Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 10:29 pm BST

PDB ID	:	7ZUH
Title	:	PENICILLIN-BINDING PROTEIN 1B (PBP-1B) Streptococcus pneumoniae R6
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Deposited on	:	2022-05-12
Resolution	:	1.47 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
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:

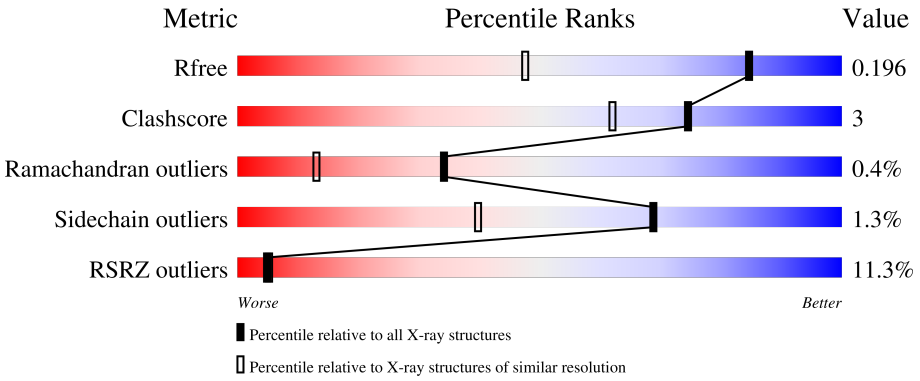
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.47 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}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 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	AAA	821	6% 52% 5% 43%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4345 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 Penicillin-binding protein 1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	469	Total	C	N	O	S	0	6	0
			3642	2286	612	728	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	656	GLY	ASN	engineered mutation	UNP Q7CRA4
AAA	686	GLN	ARG	engineered mutation	UNP Q7CRA4
AAA	687	GLN	ARG	engineered mutation	UNP Q7CRA4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	25	Total	Cl	0	0
			25	25		

- Molecule 4 is water.

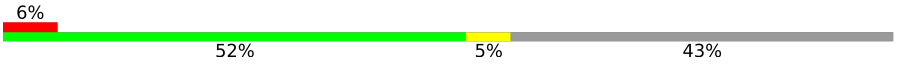
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	677	Total	O	0	0
			677	677		

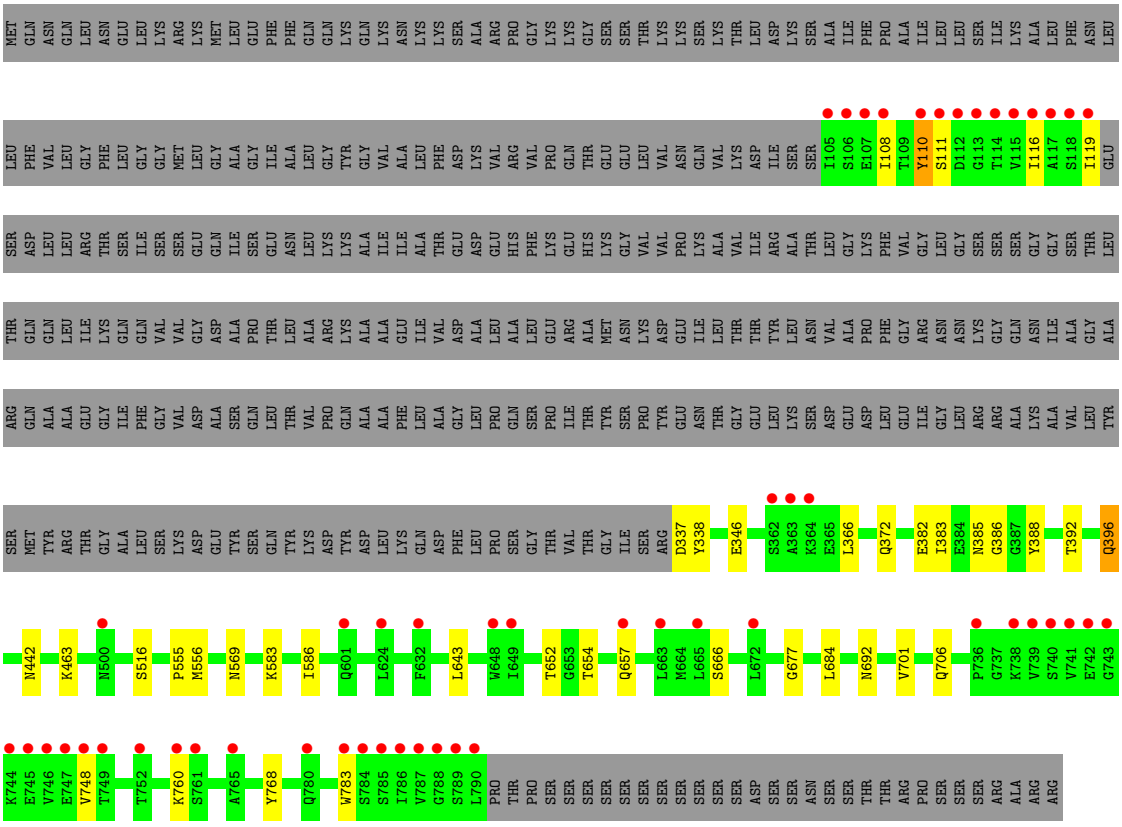
3 Residue-property plots (i)

