Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2026 – 12:14 PM EST

PDB ID	:	9Z13 / pdb_00009z13
Title	:	GH95 alpha-fucosidase from Bacteroides fragilis
Authors	:	Kowalewski, M.E.; Redinbo, M.R.
Deposited on	:	2025-11-03
Resolution	:	2.36 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:

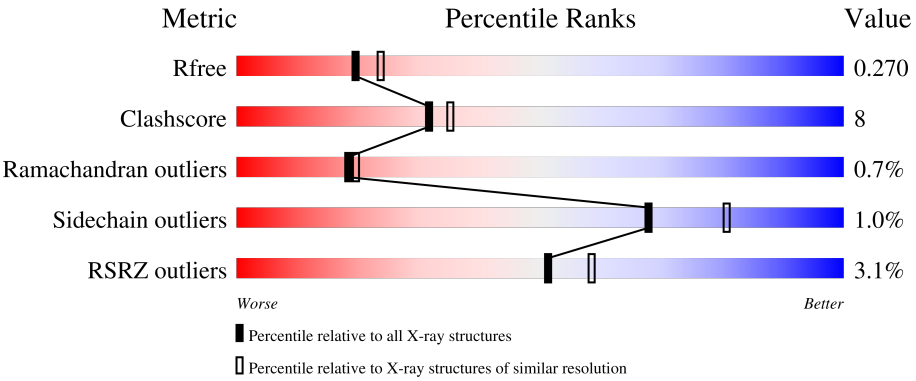
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 <=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	829	3% 80% 17% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6695 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 Glycoside hydrolase family 95 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	808	6405	4066	1104	1213	22	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP A0A412YEK4
A	2	HIS	-	expression tag	UNP A0A412YEK4
A	3	HIS	-	expression tag	UNP A0A412YEK4
A	4	HIS	-	expression tag	UNP A0A412YEK4
A	5	HIS	-	expression tag	UNP A0A412YEK4
A	6	HIS	-	expression tag	UNP A0A412YEK4
A	7	SER	-	expression tag	UNP A0A412YEK4
A	8	SER	-	expression tag	UNP A0A412YEK4
A	9	GLY	-	expression tag	UNP A0A412YEK4
A	10	VAL	-	expression tag	UNP A0A412YEK4
A	11	ASP	-	expression tag	UNP A0A412YEK4
A	12	LEU	-	expression tag	UNP A0A412YEK4
A	13	GLY	-	expression tag	UNP A0A412YEK4
A	14	THR	-	expression tag	UNP A0A412YEK4
A	15	GLU	-	expression tag	UNP A0A412YEK4
A	16	ASN	-	expression tag	UNP A0A412YEK4
A	17	LEU	-	expression tag	UNP A0A412YEK4
A	18	TYR	-	expression tag	UNP A0A412YEK4
A	19	PHE	-	expression tag	UNP A0A412YEK4
A	20	GLN	-	expression tag	UNP A0A412YEK4
A	21	SER	-	expression tag	UNP A0A412YEK4
A	22	ASN	-	expression tag	UNP A0A412YEK4
A	204	VAL	ILE	conflict	UNP A0A412YEK4

- Molecule 2 is water.

