



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2017 – 04:11 PM EDT

PDB ID : 5MS2
Title : Crystal structure of the Legionella pneumophila effector protein RavZ in complex with human LC3B
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Deposited on : 2016-12-30
Resolution : 2.47 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

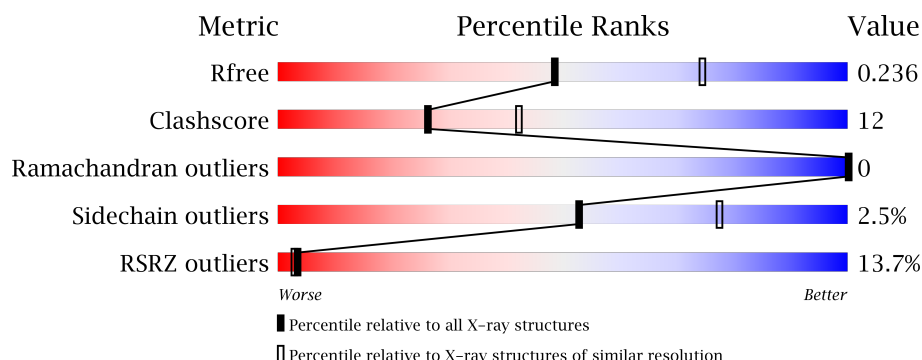
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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}	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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. 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	433	
2	B	124	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4273 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 Legionella pneumophila effector protein RavZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	2	0
			3202	2029	518	645	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q5ZUV9
A	0	PRO	-	expression tag	UNP Q5ZUV9

- Molecule 2 is a protein called Microtubule-associated proteins 1A/1B light chain 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			960	614	168	175	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9GZQ8
B	-3	HIS	-	expression tag	UNP Q9GZQ8
B	-2	MET	-	expression tag	UNP Q9GZQ8
B	-1	GLY	-	expression tag	UNP Q9GZQ8
B	0	CYS	-	expression tag	UNP Q9GZQ8

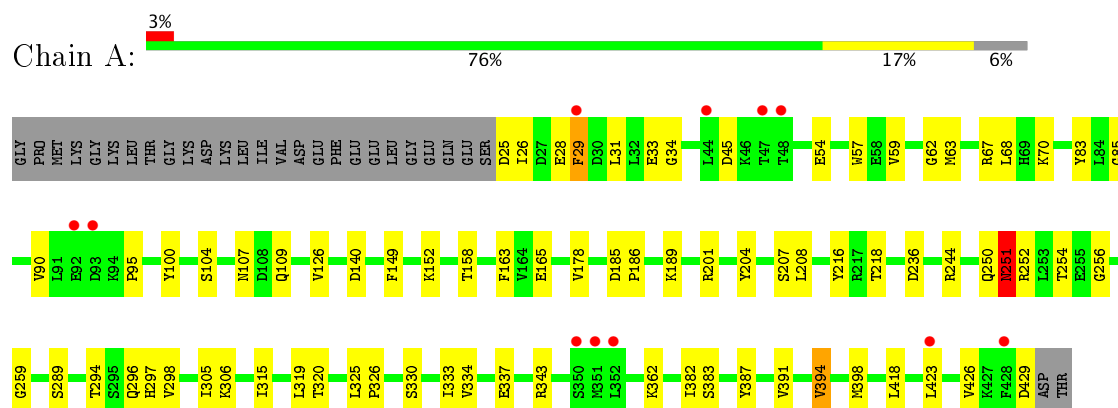
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		
3	B	5	Total	O	0	0
			5	5		

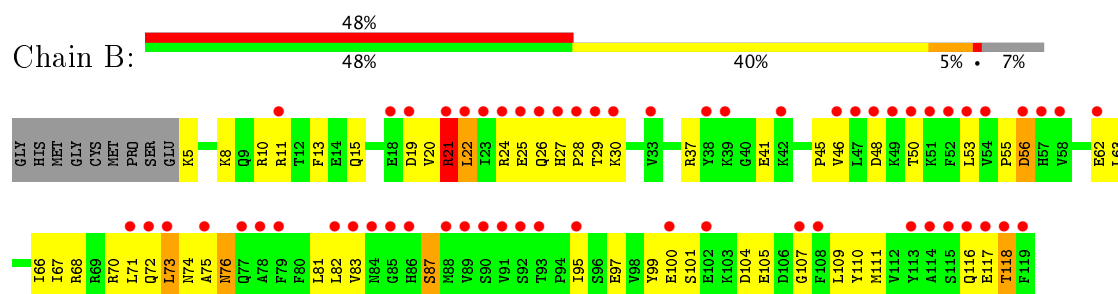
3 Residue-property plots [i](#)

