Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 10:43 pm GMT

PDB ID	:	6GYZ
Title	:	Crystal structure of GlmM from Staphylococcus aureus
Authors	:	Tosi, T.; Freemont, P.S.; Grundling, A.
Deposited on	:	2018-07-02
Resolution	:	3.00 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:

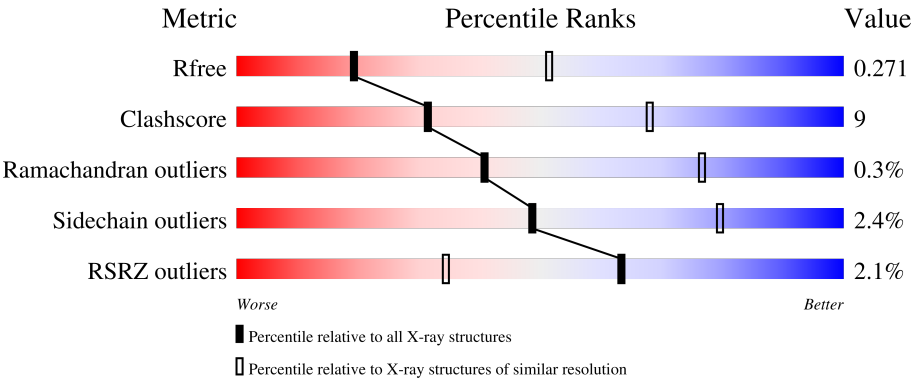
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	455	% 78% 18%
1	B	455	3% 82% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6831 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 Phosphoglucosamine mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	303	0	0
			3420	2130	577	694	19			
1	B	446	Total	C	N	O	S	464	0	0
			3411	2124	575	693	19			

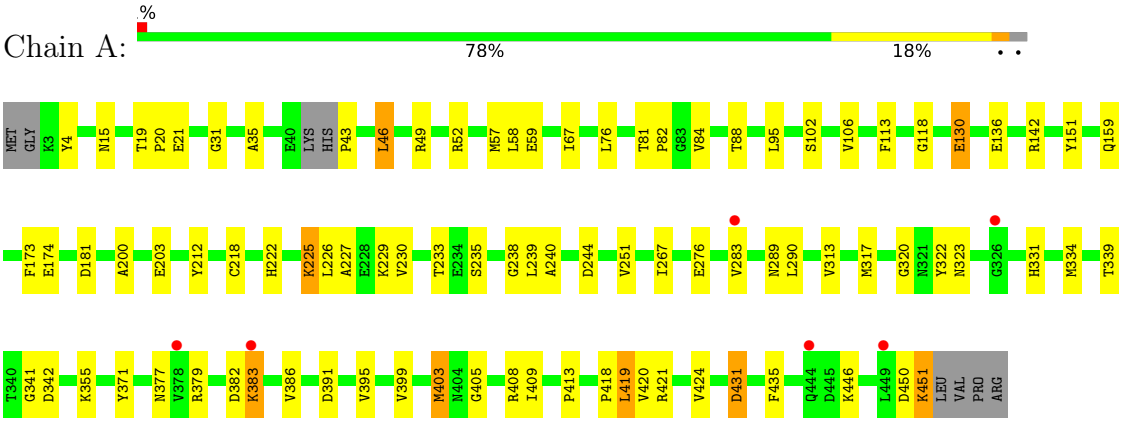
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	LEU	-	expression tag	UNP A0A0D6H967
A	453	VAL	-	expression tag	UNP A0A0D6H967
A	454	PRO	-	expression tag	UNP A0A0D6H967
A	455	ARG	-	expression tag	UNP A0A0D6H967
B	452	LEU	-	expression tag	UNP A0A0D6H967
B	453	VAL	-	expression tag	UNP A0A0D6H967
B	454	PRO	-	expression tag	UNP A0A0D6H967
B	455	ARG	-	expression tag	UNP A0A0D6H967