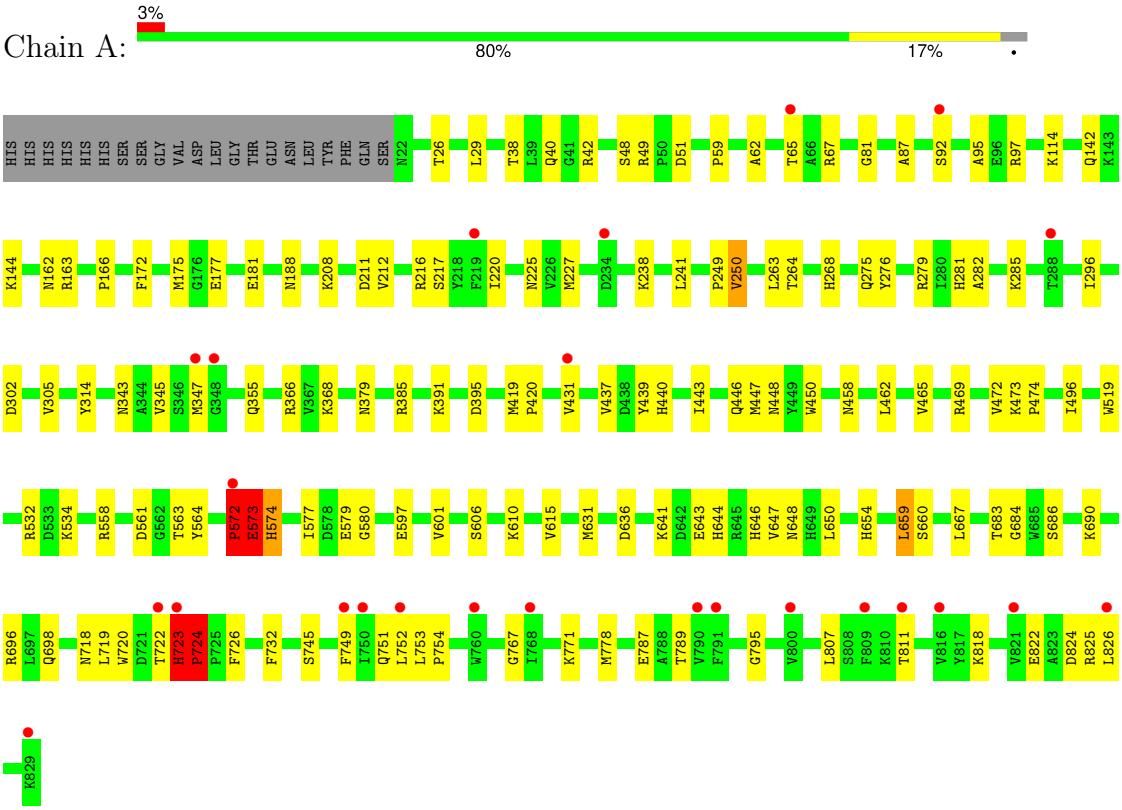
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	290	Total	O	0	0
			290	290		

3 Residue-property plots (i)

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: Glycoside hydrolase family 95 protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.80Å 86.80Å 258.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.22 – 2.36 33.22 – 2.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.22-2.36) 99.9 (33.22-2.36)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.218 , 0.269 0.218 , 0.270	Depositor DCC
R_{free} test set	2000 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.47	1/6582 (0.0%)	0.68	4/8950 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	572	PRO	N-CD	-12.20	1.30	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	724	PRO	CB-CA-C	8.89	121.77	110.92
1	A	574	HIS	CA-CB-CG	8.49	122.29	113.80
1	A	723	HIS	CB-CA-C	-7.21	95.97	110.17
1	A	573	GLU	N-CA-CB	-6.19	102.81	112.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ARG	Sidechain

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	6405	0	6132	101	0
2	A	290	0	0	16	0
All	All	6695	0	6132	101	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 8.

