



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 10, 2016 – 10:29 PM EDT

PDB ID : 5HTS  
Title : Crystal structure of shaft pilin spaA from Lactobacillus rhamnosus GG - D295N mutant  
Authors : Chaurasia, P.; Pratap, S.; von Ossowski, I.; Palva, A.; Krishnan, V.  
Deposited on : 2016-01-27  
Resolution : 2.60 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  
<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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790

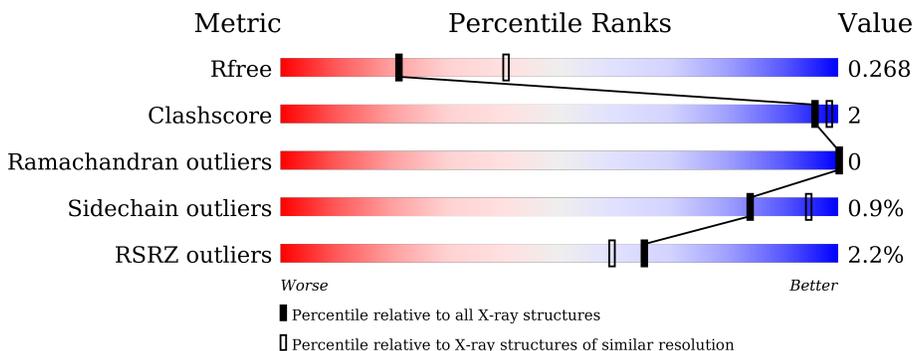
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	283	89% (8% poor fit)
1	B	283	90% (7% poor fit)
1	C	283	87% (10% poor fit)
1	D	283	87% (5% poor fit, 8% not modelled)
1	E	283	83% (13% poor fit)
1	F	283	83% (8% poor fit, 15% not modelled)

