Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:08 am BST

PDB ID	:	6J0V
Title	:	Crystal Structure of Yeast Rtt107
Authors	:	Wan, B.; Wu, J.; Lei, M.
Deposited on	:	2018-12-27
Resolution	:	2.31 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 following versions of software and data (see references ⓘ) were used in the production of this report:

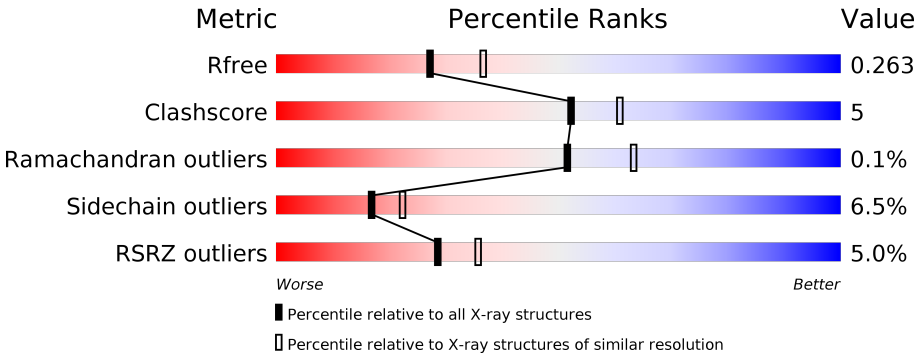
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 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	513	3% 72% 17% • 10%
1	B	513	6% 72% 15% • 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7625 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 Regulator of Ty1 transposition protein 107.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3773	2458	617	680	18			
1	B	454	Total	C	N	O	S	0	0	0
			3730	2434	610	668	18			

- Molecule 2 is water.

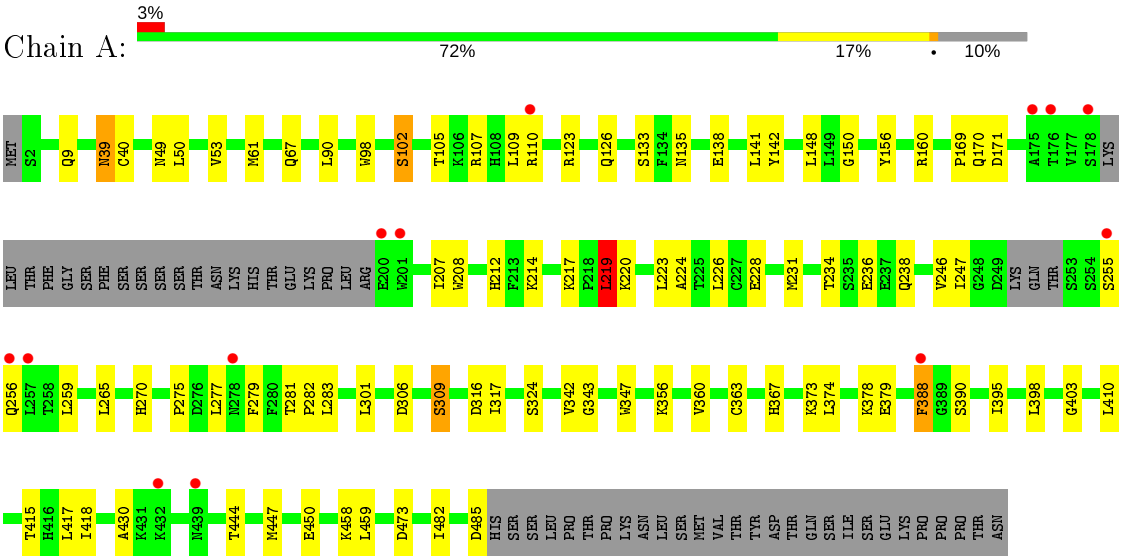
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	52	Total	O	0	0
			52	52		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

