



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:34 am GMT

PDB ID : 2J8D
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC
REACTION CENTER FROM RB. SPHAEROIDES AT PH 8 IN THE
CHARGE-SEPARATED STATE
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2006-10-24
Resolution : 2.07 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

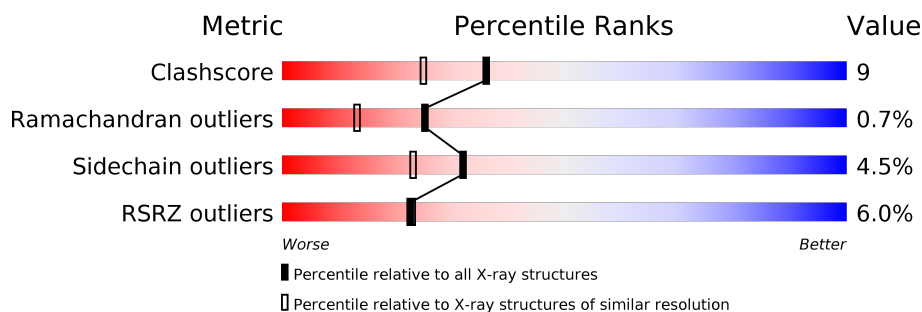
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

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
10	HTO	L	1290	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTO	L	1291	-	-	-	X
13	CDL	M	1320	-	-	-	X
4	GOL	H	1261	-	-	X	X
4	GOL	L	1293	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1283	X	-	-	-
5	BCL	M	1308	X	-	-	-
5	BCL	M	1309	X	-	-	-
6	LDA	L	1284	-	-	-	X
6	LDA	L	1285	-	-	-	X
6	LDA	L	1286	-	-	-	X
6	LDA	M	1310	-	-	-	X
6	LDA	M	1311	-	-	-	X
6	LDA	M	1312	-	-	-	X
6	LDA	M	1314	-	-	-	X
8	U10	L	1288[A]	-	-	-	X
8	U10	L	1288[B]	-	-	-	X
8	U10	M	1318	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 7895 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	260	Total	C	N	O	S	0	1	0
			1980	1271	335	363	11			

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

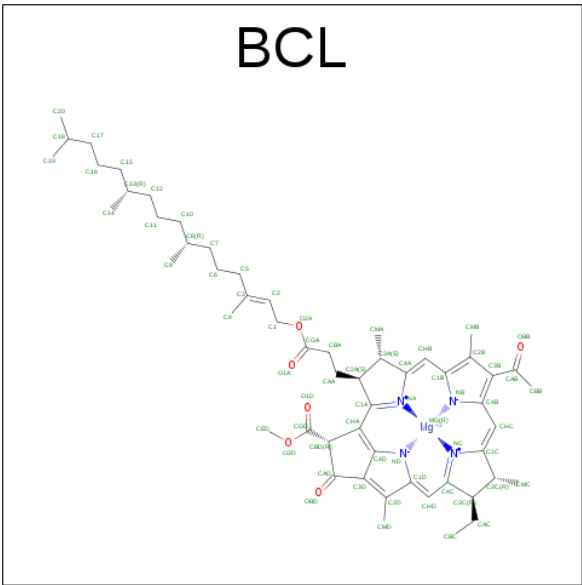
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	307	Total	C	N	O	S	0	1	0
			2451	1634	402	404	11			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

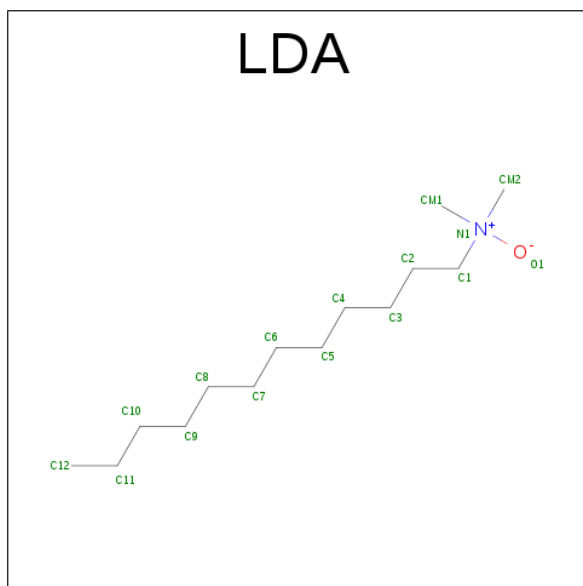
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

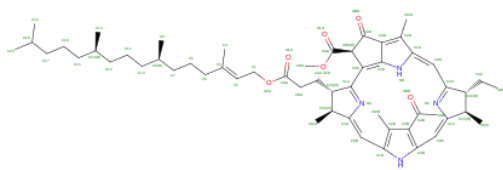
C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).

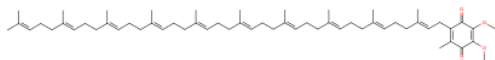
BPH



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

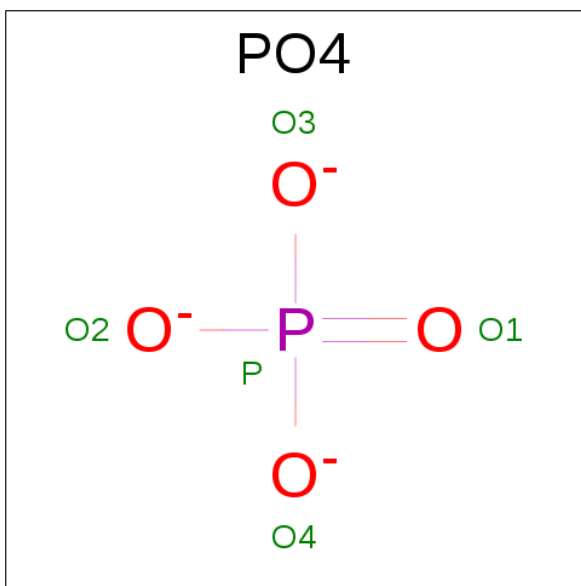
- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

U10



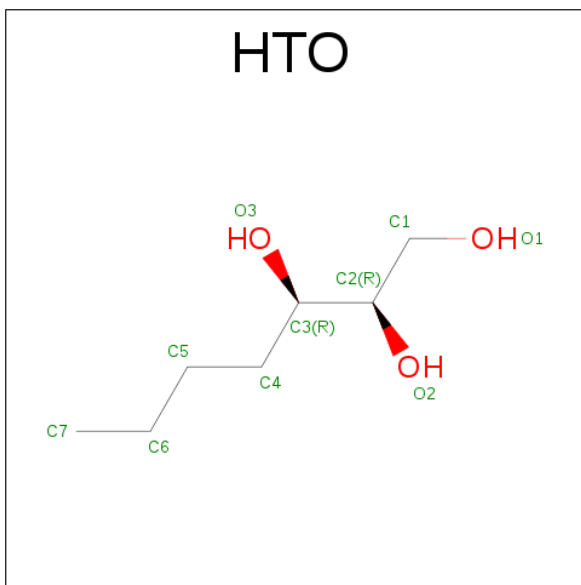
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			47	44	3		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $\text{C}_7\text{H}_{16}\text{O}_3$).

