



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 05:07 AM EDT

PDB ID : 2FHB
Title : Crystal Structure Analysis of Klebsiella pneumoniae pullulanase complexed with maltose
Authors : Mikami, B.; Iwamoto, H.; Katsuya, Y.; Yoon, H.-J.; Demirkan-Sarikaya, E.; Malle, D.
Deposited on : unknown
Resolution : 1.80 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 : rb-20030345
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) : rb-20030345

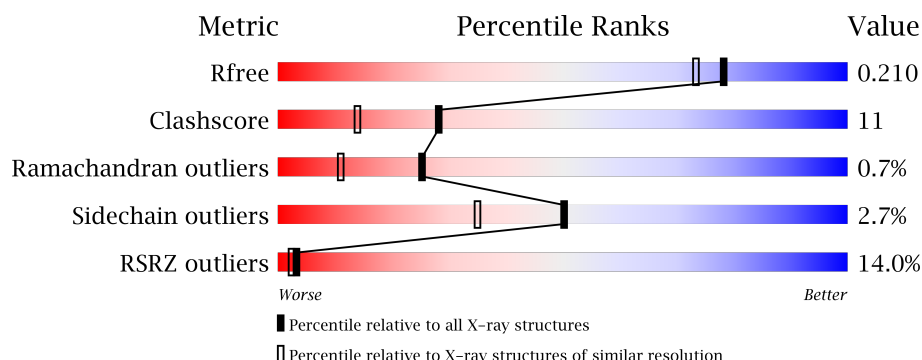
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	A	1083	<div> <div>14%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9181 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.

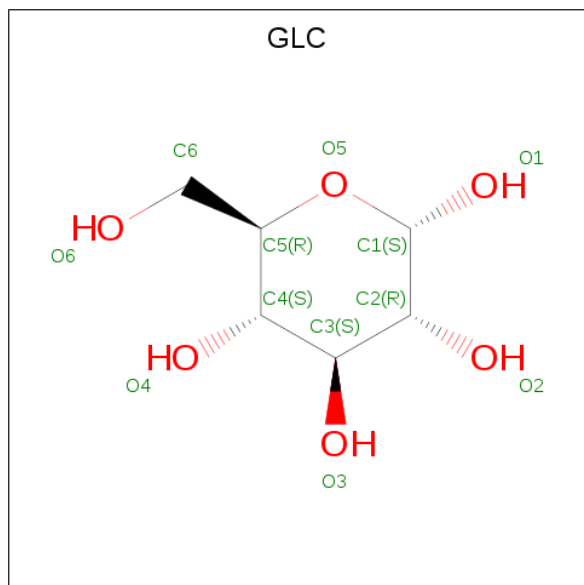
- Molecule 1 is a protein called pullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1052	8128	5076	1387	1638	27	0	17	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	ENGINEERED	GB 149300
A	882	LEU	VAL	ENGINEERED	GB 149300

