-4.83	1.48	1.53
4	1	601	CHL	CHD-C1D	-4.81	1.45	1.53
4	1	608	CHL	CHB-C1B	-4.79	1.46	1.53
4	2	605	CHL	CHD-C1D	-4.76	1.46	1.53
4	3	607	CHL	CHD-C1D	-4.74	1.46	1.53
4	3	606	CHL	CHB-C1B	-4.74	1.46	1.53
4	4	609	CHL	CHB-C1B	-4.73	1.46	1.53
4	2	607	CHL	CHC-C4B	-4.73	1.46	1.53
4	4	601	CHL	C4A-C3A	-4.73	1.48	1.53
4	2	609	CHL	CHD-C1D	-4.72	1.46	1.53
4	1	601	CHL	C4A-C3A	-4.72	1.48	1.53
4	2	606	CHL	CHC-C4B	-4.71	1.46	1.53
4	1	605	CHL	CHC-C4B	-4.71	1.46	1.53
4	3	601	CHL	CHC-C4B	-4.70	1.46	1.53
4	3	606	CHL	C3B-C4B	-4.69	1.49	1.54
4	4	606	CHL	CHB-C1B	-4.69	1.46	1.53
4	4	606	CHL	CHD-C1D	-4.66	1.46	1.53
4	1	609	CHL	CHB-C1B	-4.66	1.46	1.53
4	1	601	CHL	CHC-C4B	-4.65	1.46	1.53
4	2	607	CHL	C4A-C3A	-4.64	1.48	1.53
4	4	606	CHL	C4A-C3A	-4.64	1.48	1.53
4	4	607	CHL	C4A-C3A	-4.64	1.48	1.53
4	1	607	CHL	CHD-C1D	-4.62	1.46	1.53
4	4	608	CHL	CHC-C4B	-4.62	1.46	1.53
4	4	609	CHL	C4A-C3A	-4.62	1.48	1.53
4	2	608	CHL	CHB-C1B	-4.60	1.46	1.53
4	3	609	CHL	CHC-C4B	-4.60	1.46	1.53
4	2	606	CHL	CHB-C1B	-4.59	1.46	1.53
4	2	609	CHL	CHC-C4B	-4.58	1.46	1.53
4	3	606	CHL	C4A-C3A	-4.56	1.48	1.53
4	3	606	CHL	CHD-C1D	-4.55	1.46	1.53
4	1	605	CHL	C4A-C3A	-4.52	1.48	1.53
4	3	607	CHL	CHB-C1B	-4.52	1.46	1.53
4	2	606	CHL	CHD-C1D	-4.51	1.46	1.53
4	3	608	CHL	CHB-C1B	-4.51	1.46	1.53
4	4	607	CHL	CHD-C1D	-4.50	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	605	CHL	CHB-C1B	-4.50	1.46	1.53
4	4	609	CHL	CHC-C4B	-4.49	1.46	1.53
4	2	601	CHL	C4A-C3A	-4.46	1.48	1.53
4	1	606	CHL	C4A-C3A	-4.46	1.48	1.53
4	2	607	CHL	CHB-C1B	-4.46	1.46	1.53
4	2	609	CHL	CHB-C1B	-4.42	1.46	1.53
4	3	609	CHL	C4A-C3A	-4.42	1.48	1.53
4	3	605	CHL	CHC-C4B	-4.41	1.46	1.53
4	4	608	CHL	C4A-C3A	-4.40	1.48	1.53
4	2	608	CHL	CHC-C4B	-4.40	1.46	1.53
4	4	607	CHL	CHC-C4B	-4.39	1.46	1.53
4	2	605	CHL	C4A-C3A	-4.38	1.48	1.53
4	2	601	CHL	CHC-C4B	-4.38	1.46	1.53
4	2	605	CHL	CHB-C1B	-4.37	1.46	1.53
4	3	609	CHL	CHB-C1B	-4.36	1.46	1.53
4	1	608	CHL	C4A-C3A	-4.35	1.48	1.53
4	3	608	CHL	C4A-C3A	-4.34	1.48	1.53
4	2	609	CHL	C4A-C3A	-4.33	1.48	1.53
4	1	601	CHL	CHB-C1B	-4.33	1.46	1.53
4	3	606	CHL	C1A-C2A	-4.32	1.48	1.53
4	2	601	CHL	CHB-C1B	-4.32	1.46	1.53
4	2	608	CHL	C4A-C3A	-4.30	1.48	1.53
4	4	607	CHL	CHB-C1B	-4.28	1.46	1.53
4	3	607	CHL	CHC-C4B	-4.28	1.46	1.53
4	1	605	CHL	CHB-C1B	-4.27	1.46	1.53
4	1	601	CHL	C3D-C2D	-4.27	1.43	1.55
4	1	606	CHL	CHC-C4B	-4.26	1.46	1.53
4	2	607	CHL	CHD-C1D	-4.23	1.46	1.53
4	3	609	CHL	CHD-C1D	-4.21	1.46	1.53
4	3	606	CHL	C1A-CHA	-4.18	1.47	1.53
4	3	605	CHL	C4A-C3A	-4.17	1.48	1.53
4	1	608	CHL	CHC-C4B	-4.16	1.47	1.53
4	4	606	CHL	CHC-C4B	-4.16	1.47	1.53
4	3	608	CHL	CHC-C4B	-4.16	1.47	1.53
4	2	601	CHL	C3D-C2D	-4.11	1.44	1.55
4	4	601	CHL	CHB-C1B	-4.10	1.47	1.53
4	1	608	CHL	C3D-C2D	-4.07	1.44	1.55
4	3	606	CHL	C3D-C2D	-4.07	1.44	1.55
4	3	601	CHL	C3D-C2D	-4.06	1.44	1.55
4	3	608	CHL	C3D-C2D	-4.06	1.44	1.55
4	1	609	CHL	CHD-C1D	-4.05	1.47	1.53
4	1	607	CHL	C3D-C2D	-4.01	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	601	CHL	C1A-CHA	-4.01	1.47	1.53
4	4	608	CHL	CHB-C1B	-3.99	1.47	1.53
4	2	605	CHL	CHC-C4B	-3.99	1.47	1.53
4	3	601	CHL	C1A-CHA	-3.96	1.47	1.53
4	4	601	CHL	CHD-C1D	-3.94	1.47	1.53
4	3	606	CHL	CHC-C4B	-3.94	1.47	1.53
4	1	606	CHL	C3D-C2D	-3.93	1.44	1.55
4	2	601	CHL	C1A-CHA	-3.92	1.47	1.53
4	3	601	CHL	C1A-C2A	-3.90	1.49	1.53
4	4	601	CHL	CHC-C4B	-3.89	1.47	1.53
4	1	609	CHL	CHC-C1C	-3.86	1.46	1.53
4	2	601	CHL	CHC-C1C	-3.86	1.46	1.53
4	1	606	CHL	CHD-C4C	-3.84	1.46	1.53
4	4	608	CHL	C3D-C2D	-3.84	1.45	1.55
4	4	609	CHL	C3D-C2D	-3.83	1.45	1.55
4	1	609	CHL	C3D-C2D	-3.82	1.45	1.55
4	1	601	CHL	C1A-C2A	-3.82	1.49	1.53
4	1	608	CHL	C1A-CHA	-3.80	1.47	1.53
5	3	611	CLA	C3B-C2B	-3.80	1.35	1.40
5	3	611	CLA	CMB-C2B	-3.79	1.43	1.51
4	1	609	CHL	C1A-CHA	-3.78	1.47	1.53
4	2	606	CHL	CHC-C1C	-3.78	1.46	1.53
4	3	605	CHL	CHC-C1C	-3.77	1.46	1.53
4	2	608	CHL	C3D-C2D	-3.75	1.45	1.55
4	1	605	CHL	C1A-CHA	-3.75	1.47	1.53
4	1	605	CHL	C1A-C2A	-3.75	1.49	1.53
4	4	609	CHL	CHC-C1C	-3.75	1.46	1.53
4	2	606	CHL	C3D-C2D	-3.74	1.45	1.55
4	3	609	CHL	C1A-CHA	-3.72	1.47	1.53
4	1	607	CHL	CHC-C1C	-3.72	1.46	1.53
4	1	608	CHL	CHD-C4C	-3.72	1.46	1.53
4	4	608	CHL	C1A-CHA	-3.70	1.48	1.53
4	3	607	CHL	CHD-C4C	-3.70	1.46	1.53
4	3	607	CHL	C3D-C2D	-3.69	1.45	1.55
4	3	609	CHL	C3D-C2D	-3.68	1.45	1.55
4	3	608	CHL	C1A-CHA	-3.67	1.48	1.53
4	2	608	CHL	CHC-C1C	-3.66	1.46	1.53
4	1	601	CHL	CHC-C1C	-3.65	1.46	1.53
4	4	608	CHL	CHC-C1C	-3.64	1.46	1.53
4	4	608	CHL	CHD-C4C	-3.64	1.46	1.53
4	4	606	CHL	C3D-C2D	-3.63	1.45	1.55
4	2	609	CHL	C3D-C2D	-3.62	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	604	CLA	C3B-C2B	-3.62	1.35	1.40
4	4	606	CHL	C1A-CHA	-3.60	1.48	1.53
4	3	609	CHL	CHC-C1C	-3.59	1.46	1.53
4	4	607	CHL	C3D-C2D	-3.56	1.45	1.55
4	3	601	CHL	CHD-C4C	-3.56	1.46	1.53
4	1	605	CHL	CHC-C1C	-3.56	1.46	1.53
5	1	604	CLA	CMB-C2B	-3.55	1.44	1.51
4	4	607	CHL	C1A-CHA	-3.55	1.48	1.53
4	2	607	CHL	C3D-C2D	-3.54	1.45	1.55
4	2	605	CHL	C3D-C2D	-3.49	1.46	1.55
4	1	606	CHL	CHC-C1C	-3.48	1.46	1.53
4	1	605	CHL	C3D-C2D	-3.48	1.46	1.55
5	1	603	CLA	C3B-C2B	-3.48	1.35	1.40
4	2	609	CHL	C1A-CHA	-3.48	1.48	1.53
4	3	605	CHL	C3D-C2D	-3.47	1.46	1.55
4	3	605	CHL	C1A-CHA	-3.46	1.48	1.53
4	2	609	CHL	CHC-C1C	-3.46	1.47	1.53
4	4	609	CHL	CHD-C4C	-3.45	1.47	1.53
8	1	1623	NEX	C7-C8	-3.44	1.26	1.32
4	4	607	CHL	CHC-C1C	-3.44	1.47	1.53
5	2	612	CLA	C3B-C2B	-3.43	1.35	1.40
4	2	608	CHL	CHD-C4C	-3.42	1.47	1.53
4	1	606	CHL	C1A-CHA	-3.41	1.48	1.53
4	3	601	CHL	C3B-CAB	-3.41	1.47	1.50
4	3	608	CHL	CHD-C4C	-3.40	1.47	1.53
4	2	606	CHL	CHD-C4C	-3.40	1.47	1.53
4	2	606	CHL	C1A-CHA	-3.38	1.48	1.53
4	4	606	CHL	CHC-C1C	-3.38	1.47	1.53
4	3	605	CHL	CHD-C4C	-3.37	1.47	1.53
4	1	607	CHL	CHD-C4C	-3.36	1.47	1.53
4	1	609	CHL	C2B-C1B	-3.36	1.46	1.53
4	2	607	CHL	C3B-CAB	-3.35	1.47	1.50
4	4	606	CHL	CHD-C4C	-3.35	1.47	1.53
4	1	605	CHL	CHD-C4C	-3.34	1.47	1.53
4	1	608	CHL	C2B-C1B	-3.34	1.46	1.53
4	3	601	CHL	CHC-C1C	-3.33	1.47	1.53
4	1	607	CHL	C1A-C2A	-3.31	1.49	1.53
4	3	606	CHL	CHD-C4C	-3.30	1.47	1.53
4	2	605	CHL	C1A-CHA	-3.30	1.48	1.53
4	3	606	CHL	CHC-C1C	-3.28	1.47	1.53
4	4	609	CHL	C1A-CHA	-3.27	1.48	1.53
5	3	612	CLA	C3B-C2B	-3.27	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	605	CHL	CBD-CAD	-3.26	1.48	1.53
4	1	608	CHL	CHC-C1C	-3.25	1.47	1.53
4	3	601	CHL	CBD-CAD	-3.25	1.48	1.53
4	2	609	CHL	CHD-C4C	-3.24	1.47	1.53
4	2	607	CHL	CHC-C1C	-3.24	1.47	1.53
5	1	612	CLA	C3B-C2B	-3.21	1.36	1.40
4	2	608	CHL	C1A-CHA	-3.20	1.48	1.53
5	3	610	CLA	C3B-C2B	-3.20	1.36	1.40
8	2	1623	NEX	C7-C8	-3.18	1.26	1.32
5	3	613	CLA	C3B-C2B	-3.18	1.36	1.40
4	2	605	CHL	CHD-C4C	-3.17	1.47	1.53
4	2	601	CHL	CHD-C4C	-3.17	1.47	1.53
4	2	607	CHL	C1A-CHA	-3.17	1.48	1.53
4	1	607	CHL	C1A-CHA	-3.16	1.48	1.53
4	4	601	CHL	C3D-C2D	-3.16	1.46	1.55
4	2	605	CHL	CHC-C1C	-3.15	1.47	1.53
4	2	606	CHL	C1A-C2A	-3.12	1.50	1.53
5	3	611	CLA	CMD-C2D	-3.11	1.44	1.51
4	1	601	CHL	CHD-C4C	-3.09	1.47	1.53
4	3	607	CHL	CHC-C1C	-3.09	1.47	1.53
4	1	608	CHL	CBD-CAD	-3.08	1.48	1.53
5	2	610	CLA	C3B-C2B	-3.07	1.36	1.40
4	1	609	CHL	C1A-C2A	-3.07	1.50	1.53
5	1	603	CLA	CMB-C2B	-3.07	1.45	1.51
5	4	610	CLA	CMD-C2D	-3.06	1.45	1.51
4	2	608	CHL	C3B-CAB	-3.06	1.47	1.50
5	3	604	CLA	CMB-C2B	-3.05	1.45	1.51
4	4	608	CHL	C1A-C2A	-3.05	1.50	1.53
5	3	612	CLA	CMD-C2D	-3.04	1.45	1.51
4	2	601	CHL	C2A-C3A	-3.04	1.49	1.55
5	4	604	CLA	C3B-C2B	-3.04	1.36	1.40
5	4	604	CLA	CMB-C2B	-3.04	1.45	1.51
4	1	606	CHL	C2B-C1B	-3.04	1.47	1.53
5	3	603	CLA	CMD-C2D	-3.04	1.45	1.51
4	1	607	CHL	CBD-CAD	-3.02	1.48	1.53
4	2	607	CHL	CHD-C4C	-3.02	1.47	1.53
4	3	608	CHL	C1A-C2A	-3.02	1.50	1.53
4	1	606	CHL	CBD-CAD	-3.02	1.48	1.53
5	3	604	CLA	C3B-C2B	-3.01	1.36	1.40
4	4	608	CHL	CBD-CAD	-3.01	1.48	1.53
4	2	609	CHL	C2B-C1B	-3.00	1.47	1.53
4	2	601	CHL	C1A-C2A	-2.99	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	608	CHL	C3B-CAB	-2.98	1.47	1.50
4	1	608	CHL	C3D-CAD	-2.98	1.45	1.51
4	4	607	CHL	CHD-C4C	-2.98	1.47	1.53
4	3	608	CHL	CHC-C1C	-2.98	1.47	1.53
5	1	610	CLA	C3B-C2B	-2.97	1.36	1.40
4	1	609	CHL	C3B-CAB	-2.97	1.47	1.50
4	2	609	CHL	CBD-CAD	-2.97	1.48	1.53
5	2	603	CLA	C3B-C2B	-2.97	1.36	1.40
4	1	608	CHL	C1A-C2A	-2.96	1.50	1.53
4	1	607	CHL	C2A-C3A	-2.96	1.49	1.55
5	3	603	CLA	C3B-C2B	-2.95	1.36	1.40
4	1	601	CHL	CBD-CAD	-2.94	1.48	1.53
4	3	609	CHL	CHD-C4C	-2.94	1.47	1.53
5	2	613	CLA	CMD-C2D	-2.94	1.45	1.51
4	3	606	CHL	C2A-C3A	-2.93	1.49	1.55
5	3	610	CLA	CMB-C2B	-2.93	1.45	1.51
4	4	608	CHL	C2A-C3A	-2.93	1.49	1.55
4	2	607	CHL	C1A-C2A	-2.92	1.50	1.53
4	1	608	CHL	C2A-C3A	-2.92	1.49	1.55