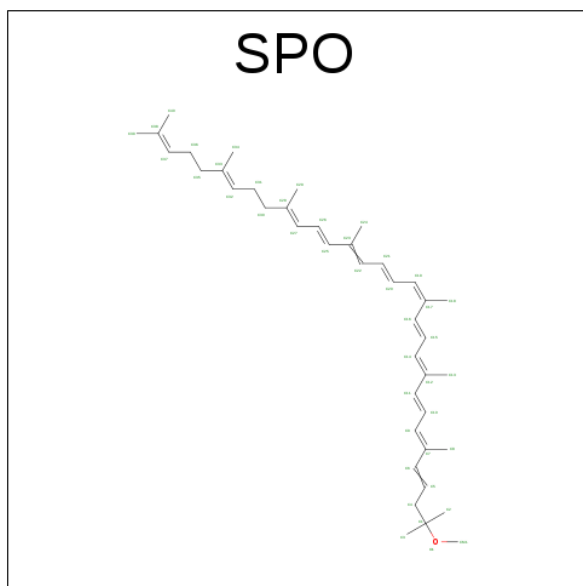


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

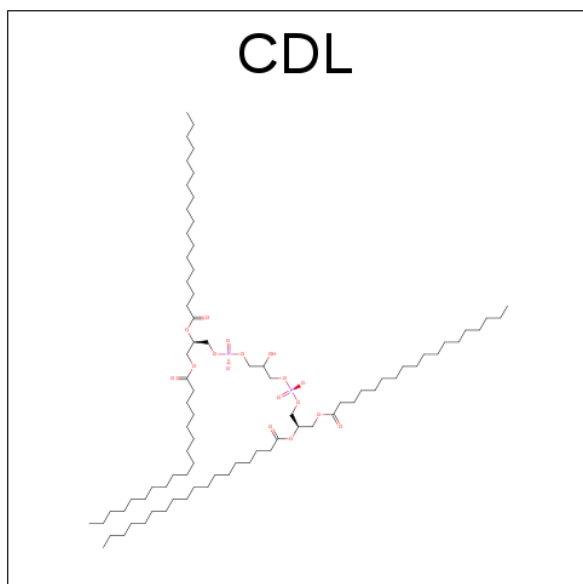
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			81	62	17	2		

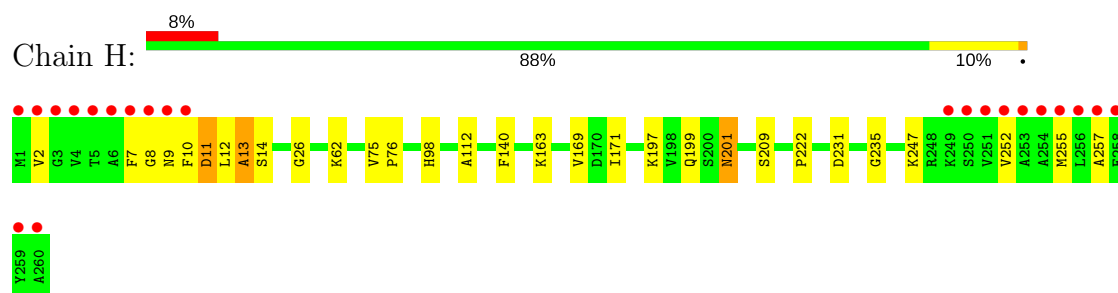
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	161	Total	O	0	0
			161	161		
14	L	121	Total	O	0	0
			121	121		
14	M	128	Total	O	0	0
			128	128		

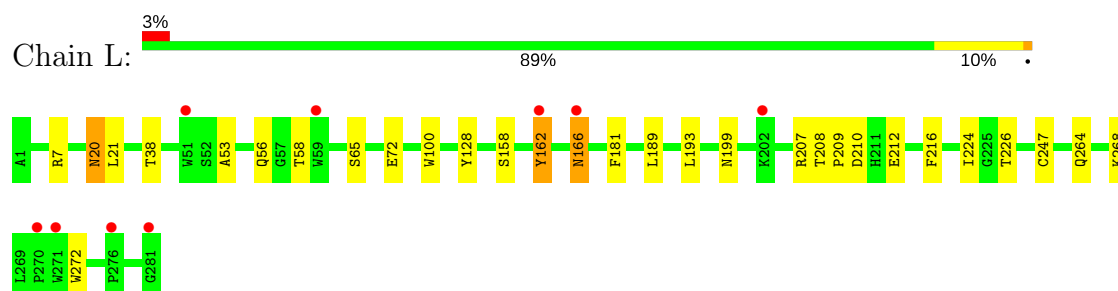
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