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: Penicillin-binding protein 1b

Chain AAA:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.68Å 147.02Å 98.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.05 – 1.47 43.05 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.05-1.47) 99.1 (43.05-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.200 0.180 , 0.196	Depositor DCC
R_{free} test set	2358 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4345	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL

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	0.64	2/3733 (0.1%)	0.66	0/5067

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	AAA	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	338	TYR	C-O	6.18	1.35	1.23
1	AAA	748	VAL	C-O	5.46	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	385	ASN	Peptide
1	AAA	666	SER	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	AAA	3642	0	3536	23	0
2	AAA	1	0	0	0	0
3	AAA	25	0	0	1	0
4	AAA	677	0	0	2	0
All	All	4345	0	3536	23	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 3.

All (23) 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:AAA:346:GLU:HG3	1:AAA:586[A]:ILE:HD12	1.61	0.81
1:AAA:569:ASN:HD21	1:AAA:583:LYS:H	1.38	0.71
1:AAA:569:ASN:ND2	1:AAA:583:LYS:H	1.95	0.64
1:AAA:346:GLU:CG	1:AAA:586[A]:ILE:HD12	2.28	0.63
1:AAA:768:TYR:CE1	1:AAA:783:TRP:CD1	2.91	0.58
1:AAA:110:TYR:CG	1:AAA:396:GLN:HB2	2.38	0.58
1:AAA:108:ILE:HG13	1:AAA:116:ILE:HB	1.86	0.55
1:AAA:382:GLU:O	1:AAA:386:GLY:HA3	2.08	0.53
1:AAA:111:SER:HA	1:AAA:392:THR:O	2.09	0.53
1:AAA:110:TYR:CE2	1:AAA:396:GLN:HG3	2.45	0.51
1:AAA:382:GLU:HG3	1:AAA:388:TYR:CE2	2.47	0.50
1:AAA:119:ILE:HG21	1:AAA:383:ILE:HG22	1.98	0.46
1:AAA:643:LEU:HD21	1:AAA:701:VAL:HG12	1.96	0.46
1:AAA:677:GLY:HA2	1:AAA:684:LEU:HD11	2.00	0.44
1:AAA:692:ASN:HD22	1:AAA:692:ASN:H	1.66	0.44
1:AAA:366:LEU:O	1:AAA:372:GLN:HG3	2.18	0.43
1:AAA:760:LYS:HD3	1:AAA:760:LYS:HA	1.81	0.43
1:AAA:652:THR:HB	1:AAA:654:THR:HG23	2.00	0.43
1:AAA:366:LEU:O	1:AAA:372:GLN:CG	2.66	0.42
1:AAA:706:GLN:HG3	4:AAA:1452:HOH:O	2.20	0.41
1:AAA:346:GLU:HG2	3:AAA:914:CL:CL	2.58	0.41
1:AAA:706:GLN:HA	4:AAA:1237:HOH:O	2.22	0.40
1:AAA:463:LYS:HG3	1:AAA:555:PRO:O	2.22	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	471/821 (57%)	458 (97%)	11 (2%)	2 (0%)	34 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	110	TYR
1	AAA	442	ASN

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	391/679 (58%)	386 (99%)	5 (1%)	69 40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	337	ASP
1	AAA	396	GLN
1	AAA	516	SER
1	AAA	556	MET
1	AAA	657	GLN