4	3	607	CHL	C1A-CHA	-2.91	1.49	1.53
4	1	606	CHL	C3B-CAB	-2.90	1.47	1.50
4	3	606	CHL	C2B-C1B	-2.89	1.47	1.53
4	1	609	CHL	CHD-C4C	-2.88	1.48	1.53
4	4	609	CHL	C3B-CAB	-2.88	1.47	1.50
4	4	608	CHL	C3D-CAD	-2.88	1.46	1.51
4	1	601	CHL	C3B-CAB	-2.88	1.47	1.50
4	2	605	CHL	C1A-C2A	-2.88	1.50	1.53
5	4	603	CLA	CMD-C2D	-2.87	1.45	1.51
4	2	606	CHL	C2B-C1B	-2.87	1.47	1.53
9	3	2630	LHG	O7-C5	-2.87	1.39	1.46
4	4	607	CHL	C1A-C2A	-2.86	1.50	1.53
4	1	607	CHL	C2B-C1B	-2.86	1.47	1.53
5	3	602	CLA	CMD-C2D	-2.86	1.45	1.51
4	2	606	CHL	C3B-CAB	-2.85	1.47	1.50
4	1	601	CHL	C3D-CAD	-2.84	1.46	1.51
4	2	609	CHL	C2A-C3A	-2.84	1.49	1.55
5	1	613	CLA	CMB-C2B	-2.84	1.45	1.51
4	3	608	CHL	C3D-CAD	-2.83	1.46	1.51
4	4	606	CHL	C2A-C3A	-2.83	1.49	1.55
5	2	610	CLA	CMB-C2B	-2.83	1.45	1.51
6	4	620	LUT	C22-C21	-2.82	1.51	1.54
5	3	610	CLA	C3B-CAB	-2.82	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	602	CLA	CMD-C2D	-2.82	1.45	1.51
4	3	601	CHL	C3D-CAD	-2.82	1.46	1.51
4	3	605	CHL	C1A-C2A	-2.82	1.50	1.53
5	3	612	CLA	CMB-C2B	-2.81	1.45	1.51
4	3	608	CHL	CBD-CAD	-2.81	1.48	1.53
5	3	613	CLA	CMB-C2B	-2.81	1.45	1.51
4	3	608	CHL	C2B-C1B	-2.81	1.47	1.53
4	1	607	CHL	C3B-CAB	-2.81	1.47	1.50
5	2	612	CLA	CMB-C2B	-2.81	1.45	1.51
5	2	604	CLA	CMB-C2B	-2.81	1.46	1.51
4	4	606	CHL	C2B-C1B	-2.81	1.47	1.53
4	4	601	CHL	CHC-C1C	-2.80	1.48	1.53
4	3	606	CHL	CBD-CAD	-2.80	1.48	1.53
4	1	609	CHL	C2A-C3A	-2.80	1.49	1.55
6	3	1620	LUT	C22-C21	-2.78	1.51	1.54
5	2	614	CLA	CMD-C2D	-2.78	1.45	1.51
4	3	607	CHL	CBD-CAD	-2.78	1.48	1.53
5	1	611	CLA	CMB-C2B	-2.78	1.46	1.51
5	1	612	CLA	CMB-C2B	-2.78	1.46	1.51
5	3	613	CLA	CMD-C2D	-2.77	1.45	1.51
5	1	614	CLA	CMD-C2D	-2.77	1.45	1.51
5	1	610	CLA	C3B-CAB	-2.77	1.42	1.47
5	4	612	CLA	CMD-C2D	-2.76	1.45	1.51
4	1	609	CHL	CBD-CAD	-2.76	1.48	1.53
5	2	603	CLA	CMD-C2D	-2.76	1.45	1.51
5	1	611	CLA	C3B-C2B	-2.76	1.36	1.40
8	3	1623	NEX	C7-C8	-2.76	1.27	1.32
5	1	602	CLA	CMD-C2D	-2.75	1.45	1.51
4	3	607	CHL	C3B-CAB	-2.75	1.48	1.50
5	3	614	CLA	CMB-C2B	-2.75	1.46	1.51
4	1	605	CHL	C3B-CAB	-2.75	1.48	1.50
4	2	606	CHL	CBD-CAD	-2.74	1.49	1.53
5	4	602	CLA	CMB-C2B	-2.74	1.46	1.51
5	1	604	CLA	CMD-C2D	-2.74	1.45	1.51
5	1	602	CLA	CMB-C2B	-2.73	1.46	1.51
5	3	603	CLA	CMB-C2B	-2.73	1.46	1.51
4	2	608	CHL	CBD-CAD	-2.72	1.49	1.53
5	1	603	CLA	CMD-C2D	-2.72	1.45	1.51
5	1	613	CLA	C3B-C2B	-2.72	1.36	1.40
7	3	1622	XAT	C10-C9	-2.72	1.32	1.35
4	2	606	CHL	C2A-C3A	-2.72	1.49	1.55
5	1	614	CLA	CMB-C2B	-2.71	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	609	CHL	C3B-CAB	-2.71	1.48	1.50
4	3	609	CHL	C1A-C2A	-2.71	1.50	1.53
5	1	613	CLA	CMD-C2D	-2.71	1.45	1.51
4	4	609	CHL	CBD-CAD	-2.70	1.49	1.53
4	2	608	CHL	C2A-C3A	-2.69	1.49	1.55
5	4	603	CLA	CMB-C2B	-2.69	1.46	1.51
4	1	607	CHL	C3D-CAD	-2.68	1.46	1.51
5	2	614	CLA	CMB-C2B	-2.68	1.46	1.51
4	3	607	CHL	C1A-C2A	-2.67	1.50	1.53
5	4	610	CLA	CMC-C2C	-2.67	1.45	1.50
4	3	608	CHL	C2A-C3A	-2.67	1.49	1.55
4	4	609	CHL	C2A-C3A	-2.66	1.49	1.55
5	1	602	CLA	C3B-C2B	-2.66	1.36	1.40
5	2	613	CLA	CMB-C2B	-2.66	1.46	1.51
4	3	609	CHL	C2B-C1B	-2.66	1.48	1.53
5	2	603	CLA	CMB-C2B	-2.65	1.46	1.51
4	3	605	CHL	C2A-C3A	-2.65	1.49	1.55
5	3	602	CLA	CMB-C2B	-2.65	1.46	1.51
5	3	610	CLA	CMD-C2D	-2.64	1.45	1.51
5	1	610	CLA	CMB-C2B	-2.64	1.46	1.51
5	4	611	CLA	CMD-C2D	-2.63	1.46	1.51
5	1	612	CLA	CMD-C2D	-2.63	1.46	1.51
5	2	610	CLA	CMD-C2D	-2.63	1.46	1.51
4	3	606	CHL	C3B-CAB	-2.63	1.48	1.50
4	2	605	CHL	CBD-CAD	-2.62	1.49	1.53
5	3	602	CLA	CMC-C2C	-2.62	1.45	1.50
5	2	611	CLA	CMD-C2D	-2.62	1.46	1.51
4	1	608	CHL	CBD-CGD	-2.62	1.47	1.52
4	4	607	CHL	CBD-CAD	-2.62	1.49	1.53
7	3	1622	XAT	C14-C13	-2.62	1.32	1.35
5	4	611	CLA	CMB-C2B	-2.61	1.46	1.51
5	2	604	CLA	CMD-C2D	-2.61	1.46	1.51
5	2	611	CLA	CMB-C2B	-2.61	1.46	1.51
5	4	604	CLA	CMD-C2D	-2.60	1.46	1.51
6	1	1621	LUT	C10-C9	-2.60	1.32	1.35
5	2	613	CLA	C3B-C2B	-2.60	1.36	1.40
4	4	607	CHL	C2A-C3A	-2.60	1.49	1.55
5	2	602	CLA	CMC-C2C	-2.60	1.45	1.50
4	3	601	CHL	C2B-C1B	-2.59	1.48	1.53
4	2	607	CHL	C2A-C3A	-2.59	1.49	1.55
4	1	606	CHL	C2A-C3A	-2.59	1.49	1.55
4	4	606	CHL	CBD-CAD	-2.58	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	602	CLA	CMB-C2B	-2.58	1.46	1.51
4	1	601	CHL	C2A-C3A	-2.57	1.49	1.55
5	4	610	CLA	CMB-C2B	-2.57	1.46	1.51
4	3	601	CHL	C2A-C3A	-2.57	1.49	1.55
4	4	601	CHL	CHD-C4C	-2.57	1.48	1.53
4	4	609	CHL	C2B-C1B	-2.57	1.48	1.53
4	2	605	CHL	C2A-C3A	-2.57	1.49	1.55
6	3	1621	LUT	C22-C21	-2.56	1.51	1.54
7	3	1622	XAT	C34-C33	-2.55	1.32	1.35
4	4	609	CHL	C1A-C2A	-2.54	1.50	1.53
4	4	606	CHL	C1A-C2A	-2.54	1.50	1.53
5	1	604	CLA	C3B-CAB	-2.53	1.42	1.47
4	2	609	CHL	C1A-C2A	-2.53	1.50	1.53
4	3	609	CHL	CBD-CAD	-2.53	1.49	1.53
4	2	601	CHL	C3D-CAD	-2.53	1.46	1.51
5	4	612	CLA	CMB-C2B	-2.52	1.46	1.51
5	1	610	CLA	CMD-C2D	-2.52	1.46	1.51
4	1	606	CHL	C3D-CAD	-2.51	1.46	1.51
6	1	1621	LUT	C1-C6	-2.51	1.50	1.53
5	3	604	CLA	CMD-C2D	-2.51	1.46	1.51
4	4	607	CHL	C2B-C1B	-2.50	1.48	1.53
5	1	611	CLA	CMD-C2D	-2.50	1.46	1.51
4	2	607	CHL	CBD-CAD	-2.50	1.49	1.53
5	2	612	CLA	CMD-C2D	-2.49	1.46	1.51
4	3	606	CHL	C3D-CAD	-2.49	1.46	1.51
4	1	607	CHL	CBD-CGD	-2.49	1.47	1.52
5	2	610	CLA	C3B-CAB	-2.49	1.42	1.47
5	1	602	CLA	C3B-CAB	-2.49	1.42	1.47
4	1	606	CHL	C1A-C2A	-2.49	1.50	1.53
6	1	1621	LUT	C22-C21	-2.49	1.51	1.54
4	3	607	CHL	C2B-C1B	-2.49	1.48	1.53
4	1	609	CHL	C3D-CAD	-2.48	1.46	1.51
4	2	601	CHL	CBD-CAD	-2.48	1.49	1.53
4	3	609	CHL	C2A-C3A	-2.47	1.50	1.55
4	2	608	CHL	C1A-C2A	-2.47	1.50	1.53
4	1	608	CHL	C3B-CAB	-2.47	1.48	1.50
4	1	601	CHL	CBD-CGD	-2.46	1.48	1.52
4	2	605	CHL	C3B-CAB	-2.46	1.48	1.50
5	3	614	CLA	CMD-C2D	-2.46	1.46	1.51
4	3	607	CHL	C2A-C3A	-2.45	1.50	1.55
4	2	608	CHL	C3D-CAD	-2.45	1.46	1.51
4	2	601	CHL	C2B-C1B	-2.45	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	602	CLA	CMC-C2C	-2.44	1.45	1.50
5	3	612	CLA	C3B-CAB	-2.44	1.43	1.47
5	3	604	CLA	C3B-CAB	-2.43	1.43	1.47
4	1	609	CHL	CBD-CGD	-2.42	1.48	1.52
5	2	604	CLA	C3B-C2B	-2.41	1.37	1.40
5	4	602	CLA	CMD-C2D	-2.39	1.46	1.51
5	4	604	CLA	C3B-CAB	-2.39	1.43	1.47
5	4	610	CLA	C3B-C2B	-2.38	1.37	1.40
4	1	601	CHL	C2B-C1B	-2.37	1.48	1.53
4	1	605	CHL	C2A-C3A	-2.36	1.50	1.55
4	3	601	CHL	CBD-CGD	-2.36	1.48	1.52
4	4	607	CHL	C3B-CAB	-2.36	1.48	1.50
4	4	609	CHL	C3D-CAD	-2.35	1.47	1.51
4	3	607	CHL	C3D-CAD	-2.34	1.47	1.51
4	3	605	CHL	C2B-C1B	-2.34	1.48	1.53
4	4	608	CHL	CBD-CGD	-2.33	1.48	1.52
9	1	2630	LHG	O7-C5	-2.33	1.40	1.46
5	1	603	CLA	C3B-CAB	-2.33	1.43	1.47
5	3	612	CLA	CMC-C2C	-2.32	1.45	1.50
4	4	608	CHL	C2B-C1B	-2.31	1.48	1.53
5	2	603	CLA	CMC-C2C	-2.29	1.45	1.50
5	4	611	CLA	C3B-C2B	-2.29	1.37	1.40
4	2	609	CHL	CBD-CGD	-2.29	1.48	1.52
5	2	610	CLA	CMC-C2C	-2.29	1.45	1.50
4	1	605	CHL	C2B-C1B	-2.28	1.48	1.53
5	1	603	CLA	CMC-C2C	-2.28	1.45	1.50
4	4	606	CHL	C3D-CAD	-2.27	1.47	1.51
5	3	611	CLA	C3B-CAB	-2.27	1.43	1.47
4	4	606	CHL	CBD-CGD	-2.27	1.48	1.52
4	2	606	CHL	C3D-CAD	-2.27	1.47	1.51
5	1	612	CLA	CMC-C2C	-2.26	1.45	1.50
4	3	607	CHL	CBD-CGD	-2.25	1.48	1.52
4	2	609	CHL	C3D-CAD	-2.25	1.47	1.51
5	2	614	CLA	C3B-C2B	-2.25	1.37	1.40
5	4	602	CLA	C3B-C2B	-2.25	1.37	1.40
4	2	607	CHL	C2B-C1B	-2.25	1.48	1.53
5	3	613	CLA	C3B-CAB	-2.25	1.43	1.47
7	3	1622	XAT	O4-C5	-2.24	1.42	1.46
4	1	605	CHL	CBD-CAD	-2.24	1.49	1.53
5	3	611	CLA	C4B-CHC	-2.24	1.34	1.40
4	3	609	CHL	C3D-CAD	-2.23	1.47	1.51
5	3	603	CLA	C3B-CAB	-2.23	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	610	CLA	CMC-C2C	-2.22	1.46	1.50
4	2	608	CHL	C2B-C1B	-2.22	1.48	1.53
5	1	610	CLA	CMC-C2C	-2.22	1.46	1.50
5	1	603	CLA	C4B-CHC	-2.22	1.34	1.40
5	4	603	CLA	C3B-C2B	-2.22	1.37	1.40
5	1	611	CLA	C3B-CAB	-2.20	1.43	1.47
5	3	613	CLA	CMC-C2C	-2.20	1.46	1.50
5	2	604	CLA	CMC-C2C	-2.20	1.46	1.50
5	3	603	CLA	CMC-C2C	-2.20	1.46	1.50
4	2	605	CHL	C2B-C1B	-2.19	1.48	1.53
5	1	603	CLA	CAC-C3C	-2.19	1.45	1.51
4	1	606	CHL	CBD-CGD	-2.19	1.48	1.52
5	1	612	CLA	C4B-CHC	-2.19	1.34	1.40
5	1	612	CLA	C3B-CAB	-2.18	1.43	1.47
5	4	602	CLA	CMC-C2C	-2.18	1.46	1.50
8	1	1623	NEX	O24-C25	-2.18	1.42	1.46
5	3	613	CLA	C4B-CHC	-2.17	1.34	1.40
5	1	614	CLA	C3B-C2B	-2.17	1.37	1.40
4	4	601	CHL	C2B-C1B	-2.17	1.48	1.53
4	3	608	CHL	CBD-CGD	-2.17	1.48	1.52
6	1	1620	LUT	C10-C9	-2.17	1.32	1.35
6	2	1621	LUT	C22-C21	-2.17	1.52	1.54
4	2	608	CHL	CBD-CGD	-2.17	1.48	1.52
5	4	611	CLA	C3B-CAB	-2.16	1.43	1.47
4	3	605	CHL	CBD-CGD	-2.16	1.48	1.52
5	3	614	CLA	C3B-C2B	-2.15	1.37	1.40
5	4	612	CLA	CMC-C2C	-2.15	1.46	1.50
4	3	609	CHL	C3B-CAB	-2.14	1.48	1.50
5	4	603	CLA	CMC-C2C	-2.14	1.46	1.50
4	3	605	CHL	C3B-CAB	-2.14	1.48	1.50
5	1	604	CLA	CMC-C2C	-2.14	1.46	1.50
