



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:05 AM UTC

PDB ID : 2FH6 / pdb_00002fh6
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

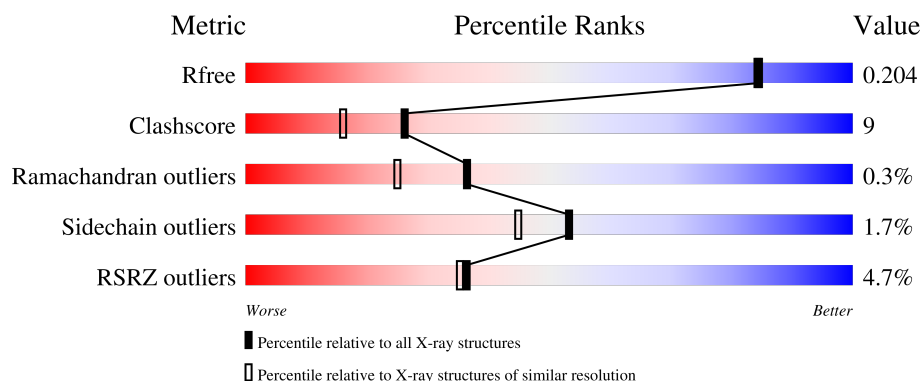
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

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.

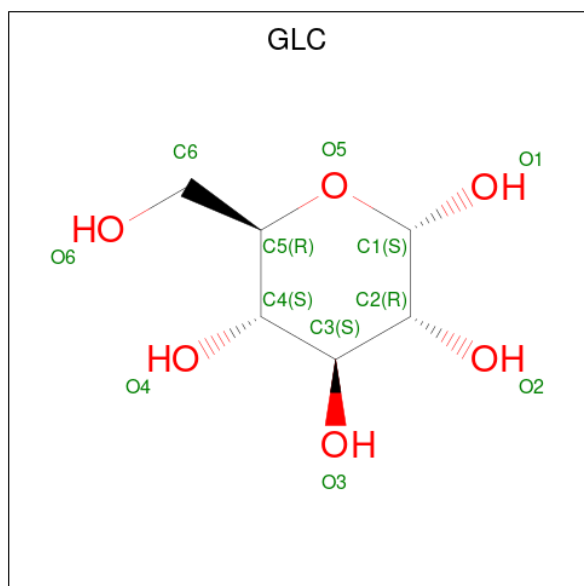
- Molecule 1 is a protein called Alpha-dextrin endo-1,6-alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	920	7107	4438	1214	1430	25	0	11	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	conflict	UNP W9BQ28

- Molecule 2 is alpha-D-glucopyranose (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

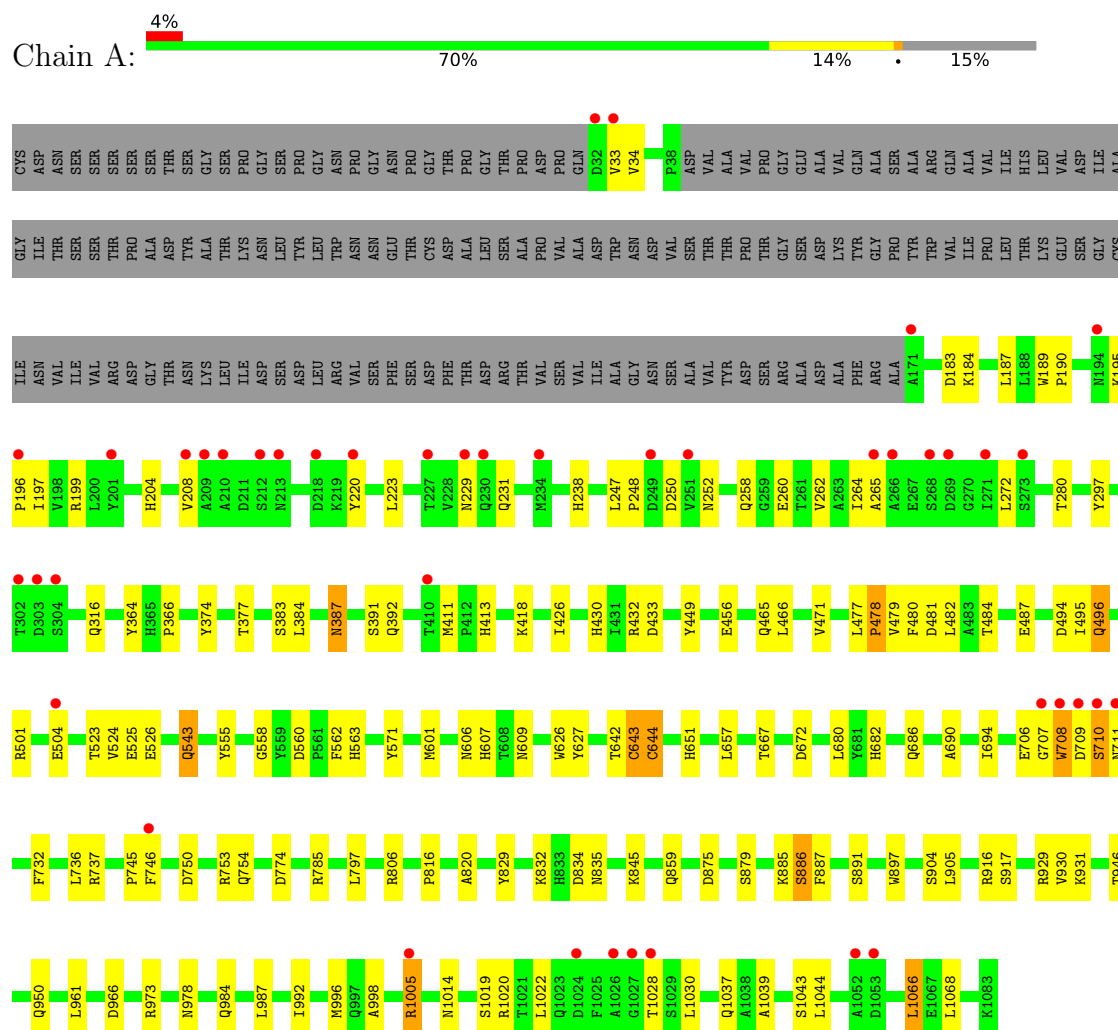
- Molecule 4 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alpha-dextrin endo-1,6-alpha-glucosidase