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: *Legionella pneumophila* effector protein RavZ



- Molecule 2: Microtubule-associated proteins 1A/1B light chain 3B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.55Å 69.55Å 90.17Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	48.08 – 2.47 48.08 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.08-2.47) 99.9 (48.08-2.47)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.177 , 0.238 0.178 , 0.236	Depositor DCC
R_{free} test set	1130 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4273	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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	0.51	0/3267	0.70	3/4413 (0.1%)
2	B	0.41	0/978	0.72	0/1316
All	All	0.49	0/4245	0.70	3/5729 (0.1%)

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
2	B	0	4
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ASN	N-CA-C	-9.06	86.54	111.00
1	A	29	PHE	CA-C-O	7.62	136.11	120.10
1	A	29	PHE	CA-C-N	-7.27	101.21	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	GLN	Peptide
2	B	21	ARG	Peptide
2	B	22	LEU	Peptide
2	B	48	ASP	Peptide
2	B	73	LEU	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	3202	0	3173	53	1
2	B	960	0	979	46	0
3	A	106	0	0	0	0
3	B	5	0	0	3	0
All	All	4273	0	4152	97	1

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 12.

All (97) 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)
2:B:24:ARG:NH1	2:B:25:GLU:OE1	1.98	0.97
2:B:82:LEU:HD12	2:B:87:SER:HB3	1.61	0.82
2:B:45:PRO:HG2	2:B:71:LEU:HD22	1.61	0.81
1:A:107:ASN:HB3	1:A:109:GLN:H	1.46	0.80
2:B:87:SER:OG	3:B:201:HOH:O	2.02	0.78
2:B:76:ASN:OD1	3:B:202:HOH:O	2.03	0.76
1:A:251:ASN:OD1	1:A:289:SER:OG	2.04	0.75
1:A:34:GLY:HA3	2:B:76:ASN:HD21	1.51	0.74
1:A:63:MET:HG3	1:A:259:GLY:HA3	1.71	0.72
2:B:70:ARG:O	2:B:72:GLN:NE2	2.23	0.71
2:B:13:PHE:HE2	2:B:105:GLU:HG3	1.58	0.69
2:B:26:GLN:N	2:B:26:GLN:OE1	2.28	0.67
2:B:10:ARG:HH22	2:B:50:THR:HG21	1.60	0.66
1:A:25:ASP:OD1	1:A:26:ILE:N	2.27	0.66
2:B:37:ARG:NH2	2:B:41:GLU:O	2.29	0.66
1:A:34:GLY:HA3	2:B:76:ASN:ND2	2.09	0.66
2:B:68:ARG:NH1	2:B:75:ALA:HA	2.14	0.63
2:B:37:ARG:HD3	2:B:46:VAL:HG22	1.81	0.61
2:B:22:LEU:HD11	2:B:25:GLU:H	1.68	0.59
2:B:11:ARG:HD3	2:B:15:GLN:HB3	1.84	0.59
2:B:24:ARG:HH11	2:B:25:GLU:CD	2.05	0.59
1:A:90:VAL:HG11	1:A:320:THR:O	2.04	0.57
2:B:25:GLU:HA	2:B:28:PRO:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLN:NE2	1:A:158:THR:OG1	2.38	0.57
1:A:83:TYR:CZ	1:A:85:GLY:HA3	2.39	0.57
1:A:204:TYR:CD2	1:A:218:THR:HG21	2.40	0.57
2:B:22:LEU:CD1	2:B:25:GLU:H	2.19	0.55
1:A:294[A]:THR:HB	1:A:297:HIS:ND1	2.22	0.55
2:B:83:VAL:HG22	2:B:111:MET:HG2	1.89	0.54
1:A:387:TYR:CZ	1:A:423:LEU:HD13	2.43	0.54
1:A:29:PHE:CD1	1:A:31:LEU:HB2	2.43	0.54
2:B:73:LEU:HD23	2:B:74:ASN:H	1.72	0.54
1:A:294[A]:THR:HG22	1:A:296:GLN:H	1.72	0.54
