



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 10:20 pm BST

PDB ID : 4Y4Q  
Title : Crystal structure of sortase B from Type II pilus of *Streptococcus pneumoniae*  
Authors : Shaik, M.M.; Dessen, A.; Di Guilmi, A.M.  
Deposited on : 2015-02-10  
Resolution : 2.16 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](mailto: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.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

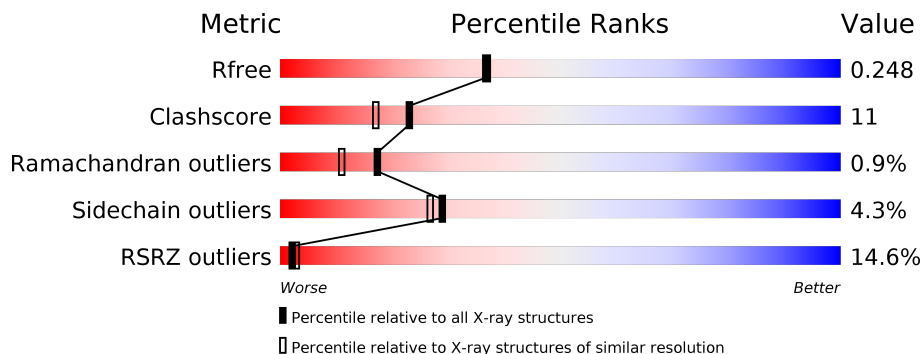
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	243	
1	B	243	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2959 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 Sortase, SrtB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	174	1398	894	230	270	4	0	0	0
1	B	175	1407	899	231	273	4	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP M7N1R6
A	19	VAL	-	expression tag	UNP M7N1R6
A	20	SER	-	expression tag	UNP M7N1R6
A	21	LEU	-	expression tag	UNP M7N1R6
A	22	SER	-	expression tag	UNP M7N1R6
A	23	PRO	-	expression tag	UNP M7N1R6
A	24	ASN	-	expression tag	UNP M7N1R6
A	25	PRO	-	expression tag	UNP M7N1R6
A	26	LEU	-	expression tag	UNP M7N1R6
A	27	LEU	-	expression tag	UNP M7N1R6
A	28	GLY	-	expression tag	UNP M7N1R6
A	29	LEU	-	expression tag	UNP M7N1R6
A	30	ASP	-	expression tag	UNP M7N1R6
A	31	SER	-	expression tag	UNP M7N1R6
A	32	THR	-	expression tag	UNP M7N1R6
A	33	GLU	-	expression tag	UNP M7N1R6
A	34	ASN	-	expression tag	UNP M7N1R6
A	35	LEU	-	expression tag	UNP M7N1R6
A	36	TYR	-	expression tag	UNP M7N1R6
A	37	PHE	-	expression tag	UNP M7N1R6
A	38	GLN	-	expression tag	UNP M7N1R6
A	39	GLY	-	expression tag	UNP M7N1R6
A	40	ILE	-	expression tag	UNP M7N1R6
A	41	ASP	-	expression tag	UNP M7N1R6
A	42	PRO	-	expression tag	UNP M7N1R6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	43	PHE	-	expression tag	UNP M7N1R6
A	44	THR	-	expression tag	UNP M7N1R6
A	45	MET	-	expression tag	UNP M7N1R6
B	18	MET	-	initiating methionine	UNP M7N1R6
B	19	VAL	-	expression tag	UNP M7N1R6
B	20	SER	-	expression tag	UNP M7N1R6
B	21	LEU	-	expression tag	UNP M7N1R6
B	22	SER	-	expression tag	UNP M7N1R6
B	23	PRO	-	expression tag	UNP M7N1R6
B	24	ASN	-	expression tag	UNP M7N1R6
B	25	PRO	-	expression tag	UNP M7N1R6
B	26	LEU	-	expression tag	UNP M7N1R6
B	27	LEU	-	expression tag	UNP M7N1R6
B	28	GLY	-	expression tag	UNP M7N1R6
B	29	LEU	-	expression tag	UNP M7N1R6
B	30	ASP	-	expression tag	UNP M7N1R6
B	31	SER	-	expression tag	UNP M7N1R6
B	32	THR	-	expression tag	UNP M7N1R6
B	33	GLU	-	expression tag	UNP M7N1R6
B	34	ASN	-	expression tag	UNP M7N1R6
B	35	LEU	-	expression tag	UNP M7N1R6
B	36	TYR	-	expression tag	UNP M7N1R6
B	37	PHE	-	expression tag	UNP M7N1R6
B	38	GLN	-	expression tag	UNP M7N1R6
B	39	GLY	-	expression tag	UNP M7N1R6
B	40	ILE	-	expression tag	UNP M7N1R6
B	41	ASP	-	expression tag	UNP M7N1R6
B	42	PRO	-	expression tag	UNP M7N1R6
B	43	PHE	-	expression tag	UNP M7N1R6
B	44	THR	-	expression tag	UNP M7N1R6
B	45	MET	-	expression tag	UNP M7N1R6

