



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 AM UTC

PDB ID : 2FPN / pdb_00002fpn
Title : The crystal structure of the ywmB protein from Bacillus subtilis
Authors : Zhang, R.; Wu, R.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-01-16
Resolution : 2.49 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

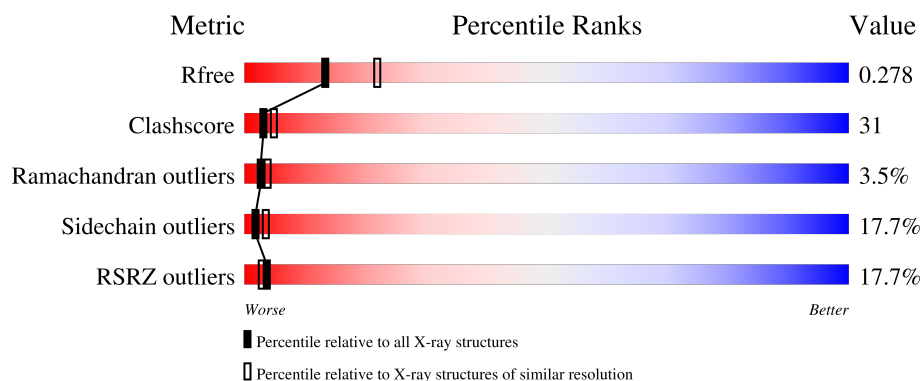
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	216	16% 59% 24% 9% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1753 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 ywmB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	205	1700	1080	287	325	1	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MSE	MET	modified residue	GB 2636202
A	11	MSE	MET	modified residue	GB 2636202
A	60	MSE	MET	modified residue	GB 2636202
A	98	MSE	MET	modified residue	GB 2636202
A	139	MSE	MET	modified residue	GB 2636202
A	182	MSE	MET	modified residue	GB 2636202
A	188	MSE	MET	modified residue	GB 2636202
A	199	MSE	MET	modified residue	GB 2636202

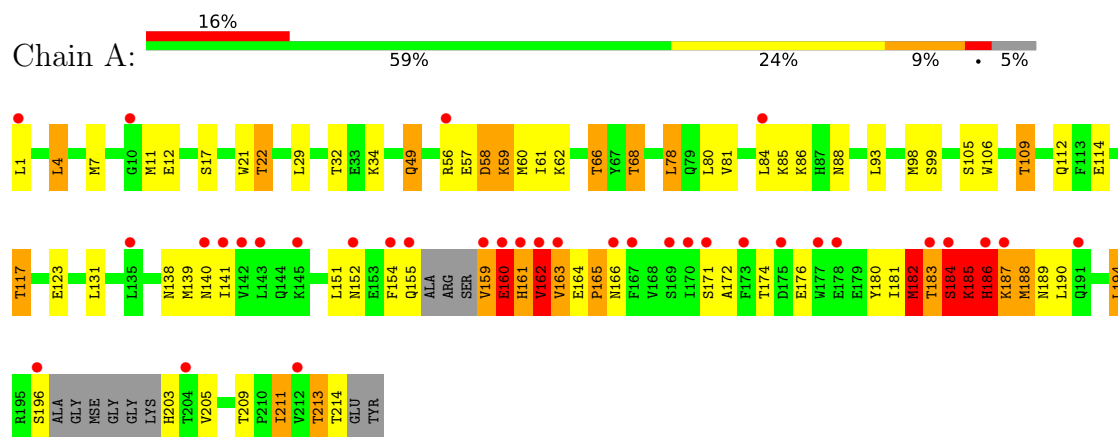
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		

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: ywmB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.79Å 50.86Å 81.26Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	80.85 – 2.49 80.74 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.4 (80.85-2.49) 96.7 (80.74-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.281 (Not available) , 0.278	Depositor DCC
R_{free} test set	625 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	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	0.90	EDS
Total number of atoms	1753	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.01% 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

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	1.29	10/1725 (0.6%)	1.04	5/2319 (0.2%)

