



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:46 PM UTC

PDB ID : 6HR4 / pdb_00006hr4
Title : Apo form of penicillin-binding protein 3 from *P. aeruginosa*
Authors : Bellini, D.; Dowson, C.G.
Deposited on : 2018-09-26
Resolution : 1.19 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

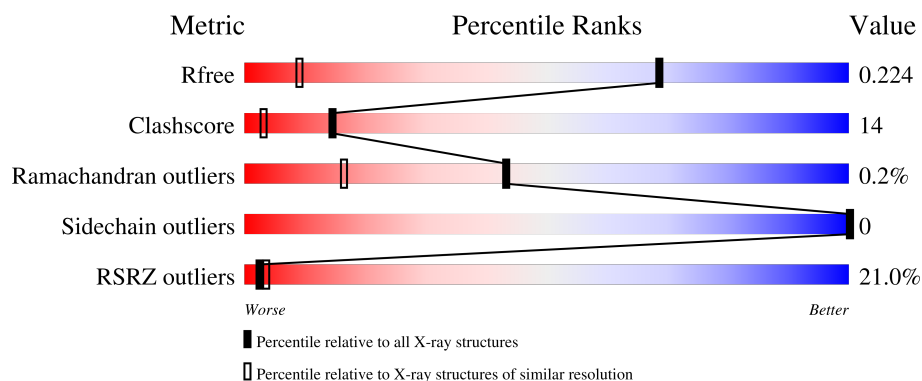
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	A	535	20% 77% 16% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4492 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	A	504	Total	C	N	O	S	0	7	0
			3864	2442	694	716	12			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP G3XD46
A	46	TYR	-	expression tag	UNP G3XD46
A	47	GLN	-	expression tag	UNP G3XD46
A	48	ASP	-	expression tag	UNP G3XD46
A	49	PRO	-	expression tag	UNP G3XD46

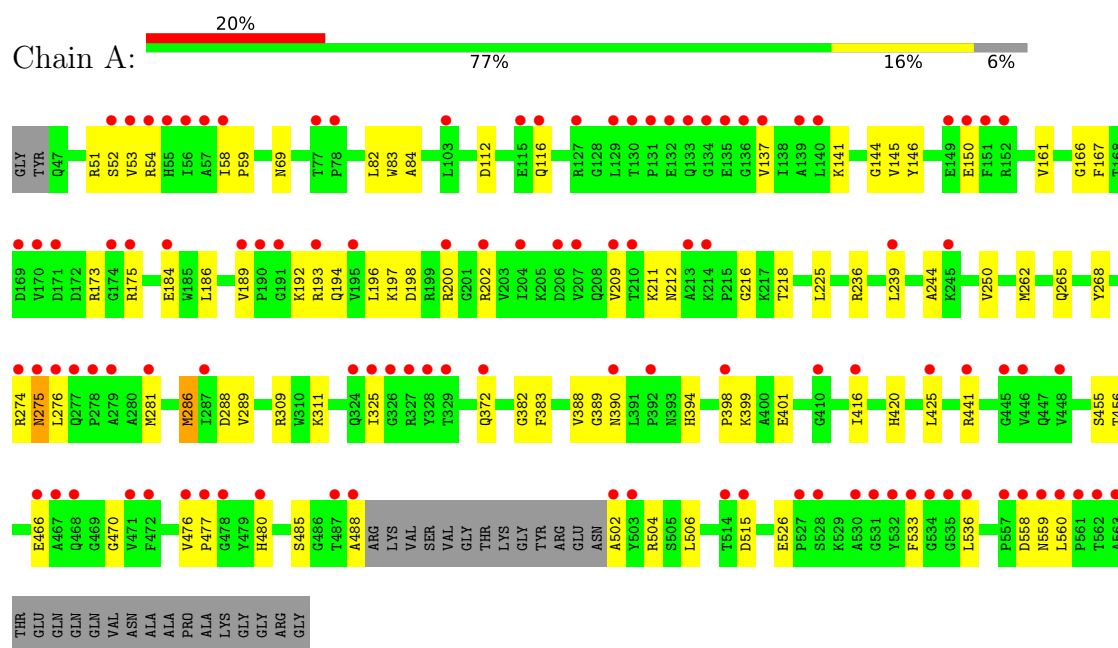
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	628	Total	O	0	0
			628	628		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.55Å 82.14Å 88.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.08 – 1.19 60.08 – 1.19	Depositor EDS
% Data completeness (in resolution range)	77.2 (60.08-1.19) 77.2 (60.08-1.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.226 0.207 , 0.224	Depositor DCC
R_{free} test set	5816 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4492	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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	A	0.74	2/3961 (0.1%)	0.87	3/5377 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	HIS	CG-ND1	-6.27	1.31	1.38
1	A	420	HIS	CD2-NE2	-5.44	1.31	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	VAL	CA-C-N	6.58	128.06	119.84
1	A	476	VAL	C-N-CA	6.58	128.06	119.84
1	A	286	MET	CG-SD-CE	-5.96	87.79	100.90

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	A	3864	0	3934	109	2
2	A	628	0	0	78	6
All	All	4492	0	3934	109	8

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 14.