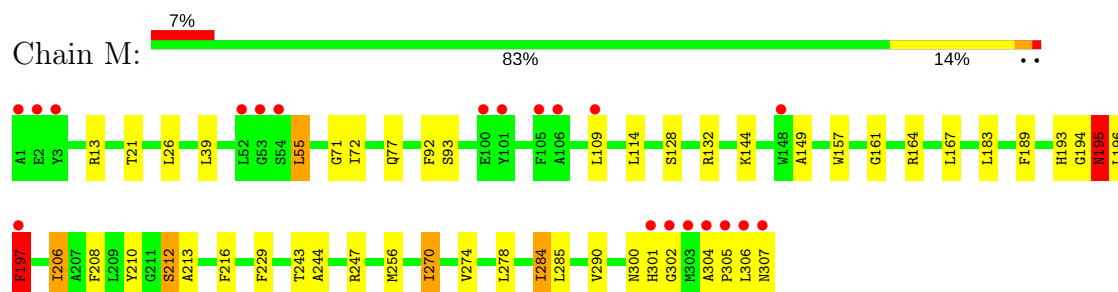
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.01Å 140.01Å 184.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.07 38.55 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.6 (119.52-2.07) 95.6 (38.55-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.218 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7895	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE, SPO, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	0.75	0/2036	0.69	0/2768
2	L	0.78	0/2320	0.67	1/3175 (0.0%)
3	M	0.80	3/2549 (0.1%)	0.69	1/3479 (0.0%)
All	All	0.78	3/6905 (0.0%)	0.69	2/9422 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	212	SER	CB-OG	-6.55	1.33	1.42
3	M	197	PHE	CE2-CZ	6.37	1.49	1.37
3	M	213	ALA	CA-CB	5.11	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	212	SER	CB-CA-C	6.03	121.56	110.10
2	L	21	LEU	CA-CB-CG	5.74	128.51	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	H	1980	0	1986	27	0
2	L	2232	0	2187	29	0
3	M	2451	0	2362	49	0
4	H	24	0	32	4	0
4	L	18	0	24	0	0
5	L	132	0	148	5	0
5	M	132	0	148	9	0
6	L	48	0	93	1	0
6	M	96	0	186	8	0
7	L	65	0	76	6	0
7	M	65	0	76	9	0
8	L	46	0	46	10	0
8	M	47	0	63	4	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	3	0
13	M	81	0	102	18	0
14	H	161	0	0	2	0
14	L	121	0	0	2	0
14	M	128	0	0	1	0
All	All	7895	0	7621	138	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 9.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1320:CDL:C36	13:M:1320:CDL:C37	1.80	1.57
13:M:1320:CDL:C33	13:M:1320:CDL:C34	1.74	1.56
13:M:1320:CDL:C34	13:M:1320:CDL:C35	1.83	1.55
6:M:1314:LDA:C8	6:M:1314:LDA:C9	1.78	1.55
13:M:1320:CDL:C17	13:M:1320:CDL:C18	1.83	1.53
1:H:10[B]:PHE:CD1	3:M:301[B]:HIS:NE2	1.87	1.41
1:H:10[B]:PHE:CE1	3:M:301[B]:HIS:NE2	2.04	1.25
1:H:10[B]:PHE:CE1	3:M:301[B]:HIS:CE1	2.32	1.18
1:H:201:ASN:HD22	1:H:201:ASN:H	1.08	1.00
1:H:10[B]:PHE:HD1	3:M:301[B]:HIS:NE2	1.38	0.95
2:L:162:TYR:CD2	14:L:2069:HOH:O	2.19	0.94
13:M:1320:CDL:C19	13:M:1320:CDL:C17	2.47	0.93
7:L:1287:BPH:HBB3	7:L:1287:BPH:HHC	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10[B]:PHE:HE1	3:M:301[B]:HIS:CE1	1.88	0.88
3:M:206:ILE:HD11	3:M:210:TYR:CE2	2.11	0.84
1:H:10[B]:PHE:CD1	3:M:301[B]:HIS:CE1	2.63	0.84
2:L:56:GLN:HE22	2:L:65:SER:H	1.27	0.81
13:M:1320:CDL:C16	13:M:1320:CDL:C18	2.58	0.81
7:L:1287:BPH:CBB	7:L:1287:BPH:HHC	2.10	0.80
3:M:206:ILE:CD1	3:M:210:TYR:CE2	2.63	0.80
13:M:1320:CDL:C37	13:M:1320:CDL:C35	2.60	0.78
2:L:158:SER:HB2	3:M:197:PHE:CE2	2.20	0.77
1:H:10[B]:PHE:HD1	3:M:301[B]:HIS:HE2	0.79	0.77
6:M:1314:LDA:C8	6:M:1314:LDA:C10	2.63	0.76
1:H:201:ASN:H	1:H:201:ASN:ND2	1.84	0.76
1:H:201:ASN:HD22	1:H:201:ASN:N	1.84	0.74
2:L:181:PHE:HB3	7:M:1317:BPH:HBB2	1.69	0.73
6:M:1314:LDA:C7	6:M:1314:LDA:C9	2.66	0.73
7:M:1317:BPH:HHC	7:M:1317:BPH:HBB3	1.70	0.73
3:M:189:PHE:O	3:M:193:HIS:HD2	1.71	0.73
2:L:264:GLN:NE2	14:L:2112:HOH:O	2.23	0.72
5:M:1309:BCL:HHC	5:M:1309:BCL:CBB	2.20	0.72
5:M:1309:BCL:HBB3	5:M:1309:BCL:HHC	1.72	0.71
5:M:1308:BCL:HHC	5:M:1308:BCL:CBB	2.22	0.70
5:M:1308:BCL:HBB3	5:M:1309:BCL:H41	1.73	0.70
3:M:157:TRP:HB2	5:M:1309:BCL:H71	1.74	0.69
13:M:1320:CDL:C36	13:M:1320:CDL:C38	2.71	0.68
4:H:1261:GOL:H32	14:H:2002:HOH:O	1.92	0.68
5:L:1283:BCL:HBB2	5:L:1283:BCL:HHC	1.77	0.67
2:L:162:TYR:C	2:L:162:TYR:CD2	2.67	0.67
2:L:181:PHE:CD2	7:M:1317:BPH:HBB1	2.29	0.67
2:L:158:SER:HB2	3:M:197:PHE:HE2	1.58	0.67
3:M:206:ILE:CD1	3:M:210:TYR:CZ	2.78	0.67
2:L:199:ASN:O	13:M:1320:CDL:HB22	1.96	0.66
2:L:224:ILE:H	8:L:1288[A]:U10:H8	1.61	0.65
1:H:12:LEU:O	1:H:13:ALA:CB	2.47	0.63
2:L:224:ILE:HG22	8:L:1288[A]:U10:H8	1.81	0.63
5:M:1308:BCL:HBB2	5:M:1308:BCL:HHC	1.82	0.62
7:M:1317:BPH:HHC	7:M:1317:BPH:CBB	2.31	0.61
7:L:1287:BPH:HBB3	7:L:1287:BPH:CHC	2.28	0.60
3:M:270:ILE:O	3:M:274:VAL:HG13	2.02	0.59
3:M:206:ILE:HD13	3:M:210:TYR:CZ	2.39	0.58
1:H:10[B]:PHE:HE1	3:M:301[B]:HIS:NE2	1.76	0.58
5:M:1308:BCL:H71	5:M:1309:BCL:H202	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:71:GLY:HA3	12:M:1319:SPO:H6	1.86	0.57
2:L:226:THR:HG22	8:L:1288[A]:U10:H3M3	1.85	0.57
1:H:10[B]:PHE:CE1	3:M:301[B]:HIS:HE1	2.13	0.57
2:L:189:LEU:HD23	7:M:1317:BPH:HMD2	1.86	0.56
7:L:1287:BPH:HBB2	3:M:210:TYR:HB3	1.87	0.56
2:L:181:PHE:HB3	7:M:1317:BPH:CBB	2.36	0.56