1:A:423:LEU:O	1:A:426:VAL:HG12	2.07	0.53
1:A:163:PHE:CE1	1:A:178:VAL:HG13	2.43	0.53
2:B:67:ILE:HD12	2:B:81:LEU:HD11	1.89	0.53
2:B:8:LYS:NZ	2:B:104:ASP:OD2	2.35	0.52
1:A:126:VAL:HG11	1:A:208:LEU:HD13	1.91	0.52
1:A:201:ARG:HG2	1:A:252:ARG:HG3	1.92	0.52
1:A:33:GLU:HB2	3:B:202:HOH:O	2.10	0.51
1:A:28:GLU:HG2	1:A:29:PHE:H	1.74	0.51
1:A:294[B]:THR:HG22	1:A:297:HIS:ND1	2.26	0.51
2:B:116:GLN:HG2	2:B:118:THR:H	1.77	0.50
2:B:22:LEU:HG	2:B:26:GLN:OE1	2.12	0.50
2:B:66:ILE:O	2:B:70:ARG:HG3	2.12	0.50
2:B:30:LYS:HE3	2:B:55:PRO:HG3	1.94	0.50
2:B:20:VAL:HG11	2:B:107:GLY:HA3	1.94	0.50
1:A:294[B]:THR:HG23	1:A:296:GLN:H	1.78	0.49
2:B:117:GLU:O	2:B:117:GLU:HG2	2.13	0.49
1:A:201:ARG:NH1	1:A:254:THR:HG22	2.28	0.49
2:B:30:LYS:HB3	2:B:53:LEU:HG	1.95	0.49
2:B:11:ARG:NH1	2:B:19:ASP:OD1	2.46	0.49
2:B:97:GLU:O	2:B:101:SER:OG	2.28	0.49
1:A:343:ARG:HH12	1:A:362:LYS:HD2	1.78	0.48
2:B:10:ARG:NH2	2:B:50:THR:HG21	2.28	0.48
1:A:62:GLY:HA2	1:A:256:GLY:HA2	1.96	0.48
2:B:25:GLU:HA	2:B:28:PRO:CA	2.44	0.48
2:B:99:TYR:HD1	2:B:109:LEU:HB2	1.78	0.48
1:A:294[B]:THR:HG22	1:A:297:HIS:H	1.78	0.47
1:A:201:ARG:CG	1:A:252:ARG:HG3	2.42	0.47
1:A:333:ILE:O	1:A:337:GLU:HG3	2.14	0.47
2:B:11:ARG:HH11	2:B:15:GLN:HB3	1.79	0.47
1:A:57:TRP:CH2	1:A:59:VAL:HA	2.50	0.47
1:A:152:LYS:HB2	1:A:152:LYS:HE2	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294[B]:THR:HG23	1:A:296:GLN:N	2.30	0.47
2:B:27:HIS:HB3	2:B:30:LYS:HB2	1.98	0.46
1:A:387:TYR:O	1:A:391:VAL:HG23	2.16	0.45
2:B:22:LEU:HA	2:B:22:LEU:HD12	1.72	0.45
1:A:189:LYS:HD3	1:A:236:ASP:HB3	1.99	0.45
1:A:59:VAL:HG21	1:A:298:VAL:HG13	1.98	0.45
2:B:21:ARG:HG3	2:B:24:ARG:HH21	1.82	0.44
2:B:56:ASP:N	2:B:56:ASP:OD1	2.50	0.43
2:B:63:LEU:HD22	2:B:95:ILE:HD13	2.00	0.43
1:A:67:ARG:HB3	1:A:305:ILE:HD12	2.00	0.43
1:A:70:LYS:HA	1:A:315:ILE:HD11	1.99	0.43
1:A:29:PHE:CE1	1:A:31:LEU:HB2	2.53	0.43
2:B:21:ARG:O	2:B:24:ARG:NH2	2.52	0.43
1:A:189:LYS:NZ	1:A:236:ASP:OD2	2.49	0.43
1:A:325:LEU:HA	1:A:326:PRO:HD2	1.88	0.43
1:A:394:VAL:O	1:A:398:MET:HG2	2.19	0.43
1:A:54:GLU:O	1:A:306:LYS:HA	2.19	0.43
1:A:104:SER:CB	1:A:107:ASN:HB2	2.49	0.42
1:A:330:SER:O	1:A:334:VAL:HG23	2.18	0.42
1:A:185:ASP:HA	1:A:186:PRO:HD3	1.77	0.42
2:B:5:LYS:HE2	2:B:5:LYS:HB2	1.86	0.42
2:B:74:ASN:O	2:B:75:ALA:HB3	2.20	0.42
1:A:63:MET:HE1	1:A:68:LEU:N	2.35	0.41
2:B:8:LYS:HE3	2:B:110:TYR:CZ	2.55	0.41
1:A:163:PHE:CZ	1:A:178:VAL:HG13	2.54	0.41
1:A:165:GLU:OE1	1:A:244:ARG:NH2	2.52	0.41
1:A:100:TYR:CD2	1:A:319:LEU:HD12	2.55	0.41
1:A:126:VAL:HG13	1:A:216:TYR:CE1	2.55	0.41
1:A:382:ILE:HD13	1:A:382:ILE:HA	1.78	0.41
1:A:394:VAL:HG22	1:A:418:LEU:HD12	2.02	0.41
2:B:62:GLU:O	2:B:66:ILE:HG13	2.21	0.41
1:A:45:ASP:OD1	1:A:45:ASP:N	2.43	0.40
1:A:95:PRO:HB2	1:A:149:PHE:HE2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD2	1:A:207:SER:OG[2_455]	2.03	0.17

