



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2019 – 10:53 AM EDT

PDB ID : 2Y1V
Title : Full length structure of RrgB Pilus protein from *Streptococcus pneumoniae*
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Deposited on : 2010-12-10
Resolution : 2.39 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

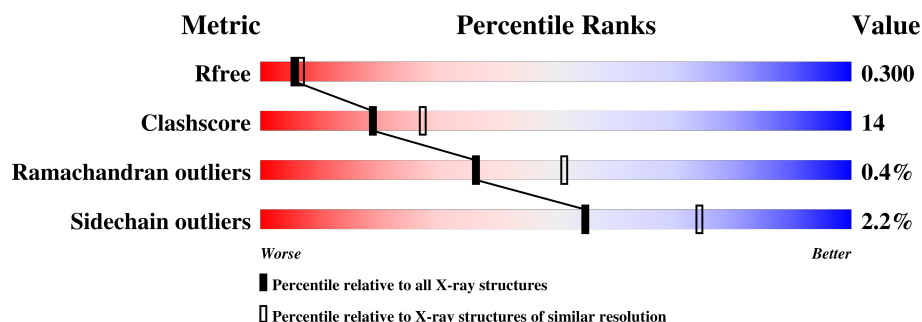
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.39 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	605	 76% 22% .
1	B	605	 77% 22% .
1	C	605	 69% 30% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14167 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 CELL WALL SURFACE ANCHOR FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	Se	0	0	0
			4576	2866	763	942	5			
1	B	604	Total	C	N	O	Se	0	0	0
			4576	2866	763	942	5			
1	C	604	Total	C	N	O	Se	0	0	0
			4576	2866	763	942	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q97SC2
B	29	GLY	-	expression tag	UNP Q97SC2
C	29	GLY	-	expression tag	UNP Q97SC2

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ni	0	0
			3	3		
2	A	3	Total	Ni	0	0
			3	3		
2	C	3	Total	Ni	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	141	Total	O	0	0
			141	141		

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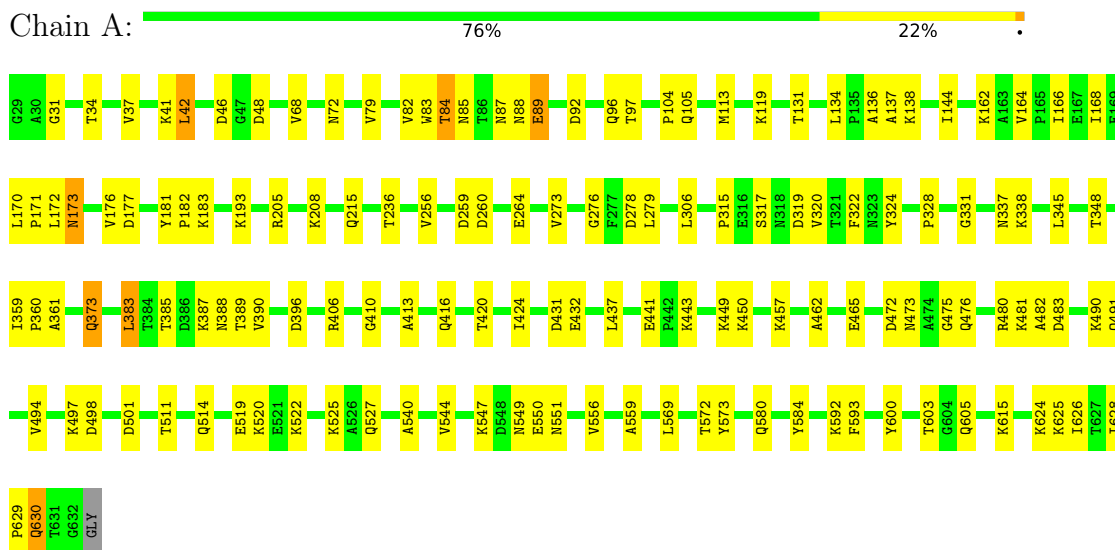
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	120	Total 120	O 120	0	0

