



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 12:55 PM GMT

PDB ID : 6TUD
Title : Crystal structure of Y. pestis penicillin-binding protein 3
Authors : Pankov, G.; Hunter, W.N.; Dawson, A.
Deposited on : 2020-01-06
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 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	:	2.16
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)	:	2.16

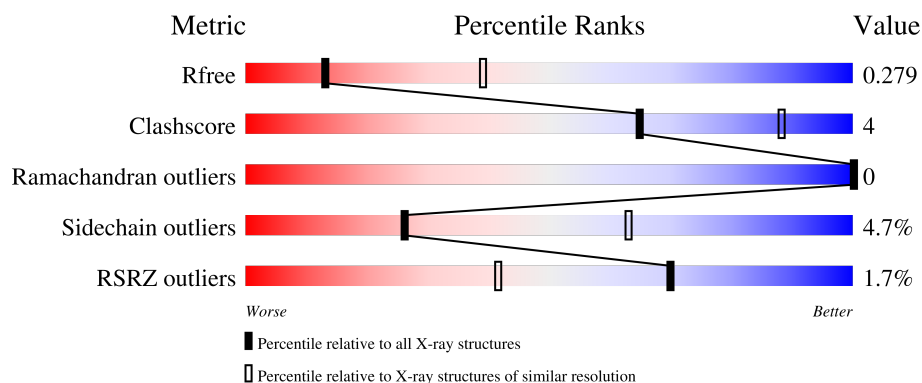
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

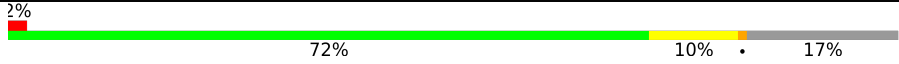

The reported resolution of this entry is 3.00 Å.

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 $\leq 5\%$. 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	AAA	549	
1	BBB	549	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7046 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 Peptidoglycan D,D-transpeptidase FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	456	Total	C	N	O	S	0	0	0
			3448	2188	612	634	14			
1	BBB	472	Total	C	N	O	S	0	0	0
			3571	2265	634	658	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	39	HIS	-	expression tag	UNP Q0WJB8
AAA	40	HIS	-	expression tag	UNP Q0WJB8
AAA	41	HIS	-	expression tag	UNP Q0WJB8
AAA	42	HIS	-	expression tag	UNP Q0WJB8
AAA	43	HIS	-	expression tag	UNP Q0WJB8
AAA	44	HIS	-	expression tag	UNP Q0WJB8
AAA	45	SER	-	expression tag	UNP Q0WJB8
AAA	46	SER	-	expression tag	UNP Q0WJB8
AAA	47	GLY	-	expression tag	UNP Q0WJB8
AAA	48	GLU	-	expression tag	UNP Q0WJB8
AAA	49	ASN	-	expression tag	UNP Q0WJB8
AAA	50	LEU	-	expression tag	UNP Q0WJB8
AAA	51	TYR	-	expression tag	UNP Q0WJB8
AAA	52	PHE	-	expression tag	UNP Q0WJB8
AAA	53	GLN	-	expression tag	UNP Q0WJB8
AAA	54	GLY	-	expression tag	UNP Q0WJB8
AAA	55	HIS	-	expression tag	UNP Q0WJB8
AAA	56	MET	-	expression tag	UNP Q0WJB8
BBB	39	HIS	-	expression tag	UNP Q0WJB8
BBB	40	HIS	-	expression tag	UNP Q0WJB8
BBB	41	HIS	-	expression tag	UNP Q0WJB8
BBB	42	HIS	-	expression tag	UNP Q0WJB8
BBB	43	HIS	-	expression tag	UNP Q0WJB8
BBB	44	HIS	-	expression tag	UNP Q0WJB8
BBB	45	SER	-	expression tag	UNP Q0WJB8

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	46	SER	-	expression tag	UNP Q0WJB8
BBB	47	GLY	-	expression tag	UNP Q0WJB8
BBB	48	GLU	-	expression tag	UNP Q0WJB8
BBB	49	ASN	-	expression tag	UNP Q0WJB8
BBB	50	LEU	-	expression tag	UNP Q0WJB8
BBB	51	TYR	-	expression tag	UNP Q0WJB8
BBB	52	PHE	-	expression tag	UNP Q0WJB8
BBB	53	GLN	-	expression tag	UNP Q0WJB8
BBB	54	GLY	-	expression tag	UNP Q0WJB8
BBB	55	HIS	-	expression tag	UNP Q0WJB8
BBB	56	MET	-	expression tag	UNP Q0WJB8