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	405/433 (94%)	398 (98%)	7 (2%)	0	100	100
2	B	113/124 (91%)	107 (95%)	6 (5%)	0	100	100
All	All	518/557 (93%)	505 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	366/388 (94%)	361 (99%)	5 (1%)	71	88
2	B	109/116 (94%)	102 (94%)	7 (6%)	20	36
All	All	475/504 (94%)	463 (98%)	12 (2%)	53	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ASP
1	A	251	ASN
1	A	383	SER
1	A	394	VAL
1	A	429	ASP
2	B	21	ARG
2	B	29	THR
2	B	56	ASP

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Mol	Chain	Res	Type
2	B	76	ASN
2	B	87	SER
2	B	100	GLU
2	B	118	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
2	B	77	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	405/433 (93%)	0.10	11 (2%) 55 56	17, 33, 74, 122	0
2	B	115/124 (92%)	2.45	60 (52%) 0 0	46, 89, 134, 147	0
All	All	520/557 (93%)	0.62	71 (13%) 3 3	17, 40, 106, 147	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	119	PHE	9.8
2	B	89	VAL	9.5
1	A	44	LEU	8.3
2	B	23	ILE	7.2
2	B	57	HIS	6.1
2	B	86	HIS	5.8
2	B	118	THR	5.8
2	B	90	SER	5.3
2	B	72	GLN	4.9
2	B	28	PRO	4.8
2	B	95	ILE	4.8
2	B	21	ARG	4.8
2	B	38	TYR	4.6
2	B	88	MET	4.6
2	B	22	LEU	4.5
2	B	25	GLU	4.5
2	B	47	LEU	4.4
2	B	24	ARG	4.3
2	B	93	THR	4.3
2	B	83	VAL	4.3
2	B	53	LEU	4.2
1	A	29	PHE	4.2
2	B	84	ASN	4.1
2	B	50	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	52	PHE	4.0
1	A	47	THR	3.9
2	B	48	ASP	3.9
2	B	73	LEU	3.9
1	A	352	LEU	3.8
2	B	117	GLU	3.7
2	B	71	LEU	3.7
2	B	26	GLN	3.5
2	B	39	LYS	3.5
2	B	56	ASP	3.4
2	B	33	VAL	3.4
2	B	92	SER	3.4
1	A	350	SER	3.3
2	B	29	THR	3.3
2	B	58	VAL	3.3
2	B	114	ALA	3.2
1	A	48	THR	3.2
2	B	49	LYS	3.2
2	B	116	GLN	3.0
2	B	115	SER	3.0
1	A	93	ASP	2.9
2	B	82	LEU	2.9
2	B	78	ALA	2.9
2	B	42	LYS	2.8
2	B	85	GLY	2.8
2	B	54	VAL	2.7
1	A	428	PHE	2.7
2	B	19	ASP	2.7
2	B	102	GLU	2.7
2	B	77	GLN	2.6
1	A	92	GLU	2.6
1	A	423	LEU	2.5
2	B	18	GLU	2.5
2	B	51	LYS	2.5
2	B	91	VAL	2.4
2	B	11	ARG	2.4
2	B	75	ALA	2.4
1	A	351	MET	2.3
2	B	79	PHE	2.3
2	B	27	HIS	2.3
2	B	113	TYR	2.2
2	B	100	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	46	VAL	2.2
2	B	30	LYS	2.1
2	B	62	GLU	2.1
2	B	107	GLY	2.1
2	B	108	PHE	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.