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		

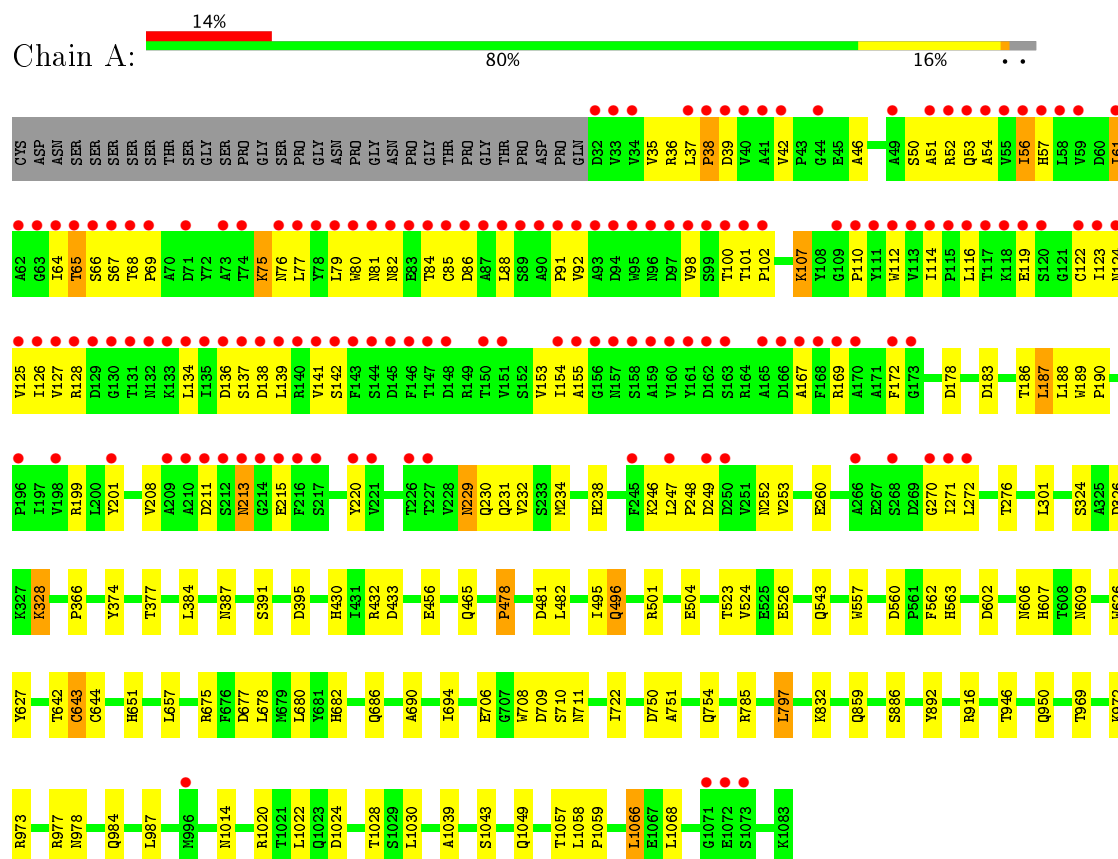
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1002	Total	O	0	0
			1002	1002		

3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: pullulanase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.26Å 60.60Å 135.10Å 90.00° 114.43° 90.00°	Depositor
Resolution (Å)	14.96 – 1.80 47.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	87.4 (14.96-1.80) 80.8 (47.62-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.205 0.179 , 0.210	Depositor DCC
R_{free} test set	9010 reflections (10.04%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/8361	0.59	0/11379

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8128	0	7824	178	0
2	A	46	0	42	2	0
3	A	5	0	0	0	0
4	A	1002	0	0	7	0
All	All	9181	0	7866	178	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 11.