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.87	0.55
1:H:26:GLY:HA3	13:M:1320:CDL:H171	1.87	0.55
7:M:1317:BPH:HHO	7:M:1317:BPH:HBC2	1.89	0.55
1:H:62:LYS:NZ	4:H:1261:GOL:H11	2.21	0.55
7:M:1317:BPH:HBB3	7:M:1317:BPH:CHC	2.35	0.55
2:L:20:ASN:C	2:L:20:ASN:HD22	2.10	0.55
3:M:208:PHE:O	3:M:212:SER:HB3	2.07	0.54
2:L:193:LEU:HD23	8:L:1288[A]:U10:C2	2.38	0.54
3:M:144:LYS:N	13:M:1320:CDL:OB3	2.31	0.54
3:M:189:PHE:O	3:M:193:HIS:CD2	2.57	0.53
8:M:1318:U10:O3	8:M:1318:U10:H4M2	2.08	0.53
3:M:149:ALA:HB2	3:M:270:ILE:HD11	1.91	0.53
1:H:209:SER:OG	1:H:247:LYS:HD3	2.09	0.53
5:M:1309:BCL:HAA2	5:M:1309:BCL:HBD	1.92	0.52
3:M:243:THR:O	3:M:247:ARG:HG3	2.10	0.52
3:M:77:GLN:HE22	3:M:93:SER:H	1.58	0.51
2:L:166:ASN:N	2:L:166:ASN:HD22	2.08	0.51
8:M:1318:U10:H33	8:M:1318:U10:H403	1.91	0.51
7:L:1287:BPH:CBB	7:L:1287:BPH:CHC	2.81	0.51
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.29	0.50
2:L:224:ILE:HG22	8:L:1288[A]:U10:C8	2.41	0.50
5:L:1282:BCL:HMB1	5:L:1282:BCL:CBB	2.42	0.50
3:M:109:LEU:O	3:M:114:LEU:HB2	2.11	0.50
3:M:77:GLN:NE2	3:M:92:PHE:HB3	2.26	0.50
1:H:112:ALA:HA	1:H:235:GLY:O	2.12	0.50
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.49
3:M:300:ASN:O	3:M:304:ALA:HB3	2.11	0.49
2:L:128:TYR:HD1	5:L:1283:BCL:HBB1	1.76	0.49
2:L:158:SER:HB2	3:M:197:PHE:CZ	2.49	0.48
2:L:212:GLU:HB3	8:L:1288[A]:U10:H4M3	1.95	0.48
6:M:1313:LDA:H51	8:M:1318:U10:H23	1.96	0.48
3:M:194:GLY:O	3:M:195:ASN:HB3	2.12	0.48
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.47
8:L:1288[A]:U10:H71	8:L:1288[A]:U10:H1M1	1.69	0.47
3:M:195:ASN:HD22	3:M:195:ASN:C	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:216:PHE:CE1	8:L:1288[B]:U10:H3M2	2.49	0.47
3:M:77:GLN:HE21	3:M:92:PHE:HB3	1.79	0.47
13:M:1320:CDL:H341	13:M:1320:CDL:C33	2.19	0.47
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.96	0.46
13:M:1320:CDL:H351	13:M:1320:CDL:C37	2.44	0.46
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.97	0.46
1:H:62:LYS:HE3	4:H:1261:GOL:H12	1.98	0.46
3:M:164:ARG:HD2	3:M:284:ILE:HD12	1.98	0.46
1:H:11:ASP:O	1:H:14:SER:HB2	2.16	0.45
6:M:1313:LDA:H22	6:M:1313:LDA:HM13	1.71	0.45
14:H:2002:HOH:O	13:M:1320:CDL:HA32	2.15	0.45
8:L:1288[B]:U10:H121	8:L:1288[B]:U10:H101	1.63	0.45
6:M:1312:LDA:H12	6:M:1313:LDA:HM22	1.98	0.45
2:L:208:THR:HB	2:L:209:PRO:HD2	1.99	0.44
3:M:132:ARG:HB2	14:M:2073:HOH:O	2.16	0.44
1:H:197:LYS:HE3	1:H:199:GLN:NE2	2.32	0.44
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.83	0.44
5:M:1308:BCL:HBB3	5:M:1308:BCL:HHC	1.99	0.44
3:M:161:GLY:HA3	12:M:1319:SPO:H292	2.00	0.44
13:M:1320:CDL:H171	13:M:1320:CDL:C19	2.43	0.44
1:H:62:LYS:HE3	4:H:1261:GOL:C1	2.48	0.43
3:M:278:LEU:HD21	13:M:1320:CDL:H782	2.00	0.43
2:L:189:LEU:CD2	7:M:1317:BPH:HMD2	2.48	0.43
13:M:1320:CDL:H322	13:M:1320:CDL:H111	2.01	0.43
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.67	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.18	0.43
3:M:305:PRO:C	3:M:307:ASN:H	2.21	0.42
5:L:1283:BCL:CAD	3:M:206:ILE:HG12	2.50	0.42
6:M:1314:LDA:C8	6:M:1314:LDA:H102	2.46	0.42
5:L:1283:BCL:HBB2	5:L:1283:BCL:CHC	2.49	0.42
3:M:196:LEU:HA	3:M:196:LEU:HD12	1.88	0.42
3:M:71:GLY:HA3	12:M:1319:SPO:C6	2.47	0.41
1:H:197:LYS:HE3	1:H:199:GLN:HE21	1.85	0.41
6:L:1286:LDA:H121	8:L:1288[A]:U10:C16	2.51	0.41
2:L:53:ALA:HB1	2:L:58:THR:O	2.20	0.41
3:M:21:THR:HG23	3:M:26:LEU:HD21	2.01	0.41
2:L:166:ASN:N	2:L:166:ASN:ND2	2.69	0.41
6:M:1312:LDA:H22	6:M:1312:LDA:HM11	1.79	0.41
3:M:256:MET:CE	8:M:1318:U10:H102	2.51	0.41
13:M:1320:CDL:C33	13:M:1320:CDL:H342	2.19	0.40
3:M:195:ASN:ND2	3:M:197:PHE:H	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:114:LEU:HA	3:M:114:LEU:HD12	1.87	0.40
7:L:1287:BPH:ND	7:L:1287:BPH:NC	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	259/260 (100%)	249 (96%)	6 (2%)	4 (2%)	12	3
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	306/307 (100%)	292 (95%)	12 (4%)	2 (1%)	25	13
All	All	844/848 (100%)	813 (96%)	25 (3%)	6 (1%)	25	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	13	ALA
1	H	252	VAL
1	H	257	ALA
3	M	195	ASN
1	H	8	GLY
3	M	302	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	209/208 (100%)	200 (96%)	9 (4%)	33	25
2	L	220/220 (100%)	211 (96%)	9 (4%)	35	27
3	M	241/240 (100%)	229 (95%)	12 (5%)	28	19
All	All	670/668 (100%)	640 (96%)	30 (4%)	32	23

