



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID : 2WAE
Title : PENICILLIN-BINDING PROTEIN 2B (PBP-2B) FROM STREPTOCOCCUS PNEUMONIAE (STRAIN 5204)
Authors : Contreras-Martel, C.; Dahout-Gonzalez, C.; Dos-Santos-Martins, A.; Kotnik, M.; Dessen, A.
Deposited on : 2009-02-05
Resolution : 2.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

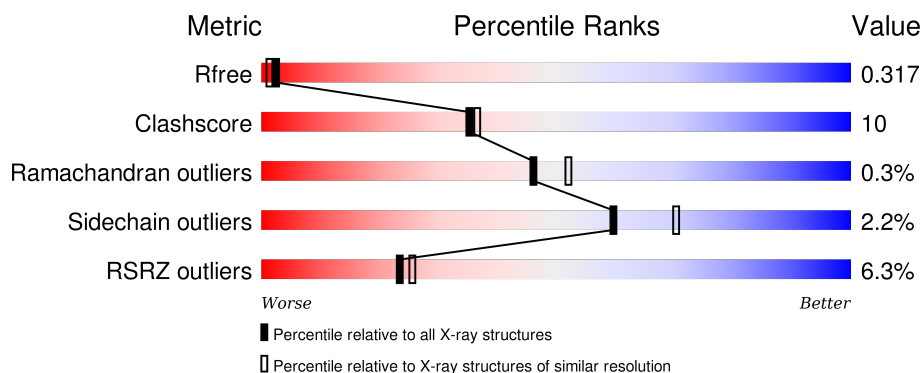
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	680	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>• 11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4800 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 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	1	0
			4613	2904	760	939	10			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	VAL	ILE	CONFLICT SEE REMARK 9	UNP P0A3M6
A	56	THR	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	96	ILE	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	130	THR	ILE	CONFLICT SEE REMARK 9	UNP P0A3M6
A	161	PRO	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	225	ILE	VAL	CONFLICT SEE REMARK 9	UNP P0A3M6
A	251	SER	ALA	CONFLICT SEE REMARK 9	UNP P0A3M6
A	275	VAL	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	281	PRO	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	290	HIS	TYR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	292	ASP	ASN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	297	GLU	ASP	CONFLICT SEE REMARK 9	UNP P0A3M6
A	298	ASN	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	306	LYS	ASN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	333	GLY	GLU	CONFLICT SEE REMARK 9	UNP P0A3M6
A	351	GLN	LYS	CONFLICT SEE REMARK 9	UNP P0A3M6
A	361	LEU	ILE	CONFLICT SEE REMARK 9	UNP P0A3M6
A	412	PRO	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	422	TYR	ASN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	426	LYS	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	427	LEU	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	438	GLU	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	446	ALA	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	448	VAL	MET	CONFLICT SEE REMARK 9	UNP P0A3M6
A	455	ILE	LEU	CONFLICT SEE REMARK 9	UNP P0A3M6
A	476	GLY	GLU	CONFLICT SEE REMARK 9	UNP P0A3M6
A	489	SER	THR	CONFLICT SEE REMARK 9	UNP P0A3M6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	502	LEU	PHE	CONFLICT SEE REMARK 9	UNP P0A3M6
A	508	ASN	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	512	PHE	TYR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	542	LEU	VAL	CONFLICT SEE REMARK 9	UNP P0A3M6
A	545	HIS	ARG	CONFLICT SEE REMARK 9	UNP P0A3M6
A	552	ASP	GLY	CONFLICT SEE REMARK 9	UNP P0A3M6
A	561	GLU	ASP	CONFLICT SEE REMARK 9	UNP P0A3M6
A	565	ALA	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	566	ILE	LEU	CONFLICT SEE REMARK 9	UNP P0A3M6
A	567	ASP	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	568	THR	PRO	CONFLICT SEE REMARK 9	UNP P0A3M6
A	569	LYS	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	571	ILE	MET	CONFLICT SEE REMARK 9	UNP P0A3M6
A	578	GLU	ASP	CONFLICT SEE REMARK 9	UNP P0A3M6
A	582	ALA	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	592	SER	ALA	CONFLICT SEE REMARK 9	UNP P0A3M6
A	597	PRO	GLY	CONFLICT SEE REMARK 9	UNP P0A3M6
A	606	ASP	ASN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	609	THR	LEU	CONFLICT SEE REMARK 9	UNP P0A3M6
A	619	GLY	ALA	CONFLICT SEE REMARK 9	UNP P0A3M6
A	625	GLY	ASP	CONFLICT SEE REMARK 9	UNP P0A3M6
A	628	GLU	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	630	ASN	THR	CONFLICT SEE REMARK 9	UNP P0A3M6
A	640	THR	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	641	GLU	ASP	CONFLICT SEE REMARK 9	UNP P0A3M6
A	659	LYS	ASN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	660	ASN	GLY	CONFLICT SEE REMARK 9	UNP P0A3M6
A	664	ALA	SER	CONFLICT SEE REMARK 9	UNP P0A3M6
A	674	ASN	GLN	CONFLICT SEE REMARK 9	UNP P0A3M6
A	675	GLN	LYS	CONFLICT SEE REMARK 9	UNP P0A3M6
A	676	HIS	TYR	CONFLICT SEE REMARK 9	UNP P0A3M6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