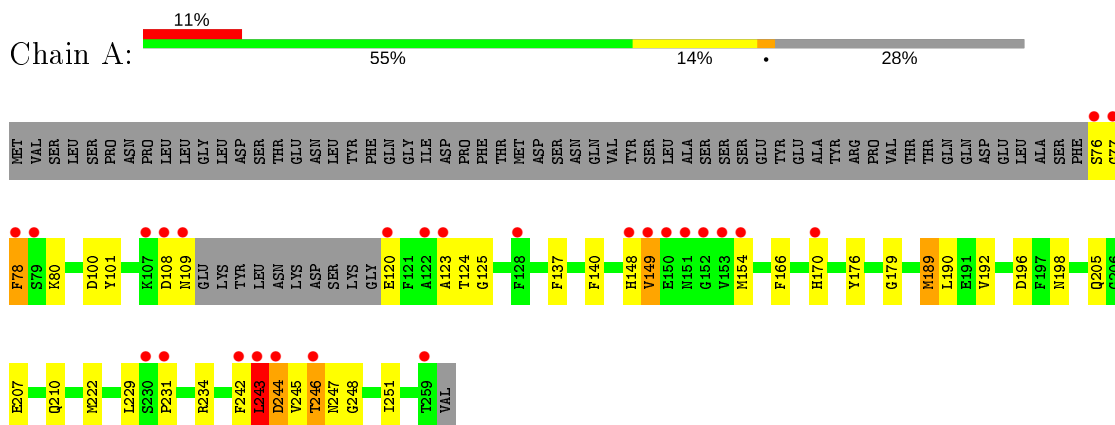
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	71	Total O 71 71	0	0
2	B	83	Total O 83 83	0	0

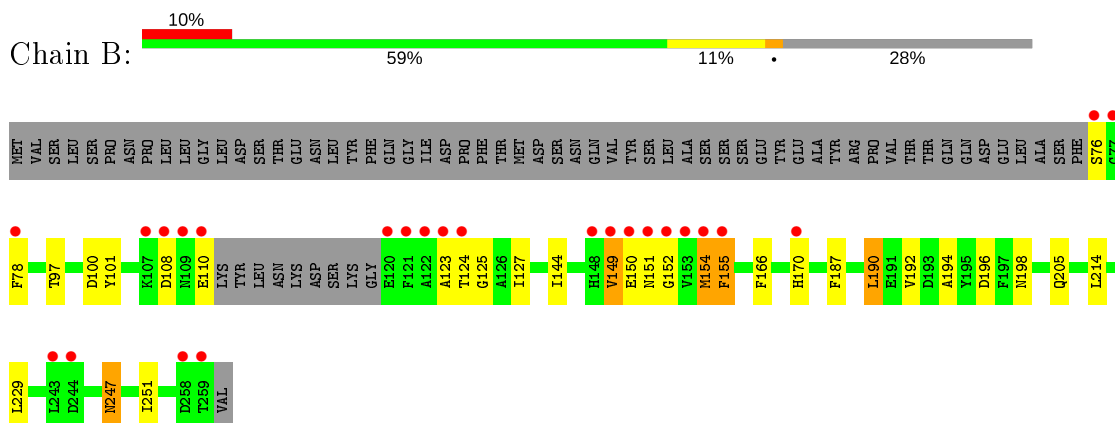
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Sortase, SrtB family



- Molecule 1: Sortase, SrtB family



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.15Å 101.14Å 143.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.31 – 2.16 41.31 – 2.16	Depositor EDS
% Data completeness (in resolution range)	95.6 (41.31-2.16) 95.7 (41.31-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.16Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.188 , 0.232 0.209 , 0.248	Depositor DCC
$R_{free}$ test set	1413 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtrriage
Anisotropy	0.539	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8187e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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	0.62	3/1430 (0.2%)	0.68	3/1937 (0.2%)
1	B	0.39	0/1439	0.57	0/1949
All	All	0.52	3/2869 (0.1%)	0.62	3/3886 (0.1%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLY	C-N	14.12	1.66	1.34
1	A	243	LEU	C-N	6.59	1.49	1.34
1	A	76	SER	C-N	-5.05	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	SER	O-C-N	-10.18	105.89	123.20
1	A	76	SER	CA-C-N	7.13	130.47	116.20
1	A	243	LEU	O-C-N	-5.90	113.25	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	LEU	Mainchain

## 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	1398	0	1326	31	1
1	B	1407	0	1332	33	1
2	A	71	0	0	1	0
2	B	83	0	0	1	0
All	All	2959	0	2658	62	1

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 11.

The worst 5 of 62 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:B:149:VAL:HG13	1:B:151:ASN:H	1.09	1.16
1:A:245:VAL:HG13	1:A:248:GLY:HA3	1.40	1.01
1:B:149:VAL:CG1	1:B:151:ASN:H	1.79	0.96
1:A:170:HIS:O	2:A:301:HOH:O	1.88	0.90
1:B:149:VAL:HG13	1:B:151:ASN:N	1.90	0.85

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PHE:CZ	1:B:76:SER:OG[7_555]	2.08	0.12

## 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	170/243 (70%)	165 (97%)	4 (2%)	1 (1%)	25	18
1	B	171/243 (70%)	163 (95%)	6 (4%)	2 (1%)	13	7
All	All	341/486 (70%)	328 (96%)	10 (3%)	3 (1%)	17	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ASP
1	B	155	PHE
1	B	125	GLY

### 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	150/213 (70%)	143 (95%)	7 (5%)	26	23
1	B	151/213 (71%)	145 (96%)	6 (4%)	31	29
All	All	301/426 (71%)	288 (96%)	13 (4%)	29	27

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	THR
1	A	247	ASN
1	B	154	MET
1	A	243	LEU
1	B	149	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS

### 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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	77:GLY	C	78:PHE	N	1.66

## 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, 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	174/243 (71%)	0.62	26 (14%) 2   3	25, 43, 104, 142	0
1	B	175/243 (72%)	0.62	25 (14%) 2   3	20, 40, 109, 135	0
All	All	349/486 (71%)	0.62	51 (14%) 2   3	20, 42, 105, 142	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	VAL	10.9
1	B	152	GLY	9.2
1	A	151	ASN	8.9
1	A	149	VAL	8.5
1	B	151	ASN	7.6

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.