



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:22 PM GMT

PDB ID : 2C6W  
Title : PENICILLIN-BINDING PROTEIN 1A (PBP-1A) FROM STREPTOCOCCUS PNEUMONIAE  
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Deposited on : 2005-11-14  
Resolution : 2.61 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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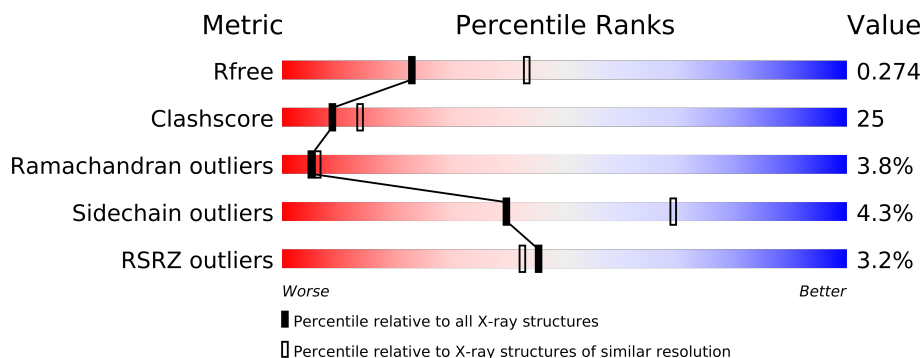
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.61 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))
$R_{free}$	66092	1940 (2.64-2.60)
Clashscore	79885	2404 (2.64-2.60)
Ramachandran outliers	78287	2360 (2.64-2.60)
Sidechain outliers	78261	2360 (2.64-2.60)
RSRZ outliers	66119	1939 (2.64-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	16	
2	B	384	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	B	702	-	X
4	CL	B	706	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3167 atoms, of which 0 are hydrogen and 0 are deuterium.

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 1A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	16	Total	C	N	O	0	0	0
			119	73	19	27			

- Molecule 2 is a protein called PENICILLIN-BINDING PROTEIN 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	384	Total	C	N	O	S	0	0	0
			3006	1904	494	595	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	388	ASP	GLU	CONFLICT	UNP Q8DR59
B	540	THR	SER	CONFLICT	UNP Q8DR59

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cl	0	0
			4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	35	Total	O	0	0
			35	35		

### 3 Residue-property plots

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.

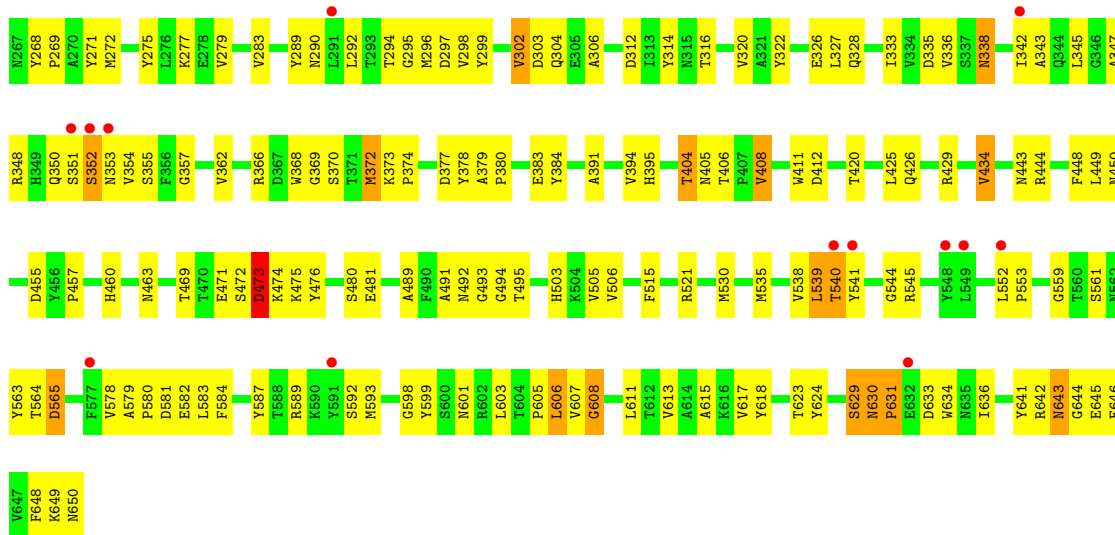
#### • Molecule 1: PENICILLIN-BINDING PROTEIN 1A

Chain A: 



#### • Molecule 2: PENICILLIN-BINDING PROTEIN 1A

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.78Å 187.26Å 51.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.99 – 2.61 44.99 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.0 (44.99-2.61) 96.1 (44.99-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.240 , 0.276 0.242 , 0.274	Depositor DCC
$R_{free}$ test set	779 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.8	EDS
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15916 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	0.34	0/119	0.51	0/159
2	B	0.40	0/3080	0.68	1/4196 (0.0%)
All	All	0.39	0/3199	0.67	1/4355 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	408	VAL	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	119	0	100	14	0
2	B	3006	0	2833	146	1
3	B	3	0	0	0	0
4	B	4	0	0	1	0
5	B	35	0	0	1	0
All	All	3167	0	2933	154	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:370:SER:HB2	2:B:559:GLY:HA2	1.47	0.96
2:B:474:LYS:CB	2:B:474:LYS:CD	2.51	0.87
2:B:275:TYR:CZ	2:B:302:VAL:HG22	2.15	0.82
2:B:404:THR:CG2	2:B:406:THR:H	1.95	0.80
2:B:297:ASP:HB2	2:B:506:VAL:HG22	1.63	0.80

All (1) 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	Distance(Å)	Clash(Å)
2:B:472:SER:OG	2:B:472:SER:OG[3_756]	2.17	0.03

## 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	A	14/16 (88%)	10 (71%)	2 (14%)	2 (14%)	0	0
2	B	382/384 (100%)	325 (85%)	44 (12%)	13 (3%)	6	8
All	All	396/400 (99%)	335 (85%)	46 (12%)	15 (4%)	5	6

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
2	B	352	SER
2	B	355	SER
2	B	473	ASP
2	B	630	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	A	11/15 (73%)	10 (91%)	1 (9%)	14	25
2	B	315/324 (97%)	302 (96%)	13 (4%)	41	71
All	All	326/339 (96%)	312 (96%)	14 (4%)	40	69

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	404	THR
2	B	426	GLN
2	B	539	LEU
2	B	377	ASP
2	B	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	427	GLN
2	B	438	ASN
2	B	571	HIS
2	B	426	GLN
2	B	503	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	16/16 (100%)	0.35	0	100	100	80, 92, 103, 109	0
2	B	384/384 (100%)	0.04	13 (3%)	43	40	40, 63, 97, 121	5 (1%)
All	All	400/400 (100%)	0.06	13 (3%)	45	41	40, 64, 98, 121	5 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	549	LEU	4.2
2	B	548	TYR	3.9
2	B	541	TYR	3.6
2	B	352	SER	3.4
2	B	353	ASN	3.4

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	706	1/1	0.25	8.78	105,105,105,105	0
3	ZN	B	702	1/1	0.21	6.53	51,51,51,51	0
3	ZN	B	703	1/1	0.15	-0.02	61,61,61,61	0
3	ZN	B	701	1/1	0.19	-0.07	100,100,100,100	0
4	CL	B	704	1/1	0.15	-0.24	73,73,73,73	0
4	CL	B	705	1/1	0.12	-1.10	99,99,99,99	0
4	CL	B	707	1/1	0.39	-	100,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.