Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2024 – 01:46 am BST

PDB ID	:	2WUI
Title	:	Crystal Structure of MexZ, a key repressor responsible for antibiotic resistance in Pseudomonas aeruginosa.
Authors	:	Alguel, Y.; Lu, D.; Quade, N.; Zhang, X.
Deposited on	:	2009-10-05
Resolution	:	2.90 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:

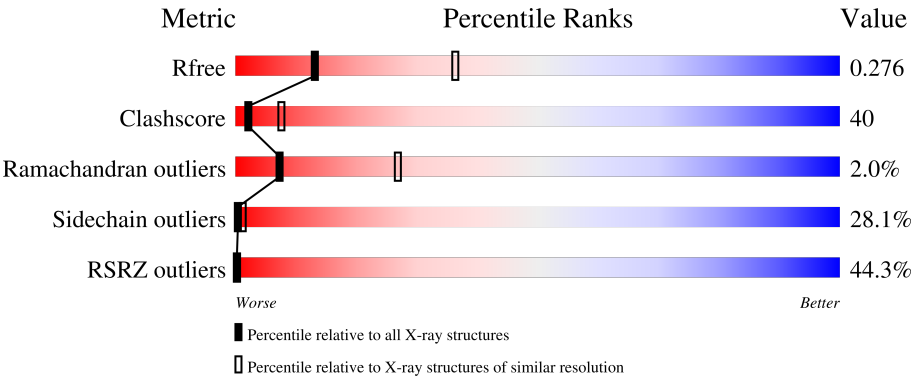
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	210	42% 39% 40% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1539 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 TRANSCRIPTIONAL REGULATOR.

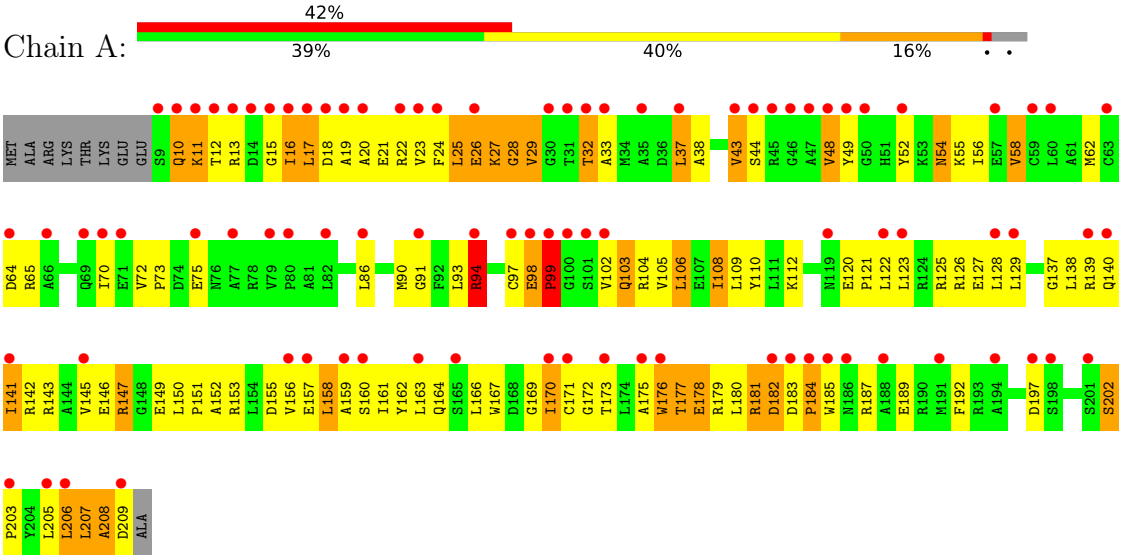
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1539	960	288	281	10	0	0	1

