



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 23, 2017 – 08:20 PM EDT

PDB ID : 5WJX
EMDB ID: : EMD-8851
Title : Cryo-EM structure of B. subtilis flagellar filaments S17P
Authors : Wang, F.; Burrage, A.M.; Orlova, A.; Kearns, D.B.; Egelman, E.H.
Deposited on : unknown
Resolution : 6.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

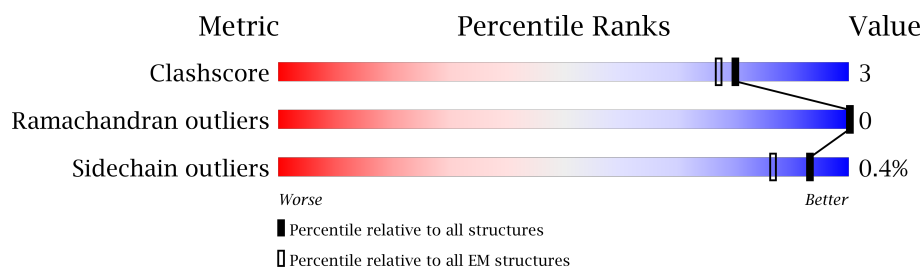
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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.
















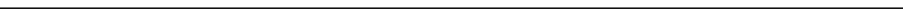




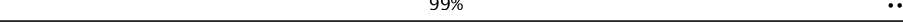
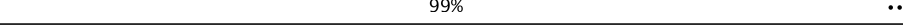
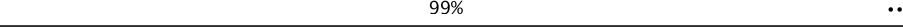
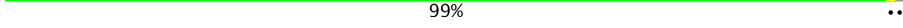
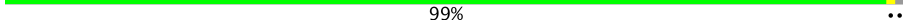
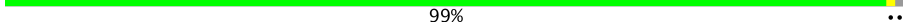
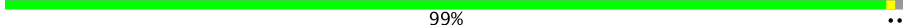
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 ≥ 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	304	85% 15% .
1	B	304	85% 14% .
1	C	304	84% 15% .
1	D	304	84% 15% .
1	E	304	85% 14% .
1	F	304	85% 15% .
1	G	304	84% 15% .
1	H	304	85% 14% .
1	I	304	85% 15% .

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Mol	Chain	Length	Quality of chain
1	J	304	 85% 15% .
1	K	304	 85% 14% .
1	L	304	 84% 15% .
1	M	304	 85% 14% .
1	N	304	 85% 15% .
1	O	304	 85% 14% .
1	P	304	 86% 14% .
1	Q	304	 85% 14% .
1	R	304	 85% 14% .
1	S	304	 85% 14% .
1	T	304	 86% 14% .
1	U	304	 86% 14% .
1	V	304	 86% 14% .
1	W	304	 85% 14% .
1	X	304	 86% 13% .
1	Y	304	 87% 12% .
1	Z	304	 87% 13% .
1	a	304	 99% ..
1	b	304	 99% ..
1	c	304	 99% ..
1	d	304	 99% ..
1	e	304	 99% ..
1	f	304	 99% ..
1	g	304	 99% ..
1	h	304	 99% ..