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 14.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (14.96-1.80) 88.2 (14.96-1.80)	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 0.179 , 0.204	Depositor DCC
R_{free} test set	9056 reflections (8.56%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.7	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	0.95	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, 0.333 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: GLC, CA

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	0.33	0/7294	0.90	23/9919 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	644	CYS	N-CA-CB	-9.25	102.99	111.59
1	A	484	THR	N-CA-C	7.70	122.06	113.21
1	A	426	ILE	N-CA-C	7.00	119.51	108.87
1	A	555	TYR	N-CA-C	6.76	120.85	109.76
1	A	845	LYS	N-CA-C	6.67	121.55	113.41
1	A	562	PHE	N-CA-C	-6.43	104.38	112.93
1	A	480	PHE	N-CA-C	-6.38	100.48	110.36
1	A	931	LYS	N-CA-C	6.30	118.67	111.11
1	A	904	SER	N-CA-C	-6.08	105.62	113.16
1	A	644	CYS	N-CA-C	6.02	117.19	108.34
1	A	891	SER	N-CA-C	5.85	119.48	112.93
1	A	905	LEU	N-CA-C	5.66	119.48	112.24
1	A	1044	LEU	N-CA-C	-5.53	106.37	113.01
1	A	1019	SER	N-CA-C	-5.52	101.48	110.20
1	A	477	LEU	N-CA-C	-5.48	102.06	110.01
1	A	297	TYR	N-CA-C	5.30	117.92	109.81
1	A	280	THR	N-CA-C	5.27	119.81	113.17
1	A	471	VAL	N-CA-C	-5.21	102.01	108.89
1	A	667	THR	N-CA-C	5.14	116.70	111.14
1	A	885	LYS	N-CA-C	-5.12	105.75	112.41
1	A	820	ALA	N-CA-C	5.04	117.97	110.52
1	A	806[A]	ARG	N-CA-C	-5.01	103.11	110.52
1	A	806[B]	ARG	N-CA-C	-5.01	103.11	110.52