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: TRANSCRIPTIONAL REGULATOR

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	177.06Å 177.06Å 54.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.38 – 2.90 39.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.38-2.90) 99.6 (39.76-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.227 , 0.277 0.231 , 0.276	Depositor DCC
R_{free} test set	346 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	74.5	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 134.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	1539	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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	0.46	0/1562	0.86	7/2111 (0.3%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ALA	CB-CA-C	-14.29	88.66	110.10
1	A	99	PRO	CB-CA-C	-12.66	80.36	112.00
1	A	94	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	A	98	GLU	CB-CA-C	-6.19	98.03	110.40
1	A	26	GLU	CB-CA-C	-6.01	98.37	110.40
1	A	94	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	26	GLU	N-CA-C	5.29	125.27	111.00

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	1539	0	1519	122	0
All	All	1539	0	1519	122	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 40.

All (122) 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:138:LEU:HA	1:A:141:ILE:HD11	1.18	1.08
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.16	1.02
1:A:183:ASP:O	1:A:187:ARG:HD3	1.61	0.99
1:A:94:ARG:NH1	1:A:185:TRP:CD2	2.36	0.93
1:A:138:LEU:CA	1:A:141:ILE:HD11	2.01	0.90
1:A:93:LEU:O	1:A:93:LEU:HD23	1.73	0.88
1:A:102:VAL:O	1:A:106:LEU:HD22	1.74	0.87
1:A:26:GLU:HG2	1:A:27:LYS:HD2	1.57	0.87
1:A:38:ALA:HB2	1:A:48:VAL:HG21	1.57	0.86
1:A:25:LEU:HA	1:A:108:ILE:HD11	1.57	0.84
1:A:28:GLY:O	1:A:32:THR:HG22	1.78	0.83
1:A:147:ARG:HH11	1:A:147:ARG:CG	1.91	0.83
1:A:25:LEU:CA	1:A:108:ILE:HD11	2.09	0.82
1:A:16:ILE:HG21	1:A:48:VAL:HG13	1.62	0.81
1:A:91:GLY:O	1:A:94:ARG:HB3	1.83	0.78
1:A:10:GLN:O	1:A:13:ARG:HB2	1.87	0.75
1:A:94:ARG:NH1	1:A:185:TRP:CE3	2.54	0.74
1:A:207:LEU:HD12	1:A:207:LEU:H	1.51	0.74
1:A:52:TYR:CD2	1:A:58:VAL:HG23	2.24	0.71
1:A:15:GLY:O	1:A:19:ALA:HB2	1.92	0.69
1:A:153:ARG:O	1:A:207:LEU:HD12	1.93	0.69