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

Mol	Chain	Res	Type
1	H	2	VAL
1	H	7	PHE
1	H	9	ASN
1	H	11	ASP
1	H	163	LYS
1	H	201	ASN
1	H	222	PRO
1	H	231	ASP
1	H	255	MET
2	L	20	ASN
2	L	72	GLU
2	L	162	TYR
2	L	166	ASN
2	L	207	ARG
2	L	210	ASP
2	L	247	CYS
2	L	268	LYS
2	L	272	TRP
3	M	39	LEU
3	M	55	LEU
3	M	72	ILE
3	M	183	LEU
3	M	195	ASN
3	M	197	PHE
3	M	206	ILE
3	M	216	PHE
3	M	270	ILE
3	M	284	ILE
3	M	290	VAL
3	M	306	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	201	ASN
2	L	20	ASN
2	L	56	GLN
2	L	153	HIS
2	L	159	ASN
2	L	166	ASN
2	L	183	ASN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	195	ASN
3	M	299	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	H	1261	-	5,5,5	0.54	0	5,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	H	1262	-	5,5,5	0.49	0	5,5,5	0.49	0
4	GOL	H	1263	-	5,5,5	0.43	0	5,5,5	0.17	0
4	GOL	H	1264	-	5,5,5	0.34	0	5,5,5	0.26	0
5	BCL	L	1282	2	55,74,74	2.30	8 (14%)	65,115,115	1.92	20 (30%)
5	BCL	L	1283	-	55,74,74	2.09	8 (14%)	65,115,115	2.18	24 (36%)
6	LDA	L	1284	-	13,15,15	2.33	1 (7%)	14,17,17	0.57	0
6	LDA	L	1285	-	13,15,15	2.32	1 (7%)	14,17,17	0.58	0
6	LDA	L	1286	-	13,15,15	2.41	1 (7%)	14,17,17	0.58	0
7	BPH	L	1287	-	65,70,70	2.80	18 (27%)	75,101,101	1.92	17 (22%)
8	U10	L	1288[A]	-	23,23,63	2.51	7 (30%)	28,31,79	1.67	7 (25%)
8	U10	L	1288[B]	-	23,23,63	2.59	7 (30%)	28,31,79	1.24	2 (7%)
9	PO4	L	1289	-	4,4,4	0.72	0	6,6,6	0.70	0
10	HTO	L	1290	-	9,9,9	0.50	0	9,10,10	0.60	0
10	HTO	L	1291	-	9,9,9	0.33	0	9,10,10	0.72	0
4	GOL	L	1292	-	5,5,5	0.38	0	5,5,5	0.94	0
4	GOL	L	1293	-	5,5,5	0.37	0	5,5,5	0.26	0
4	GOL	L	1294	-	5,5,5	0.33	0	5,5,5	0.27	0
5	BCL	M	1308	3	55,74,74	2.13	7 (12%)	65,115,115	1.93	13 (20%)
5	BCL	M	1309	3	55,74,74	2.31	7 (12%)	65,115,115	1.97	15 (23%)
6	LDA	M	1310	-	13,15,15	2.34	1 (7%)	14,17,17	0.73	1 (7%)
6	LDA	M	1311	-	13,15,15	2.32	1 (7%)	14,17,17	0.71	0
6	LDA	M	1312	-	13,15,15	2.18	1 (7%)	14,17,17	0.60	0
6	LDA	M	1313	-	13,15,15	2.39	2 (15%)	14,17,17	0.93	1 (7%)
6	LDA	M	1314	-	13,15,15	3.00	3 (23%)	14,17,17	1.45	3 (21%)
6	LDA	M	1315	-	13,15,15	2.50	2 (15%)	14,17,17	0.90	0
7	BPH	M	1317	-	65,70,70	2.75	19 (29%)	75,101,101	1.74	16 (21%)
8	U10	M	1318	-	47,47,63	2.78	14 (29%)	51,59,79	1.76	13 (25%)
12	SPO	M	1319	-	40,41,41	3.88	12 (30%)	49,50,50	2.08	13 (26%)
13	CDL	M	1320	-	80,80,99	2.09	18 (22%)	82,92,111	1.83	19 (23%)