6	1	1620	LUT	C30-C29	-2.14	1.33	1.35
5	2	613	CLA	C3B-CAB	-2.13	1.43	1.47
5	2	604	CLA	C4B-CHC	-2.13	1.34	1.40
4	4	601	CHL	C1A-CHA	-2.13	1.50	1.53
5	3	603	CLA	CAC-C3C	-2.13	1.45	1.51
5	2	603	CLA	C3B-CAB	-2.13	1.43	1.47
6	4	620	LUT	C1-C6	-2.13	1.50	1.53
4	3	609	CHL	CBD-CGD	-2.12	1.48	1.52
5	1	611	CLA	CMC-C2C	-2.12	1.46	1.50
9	2	2630	LHG	O7-C5	-2.12	1.41	1.46
8	1	1623	NEX	C22-C21	-2.12	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	613	CLA	CMC-C2C	-2.11	1.46	1.50
5	2	611	CLA	C3B-C2B	-2.11	1.37	1.40
6	3	1620	LUT	C14-C13	-2.10	1.33	1.35
5	1	613	CLA	C4B-CHC	-2.10	1.34	1.40
7	4	622	XAT	O4-C5	-2.09	1.43	1.46
5	4	610	CLA	C3B-CAB	-2.09	1.43	1.47
5	3	604	CLA	CMC-C2C	-2.09	1.46	1.50
5	1	613	CLA	C3B-CAB	-2.08	1.43	1.47
4	4	607	CHL	C3D-CAD	-2.08	1.47	1.51
5	4	604	CLA	CMC-C2C	-2.08	1.46	1.50
5	3	612	CLA	C4B-CHC	-2.08	1.34	1.40
4	1	609	CHL	CMB-C2B	-2.08	1.48	1.53
7	1	1622	XAT	O4-C5	-2.07	1.43	1.46
5	1	614	CLA	CMC-C2C	-2.07	1.46	1.50
5	3	603	CLA	C4B-CHC	-2.07	1.34	1.40
5	2	613	CLA	CMC-C2C	-2.06	1.46	1.50
8	1	1623	NEX	C30-C29	-2.06	1.33	1.35
4	2	607	CHL	C3D-CAD	-2.06	1.47	1.51
5	3	602	CLA	C3B-C2B	-2.06	1.37	1.40
6	3	1620	LUT	C30-C29	-2.05	1.33	1.35
5	2	611	CLA	CMC-C2C	-2.05	1.46	1.50
4	4	606	CHL	C3B-CAB	-2.05	1.48	1.50
8	3	1623	NEX	O24-C25	-2.05	1.43	1.46
6	4	620	LUT	C30-C29	-2.04	1.33	1.35
5	2	614	CLA	CMC-C2C	-2.03	1.46	1.50
4	4	601	CHL	C3D-CAD	-2.03	1.47	1.51
4	2	601	CHL	CBD-CGD	-2.01	1.48	1.52
5	2	604	CLA	C3B-CAB	-2.01	1.43	1.47
5	1	604	CLA	C4B-CHC	-2.01	1.34	1.40
4	3	606	CHL	CMD-C2D	-2.01	1.49	1.53
5	3	602	CLA	C3B-CAB	-2.00	1.43	1.47
4	1	606	CHL	C2D-C1D	-2.00	1.49	1.53
5	2	604	CLA	CHC-C1C	2.00	1.41	1.35
5	2	612	CLA	CHC-C1C	2.01	1.41	1.35
4	1	601	CHL	CMC-C2C	2.04	1.48	1.45
5	1	604	CLA	CHC-C1C	2.05	1.41	1.35
5	3	612	CLA	CHC-C1C	2.07	1.41	1.35
5	1	613	CLA	CHC-C1C	2.07	1.41	1.35
5	1	611	CLA	CHC-C1C	2.08	1.41	1.35
4	1	608	CHL	CMC-C2C	2.10	1.48	1.45
5	3	603	CLA	CHC-C1C	2.10	1.41	1.35
5	3	604	CLA	CHC-C1C	2.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	601	CHL	CMC-C2C	2.13	1.49	1.45
4	2	608	CHL	CMC-C2C	2.16	1.49	1.45
5	2	603	CLA	CHC-C1C	2.16	1.41	1.35
5	4	603	CLA	CHC-C1C	2.18	1.41	1.35
5	1	610	CLA	CHC-C1C	2.20	1.41	1.35
5	3	602	CLA	CHC-C1C	2.20	1.41	1.35
5	4	604	CLA	CHC-C1C	2.22	1.41	1.35
5	2	613	CLA	CHC-C1C	2.26	1.41	1.35
5	3	610	CLA	CHB-C4A	2.26	1.36	1.33
5	4	611	CLA	CHC-C1C	2.28	1.41	1.35
4	2	601	CHL	CMC-C2C	2.29	1.49	1.45
5	3	610	CLA	CHC-C1C	2.29	1.42	1.35
5	2	611	CLA	CHC-C1C	2.31	1.42	1.35
4	3	608	CHL	CMC-C2C	2.33	1.49	1.45
5	2	610	CLA	CHC-C1C	2.34	1.42	1.35
5	4	602	CLA	CHB-C4A	2.35	1.36	1.33
5	1	602	CLA	CHC-C1C	2.38	1.42	1.35
5	3	614	CLA	CHC-C1C	2.39	1.42	1.35
5	4	610	CLA	CHC-C1C	2.40	1.42	1.35
5	4	612	CLA	CHC-C1C	2.41	1.42	1.35
5	1	614	CLA	CHC-C1C	2.41	1.42	1.35
5	1	604	CLA	CHB-C4A	2.42	1.36	1.33
5	2	602	CLA	CHC-C1C	2.44	1.42	1.35
5	4	602	CLA	CHC-C1C	2.44	1.42	1.35
5	2	614	CLA	CHC-C1C	2.44	1.42	1.35
5	1	602	CLA	CHB-C4A	2.47	1.36	1.33
5	2	603	CLA	CHB-C4A	2.50	1.36	1.33
5	2	614	CLA	CHB-C4A	2.54	1.36	1.33
5	2	604	CLA	CHB-C4A	2.54	1.36	1.33
5	1	613	CLA	CHB-C4A	2.58	1.36	1.33
5	4	612	CLA	CHB-C4A	2.60	1.36	1.33
5	4	610	CLA	CHB-C4A	2.61	1.36	1.33
5	3	603	CLA	CHB-C4A	2.62	1.36	1.33
5	3	613	CLA	CHB-C4A	2.65	1.36	1.33
5	1	612	CLA	CHB-C4A	2.67	1.36	1.33
5	2	613	CLA	CHB-C4A	2.68	1.37	1.33
5	4	604	CLA	CHB-C4A	2.69	1.37	1.33
5	1	614	CLA	CHB-C4A	2.72	1.37	1.33
5	3	612	CLA	CHB-C4A	2.76	1.37	1.33
5	2	612	CLA	CHB-C4A	2.80	1.37	1.33
5	2	610	CLA	CHB-C4A	2.82	1.37	1.33
5	3	604	CLA	CHB-C4A	2.83	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	602	CLA	CHB-C4A	2.89	1.37	1.33
5	1	611	CLA	CHB-C4A	2.90	1.37	1.33
5	2	611	CLA	CHB-C4A	3.00	1.37	1.33
5	3	602	CLA	CHB-C4A	3.01	1.37	1.33
5	4	603	CLA	CHB-C4A	3.02	1.37	1.33
5	1	603	CLA	CHB-C4A	3.02	1.37	1.33
5	3	611	CLA	CHB-C4A	3.12	1.37	1.33
4	4	608	CHL	OBD-CAD	3.15	1.26	1.21
5	3	614	CLA	CHB-C4A	3.21	1.37	1.33
4	1	608	CHL	OBD-CAD	3.40	1.27	1.21
4	3	608	CHL	OBD-CAD	3.47	1.27	1.21
4	3	601	CHL	OBD-CAD	3.55	1.27	1.21
5	4	611	CLA	CHB-C4A	3.66	1.38	1.33
4	2	608	CHL	OBD-CAD	3.74	1.27	1.21
4	1	601	CHL	OBD-CAD	3.77	1.28	1.21
4	1	606	CHL	OBD-CAD	3.86	1.28	1.21
4	3	606	CHL	OBD-CAD	3.86	1.28	1.21
4	1	609	CHL	OBD-CAD	3.88	1.28	1.21
4	2	601	CHL	OBD-CAD	3.89	1.28	1.21
4	2	606	CHL	OBD-CAD	3.90	1.28	1.21
4	1	607	CHL	OBD-CAD	3.90	1.28	1.21
4	2	609	CHL	OBD-CAD	3.92	1.28	1.21
4	3	607	CHL	OBD-CAD	3.92	1.28	1.21
4	2	607	CHL	OBD-CAD	3.95	1.28	1.21
4	3	609	CHL	OBD-CAD	3.96	1.28	1.21
4	1	605	CHL	OBD-CAD	3.96	1.28	1.21
4	4	606	CHL	OBD-CAD	3.97	1.28	1.21
4	4	609	CHL	OBD-CAD	3.98	1.28	1.21
4	3	605	CHL	OBD-CAD	4.03	1.28	1.21
4	4	607	CHL	OBD-CAD	4.04	1.28	1.21
4	2	607	CHL	O2A-CGA	4.10	1.45	1.33
4	3	601	CHL	O2A-CGA	4.15	1.45	1.33
4	2	605	CHL	OBD-CAD	4.16	1.28	1.21
4	2	609	CHL	O2A-CGA	4.17	1.45	1.33
4	4	601	CHL	OBD-CAD	4.19	1.28	1.21
4	1	609	CHL	O2A-CGA	4.21	1.45	1.33
4	1	607	CHL	O2A-CGA	4.21	1.45	1.33
4	3	607	CHL	O2A-CGA	4.29	1.46	1.33
4	3	609	CHL	O2A-CGA	4.39	1.46	1.33
4	1	609	CHL	O2D-CGD	4.47	1.44	1.33
4	3	607	CHL	O2D-CGD	4.52	1.44	1.33
4	1	608	CHL	O2D-CGD	4.52	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	607	CHL	O2D-CGD	4.53	1.44	1.33
4	3	609	CHL	O2D-CGD	4.54	1.44	1.33
4	1	601	CHL	O2D-CGD	4.55	1.44	1.33
4	3	608	CHL	O2D-CGD	4.60	1.44	1.33
4	4	607	CHL	O2D-CGD	4.64	1.45	1.33
4	3	601	CHL	O2D-CGD	4.64	1.45	1.33
4	1	606	CHL	O2D-CGD	4.65	1.45	1.33
4	2	608	CHL	O2D-CGD	4.68	1.45	1.33
4	1	605	CHL	O2D-CGD	4.69	1.45	1.33
4	4	606	CHL	O2D-CGD	4.71	1.45	1.33
4	2	606	CHL	O2D-CGD	4.76	1.45	1.33
4	4	608	CHL	O2D-CGD	4.76	1.45	1.33
4	3	606	CHL	O2D-CGD	4.77	1.45	1.33
4	3	605	CHL	O2D-CGD	4.78	1.45	1.33
4	2	609	CHL	O2D-CGD	4.78	1.45	1.33
4	2	601	CHL	O2D-CGD	4.82	1.45	1.33
4	2	605	CHL	O2D-CGD	4.84	1.45	1.33
4	4	609	CHL	O2D-CGD	4.91	1.45	1.33
4	2	607	CHL	O2D-CGD	4.92	1.45	1.33
4	3	601	CHL	C3C-C2C	8.42	1.44	1.34
4	4	608	CHL	C3C-C2C	8.48	1.45	1.34
4	3	607	CHL	C3C-C2C	8.67	1.45	1.34
4	2	609	CHL	C3C-C2C	8.81	1.45	1.34
4	1	601	CHL	C3C-C2C	8.85	1.45	1.34
4	4	609	CHL	C3C-C2C	8.95	1.45	1.34
4	3	606	CHL	C3C-C2C	9.04	1.45	1.34
4	1	607	CHL	C3C-C2C	9.09	1.45	1.34
4	1	608	CHL	C3C-C2C	9.11	1.45	1.34
4	4	607	CHL	C3C-C2C	9.15	1.45	1.34
4	2	601	CHL	C3C-C2C	9.19	1.45	1.34
4	1	606	CHL	C3C-C2C	9.29	1.46	1.34
4	1	609	CHL	C3C-C2C	9.33	1.46	1.34
4	1	605	CHL	C3C-C2C	9.34	1.46	1.34
4	3	605	CHL	C3C-C2C	9.46	1.46	1.34
4	2	607	CHL	C3C-C2C	9.51	1.46	1.34
4	4	606	CHL	C3C-C2C	9.56	1.46	1.34
4	3	609	CHL	C3C-C2C	9.57	1.46	1.34
4	2	606	CHL	C3C-C2C	9.57	1.46	1.34
4	2	608	CHL	C3C-C2C	9.63	1.46	1.34
4	3	608	CHL	C3C-C2C	9.63	1.46	1.34
4	2	605	CHL	C3C-C2C	9.73	1.46	1.34
4	4	601	CHL	C3C-C2C	9.93	1.46	1.34

All (868) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	623	BCR	C24-C23-C22	-7.63	114.74	126.21
4	3	601	CHL	C1C-C2C-C3C	-7.30	104.24	111.52
4	2	601	CHL	C1C-C2C-C3C	-7.27	104.27	111.52
4	1	601	CHL	C1C-C2C-C3C	-7.06	104.48	111.52
6	4	620	LUT	C23-C24-C25	-7.04	118.63	125.22
4	2	607	CHL	CBA-CAA-C2A	-6.98	106.13	115.76
4	3	609	CHL	C1C-C2C-C3C	-6.91	104.63	111.52
4	1	609	CHL	C1C-C2C-C3C	-6.83	104.71	111.52
4	2	608	CHL	C1C-C2C-C3C	-6.78	104.76	111.52
4	2	609	CHL	C1C-C2C-C3C	-6.73	104.81	111.52
4	1	608	CHL	C1C-C2C-C3C	-6.72	104.82	111.52
4	4	608	CHL	C1C-C2C-C3C	-6.59	104.95	111.52
4	3	606	CHL	C1C-C2C-C3C	-6.57	104.97	111.52
4	3	605	CHL	C1C-C2C-C3C	-6.56	104.98	111.52
4	2	605	CHL	C1C-C2C-C3C	-6.51	105.03	111.52
4	2	606	CHL	C1C-C2C-C3C	-6.48	105.06	111.52
4	4	606	CHL	C1C-C2C-C3C	-6.41	105.14	111.52
4	4	609	CHL	C1C-C2C-C3C	-6.34	105.20	111.52
4	4	607	CHL	C1C-C2C-C3C	-6.30	105.24	111.52
4	1	606	CHL	C1C-C2C-C3C	-6.28	105.26	111.52
4	3	608	CHL	C1C-C2C-C3C	-6.25	105.29	111.52
4	4	601	CHL	C1C-C2C-C3C	-6.21	105.33	111.52
6	3	1620	LUT	C7-C8-C9	-6.13	117.00	126.21
6	1	1620	LUT	C23-C24-C25	-6.01	119.58	125.22
4	1	607	CHL	CBA-CAA-C2A	-5.96	107.54	115.76
7	4	622	XAT	C6-C7-C8	-5.84	113.64	125.99
7	3	1622	XAT	C31-C30-C29	-5.84	118.98	127.31
10	4	623	BCR	C28-C27-C26	-5.81	103.78	113.78
4	2	607	CHL	C1C-C2C-C3C	-5.79	105.75	111.52
7	3	1622	XAT	C27-C28-C29	-5.78	116.56	125.53
4	1	605	CHL	C1C-C2C-C3C	-5.75	105.78	111.52
4	3	601	CHL	CBC-CAC-C3C	-5.75	104.22	112.95
8	1	1623	NEX	C27-C28-C29	-5.62	116.81	125.53
7	3	1622	XAT	C6-C7-C8	-5.60	114.15	125.99
7	4	622	XAT	C38-C25-C26	-5.58	112.87	122.31
8	3	1623	NEX	C15-C14-C13	-5.54	119.40	127.31
7	3	1622	XAT	C15-C14-C13	-5.54	119.41	127.31
8	2	1623	NEX	C27-C28-C29	-5.51	116.98	125.53