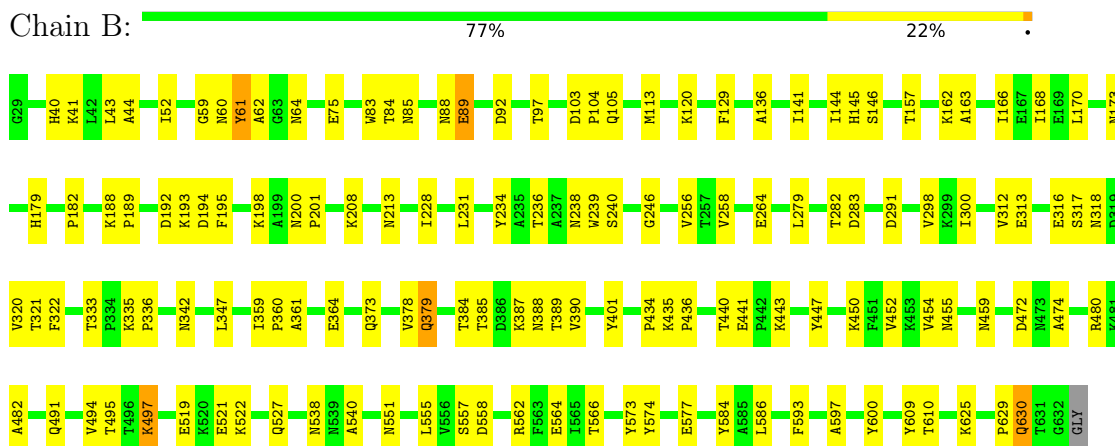
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

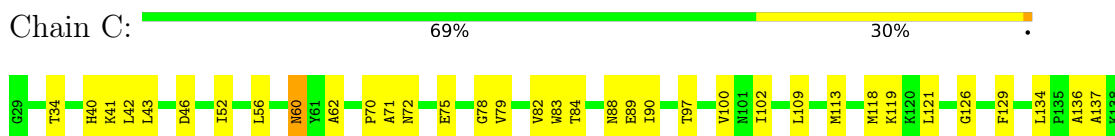
• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	74.62Å 74.62Å 340.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.53 – 2.39 19.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.7 (113.53-2.39) 93.7 (19.85-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.234 0.239 , 0.300	Depositor DCC
R_{free} test set	8066 reflections (10.32%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.097 for h,-h-k,-l 0.002 for -k,-h,-l	Xtriage
Reported twinning fraction	0.592 for H, K, L 0.408 for K, H, -L	Depositor
Outliers	0 of 78179 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14167	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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

5.1 Standard geometry

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

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	0.47	0/4646	0.62	0/6315
1	B	0.44	0/4646	0.57	0/6315
1	C	0.40	0/4646	0.57	0/6315
All	All	0.44	0/13938	0.59	0/18945

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	4576	0	4509	108	0
1	B	4576	0	4509	120	0
1	C	4576	0	4510	153	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	169	0	0	12	0
3	B	141	0	0	15	0
3	C	120	0	0	33	0
All	All	14167	0	13528	381	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 14.

The worst 5 of 381 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:84:THR:HG21	1:B:88:ASN:HA	1.24	1.15
3:A:2008:HOH:O	1:B:387:LYS:HB2	1.45	1.15
1:B:256:VAL:HG21	1:B:279:LEU:HD11	1.16	1.13
1:A:96:GLN:HB3	3:A:2012:HOH:O	1.48	1.12
1:C:168:ILE:HB	3:C:2026:HOH:O	1.47	1.11

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	602/605 (100%)	566 (94%)	34 (6%)	2 (0%)	43	58
1	B	602/605 (100%)	573 (95%)	25 (4%)	4 (1%)	24	35
1	C	602/605 (100%)	569 (94%)	31 (5%)	2 (0%)	43	58
All	All	1806/1815 (100%)	1708 (95%)	90 (5%)	8 (0%)	36	51

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	GLY
1	B	61	TYR
1	A	173	ASN
1	B	173	ASN
1	B	379	GLN

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	489/484 (101%)	475 (97%)	14 (3%)	45	66
1	B	489/484 (101%)	481 (98%)	8 (2%)	65	82
1	C	489/484 (101%)	478 (98%)	11 (2%)	55	74
All	All	1467/1452 (101%)	1434 (98%)	33 (2%)	55	74

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	ASN
1	B	342	ASN
1	C	521	GLU
1	B	89	GLU
1	B	105	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	179	HIS
1	B	491	GLN
1	C	508	ASN
1	B	214	HIS
1	B	293	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.