wwPDB EM Validation Summary Report

Nov 6, 2022 – 01:59 AM EDT

PDB ID	:	5WJY
EMDB ID	:	EMD-8852
Title	:	Cryo-EM structure of B. subtilis flagellar filaments S285P
Authors	:	Wang, F.; Burrage, A.M.; Kearns, D.B.; Egelman, E.H.
Deposited on	:	2017-07-24
Resolution	:	4.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

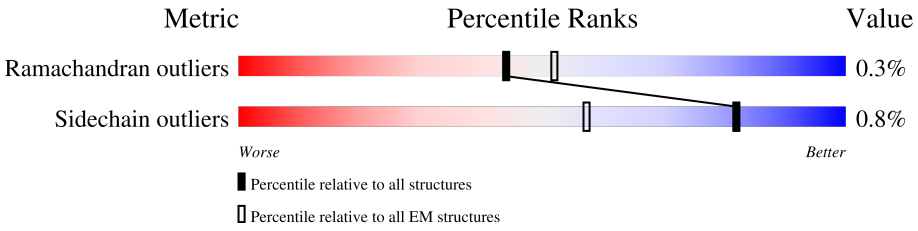
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	304	98%
1	B	304	98%
1	C	304	98%
1	D	304	98%
1	E	304	98%
1	F	304	98%
1	G	304	98%
1	H	304	98%
1	I	304	98%
1	J	304	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	304	98%
1	L	304	98%
1	M	304	98%
1	N	304	98%
1	O	304	98%
1	P	304	98%
1	Q	304	98%
1	R	304	98%
1	S	304	98%
1	T	304	98%
1	U	304	98%
1	V	304	98%
1	W	304	98%
1	X	304	98%
1	Y	304	98%
1	Z	304	98%
1	a	304	98%
1	b	304	98%
1	c	304	98%
1	d	304	98%
1	e	304	98%
1	f	304	98%
1	g	304	98%
1	h	304	98%
1	i	304	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	j	304	98%
1	k	304	98%
1	l	304	98%
1	m	304	98%
1	n	304	98%
1	o	304	98%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 184951 atoms, of which 92127 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 Flagellin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	B	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	C	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	D	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	E	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	F	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	G	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	H	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	I	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	J	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	K	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	L	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	M	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	N	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	O	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	P	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	Q	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	S	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	T	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	U	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	V	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	W	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	X	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	Y	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	Z	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	a	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	b	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	c	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	d	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	e	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	f	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	g	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	h	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	i	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	j	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	k	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	l	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	m	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	n	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		
1	o	302	Total	C	H	N	O	S	0	0
			4511	1368	2247	415	473	8		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	CYS	THR	engineered mutation	UNP A0A162QQD4
A	285	PRO	SER	engineered mutation	UNP A0A162QQD4
B	209	CYS	THR	engineered mutation	UNP A0A162QQD4