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11849 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 surface protein SpaA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	259	1981	1249	323	409	0	2	0
1	B	264	2010	1267	328	415	0	2	0
1	C	254	1942	1222	318	402	0	2	0
1	D	260	1988	1253	324	411	0	2	0
1	E	245	1862	1174	304	384	0	1	0
1	F	240	1831	1157	298	376	0	1	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP C7T9P4
A	29	GLY	-	expression tag	UNP C7T9P4
A	30	ARG	-	expression tag	UNP C7T9P4
A	31	ASP	-	expression tag	UNP C7T9P4
A	32	PRO	-	expression tag	UNP C7T9P4
A	33	ASN	-	expression tag	UNP C7T9P4
A	34	SER	-	expression tag	UNP C7T9P4
A	295	ASN	ASP	engineered mutation	UNP C7T9P4
A	303	LEU	-	expression tag	UNP C7T9P4
A	304	GLU	-	expression tag	UNP C7T9P4
A	305	HIS	-	expression tag	UNP C7T9P4
A	306	HIS	-	expression tag	UNP C7T9P4
A	307	HIS	-	expression tag	UNP C7T9P4
A	308	HIS	-	expression tag	UNP C7T9P4
A	309	HIS	-	expression tag	UNP C7T9P4
A	310	HIS	-	expression tag	UNP C7T9P4
B	28	MET	-	expression tag	UNP C7T9P4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	GLY	-	expression tag	UNP C7T9P4
B	30	ARG	-	expression tag	UNP C7T9P4
B	31	ASP	-	expression tag	UNP C7T9P4
B	32	PRO	-	expression tag	UNP C7T9P4
B	33	ASN	-	expression tag	UNP C7T9P4
B	34	SER	-	expression tag	UNP C7T9P4
B	295	ASN	ASP	engineered mutation	UNP C7T9P4
B	303	LEU	-	expression tag	UNP C7T9P4
B	304	GLU	-	expression tag	UNP C7T9P4
B	305	HIS	-	expression tag	UNP C7T9P4
B	306	HIS	-	expression tag	UNP C7T9P4
B	307	HIS	-	expression tag	UNP C7T9P4
B	308	HIS	-	expression tag	UNP C7T9P4
B	309	HIS	-	expression tag	UNP C7T9P4
B	310	HIS	-	expression tag	UNP C7T9P4
C	28	MET	-	expression tag	UNP C7T9P4
C	29	GLY	-	expression tag	UNP C7T9P4
C	30	ARG	-	expression tag	UNP C7T9P4
C	31	ASP	-	expression tag	UNP C7T9P4
C	32	PRO	-	expression tag	UNP C7T9P4
C	33	ASN	-	expression tag	UNP C7T9P4
C	34	SER	-	expression tag	UNP C7T9P4
C	295	ASN	ASP	engineered mutation	UNP C7T9P4
C	303	LEU	-	expression tag	UNP C7T9P4
C	304	GLU	-	expression tag	UNP C7T9P4
C	305	HIS	-	expression tag	UNP C7T9P4
C	306	HIS	-	expression tag	UNP C7T9P4
C	307	HIS	-	expression tag	UNP C7T9P4
C	308	HIS	-	expression tag	UNP C7T9P4
C	309	HIS	-	expression tag	UNP C7T9P4
C	310	HIS	-	expression tag	UNP C7T9P4
D	28	MET	-	expression tag	UNP C7T9P4
D	29	GLY	-	expression tag	UNP C7T9P4
D	30	ARG	-	expression tag	UNP C7T9P4
D	31	ASP	-	expression tag	UNP C7T9P4
D	32	PRO	-	expression tag	UNP C7T9P4
D	33	ASN	-	expression tag	UNP C7T9P4
D	34	SER	-	expression tag	UNP C7T9P4
D	295	ASN	ASP	engineered mutation	UNP C7T9P4
D	303	LEU	-	expression tag	UNP C7T9P4
D	304	GLU	-	expression tag	UNP C7T9P4
D	305	HIS	-	expression tag	UNP C7T9P4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	306	HIS	-	expression tag	UNP C7T9P4
D	307	HIS	-	expression tag	UNP C7T9P4
D	308	HIS	-	expression tag	UNP C7T9P4
D	309	HIS	-	expression tag	UNP C7T9P4
D	310	HIS	-	expression tag	UNP C7T9P4
E	28	MET	-	expression tag	UNP C7T9P4
E	29	GLY	-	expression tag	UNP C7T9P4
E	30	ARG	-	expression tag	UNP C7T9P4
E	31	ASP	-	expression tag	UNP C7T9P4
E	32	PRO	-	expression tag	UNP C7T9P4
E	33	ASN	-	expression tag	UNP C7T9P4
E	34	SER	-	expression tag	UNP C7T9P4
E	295	ASN	ASP	engineered mutation	UNP C7T9P4
E	303	LEU	-	expression tag	UNP C7T9P4
E	304	GLU	-	expression tag	UNP C7T9P4
E	305	HIS	-	expression tag	UNP C7T9P4
E	306	HIS	-	expression tag	UNP C7T9P4
E	307	HIS	-	expression tag	UNP C7T9P4
E	308	HIS	-	expression tag	UNP C7T9P4
E	309	HIS	-	expression tag	UNP C7T9P4
E	310	HIS	-	expression tag	UNP C7T9P4
F	28	MET	-	expression tag	UNP C7T9P4
F	29	GLY	-	expression tag	UNP C7T9P4
F	30	ARG	-	expression tag	UNP C7T9P4
F	31	ASP	-	expression tag	UNP C7T9P4
F	32	PRO	-	expression tag	UNP C7T9P4
F	33	ASN	-	expression tag	UNP C7T9P4
F	34	SER	-	expression tag	UNP C7T9P4
F	295	ASN	ASP	engineered mutation	UNP C7T9P4
F	303	LEU	-	expression tag	UNP C7T9P4
F	304	GLU	-	expression tag	UNP C7T9P4
F	305	HIS	-	expression tag	UNP C7T9P4
F	306	HIS	-	expression tag	UNP C7T9P4
F	307	HIS	-	expression tag	UNP C7T9P4
F	308	HIS	-	expression tag	UNP C7T9P4
F	309	HIS	-	expression tag	UNP C7T9P4
F	310	HIS	-	expression tag	UNP C7T9P4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	55	Total O 55 55	0	0

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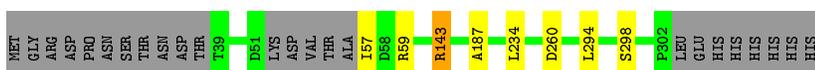
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	B	50	Total 50	O 50	0	0
2	C	50	Total 50	O 50	0	0
2	D	50	Total 50	O 50	0	0
2	E	20	Total 20	O 20	0	0
2	F	10	Total 10	O 10	0	0

