



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3J1R  
EMDB ID: : EMD-5423  
Title : Filaments from *Ignicoccus hospitalis* Show Diversity of Packing in Proteins Containing N-terminal Type IV Pilin Helices  
Authors : Yu, X.; Goforth, C.; Meyer, C.; Rachel, R.; Wirth, R.; Schroeder, G.F.; Egelman, E.H.  
Deposited on : 2012-05-18  
Resolution : 7.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

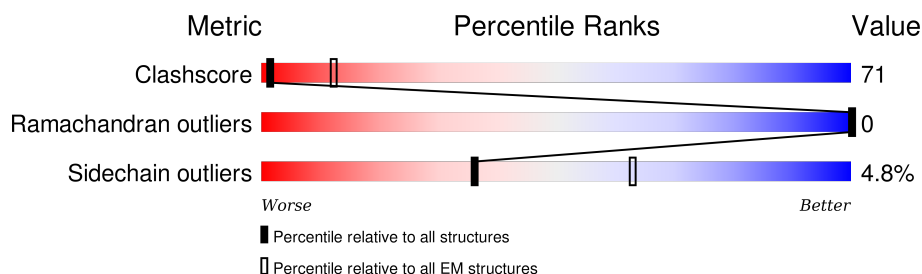
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.50 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.




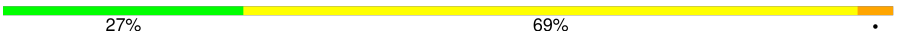



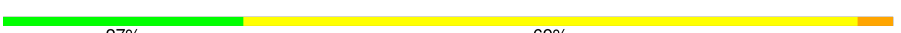
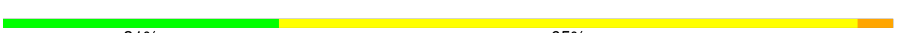





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	26	27% 69% .
1	B	26	35% 62% .
1	C	26	35% 62% .
1	D	26	27% 69% .
1	E	26	27% 69% .
1	F	26	31% 65% .
1	G	26	27% 69% .
1	H	26	35% 62% .
1	I	26	27% 69% .

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Mol	Chain	Length	Quality of chain
1	J	26	 35% 62% .
1	K	26	 27% 69% .
1	L	26	 35% 62% .
1	M	26	 35% 62% .
1	N	26	 31% 65% .
1	O	26	 27% 69% .
1	P	26	 31% 65% .
1	Q	26	 27% 69% .
1	R	26	 35% 62% .
1	S	26	 31% 65% .
1	T	26	 35% 62% .
1	U	26	 27% 69% .

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4011 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 archaeal adhesion filament core.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	26	Total	C	N	O	0	0
			191	133	27	31		
1	B	26	Total	C	N	O	0	0
			191	133	27	31		
1	C	26	Total	C	N	O	0	0
			191	133	27	31		
1	D	26	Total	C	N	O	0	0
			191	133	27	31		
1	E	26	Total	C	N	O	0	0
			191	133	27	31		
1	F	26	Total	C	N	O	0	0
			191	133	27	31		
1	G	26	Total	C	N	O	0	0
			191	133	27	31		
1	H	26	Total	C	N	O	0	0
			191	133	27	31		
1	I	26	Total	C	N	O	0	0
			191	133	27	31		
1	J	26	Total	C	N	O	0	0
			191	133	27	31		
1	K	26	Total	C	N	O	0	0
			191	133	27	31		
1	L	26	Total	C	N	O	0	0
			191	133	27	31		
1	M	26	Total	C	N	O	0	0
			191	133	27	31		
1	N	26	Total	C	N	O	0	0
			191	133	27	31		
1	O	26	Total	C	N	O	0	0
			191	133	27	31		
1	P	26	Total	C	N	O	0	0
			191	133	27	31		
1	Q	26	Total	C	N	O	0	0
			191	133	27	31		

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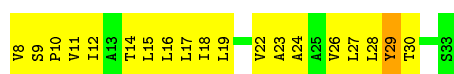
Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	26	Total 191	C 133	N 27	O 31	0	0
1	S	26	Total 191	C 133	N 27	O 31	0	0
1	T	26	Total 191	C 133	N 27	O 31	0	0
1	U	26	Total 191	C 133	N 27	O 31	0	0

### 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. 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.

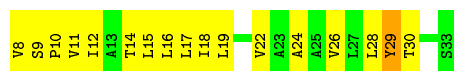
- Molecule 1: archaeal adhesion filament core

Chain A: 



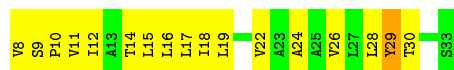
- Molecule 1: archaeal adhesion filament core

Chain B: 



- Molecule 1: archaeal adhesion filament core

Chain C: 



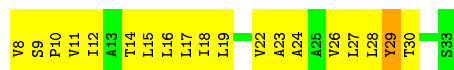
- Molecule 1: archaeal adhesion filament core

Chain D: 



- Molecule 1: archaeal adhesion filament core

Chain E: 



- Molecule 1: archaeal adhesion filament core

Chain F: 




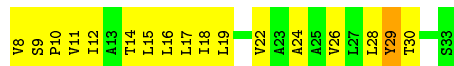
- Molecule 1: archaeal adhesion filament core

Chain G:  27% 69%



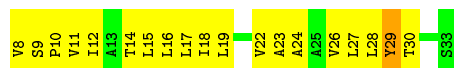
- Molecule 1: archaeal adhesion filament core

Chain H:  35% 62%



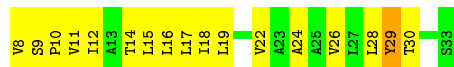
- Molecule 1: archaeal adhesion filament core