1:A:147:ARG:HG3	1:A:147:ARG:NH1	1.96	0.69
1:A:19:ALA:O	1:A:23:VAL:HG23	1.93	0.69
1:A:125:ARG:O	1:A:128:LEU:HB3	1.93	0.68
1:A:10:GLN:HB2	1:A:13:ARG:HD2	1.75	0.68
1:A:93:LEU:HD23	1:A:93:LEU:C	2.14	0.67
1:A:149:GLU:O	1:A:150:LEU:HD23	1.95	0.66
1:A:90:MET:HE3	1:A:189:GLU:N	2.09	0.66
1:A:138:LEU:HA	1:A:141:ILE:CD1	2.12	0.66
1:A:21:GLU:OE1	1:A:65:ARG:NH2	2.29	0.65
1:A:43:VAL:CG1	1:A:48:VAL:HG22	2.27	0.65
1:A:207:LEU:O	1:A:209:ASP:N	2.29	0.64
1:A:170:ILE:HD11	1:A:192:PHE:CZ	2.33	0.63
1:A:94:ARG:NH1	1:A:185:TRP:CE2	2.67	0.62
1:A:13:ARG:HA	1:A:16:ILE:HD11	1.83	0.61
1:A:16:ILE:O	1:A:19:ALA:HB3	2.01	0.61
1:A:25:LEU:N	1:A:108:ILE:HD11	2.17	0.59
1:A:24:PHE:CD1	1:A:32:THR:HG21	2.37	0.59
1:A:25:LEU:HA	1:A:108:ILE:CD1	2.29	0.59
1:A:55:LYS:HG3	1:A:56:ILE:N	2.18	0.57
1:A:141:ILE:HD12	1:A:142:ARG:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:HG2	1:A:181:ARG:O	2.05	0.56
1:A:90:MET:HE2	1:A:192:PHE:HD2	1.71	0.55
1:A:93:LEU:C	1:A:93:LEU:CD2	2.75	0.55
1:A:98:GLU:CB	1:A:99:PRO:CD	2.84	0.55
1:A:90:MET:CE	1:A:192:PHE:CD2	2.90	0.54
1:A:152:ALA:O	1:A:153:ARG:HB2	2.08	0.54
1:A:29:VAL:HA	1:A:32:THR:CG2	2.38	0.54
1:A:153:ARG:O	1:A:206:LEU:HD12	2.08	0.53
1:A:16:ILE:O	1:A:20:ALA:N	2.42	0.53
1:A:90:MET:HE2	1:A:192:PHE:CD2	2.44	0.53
1:A:169:GLY:O	1:A:173:THR:HG23	2.09	0.53
1:A:11:LYS:HD3	1:A:12:THR:N	2.24	0.53
1:A:17:LEU:O	1:A:21:GLU:HG3	2.10	0.53
1:A:94:ARG:CA	1:A:94:ARG:HE	2.23	0.52
1:A:145:VAL:HG22	1:A:146:GLU:N	2.25	0.52
1:A:155:ASP:OD1	1:A:158:LEU:HB2	2.09	0.52
1:A:120:GLU:HB3	1:A:121:PRO:HD3	1.92	0.52
1:A:94:ARG:HE	1:A:94:ARG:HA	1.74	0.52
1:A:120:GLU:N	1:A:121:PRO:CD	2.72	0.51
1:A:43:VAL:HG13	1:A:44:SER:N	2.26	0.51
1:A:38:ALA:HB2	1:A:48:VAL:CG2	2.33	0.51
1:A:55:LYS:O	1:A:58:VAL:HG12	2.10	0.51
1:A:138:LEU:O	1:A:141:ILE:HD12	2.11	0.51
1:A:90:MET:CE	1:A:192:PHE:HD2	2.22	0.50
1:A:90:MET:HE1	1:A:192:PHE:CE2	2.46	0.50
1:A:110:TYR:HE1	1:A:126:ARG:HG3	1.76	0.50
1:A:173:THR:HA	1:A:177:THR:HG23	1.93	0.50
1:A:25:LEU:HD12	1:A:104:ARG:HG2	1.93	0.50
1:A:23:VAL:HG21	1:A:37:LEU:HD12	1.94	0.50
1:A:98:GLU:CB	1:A:99:PRO:HD3	2.43	0.49
1:A:13:ARG:O	1:A:16:ILE:HG12	2.13	0.49
1:A:147:ARG:CG	1:A:147:ARG:NH1	2.60	0.49