All (178) 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)
1:A:81:ASN:HB2	1:A:86:ASP:HA	1.46	0.98
1:A:81:ASN:HD22	1:A:88:LEU:HB2	1.35	0.91
1:A:972[B]:LYS:HE3	1:A:973:ARG:HE	1.36	0.90
1:A:606:ASN:HD21	1:A:607:HIS:HD2	1.20	0.90
1:A:81:ASN:HB3	1:A:88:LEU:HD13	1.55	0.86
1:A:978:ASN:HD21	1:A:984:GLN:H	1.21	0.84
1:A:680:LEU:HD11	4:A:1543:HOH:O	1.77	0.82
1:A:229:ASN:HD21	1:A:232:VAL:HG23	1.47	0.80
1:A:972[B]:LYS:HG3	1:A:973:ARG:HG3	1.64	0.79
1:A:606:ASN:ND2	1:A:607:HIS:HD2	1.80	0.79
1:A:88:LEU:HD12	1:A:88:LEU:H	1.50	0.76
1:A:969:THR:HG23	1:A:972[B]:LYS:HE2	1.68	0.76
1:A:324:SER:OG	1:A:328[A]:LYS:HG3	1.87	0.75
1:A:229:ASN:HD21	1:A:232:VAL:CG2	2.01	0.73
1:A:972[B]:LYS:HE3	1:A:973:ARG:NE	2.02	0.73
1:A:64:ILE:HD12	1:A:64:ILE:H	1.54	0.73
1:A:213:ASN:HD22	1:A:213:ASN:C	1.92	0.72
1:A:680:LEU:HG	1:A:710:SER:HB3	1.72	0.71
1:A:134:LEU:HD21	1:A:155:ALA:HA	1.74	0.70
1:A:37:LEU:HD13	1:A:169:ARG:HB3	1.75	0.69
1:A:79:LEU:HB3	1:A:88:LEU:HD23	1.74	0.69
1:A:123:ILE:HG12	1:A:141:VAL:HB	1.73	0.69
1:A:501:ARG:O	1:A:504:GLU:HG2	1.92	0.69
1:A:42:VAL:HG11	1:A:169:ARG:HH11	1.59	0.68
1:A:627:TYR:O	1:A:651:HIS:HD2	1.79	0.65
1:A:76:ASN:HD21	1:A:128:ARG:HH21	1.44	0.65
1:A:39:ASP:HA	1:A:42:VAL:HG13	1.78	0.65
1:A:39:ASP:HA	1:A:42:VAL:CG1	2.27	0.65
1:A:560:ASP:HB3	1:A:609:ASN:ND2	2.12	0.65
1:A:85:CYS:HB3	1:A:122:CYS:O	1.97	0.64
1:A:1039:ALA:HB3	1:A:1043:SER:HB2	1.80	0.64
1:A:750:ASP:HB3	1:A:754:GLN:HE21	1.63	0.63
1:A:523:THR:OG1	1:A:526:GLU:HG3	1.99	0.62
1:A:750:ASP:HB3	1:A:754:GLN:NE2	2.15	0.62
1:A:42:VAL:HG11	1:A:169:ARG:NH1	2.15	0.61
1:A:680:LEU:HD23	1:A:680:LEU:H	1.65	0.60
1:A:54:ALA:HB2	1:A:116:LEU:HD11	1.83	0.60
1:A:208:VAL:HG22	1:A:260:GLU:OE2	2.02	0.60
1:A:706[B]:GLU:OE1	1:A:832:LYS:NZ	2.33	0.60
1:A:680:LEU:HD13	1:A:708:TRP:HB2	1.84	0.59
1:A:606:ASN:ND2	1:A:607:HIS:CD2	2.67	0.58
1:A:56:ILE:HG22	1:A:112:TRP:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:LEU:HG	1:A:1066:LEU:HB3	1.86	0.57
1:A:56:ILE:HD13	1:A:57:HIS:N	2.20	0.57
1:A:134:LEU:HD23	1:A:134:LEU:O	2.03	0.57
1:A:680:LEU:HD23	1:A:680:LEU:N	2.18	0.57
1:A:675:ARG:NH2	1:A:706[B]:GLU:OE1	2.37	0.57
1:A:107:LYS:HD2	1:A:107:LYS:H	1.70	0.57
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.87	0.57