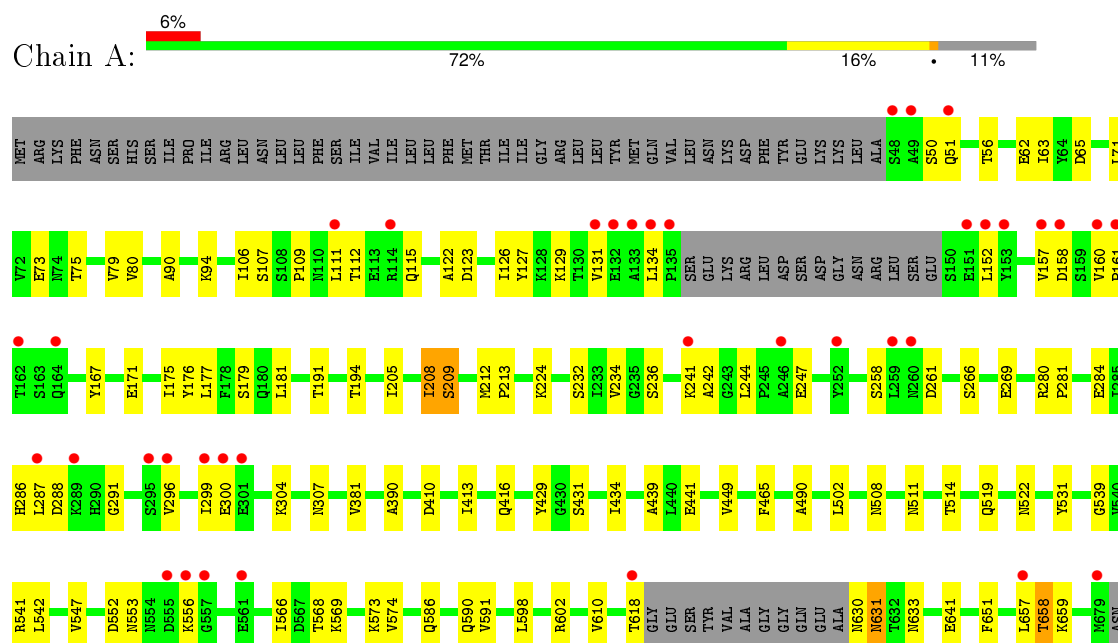
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total 186	O 186	0	0

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 errors 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 2B



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	127.95Å 127.95Å 280.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.39 – 2.26 54.36 – 2.26	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.39-2.26) 96.9 (54.36-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.244 , 0.301 0.260 , 0.317	Depositor DCC
R_{free} test set	2014 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 40258 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4800	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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:
ZN

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	0.34	0/4701	0.60	0/6389

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

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	4613	0	4536	90	0
2	A	1	0	0	0	0
3	A	186	0	0	14	0
All	All	4800	0	4536	90	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 10.

The worst 5 of 90 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:51:GLN:OE1	1:A:286[A]:HIS:HE1	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:OD2	1:A:280:ARG:NH2	2.00	0.93
1:A:56:THR:HG23	1:A:281:PRO:HG2	1.49	0.92
1:A:123:ASP:HB3	1:A:126:ILE:HG22	1.53	0.90
1:A:56:THR:O	1:A:281:PRO:HD2	1.73	0.87

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	602/680 (88%)	577 (96%)	23 (4%)	2 (0%)	46 52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	631	ASN
1	A	658	THR

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	509/573 (89%)	498 (98%)	11 (2%)	60 70

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	SER
1	A	232	SER
1	A	556	LYS
1	A	208	ILE
1	A	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	307	ASN
1	A	511	ASN
1	A	590	GLN
1	A	631	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	A	607/680 (89%)	0.56	38 (6%) 23 25	4, 20, 40, 67	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	SER	14.9
1	A	153	TYR	7.6
1	A	162	THR	7.3
1	A	49	ALA	6.0
1	A	152	LEU	4.7

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	1680	1/1	0.99	0.08	-	73,73,73,73	1

6.5 Other polymers [i](#)

There are no such residues in this entry.