



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 AM GMT

PDB ID : 2FH6
Title : Crystal Structure Analysis of Klebsiella pneumoniae pullulanase complexed with glucose
Authors : Mikami, B.; Iwamoto, H.; Katsuya, Y.; Yoon, H.-J.; Demirkan-Sarikaya, E.; Malle, D.
Deposited on : 2005-12-23
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

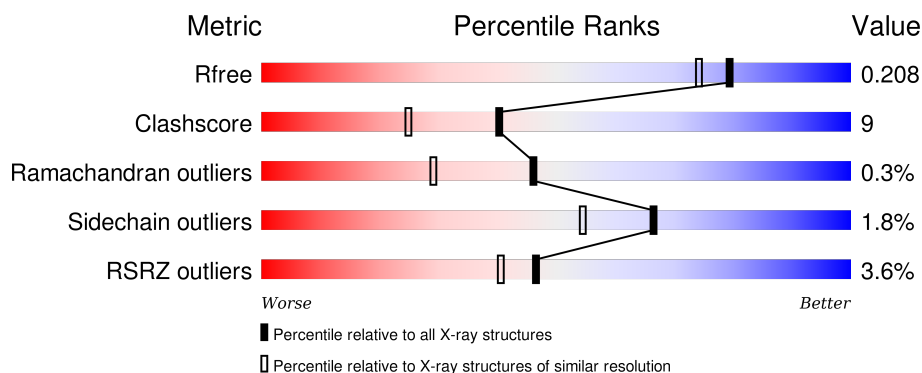
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

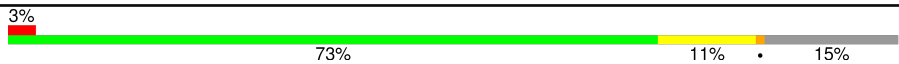
The reported resolution of this entry is 1.80 Å.

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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	

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
2	GLC	A	1097	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8068 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.

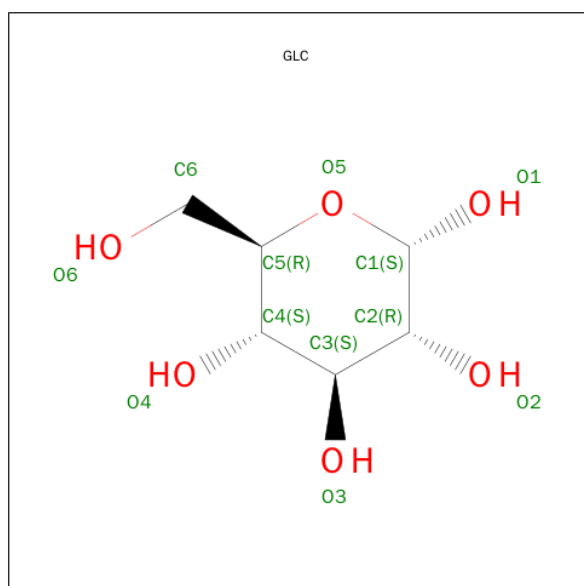
- Molecule 1 is a protein called pullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	920	7107	4438	1214	1430	25	0	11	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 SUGAR (GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	Ca 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	945	Total 945	O 945	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.26Å 60.42Å 133.65Å 90.00° 111.98° 90.00°	Depositor
Resolution (Å)	14.96 – 1.80 19.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.4 (14.96-1.80) 87.0 (19.93-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.212 0.183 , 0.208	Depositor DCC
R_{free} test set	9056 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105742 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8068	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.29	0/7294	0.60	0/9919