1:A:722:ILE:HG12	4:A:1665:HOH:O	2.05	0.56
1:A:64:ILE:HD12	1:A:64:ILE:N	2.18	0.56
1:A:35:VAL:HA	1:A:270:GLY:O	2.05	0.56
1:A:98:VAL:O	1:A:98:VAL:HG22	2.06	0.56
1:A:495:ILE:HA	1:A:524:VAL:HB	1.89	0.55
1:A:642:THR:O	1:A:643:CYS:HB3	2.06	0.55
1:A:969:THR:HA	1:A:972[B]:LYS:HG2	1.87	0.55
1:A:682:HIS:HD2	1:A:686:GLN:HE22	1.54	0.55
1:A:213:ASN:C	1:A:213:ASN:ND2	2.57	0.55
1:A:187:LEU:HD13	1:A:188:LEU:N	2.22	0.54
1:A:77:LEU:HD23	1:A:127:VAL:HA	1.90	0.54
1:A:972[B]:LYS:CE	1:A:973:ARG:HE	2.14	0.54
1:A:79:LEU:H	1:A:92:VAL:HG22	1.72	0.54
1:A:56:ILE:CG2	1:A:112:TRP:HB2	2.38	0.54
1:A:199:ARG:HD3	1:A:220:TYR:CE2	2.43	0.54
1:A:36:ARG:HA	1:A:215:GLU:HA	1.89	0.53
1:A:560:ASP:HB3	1:A:609:ASN:HD22	1.73	0.53
1:A:272:LEU:C	1:A:272:LEU:HD23	2.29	0.53
1:A:680:LEU:HD12	1:A:710:SER:N	2.23	0.53
1:A:134:LEU:CD2	1:A:155:ALA:HA	2.37	0.53
1:A:229:ASN:ND2	1:A:232:VAL:HB	2.24	0.53
1:A:465:GLN:HG3	1:A:950:GLN:HE22	1.72	0.53
1:A:229:ASN:HD21	1:A:232:VAL:CB	2.22	0.53
1:A:680:LEU:HD12	1:A:709:ASP:C	2.30	0.53
1:A:680:LEU:CD2	1:A:680:LEU:H	2.22	0.52
1:A:37:LEU:O	1:A:39:ASP:N	2.43	0.52
1:A:1014:ASN:HD21	1:A:1020:ARG:HH11	1.57	0.52
1:A:139:LEU:HD12	1:A:139:LEU:N	2.25	0.51
1:A:64:ILE:CD1	1:A:64:ILE:H	2.21	0.51
1:A:977:ARG:NH1	1:A:1024:ASP:HB3	2.26	0.51
1:A:76:ASN:ND2	1:A:128:ARG:HH21	2.07	0.51
1:A:229:ASN:ND2	1:A:232:VAL:H	2.10	0.50
1:A:154:ILE:HG12	1:A:167:ALA:HB1	1.92	0.50
1:A:643:CYS:SG	1:A:644:CYS:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD11	1:A:138:ASP:HA	1.93	0.50
1:A:326:ASP:HB2	1:A:328[A]:LYS:HE2	1.94	0.50
1:A:229:ASN:N	1:A:229:ASN:HD22	2.09	0.50
1:A:785:ARG:NH2	4:A:1360:HOH:O	2.45	0.49
1:A:125:VAL:HG12	1:A:126:ILE:N	2.27	0.49
1:A:1028:THR:HG22	1:A:1068:LEU:CD2	2.43	0.49
1:A:68:THR:HG23	1:A:69:PRO:HD2	1.95	0.49
1:A:76:ASN:HD21	1:A:128:ARG:NH2	2.10	0.49
1:A:682:HIS:HD2	1:A:686:GLN:NE2	2.10	0.49
1:A:1066:LEU:N	1:A:1066:LEU:HD22	2.27	0.49
1:A:56:ILE:HD13	1:A:56:ILE:C	2.33	0.49
1:A:102:PRO:HB3	1:A:110:PRO:HB2	1.95	0.49
1:A:642:THR:O	1:A:643:CYS:CB	2.61	0.48
1:A:465:GLN:HG3	1:A:950:GLN:NE2	2.29	0.48
1:A:50:SER:H	1:A:53:GLN:NE2	2.11	0.48
1:A:51:ALA:HA	1:A:119:GLU:OE1	2.15	0.47
1:A:677:ASP:OD1	2:A:1098:GLC:H1	2.15	0.47
1:A:430:HIS:HD2	1:A:433:ASP:H	1.62	0.47