All (109) 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:325:ILE:HB	2:A:917:HOH:O	1.23	1.36
1:A:200:ARG:HD3	2:A:601:HOH:O	1.39	1.18
1:A:58:ILE:HD12	2:A:610:HOH:O	1.41	1.15
1:A:390:ASN:HB3	2:A:692:HOH:O	1.46	1.14
1:A:51:ARG:HD3	2:A:612:HOH:O	1.51	1.09
1:A:198:ASP:HA	2:A:612:HOH:O	1.55	1.06
1:A:189:VAL:HB	2:A:632:HOH:O	1.55	1.05
1:A:202:ARG:NH1	2:A:601:HOH:O	1.88	1.04
1:A:145:VAL:HG13	2:A:756:HOH:O	1.57	1.03
1:A:202:ARG:HD3	2:A:1105:HOH:O	1.63	0.95
1:A:388:VAL:HG23	2:A:629:HOH:O	1.65	0.95
1:A:276:LEU:HD21	1:A:281:MET:HE3	1.47	0.94
1:A:161:VAL:HB	2:A:1080:HOH:O	1.66	0.94
1:A:382:GLY:HA2	2:A:626:HOH:O	1.70	0.92
1:A:372:GLN:HG3	2:A:861:HOH:O	1.72	0.90
1:A:146:TYR:HB3	2:A:636:HOH:O	1.75	0.87
1:A:288:ASP:HB3	2:A:652:HOH:O	1.73	0.87
1:A:202:ARG:CZ	2:A:601:HOH:O	2.18	0.87
1:A:398:PRO:HB2	1:A:401:GLU:OE1	1.75	0.86
1:A:212:ASN:HA	2:A:1034:HOH:O	1.76	0.85
1:A:309:ARG:NH1	2:A:604:HOH:O	1.94	0.85
1:A:515:ASP:CG	2:A:619:HOH:O	2.19	0.85
1:A:560:LEU:HG	2:A:770:HOH:O	1.76	0.84
1:A:166:GLY:HA2	2:A:607:HOH:O	1.78	0.84
1:A:488:ALA:HB3	1:A:504:ARG:HB2	1.58	0.83
1:A:425:LEU:HD13	2:A:1081:HOH:O	1.78	0.83
1:A:559:ASN:ND2	2:A:603:HOH:O	1.92	0.80
1:A:276:LEU:HD21	1:A:281:MET:CE	2.12	0.80
1:A:477:PRO:O	2:A:605:HOH:O	2.00	0.79
1:A:54:ARG:HG3	1:A:197:LYS:HD2	1.65	0.78
1:A:82:LEU:HB3	2:A:756:HOH:O	1.81	0.78
1:A:54:ARG:HD3	2:A:606:HOH:O	1.83	0.77
1:A:53:VAL:O	2:A:606:HOH:O	2.04	0.74
1:A:200:ARG:CD	2:A:601:HOH:O	2.14	0.74
1:A:192:LYS:N	2:A:610:HOH:O	2.20	0.74
1:A:289:VAL:HG21	2:A:740:HOH:O	1.87	0.73
1:A:389:GLY:HA2	2:A:740:HOH:O	1.90	0.72
1:A:173:ARG:HB3	2:A:669:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD12	2:A:609:HOH:O	1.91	0.70
1:A:54:ARG:HA	2:A:606:HOH:O	1.95	0.67
1:A:69:ASN:ND2	2:A:602:HOH:O	1.89	0.67
1:A:196:LEU:CD1	2:A:609:HOH:O	2.43	0.65
1:A:236:ARG:NH2	2:A:613:HOH:O	2.28	0.65
1:A:325:ILE:HG21	1:A:399:LYS:HB3	1.79	0.65
1:A:209:VAL:HG21	2:A:1034:HOH:O	1.96	0.64
1:A:274:ARG:O	1:A:275:ASN:HB2	1.97	0.64
1:A:488:ALA:HB2	1:A:506:LEU:HD11	1.79	0.62
1:A:197:LYS:HG2	2:A:618:HOH:O	2.00	0.61
1:A:53:VAL:C	2:A:606:HOH:O	2.44	0.60
1:A:274:ARG:O	1:A:275:ASN:CB	2.49	0.60
1:A:218[B]:THR:CG2	2:A:987:HOH:O	2.48	0.60
1:A:82:LEU:CD1	1:A:137:VAL:HG11	2.32	0.59
1:A:145:VAL:CG1	2:A:756:HOH:O	2.32	0.59
1:A:504:ARG:NH2	2:A:622:HOH:O	2.35	0.59