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Mol	Chain	Length	Quality of chain
1	i	304	<div><div></div><div>99%</div><div>..</div></div>
1	j	304	<div><div></div><div>99%</div><div>..</div></div>
1	k	304	<div><div></div><div>99%</div><div>..</div></div>
1	l	304	<div><div></div><div>99%</div><div>..</div></div>
1	m	304	<div><div></div><div>99%</div><div>..</div></div>
1	n	304	<div><div></div><div>99%</div><div>..</div></div>
1	o	304	<div><div></div><div>99%</div><div>..</div></div>
1	p	304	<div><div></div><div>99%</div><div>..</div></div>
1	q	304	<div><div></div><div>99%</div><div>..</div></div>
1	r	304	<div><div></div><div>99%</div><div>..</div></div>
1	s	304	<div><div></div><div>99%</div><div>..</div></div>
1	t	304	<div><div></div><div>99%</div><div>..</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 207736 atoms, of which 103592 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 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	B	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	C	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	D	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	E	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	F	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	G	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	H	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	I	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	J	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	K	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	L	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	M	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	N	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	O	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	P	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	Q	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	S	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	T	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	U	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	V	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	W	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	X	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	Y	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	Z	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	a	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	b	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	c	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	d	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	e	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	f	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	g	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	h	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	i	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	j	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	k	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0
1	l	302	Total 4516	C 1368	H 2252	N 415	O 473	S 8	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	m	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	n	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	o	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	p	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	q	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	r	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	s	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		
1	t	302	Total	C	H	N	O	S	0	0
			4516	1368	2252	415	473	8		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	PRO	SER	engineered mutation	UNP A0A162QQD4
A	209	CYS	THR	engineered mutation	UNP A0A162QQD4
B	17	PRO	SER	engineered mutation	UNP A0A162QQD4
B	209	CYS	THR	engineered mutation	UNP A0A162QQD4
C	17	PRO	SER	engineered mutation	UNP A0A162QQD4
C	209	CYS	THR	engineered mutation	UNP A0A162QQD4
D	17	PRO	SER	engineered mutation	UNP A0A162QQD4
D	209	CYS	THR	engineered mutation	UNP A0A162QQD4
E	17	PRO	SER	engineered mutation	UNP A0A162QQD4
E	209	CYS	THR	engineered mutation	UNP A0A162QQD4
F	17	PRO	SER	engineered mutation	UNP A0A162QQD4
F	209	CYS	THR	engineered mutation	UNP A0A162QQD4
G	17	PRO	SER	engineered mutation	UNP A0A162QQD4
G	209	CYS	THR	engineered mutation	UNP A0A162QQD4
H	17	PRO	SER	engineered mutation	UNP A0A162QQD4
H	209	CYS	THR	engineered mutation	UNP A0A162QQD4
I	17	PRO	SER	engineered mutation	UNP A0A162QQD4
I	209	CYS	THR	engineered mutation	UNP A0A162QQD4
J	17	PRO	SER	engineered mutation	UNP A0A162QQD4
J	209	CYS	THR	engineered mutation	UNP A0A162QQD4
K	17	PRO	SER	engineered mutation	UNP A0A162QQD4
K	209	CYS	THR	engineered mutation	UNP A0A162QQD4
L	17	PRO	SER	engineered mutation	UNP A0A162QQD4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	209	CYS	THR	engineered mutation	UNP A0A162QQD4
M	17	PRO	SER	engineered mutation	UNP A0A162QQD4
M	209	CYS	THR	engineered mutation	UNP A0A162QQD4
N	17	PRO	SER	engineered mutation	UNP A0A162QQD4
N	209	CYS	THR	engineered mutation	UNP A0A162QQD4
O	17	PRO	SER	engineered mutation	UNP A0A162QQD4
O	209	CYS	THR	engineered mutation	UNP A0A162QQD4
P	17	PRO	SER	engineered mutation	UNP A0A162QQD4
P	209	CYS	THR	engineered mutation	UNP A0A162QQD4
Q	17	PRO	SER	engineered mutation	UNP A0A162QQD4
Q	209	CYS	THR	engineered mutation	UNP A0A162QQD4
R	17	PRO	SER	engineered mutation	UNP A0A162QQD4
R	209	CYS	THR	engineered mutation	UNP A0A162QQD4
S	17	PRO	SER	engineered mutation	UNP A0A162QQD4
S	209	CYS	THR	engineered mutation	UNP A0A162QQD4
T	17	PRO	SER	engineered mutation	UNP A0A162QQD4
T	209	CYS	THR	engineered mutation	UNP A0A162QQD4
U	17	PRO	SER	engineered mutation	UNP A0A162QQD4
U	209	CYS	THR	engineered mutation	UNP A0A162QQD4
V	17	PRO	SER	engineered mutation	UNP A0A162QQD4
V	209	CYS	THR	engineered mutation	UNP A0A162QQD4
W	17	PRO	SER	engineered mutation	UNP A0A162QQD4
W	209	CYS	THR	engineered mutation	UNP A0A162QQD4
X	17	PRO	SER	engineered mutation	UNP A0A162QQD4
X	209	CYS	THR	engineered mutation	UNP A0A162QQD4
Y	17	PRO	SER	engineered mutation	UNP A0A162QQD4
Y	209	CYS	THR	engineered mutation	UNP A0A162QQD4
Z	17	PRO	SER	engineered mutation	UNP A0A162QQD4
Z	209	CYS	THR	engineered mutation	UNP A0A162QQD4
a	17	PRO	SER	engineered mutation	UNP A0A162QQD4
a	209	CYS	THR	engineered mutation	UNP A0A162QQD4
b	17	PRO	SER	engineered mutation	UNP A0A162QQD4
b	209	CYS	THR	engineered mutation	UNP A0A162QQD4
c	17	PRO	SER	engineered mutation	UNP A0A162QQD4
c	209	CYS	THR	engineered mutation	UNP A0A162QQD4
d	17	PRO	SER	engineered mutation	UNP A0A162QQD4
d	209	CYS	THR	engineered mutation	UNP A0A162QQD4
e	17	PRO	SER	engineered mutation	UNP A0A162QQD4
e	209	CYS	THR	engineered mutation	UNP A0A162QQD4
f	17	PRO	SER	engineered mutation	UNP A0A162QQD4
f	209	CYS	THR	engineered mutation	UNP A0A162QQD4
g	17	PRO	SER	engineered mutation	UNP A0A162QQD4