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7107	0	6837	121	0
2	A	12	0	12	0	0
3	A	4	0	0	0	0
4	A	945	0	0	11	0
All	All	8068	0	6849	121	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 (121) 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:680:LEU:HD13	1:A:708:TRP:H	1.34	0.91
1:A:978:ASN:HD21	1:A:984:GLN:H	1.12	0.91
1:A:606:ASN:HD21	1:A:607:HIS:HD2	1.23	0.83
1:A:1005:ARG:HH21	1:A:1005:ARG:HB3	1.46	0.80
1:A:680:LEU:HD11	1:A:710:SER:H	1.47	0.80
1:A:606:ASN:ND2	1:A:607:HIS:HD2	1.84	0.75
1:A:706:GLU:HG2	1:A:707:GLY:H	1.53	0.73
1:A:680:LEU:HD21	4:A:1411:HOH:O	1.89	0.72
1:A:680:LEU:HD22	1:A:707:GLY:HA3	1.72	0.71
1:A:706:GLU:HG2	1:A:707:GLY:N	2.05	0.71
1:A:816:PRO:HG2	4:A:1809:HOH:O	1.89	0.71
1:A:680:LEU:CD1	1:A:710:SER:H	2.04	0.70
1:A:680:LEU:HD13	1:A:708:TRP:N	2.06	0.68
1:A:627:TYR:O	1:A:651:HIS:HD2	1.77	0.68
1:A:1030:LEU:HG	1:A:1066:LEU:HB3	1.77	0.66
1:A:1039:ALA:HB3	1:A:1043:SER:HB2	1.78	0.65
1:A:229:ASN:ND2	1:A:231:GLN:HB2	2.10	0.65
1:A:1028:THR:HG22	1:A:1068:LEU:HD21	1.80	0.64
1:A:495:ILE:HA	1:A:524:VAL:HB	1.80	0.63
1:A:523:THR:OG1	1:A:526:GLU:HG3	1.99	0.63
1:A:1005:ARG:HB3	1:A:1005:ARG:NH2	2.15	0.62
1:A:1028:THR:HG22	1:A:1068:LEU:CD2	2.30	0.60
1:A:465:GLN:HG3	1:A:950:GLN:HE22	1.66	0.60
1:A:680:LEU:CD1	1:A:708:TRP:H	2.13	0.59
1:A:229:ASN:HD21	1:A:231:GLN:HB2	1.67	0.59
1:A:708:TRP:N	1:A:708:TRP:CE3	2.71	0.59
1:A:560:ASP:HB3	1:A:609:ASN:ND2	2.18	0.59
1:A:680:LEU:HD11	1:A:710:SER:N	2.19	0.57
1:A:708:TRP:HB2	4:A:1786:HOH:O	2.04	0.57
1:A:774:ASP:HB3	4:A:2186:HOH:O	2.04	0.56
1:A:496:GLN:NE2	1:A:496:GLN:H	2.03	0.56
1:A:642:THR:O	1:A:643:CYS:HB3	2.06	0.55
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.89	0.55
1:A:606:ASN:ND2	1:A:607:HIS:CD2	2.71	0.55
1:A:682:HIS:HD2	1:A:686:GLN:NE2	2.06	0.54
1:A:690:ALA:O	1:A:694:ILE:HG12	2.07	0.54
1:A:706:GLU:CG	1:A:707:GLY:H	2.21	0.54
1:A:682:HIS:HD2	1:A:686:GLN:HE22	1.55	0.54
1:A:946:THR:O	1:A:950:GLN:HG3	2.09	0.53
1:A:238:HIS:HE1	4:A:1438:HOH:O	1.91	0.52
1:A:682:HIS:CD2	1:A:686:GLN:HE22	2.28	0.52
1:A:465:GLN:HG3	1:A:950:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ARG:O	1:A:504:GLU:HG2	2.08	0.52
1:A:643:CYS:SG	1:A:644:CYS:N	2.83	0.51
1:A:706:GLU:CG	1:A:707:GLY:N	2.74	0.51
1:A:501:ARG:HA	1:A:504:GLU:OE1	2.11	0.51
1:A:197:ILE:O	1:A:265:ALA:HA	2.10	0.51
1:A:430:HIS:CD2	1:A:432:ARG:H	2.28	0.51
1:A:680:LEU:HD11	1:A:709:ASP:N	2.27	0.50
1:A:252:ASN:C	1:A:252:ASN:HD22	2.14	0.50
1:A:785:ARG:NH2	4:A:1603:HOH:O	2.45	0.50
1:A:223:LEU:CD2	1:A:247:LEU:HG	2.42	0.50
1:A:680:LEU:CD2	1:A:680:LEU:H	2.24	0.50
1:A:272:LEU:HD13	1:A:272:LEU:C	2.32	0.50
1:A:377:THR:OG1	1:A:563:HIS:HE1	1.93	0.50
1:A:642:THR:O	1:A:643:CYS:CB	2.60	0.50
1:A:606:ASN:HD21	1:A:607:HIS:CD2	2.15	0.49
1:A:208:VAL:CG2	1:A:262:VAL:HG21	2.42	0.49
1:A:430:HIS:HD2	1:A:433:ASP:H	1.59	0.49
1:A:387:ASN:ND2	1:A:487:GLU:H	2.10	0.49
1:A:750:ASP:O	1:A:754:GLN:HG3	2.13	0.48
1:A:229:ASN:HD22	1:A:231:GLN:CD	2.16	0.48
1:A:418:LYS:HD2	1:A:966[B]:ASP:OD1	2.13	0.48