1:A:239:LEU:HG	1:A:244:ALA:HB3	1.85	0.59
1:A:202:ARG:NH1	2:A:611:HOH:O	2.22	0.58
1:A:167:PHE:CE1	1:A:175:ARG:HD3	2.38	0.58
1:A:325:ILE:HD11	2:A:886:HOH:O	2.04	0.57
1:A:236:ARG:NE	2:A:613:HOH:O	2.36	0.57
1:A:211:LYS:HE3	2:A:685:HOH:O	2.05	0.56
1:A:59:PRO:HG2	1:A:150:GLU:HG2	1.88	0.55
1:A:236:ARG:CZ	2:A:613:HOH:O	2.56	0.54
1:A:455[B]:SER:OG	2:A:608:HOH:O	2.18	0.54
1:A:202:ARG:NH2	2:A:625:HOH:O	2.41	0.53
1:A:225:LEU:CD1	2:A:1080:HOH:O	2.57	0.52
1:A:268:TYR:OH	2:A:607:HOH:O	2.16	0.52
1:A:250:VAL:HG21	1:A:416:ILE:HD13	1.92	0.51
1:A:383:PHE:HE1	2:A:991:HOH:O	1.94	0.51
1:A:276:LEU:CD2	1:A:281:MET:HE3	2.30	0.51
1:A:441:ARG:NH1	2:A:617:HOH:O	2.33	0.50
1:A:456:THR:HG21	2:A:1112:HOH:O	2.12	0.50
1:A:311:LYS:HE2	2:A:933:HOH:O	2.11	0.49
1:A:218[B]:THR:HG22	2:A:1088:HOH:O	2.11	0.49
1:A:58:ILE:HD11	1:A:193:ARG:HB3	1.95	0.49
1:A:193:ARG:HA	1:A:209:VAL:HA	1.95	0.49
1:A:558:ASP:CB	2:A:1094:HOH:O	2.60	0.48
1:A:52:SER:N	2:A:609:HOH:O	2.42	0.48
1:A:200:ARG:NE	2:A:601:HOH:O	2.39	0.47
1:A:325:ILE:HG21	1:A:399:LYS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:O	2:A:609:HOH:O	2.20	0.47
1:A:141:LYS:N	2:A:614:HOH:O	2.47	0.46
1:A:558:ASP:HB3	2:A:1094:HOH:O	2.15	0.46
1:A:202:ARG:NH2	2:A:601:HOH:O	2.41	0.46
1:A:268:TYR:CB	1:A:276:LEU:HD13	2.46	0.46
1:A:262:MET:SD	1:A:286:MET:HE3	2.56	0.46
1:A:533:PHE:CD2	2:A:1130:HOH:O	2.56	0.45
1:A:197:LYS:CG	2:A:618:HOH:O	2.62	0.45
1:A:239:LEU:HD22	1:A:265:GLN:CB	2.47	0.44
1:A:202:ARG:HD2	2:A:611:HOH:O	2.17	0.44
1:A:83:TRP:NE1	2:A:636:HOH:O	2.51	0.43
1:A:502:ALA:N	2:A:638:HOH:O	2.51	0.43
1:A:144:GLY:N	2:A:628:HOH:O	2.51	0.43
1:A:202:ARG:CD	2:A:1105:HOH:O	2.41	0.43
1:A:466:GLU:OE2	1:A:480:HIS:ND1	2.52	0.43
1:A:218[B]:THR:HG22	2:A:987:HOH:O	2.15	0.43
1:A:325:ILE:HG23	1:A:399:LYS:HD3	1.99	0.43
1:A:84:ALA:HA	1:A:144:GLY:O	2.19	0.42
1:A:276:LEU:CD2	1:A:281:MET:CE	2.92	0.42
1:A:559:ASN:HB3	2:A:678:HOH:O	2.20	0.42
1:A:53:VAL:HG13	1:A:194:GLN:HB3	2.02	0.42
1:A:186:LEU:O	1:A:216:GLY:HA3	2.19	0.41
1:A:502:ALA:HA	1:A:526:GLU:HG2	2.01	0.41
1:A:394:HIS:HD2	2:A:1095:HOH:O	2.02	0.41
1:A:558:ASP:HB2	2:A:1094:HOH:O	2.19	0.41
1:A:470:GLY:HA3	2:A:778:HOH:O	2.21	0.41
1:A:485:SER:CB	1:A:536:LEU:HD22	2.50	0.41
1:A:325:ILE:CG2	1:A:399:LYS:HD3	2.52	0.40
1:A:112:ASP:O	1:A:116:GLN:HG2	2.20	0.40
1:A:175:ARG:NH1	2:A:642:HOH:O	2.53	0.40