All (101) 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:722:THR:O	1:A:723:HIS:C	2.12	0.92
1:A:92:SER:OG	1:A:95:ALA:O	1.93	0.86
1:A:29:LEU:HD21	2:A:1154:HOH:O	1.87	0.74
1:A:723:HIS:O	1:A:724:PRO:C	2.32	0.70
1:A:789:THR:HG22	1:A:818:LYS:HG3	1.74	0.70
1:A:572:PRO:HG2	1:A:648:ASN:OD1	1.93	0.69
1:A:690:LYS:NZ	2:A:906:HOH:O	2.24	0.69
1:A:722:THR:O	1:A:724:PRO:N	2.27	0.68
1:A:787:GLU:OE2	1:A:789:THR:HG23	1.94	0.68
1:A:268:HIS:CD2	1:A:275:GLN:HG2	2.32	0.65
1:A:684:GLY:HA3	1:A:723:HIS:HB2	1.81	0.63
1:A:38:THR:HG21	1:A:40:GLN:OE1	1.99	0.62
1:A:29:LEU:CD2	2:A:1154:HOH:O	2.46	0.61
1:A:752:LEU:HD22	1:A:778:MET:HE3	1.83	0.61
1:A:264:THR:HG22	1:A:279:ARG:HG2	1.83	0.60
1:A:263:LEU:HD11	1:A:296:ILE:HG13	1.84	0.60
1:A:643:GLU:OE1	2:A:901:HOH:O	2.17	0.60
1:A:751:GLN:HG2	1:A:754:PRO:HB3	1.83	0.59
1:A:65:THR:CG2	1:A:67:ARG:O	2.50	0.59
1:A:114:LYS:HE2	1:A:166:PRO:HD2	1.85	0.59
1:A:644:HIS:CE1	1:A:646:HIS:HB2	2.37	0.59
1:A:579:GLU:OE1	2:A:902:HOH:O	2.17	0.58
1:A:162:ASN:HB3	2:A:1148:HOH:O	2.03	0.58
1:A:97:ARG:NH1	1:A:177:GLU:OE2	2.33	0.57
1:A:38:THR:HG22	2:A:995:HOH:O	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:HIS:HB2	1:A:696:ARG:HG3	1.87	0.55
1:A:573:GLU:O	1:A:574:HIS:HB3	2.06	0.54
1:A:225:ASN:ND2	2:A:921:HOH:O	2.40	0.54
1:A:144:LYS:NZ	2:A:922:HOH:O	2.40	0.54
1:A:65:THR:HG21	1:A:67:ARG:O	2.08	0.54
1:A:49:ARG:NH2	2:A:923:HOH:O	2.41	0.53
1:A:208:LYS:HE2	1:A:211:ASP:HA	1.90	0.52
1:A:564:TYR:CD2	1:A:615:VAL:HG23	2.44	0.52
1:A:446:GLN:HG2	1:A:519:TRP:CD1	2.45	0.51
1:A:795:GLY:HA2	1:A:811:THR:HG23	1.92	0.51
1:A:220:ILE:HG12	1:A:227:MET:HE3	1.91	0.51
1:A:347:MET:HE1	1:A:355:GLN:OE1	2.11	0.51
1:A:250:VAL:HG21	1:A:431:VAL:HG13	1.92	0.50
1:A:343:ASN:O	1:A:347:MET:HG3	2.11	0.50
1:A:163:ARG:HD3	2:A:1112:HOH:O	2.11	0.50
1:A:212:VAL:HG11	1:A:238:LYS:HG3	1.93	0.50
1:A:65:THR:HG23	1:A:67:ARG:O	2.12	0.50
1:A:722:THR:HA	1:A:726:PHE:HA	1.93	0.49
1:A:87:ALA:HB3	1:A:227:MET:HE1	1.94	0.49
1:A:142:GLN:NE2	1:A:577:ILE:O	2.42	0.49
1:A:175:MET:HE2	1:A:276:TYR:CD2	2.47	0.49
1:A:285:LYS:O	1:A:302:ASP:HB2	2.12	0.49
1:A:597:GLU:O	1:A:601:VAL:HG23	2.12	0.49
1:A:789:THR:HG22	1:A:818:LYS:CG	2.42	0.48
1:A:698:GLN:HG2	1:A:754:PRO:HB2	1.95	0.48
1:A:181:GLU:O	1:A:241:LEU:HA	2.14	0.48
1:A:745:SER:HA	1:A:749:PHE:O	2.14	0.48
1:A:49:ARG:NH1	1:A:51:ASP:OD2	2.47	0.47
1:A:368:LYS:HD3	1:A:368:LYS:HA	1.63	0.47
1:A:558:ARG:HB2	1:A:564:TYR:CE1	2.51	0.46
1:A:573:GLU:HG3	1:A:646:HIS:CE1	2.50	0.46
1:A:282:ALA:HA	1:A:305:VAL:O	2.16	0.46
1:A:220:ILE:CG1	1:A:227:MET:HE3	2.45	0.46
1:A:250:VAL:HG21	1:A:431:VAL:CG1	2.47	0.45
1:A:458:ASN:ND2	2:A:925:HOH:O	2.50	0.45
1:A:263:LEU:CD1	1:A:296:ILE:HG13	2.46	0.45
1:A:641:LYS:HE2	1:A:641:LYS:HB2	1.74	0.45
1:A:81:GLY:HA2	1:A:220:ILE:HD12	1.98	0.44
1:A:188:ASN:OD1	2:A:903:HOH:O	2.21	0.44