1:A:21:GLU:O	1:A:25:LEU:HB2	2.14	0.48
1:A:167:TRP:HA	1:A:170:ILE:CD1	2.44	0.48
1:A:178:GLU:OE2	1:A:178:GLU:HA	2.13	0.48
1:A:11:LYS:HB2	1:A:11:LYS:HE2	1.58	0.48
1:A:138:LEU:O	1:A:142:ARG:HG3	2.14	0.47
1:A:180:LEU:O	1:A:184:PRO:HB3	2.15	0.47
1:A:16:ILE:HG12	1:A:17:LEU:HD23	1.96	0.47
1:A:10:GLN:CD	1:A:10:GLN:C	2.73	0.46
1:A:17:LEU:HD13	1:A:62:MET:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG13	1:A:44:SER:O	2.16	0.46
1:A:54:ASN:ND2	1:A:54:ASN:N	2.63	0.46
1:A:167:TRP:HA	1:A:170:ILE:HD11	1.96	0.46
1:A:158:LEU:HA	1:A:158:LEU:HD23	1.67	0.45
1:A:12:THR:O	1:A:16:ILE:HD13	2.16	0.45
1:A:166:LEU:O	1:A:166:LEU:HD23	2.17	0.45
1:A:103:GLN:HG3	1:A:104:ARG:N	2.31	0.45
1:A:49:TYR:O	1:A:52:TYR:O	2.35	0.44
1:A:202:SER:HA	1:A:203:PRO:HD2	1.57	0.44
1:A:172:GLY:HA2	1:A:175:ALA:O	2.17	0.44
1:A:175:ALA:HA	1:A:176:TRP:HA	1.74	0.44
1:A:160:SER:O	1:A:161:ILE:C	2.54	0.44
1:A:166:LEU:O	1:A:170:ILE:HD13	2.17	0.44
1:A:18:ASP:OD2	1:A:19:ALA:N	2.52	0.43
1:A:138:LEU:O	1:A:141:ILE:CD1	2.66	0.43
1:A:90:MET:HE1	1:A:192:PHE:CD2	2.53	0.43
1:A:64:ASP:O	1:A:65:ARG:C	2.57	0.43
1:A:150:LEU:HB3	1:A:151:PRO:HD2	2.00	0.43
1:A:21:GLU:OE2	1:A:104:ARG:NH1	2.47	0.43
1:A:145:VAL:CG2	1:A:146:GLU:N	2.81	0.43
1:A:43:VAL:HG11	1:A:48:VAL:HG22	1.98	0.43
1:A:17:LEU:HD23	1:A:17:LEU:N	2.34	0.42
1:A:137:GLY:O	1:A:141:ILE:HG13	2.18	0.42
1:A:90:MET:HE2	1:A:189:GLU:HA	2.02	0.42
1:A:29:VAL:HA	1:A:32:THR:HG22	2.01	0.42
1:A:105:VAL:O	1:A:108:ILE:HB	2.19	0.42
1:A:159:ALA:O	1:A:162:TYR:HB3	2.19	0.42
1:A:143:ARG:O	1:A:147:ARG:N	2.49	0.41
1:A:152:ALA:O	1:A:153:ARG:CB	2.67	0.41
1:A:182:ASP:O	1:A:183:ASP:C	2.58	0.41
1:A:16:ILE:HA	1:A:19:ALA:HB3	2.03	0.41
1:A:37:LEU:HD21	1:A:58:VAL:HG11	2.03	0.41
1:A:153:ARG:HH12	1:A:208:ALA:HB3	1.84	0.41
1:A:20:ALA:O	1:A:21:GLU:C	2.59	0.41
1:A:110:TYR:CE1	1:A:126:ARG:HD2	2.56	0.41
1:A:29:VAL:HG12	1:A:112:LYS:O	2.21	0.40
1:A:123:LEU:O	1:A:127:GLU:HG3	2.21	0.40
1:A:75:GLU:OE1	1:A:139:ARG:NH2	2.54	0.40
1:A:156:VAL:O	1:A:157:GLU:C	2.57	0.40
1:A:72:VAL:HA	1:A:73:PRO:HD3	1.97	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	199/210 (95%)	171 (86%)	24 (12%)	4 (2%)	7 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ALA
1	A	99	PRO
1	A	184	PRO
1	A	28	GLY