All (8) 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)
2:A:857:HOH:O	2:A:1083:HOH:O[4_545]	1.62	0.58
2:A:852:HOH:O	2:A:1106:HOH:O[4_445]	1.65	0.55
1:A:184:GLU:OE2	1:A:533:PHE:CE1[4_545]	1.79	0.41
2:A:982:HOH:O	2:A:1118:HOH:O[2_554]	2.09	0.11
2:A:651:HOH:O	2:A:676:HOH:O[3_554]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1083:HOH:O	2:A:1210:HOH:O[4_445]	2.11	0.09
1:A:184:GLU:OE2	1:A:533:PHE:CZ[4_545]	2.14	0.06
2:A:630:HOH:O	2:A:1019:HOH:O[1_556]	2.18	0.02

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	507/535 (95%)	500 (99%)	6 (1%)	1 (0%)	43 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ASN

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	408/423 (96%)	408 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	194	GLN
1	A	212	ASN
1	A	275	ASN
1	A	420	HIS
1	A	462	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 oligosaccharides 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	504/535 (94%)	1.12	106 (21%) 2 3	4, 12, 25, 104	7 (1%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	LEU	10.5
1	A	563	ALA	9.6
1	A	488	ALA	8.1
1	A	562	THR	7.9
1	A	533	PHE	7.9
1	A	170	VAL	7.7
1	A	53	VAL	7.4
1	A	561	PRO	7.3
1	A	502	ALA	7.3
1	A	275	ASN	6.8
1	A	276	LEU	5.9
1	A	558	ASP	5.4
1	A	503	TYR	5.3
1	A	534	GLY	5.1
1	A	472	PHE	5.0
1	A	54	ARG	4.9
1	A	559	ASN	4.9
1	A	209	VAL	4.9
1	A	532	TYR	4.8
1	A	327	ARG	4.7
1	A	274	ARG	4.6
1	A	468	GLN	4.5
1	A	189	VAL	4.3
1	A	207	VAL	4.3
1	A	132	GLU	4.3
1	A	325	ILE	4.2
1	A	528	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	3.9
1	A	536	LEU	3.9
1	A	171	ASP	3.8
1	A	478	GLY	3.8
1	A	169	ASP	3.8
1	A	152	ARG	3.7
1	A	477	PRO	3.4
1	A	530	ALA	3.3
1	A	279	ALA	3.3
1	A	392	PRO	3.3
1	A	277	GLN	3.3
1	A	184	GLU	3.2
1	A	487	THR	3.2
1	A	535	GLY	3.2
1	A	278	PRO	3.2
1	A	214	LYS	3.2
1	A	135	GLU	3.0
1	A	149	GLU	3.0
1	A	55	HIS	3.0
1	A	328	TYR	3.0
1	A	58	ILE	3.0
1	A	527	PRO	2.9
1	A	287	ILE	2.9
1	A	245	LYS	2.9
1	A	531	GLY	2.9
1	A	56	ILE	2.8
1	A	103	LEU	2.8
1	A	448	VAL	2.8
1	A	441	ARG	2.8
1	A	139	ALA	2.7
1	A	467	ALA	2.7
1	A	175	ARG	2.7
1	A	130	THR	2.7
1	A	131	PRO	2.7
1	A	136	GLY	2.7
1	A	190	PRO	2.7
1	A	210	THR	2.7
1	A	445	GLY	2.7
1	A	416	ILE	2.7
1	A	52	SER	2.7
1	A	78	PRO	2.6
1	A	195	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	206	ASP	2.6
1	A	515	ASP	2.6
1	A	390	ASN	2.6
1	A	150	GLU	2.6
1	A	202	ARG	2.5
1	A	324	GLN	2.5
1	A	466	GLU	2.5
1	A	557	PRO	2.5
1	A	77	THR	2.5
1	A	480	HIS	2.5
1	A	127	ARG	2.5
1	A	151	PHE	2.5
1	A	514	THR	2.4
1	A	193	ARG	2.4
1	A	425	LEU	2.4
1	A	115	GLU	2.4
1	A	446	VAL	2.4
1	A	137	VAL	2.3
1	A	326	GLY	2.3
1	A	200	ARG	2.3
1	A	471	VAL	2.3
1	A	476	VAL	2.3
1	A	134	GLY	2.2
1	A	281	MET	2.2
1	A	129	LEU	2.2
1	A	398	PRO	2.2
1	A	116	GLN	2.2
1	A	213	ALA	2.2
1	A	204	ILE	2.2
1	A	410	GLY	2.1
1	A	140	LEU	2.1
1	A	133	GLN	2.1
1	A	372	GLN	2.1
1	A	191	GLY	2.1
1	A	329	THR	2.1
1	A	57	ALA	2.0
1	A	174	GLY	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 oligosaccharides 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.