1:A:127:VAL:HG12	1:A:134:LEU:HD13	1.97	0.47
1:A:211:ASP:OD1	1:A:213:ASN:HB3	2.13	0.47
1:A:324:SER:OG	1:A:328[A]:LYS:HE3	2.15	0.47
1:A:430:HIS:CD2	1:A:432:ARG:H	2.32	0.47
1:A:102:PRO:HG3	1:A:112:TRP:CZ2	2.50	0.46
1:A:61:ILE:HG23	1:A:61:ILE:O	2.15	0.46
1:A:81:ASN:HD21	1:A:91:PRO:HD3	1.80	0.46
1:A:183:ASP:OD2	1:A:186:THR:N	2.48	0.46
1:A:52:ARG:HH11	1:A:52:ARG:HG3	1.81	0.46
1:A:231:GLN:N	1:A:231:GLN:OE1	2.48	0.46
1:A:38:PRO:HG2	1:A:172:PHE:CD2	2.51	0.46
1:A:88:LEU:H	1:A:88:LEU:CD1	2.25	0.46
1:A:122:CYS:HB3	1:A:142:SER:HA	1.97	0.46
1:A:88:LEU:HD12	1:A:88:LEU:N	2.26	0.46
1:A:651:HIS:HE1	4:A:1186:HOH:O	1.99	0.45
1:A:246:LYS:HD3	1:A:247:LEU:O	2.17	0.45
1:A:384:LEU:HD23	1:A:391:SER:HA	1.99	0.45
1:A:85:CYS:HB3	1:A:122:CYS:C	2.36	0.45
1:A:1028:THR:HG22	1:A:1068:LEU:HD21	1.98	0.45
1:A:38:PRO:CB	1:A:271:ILE:HD11	2.47	0.45
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.82	0.45
1:A:127:VAL:HG21	1:A:153:VAL:HG21	1.97	0.44
1:A:246:LYS:HD3	1:A:247:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HB3	1:A:125:VAL:CG1	2.47	0.44
1:A:38:PRO:HG3	1:A:271:ILE:HD11	1.99	0.44
1:A:123:ILE:CG1	1:A:141:VAL:HB	2.45	0.44
1:A:657:LEU:C	1:A:657:LEU:HD23	2.38	0.44
1:A:682:HIS:CD2	1:A:686:GLN:HE22	2.34	0.44
1:A:75:LYS:O	1:A:102:PRO:HD3	2.18	0.44
1:A:677:ASP:OD1	2:A:1098:GLC:C1	2.66	0.43
1:A:136:ASP:O	1:A:137:SER:HB2	2.17	0.43
1:A:37:LEU:CD1	1:A:169:ARG:HB3	2.46	0.43
1:A:199:ARG:HB2	1:A:201:TYR:HE1	1.83	0.43
1:A:946:THR:O	1:A:950:GLN:HG3	2.19	0.43
1:A:100:THR:O	1:A:100:THR:HG22	2.18	0.43
1:A:230:GLN:O	1:A:234:MET:HG3	2.18	0.43
1:A:301:LEU:HD23	1:A:395:ASP:HB2	2.01	0.43
1:A:124:ASN:HA	1:A:139:LEU:O	2.19	0.43
1:A:229:ASN:N	1:A:229:ASN:ND2	2.67	0.43
1:A:238:HIS:CD2	1:A:238:HIS:H	2.35	0.43
1:A:189:TRP:HA	1:A:190:PRO:HD3	1.89	0.43
1:A:481:ASP:OD2	1:A:563:HIS:HD2	2.01	0.42
1:A:126:ILE:HD11	1:A:138:ASP:OD1	2.19	0.42
1:A:751:ALA:HB1	4:A:2323:HOH:O	2.19	0.42
1:A:81:ASN:CB	1:A:86:ASP:HA	2.33	0.42
1:A:1028:THR:O	1:A:1028:THR:HG22	2.19	0.42
1:A:456:GLU:CD	1:A:456:GLU:H	2.20	0.42
1:A:678:LEU:C	1:A:680:LEU:HD23	2.39	0.42
1:A:680:LEU:HD13	1:A:708:TRP:C	2.40	0.42
1:A:56:ILE:HG21	1:A:77:LEU:HD11	2.00	0.42
1:A:46:ALA:HB3	1:A:57:HIS:CE1	2.55	0.42
1:A:38:PRO:HG2	1:A:172:PHE:CE2	2.54	0.42
