



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:35 AM GMT

PDB ID : 3PG2  
Title : The Crystal structure of the major pilin GBS80 of Streptococcus agalactiae  
35 kDa C-terminal fragment  
Authors : Vengadesan, K.; Narayana, S.V.L.  
Deposited on : 2010-10-29  
Resolution : 1.80 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](mailto: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.

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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 : 1.7 (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

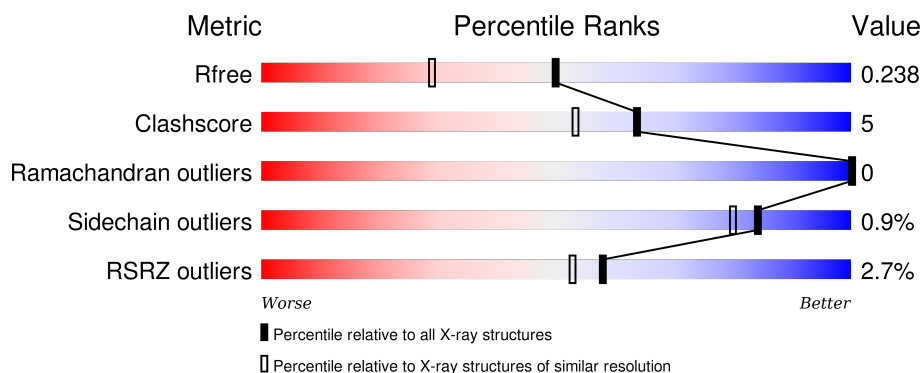
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	319	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 89%, yellow 89%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>9% ..</span> </div> </div>
1	B	319	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, orange 5%, orange 88%, yellow 88%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>88%</span> <span>9% ..</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5733 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	315	Total	C	N	O	S	0	0	0
			2438	1539	396	502	1			
1	B	313	Total	C	N	O	S	0	0	0
			2424	1530	393	500	1			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

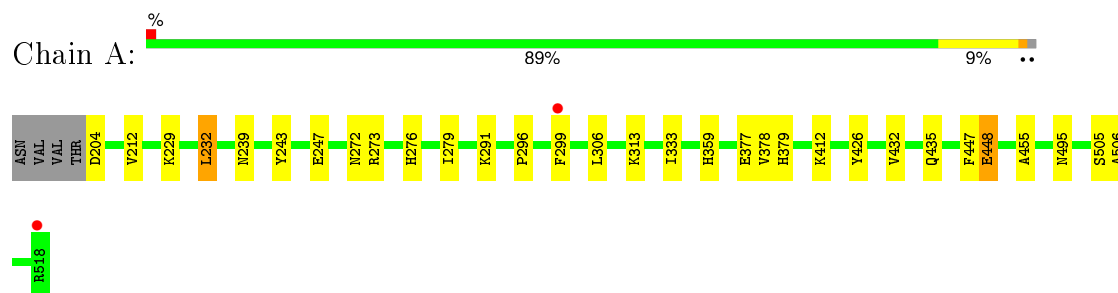
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	550	Total	O	0	0
			550	550		
3	B	317	Total	O	0	0
			317	317		

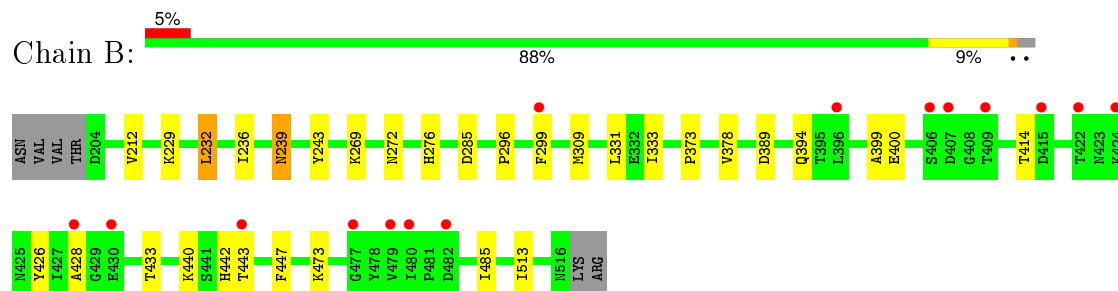
### 3 Residue-property plots

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: 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 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.87Å 60.27Å 80.37Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	37.15 – 1.80 37.15 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.15-1.80) 99.6 (37.15-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.200 , 0.234 0.204 , 0.238	Depositor DCC
$R_{free}$ test set	3068 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 60618 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.20 % 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 1.0897e-06. 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, 0.375 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:  
CA

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	0.58	0/2483	0.63	1/3363 (0.0%)
1	B	0.50	0/2469	0.61	0/3345
All	All	0.54	0/4952	0.62	1/6708 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	LEU	CA-CB-CG	5.49	127.92	115.30

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	2438	0	2405	27	0
1	B	2424	0	2393	23	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	550	0	0	7	0
3	B	317	0	0	2	0
All	All	5733	0	4798	50	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 5.