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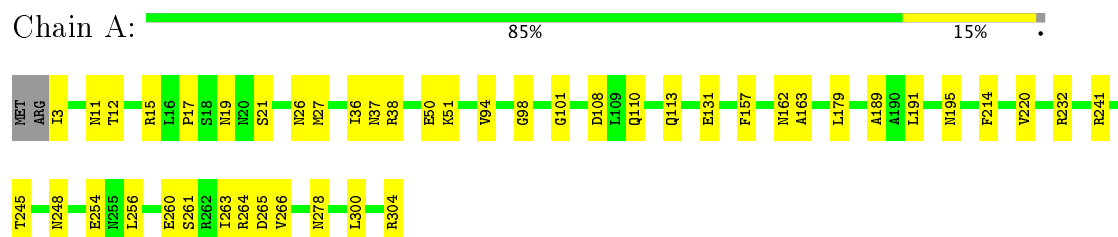
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Chain	Residue	Modelled	Actual	Comment	Reference
g	209	CYS	THR	engineered mutation	UNP A0A162QQD4
h	17	PRO	SER	engineered mutation	UNP A0A162QQD4
h	209	CYS	THR	engineered mutation	UNP A0A162QQD4
i	17	PRO	SER	engineered mutation	UNP A0A162QQD4
i	209	CYS	THR	engineered mutation	UNP A0A162QQD4
j	17	PRO	SER	engineered mutation	UNP A0A162QQD4
j	209	CYS	THR	engineered mutation	UNP A0A162QQD4
k	17	PRO	SER	engineered mutation	UNP A0A162QQD4
k	209	CYS	THR	engineered mutation	UNP A0A162QQD4
l	17	PRO	SER	engineered mutation	UNP A0A162QQD4
l	209	CYS	THR	engineered mutation	UNP A0A162QQD4
m	17	PRO	SER	engineered mutation	UNP A0A162QQD4
m	209	CYS	THR	engineered mutation	UNP A0A162QQD4
n	17	PRO	SER	engineered mutation	UNP A0A162QQD4
n	209	CYS	THR	engineered mutation	UNP A0A162QQD4
o	17	PRO	SER	engineered mutation	UNP A0A162QQD4
o	209	CYS	THR	engineered mutation	UNP A0A162QQD4
p	17	PRO	SER	engineered mutation	UNP A0A162QQD4
p	209	CYS	THR	engineered mutation	UNP A0A162QQD4
q	17	PRO	SER	engineered mutation	UNP A0A162QQD4
q	209	CYS	THR	engineered mutation	UNP A0A162QQD4
r	17	PRO	SER	engineered mutation	UNP A0A162QQD4
r	209	CYS	THR	engineered mutation	UNP A0A162QQD4
s	17	PRO	SER	engineered mutation	UNP A0A162QQD4
s	209	CYS	THR	engineered mutation	UNP A0A162QQD4
t	17	PRO	SER	engineered mutation	UNP A0A162QQD4
t	209	CYS	THR	engineered mutation	UNP A0A162QQD4