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	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	MSE	CG-SE	36.30	3.04	1.95
1	A	188	MSE	CG-SE	14.88	2.40	1.95
1	A	182	MSE	SE-CE	14.04	2.37	1.95
1	A	188	MSE	SE-CE	13.93	2.37	1.95
1	A	7	MSE	SE-CE	-5.79	1.78	1.95
1	A	11	MSE	SE-CE	-5.21	1.79	1.95
1	A	60	MSE	SE-CE	-5.16	1.79	1.95
1	A	11	MSE	CG-SE	-5.09	1.80	1.95
1	A	139	MSE	SE-CE	-5.08	1.80	1.95
1	A	7	MSE	CG-SE	-5.06	1.80	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	MSE	CB-CG-SE	-16.72	62.55	112.70
1	A	182	MSE	CG-SE-CE	-16.21	63.26	98.92
1	A	188	MSE	CG-SE-CE	-5.73	86.32	98.92
1	A	209	THR	CB-CA-C	-5.60	102.72	110.16
1	A	58	ASP	N-CA-C	5.33	117.59	110.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLU	Peptide
1	A	185	LYS	Peptide
1	A	186	HIS	Peptide

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	1700	0	1687	106	0
2	A	53	0	0	9	0
All	All	1753	0	1687	106	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 31.