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	153/172 (89%)	110 (72%)	43 (28%)	0 1

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	LYS
1	A	16	ILE
1	A	17	LEU
1	A	22	ARG
1	A	25	LEU
1	A	27	LYS

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Mol	Chain	Res	Type
1	A	29	VAL
1	A	32	THR
1	A	37	LEU
1	A	43	VAL
1	A	48	VAL
1	A	54	ASN
1	A	58	VAL
1	A	70	ILE
1	A	86	LEU
1	A	94	ARG
1	A	97	CYS
1	A	103	GLN
1	A	106	LEU
1	A	108	ILE
1	A	109	LEU
1	A	122	LEU
1	A	129	LEU
1	A	140	GLN
1	A	141	ILE
1	A	147	ARG
1	A	158	LEU
1	A	163	LEU
1	A	164	GLN
1	A	170	ILE
1	A	171	CYS
1	A	176	TRP
1	A	177	THR
1	A	178	GLU
1	A	179	ARG
1	A	181	ARG
1	A	182	ASP
1	A	197	ASP
1	A	202	SER
1	A	205	LEU
1	A	206	LEU
1	A	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	76	ASN
1	A	103	GLN
1	A	140	GLN

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 monosaccharides 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	201/210 (95%)	1.99	89 (44%) 0 0	112, 138, 158, 176	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	SER	9.2
1	A	12	THR	7.1
1	A	44	SER	5.2
1	A	15	GLY	5.1
1	A	22	ARG	5.0
1	A	16	ILE	4.9
1	A	10	GLN	4.7
1	A	18	ASP	4.4
1	A	47	ALA	4.3
1	A	14	ASP	4.1
1	A	188	ALA	4.1
1	A	209	ASP	4.0
1	A	43	VAL	4.0
1	A	184	PRO	3.9
1	A	182	ASP	3.9
1	A	31	THR	3.7
1	A	176	TRP	3.6
1	A	11	LYS	3.6
1	A	175	ALA	3.6
1	A	173	THR	3.5
1	A	94	ARG	3.3
1	A	80	PRO	3.2
1	A	24	PHE	3.2
1	A	69	GLN	3.2
1	A	50	GLY	3.2
1	A	66	ALA	3.2
1	A	128	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	48	VAL	3.1
1	A	59	CYS	3.1
1	A	170	ILE	3.0
1	A	20	ALA	2.9
1	A	171	CYS	2.9
1	A	186	ASN	2.8
1	A	46	GLY	2.8
1	A	70	ILE	2.7
1	A	129	LEU	2.7
1	A	183	ASP	2.7
1	A	30	GLY	2.7
1	A	185	TRP	2.7
1	A	159	ALA	2.7
1	A	98	GLU	2.6
1	A	198	SER	2.6
1	A	45	ARG	2.6
1	A	119	ASN	2.5
1	A	156	VAL	2.5
1	A	37	LEU	2.5
1	A	101	SER	2.5
1	A	100	GLY	2.5
1	A	17	LEU	2.4
1	A	23	VAL	2.4
1	A	191	MET	2.4
1	A	35	ALA	2.4
1	A	13	ARG	2.4
1	A	86	LEU	2.4
1	A	75	GLU	2.4
1	A	97	CYS	2.4
1	A	123	LEU	2.3
1	A	206	LEU	2.3
1	A	64	ASP	2.3
1	A	33	ALA	2.3
1	A	57	GLU	2.3
1	A	197	ASP	2.3
1	A	63	CYS	2.3
1	A	26	GLU	2.3
1	A	122	LEU	2.2
1	A	49	TYR	2.2
1	A	139	ARG	2.2
1	A	91	GLY	2.2
1	A	60	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	ILE	2.2
1	A	205	LEU	2.2
1	A	77	ALA	2.2
1	A	82	LEU	2.1
1	A	203	PRO	2.1
1	A	19	ALA	2.1
1	A	201	SER	2.1
1	A	52	TYR	2.1
1	A	157	GLU	2.1
1	A	145	VAL	2.1
1	A	32	THR	2.1
1	A	79	VAL	2.1
1	A	71	GLU	2.1
1	A	163	LEU	2.1
1	A	165	SER	2.0
1	A	102	VAL	2.0
1	A	160	SER	2.0
1	A	99	PRO	2.0
1	A	194	ALA	2.0
1	A	140	GLN	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 monosaccharides 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.