7	4	622	XAT	C18-C5-C6	-5.25	113.43	122.31
6	2	1620	LUT	C23-C24-C25	-5.19	120.36	125.22
7	4	622	XAT	C26-C27-C28	-5.16	115.09	125.99
8	3	1623	NEX	C38-C25-C26	-4.99	113.88	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	623	BCR	C11-C10-C9	-4.98	120.21	127.31
10	4	623	BCR	C15-C14-C13	-4.96	120.23	127.31
4	1	607	CHL	C1C-C2C-C3C	-4.96	106.58	111.52
5	3	602	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
7	3	1622	XAT	C38-C25-C26	-4.93	113.96	122.31
7	2	1622	XAT	C38-C25-C26	-4.93	113.97	122.31
7	2	1622	XAT	C31-C30-C29	-4.88	120.35	127.31
6	4	620	LUT	C35-C34-C33	-4.86	120.38	127.31
4	3	607	CHL	C1C-C2C-C3C	-4.85	106.69	111.52
6	1	1620	LUT	C35-C34-C33	-4.83	120.42	127.31
7	3	1622	XAT	C11-C10-C9	-4.81	120.44	127.31
7	1	1622	XAT	C15-C14-C13	-4.80	120.46	127.31
7	1	1622	XAT	C27-C28-C29	-4.76	118.15	125.53
7	2	1622	XAT	C27-C28-C29	-4.74	118.17	125.53
7	2	1622	XAT	C15-C35-C34	-4.72	113.38	123.46
6	4	620	LUT	C7-C8-C9	-4.71	119.13	126.21
8	2	1623	NEX	C15-C14-C13	-4.71	120.59	127.31
7	2	1622	XAT	C7-C8-C9	-4.70	118.23	125.53
4	2	601	CHL	CBA-CAA-C2A	-4.69	108.91	115.66
5	2	602	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
6	4	620	LUT	C15-C14-C13	-4.67	120.65	127.31
4	3	607	CHL	CBA-CAA-C2A	-4.66	109.33	115.76
5	4	612	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
4	1	605	CHL	OMC-CMC-C2C	-4.63	118.39	124.29
8	2	1623	NEX	C38-C25-C26	-4.62	114.50	122.31
8	1	1623	NEX	C35-C34-C33	-4.61	120.74	127.31
4	1	607	CHL	OMC-CMC-C2C	-4.54	118.49	124.29
5	4	602	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
4	1	606	CHL	CBA-CAA-C2A	-4.50	109.18	115.66
10	4	623	BCR	C16-C17-C18	-4.48	120.92	127.31
6	1	1621	LUT	C15-C14-C13	-4.46	120.94	127.31
4	2	609	CHL	CHA-CBD-CGD	-4.46	104.66	115.00
5	2	604	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
7	1	1622	XAT	C31-C30-C29	-4.44	120.97	127.31
7	4	622	XAT	C35-C34-C33	-4.43	120.99	127.31
7	2	1622	XAT	C15-C14-C13	-4.42	121.00	127.31
8	1	1623	NEX	C38-C25-C26	-4.39	114.89	122.31
5	4	602	CLA	O2D-CGD-O1D	-4.36	115.05	123.82
7	1	1622	XAT	C38-C25-C26	-4.35	114.95	122.31
5	1	614	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
4	4	609	CHL	OMC-CMC-C2C	-4.31	118.79	124.29
4	2	606	CHL	CBA-CAA-C2A	-4.29	109.48	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	610	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
7	1	1622	XAT	C18-C5-C6	-4.24	115.14	122.31
8	1	1623	NEX	C17-C1-C6	-4.22	106.69	110.47
7	1	1622	XAT	C11-C10-C9	-4.22	121.29	127.31
7	4	622	XAT	C15-C14-C13	-4.20	121.31	127.31
5	1	613	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
4	4	608	CHL	CBC-CAC-C3C	-4.15	106.64	112.95
5	4	603	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
5	3	614	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
6	3	1621	LUT	C10-C11-C12	-4.13	110.56	123.23
6	2	1621	LUT	C35-C34-C33	-4.10	121.46	127.31
6	2	1621	LUT	C22-C23-C24	-4.08	107.11	111.73
7	2	1622	XAT	C18-C5-C6	-4.07	115.42	122.31
5	1	610	CLA	C1B-CHB-C4A	-4.05	122.09	130.12
4	2	605	CHL	C4A-C3A-C2A	-4.04	97.69	103.86
5	1	610	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
6	2	1620	LUT	C15-C14-C13	-4.01	121.58	127.31
5	2	614	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
4	2	609	CHL	CBC-CAC-C3C	-3.99	106.90	112.95
8	3	1623	NEX	C11-C10-C9	-3.96	121.65	127.31
6	2	1621	LUT	C23-C24-C25	-3.96	121.51	125.22
7	3	1622	XAT	C18-C5-C6	-3.96	115.62	122.31
6	1	1621	LUT	C35-C34-C33	-3.95	121.67	127.31
5	1	602	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
4	3	606	CHL	CBA-CAA-C2A	-3.94	109.98	115.66
8	3	1623	NEX	C27-C28-C29	-3.93	119.43	125.53
5	2	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
7	3	1622	XAT	C4-C3-C2	-3.88	102.78	110.68
5	4	604	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
5	1	604	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
4	1	609	CHL	CHA-CBD-CGD	-3.83	106.12	115.00
5	2	613	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
4	3	609	CHL	CHA-CBD-CGD	-3.79	106.22	115.00
6	1	1620	LUT	C10-C11-C12	-3.77	111.66	123.23
7	3	1622	XAT	C15-C35-C34	-3.73	115.50	123.46
7	1	1622	XAT	C6-C7-C8	-3.73	118.12	125.99
7	4	622	XAT	C4-C3-C2	-3.72	103.09	110.68
6	3	1620	LUT	C35-C34-C33	-3.72	122.01	127.31
5	2	613	CLA	C1B-CHB-C4A	-3.71	122.76	130.12
4	3	601	CHL	CBA-CAA-C2A	-3.70	110.66	115.76
5	1	604	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
7	3	1622	XAT	C35-C34-C33	-3.68	122.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	604	CLA	C1B-CHB-C4A	-3.68	122.82	130.12
7	2	1622	XAT	C11-C10-C9	-3.68	122.05	127.31
8	3	1623	NEX	C19-C9-C10	-3.68	117.77	122.92
6	1	1620	LUT	C15-C14-C13	-3.62	122.14	127.31
6	3	1620	LUT	C16-C1-C6	-3.62	104.44	110.31
5	2	614	CLA	C1B-CHB-C4A	-3.61	122.96	130.12
5	1	613	CLA	C1B-CHB-C4A	-3.61	122.96	130.12
5	1	611	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
5	2	614	CLA	O2D-CGD-O1D	-3.58	116.61	123.82
5	4	610	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
6	4	620	LUT	C31-C30-C29	-3.55	122.24	127.31
6	1	1620	LUT	C35-C15-C14	-3.54	115.91	123.46
4	3	607	CHL	OMC-CMC-C2C	-3.52	119.80	124.29
5	3	610	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
4	4	608	CHL	OMC-CMC-C2C	-3.50	119.82	124.29
5	2	610	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
5	3	612	CLA	OBD-CAD-CBD	-3.49	120.66	125.94
8	2	1623	NEX	C11-C10-C9	-3.46	122.37	127.31
5	2	612	CLA	C1B-CHB-C4A	-3.44	123.30	130.12
6	3	1621	LUT	C23-C24-C25	-3.43	122.00	125.22
5	4	602	CLA	C1B-CHB-C4A	-3.43	123.32	130.12
8	1	1623	NEX	C15-C35-C34	-3.43	116.14	123.46
5	3	613	CLA	C1B-CHB-C4A	-3.42	123.34	130.12
5	4	604	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
8	1	1623	NEX	C39-C29-C30	-3.40	118.16	122.92
6	2	1620	LUT	C35-C34-C33	-3.39	122.47	127.31
6	1	1620	LUT	C30-C31-C32	-3.39	112.84	123.23
6	1	1621	LUT	C18-C5-C6	-3.39	120.72	124.51
6	3	1620	LUT	C11-C10-C9	-3.37	122.49	127.31
5	3	610	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
5	3	604	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
5	3	612	CLA	O2D-CGD-O1D	-3.37	117.04	123.82
5	1	612	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
6	3	1621	LUT	C7-C8-C9	-3.36	121.16	126.21
8	2	1623	NEX	C39-C29-C30	-3.36	118.22	122.92
4	2	605	CHL	CBA-CAA-C2A	-3.36	110.82	115.66
4	3	606	CHL	CHA-CBD-CGD	-3.36	107.22	115.00
8	3	1623	NEX	C39-C29-C30	-3.35	118.23	122.92
10	4	623	BCR	C11-C12-C13	-3.34	117.02	126.42
8	1	1623	NEX	C11-C10-C9	-3.34	122.54	127.31
4	1	601	CHL	CBA-CAA-C2A	-3.34	110.85	115.66
7	4	622	XAT	C24-C23-C22	-3.32	103.92	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	3	1622	XAT	C35-C15-C14	-3.32	116.39	123.46
7	1	1622	XAT	C4-C3-C2	-3.31	103.93	110.68
5	1	602	CLA	OBD-CAD-CBD	-3.31	120.95	125.94
5	2	612	CLA	CAA-C2A-C3A	-3.30	103.77	112.81
6	3	1621	LUT	C35-C34-C33	-3.29	122.62	127.31
4	2	605	CHL	OMC-CMC-C2C	-3.28	120.10	124.29
5	1	614	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
5	2	603	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
6	1	1621	LUT	C10-C11-C12	-3.26	113.25	123.23
6	4	620	LUT	C11-C10-C9	-3.25	122.67	127.31
7	3	1622	XAT	C30-C31-C32	-3.24	113.29	123.23
6	3	1620	LUT	C15-C14-C13	-3.24	122.69	127.31
5	4	612	CLA	CAA-C2A-C3A	-3.22	103.98	112.81
5	3	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
5	1	603	CLA	OBD-CAD-CBD	-3.20	121.11	125.94
7	4	622	XAT	C10-C11-C12	-3.20	113.42	123.23
6	3	1620	LUT	C30-C31-C32	-3.20	113.43	123.23
6	1	1620	LUT	C31-C30-C29	-3.19	122.76	127.31
5	4	611	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
5	3	611	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
5	3	614	CLA	O2D-CGD-O1D	-3.16	117.47	123.82
6	3	1620	LUT	C35-C15-C14	-3.15	116.74	123.46
5	2	611	CLA	O2D-CGD-O1D	-3.15	117.49	123.82
5	3	603	CLA	CBC-CAC-C3C	-3.14	103.49	112.41
8	1	1623	NEX	C15-C14-C13	-3.13	122.84	127.31
6	1	1621	LUT	C15-C35-C34	-3.12	116.79	123.46
5	2	603	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
7	1	1622	XAT	C35-C34-C33	-3.09	122.89	127.31
5	2	611	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
4	2	607	CHL	C3B-CAB-CBB	-3.09	118.27	125.20
8	2	1623	NEX	C35-C34-C33	-3.09	122.91	127.31
4	3	608	CHL	C3B-CAB-CBB	-3.08	118.28	125.20
4	4	608	CHL	CMA-C3A-C2A	-3.08	105.59	115.84
5	1	603	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
7	1	1622	XAT	C7-C8-C9	-3.07	120.77	125.53
5	1	610	CLA	OBD-CAD-CBD	-3.07	121.31	125.94
8	3	1623	NEX	C11-C12-C13	-3.06	117.82	126.42
6	2	1621	LUT	C10-C11-C12	-3.05	113.86	123.23