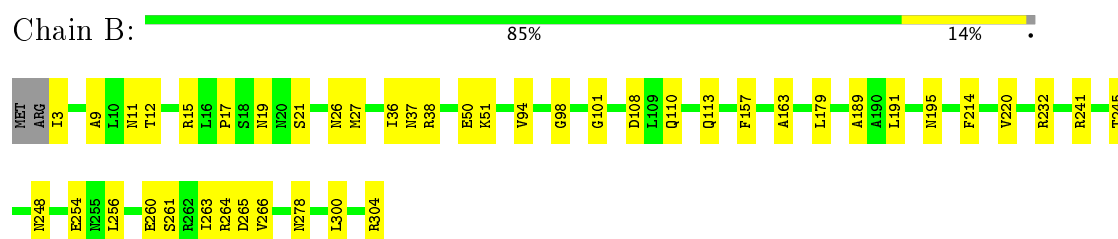
3 Residue-property plots

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.

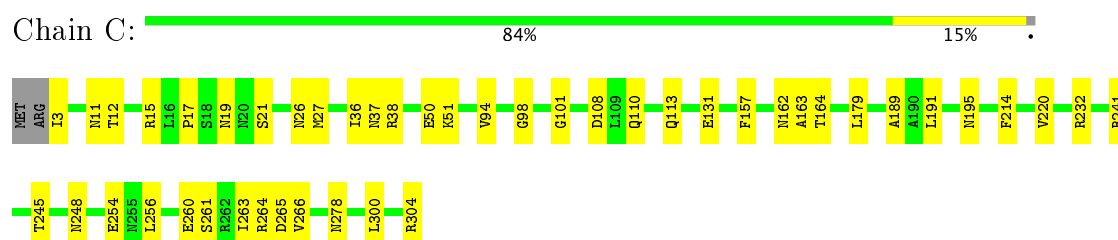
• Molecule 1: Flagellin



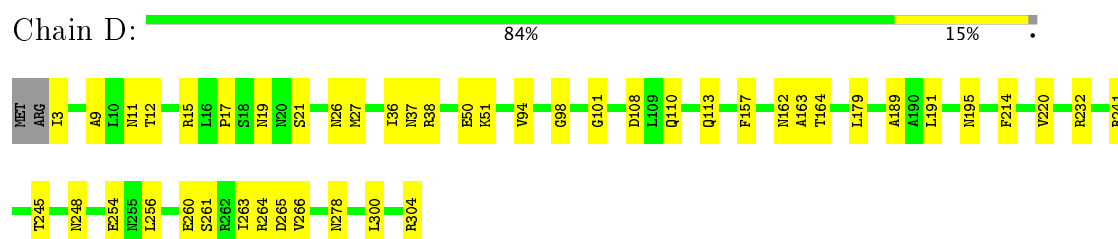
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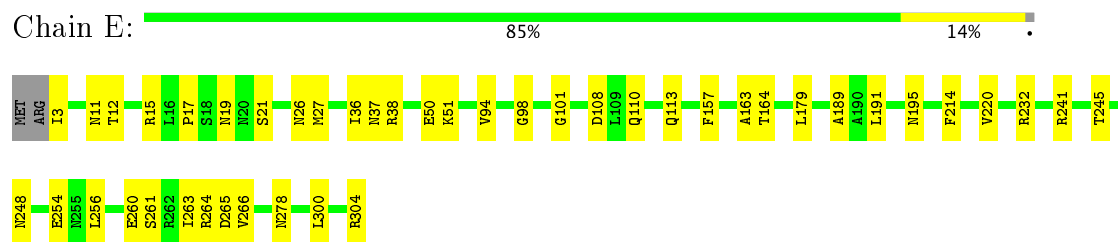