1:A:385:ARG:NH1	1:A:395:ASP:OD2	2.43	0.44
1:A:683:THR:O	1:A:686:SER:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:MET:HE3	1:A:636:ASP:HA	1.99	0.44
1:A:807:LEU:HD22	1:A:826:LEU:HG	1.98	0.44
1:A:462:LEU:HD13	1:A:462:LEU:HA	1.78	0.44
1:A:745:SER:O	1:A:771:LYS:HD2	2.18	0.44
1:A:250:VAL:CG2	1:A:431:VAL:HG13	2.48	0.44
1:A:684:GLY:CA	1:A:723:HIS:HB2	2.45	0.44
1:A:447:MET:HE2	1:A:450:TRP:CZ3	2.53	0.43
1:A:753:LEU:H	1:A:778:MET:HE1	1.82	0.43
1:A:281:HIS:CD2	1:A:345:VAL:HG22	2.52	0.43
1:A:420:PRO:HG2	1:A:439:TYR:CE1	2.53	0.43
1:A:824:ASP:O	1:A:825:ARG:HD3	2.18	0.43
1:A:59:PRO:HB2	1:A:62:ALA:HB2	1.99	0.43
1:A:573:GLU:HG3	1:A:646:HIS:NE2	2.34	0.43
1:A:465:VAL:O	1:A:469:ARG:HG3	2.19	0.43
1:A:249:PRO:HG2	1:A:431:VAL:HG21	2.02	0.42
1:A:314:TYR:OH	1:A:419:MET:HE2	2.20	0.42
1:A:534:LYS:N	2:A:939:HOH:O	2.49	0.42
1:A:659:LEU:HD11	1:A:667:LEU:HB3	2.01	0.42
1:A:561:ASP:OD1	1:A:563:THR:HG22	2.19	0.42
1:A:724:PRO:HD3	2:A:1074:HOH:O	2.19	0.42
1:A:42:ARG:O	1:A:48:SER:HA	2.20	0.42
1:A:532:ARG:HA	1:A:532:ARG:HD3	1.69	0.42
1:A:472:VAL:HG21	2:A:1164:HOH:O	2.19	0.42
1:A:366:ARG:O	1:A:767:GLY:HA3	2.19	0.42
1:A:391:LYS:HB2	1:A:391:LYS:HE3	1.96	0.41
1:A:647:VAL:HG12	1:A:650:LEU:HG	2.01	0.41
1:A:469:ARG:O	1:A:472:VAL:HG22	2.20	0.41
1:A:472:VAL:HG23	1:A:473:LYS:N	2.36	0.41
1:A:718:ASN:O	1:A:719:LEU:HB2	2.20	0.41
1:A:172:PHE:HB3	1:A:437:VAL:HB	2.03	0.41
1:A:448:ASN:HA	1:A:732:PHE:CD2	2.56	0.41
1:A:473:LYS:HB3	1:A:474:PRO:HD3	2.03	0.41
1:A:606:SER:O	1:A:610:LYS:HD3	2.20	0.41
1:A:26:THR:CB	1:A:379:ASN:HD21	2.34	0.40
1:A:314:TYR:CE1	1:A:496:ILE:HD12	2.57	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	806/829 (97%)	759 (94%)	41 (5%)	6 (1%)	18 20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	ILE
1	A	724	PRO
1	A	572	PRO
1	A	723	HIS
1	A	580	GLY
1	A	250	VAL

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	675/699 (97%)	668 (99%)	7 (1%)	68 81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	SER
1	A	440	HIS
1	A	573	GLU
1	A	659	LEU
1	A	660	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	720	TRP
1	A	822	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	225	ASN
1	A	275	GLN
1	A	379	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	808/829 (97%)	0.43	25 (3%) 51 58	30, 51, 73, 100	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	821	VAL	3.3
1	A	829	LYS	3.1
1	A	816	VAL	3.0
1	A	826	LEU	3.0
1	A	790	VAL	3.0
1	A	288	THR	2.9
1	A	572	PRO	2.8
1	A	723	HIS	2.6
1	A	219	PHE	2.6
1	A	800	VAL	2.4
1	A	760	TRP	2.4
1	A	809	PHE	2.4
1	A	750	ILE	2.3
1	A	431	VAL	2.3
1	A	791	PHE	2.3
1	A	65	THR	2.3
1	A	811	THR	2.2
1	A	768	ILE	2.2
1	A	234	ASP	2.2
1	A	749	PHE	2.2
1	A	722	THR	2.2
1	A	347	MET	2.1
1	A	752	LEU	2.1
1	A	92	SER	2.1
1	A	348	GLY	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.