1:A:1049:GLN:HG3	1:A:1057:THR:HB	2.02	0.42
1:A:1058:LEU:HA	1:A:1059:PRO:HD3	1.89	0.42
1:A:675:ARG:NE	4:A:1365:HOH:O	2.53	0.42
1:A:377:THR:OG1	1:A:563:HIS:HE1	2.01	0.42
1:A:88:LEU:HD12	1:A:123:ILE:HG22	2.01	0.42
1:A:366:PRO:HB2	1:A:626:TRP:CE2	2.55	0.41
1:A:247:LEU:HD23	1:A:248:PRO:HD2	2.02	0.41
1:A:710:SER:O	1:A:711:ASN:HB2	2.20	0.41
1:A:101:THR:C	1:A:112:TRP:HE1	2.24	0.41
1:A:690:ALA:O	1:A:694:ILE:HG12	2.21	0.41
1:A:79:LEU:HD23	1:A:125:VAL:HG22	2.01	0.41
1:A:80:TRP:CZ3	1:A:126:ILE:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:N	1:A:92:VAL:HG22	2.35	0.41
1:A:178:ASP:OD1	1:A:276:THR:HG21	2.21	0.40
1:A:238:HIS:HE1	4:A:1434:HOH:O	2.03	0.40
1:A:79:LEU:H	1:A:92:VAL:CG2	2.33	0.40
1:A:79:LEU:CD2	1:A:125:VAL:HG22	2.51	0.40
1:A:39:ASP:CA	1:A:42:VAL:HG13	2.48	0.40
1:A:496:GLN:NE2	1:A:496:GLN:H	2.20	0.40
1:A:79:LEU:HD21	1:A:114:ILE:HD13	2.03	0.40
1:A:38:PRO:HB3	1:A:271:ILE:HD11	2.04	0.40
1:A:557:TRP:CE3	1:A:892:TYR:HB3	2.57	0.40
1:A:65:THR:O	1:A:67:SER:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1067/1083 (98%)	1016 (95%)	44 (4%)	7 (1%)	25 11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	84	THR
1	A	643	CYS
1	A	38	PRO
1	A	66	SER
1	A	82	ASN
1	A	478	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	883/891 (99%)	857 (97%)	26 (3%)	48 32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ILE
1	A	65	THR
1	A	75	LYS
1	A	107	LYS
1	A	187	LEU
1	A	213	ASN
1	A	229	ASN
1	A	249	ASP
1	A	252	ASN
1	A	328[A]	LYS
1	A	328[B]	LYS
1	A	374	TYR
1	A	387	ASN
1	A	478	PRO
1	A	482	LEU
1	A	496	GLN
1	A	543	GLN
1	A	562	PHE
1	A	602[A]	ASP
1	A	602[B]	ASP
1	A	797[A]	LEU
1	A	797[B]	LEU
1	A	859	GLN
1	A	886	SER
1	A	916	ARG
1	A	1066	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	GLN
1	A	76	ASN
1	A	81	ASN
1	A	204	HIS
1	A	213	ASN
1	A	229	ASN
1	A	230	GLN
1	A	238	HIS
1	A	252	ASN
1	A	258	GLN
1	A	279	GLN
1	A	316	GLN
1	A	387	ASN
1	A	392	GLN
1	A	413	HIS
1	A	430	HIS
1	A	439	GLN
1	A	455	GLN
1	A	458	ASN
1	A	465	GLN
1	A	496	GLN
1	A	533	GLN
1	A	534	ASN
1	A	541	GLN
1	A	543	GLN
1	A	551	GLN
1	A	563	HIS
1	A	606	ASN
1	A	607	HIS
1	A	609	ASN
1	A	651	HIS
1	A	682	HIS
1	A	686	GLN
1	A	754	GLN
1	A	859	GLN
1	A	899	ASN
1	A	911	ASN
1	A	950	GLN
1	A	978	ASN
1	A	983	GLN
1	A	984	GLN
1	A	1014	ASN