B	285	PRO	SER	engineered mutation	UNP A0A162QQD4
C	209	CYS	THR	engineered mutation	UNP A0A162QQD4
C	285	PRO	SER	engineered mutation	UNP A0A162QQD4
D	209	CYS	THR	engineered mutation	UNP A0A162QQD4
D	285	PRO	SER	engineered mutation	UNP A0A162QQD4
E	209	CYS	THR	engineered mutation	UNP A0A162QQD4
E	285	PRO	SER	engineered mutation	UNP A0A162QQD4
F	209	CYS	THR	engineered mutation	UNP A0A162QQD4
F	285	PRO	SER	engineered mutation	UNP A0A162QQD4
G	209	CYS	THR	engineered mutation	UNP A0A162QQD4
G	285	PRO	SER	engineered mutation	UNP A0A162QQD4
H	209	CYS	THR	engineered mutation	UNP A0A162QQD4
H	285	PRO	SER	engineered mutation	UNP A0A162QQD4
I	209	CYS	THR	engineered mutation	UNP A0A162QQD4
I	285	PRO	SER	engineered mutation	UNP A0A162QQD4
J	209	CYS	THR	engineered mutation	UNP A0A162QQD4
J	285	PRO	SER	engineered mutation	UNP A0A162QQD4
K	209	CYS	THR	engineered mutation	UNP A0A162QQD4
K	285	PRO	SER	engineered mutation	UNP A0A162QQD4
L	209	CYS	THR	engineered mutation	UNP A0A162QQD4
L	285	PRO	SER	engineered mutation	UNP A0A162QQD4
M	209	CYS	THR	engineered mutation	UNP A0A162QQD4
M	285	PRO	SER	engineered mutation	UNP A0A162QQD4
N	209	CYS	THR	engineered mutation	UNP A0A162QQD4
N	285	PRO	SER	engineered mutation	UNP A0A162QQD4
O	209	CYS	THR	engineered mutation	UNP A0A162QQD4
O	285	PRO	SER	engineered mutation	UNP A0A162QQD4
P	209	CYS	THR	engineered mutation	UNP A0A162QQD4
P	285	PRO	SER	engineered mutation	UNP A0A162QQD4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	209	CYS	THR	engineered mutation	UNP A0A162QQD4
Q	285	PRO	SER	engineered mutation	UNP A0A162QQD4
R	209	CYS	THR	engineered mutation	UNP A0A162QQD4
R	285	PRO	SER	engineered mutation	UNP A0A162QQD4
S	209	CYS	THR	engineered mutation	UNP A0A162QQD4
S	285	PRO	SER	engineered mutation	UNP A0A162QQD4
T	209	CYS	THR	engineered mutation	UNP A0A162QQD4
T	285	PRO	SER	engineered mutation	UNP A0A162QQD4
U	209	CYS	THR	engineered mutation	UNP A0A162QQD4
U	285	PRO	SER	engineered mutation	UNP A0A162QQD4
V	209	CYS	THR	engineered mutation	UNP A0A162QQD4
V	285	PRO	SER	engineered mutation	UNP A0A162QQD4
W	209	CYS	THR	engineered mutation	UNP A0A162QQD4
W	285	PRO	SER	engineered mutation	UNP A0A162QQD4
X	209	CYS	THR	engineered mutation	UNP A0A162QQD4
X	285	PRO	SER	engineered mutation	UNP A0A162QQD4
Y	209	CYS	THR	engineered mutation	UNP A0A162QQD4
Y	285	PRO	SER	engineered mutation	UNP A0A162QQD4
Z	209	CYS	THR	engineered mutation	UNP A0A162QQD4
Z	285	PRO	SER	engineered mutation	UNP A0A162QQD4
a	209	CYS	THR	engineered mutation	UNP A0A162QQD4
a	285	PRO	SER	engineered mutation	UNP A0A162QQD4
b	209	CYS	THR	engineered mutation	UNP A0A162QQD4
b	285	PRO	SER	engineered mutation	UNP A0A162QQD4
c	209	CYS	THR	engineered mutation	UNP A0A162QQD4
c	285	PRO	SER	engineered mutation	UNP A0A162QQD4
d	209	CYS	THR	engineered mutation	UNP A0A162QQD4
d	285	PRO	SER	engineered mutation	UNP A0A162QQD4
e	209	CYS	THR	engineered mutation	UNP A0A162QQD4
e	285	PRO	SER	engineered mutation	UNP A0A162QQD4
f	209	CYS	THR	engineered mutation	UNP A0A162QQD4
f	285	PRO	SER	engineered mutation	UNP A0A162QQD4
g	209	CYS	THR	engineered mutation	UNP A0A162QQD4
g	285	PRO	SER	engineered mutation	UNP A0A162QQD4
h	209	CYS	THR	engineered mutation	UNP A0A162QQD4
h	285	PRO	SER	engineered mutation	UNP A0A162QQD4
i	209	CYS	THR	engineered mutation	UNP A0A162QQD4
i	285	PRO	SER	engineered mutation	UNP A0A162QQD4
j	209	CYS	THR	engineered mutation	UNP A0A162QQD4
j	285	PRO	SER	engineered mutation	UNP A0A162QQD4
k	209	CYS	THR	engineered mutation	UNP A0A162QQD4
k	285	PRO	SER	engineered mutation	UNP A0A162QQD4

Continued on next page...

Continued from previous page...