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
4	GOL	H	1261	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1262	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	1263	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1264	-	-	0/4/4/4	0/0/0/0
5	BCL	L	1282	2	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	L	1283	-	2/2/21/25	0/37/137/137	0/0/9/9
6	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1285	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1286	-	-	0/13/13/13	0/0/0/0
7	BPH	L	1287	-	-	0/54/105/105	0/1/6/6
8	U10	L	1288[A]	-	-	0/15/39/87	0/1/1/1
8	U10	L	1288[B]	-	-	0/15/39/87	0/1/1/1
9	PO4	L	1289	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1290	-	-	0/10/10/10	0/0/0/0
10	HTO	L	1291	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1292	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1293	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1294	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1308	3	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	1309	3	2/2/21/25	0/37/137/137	0/0/9/9
6	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1311	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1312	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1313	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1314	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1315	-	-	0/13/13/13	0/0/0/0
7	BPH	M	1317	-	-	0/54/105/105	0/1/6/6
8	U10	M	1318	-	-	0/45/65/87	0/1/1/1
12	SPO	M	1319	-	-	0/47/47/47	0/0/0/0
13	CDL	M	1320	-	-	0/91/91/110	0/0/0/0

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1286	LDA	O1-N1	-8.41	1.25	1.42
6	M	1313	LDA	O1-N1	-8.32	1.25	1.42
6	M	1315	LDA	O1-N1	-8.28	1.25	1.42
6	M	1314	LDA	O1-N1	-8.20	1.26	1.42
6	L	1285	LDA	O1-N1	-8.17	1.26	1.42
6	M	1310	LDA	O1-N1	-8.17	1.26	1.42
6	L	1284	LDA	O1-N1	-8.16	1.26	1.42
6	M	1311	LDA	O1-N1	-8.10	1.26	1.42
6	M	1312	LDA	O1-N1	-7.63	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1288[B]	U10	O4-C4	-5.05	1.24	1.36
8	L	1288[B]	U10	O3-C3	-5.02	1.24	1.36
13	M	1320	CDL	C11-CA5	-4.98	1.36	1.50
8	L	1288[A]	U10	O4-C4	-4.96	1.24	1.36
7	L	1287	BPH	C3D-C4D	-4.18	1.36	1.41
13	M	1320	CDL	C20-C19	-4.06	1.28	1.51
8	L	1288[A]	U10	O3-C3	-4.05	1.26	1.36
8	M	1318	U10	C5-C4	-3.81	1.42	1.49
7	M	1317	BPH	C3D-CAD	-3.63	1.38	1.47
7	L	1287	BPH	C3D-CAD	-3.58	1.38	1.47
7	L	1287	BPH	O2D-CGD	-3.39	1.24	1.33
8	L	1288[A]	U10	C3-C2	-3.26	1.39	1.48
8	M	1318	U10	O3-C3	-3.19	1.28	1.36
8	L	1288[B]	U10	C3-C2	-3.05	1.40	1.48
7	L	1287	BPH	CBB-CAB	-3.05	1.43	1.50
7	M	1317	BPH	O2D-CGD	-2.95	1.25	1.33
13	M	1320	CDL	C79-C78	-2.95	1.34	1.51
13	M	1320	CDL	C22-C21	-2.89	1.35	1.51
13	M	1320	CDL	C80-C79	-2.89	1.35	1.51
8	M	1318	U10	O4-C4	-2.87	1.27	1.35
8	L	1288[B]	U10	C4-C5	-2.81	1.40	1.48
7	M	1317	BPH	C3D-C4D	-2.80	1.38	1.41
7	L	1287	BPH	C1B-C2B	-2.73	1.39	1.45
5	L	1282	BCL	O2D-CGD	-2.71	1.26	1.33
5	M	1308	BCL	O2D-CGD	-2.70	1.26	1.33
8	M	1318	U10	C5-C6	-2.64	1.44	1.50
5	M	1309	BCL	O2D-CGD	-2.63	1.26	1.33
5	L	1282	BCL	O2A-CGA	-2.58	1.25	1.33
7	L	1287	BPH	O2A-CGA	-2.50	1.25	1.33
8	L	1288[A]	U10	C4-C5	-2.49	1.41	1.48
7	M	1317	BPH	C1B-C2B	-2.47	1.40	1.45
5	L	1283	BCL	O2D-CGD	-2.37	1.27	1.33
8	M	1318	U10	C1-C2	-2.36	1.37	1.47
5	L	1282	BCL	C3D-CAD	-2.34	1.39	1.46
7	M	1317	BPH	O2A-CGA	-2.32	1.26	1.33
5	M	1308	BCL	C3D-CAD	-2.29	1.39	1.46
5	L	1283	BCL	O2A-CGA	-2.29	1.26	1.33
13	M	1320	CDL	C13-C12	-2.08	1.39	1.51
7	M	1317	BPH	C1C-NC	-2.08	1.32	1.37
6	M	1313	LDA	C1-N1	-2.08	1.46	1.51
7	M	1317	BPH	CBB-CAB	-2.05	1.46	1.50
8	L	1288[A]	U10	C6-C1	2.09	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1309	BCL	OBB-CAB	2.12	1.29	1.22
5	L	1283	BCL	O1D-CGD	2.15	1.26	1.21
7	L	1287	BPH	C1D-CHD	2.15	1.48	1.40
6	M	1315	LDA	C3-C2	2.18	1.64	1.51
13	M	1320	CDL	C33-C32	2.22	1.64	1.51
13	M	1320	CDL	C36-C35	2.29	1.64	1.51
13	M	1320	CDL	C32-C31	2.48	1.61	1.52
7	M	1317	BPH	C1D-CHD	2.50	1.49	1.40
7	L	1287	BPH	CHB-C4A	2.70	1.46	1.40
8	L	1288[B]	U10	C6-C1	2.74	1.41	1.35
5	M	1309	BCL	C2-C3	2.87	1.40	1.33
7	M	1317	BPH	CHB-C4A	2.94	1.47	1.40
5	M	1308	BCL	C2-C3	2.95	1.40	1.33
5	L	1283	BCL	C2-C3	3.14	1.40	1.33
7	M	1317	BPH	CHD-C4C	3.14	1.46	1.38
7	L	1287	BPH	CHD-C4C	3.19	1.46	1.38
5	L	1282	BCL	C2-C3	3.23	1.41	1.33
5	M	1308	BCL	CHC-C1C	3.29	1.37	1.33
7	L	1287	BPH	C3D-C2D	3.41	1.47	1.39
12	M	1319	SPO	C21-C20	3.75	1.45	1.35
12	M	1319	SPO	C26-C25	3.89	1.44	1.34
6	M	1314	LDA	C8-C7	3.90	1.73	1.51
5	L	1283	BCL	CHB-C4A	3.91	1.38	1.33
7	M	1317	BPH	C3D-C2D	3.93	1.48	1.39
13	M	1320	CDL	C12-C11	3.94	1.66	1.52
7	M	1317	BPH	CHC-C4B	4.06	1.50	1.40
13	M	1320	CDL	C34-C33	4.08	1.74	1.51
12	M	1319	SPO	C15-C16	4.08	1.45	1.34
7	L	1287	BPH	CHC-C4B	4.36	1.50	1.40
12	M	1319	SPO	C10-C11	4.56	1.46	1.34
5	L	1283	BCL	CHC-C1C	4.62	1.39	1.33
6	M	1314	LDA	C9-C8	4.63	1.78	1.51
13	M	1320	CDL	OB6-CB5	4.86	1.48	1.34
7	L	1287	BPH	CHB-C1B	4.91	1.48	1.38
7	M	1317	BPH	CHB-C1B	4.91	1.48	1.38
13	M	1320	CDL	OB8-CB7	4.93	1.47	1.33
5	L	1282	BCL	CHB-C4A	4.94	1.39	1.33
5	M	1308	BCL	CHB-C4A	4.94	1.39	1.33
7	L	1287	BPH	CHC-C1C	4.98	1.46	1.36
13	M	1320	CDL	C37-C36	4.99	1.80	1.51
13	M	1320	CDL	OA8-CA7	5.15	1.48	1.33
8	M	1318	U10	C18-C19	5.20	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1288[B]	U10	C13-C14	5.21	1.47	1.32
12	M	1319	SPO	C6-C5	5.27	1.46	1.31
5	L	1283	BCL	O1A-CGA	5.38	1.38	1.22
8	M	1318	U10	C38-C39	5.44	1.48	1.32
8	L	1288[A]	U10	C13-C14	5.46	1.48	1.32
8	M	1318	U10	C13-C14	5.47	1.46	1.33
5	M	1309	BCL	O1A-CGA	5.50	1.39	1.22
13	M	1320	CDL	C35-C34	5.51	1.83	1.51
5	M	1309	BCL	CHB-C4A	5.53	1.40	1.33
5	L	1282	BCL	CHC-C1C	5.53	1.40	1.33
13	M	1320	CDL	C18-C17	5.54	1.83	1.51
8	M	1318	U10	C28-C29	5.56	1.46	1.33
8	M	1318	U10	C23-C24	5.64	1.47	1.33
5	M	1308	BCL	O1A-CGA	5.67	1.39	1.22
7	M	1317	BPH	O1A-CGA	5.67	1.39	1.22
8	M	1318	U10	C8-C9	5.67	1.47	1.33
8	M	1318	U10	C6-C1	5.68	1.42	1.34
13	M	1320	CDL	OA6-CA5	5.71	1.50	1.34
12	M	1319	SPO	C37-C38	5.77	1.49	1.32
5	M	1309	BCL	CHC-C1C	5.77	1.40	1.33
7	M	1317	BPH	CHC-C1C	5.80	1.47	1.36
7	M	1317	BPH	C2-C3	5.84	1.47	1.33
12	M	1319	SPO	C32-C33	5.90	1.47	1.33
7	L	1287	BPH	O1A-CGA	5.98	1.40	1.22
7	L	1287	BPH	C2-C3	6.04	1.48	1.33
8	L	1288[A]	U10	C8-C9	6.11	1.48	1.33
8	M	1318	U10	C33-C34	6.12	1.48	1.33
8	L	1288[B]	U10	C8-C9	6.19	1.48	1.33
5	L	1282	BCL	O1A-CGA	6.66	1.42	1.22
7	M	1317	BPH	O1D-CGD	6.86	1.38	1.21
7	L	1287	BPH	O1D-CGD	6.96	1.38	1.21
8	M	1318	U10	C3-C4	7.25	1.43	1.36
12	M	1319	SPO	C14-C12	8.06	1.46	1.35
7	M	1317	BPH	OBB-CAB	8.12	1.41	1.23
12	M	1319	SPO	C22-C23	8.32	1.46	1.35
12	M	1319	SPO	C19-C17	9.07	1.47	1.35
12	M	1319	SPO	C9-C7	9.15	1.47	1.35
7	L	1287	BPH	OBB-CAB	9.18	1.43	1.23
5	L	1283	BCL	OBD-CAD	11.04	1.38	1.22
7	L	1287	BPH	OBD-CAD	11.09	1.38	1.22
5	M	1308	BCL	OBD-CAD	11.23	1.38	1.22
7	M	1317	BPH	OBD-CAD	11.28	1.38	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1319	SPO	C27-C28	11.50	1.46	1.34
5	L	1282	BCL	OBD-CAD	11.59	1.39	1.22
5	M	1309	BCL	OBD-CAD	12.41	1.40	1.22