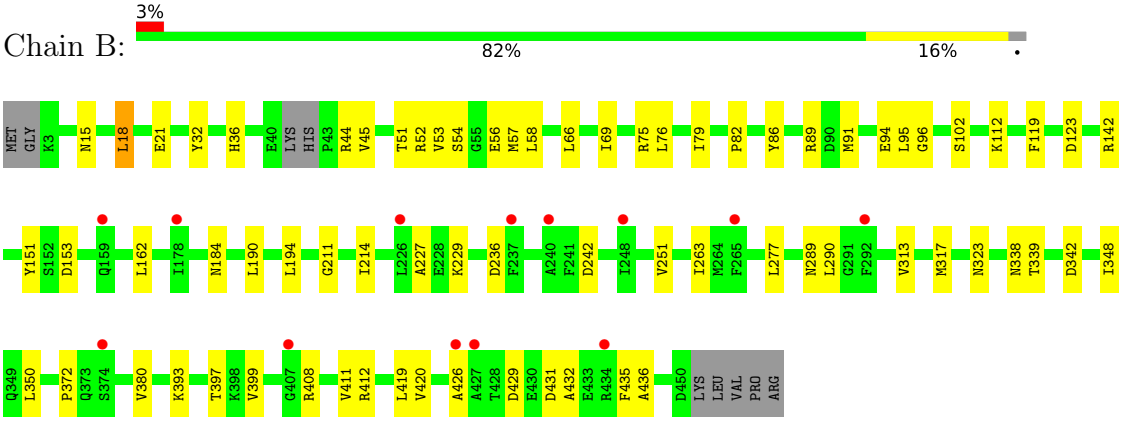
3 Residue-property plots (i)

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: Phosphoglucosamine mutase



• Molecule 1: Phosphoglucosamine mutase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.65Å 93.88Å 156.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.48 – 3.00 80.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (80.48-3.00) 99.7 (80.48-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.222 , 0.273 0.222 , 0.271	Depositor DCC
R_{free} test set	1341 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	97.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 112.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6831	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0.28	0/3467	0.52	1/4674 (0.0%)
1	B	0.28	0/3458	0.50	1/4663 (0.0%)
All	All	0.28	0/6925	0.51	2/9337 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	18	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	403	MET	N-CA-C	-5.03	97.41	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	3420	0	3356	63	0
1	B	3411	0	3345	49	0
All	All	6831	0	6701	105	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 9.