1:A:1005:ARG:HH21	1:A:1005:ARG:CB	2.23	0.48
1:A:494:ASP:HB3	1:A:496:GLN:HE22	1.78	0.48
1:A:834:ASP:O	1:A:835:ASN:HB2	2.12	0.48
1:A:710:SER:O	1:A:711:ASN:CB	2.62	0.48
1:A:543:GLN:HE21	1:A:916:ARG:HA	1.78	0.48
1:A:706:GLU:HB2	1:A:732:PHE:CD2	2.49	0.48
1:A:680:LEU:CD1	1:A:708:TRP:N	2.75	0.48
1:A:199:ARG:HD3	1:A:220:TYR:CD2	2.49	0.48
1:A:481:ASP:OD2	1:A:563:HIS:HD2	1.97	0.47
1:A:1028:THR:HG22	1:A:1028:THR:O	2.14	0.47
1:A:753:ARG:HD2	1:A:930:VAL:HG11	1.95	0.47
1:A:680:LEU:N	1:A:680:LEU:HD23	2.30	0.47
1:A:929:ARG:HD2	4:A:1629:HOH:O	2.15	0.47
1:A:33:VAL:HG12	1:A:34:VAL:N	2.29	0.47
1:A:710:SER:O	1:A:711:ASN:HB3	2.15	0.46
1:A:560:ASP:HB3	1:A:609:ASN:HD22	1.80	0.46
1:A:1066:LEU:N	1:A:1066:LEU:HD22	2.30	0.46
1:A:466:LEU:HD23	1:A:950:GLN:HE21	1.81	0.45
1:A:258:GLN:HE22	1:A:316:GLN:HA	1.81	0.45
1:A:465:GLN:CG	1:A:950:GLN:HE22	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ASP:OD1	1:A:879:SER:HB2	2.17	0.45
1:A:710:SER:HA	4:A:1414:HOH:O	2.15	0.44
1:A:745:PRO:HG2	1:A:746:PHE:CD1	2.52	0.44
1:A:264:ILE:HG23	1:A:272:LEU:HD23	1.99	0.44
1:A:543:GLN:NE2	1:A:917:SER:H	2.15	0.44
1:A:886:SER:O	1:A:887:PHE:HB2	2.18	0.44
1:A:651:HIS:HE1	4:A:1205:HOH:O	2.01	0.44
1:A:978:ASN:ND2	1:A:984:GLN:H	1.95	0.43
1:A:413:HIS:HD2	4:A:1488:HOH:O	2.01	0.43
1:A:231:GLN:N	1:A:231:GLN:OE1	2.49	0.43
1:A:737:ARG:HD3	1:A:829:TYR:CZ	2.54	0.43
1:A:238:HIS:CD2	1:A:238:HIS:H	2.37	0.42
1:A:525[B]:GLU:HG3	1:A:897:TRP:HZ3	1.84	0.42
1:A:384:LEU:HD23	1:A:391:SER:HA	2.01	0.42
1:A:248:PRO:HB2	1:A:250:ASP:OD1	2.19	0.42
1:A:247:LEU:HD12	1:A:247:LEU:N	2.35	0.42
1:A:260:GLU:HB2	1:A:364:TYR:CE1	2.55	0.42
1:A:449:TYR:CZ	1:A:571:TYR:HB2	2.55	0.42
1:A:264:ILE:HG23	1:A:272:LEU:CD2	2.49	0.42
1:A:208:VAL:HG21	1:A:262:VAL:HG21	2.02	0.42
1:A:680:LEU:N	1:A:680:LEU:CD2	2.83	0.42
1:A:961:LEU:HB3	1:A:992:ILE:HG21	2.02	0.42
1:A:706:GLU:OE1	1:A:832:LYS:HE2	2.20	0.41
1:A:680:LEU:CD1	1:A:710:SER:N	2.78	0.41
1:A:1014:ASN:HD21	1:A:1020:ARG:HH11	1.68	0.41
1:A:501:ARG:HA	1:A:504:GLU:HG2	2.02	0.41
1:A:189:TRP:HA	1:A:190:PRO:HD3	1.93	0.41
1:A:204:HIS:HE1	4:A:1651:HOH:O	2.02	0.41
1:A:657:LEU:HD23	1:A:657:LEU:C	2.40	0.41
1:A:1028:THR:O	1:A:1068:LEU:HD22	2.20	0.41
1:A:411[A]:MET:HG2	1:A:672:ASP:OD1	2.20	0.41
1:A:973:ARG:HG2	1:A:998:ALA:HB1	2.02	0.41
1:A:366:PRO:HB2	1:A:626:TRP:CE2	2.56	0.41
1:A:383:SER:HB3	1:A:392:GLN:HB3	2.02	0.41
1:A:680:LEU:HD23	1:A:680:LEU:H	1.85	0.41
1:A:680:LEU:HD12	1:A:710:SER:HB3	2.03	0.40
1:A:195:LYS:HA	1:A:196:PRO:HD3	1.85	0.40
1:A:1028:THR:HG22	1:A:1068:LEU:HD22	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 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	927/1083 (86%)	903 (97%)	21 (2%)	3 (0%)	46 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	SER
1	A	643	CYS
1	A	478	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	768/891 (86%)	754 (98%)	14 (2%)	66 54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
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