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1308	BCL	CMB-C2B-C1B	-7.19	117.42	128.46
5	M	1309	BCL	CMB-C2B-C1B	-6.78	118.04	128.46
5	L	1282	BCL	CMB-C2B-C1B	-6.66	118.23	128.46
5	L	1283	BCL	CMB-C2B-C1B	-6.07	119.13	128.46
12	M	1319	SPO	C15-C14-C12	-4.68	120.63	127.31
5	L	1283	BCL	CHD-C4C-NC	-4.65	119.91	125.08
12	M	1319	SPO	C10-C9-C7	-4.61	120.73	127.31
5	L	1283	BCL	OBD-CAD-CBD	-4.44	119.24	125.94
7	M	1317	BPH	OBD-CAD-CBD	-4.39	119.32	125.94
12	M	1319	SPO	C21-C22-C23	-4.26	121.23	127.31
12	M	1319	SPO	C20-C19-C17	-4.25	121.24	127.31
5	M	1308	BCL	C1D-CHD-C4C	-4.08	119.84	125.92
13	M	1320	CDL	CA4-OA6-CA5	-4.02	108.37	117.88
8	M	1318	U10	O4-C4-C3	-3.85	119.65	127.45
8	L	1288[A]	U10	C7-C6-C1	-3.47	116.65	123.47
13	M	1320	CDL	C19-C18-C17	-3.46	96.61	114.45
12	M	1319	SPO	C4-C5-C6	-3.34	119.78	124.57
5	L	1282	BCL	OBD-CAD-CBD	-3.33	120.92	125.94
5	M	1308	BCL	O1D-CGD-CBD	-3.31	118.65	124.60
5	L	1283	BCL	O1D-CGD-CBD	-3.29	118.70	124.60
5	L	1283	BCL	C4B-CHC-C1C	-3.20	123.79	130.12
12	M	1319	SPO	C25-C23-C22	-3.19	114.04	118.94
13	M	1320	CDL	OA6-CA5-OA7	-3.17	115.76	123.68
5	L	1282	BCL	CHD-C4C-NC	-3.17	121.56	125.08
5	M	1308	BCL	CMA-C3A-C4A	-3.13	103.36	111.77
13	M	1320	CDL	C37-C36-C35	-3.13	98.35	114.45
7	L	1287	BPH	CBB-CAB-C3B	-3.12	113.84	120.52
5	M	1309	BCL	C1D-CHD-C4C	-3.12	121.27	125.92
6	M	1314	LDA	C9-C8-C7	-3.07	98.62	114.45
5	L	1283	BCL	C6-C5-C3	-3.07	105.69	112.66
7	L	1287	BPH	C1C-NC-C4C	-2.99	107.85	110.54
5	M	1309	BCL	C16-C15-C13	-2.99	105.92	115.73
7	M	1317	BPH	CHC-C4B-NB	-2.98	119.24	124.97
8	L	1288[A]	U10	C1M-C1-C6	-2.95	118.21	124.20
7	M	1317	BPH	CBA-CAA-C2A	-2.90	105.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1319	SPO	C14-C15-C16	-2.86	114.46	123.23
5	L	1282	BCL	C4B-CHC-C1C	-2.86	124.46	130.12
8	M	1318	U10	C27-C28-C29	-2.84	120.56	127.68
5	L	1282	BCL	CMA-C3A-C4A	-2.80	104.26	111.77
7	L	1287	BPH	O2A-CGA-O1A	-2.78	116.65	123.55
5	L	1283	BCL	O2A-CGA-O1A	-2.76	116.70	123.55
7	M	1317	BPH	O2D-CGD-O1D	-2.75	118.29	123.82
5	M	1308	BCL	C1B-CHB-C4A	-2.75	124.67	130.12
5	L	1283	BCL	C1-C2-C3	-2.74	120.91	125.96
8	M	1318	U10	C22-C23-C24	-2.73	120.82	127.68
5	L	1282	BCL	O2A-CGA-O1A	-2.71	116.81	123.55
5	L	1282	BCL	CMD-C2D-C3D	-2.71	119.87	124.89
5	L	1282	BCL	CAA-C2A-C1A	-2.68	103.18	111.97
7	M	1317	BPH	O1D-CGD-CBD	-2.67	119.80	124.60
6	M	1314	LDA	C8-C7-C6	-2.66	100.73	114.45
8	M	1318	U10	C5-C4-C3	-2.66	121.51	125.68
8	L	1288[A]	U10	O2-C2-C3	-2.62	115.37	120.95
5	L	1283	BCL	CAC-C3C-C4C	-2.62	106.77	112.58
5	M	1309	BCL	O1D-CGD-CBD	-2.62	119.90	124.60
7	M	1317	BPH	OBD-CAD-C3D	-2.60	123.24	128.03
5	L	1282	BCL	C3C-C4C-CHD	-2.59	117.89	123.34
8	M	1318	U10	C12-C13-C14	-2.59	121.18	127.68
7	L	1287	BPH	O1D-CGD-CBD	-2.58	119.97	124.60
6	M	1313	LDA	CM2-N1-CM1	-2.56	106.10	110.99
7	M	1317	BPH	C1C-NC-C4C	-2.54	108.26	110.54
5	L	1283	BCL	CAA-C2A-C1A	-2.52	103.70	111.97
7	L	1287	BPH	C7-C6-C5	-2.52	106.10	113.11
5	L	1282	BCL	O2D-CGD-O1D	-2.51	118.76	123.82
5	L	1283	BCL	C3C-C4C-CHD	-2.51	118.07	123.34
13	M	1320	CDL	C18-C17-C16	-2.48	101.70	114.45
12	M	1319	SPO	C5-C6-C7	-2.47	122.16	125.89
5	M	1309	BCL	OBD-CAD-CBD	-2.43	122.28	125.94
5	M	1308	BCL	OBD-CAD-CBD	-2.40	122.32	125.94
7	M	1317	BPH	C3B-C2B-C1B	-2.37	102.30	105.82
7	L	1287	BPH	C1B-NB-C4B	-2.36	101.85	106.52
5	M	1309	BCL	CBB-CAB-C3B	-2.35	113.56	120.39
7	L	1287	BPH	OBD-CAD-C3D	-2.34	123.72	128.03
5	M	1308	BCL	C3C-C4C-CHD	-2.32	118.46	123.34
5	M	1308	BCL	CAA-C2A-C3A	-2.30	106.51	112.81
13	M	1320	CDL	OB8-CB7-OB9	-2.29	117.86	123.55
7	L	1287	BPH	C3B-C2B-C1B	-2.29	102.42	105.82
5	M	1309	BCL	C1B-CHB-C4A	-2.29	125.59	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1320	CDL	OA8-CA7-OA9	-2.27	117.92	123.55
5	L	1283	BCL	C3C-C2C-C1C	-2.25	98.24	101.87
5	L	1283	BCL	CHB-C4A-NA	-2.21	121.45	124.51
5	L	1283	BCL	C1D-CHD-C4C	-2.20	122.65	125.92
8	M	1318	U10	C26-C27-C28	-2.17	104.52	111.97
7	L	1287	BPH	C1-C2-C3	-2.14	122.01	125.96
7	L	1287	BPH	CHB-C1B-NB	-2.12	120.49	124.64
5	L	1282	BCL	CHB-C4A-NA	-2.11	121.59	124.51
5	L	1283	BCL	O2D-CGD-O1D	-2.10	119.59	123.82
8	L	1288[A]	U10	C4-C3-C2	-2.10	116.31	120.67
5	L	1283	BCL	CHA-C1A-NA	-2.08	121.36	126.18
5	M	1309	BCL	C3C-C4C-CHD	-2.06	119.00	123.34
6	M	1314	LDA	C10-C9-C8	-2.06	103.86	114.45
5	L	1283	BCL	CMD-C2D-C3D	-2.05	121.08	124.89
8	M	1318	U10	C17-C18-C19	-2.04	122.55	127.68
5	L	1282	BCL	C1D-CHD-C4C	-2.04	122.89	125.92
8	M	1318	U10	C22-C21-C19	-2.03	106.06	112.93
5	M	1309	BCL	C1-C2-C3	-2.02	122.23	125.96
8	L	1288[A]	U10	C12-C13-C14	-2.02	120.59	127.80
5	M	1308	BCL	CHA-C1A-NA	-2.01	121.52	126.18
5	M	1309	BCL	OB B-CAB-C3B	2.02	123.79	119.95
6	M	1310	LDA	O1-N1-C1	2.02	114.23	109.27
5	L	1283	BCL	C4-C3-C5	2.05	118.84	115.29
5	L	1283	BCL	C2A-C3A-C4A	2.11	105.28	101.87
8	L	1288[B]	U10	C16-C14-C15	2.14	119.59	114.60
13	M	1320	CDL	C80-C79-C78	2.14	125.48	114.45
12	M	1319	SPO	C24-C23-C25	2.20	121.60	118.10
13	M	1320	CDL	C34-C33-C32	2.24	125.97	114.45
13	M	1320	CDL	C12-C11-CA5	2.27	121.86	113.58
12	M	1319	SPO	C40-C38-C39	2.31	119.99	114.60
13	M	1320	CDL	CA6-OA8-CA7	2.31	124.08	117.13
8	L	1288[B]	U10	C10-C9-C11	2.33	119.33	115.29
8	M	1318	U10	C25-C24-C26	2.34	119.36	115.29
5	M	1309	BCL	CHD-C4C-NC	2.37	127.71	125.08
7	M	1317	BPH	CED-O2D-CGD	2.38	121.56	115.97
5	L	1282	BCL	C2A-C3A-C4A	2.44	105.81	101.87
5	L	1283	BCL	C4A-NA-C1A	2.44	109.48	106.45
12	M	1319	SPO	C34-C33-C35	2.45	119.54	115.29
5	L	1282	BCL	C14-C13-C12	2.46	120.33	111.36
7	M	1317	BPH	O2A-CGA-CBA	2.59	119.45	111.90
7	M	1317	BPH	C1-O2A-CGA	2.61	123.04	116.77
5	L	1283	BCL	CED-O2D-CGD	2.67	122.24	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1288[A]	U10	C3M-O3-C3	2.68	126.02	116.44
5	L	1282	BCL	C1-O2A-CGA	2.70	123.24	116.77
12	M	1319	SPO	C13-C12-C11	2.76	122.50	118.10
7	L	1287	BPH	O2A-CGA-CBA	2.80	120.03	111.90
8	M	1318	U10	C15-C14-C16	2.93	120.37	115.29
13	M	1320	CDL	OB8-CB7-C71	2.98	120.57	111.90
5	L	1282	BCL	CED-O2D-CGD	3.00	123.00	115.97
5	L	1282	BCL	C11-C12-C13	3.03	125.68	115.73
5	M	1308	BCL	O2A-CGA-CBA	3.08	120.87	111.90
5	L	1282	BCL	O2A-CGA-CBA	3.13	121.01	111.90
7	M	1317	BPH	C4D-C3D-CAD	3.13	109.57	107.78
8	M	1318	U10	C35-C34-C36	3.15	120.76	115.29
7	L	1287	BPH	CMB-C2B-C1B	3.16	129.97	125.04
5	L	1282	BCL	O2D-CGD-CBD	3.20	117.02	111.30
8	L	1288[A]	U10	C10-C9-C11	3.25	120.94	115.29
13	M	1320	CDL	C33-C32-C31	3.28	125.26	113.24
13	M	1320	CDL	OA8-CA7-C31	3.31	121.54	111.90
7	M	1317	BPH	C2B-C1B-NB	3.32	114.74	109.82
13	M	1320	CDL	C35-C34-C33	3.40	131.99	114.45
8	M	1318	U10	C30-C29-C31	3.49	121.35	115.29
5	L	1283	BCL	CMB-C2B-C3B	3.53	131.43	124.89
7	L	1287	BPH	C2B-C1B-NB	3.58	115.12	109.82
12	M	1319	SPO	C29-C28-C30	3.65	121.62	115.29
13	M	1320	CDL	OB6-CB5-C51	3.65	119.13	111.55
5	L	1282	BCL	CMB-C2B-C3B	3.66	131.69	124.89
5	M	1309	BCL	O2A-CGA-CBA	3.88	123.18	111.90
8	M	1318	U10	C10-C9-C11	3.93	122.11	115.29
7	M	1317	BPH	CAC-C3C-C4C	4.10	123.20	112.67
5	L	1283	BCL	O2A-CGA-CBA	4.10	123.83	111.90
5	M	1309	BCL	CMB-C2B-C3B	4.16	132.61	124.89
7	M	1317	BPH	C3C-C4C-NC	4.31	112.03	107.97
7	L	1287	BPH	CED-O2D-CGD	4.34	126.15	115.97
5	M	1308	BCL	CMB-C2B-C3B	4.59	133.41	124.89
7	L	1287	BPH	O2D-CGD-CBD	4.65	119.61	111.30
5	M	1309	BCL	CED-O2D-CGD	4.73	127.05	115.97
13	M	1320	CDL	C20-C19-C18	4.79	139.15	114.45
5	M	1309	BCL	O2D-CGD-CBD	4.85	119.97	111.30
5	M	1308	BCL	O2D-CGD-CBD	4.94	120.12	111.30
5	M	1308	BCL	C1-O2A-CGA	5.23	129.32	116.77
13	M	1320	CDL	OA6-CA5-C11	5.67	123.33	111.55
13	M	1320	CDL	C13-C12-C11	5.77	134.38	113.24
7	L	1287	BPH	C3C-C4C-NC	5.81	113.44	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1283	BCL	O2D-CGD-CBD	5.82	121.71	111.30
7	M	1317	BPH	O2D-CGD-CBD	5.92	121.87	111.30
7	L	1287	BPH	C4D-C3D-CAD	7.09	111.83	107.78