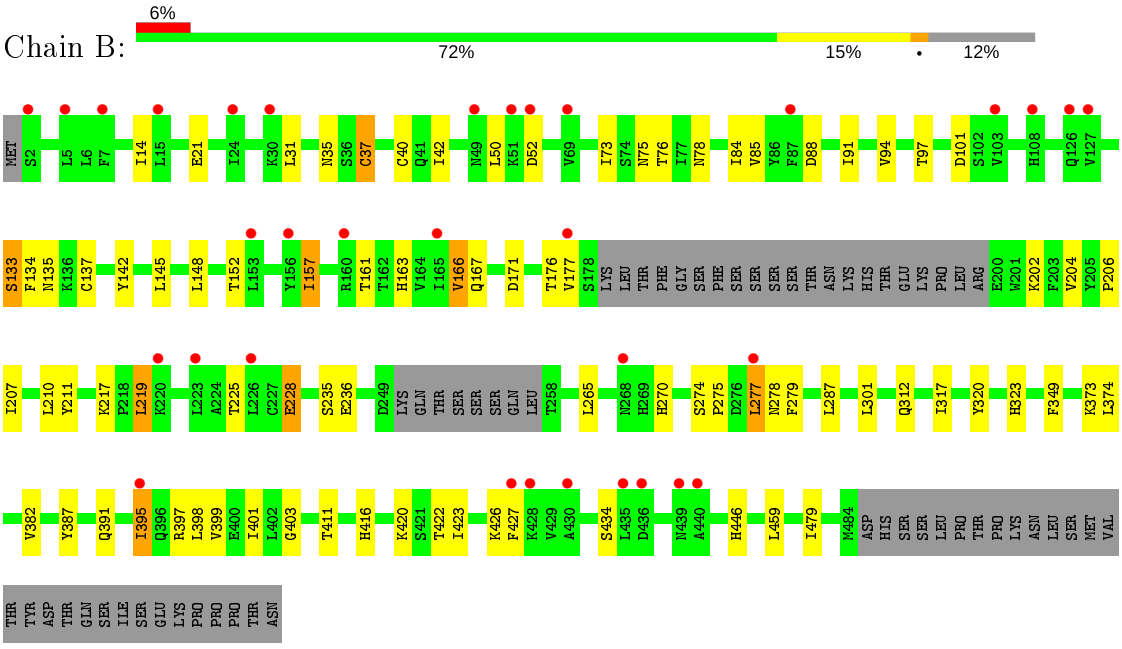
- Molecule 1: Regulator of Ty1 transposition protein 107

Chain A:



- Molecule 1: Regulator of Ty1 transposition protein 107

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.40Å 98.91Å 87.46Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	49.45 – 2.31 63.93 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.45-2.31) 97.5 (63.93-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.215 , 0.266 0.215 , 0.263	Depositor DCC
R_{free} test set	2482 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7625	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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	0.42	0/3879	0.60	1/5263 (0.0%)
1	B	0.40	0/3836	0.54	0/5205
All	All	0.41	0/7715	0.57	1/10468 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	LEU	CA-CB-CG	5.89	128.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	PHE	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	3773	0	3740	46	0
1	B	3730	0	3704	36	0
2	A	70	0	0	4	0
2	B	52	0	0	2	0
All	All	7625	0	7444	82	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 5.