All (106) 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:162:VAL:O	1:A:163:VAL:HG23	1.14	1.27
1:A:188:MSE:SE	1:A:188:MSE:CE	2.37	1.23
1:A:182:MSE:SE	1:A:182:MSE:CE	2.37	1.23
1:A:182:MSE:SE	1:A:182:MSE:HB2	1.88	1.22
1:A:188:MSE:SE	1:A:188:MSE:CG	2.40	1.20
1:A:151:LEU:CD2	1:A:159:VAL:HG11	1.73	1.19
1:A:151:LEU:HD21	1:A:159:VAL:CG1	1.78	1.11
1:A:162:VAL:HG13	1:A:163:VAL:N	1.64	1.10
1:A:151:LEU:HD11	1:A:159:VAL:HG13	1.38	1.06
1:A:185:LYS:O	1:A:185:LYS:HG3	1.51	1.05
1:A:151:LEU:HD11	1:A:159:VAL:CG1	1.87	1.04
1:A:162:VAL:O	1:A:163:VAL:CG2	2.03	1.04
1:A:155:GLN:HB2	1:A:174:THR:CG2	1.92	1.00
1:A:162:VAL:CG1	1:A:163:VAL:N	2.24	1.00
1:A:185:LYS:O	1:A:186:HIS:CD2	2.17	0.97
1:A:155:GLN:HB2	1:A:174:THR:HG21	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MSE:SE	1:A:182:MSE:CB	2.70	0.90
1:A:182:MSE:CG	2:A:254:HOH:O	2.21	0.88
1:A:151:LEU:CD1	1:A:159:VAL:CG1	2.52	0.86
1:A:49:GLN:H	1:A:49:GLN:HE21	1.20	0.86
1:A:151:LEU:HD21	1:A:159:VAL:HG11	0.88	0.86
1:A:180:TYR:CE2	1:A:182:MSE:SE	2.79	0.86
1:A:180:TYR:HE2	1:A:182:MSE:SE	2.10	0.83
1:A:185:LYS:O	1:A:186:HIS:CG	2.31	0.83
1:A:68:THR:HG22	2:A:229:HOH:O	1.80	0.82
1:A:182:MSE:HG2	2:A:254:HOH:O	1.80	0.81
1:A:162:VAL:HG13	1:A:163:VAL:H	1.43	0.80
1:A:159:VAL:C	1:A:171:SER:O	2.25	0.80
1:A:154:PHE:O	1:A:155:GLN:CG	2.30	0.79
1:A:154:PHE:O	1:A:155:GLN:CB	2.31	0.79
1:A:182:MSE:HG3	2:A:254:HOH:O	1.82	0.78
1:A:151:LEU:CD2	1:A:159:VAL:CG1	2.46	0.77
1:A:188:MSE:HE2	1:A:211:ILE:HG22	1.67	0.75
1:A:185:LYS:O	1:A:185:LYS:CG	2.30	0.74
1:A:184:SER:O	1:A:185:LYS:C	2.32	0.73
1:A:151:LEU:CD1	1:A:159:VAL:HG12	2.19	0.72
1:A:155:GLN:HB2	1:A:174:THR:HG22	1.72	0.68
1:A:159:VAL:O	1:A:160:GLU:CB	2.40	0.68
1:A:196:SER:HA	1:A:203:HIS:CD2	2.29	0.67
1:A:159:VAL:O	1:A:160:GLU:CG	2.42	0.67
1:A:162:VAL:C	1:A:163:VAL:HG23	2.15	0.66
1:A:154:PHE:O	1:A:155:GLN:HB2	1.94	0.66
1:A:155:GLN:CB	1:A:174:THR:CG2	2.71	0.66
1:A:58:ASP:HB3	1:A:59:LYS:HE3	1.77	0.66
1:A:32:THR:HG22	1:A:34:LYS:H	1.61	0.65
1:A:154:PHE:O	1:A:155:GLN:HG3	1.94	0.65
1:A:49:GLN:H	1:A:49:GLN:NE2	1.92	0.65
1:A:159:VAL:HA	1:A:171:SER:O	1.98	0.64
1:A:160:GLU:HA	1:A:161:HIS:ND1	2.13	0.64
1:A:159:VAL:O	1:A:160:GLU:HG2	1.99	0.63
1:A:188:MSE:CE	1:A:211:ILE:HG22	2.28	0.62
1:A:21:TRP:HB3	1:A:131:LEU:HD13	1.81	0.62
1:A:155:GLN:CB	1:A:174:THR:HG22	2.29	0.61
1:A:183:THR:O	1:A:184:SER:C	2.44	0.61
1:A:159:VAL:CA	1:A:171:SER:O	2.49	0.60
1:A:159:VAL:O	1:A:160:GLU:HB3	2.02	0.59
1:A:66:THR:HG22	2:A:233:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TYR:CD2	1:A:182:MSE:SE	3.06	0.59
1:A:105:SER:O	1:A:109:THR:HG23	2.03	0.58
1:A:49:GLN:HE21	1:A:49:GLN:N	1.96	0.58
1:A:160:GLU:HA	1:A:161:HIS:CE1	2.39	0.57
1:A:185:LYS:C	1:A:186:HIS:CG	2.77	0.57
1:A:160:GLU:HG3	1:A:171:SER:HB2	1.88	0.56
1:A:78:LEU:HD22	1:A:93:LEU:HD11	1.88	0.56
1:A:182:MSE:SE	1:A:182:MSE:CG	3.04	0.56
1:A:183:THR:OG1	1:A:184:SER:N	2.35	0.55
1:A:22:THR:HG23	2:A:219:HOH:O	2.07	0.55
1:A:164:GLU:HB3	1:A:165:PRO:HD2	1.89	0.55
1:A:181:ILE:HD11	1:A:211:ILE:CG2	2.38	0.54
1:A:160:GLU:N	1:A:171:SER:O	2.41	0.54
1:A:160:GLU:CD	1:A:171:SER:HB2	2.33	0.53
1:A:154:PHE:C	1:A:155:GLN:HG3	2.32	0.53
1:A:86:LYS:HD2	1:A:88:ASN:O	2.08	0.53
1:A:194:LEU:HD13	1:A:205:VAL:HG22	1.91	0.52
1:A:194:LEU:CD1	1:A:205:VAL:HG22	2.40	0.52
1:A:98:MSE:HG3	2:A:236:HOH:O	2.10	0.51
1:A:182:MSE:CE	1:A:182:MSE:CG	2.89	0.50
1:A:174:THR:C	1:A:176:GLU:H	2.18	0.49
1:A:187:LYS:HB2	2:A:254:HOH:O	2.11	0.49
1:A:180:TYR:HA	1:A:189:ASN:HB3	1.94	0.49
1:A:186:HIS:HB2	1:A:187:LYS:H	1.58	0.48
1:A:32:THR:HG22	1:A:34:LYS:N	2.29	0.47
1:A:162:VAL:HG13	1:A:163:VAL:CA	2.42	0.47
1:A:151:LEU:HD13	1:A:159:VAL:HG12	1.96	0.47
1:A:188:MSE:HB2	1:A:188:MSE:HE3	1.97	0.46
1:A:152:ASN:C	1:A:154:PHE:N	2.73	0.46
1:A:159:VAL:N	1:A:172:ALA:HA	2.31	0.46
1:A:196:SER:C	1:A:203:HIS:HD2	2.22	0.46
1:A:159:VAL:C	1:A:160:GLU:CG	2.89	0.46
1:A:160:GLU:CG	1:A:171:SER:HB2	2.46	0.46
1:A:21:TRP:CE2	1:A:99:SER:HB3	2.51	0.45
1:A:181:ILE:HD11	1:A:211:ILE:HG23	1.98	0.45
1:A:66:THR:HB	2:A:217:HOH:O	2.16	0.45
1:A:114:GLU:O	1:A:117:THR:HB	2.17	0.44
1:A:151:LEU:CG	1:A:159:VAL:CG1	2.96	0.44
1:A:138:ASN:O	1:A:141:ILE:HG22	2.18	0.44
1:A:188:MSE:SE	1:A:188:MSE:CB	3.12	0.44
1:A:162:VAL:HG12	1:A:163:VAL:N	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LYS:HG3	1:A:81:VAL:HG22	2.00	0.43
1:A:160:GLU:HG3	1:A:171:SER:O	2.19	0.43
1:A:160:GLU:HA	1:A:161:HIS:CG	2.54	0.42
1:A:59:LYS:HG3	1:A:85:LYS:HD3	2.01	0.42
1:A:56:ARG:NH2	1:A:84:LEU:HD11	2.34	0.42
1:A:213:THR:HB	1:A:214:THR:H	1.72	0.42
1:A:4:LEU:HD13	1:A:106:TRP:HE3	1.86	0.41
1:A:182:MSE:SE	1:A:182:MSE:N	3.03	0.41