5	1	612	CLA	CAA-C2A-C3A	-3.05	104.46	112.81
4	3	608	CHL	C4A-C3A-C2A	-3.04	99.20	103.86
5	3	612	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
6	2	1621	LUT	C30-C31-C32	-3.04	113.90	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	3	1622	XAT	C7-C8-C9	-3.03	120.82	125.53
8	1	1623	NEX	C24-C23-C22	-3.03	104.50	110.68
4	3	605	CHL	C4A-C3A-C2A	-3.03	99.23	103.86
8	2	1623	NEX	C24-C23-C22	-3.03	104.51	110.68
5	2	603	CLA	CAA-C2A-C3A	-3.03	104.50	112.81
5	3	612	CLA	CAA-C2A-C3A	-3.03	104.50	112.81
5	3	604	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
5	3	603	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
6	4	620	LUT	C30-C31-C32	-3.00	114.04	123.23
4	3	605	CHL	CHA-CBD-CGD	-3.00	108.05	115.00
4	3	609	CHL	CBC-CAC-C3C	-2.99	108.42	112.95
6	1	1621	LUT	C23-C24-C25	-2.98	122.42	125.22
5	1	602	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
6	4	620	LUT	C18-C5-C6	-2.97	121.18	124.51
6	2	1620	LUT	C31-C30-C29	-2.97	123.07	127.31
5	3	610	CLA	OBD-CAD-CBD	-2.96	121.47	125.94
5	2	602	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
5	1	604	CLA	O2D-CGD-O1D	-2.95	117.89	123.82
6	2	1621	LUT	C15-C14-C13	-2.94	123.11	127.31
6	3	1620	LUT	C10-C11-C12	-2.94	114.20	123.23
5	3	611	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
5	4	611	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
6	3	1621	LUT	C15-C14-C13	-2.93	123.12	127.31
5	1	611	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
7	1	1622	XAT	C15-C35-C34	-2.92	117.22	123.46
7	4	622	XAT	C31-C30-C29	-2.92	123.14	127.31
9	3	2630	LHG	O8-C6-C5	-2.91	101.33	108.66
5	1	603	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
8	1	1623	NEX	C26-C27-C28	-2.91	119.84	125.99
4	4	601	CHL	OMC-CMC-C2C	-2.90	120.58	124.29
10	4	623	BCR	C20-C21-C22	-2.90	123.17	127.31
6	1	1620	LUT	C8-C9-C10	-2.88	114.52	118.94
6	4	620	LUT	C15-C35-C34	-2.88	117.31	123.46
5	4	612	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
5	2	604	CLA	O2D-CGD-O1D	-2.87	118.04	123.82
6	2	1620	LUT	C30-C31-C32	-2.87	114.42	123.23
5	3	602	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
5	3	613	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
4	3	605	CHL	OMC-CMC-C2C	-2.86	120.64	124.29
4	4	607	CHL	OMC-CMC-C2C	-2.86	120.64	124.29
5	2	610	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
4	3	605	CHL	CBA-CAA-C2A	-2.82	111.59	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	1623	NEX	C31-C30-C29	-2.81	123.30	127.31
4	4	601	CHL	C4A-C3A-C2A	-2.79	99.59	103.86
7	2	1622	XAT	C35-C34-C33	-2.79	123.32	127.31
6	2	1620	LUT	C10-C11-C12	-2.79	114.69	123.23
8	1	1623	NEX	C30-C31-C32	-2.78	114.71	123.23
7	3	1622	XAT	C24-C23-C22	-2.77	105.04	110.68
8	1	1623	NEX	C11-C12-C13	-2.76	118.66	126.42
5	3	614	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
5	4	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
5	3	612	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
8	3	1623	NEX	C35-C34-C33	-2.75	123.38	127.31
5	2	613	CLA	O2D-CGD-O1D	-2.75	118.30	123.82
4	3	606	CHL	C4A-C3A-C2A	-2.74	99.67	103.86
5	2	612	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
4	4	606	CHL	CBC-CAC-C3C	-2.72	108.81	112.95
6	1	1621	LUT	C31-C30-C29	-2.71	123.44	127.31
7	3	1622	XAT	C10-C11-C12	-2.71	114.92	123.23
5	3	602	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
4	2	609	CHL	O1D-CGD-CBD	-2.69	118.97	124.53
4	3	609	CHL	OMC-CMC-C2C	-2.69	120.86	124.29
4	3	601	CHL	C3B-CAB-CBB	-2.69	119.17	125.20
6	2	1620	LUT	C15-C35-C34	-2.68	117.74	123.46
5	1	612	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
5	4	603	CLA	CAA-C2A-C3A	-2.67	105.49	112.81
4	1	605	CHL	O2D-CGD-O1D	-2.66	118.46	123.82
4	3	605	CHL	CBC-CAC-C3C	-2.66	108.91	112.95
5	1	603	CLA	CBC-CAC-C3C	-2.66	104.87	112.41
8	3	1623	NEX	C15-C35-C34	-2.66	117.79	123.46
4	2	606	CHL	CBC-CAC-C3C	-2.65	108.93	112.95
4	2	606	CHL	C4A-C3A-C2A	-2.65	99.81	103.86
5	2	610	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
4	4	601	CHL	CBC-CAC-C3C	-2.63	108.95	112.95
4	4	607	CHL	CHA-CBD-CGD	-2.63	108.90	115.00
6	1	1621	LUT	C8-C7-C6	-2.63	119.90	127.25
10	4	623	BCR	C7-C8-C9	-2.62	122.27	126.21
4	4	606	CHL	OMC-CMC-C2C	-2.62	120.94	124.29
6	3	1621	LUT	C30-C31-C32	-2.62	115.20	123.23
10	4	623	BCR	C1-C6-C5	-2.60	118.93	122.59
6	4	620	LUT	C35-C15-C14	-2.59	117.92	123.46
5	3	603	CLA	CAA-C2A-C3A	-2.59	105.70	112.81
4	1	606	CHL	CBC-CAC-C3C	-2.59	109.02	112.95
5	2	602	CLA	O2D-CGD-O1D	-2.58	118.62	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	609	CHL	CHA-CBD-CGD	-2.58	109.01	115.00
5	1	612	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
5	1	603	CLA	CAA-C2A-C3A	-2.58	105.75	112.81
7	2	1622	XAT	C6-C7-C8	-2.57	120.55	125.99
5	1	602	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
5	4	610	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
6	1	1621	LUT	C30-C31-C32	-2.57	115.35	123.23
6	3	1620	LUT	C31-C30-C29	-2.57	123.65	127.31
6	3	1621	LUT	C38-C25-C24	-2.57	118.15	123.68
4	3	609	CHL	O1D-CGD-CBD	-2.57	119.23	124.53
6	2	1620	LUT	C8-C7-C6	-2.56	120.07	127.25
5	2	603	CLA	O2D-CGD-O1D	-2.56	118.66	123.82
6	4	620	LUT	C8-C7-C6	-2.56	120.08	127.25
7	4	622	XAT	C15-C35-C34	-2.56	118.00	123.46
5	4	604	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
4	1	608	CHL	CBC-CAC-C3C	-2.55	109.08	112.95
4	1	601	CHL	C3B-CAB-CBB	-2.54	119.49	125.20
4	2	608	CHL	C3B-CAB-CBB	-2.54	119.50	125.20
5	2	612	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
6	3	1620	LUT	C23-C24-C25	-2.53	122.85	125.22
5	3	611	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
6	3	1620	LUT	C38-C25-C24	-2.52	118.26	123.68
9	3	2630	LHG	C11-C10-C9	-2.52	101.49	114.45
7	1	1622	XAT	C5-C4-C3	-2.51	107.82	112.64
8	3	1623	NEX	C24-C23-C22	-2.50	105.58	110.68
4	3	601	CHL	O1D-CGD-CBD	-2.50	119.37	124.53
6	3	1620	LUT	C37-C21-C22	-2.50	104.65	109.42
5	2	602	CLA	OBD-CAD-CBD	-2.49	122.18	125.94
5	3	604	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
4	2	607	CHL	C4A-C3A-C2A	-2.48	100.07	103.86
6	1	1621	LUT	O3-C3-C2	-2.48	104.83	109.86
7	2	1622	XAT	C10-C11-C12	-2.47	115.65	123.23
8	3	1623	NEX	C20-C13-C14	-2.47	119.46	122.92
4	1	601	CHL	CBC-CAC-C3C	-2.47	109.20	112.95
4	2	605	CHL	O1D-CGD-CBD	-2.47	119.44	124.53
5	4	611	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
6	2	1621	LUT	C8-C7-C6	-2.46	120.38	127.25
5	4	603	CLA	O2D-CGD-O1D	-2.45	118.88	123.82
8	1	1623	NEX	C19-C9-C10	-2.44	119.51	122.92
4	2	605	CHL	CHA-CBD-CGD	-2.43	109.36	115.00
9	1	2630	LHG	C18-C17-C16	-2.43	101.96	114.45
5	1	604	CLA	OBD-CAD-CBD	-2.43	122.28	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	608	CHL	CHA-CBD-CGD	-2.42	109.38	115.00
6	2	1621	LUT	C31-C30-C29	-2.42	123.86	127.31
4	1	609	CHL	O1D-CGD-CBD	-2.42	119.54	124.53
4	3	609	CHL	O2D-CGD-O1D	-2.41	118.96	123.82
7	1	1622	XAT	C31-C32-C33	-2.41	119.64	126.42
5	1	604	CLA	C1-C2-C3	-2.41	122.87	126.68
5	4	612	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
7	3	1622	XAT	C39-C29-C30	-2.40	119.56	122.92
4	3	606	CHL	O1D-CGD-CBD	-2.40	119.57	124.53
7	3	1622	XAT	C25-C24-C23	-2.40	108.04	112.64
6	4	620	LUT	C1-C6-C5	-2.39	119.23	122.59
4	4	608	CHL	C4A-C3A-C2A	-2.39	100.21	103.86
4	1	605	CHL	C3B-CAB-CBB	-2.39	119.84	125.20
7	2	1622	XAT	C39-C29-C30	-2.39	119.58	122.92
5	1	611	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
5	1	613	CLA	O2D-CGD-O1D	-2.38	119.02	123.82
4	3	606	CHL	O2D-CGD-O1D	-2.38	119.03	123.82
6	1	1621	LUT	C8-C9-C10	-2.38	115.29	118.94
5	3	603	CLA	O2D-CGD-O1D	-2.38	119.04	123.82
6	1	1621	LUT	C7-C8-C9	-2.37	122.65	126.21
4	1	606	CHL	O1D-CGD-CBD	-2.37	119.63	124.53
9	1	2630	LHG	C20-C19-C18	-2.37	102.24	114.45
4	4	609	CHL	C4A-C3A-C2A	-2.37	100.24	103.86
5	2	602	CLA	CAA-CBA-CGA	-2.37	106.22	113.35
5	1	604	CLA	O2A-CGA-O1A	-2.37	117.68	123.55
10	4	623	BCR	C27-C26-C25	-2.36	119.27	122.74
4	4	609	CHL	O1D-CGD-CBD	-2.35	119.67	124.53
4	1	605	CHL	CHA-CBD-CGD	-2.35	109.55	115.00
6	2	1620	LUT	C35-C15-C14	-2.35	118.46	123.46
5	1	610	CLA	O2D-CGD-O1D	-2.34	119.10	123.82
9	2	2630	LHG	C11-C10-C9	-2.34	102.39	114.45
6	2	1621	LUT	C35-C15-C14	-2.34	118.47	123.46
7	3	1622	XAT	C32-C33-C34	-2.34	115.35	118.94
5	2	602	CLA	C1-C2-C3	-2.33	121.67	125.96
6	2	1621	LUT	C7-C8-C9	-2.33	122.72	126.21
5	1	610	CLA	O2A-CGA-O1A	-2.33	117.78	123.55
7	3	1622	XAT	C26-C27-C28	-2.32	121.08	125.99
6	3	1620	LUT	C18-C5-C6	-2.31	121.92	124.51
5	3	610	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