All (50) 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:243:TYR:O	1:A:299:PHE:HD2	1.34	1.09
1:B:243:TYR:O	1:B:299:PHE:HD2	1.52	0.91
1:A:272:ASN:H	1:A:276:HIS:HD2	1.16	0.90
1:A:243:TYR:O	1:A:299:PHE:CD2	2.25	0.89
1:B:239:ASN:H	1:B:239:ASN:HD22	1.19	0.89
1:B:272:ASN:H	1:B:276:HIS:HD2	1.22	0.87
1:A:247:GLU:OE2	1:A:291:LYS:HD3	1.78	0.83
1:A:229:LYS:HE3	3:A:563:HOH:O	1.80	0.82
1:B:243:TYR:O	1:B:299:PHE:CD2	2.40	0.74
1:A:432:VAL:HG23	1:A:435:GLN:CG	2.21	0.71
1:A:377:GLU:OE2	1:A:379:HIS:HD2	1.79	0.64
1:A:313:LYS:HE2	3:A:799:HOH:O	1.99	0.62
1:A:432:VAL:CG2	1:A:435:GLN:HG3	2.30	0.61
1:A:204:ASP:N	3:A:578:HOH:O	2.36	0.59
1:A:272:ASN:H	1:A:276:HIS:CD2	2.09	0.57
1:B:272:ASN:H	1:B:276:HIS:CD2	2.13	0.56
1:B:485:ILE:HG21	1:B:513:ILE:HD12	1.89	0.55
1:B:389:ASP:OD2	1:B:394:GLN:HB3	2.08	0.55
1:A:296:PRO:HA	1:A:299:PHE:CE2	2.43	0.54
1:A:432:VAL:HG23	1:A:435:GLN:HG2	1.89	0.54
1:A:239:ASN:ND2	3:A:725:HOH:O	2.40	0.54
1:A:379:HIS:HE1	1:A:455:ALA:O	1.91	0.52
1:B:414:THR:HA	1:B:433:THR:HG23	1.92	0.51
1:A:432:VAL:CG2	1:A:435:GLN:CG	2.88	0.51
1:B:212:VAL:HG21	1:B:378:VAL:CG1	2.42	0.49
1:A:495:ASN:ND2	1:A:505:SER:H	2.11	0.49
1:B:229:LYS:HE3	3:B:703:HOH:O	2.12	0.48
1:B:442:HIS:CG	1:B:443:THR:H	2.31	0.48
1:A:273:ARG:HD2	1:A:279:ILE:HD12	1.96	0.48
1:B:400:GLU:HB2	1:B:473:LYS:HB3	1.96	0.48
1:A:495:ASN:ND2	1:A:506:ALA:H	2.11	0.48
1:A:232:LEU:HB2	1:A:333:ILE:HB	1.97	0.47
1:B:239:ASN:N	1:B:239:ASN:HD22	1.94	0.47
1:B:399:ALA:O	1:B:440:LYS:HA	2.16	0.45
1:B:239:ASN:ND2	1:B:239:ASN:H	1.99	0.45
1:A:412:LYS:NZ	3:A:868:HOH:O	2.45	0.45
1:B:232:LEU:HB2	1:B:333:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PRO:HA	1:B:299:PHE:CE2	2.52	0.44
1:A:426:TYR:CD1	1:A:447:PHE:HA	2.52	0.44
1:A:296:PRO:HA	1:A:299:PHE:CD2	2.54	0.43
1:A:359:HIS:HD2	3:A:524:HOH:O	2.01	0.43
1:B:373:PRO:HD2	3:B:556:HOH:O	2.19	0.42
1:A:426:TYR:CE2	1:A:448:GLU:HG3	2.55	0.42
1:B:442:HIS:CG	1:B:443:THR:N	2.88	0.41
1:B:236:ILE:HD11	1:B:331:LEU:HB2	2.01	0.41
1:A:212:VAL:HG21	1:A:378:VAL:CG1	2.50	0.41
1:B:269:LYS:CG	1:B:309:MET:HE1	2.51	0.41
1:B:426:TYR:CD1	1:B:447:PHE:HA	2.56	0.41
1:B:428:ALA:HB2	1:B:440:LYS:HB2	2.02	0.40
1:A:432:VAL:HG22	3:A:679:HOH:O	2.20	0.40

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	313/319 (98%)	304 (97%)	9 (3%)	0	100	100
1	B	311/319 (98%)	301 (97%)	10 (3%)	0	100	100
All	All	624/638 (98%)	605 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	266/271 (98%)	264 (99%)	2 (1%)	86	83
1	B	265/271 (98%)	262 (99%)	3 (1%)	80	74
All	All	531/542 (98%)	526 (99%)	5 (1%)	84	80

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

Mol	Chain	Res	Type
1	A	232	LEU
1	A	448	GLU
1	B	232	LEU
1	B	239	ASN
1	B	285	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	276	HIS
1	A	359	HIS
1	A	371	ASN
1	A	379	HIS
1	A	495	ASN
1	B	239	ASN
1	B	272	ASN
1	B	276	HIS
1	B	314	ASN
1	B	371	ASN
1	B	394	GLN
1	B	516	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 4 ligands modelled in this entry, 4 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 ⓘ

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	315/319 (98%)	-0.31	2 (0%) 90 88	7, 14, 23, 33	0
1	B	313/319 (98%)	0.11	15 (4%) 34 28	10, 19, 37, 41	0
All	All	628/638 (98%)	-0.10	17 (2%) 58 53	7, 16, 35, 41	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	PHE	4.2
1	B	443	THR	3.7
1	B	480	ILE	3.7
1	B	299	PHE	3.6
1	B	406	SER	3.5
1	B	482	ASP	3.4
1	B	477	GLY	3.2
1	A	518	ARG	3.2
1	B	409	THR	3.1
1	B	396	LEU	3.1
1	B	407	ASP	2.8
1	B	415	ASP	2.5
1	B	428	ALA	2.5
1	B	422	THR	2.5
1	B	424	LYS	2.4
1	B	479	VAL	2.4
1	B	430	GLU	2.2

### 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 [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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1	1/1	1.00	0.09	-0.71	9,9,9,9	0
2	CA	B	1	1/1	1.00	0.08	-0.85	12,12,12,12	0
2	CA	B	2	1/1	0.98	0.06	-1.48	18,18,18,18	0
2	CA	A	2	1/1	0.99	0.07	-1.55	14,14,14,14	0

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

There are no such residues in this entry.