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1308	BCL	C8
5	M	1308	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1283	BCL	C8
5	L	1283	BCL	C13
5	M	1309	BCL	C8
5	M	1309	BCL	C13

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1261	GOL	4	0
5	L	1282	BCL	1	0
5	L	1283	BCL	4	0
6	L	1286	LDA	1	0
7	L	1287	BPH	6	0
8	L	1288[A]	U10	8	0
8	L	1288[B]	U10	2	0
5	M	1308	BCL	5	0
5	M	1309	BCL	6	0
6	M	1312	LDA	2	0
6	M	1313	LDA	3	0
6	M	1314	LDA	4	0
7	M	1317	BPH	9	0
8	M	1318	U10	4	0
12	M	1319	SPO	3	0
13	M	1320	CDL	18	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	260/260 (100%)	0.28	22 (8%) 11 11	17, 26, 108, 129	0
2	L	281/281 (100%)	-0.36	9 (3%) 48 51	16, 24, 45, 56	0
3	M	307/307 (100%)	0.03	20 (6%) 20 20	14, 28, 52, 100	0
All	All	848/848 (100%)	-0.02	51 (6%) 23 23	14, 26, 53, 129	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	7	PHE	16.0
1	H	6	ALA	14.4
1	H	260	ALA	12.9
1	H	5	THR	12.8
1	H	4	VAL	12.2
1	H	257	ALA	11.4
1	H	3	GLY	11.4
3	M	305	PRO	11.3
1	H	259	TYR	11.2
1	H	2	VAL	10.9
3	M	304	ALA	10.6
3	M	306	LEU	9.9
1	H	1	MET	9.6
1	H	9	ASN	9.6
1	H	256	LEU	9.5
1	H	10[A]	PHE	8.9
3	M	307	ASN	8.5
3	M	1	ALA	8.3
1	H	251	VAL	8.1
1	H	253	ALA	7.5
1	H	255	MET	7.0
1	H	8	GLY	7.0
2	L	162	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	H	254	ALA	5.9
1	H	258	GLU	5.9
1	H	250	SER	5.8
3	M	197	PHE	4.9
3	M	303	MET	4.8
1	H	252	VAL	4.6
1	H	249	LYS	4.4
3	M	106	ALA	3.6
3	M	301[A]	HIS	3.4
3	M	302	GLY	3.3
2	L	281	GLY	3.2
2	L	59	TRP	3.0
3	M	2	GLU	2.8
3	M	52	LEU	2.7
3	M	148	TRP	2.7
3	M	101	TYR	2.7
2	L	271	TRP	2.5
2	L	270	PRO	2.5
3	M	3	TYR	2.4
3	M	54	SER	2.3
3	M	100	GLU	2.3
2	L	276	PRO	2.2
3	M	53	GLY	2.2
3	M	109	LEU	2.1
2	L	166	ASN	2.1
2	L	51	TRP	2.1
3	M	105	PHE	2.1
2	L	202	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	H	1261	6/6	0.77	0.29	19.35	35,46,50,52	0
10	HTO	L	1290	10/10	0.71	0.31	15.83	55,59,60,61	0
6	LDA	L	1285	16/16	0.19	0.43	14.51	88,89,95,95	0
10	HTO	L	1291	10/10	0.74	0.51	12.78	100,101,102,102	0
6	LDA	L	1286	16/16	0.36	0.42	12.39	96,98,102,102	0
6	LDA	L	1284	16/16	0.53	0.34	10.78	55,79,92,92	0
8	U10	L	1288[A]	23/63	0.79	0.33	5.96	33,42,54,55	23
8	U10	L	1288[B]	23/63	0.79	0.33	5.84	32,34,35,35	23
4	GOL	L	1293	6/6	0.87	0.26	5.45	75,76,76,77	0
13	CDL	M	1320	81/100	0.70	0.40	5.28	49,79,102,105	0
6	LDA	M	1310	16/16	0.90	0.16	5.14	29,47,53,54	0
6	LDA	M	1311	16/16	0.79	0.21	4.55	55,60,71,72	0
6	LDA	M	1312	16/16	0.86	0.15	3.64	47,52,54,55	0
6	LDA	M	1314	16/16	0.53	0.25	2.61	66,72,84,85	0
8	U10	M	1318	47/63	0.92	0.17	2.43	15,26,55,57	0
12	SPO	M	1319	42/42	0.90	0.14	1.23	19,33,53,58	0
7	BPH	M	1317	65/65	0.93	0.15	1.16	16,26,84,85	0
4	GOL	L	1292	6/6	0.87	0.16	0.72	34,38,39,45	0
5	BCL	M	1308	66/66	0.97	0.14	0.66	13,21,67,68	0
7	BPH	L	1287	65/65	0.97	0.10	0.36	10,17,31,34	0
5	BCL	L	1283	66/66	0.96	0.11	0.32	14,19,45,50	0
5	BCL	M	1309	66/66	0.96	0.14	0.15	13,18,39,47	0
5	BCL	L	1282	66/66	0.97	0.11	0.01	15,18,32,37	0
9	PO4	L	1289	5/5	0.97	0.12	-0.23	58,60,60,61	0
11	FE	M	1316	1/1	1.00	0.08	-4.99	16,16,16,16	0
4	GOL	H	1264	6/6	0.73	0.30	-	71,74,74,76	0
4	GOL	H	1262	6/6	0.75	0.21	-	66,67,67,68	0
4	GOL	L	1294	6/6	0.80	0.19	-	94,95,95,95	0
6	LDA	M	1313	16/16	0.87	0.19	-	68,71,72,72	0
4	GOL	H	1263	6/6	0.79	0.26	-	72,74,74,75	0
6	LDA	M	1315	16/16	0.34	0.38	-	77,85,92,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.