All (105) 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:181:ASP:OD2	1:A:225:LYS:NZ	1.94	1.00
1:A:46:LEU:HB2	1:A:76:LEU:HD21	1.50	0.93
1:A:218:CYS:HA	1:A:225:LYS:HE2	1.57	0.86
1:A:386:VAL:HG21	1:A:420:VAL:HG11	1.59	0.84
1:A:225:LYS:HD2	1:A:226:LEU:N	1.97	0.78
1:A:225:LYS:HD2	1:A:226:LEU:H	1.51	0.73
1:A:174:GLU:O	1:A:355:LYS:NZ	2.23	0.70
1:A:377:ASN:OD1	1:A:421:ARG:NE	2.25	0.69
1:B:399:VAL:HG22	1:B:435:PHE:HD1	1.56	0.68
1:A:399:VAL:O	1:A:403:MET:HG2	1.94	0.67
1:A:222:HIS:O	1:A:225:LYS:HE3	1.95	0.66
1:B:432:ALA:O	1:B:436:ALA:N	2.26	0.65
1:B:36:HIS:HE1	1:B:69:ILE:HG22	1.61	0.65
1:A:218:CYS:HA	1:A:225:LYS:CE	2.26	0.64
1:B:86:TYR:HA	1:B:89:ARG:HH21	1.64	0.62
1:B:89:ARG:NH1	1:B:339:THR:HG23	2.13	0.62
1:A:320:GLY:HA3	1:A:322:TYR:HE1	1.64	0.62
1:B:313:VAL:O	1:B:317:MET:HG3	2.00	0.62
1:A:49:ARG:NH1	1:A:59:GLU:OE1	2.32	0.62
1:A:379:ARG:HA	1:A:419:LEU:HB3	1.82	0.61
1:B:45:VAL:HG21	1:B:66:LEU:HD13	1.82	0.61
1:B:52:ARG:NH2	1:B:102:SER:O	2.33	0.60
1:B:194:LEU:HD21	1:B:348:ILE:HD11	1.83	0.60
1:A:95:LEU:HD11	1:A:113:PHE:HD2	1.64	0.59
1:B:277:LEU:HA	1:B:323:ASN:HD21	1.66	0.59
1:A:379:ARG:HB3	1:A:450:ASP:OD2	2.02	0.59
1:A:290:LEU:HB3	1:A:371:TYR:HD1	1.69	0.58
1:B:36:HIS:CE1	1:B:69:ILE:HG22	2.39	0.58
1:A:52:ARG:NH2	1:A:102:SER:O	2.37	0.56
1:B:380:VAL:HG11	1:B:420:VAL:HG23	1.89	0.55
1:B:32:TYR:HA	1:B:36:HIS:ND1	2.21	0.55
1:A:320:GLY:HA3	1:A:322:TYR:CE1	2.42	0.54
1:A:451:LYS:HE3	1:A:451:LYS:O	2.08	0.54
1:B:44:ARG:H	1:B:94:GLU:HG2	1.73	0.54
1:A:142:ARG:NH2	1:B:21:GLU:OE1	2.29	0.53
1:B:89:ARG:HH11	1:B:339:THR:HG23	1.73	0.52
1:A:118:GLY:O	1:A:339:THR:OG1	2.25	0.52
1:B:75:ARG:NH2	1:B:153:ASP:OD2	2.43	0.52
1:A:20:PRO:HG3	1:A:57:MET:HE1	1.92	0.52
1:A:106:VAL:HG21	1:A:212:TYR:HA	1.92	0.51
1:B:52:ARG:HG2	1:B:214:ILE:HG21	1.92	0.51
1:B:82:PRO:HG2	1:B:342:ASP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:HA	1:B:89:ARG:HE	1.76	0.50
1:A:46:LEU:HB2	1:A:76:LEU:CD2	2.34	0.50
1:B:53:VAL:O	1:B:54:SER:OG	2.18	0.50
1:B:184:ASN:HB2	1:B:214:ILE:HA	1.93	0.50
1:B:399:VAL:HG22	1:B:435:PHE:CD1	2.44	0.50
1:A:383:LYS:HB2	1:A:413:PRO:HB3	1.94	0.50
1:A:313:VAL:O	1:A:317:MET:HG3	2.12	0.49
1:A:67:ILE:HG21	1:B:57:MET:HB2	1.95	0.49
1:B:36:HIS:HE1	1:B:69:ILE:CG2	2.25	0.49
1:B:44:ARG:NH2	1:B:91:MET:O	2.45	0.49
1:A:290:LEU:HB3	1:A:371:TYR:CD1	2.47	0.49
1:A:31:GLY:O	1:A:35:ALA:N	2.46	0.48
1:A:431:ASP:HB3	1:A:435:PHE:HE2	1.78	0.48
1:A:46:LEU:HD21	1:A:88:THR:HA	1.95	0.48
1:A:4:TYR:N	1:A:130:GLU:OE1	2.45	0.48
1:A:409:ILE:HG22	1:A:424:VAL:HG13	1.95	0.48
1:B:289:ASN:OD1	1:B:290:LEU:N	2.46	0.48
1:A:289:ASN:OD1	1:A:290:LEU:N	2.47	0.47
1:B:123:ASP:N	1:B:123:ASP:OD1	2.46	0.47
1:B:95:LEU:HG	1:B:96:GLY:N	2.29	0.47
1:A:81:THR:OG1	1:A:244:ASP:HB2	2.15	0.47
1:A:57:MET:HG3	1:A:58:LEU:N	2.30	0.46
1:A:290:LEU:HD13	1:A:408:ARG:HD3	1.97	0.46
1:A:233:THR:OG1	1:A:235:SER:OG	2.13	0.46
1:A:15:ASN:O	1:B:142:ARG:HD2	2.15	0.46
1:A:151:TYR:CE2	1:B:56:GLU:HB3	2.51	0.46
1:A:276:GLU:O	1:A:323:ASN:ND2	2.49	0.46
1:A:379:ARG:HB3	1:A:450:ASP:HB2	1.98	0.46
1:A:151:TYR:HE2	1:B:56:GLU:HB3	1.81	0.45
1:A:21:GLU:OE2	1:B:142:ARG:NH2	2.41	0.45
1:B:162:LEU:HD21	1:B:190:LEU:HB3	1.97	0.45
1:A:35:ALA:HB1	1:A:43:PRO:HG2	1.98	0.45
1:B:119:PHE:CE1	1:B:339:THR:HB	2.52	0.45
1:B:393:LYS:O	1:B:397:THR:OG1	2.25	0.45
1:B:411:VAL:C	1:B:412:ARG:HE	2.16	0.45
1:A:173:PHE:HB2	1:A:200:ALA:HB2	1.99	0.44
1:A:227:ALA:HA	1:A:251:VAL:HG11	2.00	0.44
1:B:89:ARG:NH2	1:B:338:ASN:OD1	2.50	0.44
1:A:226:LEU:O	1:A:230:VAL:HG23	2.17	0.44
1:A:267:ILE:HD13	1:A:334:MET:HE1	1.99	0.44
1:B:242:ASP:OD1	1:B:242:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:HG21	1:A:317:MET:HG2	2.00	0.43
1:B:76:LEU:HB3	1:B:79:ILE:CD1	2.48	0.43
1:B:51:THR:O	1:B:211:GLY:HA2	2.19	0.43
1:A:379:ARG:HG3	1:A:419:LEU:HD23	1.99	0.43
1:A:82:PRO:HG2	1:A:342:ASP:HA	2.00	0.43
1:A:203:GLU:HB3	1:A:229:LYS:HE2	2.00	0.42
1:B:86:TYR:CA	1:B:89:ARG:HH21	2.32	0.42
1:A:142:ARG:HD2	1:B:15:ASN:O	2.19	0.42
1:A:84:VAL:O	1:A:88:THR:OG1	2.34	0.42
1:A:290:LEU:HD22	1:A:408:ARG:HB3	2.01	0.42
1:A:331:HIS:CE1	1:A:341:GLY:HA3	2.55	0.42
1:A:391:ASP:O	1:A:395:VAL:HG12	2.19	0.42
1:B:227:ALA:HA	1:B:251:VAL:HG11	2.01	0.41
1:B:36:HIS:CE1	1:B:69:ILE:CG2	3.02	0.41
1:A:19:THR:HB	1:A:21:GLU:OE1	2.21	0.41
1:B:18:LEU:HD11	1:B:58:LEU:HD13	2.03	0.41
1:B:263:ILE:HG23	1:B:350:LEU:HD13	2.03	0.41
1:B:372:PRO:HD2	1:B:426:ALA:O	2.20	0.41
1:A:226:LEU:HD22	1:A:240:ALA:HB2	2.02	0.40
1:A:238:GLY:O	1:A:239:LEU:HD23	2.21	0.40
1:B:323:ASN:OD1	1:B:323:ASN:N	2.45	0.40
1:A:424:VAL:HG11	1:A:435:PHE:HB2	2.03	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	445/455 (98%)	430 (97%)	12 (3%)	3 (1%)	22 60
1	B	444/455 (98%)	434 (98%)	10 (2%)	0	100 100
All	All	889/910 (98%)	864 (97%)	22 (2%)	3 (0%)	41 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	ASP
1	A	405	GLY
1	A	418	PRO