Chain I:  27% 69%

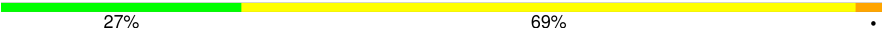


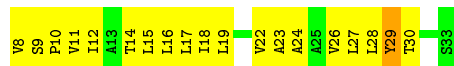
- Molecule 1: archaeal adhesion filament core

Chain J:  35% 62%



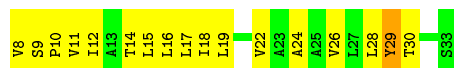
- Molecule 1: archaeal adhesion filament core

Chain K:  27% 69%



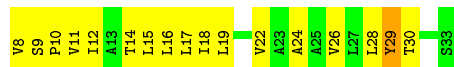
- Molecule 1: archaeal adhesion filament core

Chain L:  35% 62%



- Molecule 1: archaeal adhesion filament core

Chain M:  35% 62%

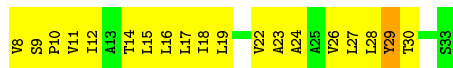
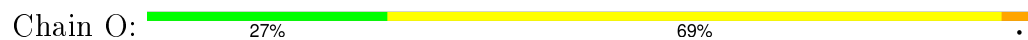


- Molecule 1: archaeal adhesion filament core

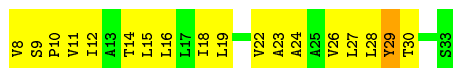
Chain N:  31% 65%



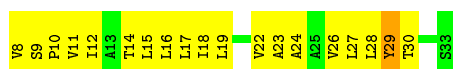
- Molecule 1: archaeal adhesion filament core



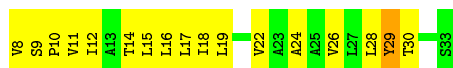
- Molecule 1: archaeal adhesion filament core



- Molecule 1: archaeal adhesion filament core



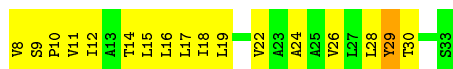
- Molecule 1: archaeal adhesion filament core



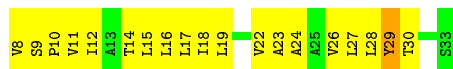
- Molecule 1: archaeal adhesion filament core



- Molecule 1: archaeal adhesion filament core



- Molecule 1: archaeal adhesion filament core





## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Each image was multiplied by the CTF. The final volume was amplitude-corrected in Fourier space by dividing by the sum of the squared CTFs.	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	55000	Depositor
Image detector	Kodak SO163 film	Depositor

## 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  >2	RMSZ	# Z  >2
1	A	0.24	0/194	0.53	0/270
1	B	0.24	0/194	0.53	0/270
1	C	0.24	0/194	0.53	0/270
1	D	0.24	0/194	0.53	0/270
1	E	0.24	0/194	0.53	0/270
1	F	0.24	0/194	0.53	0/270
1	G	0.24	0/194	0.53	0/270
1	H	0.24	0/194	0.53	0/270
1	I	0.24	0/194	0.53	0/270
1	J	0.24	0/194	0.53	0/270
1	K	0.24	0/194	0.53	0/270
1	L	0.24	0/194	0.53	0/270
1	M	0.24	0/194	0.53	0/270
1	N	0.24	0/194	0.53	0/270
1	O	0.24	0/194	0.53	0/270
1	P	0.24	0/194	0.53	0/270
1	Q	0.25	0/194	0.53	0/270
1	R	0.24	0/194	0.53	0/270
1	S	0.24	0/194	0.53	0/270
1	T	0.24	0/194	0.53	0/270
1	U	0.24	0/194	0.53	0/270
All	All	0.24	0/4074	0.53	0/5670

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	191	0	218	30	0
1	B	191	0	218	34	0
1	C	191	0	218	33	0
1	D	191	0	218	37	0
1	E	191	0	218	37	0
1	F	191	0	218	37	0
1	G	191	0	218	38	0
1	H	191	0	218	36	0
1	I	191	0	218	38	0
1	J	191	0	218	37	0
1	K	191	0	218	38	0
1	L	191	0	218	35	0
1	M	191	0	218	38	0
1	N	191	0	218	37	0
1	O	191	0	218	38	0
1	P	191	0	218	38	0
1	Q	191	0	218	39	0
1	R	191	0	218	38	0
1	S	191	0	218	32	0
1	T	191	0	218	33	0
1	U	191	0	218	31	0
All	All	4011	0	4578	611	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 71.

The worst 5 of 611 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:H:11:VAL:HG12	1:I:8:VAL:CG2	1.91	1.01
1:R:11:VAL:HG12	1:S:8:VAL:CG2	1.91	1.01
1:A:11:VAL:HG12	1:B:8:VAL:CG2	1.91	1.01
1:K:11:VAL:HG12	1:L:8:VAL:CG2	1.91	1.01
1:E:11:VAL:HG12	1:F:8:VAL:CG2	1.91	1.00

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	B	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	C	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	D	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	E	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	F	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	G	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	H	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	I	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	J	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	K	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	L	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	M	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	N	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	O	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	P	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	Q	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	R	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	S	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	T	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
1	U	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
All	All	504/546 (92%)	441 (88%)	63 (12%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	B	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	C	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	D	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	E	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	F	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	G	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	H	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	I	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	J	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	K	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	L	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	M	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	N	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	O	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	P	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	Q	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	R	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	S	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	T	21/21 (100%)	20 (95%)	1 (5%)	31	67
1	U	21/21 (100%)	20 (95%)	1 (5%)	31	67
All	All	441/441 (100%)	420 (95%)	21 (5%)	36	67

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	29	TYR
1	L	29	TYR

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Mol	Chain	Res	Type
1	R	29	TYR
1	I	29	TYR
1	S	29	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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.