### 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: Cell surface protein SpaA

Chain A:  89% 8%



- Molecule 1: Cell surface protein SpaA

Chain B:  90% 7%



- Molecule 1: Cell surface protein SpaA

Chain C:  87% 10%



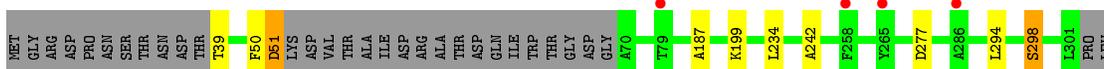
- Molecule 1: Cell surface protein SpaA

Chain D:  87% 5% 8%



- Molecule 1: Cell surface protein SpaA

Chain E:  83% 13%



- Molecule 1: Cell surface protein SpaA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.33Å 75.16Å 176.48Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	37.90 – 2.60 37.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.90-2.60) 98.7 (37.90-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.242 , 0.265 0.244 , 0.268	Depositor DCC
$R_{free}$ test set	3262 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	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 40.23 % 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 2.8228e-04. 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	0.77	0/2029	0.81	0/2761
1	B	0.78	0/2059	0.81	0/2805
1	C	0.77	0/1989	0.80	0/2705
1	D	0.82	0/2036	0.80	0/2771
1	E	0.62	0/1903	0.73	0/2588
1	F	0.57	0/1873	0.72	0/2547
All	All	0.73	0/11889	0.78	0/16177

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 [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	1981	0	1889	5	0
1	B	2010	0	1914	6	0
1	C	1942	0	1845	6	0
1	D	1988	0	1895	9	0
1	E	1862	0	1780	6	0
1	F	1831	0	1747	4	0
2	A	55	0	0	1	0
2	B	50	0	0	0	0
2	C	50	0	0	0	0
2	D	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	20	0	0	0	0
2	F	10	0	0	0	0
All	All	11849	0	11070	34	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 2.

The worst 5 of 34 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:F:143:ARG:NH1	1:F:231:ASN:HB2	1.79	0.98
1:C:277:ASP:OD1	1:C:298:SER:HB3	1.66	0.95
1:C:59:ARG:HB3	1:C:63:GLN:HE21	1.48	0.77
1:E:51:ASP:OD1	1:E:51:ASP:N	2.29	0.65
1:E:277:ASP:OD1	1:E:298:SER:HB3	1.98	0.64

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	257/283 (91%)	252 (98%)	5 (2%)	0	100	100
1	B	264/283 (93%)	259 (98%)	5 (2%)	0	100	100
1	C	252/283 (89%)	248 (98%)	4 (2%)	0	100	100
1	D	258/283 (91%)	252 (98%)	6 (2%)	0	100	100
1	E	242/283 (86%)	237 (98%)	5 (2%)	0	100	100
1	F	237/283 (84%)	233 (98%)	4 (2%)	0	100	100
All	All	1510/1698 (89%)	1481 (98%)	29 (2%)	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	211/231 (91%)	209 (99%)	2 (1%)	84	95
1	B	213/231 (92%)	211 (99%)	2 (1%)	84	95
1	C	206/231 (89%)	205 (100%)	1 (0%)	92	98
1	D	212/231 (92%)	211 (100%)	1 (0%)	92	98
1	E	198/231 (86%)	195 (98%)	3 (2%)	72	90
1	F	195/231 (84%)	193 (99%)	2 (1%)	82	94
All	All	1235/1386 (89%)	1224 (99%)	11 (1%)	84	95

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

Mol	Chain	Res	Type
1	C	298	SER
1	D	38	THR
1	E	298	SER
1	B	298	SER
1	E	51	ASP

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

Mol	Chain	Res	Type
1	C	63	GLN

### 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](#)

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, 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	259/283 (91%)	-0.05	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	35, 54, 81, 94	0
1	B	264/283 (93%)	-0.04	1 (0%) <span style="border: 1px solid blue; padding: 2px;">93</span> <span style="border: 1px solid blue; padding: 2px;">91</span>	33, 52, 84, 114	0
1	C	254/283 (89%)	0.06	3 (1%) <span style="border: 1px solid blue; padding: 2px;">81</span> <span style="border: 1px solid blue; padding: 2px;">77</span>	29, 51, 91, 124	0
1	D	260/283 (91%)	-0.03	2 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">85</span>	31, 48, 82, 104	0
1	E	245/283 (86%)	0.17	4 (1%) <span style="border: 1px solid blue; padding: 2px;">74</span> <span style="border: 1px solid blue; padding: 2px;">69</span>	59, 78, 96, 112	0
1	F	240/283 (84%)	0.66	23 (9%) <span style="border: 1px solid red; padding: 2px;">10</span> <span style="border: 1px solid red; padding: 2px;">6</span>	71, 95, 121, 137	0
All	All	1522/1698 (89%)	0.12	33 (2%) <span style="border: 1px solid blue; padding: 2px;">65</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	29, 61, 103, 137	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	PHE	5.6
1	F	258	PHE	4.2
1	F	265	TYR	3.5
1	F	154	LEU	3.3
1	C	68[B]	ASP	3.2

### 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

There are no such residues in this entry.