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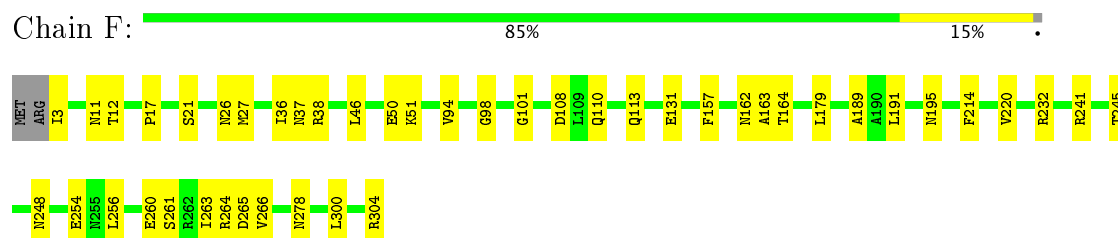
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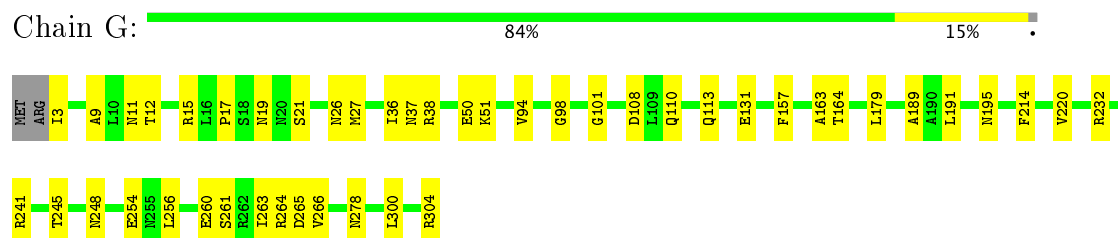
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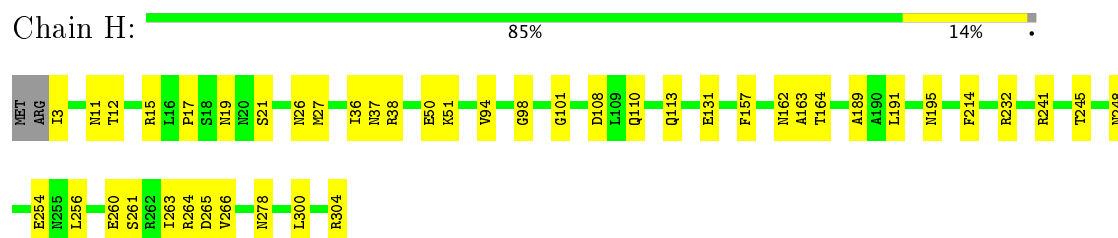
- Molecule 1: Flagellin