All (82) 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:B:101:ASP:OD2	2:B:601:HOH:O	1.98	0.81
1:A:110:ARG:HA	1:A:388:PHE:CE1	2.19	0.77
1:A:379:GLU:OE1	1:A:458:LYS:NZ	2.24	0.70
1:A:208:TRP:HD1	1:A:219:LEU:HD12	1.59	0.67
1:B:76:THR:HG23	1:B:78:ASN:H	1.59	0.67
1:A:110:ARG:HA	1:A:388:PHE:HE1	1.64	0.61
1:B:270:HIS:HB3	1:B:317:ILE:HA	1.82	0.60
1:A:105:THR:HG21	1:A:109:LEU:HD21	1.84	0.59
1:B:135:ASN:ND2	1:B:278:ASN:OD1	2.35	0.59
1:B:73:ILE:HA	1:B:94:VAL:O	2.03	0.58
1:A:110:ARG:HA	1:A:388:PHE:CZ	2.40	0.57
1:A:395:ILE:HD11	1:A:418:ILE:HG21	1.89	0.55
1:A:212:HIS:CE1	1:A:219:LEU:HB2	2.41	0.55
1:B:391:GLN:O	1:B:395:ILE:HG13	2.07	0.55
1:B:397:ARG:O	1:B:401:ILE:HG12	2.07	0.54
1:A:98:TRP:O	1:A:102:SER:HB2	2.08	0.54
1:A:410:LEU:HD21	1:A:430:ALA:HB2	1.91	0.53
1:A:219:LEU:HD13	1:A:224:ALA:HA	1.91	0.52
1:A:342:VAL:O	1:A:360:VAL:HG21	2.09	0.52
1:B:163:HIS:HD2	1:B:204:VAL:HG21	1.75	0.52
1:A:270:HIS:HB3	1:A:317:ILE:HA	1.92	0.52
1:B:373:LYS:HD3	1:B:403:GLY:HA2	1.93	0.50
1:A:417:LEU:HD22	1:A:430:ALA:HB3	1.94	0.50
1:A:208:TRP:CD1	1:A:219:LEU:HD12	2.45	0.50
1:A:214:LYS:NZ	1:A:247:ILE:O	2.41	0.49
1:A:398:LEU:HD11	1:A:450:GLU:HG2	1.95	0.49
1:B:277:LEU:HD23	1:B:323:HIS:HB2	1.95	0.49
1:A:316:ASP:N	1:A:316:ASP:OD1	2.43	0.49
1:A:207:ILE:HD12	1:A:246:VAL:HG21	1.95	0.49
1:B:382:VAL:HG12	1:B:416:HIS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:HG2	1:A:473:ASP:HA	1.95	0.48
1:A:373:LYS:HD3	1:A:403:GLY:HA2	1.95	0.48
1:A:171:ASP:HB3	2:A:615:HOH:O	2.12	0.48
1:B:84:ILE:O	1:B:88:ASP:HB3	2.14	0.48
1:B:211:TYR:CD1	1:B:219:LEU:HG	2.48	0.48
1:B:14:ILE:HB	1:B:42:ILE:HD13	1.96	0.48
1:A:256:GLN:HB3	1:A:259:LEU:HG	1.96	0.47
1:A:90:LEU:HD22	1:A:390:SER:HB3	1.96	0.47
1:B:225:THR:O	1:B:228:GLU:HG3	2.16	0.46
1:B:31:LEU:O	1:B:35:ASN:ND2	2.45	0.45
1:B:387:TYR:CB	1:B:395:ILE:HD11	2.46	0.45
1:B:76:THR:HG23	1:B:78:ASN:N	2.30	0.45
1:A:135:ASN:OD1	1:A:138:GLU:HG3	2.17	0.45
1:B:142:TYR:CE1	1:B:206:PRO:HB3	2.51	0.45
1:B:166:VAL:HG12	1:B:171:ASP:OD2	2.17	0.45
1:B:157:ILE:HD12	1:B:157:ILE:H	1.81	0.45
1:B:446:HIS:HB2	1:B:479:ILE:HD12	1.99	0.45
1:A:142:TYR:OH	1:A:283:LEU:HD22	2.16	0.45
1:A:281:THR:HB	1:A:282:PRO:HD3	1.99	0.45
1:A:343:GLY:HA3	1:A:347:TRP:CE3	2.52	0.44
1:A:170:GLN:NE2	2:A:606:HOH:O	2.51	0.44
1:A:123:ARG:HA	1:A:150:GLY:O	2.18	0.43
1:A:223:LEU:HD23	1:A:226:LEU:HD12	2.01	0.43
1:B:382:VAL:HG21	1:B:399:VAL:HG21	2.00	0.43
1:A:141:LEU:C	1:A:141:LEU:HD23	2.39	0.43
1:B:85:VAL:HG13	1:B:91:ILE:HB	2.00	0.43
1:A:207:ILE:HG22	1:A:247:ILE:HD13	2.00	0.43
1:B:422:THR:HG22	1:B:427:PHE:CZ	2.54	0.43
1:A:105:THR:HG23	1:A:107:ARG:HG2	2.01	0.43
1:B:133:SER:HB3	1:B:134:PHE:CD2	2.54	0.43
1:A:447:MET:HE2	1:A:482:ILE:HD11	2.00	0.43
1:B:279:PHE:HE2	1:B:287:LEU:HD22	1.84	0.43
1:B:426:LYS:NZ	2:B:606:HOH:O	2.46	0.42
1:A:363:CYS:HB3	1:A:367:HIS:ND1	2.34	0.42
1:A:219:LEU:CD1	1:A:224:ALA:HA	2.48	0.42
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.89	0.42
1:A:169:PRO:HB3	1:A:231:MET:SD	2.59	0.42
1:A:39:ASN:ND2	2:A:608:HOH:O	2.53	0.42
1:A:306:ASP:OD2	1:A:309:SER:HB3	2.19	0.42
1:B:148:LEU:HD12	1:B:148:LEU:HA	1.80	0.42
1:B:37:CYS:SG	1:B:40:CYS:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HA	1:A:444:THR:O	2.20	0.41
1:B:207:ILE:HA	1:B:210:LEU:HB2	2.02	0.41
1:B:275:PRO:HD3	1:B:301:LEU:HB2	2.02	0.41
1:A:238:GLN:N	2:A:609:HOH:O	2.54	0.41
1:B:274:SER:HB2	1:B:320:TYR:CZ	2.56	0.41
1:B:145:LEU:HD21	1:B:349:PHE:CZ	2.56	0.41
1:A:126:GLN:OE1	1:A:160:ARG:HB3	2.20	0.41
1:A:378:LYS:O	1:A:415:THR:HG21	2.21	0.40
1:A:275:PRO:HD3	1:A:301:LEU:HB2	2.04	0.40
1:B:134:PHE:CE1	1:B:167:GLN:HB2	2.57	0.40
1:B:21:GLU:OE2	1:B:75:ASN:ND2	2.54	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	454/513 (88%)	436 (96%)	18 (4%)	0	100	100
1	B	448/513 (87%)	426 (95%)	21 (5%)	1 (0%)	47	58
All	All	902/1026 (88%)	862 (96%)	39 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	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	428/480 (89%)	401 (94%)	27 (6%)	18 24
1	B	422/480 (88%)	394 (93%)	28 (7%)	16 22
All	All	850/960 (88%)	795 (94%)	55 (6%)	17 22