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

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

Of 26 ligands modelled in this entry, 26 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	469/821 (57%)	0.47	53 (11%)	5 5	34, 43, 84, 137	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	105	ILE	11.5
1	AAA	110	TYR	8.2
1	AAA	114	THR	7.7
1	AAA	118	SER	7.5
1	AAA	116	ILE	7.3
1	AAA	112	ASP	7.3
1	AAA	790	LEU	6.8
1	AAA	119	ILE	6.6
1	AAA	113	GLY	6.4
1	AAA	363	ALA	6.1
1	AAA	742	GLU	5.8
1	AAA	789	SER	5.5
1	AAA	364	LYS	5.5
1	AAA	117	ALA	5.4
1	AAA	108	ILE	5.1
1	AAA	115	VAL	4.4
1	AAA	787	VAL	4.3
1	AAA	738	LYS	4.1
1	AAA	741	VAL	4.0
1	AAA	740	SER	3.9
1	AAA	746	VAL	3.9
1	AAA	743	GLY	3.9
1	AAA	744	LYS	3.8
1	AAA	106	SER	3.7
1	AAA	788	GLY	3.7
1	AAA	747	GLU	3.7
1	AAA	785	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	745	GLU	3.4
1	AAA	749	THR	3.4
1	AAA	107	GLU	3.3
1	AAA	752	THR	3.3
1	AAA	748	VAL	3.2
1	AAA	362	SER	2.9
1	AAA	784	SER	2.9
1	AAA	739	VAL	2.8
1	AAA	601	GLN	2.7
1	AAA	649	ILE	2.7
1	AAA	786	ILE	2.7
1	AAA	665	LEU	2.6
1	AAA	760	LYS	2.6
1	AAA	657	GLN	2.6
1	AAA	780	GLN	2.5
1	AAA	672	LEU	2.4
1	AAA	783	TRP	2.3
1	AAA	111	SER	2.2
1	AAA	500	ASN	2.2
1	AAA	632	PHE	2.2
1	AAA	624	LEU	2.2
1	AAA	648	TRP	2.2
1	AAA	736	PRO	2.2
1	AAA	765	ALA	2.1
1	AAA	663	LEU	2.1
1	AAA	761	SER	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	AAA	926	1/1	0.89	0.06	62,62,62,62	0
3	CL	AAA	906	1/1	0.91	0.06	69,69,69,69	0
3	CL	AAA	920	1/1	0.93	0.10	68,68,68,68	0
3	CL	AAA	921	1/1	0.93	0.08	67,67,67,67	0
3	CL	AAA	910	1/1	0.93	0.18	62,62,62,62	0
3	CL	AAA	908	1/1	0.94	0.15	61,61,61,61	0
3	CL	AAA	916	1/1	0.95	0.05	52,52,52,52	0
2	MG	AAA	901	1/1	0.96	0.30	55,55,55,55	0
3	CL	AAA	909	1/1	0.96	0.13	57,57,57,57	0
3	CL	AAA	907	1/1	0.96	0.23	63,63,63,63	0
3	CL	AAA	923	1/1	0.96	0.07	53,53,53,53	0
3	CL	AAA	924	1/1	0.96	0.06	55,55,55,55	0
3	CL	AAA	915	1/1	0.96	0.09	57,57,57,57	0
3	CL	AAA	911	1/1	0.97	0.11	55,55,55,55	0
3	CL	AAA	922	1/1	0.97	0.08	53,53,53,53	0
3	CL	AAA	918	1/1	0.97	0.06	49,49,49,49	0
3	CL	AAA	919	1/1	0.97	0.04	52,52,52,52	0
3	CL	AAA	925	1/1	0.97	0.08	57,57,57,57	0
3	CL	AAA	905	1/1	0.97	0.04	51,51,51,51	0
3	CL	AAA	914	1/1	0.98	0.03	50,50,50,50	0
3	CL	AAA	913	1/1	0.98	0.05	46,46,46,46	0
3	CL	AAA	903	1/1	0.99	0.07	41,41,41,41	0
3	CL	AAA	912	1/1	0.99	0.03	42,42,42,42	0
3	CL	AAA	904	1/1	0.99	0.07	40,40,40,40	0
3	CL	AAA	917	1/1	1.00	0.12	37,37,37,37	1
3	CL	AAA	902	1/1	1.00	0.09	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.