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	7107	0	6837	131	0
2	A	12	0	12	0	0
3	A	4	0	0	0	0
4	A	945	0	0	12	0
All	All	8068	0	6849	131	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 (131) 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:HB3	1:A:1005:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:560:ASP:HB3	1:A:609:ASN:ND2	2.18	0.59
1:A:708:TRP:N	1:A:708:TRP:CE3	2.71	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:252:ASN:C	1:A:252:ASN:HD22	2.14	0.55
1:A:987:LEU:HD21	1:A:1022:LEU:HD21	1.89	0.55
1:A:272:LEU:C	1:A:272:LEU:HD13	2.32	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:229:ASN:HD22	1:A:231:GLN:CD	2.16	0.53
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
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:197:ILE:O	1:A:265:ALA:HA	2.10	0.51
1:A:501:ARG:HA	1:A:504:GLU:OE1	2.11	0.51
1:A:706:GLU:CG	1:A:707:GLY:N	2.74	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: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:H	1:A:680:LEU:CD2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:LYS:HD2	1:A:966[B]:ASP:OD1	2.13	0.48
1:A:494:ASP:HB3	1:A:496:GLN:HE22	1.78	0.48
1:A:1005:ARG:HH21	1:A:1005:ARG:CB	2.23	0.48
1:A:834:ASP:O	1:A:835:ASN:HB2	2.12	0.48
1:A:543:GLN:HE21	1:A:916:ARG:HA	1.78	0.48
1:A:710:SER:O	1:A:711:ASN:CB	2.62	0.48
1:A:706:GLU:HB2	1:A:732:PHE:CD2	2.49	0.48
1:A:199:ARG:HD3	1:A:220:TYR:CD2	2.49	0.48
1:A:680:LEU:CD1	1:A:708:TRP:N	2.75	0.48
1:A:481:ASP:OD2	1:A:563:HIS:HD2	1.97	0.47
1:A:753:ARG:HD2	1:A:930:VAL:HG11	1.95	0.47
1:A:1028:THR:HG22	1:A:1028:THR:O	2.14	0.47
1:A:680:LEU:HD23	1:A:680:LEU:N	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:657:LEU:C	1:A:657:LEU:HD23	2.40	0.46
1:A:411[B]:MET:HE2	1:A:413:HIS:O	2.15	0.46
1:A:560:ASP:HB3	1:A:609:ASN:HD22	1.80	0.46
1:A:1066:LEU:HD22	1:A:1066:LEU:N	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
1:A:996:MET:HE3	4:A:1846:HOH:O	2.17	0.45
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:797:LEU:HD12	1:A:797:LEU:C	2.42	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:OE1	1:A:231:GLN:N	2.49	0.43
1:A:479:VAL:HG23	1:A:601:MET:HE3	2.00	0.43
1:A:737:ARG:HD3	1:A:829:TYR:CZ	2.54	0.43
1:A:187:LEU:C	1:A:187:LEU:HD13	2.43	0.42
1:A:238:HIS:H	1:A:238:HIS:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD23	1:A:391:SER:HA	2.01	0.42
1:A:525[B]:GLU:HG3	1:A:897:TRP:HZ3	1.84	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:252:ASN:C	1:A:252:ASN:ND2	2.77	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:CD2	1:A:680:LEU:N	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: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:501:ARG:HA	1:A:504:GLU:HG2	2.02	0.41
1:A:558:GLY:C	1:A:560:ASP:H	2.27	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:411[A]:MET:HG2	1:A:672:ASP:OD1	2.20	0.41
1:A:456:GLU:H	1:A:456:GLU:CD	2.27	0.41
1:A:973:ARG:HG2	1:A:998:ALA:HB1	2.02	0.41
1:A:1028:THR:O	1:A:1068:LEU:HD22	2.20	0.41
1:A:680:LEU:H	1:A:680:LEU:HD23	1.85	0.41
1:A:736:LEU:HD23	1:A:736:LEU:C	2.45	0.41
1:A:680:LEU:HD12	1:A:710:SER:HB3	2.03	0.40
1:A:183:ASP:OD2	1:A:183:ASP:C	2.65	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 ⓘ

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	927/1083 (86%)	903 (97%)	21 (2%)	3 (0%)	36 25

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 ⓘ

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%)	51 43

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

Mol	Chain	Res	Type
1	A	184	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	708	TRP
1	A	859	GLN
1	A	886	SER
1	A	1005	ARG
1	A	1037[A]	GLN
1	A	1037[B]	GLN
1	A	1066	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47)

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	277	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	439	GLN
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	712	GLN
1	A	848	GLN
1	A	859	GLN
1	A	899	ASN
1	A	906	GLN
1	A	911	ASN
1	A	944	GLN
1	A	950	GLN
1	A	978	ASN
1	A	984	GLN

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Mol	Chain	Res	Type
1	A	997	GLN
1	A	1014	ASN
1	A	1023	GLN
1	A	1031	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 oligosaccharides 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	0.39	0	17,17,17	0.33	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 [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	920/1083 (84%)	-0.11	43 (4%) 36 35	12, 18, 43, 56	11 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	SER	4.9
1	A	708	TRP	4.5
1	A	302	THR	4.4
1	A	303	ASP	4.4
1	A	707	GLY	4.1
1	A	1024	ASP	3.7
1	A	229	ASN	3.2
1	A	1027	GLY	3.2
1	A	32	ASP	3.1
1	A	746	PHE	3.1
1	A	1052	ALA	3.0
1	A	209	ALA	3.0
1	A	269	ASP	2.9
1	A	304	SER	2.9
1	A	210	ALA	2.8
1	A	271	ILE	2.8
1	A	711	ASN	2.8
1	A	504	GLU	2.8
1	A	208	VAL	2.8
1	A	227	THR	2.7
1	A	171	ALA	2.6
1	A	230	GLN	2.5
1	A	709	ASP	2.5
1	A	410	THR	2.5
1	A	213	ASN	2.5
1	A	1005	ARG	2.5
1	A	265	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	SER	2.4
1	A	218	ASP	2.4
1	A	1028	THR	2.3
1	A	1026	ALA	2.2
1	A	249	ASP	2.2
1	A	1053	ASP	2.2
1	A	194	ASN	2.2
1	A	273	SER	2.1
1	A	234	MET	2.1
1	A	33	VAL	2.1
1	A	266	ALA	2.1
1	A	251	VAL	2.0
1	A	268	SER	2.0
1	A	201	TYR	2.0
1	A	220	TYR	2.0
1	A	196	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	A	1097	12/12	0.92	0.07	23,26,28,28	0
3	CA	A	2402	1/1	0.97	0.17	40,40,40,40	0
3	CA	A	2403	1/1	0.97	0.06	35,35,35,35	0
3	CA	A	2401	1/1	1.00	0.02	14,14,14,14	0
3	CA	A	2404	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.