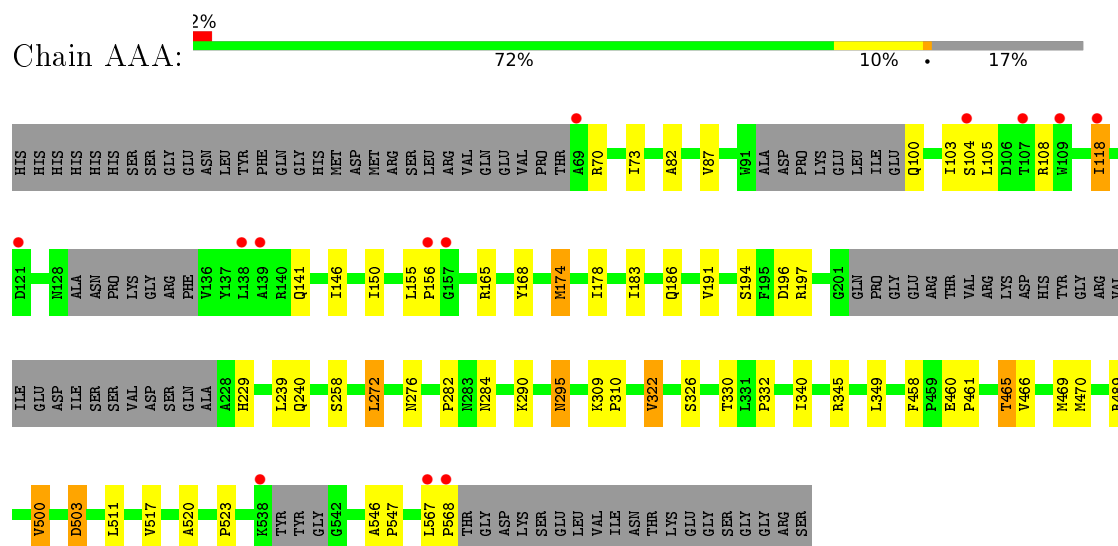
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	18	Total O 18 18	0	0
2	BBB	9	Total O 9 9	0	0

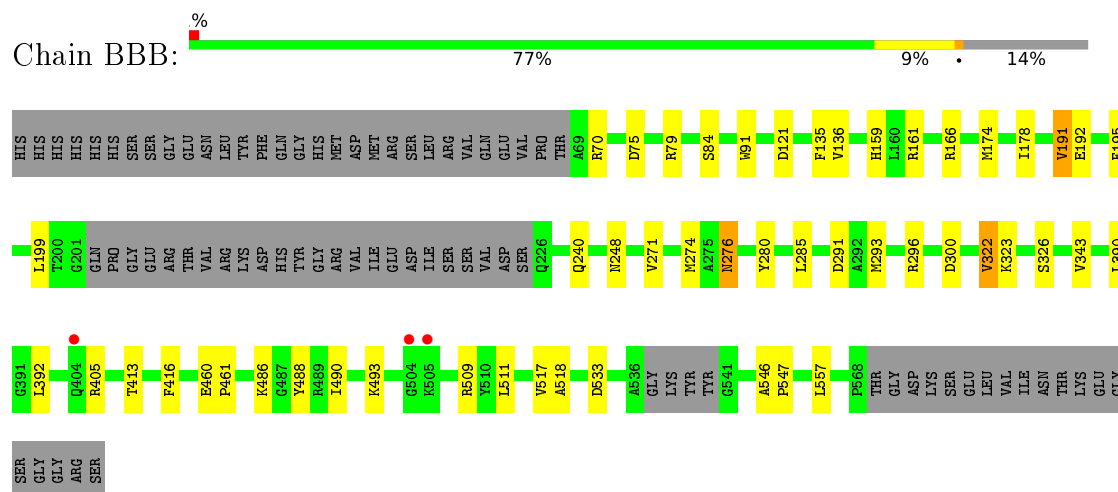
3 Residue-property plots [i](#)

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: Peptidoglycan D,D-transpeptidase FtsI