6	3	1621	LUT	C15-C35-C34	-2.31	118.53	123.46
6	3	1621	LUT	C18-C5-C6	-2.31	121.92	124.51
9	1	2630	LHG	C11-C10-C9	-2.30	102.59	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	609	CHL	CBA-CAA-C2A	-2.30	112.59	115.76
4	2	605	CHL	C3B-CAB-CBB	-2.29	120.05	125.20
4	2	609	CHL	OMC-CMC-C2C	-2.29	121.36	124.29
6	1	1620	LUT	C8-C7-C6	-2.29	120.83	127.25
6	2	1621	LUT	C38-C25-C24	-2.29	118.74	123.68
5	3	613	CLA	O2D-CGD-O1D	-2.27	119.26	123.82
8	2	1623	NEX	C20-C13-C14	-2.27	119.75	122.92
4	1	601	CHL	O1D-CGD-CBD	-2.26	119.86	124.53
7	4	622	XAT	C8-C9-C10	-2.25	115.48	118.94
6	4	620	LUT	C10-C11-C12	-2.25	116.32	123.23
4	3	606	CHL	CBC-CAC-C3C	-2.24	109.55	112.95
7	1	1622	XAT	C24-C23-C22	-2.24	106.12	110.68
4	1	608	CHL	O1D-CGD-CBD	-2.24	119.91	124.53
6	1	1620	LUT	C38-C25-C24	-2.23	118.87	123.68
7	1	1622	XAT	C39-C29-C30	-2.23	119.79	122.92
4	4	607	CHL	CBC-CAC-C3C	-2.23	109.56	112.95
4	2	609	CHL	C1-C2-C3	-2.23	121.85	125.96
4	1	608	CHL	C4A-C3A-C2A	-2.23	100.45	103.86
6	2	1620	LUT	C38-C25-C24	-2.22	118.90	123.68
5	3	610	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
4	4	608	CHL	O1D-CGD-CBD	-2.20	120.00	124.53
5	1	614	CLA	O2D-CGD-O1D	-2.19	119.42	123.82
5	1	612	CLA	CHA-C1A-NA	-2.19	121.10	126.18
4	2	607	CHL	C1-C2-C3	-2.18	121.94	125.96
5	3	611	CLA	CAA-C2A-C3A	-2.18	106.84	112.81
4	2	609	CHL	C6-C5-C3	-2.17	107.74	112.66
9	3	2630	LHG	C18-C17-C16	-2.17	103.28	114.45
6	2	1620	LUT	C8-C9-C10	-2.17	115.61	118.94
4	1	609	CHL	CBC-CAC-C3C	-2.17	109.66	112.95
5	3	611	CLA	C1C-NC-C4C	-2.16	105.81	107.06
6	2	1621	LUT	C16-C1-C6	-2.16	106.80	110.31
7	2	1622	XAT	C16-C1-C2	-2.15	105.16	108.97
8	2	1623	NEX	C30-C31-C32	-2.14	116.67	123.23
10	4	623	BCR	C21-C20-C19	-2.13	116.69	123.23
7	2	1622	XAT	C4-C3-C2	-2.13	106.34	110.68
4	4	606	CHL	O1D-CGD-CBD	-2.13	120.14	124.53
8	3	1623	NEX	C30-C31-C32	-2.13	116.71	123.23
9	2	2630	LHG	C27-C26-C25	-2.13	103.50	114.45
6	2	1621	LUT	C11-C10-C9	-2.13	124.28	127.31
6	1	1621	LUT	C22-C23-C24	-2.13	109.33	111.73
5	1	603	CLA	O2D-CGD-O1D	-2.12	119.56	123.82
4	3	607	CHL	CHA-CBD-CGD	-2.12	110.09	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	1621	LUT	C38-C25-C24	-2.12	119.12	123.68
5	2	603	CLA	O2A-CGA-O1A	-2.11	118.30	123.55
6	1	1621	LUT	C31-C32-C33	-2.11	120.48	126.42
9	1	2630	LHG	C27-C26-C25	-2.11	103.57	114.45
4	4	606	CHL	C4A-C3A-C2A	-2.11	100.64	103.86
10	4	623	BCR	C3-C4-C5	-2.10	110.17	113.78
5	2	612	CLA	C1C-NC-C4C	-2.08	105.86	107.06
7	3	1622	XAT	C11-C12-C13	-2.07	120.61	126.42
4	3	608	CHL	CMA-C3A-C2A	-2.06	108.98	115.84
4	2	609	CHL	CMA-C3A-C2A	-2.06	108.98	115.84
4	1	605	CHL	C4A-C3A-C2A	-2.06	100.71	103.86
7	1	1622	XAT	C10-C11-C12	-2.05	116.94	123.23
5	3	610	CLA	C1-C2-C3	-2.05	122.18	125.96
7	2	1622	XAT	C24-C23-C22	-2.05	106.51	110.68
5	3	611	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
6	3	1620	LUT	C15-C35-C34	-2.04	119.11	123.46
7	4	622	XAT	C30-C31-C32	-2.04	116.99	123.23
4	4	607	CHL	O2D-CGD-O1D	-2.03	119.73	123.82
6	3	1621	LUT	C31-C30-C29	-2.03	124.41	127.31
4	1	607	CHL	C4A-C3A-C2A	-2.03	100.76	103.86
5	3	603	CLA	CHA-C1A-NA	-2.03	121.47	126.18
9	2	2630	LHG	O8-C6-C5	-2.02	103.57	108.66
5	1	602	CLA	CHA-C1A-NA	-2.02	121.48	126.18
5	1	602	CLA	C1-C2-C3	-2.01	122.25	125.96
6	2	1620	LUT	C11-C10-C9	-2.01	124.44	127.31
7	2	1622	XAT	C19-C9-C10	-2.01	120.11	122.92
10	4	623	BCR	C4-C5-C6	-2.01	119.80	122.74
4	4	601	CHL	C3B-CAB-CBB	-2.01	120.69	125.20
4	3	601	CHL	O2D-CGD-O1D	-2.00	119.78	123.82
4	1	609	CHL	C4A-C3A-C2A	-2.00	100.80	103.86
7	2	1622	XAT	C31-C32-C33	-2.00	120.79	126.42
4	1	607	CHL	CAA-CBA-CGA	-2.00	107.32	113.35
5	4	612	CLA	O1D-CGD-CBD	2.00	128.20	124.60
5	2	603	CLA	C2A-C1A-CHA	2.00	127.47	123.92
4	1	607	CHL	C4-C3-C5	2.02	118.79	115.29
6	4	620	LUT	C20-C13-C12	2.02	121.33	118.10
5	2	603	CLA	C4A-NA-C1A	2.04	108.98	106.45
6	3	1621	LUT	C39-C29-C28	2.06	121.38	118.10
4	4	608	CHL	C4D-C3D-CAD	2.06	109.50	104.71
4	3	609	CHL	C4D-C3D-CAD	2.06	109.50	104.71
5	1	613	CLA	C4A-NA-C1A	2.06	109.01	106.45
5	3	613	CLA	C4A-NA-C1A	2.07	109.02	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1620	LUT	C1-C2-C3	2.07	117.88	113.40
5	2	602	CLA	O1D-CGD-CBD	2.07	128.33	124.60
4	2	606	CHL	CED-O2D-CGD	2.08	120.85	115.97
6	1	1620	LUT	C1-C2-C3	2.09	117.91	113.40
4	3	601	CHL	C1-O2A-CGA	2.09	121.78	116.77
4	1	606	CHL	CHB-C1B-C2B	2.09	122.77	116.99
6	2	1621	LUT	C1-C2-C3	2.10	117.94	113.40
5	3	611	CLA	CAA-CBA-CGA	2.10	119.68	113.35
5	3	604	CLA	C4A-NA-C1A	2.10	109.06	106.45
5	2	610	CLA	O1D-CGD-CBD	2.11	128.38	124.60
5	3	612	CLA	O1D-CGD-CBD	2.11	128.40	124.60
5	4	603	CLA	CMD-C2D-C3D	2.11	128.81	124.89
6	1	1620	LUT	C20-C13-C12	2.12	121.47	118.10
5	3	610	CLA	CHB-C4A-NA	2.12	127.45	124.51
4	1	609	CHL	C4D-C3D-CAD	2.13	109.65	104.71
6	3	1620	LUT	C17-C1-C6	2.14	113.77	110.31
4	4	607	CHL	C4D-C3D-CAD	2.14	109.68	104.71
5	2	611	CLA	C4A-NA-C1A	2.14	109.11	106.45
4	2	608	CHL	CHC-C4B-C3B	2.15	123.31	118.23
4	2	609	CHL	C4D-C3D-CAD	2.15	109.71	104.71
6	2	1620	LUT	C2-C3-C4	2.15	113.29	110.32
4	3	605	CHL	CHB-C1B-C2B	2.16	122.96	116.99
4	3	609	CHL	C4-C3-C5	2.16	119.03	115.29
5	1	612	CLA	O2D-CGD-CBD	2.16	115.16	111.30
4	4	609	CHL	CHB-C1B-C2B	2.17	122.99	116.99
4	2	601	CHL	CED-O2D-CGD	2.17	121.06	115.97
5	4	611	CLA	CMD-C2D-C3D	2.17	128.92	124.89
4	2	607	CHL	C4-C3-C5	2.17	119.06	115.29
5	1	602	CLA	CHB-C4A-NA	2.18	127.52	124.51
5	2	614	CLA	O1D-CGD-CBD	2.18	128.52	124.60
4	2	608	CHL	CHB-C1B-C2B	2.18	123.04	116.99
4	2	607	CHL	C4D-C3D-CAD	2.19	109.79	104.71
5	1	603	CLA	C2A-C1A-CHA	2.19	127.80	123.92
4	4	608	CHL	CHB-C1B-C2B	2.19	123.07	116.99
5	4	603	CLA	C4A-NA-C1A	2.19	109.18	106.45
4	3	601	CHL	C4-C3-C5	2.20	119.10	115.29
5	3	614	CLA	C4A-NA-C1A	2.21	109.19	106.45
6	2	1621	LUT	C36-C21-C26	2.21	113.01	109.59
4	3	605	CHL	C4D-C3D-CAD	2.21	109.84	104.71
5	3	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
5	3	613	CLA	CMD-C2D-C3D	2.22	129.01	124.89
4	4	609	CHL	C4D-C3D-CAD	2.23	109.89	104.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	612	CLA	CMB-C2B-C3B	2.23	129.03	124.89
5	2	612	CLA	C2C-C1C-NC	2.23	111.76	110.22
4	2	605	CHL	C4D-C3D-CAD	2.23	109.90	104.71
5	3	611	CLA	C4A-NA-C1A	2.24	109.23	106.45
4	3	601	CHL	CMD-C2D-C3D	2.24	119.94	114.27
5	4	604	CLA	CMD-C2D-C3D	2.24	129.05	124.89
5	3	602	CLA	O1D-CGD-CBD	2.24	128.63	124.60
5	4	612	CLA	CMD-C2D-C3D	2.25	129.07	124.89
5	4	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
6	2	1620	LUT	C39-C29-C28	2.26	121.70	118.10
4	3	608	CHL	C4D-C3D-CAD	2.26	109.97	104.71
6	1	1620	LUT	C40-C33-C32	2.27	121.72	118.10
4	1	607	CHL	CMD-C2D-C3D	2.28	120.03	114.27
4	3	601	CHL	O2A-CGA-CBA	2.28	118.53	111.90
4	1	608	CHL	C4D-C3D-CAD	2.28	110.00	104.71
5	2	613	CLA	O1D-CGD-CBD	2.28	128.70	124.60
7	4	622	XAT	C38-C25-C24	2.29	116.90	114.28
5	2	612	CLA	C2A-C1A-CHA	2.29	127.98	123.92
7	4	622	XAT	C19-C9-C8	2.29	121.75	118.10
7	1	1622	XAT	C18-C5-C4	2.30	116.91	114.28
4	4	606	CHL	C4D-C3D-CAD	2.30	110.05	104.71
10	4	623	BCR	C29-C30-C25	2.30	114.08	110.48
6	3	1620	LUT	C39-C29-C28	2.31	121.77	118.10
4	4	601	CHL	CHB-C4A-C3A	2.31	123.37	117.08
5	2	611	CLA	CHB-C4A-NA	2.32	127.71	124.51
5	3	612	CLA	OBD-CAD-C3D	2.32	132.30	128.03
4	2	609	CHL	CHB-C1B-C2B	2.32	123.42	116.99
5	3	603	CLA	C4A-NA-C1A	2.33	109.34	106.45
4	2	601	CHL	CHB-C1B-C2B	2.33	123.43	116.99
4	2	606	CHL	CHC-C4B-C3B	2.33	123.74	118.23
5	3	603	CLA	C2A-C1A-CHA	2.33	128.05	123.92
4	3	607	CHL	C4D-C3D-CAD	2.34	110.14	104.71
4	2	608	CHL	C4D-C3D-CAD	2.34	110.14	104.71
5	2	610	CLA	CMD-C2D-C3D	2.34	129.23	124.89
4	4	609	CHL	CMD-C2D-C3D	2.34	120.19	114.27
4	2	606	CHL	C4D-C3D-CAD	2.34	110.16	104.71
6	3	1620	LUT	C20-C13-C12	2.35	121.84	118.10
5	4	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
4	1	609	CHL	CHB-C1B-C2B	2.37	123.56	116.99
5	1	613	CLA	CMD-C2D-C3D	2.37	129.29	124.89
5	2	604	CLA	CMD-C2D-C3D	2.38	129.31	124.89
5	2	602	CLA	CHB-C4A-NA	2.38	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	609	CHL	CHC-C4B-C3B	2.39	123.90	118.23
6	1	1620	LUT	C39-C29-C28	2.42	121.95	118.10
5	1	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
6	2	1620	LUT	C19-C9-C8	2.43	121.97	118.10
8	1	1623	NEX	C2-C1-C6	2.45	111.59	109.21
5	1	603	CLA	C4A-NA-C1A	2.45	109.49	106.45
5	3	614	CLA	CMD-C2D-C3D	2.46	129.47	124.89
6	3	1621	LUT	C1-C2-C3	2.46	118.73	113.40
8	3	1623	NEX	C12-C13-C14	2.47	122.73	118.94
5	3	613	CLA	CMB-C2B-C3B	2.47	129.47	124.89
4	3	601	CHL	CHB-C1B-C2B	2.48	123.85	116.99
4	1	606	CHL	CHC-C4B-C3B	2.48	124.10	118.23