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	199/216 (92%)	181 (91%)	11 (6%)	7 (4%)	3 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	A	163	VAL
1	A	186	HIS
1	A	185	LYS
1	A	184	SER
1	A	165	PRO
1	A	162	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	192/190 (101%)	158 (82%)	34 (18%)	2 3

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	4	LEU
1	A	12	GLU
1	A	17	SER
1	A	22	THR
1	A	29	LEU
1	A	49	GLN
1	A	57	GLU
1	A	59	LYS
1	A	61	ILE
1	A	66	THR
1	A	68	THR
1	A	78	LEU
1	A	80	LEU
1	A	109	THR
1	A	112	GLN
1	A	117	THR
1	A	123	GLU
1	A	140	ASN
1	A	159	VAL
1	A	160	GLU
1	A	161	HIS
1	A	162	VAL
1	A	166	ASN
1	A	182	MSE
1	A	183	THR
1	A	184	SER
1	A	185	LYS
1	A	186	HIS
1	A	187	LYS
1	A	190	LEU
1	A	194	LEU
1	A	211	ILE
1	A	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	38	GLN
1	A	49	GLN
1	A	122	GLN
1	A	140	ASN
1	A	144	GLN
1	A	148	ASN
1	A	152	ASN
1	A	166	ASN
1	A	203	HIS

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, 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	198/216 (91%)	1.00	35 (17%) 4 3	8, 27, 66, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	9.1
1	A	160	GLU	6.6
1	A	162	VAL	5.7
1	A	163	VAL	4.2
1	A	143	LEU	3.8
1	A	84	LEU	3.5
1	A	212	VAL	3.5
1	A	183	THR	3.3
1	A	184	SER	3.1
1	A	166	ASN	3.1
1	A	169	SER	3.0
1	A	154	PHE	3.0
1	A	175	ASP	2.9
1	A	155	GLN	2.9
1	A	196	SER	2.8
1	A	152	ASN	2.7
1	A	145	LYS	2.7
1	A	171	SER	2.6
1	A	173	PHE	2.6
1	A	161	HIS	2.6
1	A	56	ARG	2.4
1	A	170	ILE	2.4
1	A	186	HIS	2.3
1	A	191	GLN	2.3
1	A	1	LEU	2.3
1	A	167	PHE	2.3
1	A	10	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	177	TRP	2.2
1	A	140	ASN	2.2
1	A	142	VAL	2.1
1	A	178	GLU	2.1
1	A	204	THR	2.1
1	A	141	ILE	2.1
1	A	135	LEU	2.0
1	A	187	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 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.