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Mol	Chain	Res	Type
1	A	680	LEU
1	A	708	TRP
1	A	797	LEU
1	A	859	GLN
1	A	886	SER
1	A	1005	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	213	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	373	GLN
1	A	387	ASN
1	A	392	GLN
1	A	413	HIS
1	A	430	HIS
1	A	455	GLN
1	A	458	ASN
1	A	461	GLN
1	A	465	GLN
1	A	496	GLN
1	A	533	GLN
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	629	GLN
1	A	651	HIS
1	A	682	HIS
1	A	686	GLN
1	A	711	ASN
1	A	859	GLN

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Mol	Chain	Res	Type
1	A	899	ASN
1	A	911	ASN
1	A	944	GLN
1	A	950	GLN
1	A	978	ASN
1	A	983	GLN
1	A	1014	ASN
1	A	1023	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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	1097	-	12,12,12	0.37	0	17,17,17	0.35	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	1097	-	-	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.

No monomer is involved in short contacts.

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	A	920/1083 (84%)	-0.23	33 (3%) 46 40	12, 18, 43, 56	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	SER	5.2
1	A	303	ASP	5.1
1	A	1027	GLY	4.7
1	A	213	ASN	4.5
1	A	32	ASP	4.3
1	A	268	SER	4.1
1	A	746	PHE	3.9
1	A	172	PHE	3.9
1	A	1026	ALA	3.8
1	A	249	ASP	3.8
1	A	250	ASP	3.7
1	A	38	PRO	3.7
1	A	230	GLN	3.5
1	A	1052	ALA	3.4
1	A	1028	THR	3.3
1	A	708	TRP	3.2
1	A	1024	ASP	3.0
1	A	711	ASN	2.9
1	A	227	THR	2.8
1	A	251	VAL	2.8
1	A	234	MET	2.8
1	A	171	ALA	2.8
1	A	302	THR	2.7
1	A	1082	SER	2.7
1	A	710	SER	2.6
1	A	981	ALA	2.5
1	A	269	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1053	ASP	2.4
1	A	194	ASN	2.3
1	A	1073	SER	2.3
1	A	208	VAL	2.2
1	A	1072	GLU	2.1
1	A	304	SER	2.1

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(\AA^2)	Q<0.9
2	GLC	A	1097	12/12	0.91	0.11	2.98	23,26,28,28	0
3	CA	A	2402	1/1	0.95	0.15	0.63	40,40,40,40	0
3	CA	A	2403	1/1	0.98	0.07	-0.57	35,35,35,35	0
3	CA	A	2404	1/1	1.00	0.04	-1.68	12,12,12,12	0
3	CA	A	2401	1/1	1.00	0.03	-4.33	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.