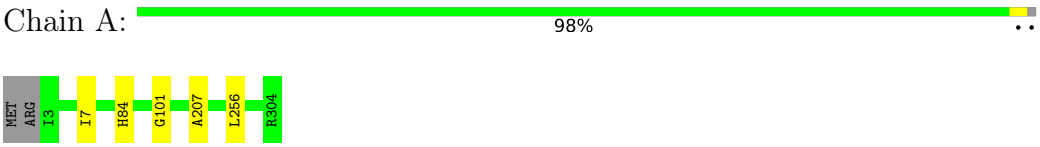
Chain	Residue	Modelled	Actual	Comment	Reference
l	209	CYS	THR	engineered mutation	UNP A0A162QQD4
l	285	PRO	SER	engineered mutation	UNP A0A162QQD4
m	209	CYS	THR	engineered mutation	UNP A0A162QQD4
m	285	PRO	SER	engineered mutation	UNP A0A162QQD4
n	209	CYS	THR	engineered mutation	UNP A0A162QQD4
n	285	PRO	SER	engineered mutation	UNP A0A162QQD4
o	209	CYS	THR	engineered mutation	UNP A0A162QQD4
o	285	PRO	SER	engineered mutation	UNP A0A162QQD4

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

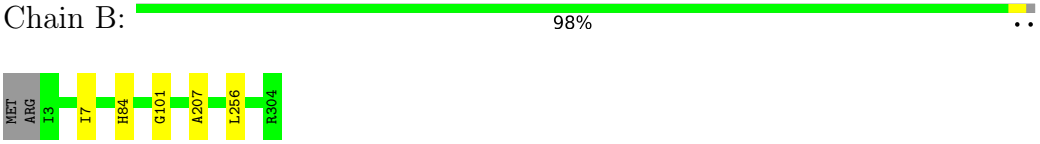
- Molecule 1: Flagellin

Chain A:



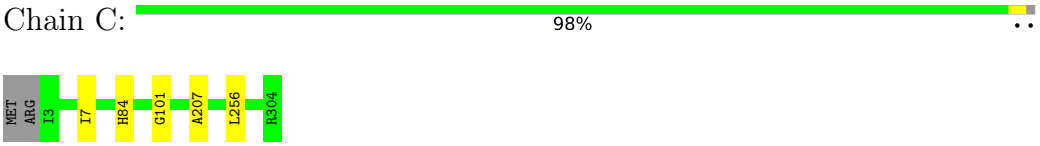
- Molecule 1: Flagellin

Chain B:



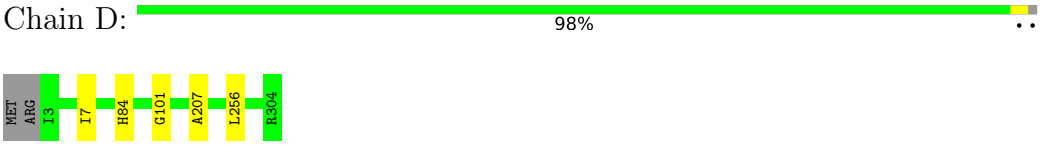
- Molecule 1: Flagellin

Chain C:



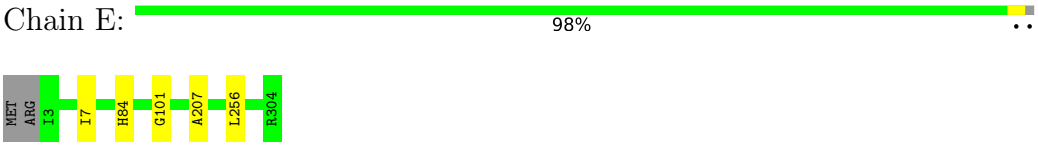
- Molecule 1: Flagellin

Chain D:



- Molecule 1: Flagellin

Chain E:

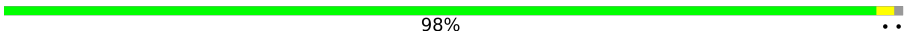


- Molecule 1: Flagellin

Chain F:

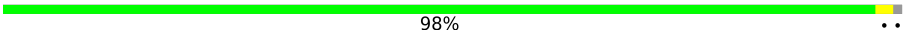
• Molecule 1: Flagellin

Chain G:



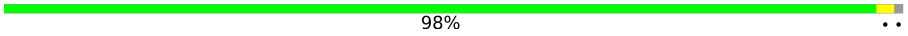
• Molecule 1: Flagellin

Chain H:



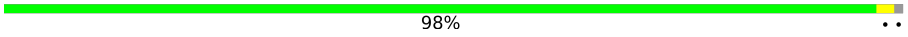
• Molecule 1: Flagellin

Chain I:



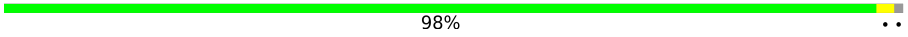
• Molecule 1: Flagellin

Chain J:



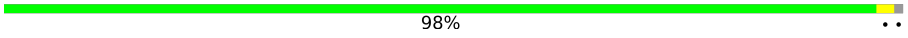
• Molecule 1: Flagellin

Chain K:



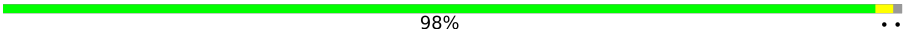
• Molecule 1: Flagellin

Chain L:

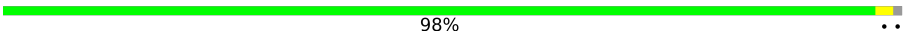


• Molecule 1: Flagellin

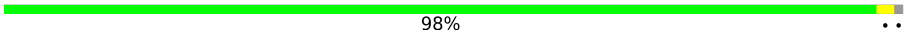
Chain M:



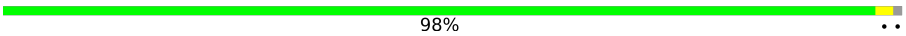
• Molecule 1: Flagellin

Chain N: 

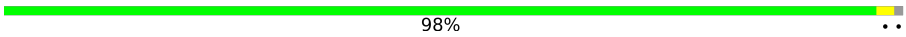
• Molecule 1: Flagellin

Chain O: 

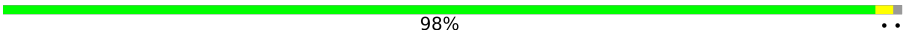
• Molecule 1: Flagellin

Chain P: 

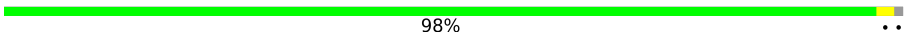
• Molecule 1: Flagellin

Chain Q: 

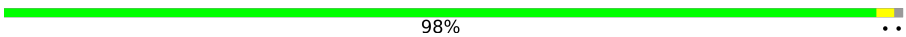
• Molecule 1: Flagellin

Chain R: 

• Molecule 1: Flagellin

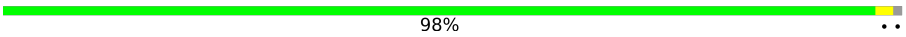
Chain S: 

• Molecule 1: Flagellin

Chain T: 

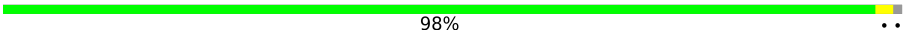
• Molecule 1: Flagellin

Chain U:



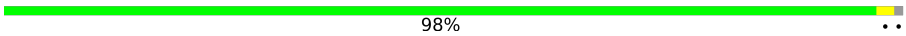
• Molecule 1: Flagellin

Chain V:



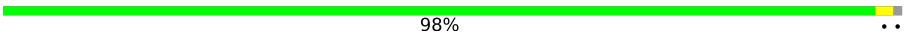
• Molecule 1: Flagellin

Chain W:



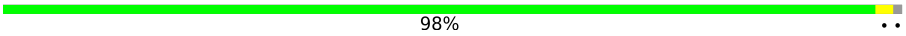
• Molecule 1: Flagellin

Chain X:



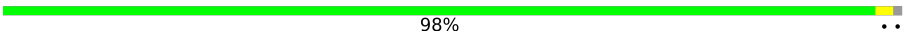
• Molecule 1: Flagellin

Chain Y:



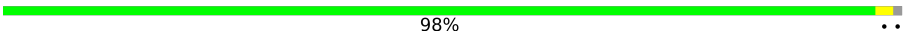
• Molecule 1: Flagellin

Chain Z:



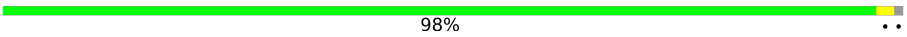
• Molecule 1: Flagellin

Chain a:



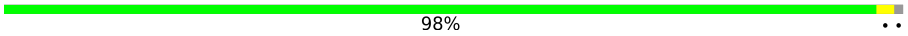
• Molecule 1: Flagellin

Chain b:



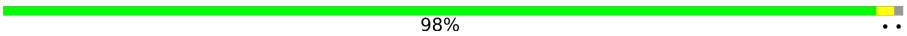
• Molecule 1: Flagellin

Chain c:



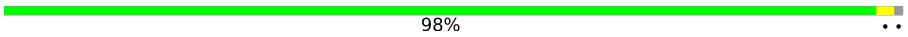
• Molecule 1: Flagellin

Chain d:



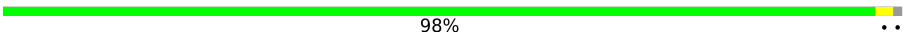
• Molecule 1: Flagellin

Chain e:



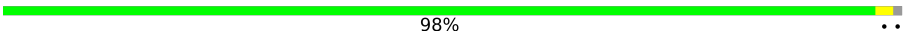
• Molecule 1: Flagellin

Chain f:



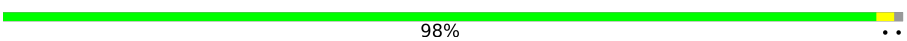
• Molecule 1: Flagellin

Chain g:



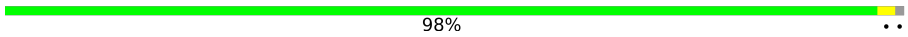
• Molecule 1: Flagellin

Chain h:



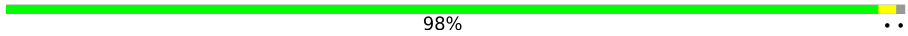
• Molecule 1: Flagellin

Chain i:



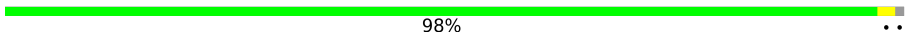
• Molecule 1: Flagellin

Chain j:



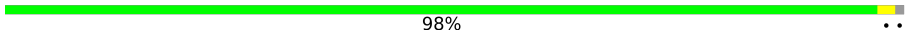
• Molecule 1: Flagellin

Chain k:



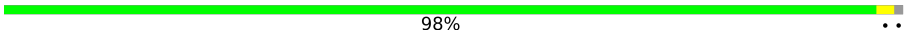
• Molecule 1: Flagellin

Chain l:



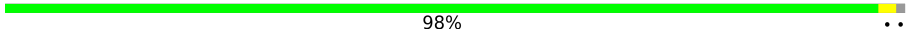
• Molecule 1: Flagellin

Chain m:



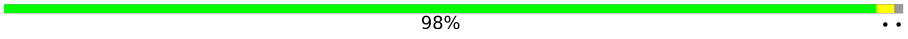
• Molecule 1: Flagellin

Chain n:



• Molecule 1: Flagellin

Chain o:




MET
ARG
I3
I7
H84
G101
A207
L256
R304

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=65.3°, rise=4.72 Å, axial sym=C1	Depositor
Number of segments used	55403	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.40	0/2276	0.62	0/3070
1	B	0.40	0/2276	0.62	0/3070
1	C	0.40	0/2276	0.62	0/3070
1	D	0.40	0/2276	0.62	0/3070
1	E	0.40	0/2276	0.62	0/3070
1	F	0.40	0/2276	0.62	0/3070
1	G	0.40	0/2276	0.62	0/3070
1	H	0.40	0/2276	0.62	0/3070
1	I	0.40	0/2276	0.62	0/3070
1	J	0.40	0/2276	0.62	0/3070
1	K	0.40	0/2276	0.62	0/3070
1	L	0.40	0/2276	0.62	0/3070
1	M	0.40	0/2276	0.62	0/3070
1	N	0.40	0/2276	0.62	0/3070
1	O	0.40	0/2276	0.62	0/3070
1	P	0.40	0/2276	0.62	0/3070
1	Q	0.40	0/2276	0.62	0/3070
1	R	0.40	0/2276	0.62	0/3070
1	S	0.40	0/2276	0.62	0/3070
1	T	0.40	0/2276	0.62	0/3070
1	U	0.40	0/2276	0.62	0/3070
1	V	0.40	0/2276	0.62	0/3070
1	W	0.40	0/2276	0.62	0/3070
1	X	0.40	0/2276	0.62	0/3070
1	Y	0.40	0/2276	0.62	0/3070
1	Z	0.40	0/2276	0.62	0/3070
1	a	0.40	0/2276	0.62	0/3070
1	b	0.40	0/2276	0.62	0/3070
1	c	0.40	0/2276	0.62	0/3070
1	d	0.40	0/2276	0.62	0/3070
1	e	0.40	0/2276	0.62	0/3070
1	f	0.40	0/2276	0.62	0/3070
1	g	0.40	0/2276	0.62	0/3070
1	h	0.40	0/2276	0.62	0/3070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	i	0.40	0/2276	0.62	0/3070
1	j	0.40	0/2276	0.62	0/3070
1	k	0.40	0/2276	0.62	0/3070
1	l	0.40	0/2276	0.62	0/3070
1	m	0.40	0/2276	0.62	0/3070
1	n	0.40	0/2276	0.62	0/3070
1	o	0.40	0/2276	0.62	0/3070
All	All	0.40	0/93316	0.62	0/125870

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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
1	a	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	2
1	c	0	2
1	d	0	2
1	e	0	2
1	f	0	2
1	g	0	2
1	h	0	2
1	i	0	2
1	j	0	2
1	k	0	2
1	l	0	2
1	m	0	2
1	n	0	2
1	o	0	2
All	All	0	82

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLY	Peptide
1	A	207	ALA	Peptide
1	B	101	GLY	Peptide
1	B	207	ALA	Peptide
1	C	101	GLY	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	B	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	C	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	D	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	E	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	F	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	G	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	H	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	I	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	J	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	K	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	L	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	M	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	N	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	O	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	P	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	Q	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	R	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	S	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	T	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	U	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	V	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	W	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	X	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	Y	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	Z	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	a	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	b	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76
1	c	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41	76
1	d	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	e	300/304 (99%)	264 (88%)	35 (12%)	1 (0%)	41 76
1	f	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	g	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	h	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	i	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41 76
1	j	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	k	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	l	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	m	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
1	n	300/304 (99%)	262 (87%)	37 (12%)	1 (0%)	41 76
1	o	300/304 (99%)	263 (88%)	36 (12%)	1 (0%)	41 76
All	All	12300/12464 (99%)	10773 (88%)	1486 (12%)	41 (0%)	44 76

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	B	7	ILE
1	C	7	ILE
1	D	7	ILE
1	E	7	ILE

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 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	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	B	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	C	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	D	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	E	244/246 (99%)	242 (99%)	2 (1%)	81 89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	G	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	H	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	I	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	J	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	K	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	L	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	M	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	N	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	O	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	P	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	Q	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	R	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	S	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	T	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	U	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	V	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	W	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	X	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	Y	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	Z	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	a	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	b	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	c	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	d	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	e	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	f	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	g	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	h	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	i	244/246 (99%)	242 (99%)	2 (1%)	81	89
1	j	244/246 (99%)	242 (99%)	2 (1%)	81	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	k	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	l	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	m	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	n	244/246 (99%)	242 (99%)	2 (1%)	81 89
1	o	244/246 (99%)	242 (99%)	2 (1%)	81 89
All	All	10004/10086 (99%)	9922 (99%)	82 (1%)	82 89

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	256	LEU
1	j	256	LEU
1	d	256	LEU
1	g	256	LEU
1	l	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 287 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	74	GLN
1	o	67	GLN
1	f	298	ASN
1	j	298	ASN
1	M	24	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 monosaccharides 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-8852. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.