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Mol	Chain	Res	Type
1	A	1023	GLN
1	A	1037	GLN
1	A	1049	GLN
1	A	1074	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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\# Z > 2$
2	GLC	A	1093	2	11,11,12	0.49	0	13,15,17	0.59	0
2	GLC	A	1094	2	12,12,12	0.43	0	17,17,17	0.34	0
2	GLC	A	1097	2	11,11,12	0.53	0	13,15,17	0.65	0
2	GLC	A	1098	2	12,12,12	0.45	0	17,17,17	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	1093	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1094	2	-	0/2/22/22	0/1/1/1
2	GLC	A	1097	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1098	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1098	GLC	2	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.

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	A	1052/1083 (97%)	0.52	147 (13%) 3 2	19, 27, 82, 96	125 (11%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	THR	28.3
1	A	64	ILE	13.7
1	A	80	TRP	13.2
1	A	81	ASN	11.7
1	A	79	LEU	10.9
1	A	78	TYR	10.6
1	A	56	ILE	10.5
1	A	84	THR	10.1
1	A	92	VAL	9.9
1	A	98	VAL	9.7
1	A	95	TRP	9.6
1	A	133	LYS	9.6
1	A	85	CYS	9.5
1	A	82	ASN	9.5
1	A	83	GLU	9.2
1	A	143	PHE	9.2
1	A	142	SER	9.0
1	A	136	ASP	8.9
1	A	90	ALA	8.9
1	A	94	ASP	8.4
1	A	86	ASP	7.9
1	A	123	ILE	7.8
1	A	144	SER	7.7
1	A	91	PRO	7.7
1	A	87	ALA	7.6
1	A	169	ARG	7.5
1	A	67	SER	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	7.4
1	A	93	ALA	7.4
1	A	134	LEU	7.4
1	A	128	ARG	7.4
1	A	139	LEU	7.2
1	A	122	CYS	7.0
1	A	125	VAL	7.0
1	A	131	THR	7.0
1	A	39	ASP	6.9
1	A	40	VAL	6.5
1	A	157	ASN	6.5
1	A	117	THR	6.3
1	A	130	GLY	6.3
1	A	127	VAL	6.1
1	A	271	ILE	5.9
1	A	214	GLY	5.8
1	A	135	ILE	5.8
1	A	116	LEU	5.7
1	A	156	GLY	5.7
1	A	77	LEU	5.7
1	A	114	ILE	5.6
1	A	158	SER	5.5
1	A	68	THR	5.5
1	A	154	ILE	5.5
1	A	141	VAL	5.4
1	A	55	VAL	5.4
1	A	129	ASP	5.2
1	A	216	PHE	5.2
1	A	132	ASN	5.1
1	A	159	ALA	5.1
1	A	161	TYR	5.1
1	A	140	ARG	5.0
1	A	155	ALA	4.9
1	A	166	ASP	4.9
1	A	112	TRP	4.8
1	A	137	SER	4.8
1	A	59	VAL	4.8
1	A	97	ASP	4.7
1	A	120	SER	4.7
1	A	126	ILE	4.6
1	A	146	PHE	4.5
1	A	170	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	160	VAL	4.5
1	A	167	ALA	4.4
1	A	101	THR	4.4
1	A	51	ALA	4.4
1	A	54	ALA	4.4
1	A	74	THR	4.4
1	A	69	PRO	4.3
1	A	270	GLY	4.2
1	A	99	SER	4.2
1	A	168	PHE	4.1
1	A	96	ASN	4.0
1	A	61	ILE	3.9
1	A	147	THR	3.9
1	A	151	VAL	3.9
1	A	33	VAL	3.8
1	A	89	SER	3.7
1	A	100	THR	3.6
1	A	119	GLU	3.6
1	A	213	ASN	3.5
1	A	162	ASP	3.4
1	A	49	ALA	3.4
1	A	266	ALA	3.4
1	A	172	PHE	3.4
1	A	1072	GLU	3.4
1	A	148	ASP	3.4
1	A	58	LEU	3.4
1	A	272	LEU	3.4
1	A	62	ALA	3.4
1	A	38	PRO	3.3
1	A	37	LEU	3.3
1	A	145	ASP	3.2
1	A	198	VAL	3.2
1	A	250	ASP	3.1
1	A	76	ASN	3.1
1	A	118	LYS	3.1
1	A	53	GLN	3.0
1	A	138	ASP	3.0
1	A	173	GLY	3.0
1	A	52	ARG	3.0
1	A	165	ALA	3.0
1	A	247	LEU	2.9
1	A	210	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	268	SER	2.9
1	A	57	HIS	2.9
1	A	113	VAL	2.9
1	A	110	PRO	2.9
1	A	196	PRO	2.9
1	A	209	ALA	2.9
1	A	66	SER	2.8
1	A	212	SER	2.8
1	A	1073	SER	2.8
1	A	115	PRO	2.8
1	A	63	GLY	2.8
1	A	42	VAL	2.8
1	A	217	SER	2.7
1	A	124	ASN	2.7
1	A	215	GLU	2.7
1	A	996	MET	2.6
1	A	34	VAL	2.6
1	A	71	ASP	2.6
1	A	201	TYR	2.5
1	A	163	SER	2.4
1	A	249	ASP	2.4
1	A	109	GLY	2.4
1	A	73	ALA	2.3
1	A	226	THR	2.3
1	A	41	ALA	2.3
1	A	111	TYR	2.2
1	A	150	THR	2.2
1	A	220	TYR	2.2
1	A	227	THR	2.2
1	A	44	GLY	2.2
1	A	32	ASP	2.2
1	A	211	ASP	2.1
1	A	1071	GLY	2.1
1	A	221	VAL	2.1
1	A	102	PRO	2.1
1	A	245	PHE	2.0

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

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(\AA^2)	Q<0.9
3	CA	A	2402	1/1	0.87	0.16	1.38	48,48,48,48	0
3	CA	A	2401	1/1	1.00	0.08	1.13	22,22,22,22	0
2	GLC	A	1093	11/12	0.83	0.14	-0.42	36,38,42,45	0
2	GLC	A	1094	12/12	0.95	0.09	-0.57	28,31,33,35	0
3	CA	A	2408	1/1	0.74	0.21	-0.68	97,97,97,97	0
2	GLC	A	1097	11/12	0.97	0.07	-0.69	25,26,28,28	0
3	CA	A	2404	1/1	1.00	0.05	-0.96	23,23,23,23	0
2	GLC	A	1098	12/12	0.90	0.10	-0.97	32,37,39,44	0
3	CA	A	2403	1/1	0.98	0.04	-1.65	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.