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	39	ASN
1	A	40	CYS
1	A	49	ASN
1	A	50	LEU
1	A	53	VAL
1	A	61	MET
1	A	102	SER
1	A	133	SER
1	A	148	LEU
1	A	156	TYR
1	A	217	LYS
1	A	219	LEU
1	A	220	LYS
1	A	228	GLU
1	A	234	THR
1	A	236	GLU
1	A	255	SER
1	A	265	LEU
1	A	277	LEU
1	A	309	SER
1	A	324	SER
1	A	356	LYS
1	A	374	LEU
1	A	388	PHE
1	A	459	LEU
1	A	485	ASP
1	B	37	CYS
1	B	50	LEU
1	B	52	ASP
1	B	97	THR
1	B	133	SER
1	B	137	CYS

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Mol	Chain	Res	Type
1	B	152	THR
1	B	157	ILE
1	B	161	THR
1	B	166	VAL
1	B	176	THR
1	B	202	LYS
1	B	217	LYS
1	B	219	LEU
1	B	228	GLU
1	B	235	SER
1	B	236	GLU
1	B	265	LEU
1	B	277	LEU
1	B	312	GLN
1	B	374	LEU
1	B	395	ILE
1	B	398	LEU
1	B	411	THR
1	B	420	LYS
1	B	423	ILE
1	B	434	SER
1	B	459	LEU

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

Mol	Chain	Res	Type
1	A	78	ASN
1	A	474	ASN
1	B	100	GLN
1	B	135	ASN
1	B	163	HIS

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

There are no carbohydrates 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	460/513 (89%)	0.37	13 (2%)	53	60	32, 60, 109, 164	0
1	B	454/513 (88%)	0.65	33 (7%)	15	20	38, 76, 124, 194	0
All	All	914/1026 (89%)	0.51	46 (5%)	28	36	32, 68, 117, 194	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	TRP	5.8
1	B	160	ARG	5.0
1	B	15	LEU	5.0
1	B	5	LEU	4.8
1	B	226	LEU	4.4
1	B	103	VAL	4.1
1	B	51	LYS	3.8
1	A	175	ALA	3.8
1	B	439	ASN	3.7
1	B	52	ASP	3.6
1	B	435	LEU	3.4
1	B	268	ASN	3.2
1	B	7	PHE	3.0
1	B	277	LEU	2.9
1	B	87	PHE	2.8
1	A	439	ASN	2.8
1	B	2	SER	2.8
1	A	200	GLU	2.7
1	B	126	GLN	2.6
1	A	388	PHE	2.6
1	A	432	LYS	2.6
1	B	108	HIS	2.6
1	B	220	LYS	2.6
1	B	427	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	395	ILE	2.5
1	B	24	ILE	2.4
1	B	177	VAL	2.4
1	B	69	VAL	2.4
1	A	178	SER	2.4
1	B	430	ALA	2.3
1	B	440	ALA	2.3
1	B	127	VAL	2.3
1	A	257	LEU	2.2
1	B	49	ASN	2.2
1	B	156	TYR	2.2
1	A	176	THR	2.2
1	B	428	LYS	2.1
1	A	110	ARG	2.1
1	B	165	ILE	2.1
1	B	153	LEU	2.1
1	A	278	ASN	2.1
1	B	223	LEU	2.0
1	A	255	SER	2.0
1	B	436	ASP	2.0
1	A	256	GLN	2.0
1	B	30	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 carbohydrates 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.