4	1	606	CHL	C4D-C3D-CAD	2.48	110.48	104.71
4	1	607	CHL	C4D-C3D-CAD	2.48	110.48	104.71
5	2	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
5	2	611	CLA	O2D-CGD-CBD	2.49	115.75	111.30
4	3	609	CHL	CMD-C2D-C3D	2.49	120.58	114.27
8	2	1623	NEX	C28-C29-C30	2.49	122.77	118.94
7	3	1622	XAT	C19-C9-C8	2.50	122.08	118.10
4	2	607	CHL	CED-O2D-CGD	2.50	121.82	115.97
5	1	602	CLA	CMD-C2D-C3D	2.50	129.53	124.89
4	3	605	CHL	CHC-C4B-C3B	2.50	124.15	118.23
4	3	601	CHL	C4D-C3D-CAD	2.50	110.53	104.71
5	1	603	CLA	CMB-C2B-C3B	2.51	129.55	124.89
5	1	611	CLA	C4A-NA-C1A	2.51	109.57	106.45
5	3	603	CLA	CMD-C2D-C3D	2.52	129.56	124.89
5	4	602	CLA	CMD-C2D-C3D	2.52	129.57	124.89
4	3	607	CHL	C4-C3-C5	2.52	119.67	115.29
5	4	612	CLA	CHB-C4A-NA	2.52	128.00	124.51
5	2	610	CLA	CMB-C2B-C3B	2.53	129.59	124.89
4	1	605	CHL	CHB-C1B-C2B	2.54	124.02	116.99
5	2	602	CLA	CMD-C2D-C3D	2.55	129.62	124.89
4	2	609	CHL	C4-C3-C5	2.55	119.72	115.29
5	3	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
4	3	606	CHL	C4D-C3D-CAD	2.56	110.66	104.71
4	1	601	CHL	C4D-C3D-CAD	2.57	110.68	104.71
5	3	604	CLA	CHB-C4A-NA	2.58	128.08	124.51
5	3	611	CLA	CHB-C4A-NA	2.58	128.08	124.51
5	3	604	CLA	CMB-C2B-C3B	2.58	129.69	124.89
4	2	605	CHL	CHB-C1B-C2B	2.58	124.15	116.99
8	2	1623	NEX	C16-C1-C6	2.59	112.79	110.47
4	1	609	CHL	CMD-C2D-C3D	2.59	120.83	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	604	CLA	CHB-C4A-NA	2.60	128.10	124.51
5	1	612	CLA	CMD-C2D-C3D	2.60	129.72	124.89
5	1	612	CLA	C2A-C1A-CHA	2.60	128.53	123.92
5	3	611	CLA	C2C-C1C-NC	2.61	112.02	110.22
4	1	601	CHL	CHB-C1B-C2B	2.62	124.24	116.99
4	1	601	CHL	CHC-C4B-C3B	2.62	124.43	118.23
5	2	613	CLA	CHB-C4A-NA	2.63	128.15	124.51
8	1	1623	NEX	C16-C1-C6	2.63	112.83	110.47
5	1	603	CLA	CMD-C2D-C3D	2.65	129.81	124.89
6	1	1620	LUT	C19-C9-C8	2.65	122.32	118.10
4	3	608	CHL	CHC-C4B-C3B	2.65	124.51	118.23
5	2	612	CLA	CMD-C2D-C3D	2.66	129.82	124.89
5	1	604	CLA	CMB-C2B-C3B	2.66	129.83	124.89
9	1	2630	LHG	O8-C23-C24	2.67	119.67	111.90
4	1	609	CHL	C4-C3-C5	2.67	119.92	115.29
4	2	601	CHL	C4D-C3D-CAD	2.68	110.92	104.71
4	4	607	CHL	CHB-C1B-C2B	2.68	124.41	116.99
5	3	604	CLA	CMD-C2D-C3D	2.68	129.87	124.89
6	2	1621	LUT	C39-C29-C28	2.68	122.37	118.10
5	3	612	CLA	CHB-C4A-NA	2.69	128.23	124.51
5	1	604	CLA	CMD-C2D-C3D	2.69	129.88	124.89
4	2	609	CHL	CHC-C4B-C3B	2.69	124.60	118.23
4	1	605	CHL	CHC-C4B-C3B	2.69	124.60	118.23
4	1	606	CHL	CMD-C2D-C3D	2.70	121.10	114.27
4	2	605	CHL	CHC-C4B-C3B	2.72	124.67	118.23
5	1	611	CLA	CHB-C4A-NA	2.72	128.27	124.51
5	3	612	CLA	CMB-C2B-C3B	2.73	129.97	124.89
5	3	611	CLA	CMD-C2D-C3D	2.74	129.97	124.89
4	3	607	CHL	CHB-C1B-C2B	2.74	124.57	116.99
5	1	613	CLA	CHB-C4A-NA	2.74	128.31	124.51
9	2	2630	LHG	O8-C23-C24	2.75	119.89	111.90
4	2	607	CHL	O2A-CGA-CBA	2.75	119.90	111.90
5	2	603	CLA	CMB-C2B-C3B	2.76	130.01	124.89
4	3	607	CHL	O2A-CGA-CBA	2.77	119.96	111.90
7	4	622	XAT	C18-C5-C4	2.77	117.45	114.28
5	1	611	CLA	CMB-C2B-C3B	2.77	130.03	124.89
5	2	603	CLA	CMD-C2D-C3D	2.77	130.03	124.89
5	1	612	CLA	CHB-C4A-NA	2.78	128.35	124.51
5	1	611	CLA	CMD-C2D-C3D	2.78	130.05	124.89
5	4	611	CLA	CMB-C2B-C3B	2.79	130.07	124.89
4	2	607	CHL	CMD-C2D-C3D	2.80	121.36	114.27
7	3	1622	XAT	C38-C25-C24	2.80	117.49	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	609	CHL	CHB-C1B-C2B	2.82	124.79	116.99
5	3	614	CLA	CMB-C2B-C3B	2.82	130.13	124.89
7	2	1622	XAT	C40-C33-C32	2.83	122.61	118.10
4	1	607	CHL	O2A-CGA-CBA	2.83	120.14	111.90
4	4	606	CHL	CHC-C4B-C3B	2.84	124.95	118.23
4	3	609	CHL	O2A-CGA-CBA	2.84	120.17	111.90
4	4	607	CHL	CHC-C4B-C3B	2.85	124.98	118.23
4	3	607	CHL	CMD-C2D-C3D	2.85	121.49	114.27
5	4	603	CLA	CHB-C4A-NA	2.86	128.47	124.51
4	4	607	CHL	CMD-C2D-C3D	2.86	121.52	114.27
4	4	608	CHL	CHC-C4B-C3B	2.87	125.02	118.23
4	1	609	CHL	CHC-C4B-C3B	2.87	125.03	118.23
5	2	604	CLA	CHB-C4A-NA	2.88	128.49	124.51
4	1	608	CHL	CMD-C2D-C3D	2.88	121.55	114.27
4	2	606	CHL	CMD-C2D-C3D	2.88	121.56	114.27
5	1	610	CLA	CMD-C2D-C3D	2.89	130.26	124.89
5	2	612	CLA	CHB-C4A-NA	2.91	128.53	124.51
4	2	609	CHL	CMD-C2D-C3D	2.92	121.65	114.27
5	2	614	CLA	CHB-C4A-NA	2.92	128.55	124.51
8	3	1623	NEX	C28-C29-C30	2.92	123.43	118.94
4	2	601	CHL	O2D-CGD-CBD	2.94	118.38	111.20
5	4	602	CLA	CHB-C4A-NA	2.94	128.58	124.51
5	3	602	CLA	CMD-C2D-C3D	2.95	130.36	124.89
5	1	614	CLA	CHB-C4A-NA	2.95	128.59	124.51
7	3	1622	XAT	C40-C33-C32	2.95	122.81	118.10
5	3	610	CLA	CMB-C2B-C3B	2.96	130.38	124.89
5	3	603	CLA	CMB-C2B-C3B	2.96	130.39	124.89
4	4	608	CHL	O2D-CGD-CBD	2.97	118.44	111.20
5	3	613	CLA	CHB-C4A-NA	2.97	128.61	124.51
4	3	601	CHL	CHC-C4B-C3B	2.98	125.28	118.23
4	2	609	CHL	O2A-CGA-CBA	2.98	120.58	111.90
4	2	608	CHL	O2D-CGD-CBD	2.99	118.49	111.20
4	3	608	CHL	CMD-C2D-C3D	2.99	121.84	114.27
4	2	608	CHL	CMD-C2D-C3D	3.00	121.87	114.27
4	4	606	CHL	O2D-CGD-CBD	3.01	118.53	111.20
4	2	607	CHL	O2D-CGD-CBD	3.01	118.54	111.20
6	4	620	LUT	C18-C5-C4	3.01	119.83	114.33
4	1	606	CHL	CHD-C1D-C2D	3.02	125.37	116.99
4	1	608	CHL	CHD-C1D-C2D	3.03	125.38	116.99
4	4	608	CHL	CHD-C1D-C2D	3.03	125.39	116.99
4	2	607	CHL	CHB-C1B-C2B	3.03	125.39	116.99
4	3	605	CHL	CMD-C2D-C3D	3.03	121.94	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	609	CHL	O2A-CGA-CBA	3.04	120.74	111.90
4	1	605	CHL	CMD-C2D-C3D	3.05	121.99	114.27
5	1	603	CLA	CHB-C4A-NA	3.05	128.73	124.51
5	4	604	CLA	CHB-C4A-NA	3.05	128.73	124.51
4	2	607	CHL	CHC-C4B-C3B	3.05	125.46	118.23
4	4	606	CHL	CMD-C2D-C3D	3.06	122.00	114.27
4	3	608	CHL	O2D-CGD-CBD	3.06	118.66	111.20
5	4	604	CLA	CMB-C2B-C3B	3.06	130.57	124.89
4	2	605	CHL	CMD-C2D-C3D	3.06	122.02	114.27
5	1	612	CLA	CMB-C2B-C3B	3.06	130.58	124.89
4	3	608	CHL	CHD-C1D-C2D	3.07	125.48	116.99
4	3	609	CHL	CHC-C4B-C3B	3.07	125.50	118.23
4	2	608	CHL	CHD-C1D-C2D	3.09	125.54	116.99
4	1	607	CHL	O2D-CGD-CBD	3.09	118.74	111.20
4	4	608	CHL	CMD-C2D-C3D	3.10	122.11	114.27
5	2	613	CLA	CMB-C2B-C3B	3.11	130.66	124.89
4	4	601	CHL	CMD-C2D-C3D	3.11	122.14	114.27
4	2	605	CHL	CHD-C1D-C2D	3.13	125.67	116.99
7	1	1622	XAT	O24-C25-C38	3.13	118.94	115.02
6	3	1620	LUT	C22-C23-C24	3.14	115.27	111.73
4	1	607	CHL	CHC-C4B-C3B	3.17	125.73	118.23
5	2	603	CLA	CHB-C4A-NA	3.21	128.96	124.51
4	1	608	CHL	O2D-CGD-CBD	3.22	119.06	111.20
4	2	606	CHL	CHD-C1D-C2D	3.22	125.92	116.99
7	2	1622	XAT	O4-C5-C18	3.22	119.06	115.02
5	2	611	CLA	CMB-C2B-C3B	3.23	130.89	124.89
7	1	1622	XAT	O4-C5-C18	3.24	119.07	115.02
4	2	601	CHL	CHC-C4B-C3B	3.25	125.94	118.23
4	3	605	CHL	CHD-C1D-C2D	3.26	126.02	116.99
4	1	601	CHL	O2D-CGD-CBD	3.27	119.18	111.20
7	3	1622	XAT	O4-C5-C18	3.28	119.13	115.02
5	2	614	CLA	CMB-C2B-C3B	3.29	131.00	124.89
4	4	606	CHL	CHD-C1D-C2D	3.30	126.14	116.99
4	2	606	CHL	O2D-CGD-CBD	3.32	119.31	111.20
5	4	603	CLA	CMB-C2B-C3B	3.33	131.07	124.89
4	3	607	CHL	O2D-CGD-CBD	3.33	119.33	111.20
4	1	605	CHL	O2D-CGD-CBD	3.37	119.42	111.20
5	1	613	CLA	CMB-C2B-C3B	3.38	131.16	124.89
5	3	603	CLA	CHB-C4A-NA	3.41	129.23	124.51
4	3	605	CHL	O2D-CGD-CBD	3.42	119.53	111.20
4	1	608	CHL	CHC-C4B-C3B	3.43	126.35	118.23
6	1	1621	LUT	C19-C9-C8	3.43	123.57	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	609	CHL	CHD-C1D-C2D	3.48	126.64	116.99
7	4	622	XAT	O4-C5-C18	3.49	119.39	115.02
5	4	602	CLA	O2D-CGD-CBD	3.51	117.56	111.30
4	4	607	CHL	O2D-CGD-CBD	3.51	119.76	111.20
4	4	601	CHL	CHB-C1B-C2B	3.51	126.71	116.99
5	2	611	CLA	CMD-C2D-C3D	3.51	131.41	124.89
4	4	609	CHL	O2D-CGD-CBD	3.52	119.80	111.20
4	4	601	CHL	CHC-C4B-C3B	3.54	126.61	118.23
4	1	607	CHL	CHD-C1D-C2D	3.55	126.82	116.99
8	1	1623	NEX	O24-C25-C38	3.55	119.46	115.02
4	2	601	CHL	CHD-C1D-C2D	3.56	126.84	116.99
4	4	609	CHL	CHD-C1D-C2D	3.56	126.85	116.99
5	1	602	CLA	CMB-C2B-C3B	3.57	131.51	124.89
8	2	1623	NEX	O24-C25-C38	3.57	119.49	115.02
4	1	606	CHL	O2D-CGD-CBD	3.58	119.94	111.20
4	1	601	CHL	CHD-C1D-C2D	3.59	126.94	116.99
5	4	610	CLA	CMB-C2B-C3B	3.60	131.58	124.89
4	3	607	CHL	CHD-C1D-C2D	3.61	127.00	116.99
5	1	614	CLA	CMB-C2B-C3B	3.61	131.60	124.89
5	2	604	CLA	CMB-C2B-C3B	3.62	131.60	124.89
8	3	1623	NEX	O24-C25-C38	3.63	119.57	115.02
4	3	601	CHL	CHD-C1D-C2D	3.64	127.07	116.99
4	2	605	CHL	O2D-CGD-CBD	3.66	120.13	111.20
4	3	607	CHL	CHC-C4B-C3B	3.70	126.99	118.23
4	1	605	CHL	CHD-C1D-C2D	3.76	127.41	116.99
4	3	606	CHL	CHC-C4B-C3B	3.77	127.17	118.23
5	1	610	CLA	CMB-C2B-C3B	3.80	131.95	124.89
4	2	607	CHL	CHD-C1D-C2D	3.82	127.58	116.99
4	1	609	CHL	O2D-CGD-CBD	3.83	120.54	111.20
4	4	607	CHL	CHD-C1D-C2D	3.83	127.59	116.99
4	3	606	CHL	CHD-C1D-C2D	3.83	127.60	116.99