- Molecule 1: Peptidoglycan D,D-transpeptidase FtsI



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.80 Å 100.80 Å 314.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 3.00 29.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.64-3.00) 100.0 (29.62-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.00 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.244 , 0.276 0.248 , 0.279	Depositor DCC
R_{free} test set	1713 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.9	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	0.92	EDS
Total number of atoms	7046	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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 [i](#)

5.1 Standard geometry [i](#)

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	AAA	0.66	0/3513	0.72	0/4768
1	BBB	0.66	0/3641	0.73	0/4945
All	All	0.66	0/7154	0.73	0/9713

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	AAA	3448	0	3522	33	0
1	BBB	3571	0	3643	25	0
2	AAA	18	0	0	0	0
2	BBB	9	0	0	0	0
All	All	7046	0	7165	58	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 4.

All (58) 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:BBB:178:ILE:HA	1:BBB:191:VAL:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:285:LEU:H	1:BBB:285:LEU:HD23	1.59	0.67
1:BBB:178:ILE:HA	1:BBB:191:VAL:HG22	1.79	0.64
1:AAA:155:LEU:HB3	1:AAA:156:PRO:HD2	1.86	0.56
1:AAA:87:VAL:CG1	1:AAA:141:GLN:HA	2.37	0.55
1:AAA:141:GLN:HG3	1:AAA:183:ILE:CD1	2.36	0.55
1:AAA:332:PRO:HG3	1:AAA:345:ARG:HD2	1.89	0.54
1:BBB:546:ALA:HB3	1:BBB:547:PRO:HD3	1.90	0.53
1:AAA:191:VAL:HA	1:AAA:194:SER:HB3	1.91	0.53
1:AAA:546:ALA:HB3	1:AAA:547:PRO:HD3	1.92	0.52
1:BBB:509:ARG:NH1	1:BBB:533:ASP:OD2	2.43	0.52
1:AAA:108:ARG:HD2	1:AAA:155:LEU:CD2	2.40	0.51
1:AAA:517:VAL:HG13	1:AAA:523:PRO:HB3	1.92	0.51
1:AAA:503:ASP:N	1:AAA:503:ASP:OD1	2.43	0.51
1:BBB:70:ARG:NH2	1:BBB:192:GLU:HG3	2.26	0.51
1:BBB:174:MET:HG2	1:BBB:240:GLN:HG2	1.94	0.50
1:AAA:108:ARG:HD2	1:AAA:155:LEU:HD21	1.94	0.49
1:AAA:322:VAL:HG22	1:AAA:326:SER:HB2	1.95	0.49
1:AAA:103:ILE:HD12	1:AAA:103:ILE:N	2.28	0.48
1:BBB:413:THR:HA	1:BBB:416:PHE:CD2	2.49	0.48
1:AAA:460:GLU:N	1:AAA:461:PRO:HD2	2.29	0.48
1:AAA:87:VAL:HG11	1:AAA:141:GLN:HA	1.95	0.48
1:AAA:141:GLN:HG3	1:AAA:183:ILE:HD11	1.95	0.47
1:BBB:75:ASP:OD2	1:BBB:79:ARG:NH1	2.47	0.47
1:AAA:489:ARG:HB3	1:AAA:520:ALA:HB3	1.95	0.47
1:AAA:239:LEU:CD1	1:AAA:272:LEU:HD12	2.44	0.47
1:BBB:271:VAL:HG11	1:BBB:274:MET:HE3	1.97	0.47
1:BBB:195:PHE:O	1:BBB:199:LEU:HG	2.15	0.47
1:BBB:322:VAL:HG22	1:BBB:326:SER:HB2	1.97	0.47
1:AAA:70:ARG:NH2	1:AAA:196:ASP:OD1	2.47	0.47
1:AAA:500:VAL:HG11	1:AAA:511:LEU:HD13	1.97	0.46
1:BBB:276:ASN:HD22	1:BBB:276:ASN:N	2.13	0.46
1:AAA:465:THR:O	1:AAA:469:MET:HG3	2.16	0.46
1:BBB:91:TRP:CE2	1:BBB:159:HIS:HB2	2.51	0.46
1:AAA:103:ILE:H	1:AAA:103:ILE:HD12	1.81	0.45
1:AAA:73:ILE:HB	1:AAA:82:ALA:HB3	1.99	0.45
1:AAA:146:ILE:O	1:AAA:150:ILE:HG12	2.16	0.45
1:BBB:70:ARG:HH21	1:BBB:192:GLU:HG3	1.81	0.45
1:AAA:567:LEU:O	1:AAA:568:PRO:C	2.54	0.44
1:AAA:168:TYR:CD2	1:AAA:282:PRO:HB2	2.53	0.44
1:BBB:285:LEU:H	1:BBB:285:LEU:CD2	2.27	0.44
1:AAA:276:ASN:OD1	1:AAA:295:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:296:ARG:NH1	1:BBB:300:ASP:OD2	2.49	0.43
1:BBB:490:ILE:HG22	1:BBB:518:ALA:HB2	2.00	0.43
1:AAA:118:ILE:HG23	1:AAA:118:ILE:O	2.19	0.43
1:AAA:309:LYS:N	1:AAA:310:PRO:CD	2.81	0.43
1:AAA:178:ILE:HA	1:AAA:191:VAL:HG22	2.00	0.43
1:AAA:330:THR:HG21	1:AAA:349:LEU:HB2	2.02	0.42
1:BBB:276:ASN:N	1:BBB:276:ASN:ND2	2.67	0.42
1:BBB:390:LEU:HB3	1:BBB:392:LEU:HD13	2.02	0.42
1:BBB:460:GLU:N	1:BBB:461:PRO:HD2	2.35	0.42
1:BBB:70:ARG:HB3	1:BBB:84:SER:OG	2.20	0.41
1:BBB:280:TYR:CE1	1:BBB:293:MET:HA	2.56	0.41
1:AAA:174:MET:SD	1:AAA:240:GLN:HG2	2.61	0.41
1:AAA:466:VAL:O	1:AAA:470:MET:HG3	2.21	0.40
1:AAA:340:ILE:N	1:AAA:340:ILE:HD12	2.37	0.40
1:BBB:91:TRP:CG	1:BBB:135:PHE:HE1	2.39	0.40
1:BBB:488:TYR:CD2	1:BBB:557:LEU:HD13	2.57	0.40