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	371/378 (98%)	361 (97%)	10 (3%)	44	77
1	B	370/378 (98%)	362 (98%)	8 (2%)	52	81
All	All	741/756 (98%)	723 (98%)	18 (2%)	49	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	130	GLU
1	A	136	GLU
1	A	159	GLN
1	A	225	LYS
1	A	383	LYS
1	A	419	LEU
1	A	431	ASP
1	A	446	LYS
1	A	451	LYS
1	B	112	LYS
1	B	151	TYR
1	B	229	LYS
1	B	236	ASP
1	B	408	ARG
1	B	419	LEU
1	B	429	ASP
1	B	431	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	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 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	447/455 (98%)	0.14	6 (1%) 77 51	65, 99, 151, 203	66 (14%)
1	B	446/455 (98%)	0.10	13 (2%) 51 23	63, 114, 160, 189	103 (23%)
All	All	893/910 (98%)	0.12	19 (2%) 63 34	63, 105, 159, 203	169 (18%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	3.3
1	B	426	ALA	3.2
1	A	449	LEU	3.1
1	B	237	PHE	3.0
1	B	178	ILE	3.0
1	B	427	ALA	2.9
1	B	240	ALA	2.8
1	B	407	GLY	2.6
1	B	159	GLN	2.6
1	B	248	ILE	2.5
1	B	226	LEU	2.4
1	B	265	PHE	2.4
1	B	292	PHE	2.4
1	A	444	GLN	2.3
1	A	383	LYS	2.2
1	B	374	SER	2.1
1	B	434	ARG	2.1
1	A	378	VAL	2.1
1	A	283	VAL	2.0

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

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.