9	3	2630	LHG	O4-P-O5	3.83	132.11	112.28
4	3	609	CHL	CHD-C1D-C2D	3.88	127.75	116.99
5	2	602	CLA	CMB-C2B-C3B	3.94	132.20	124.89
4	3	601	CHL	O2D-CGD-CBD	3.95	120.84	111.20
9	1	2630	LHG	O4-P-O5	3.96	132.80	112.28
5	4	602	CLA	CMB-C2B-C3B	3.97	132.26	124.89
7	2	1622	XAT	O24-C25-C38	3.98	120.00	115.02
4	1	609	CHL	CHD-C1D-C2D	3.98	128.03	116.99
5	4	612	CLA	CMB-C2B-C3B	4.00	132.31	124.89
9	2	2630	LHG	O4-P-O5	4.01	133.02	112.28
5	3	602	CLA	CMB-C2B-C3B	4.03	132.36	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	609	CHL	O2D-CGD-CBD	4.06	121.11	111.20
9	4	2630	LHG	O4-P-O5	4.12	133.59	112.28
4	4	601	CHL	CHD-C1D-C2D	4.15	128.48	116.99
6	1	1621	LUT	C2-C3-C4	4.17	116.07	110.32
4	3	606	CHL	O2D-CGD-CBD	4.18	121.39	111.20
5	3	612	CLA	CMD-C2D-C3D	4.21	132.70	124.89
7	4	622	XAT	O24-C25-C38	4.23	120.31	115.02
4	3	609	CHL	O2D-CGD-CBD	4.34	121.80	111.20
7	3	1622	XAT	O24-C25-C38	4.38	120.50	115.02
4	4	608	CHL	C1D-CHD-C4C	4.40	121.75	112.37
4	4	609	CHL	C1D-CHD-C4C	4.43	121.82	112.37
4	3	609	CHL	C1D-CHD-C4C	4.49	121.94	112.37
4	4	601	CHL	C1D-CHD-C4C	4.75	122.50	112.37
4	3	607	CHL	C1D-CHD-C4C	4.76	122.51	112.37
4	2	609	CHL	C1D-CHD-C4C	4.76	122.52	112.37
4	3	606	CHL	C1D-CHD-C4C	4.80	122.60	112.37
4	2	607	CHL	C1D-CHD-C4C	4.84	122.69	112.37
4	2	605	CHL	C1D-CHD-C4C	4.95	122.93	112.37
4	1	606	CHL	C1D-CHD-C4C	4.97	122.97	112.37
4	1	605	CHL	C1D-CHD-C4C	4.99	123.00	112.37
4	1	607	CHL	C1D-CHD-C4C	5.00	123.02	112.37
4	4	607	CHL	C1D-CHD-C4C	5.00	123.02	112.37
4	2	606	CHL	C1D-CHD-C4C	5.05	123.13	112.37
4	1	609	CHL	C1D-CHD-C4C	5.08	123.19	112.37
4	1	608	CHL	C1D-CHD-C4C	5.10	123.23	112.37
4	1	608	CHL	C3B-C4B-NB	5.17	112.56	103.55
4	2	608	CHL	C1D-CHD-C4C	5.17	123.39	112.37
4	4	601	CHL	C3B-C4B-NB	5.23	112.67	103.55
4	3	605	CHL	C1D-CHD-C4C	5.25	123.56	112.37
4	4	606	CHL	C1D-CHD-C4C	5.32	123.70	112.37
4	3	606	CHL	C3B-C4B-NB	5.32	112.82	103.55
4	2	601	CHL	C1D-CHD-C4C	5.32	123.71	112.37
4	1	601	CHL	C1D-CHD-C4C	5.34	123.75	112.37
4	3	608	CHL	C1D-CHD-C4C	5.34	123.76	112.37
4	3	601	CHL	C1D-CHD-C4C	5.35	123.76	112.37
4	3	607	CHL	C3B-C4B-NB	5.41	112.98	103.55
4	3	608	CHL	C3B-C4B-NB	5.44	113.04	103.55
4	4	606	CHL	C3B-C4B-NB	5.44	113.04	103.55
4	1	606	CHL	C3B-C4B-NB	5.50	113.13	103.55
4	4	607	CHL	C3B-C4B-NB	5.56	113.23	103.55
4	2	605	CHL	C3B-C4B-NB	5.56	113.24	103.55
4	2	607	CHL	C3B-C4B-NB	5.59	113.30	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	601	CHL	C3B-C4B-NB	5.62	113.34	103.55
4	1	601	CHL	C3B-C4B-NB	5.62	113.36	103.55
4	3	601	CHL	C3B-C4B-NB	5.63	113.37	103.55
4	1	605	CHL	C3B-C4B-NB	5.64	113.37	103.55
4	2	608	CHL	C3B-C4B-NB	5.66	113.41	103.55
4	2	609	CHL	C3B-C4B-NB	5.69	113.47	103.55
4	2	606	CHL	C3B-C4B-NB	5.74	113.55	103.55
4	3	609	CHL	C3B-C4B-NB	5.78	113.63	103.55
7	3	1622	XAT	O24-C25-C24	5.82	117.55	113.33
4	4	609	CHL	C3B-C4B-NB	5.83	113.72	103.55
4	1	607	CHL	C3B-C4B-NB	5.84	113.73	103.55
4	3	605	CHL	C3B-C4B-NB	5.85	113.75	103.55
4	4	608	CHL	C3B-C4B-NB	5.86	113.76	103.55
4	3	601	CHL	C4B-CHC-C1C	5.89	124.91	112.37
4	1	609	CHL	C3B-C4B-NB	5.95	113.92	103.55
4	4	608	CHL	CMB-C2B-C3B	6.12	127.93	113.69
4	3	607	CHL	C4B-CHC-C1C	6.24	125.66	112.37
4	4	601	CHL	C4B-CHC-C1C	6.25	125.69	112.37
4	1	606	CHL	C4B-CHC-C1C	6.35	125.90	112.37
4	1	601	CHL	C4B-CHC-C1C	6.35	125.91	112.37
4	1	605	CHL	C4B-CHC-C1C	6.37	125.94	112.37
4	2	607	CHL	C4B-CHC-C1C	6.39	125.98	112.37
4	2	606	CHL	C4B-CHC-C1C	6.52	126.27	112.37
4	1	601	CHL	CMB-C2B-C3B	6.54	128.89	113.69
4	2	601	CHL	CMB-C2B-C3B	6.57	128.98	113.69
4	3	607	CHL	CMB-C2B-C3B	6.59	129.01	113.69
4	1	608	CHL	CMB-C2B-C3B	6.61	129.06	113.69
4	3	605	CHL	C4B-CHC-C1C	6.62	126.48	112.37
4	4	609	CHL	CMB-C2B-C3B	6.64	129.13	113.69
4	4	607	CHL	C4B-CHC-C1C	6.65	126.53	112.37
4	2	605	CHL	C4B-CHC-C1C	6.65	126.54	112.37
4	2	608	CHL	CMB-C2B-C3B	6.66	129.19	113.69
7	4	622	XAT	O24-C25-C24	6.68	118.18	113.33
4	3	601	CHL	CMB-C2B-C3B	6.69	129.25	113.69
4	2	605	CHL	CMB-C2B-C3B	6.69	129.25	113.69
4	3	605	CHL	CMB-C2B-C3B	6.69	129.25	113.69
4	4	606	CHL	C4B-CHC-C1C	6.69	126.63	112.37
4	1	609	CHL	C4B-CHC-C1C	6.70	126.66	112.37
4	2	609	CHL	C4B-CHC-C1C	6.77	126.80	112.37
4	1	606	CHL	CMB-C2B-C3B	6.78	129.46	113.69
7	4	622	XAT	O4-C5-C4	6.78	118.25	113.33
4	4	601	CHL	CMB-C2B-C3B	6.79	129.47	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	607	CHL	CMB-C2B-C3B	6.81	129.54	113.69
4	1	605	CHL	CMB-C2B-C3B	6.82	129.54	113.69
4	2	608	CHL	C4B-CHC-C1C	6.82	126.91	112.37
4	1	607	CHL	CMB-C2B-C3B	6.83	129.57	113.69
4	4	607	CHL	CMB-C2B-C3B	6.85	129.63	113.69
4	4	609	CHL	C4B-CHC-C1C	6.90	127.08	112.37
4	3	609	CHL	CMB-C2B-C3B	6.91	129.75	113.69
4	1	607	CHL	C4B-CHC-C1C	6.92	127.11	112.37
4	3	608	CHL	CMB-C2B-C3B	6.96	129.87	113.69
4	3	606	CHL	CMB-C2B-C3B	6.98	129.92	113.69
4	3	609	CHL	C4B-CHC-C1C	7.01	127.30	112.37
4	4	606	CHL	CMB-C2B-C3B	7.03	130.04	113.69
4	2	606	CHL	CMB-C2B-C3B	7.05	130.08	113.69
4	2	609	CHL	CMB-C2B-C3B	7.14	130.29	113.69
4	3	608	CHL	C4B-CHC-C1C	7.19	127.70	112.37
4	2	601	CHL	C4B-CHC-C1C	7.23	127.78	112.37
4	4	608	CHL	C4B-CHC-C1C	7.34	128.01	112.37
4	1	609	CHL	CMB-C2B-C3B	7.68	131.55	113.69
4	1	608	CHL	C4B-CHC-C1C	7.72	128.82	112.37
4	3	606	CHL	C4B-CHC-C1C	8.03	129.47	112.37
7	1	1622	XAT	O4-C5-C4	8.21	119.28	113.33
7	3	1622	XAT	O4-C5-C4	9.18	119.99	113.33
8	3	1623	NEX	O24-C25-C24	9.68	120.35	113.33
7	2	1622	XAT	O24-C25-C24	9.84	120.47	113.33
8	1	1623	NEX	O24-C25-C24	9.88	120.49	113.33
8	2	1623	NEX	O24-C25-C24	10.11	120.67	113.33
7	2	1622	XAT	O4-C5-C4	10.29	120.79	113.33
7	1	1622	XAT	O24-C25-C24	10.93	121.26	113.33

All (85) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	4	612	CLA	NC
5	4	612	CLA	ND
5	4	612	CLA	NA
5	3	614	CLA	NC
5	3	614	CLA	ND
5	3	614	CLA	NA
5	1	603	CLA	NC
5	1	603	CLA	NA
5	1	603	CLA	ND
5	1	611	CLA	NC

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Mol	Chain	Res	Type	Atom
5	1	611	CLA	ND
5	1	611	CLA	NA
5	2	613	CLA	NC
5	2	613	CLA	NA
5	1	614	CLA	NC
5	1	614	CLA	ND
5	1	614	CLA	NA
5	4	602	CLA	NC
5	4	602	CLA	ND
5	4	602	CLA	NA
5	4	611	CLA	NC
5	4	611	CLA	ND
5	4	611	CLA	NA
5	2	602	CLA	NC
5	2	602	CLA	ND
5	2	602	CLA	NA
5	1	613	CLA	NC
5	1	613	CLA	NA
5	4	603	CLA	NC
5	4	603	CLA	ND
5	4	603	CLA	NA
5	1	612	CLA	NC
5	1	612	CLA	NA
5	1	612	CLA	ND
5	2	614	CLA	NC
5	2	614	CLA	NA
5	4	610	CLA	NC
5	4	610	CLA	ND
5	4	610	CLA	NA
5	1	602	CLA	NC
5	1	602	CLA	ND
5	1	602	CLA	NA
5	2	603	CLA	NC
5	2	603	CLA	NA
5	2	603	CLA	ND
5	2	611	CLA	NC
5	2	611	CLA	ND
5	2	611	CLA	NA
5	2	610	CLA	NC
5	2	610	CLA	ND
5	2	610	CLA	NA
5	3	602	CLA	NC

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Mol	Chain	Res	Type	Atom
5	3	602	CLA	ND
5	3	602	CLA	NA
5	2	612	CLA	NC
5	2	612	CLA	ND
5	2	612	CLA	NA
5	3	604	CLA	NC
5	3	604	CLA	ND
5	3	604	CLA	NA
5	3	613	CLA	NC
5	3	613	CLA	ND
5	3	613	CLA	NA
5	3	603	CLA	NC
5	3	603	CLA	ND
5	3	603	CLA	NA
5	3	610	CLA	NC
5	3	610	CLA	ND
5	3	610	CLA	NA
5	3	612	CLA	NC
5	3	612	CLA	ND
5	3	612	CLA	NA
5	3	611	CLA	NC
5	3	611	CLA	ND
5	3	611	CLA	NA
5	4	604	CLA	NC
5	4	604	CLA	NA
5	1	604	CLA	NC
5	1	604	CLA	ND
5	1	604	CLA	NA
5	2	604	CLA	NC
5	2	604	CLA	NA
5	1	610	CLA	NC
5	1	610	CLA	ND
5	1	610	CLA	NA

There are no torsion outliers.

There are no ring outliers.

64 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	1620	LUT	5	0
6	1	1621	LUT	4	0
7	1	1622	XAT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	1	1623	NEX	2	0
4	1	601	CHL	1	0
5	1	602	CLA	5	0
5	1	603	CLA	3	0
5	1	604	CLA	1	0
4	1	606	CHL	1	0
4	1	607	CHL	4	0
4	1	608	CHL	1	0
4	1	609	CHL	3	0
5	1	610	CLA	2	0
5	1	612	CLA	2	0
5	1	613	CLA	2	0
5	1	614	CLA	1	0
6	2	1620	LUT	4	0
6	2	1621	LUT	3	0
7	2	1622	XAT	6	0
8	2	1623	NEX	1	0
9	2	2630	LHG	2	0
4	2	601	CHL	1	0
5	2	602	CLA	3	0
5	2	603	CLA	3	0
5	2	604	CLA	1	0
4	2	605	CHL	1	0
4	2	606	CHL	3	0
4	2	607	CHL	2	0
4	2	608	CHL	2	0
4	2	609	CHL	5	0
5	2	610	CLA	3	0
5	2	612	CLA	2	0
5	2	613	CLA	3	0
5	2	614	CLA	1	0
6	3	1620	LUT	8	0
6	3	1621	LUT	3	0
7	3	1622	XAT	5	0
8	3	1623	NEX	3	0
9	3	2630	LHG	5	0
4	3	601	CHL	2	0
5	3	602	CLA	5	0
5	3	603	CLA	2	0
5	3	604	CLA	1	0
4	3	605	CHL	1	0
4	3	606	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	607	CHL	6	0
4	3	608	CHL	3	0
4	3	609	CHL	5	0
5	3	610	CLA	2	0
5	3	611	CLA	5	0
5	3	613	CLA	4	0
5	3	614	CLA	1	0
9	4	2630	LHG	1	0
4	4	601	CHL	1	0
5	4	603	CLA	1	0
4	4	606	CHL	1	0
4	4	607	CHL	1	0
4	4	608	CHL	1	0
5	4	610	CLA	1	0
5	4	611	CLA	1	0
5	4	612	CLA	2	0
6	4	620	LUT	4	0
7	4	622	XAT	3	0
10	4	623	BCR	3	0

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.