There are no symmetry-related clashes.

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	AAA	446/549 (81%)	433 (97%)	13 (3%)	0	100	100
1	BBB	466/549 (85%)	451 (97%)	15 (3%)	0	100	100
All	All	912/1098 (83%)	884 (97%)	28 (3%)	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	AAA	366/446 (82%)	347 (95%)	19 (5%)	23	59
1	BBB	378/446 (85%)	362 (96%)	16 (4%)	30	66
All	All	744/892 (83%)	709 (95%)	35 (5%)	26	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	100	GLN
1	AAA	104	SER
1	AAA	105	LEU
1	AAA	118	ILE
1	AAA	165	ARG
1	AAA	174	MET
1	AAA	186	GLN
1	AAA	197	ARG
1	AAA	229	HIS
1	AAA	258	SER
1	AAA	272	LEU
1	AAA	284	ASN
1	AAA	290	LYS
1	AAA	295	ASN
1	AAA	322	VAL
1	AAA	458	PHE
1	AAA	465	THR
1	AAA	500	VAL
1	AAA	503	ASP
1	BBB	121	ASP
1	BBB	136	VAL
1	BBB	161	ARG
1	BBB	166	ARG
1	BBB	191	VAL
1	BBB	248	ASN
1	BBB	276	ASN
1	BBB	291	ASP

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Mol	Chain	Res	Type
1	BBB	322	VAL
1	BBB	323	LYS
1	BBB	343	VAL
1	BBB	405	ARG
1	BBB	486	LYS
1	BBB	493	LYS
1	BBB	511	LEU
1	BBB	517	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	456/549 (83%)	-0.14	13 (2%)	51	23	58, 79, 160, 195	0
1	BBB	472/549 (85%)	-0.21	3 (0%)	89	72	65, 87, 113, 136	0
All	All	928/1098 (84%)	-0.18	16 (1%)	70	41	58, 82, 136, 195	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	568	PRO	3.6
1	AAA	156	PRO	3.6
1	AAA	118	ILE	3.1
1	AAA	109	TRP	2.7
1	BBB	404	GLN	2.6
1	AAA	567	LEU	2.5
1	AAA	104	SER	2.5
1	AAA	157	GLY	2.5
1	BBB	505	LYS	2.4
1	AAA	139	ALA	2.4
1	AAA	538	LYS	2.2
1	AAA	138	LEU	2.2
1	AAA	107	THR	2.2
1	BBB	504	GLY	2.2
1	AAA	121	ASP	2.1
1	AAA	69	ALA	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.