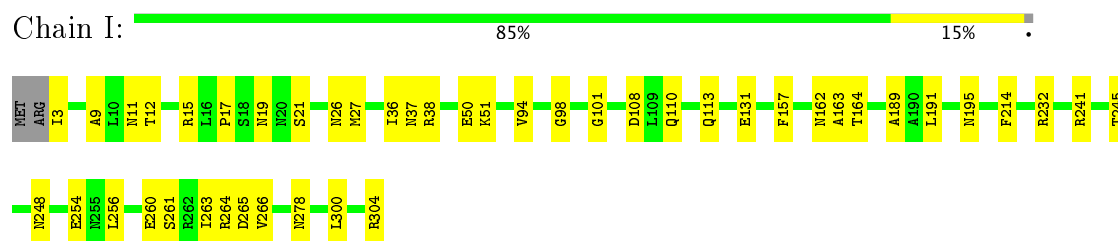
- Molecule 1: Flagellin



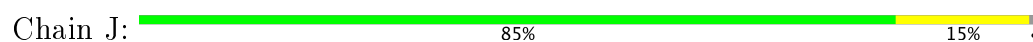
- Molecule 1: Flagellin

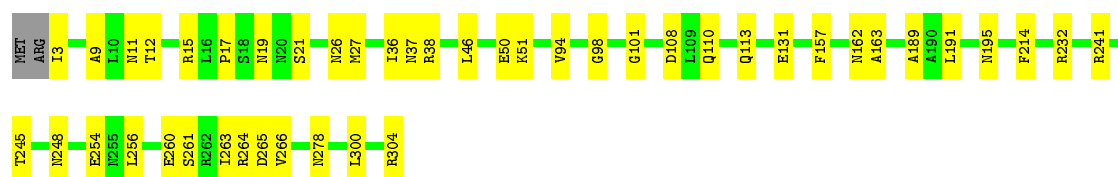


- Molecule 1: Flagellin



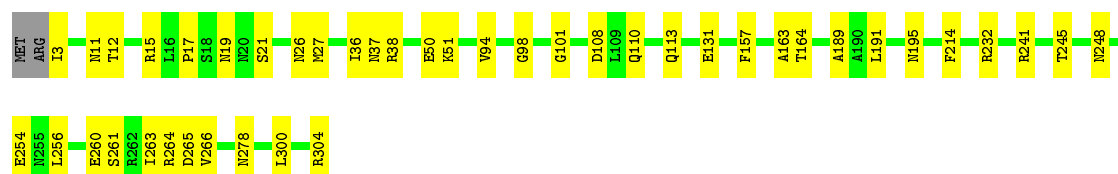
- Molecule 1: Flagellin





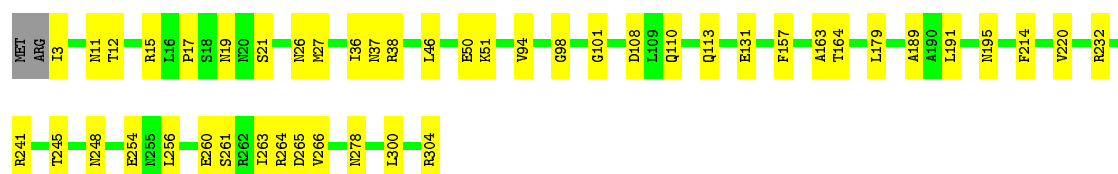
- Molecule 1: Flagellin

Chain K: 85% 14%



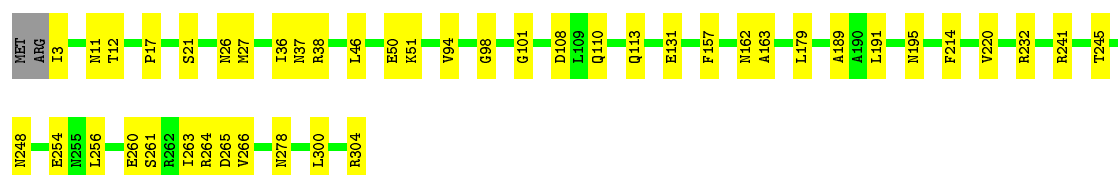
- Molecule 1: Flagellin

Chain L: 84% 15%



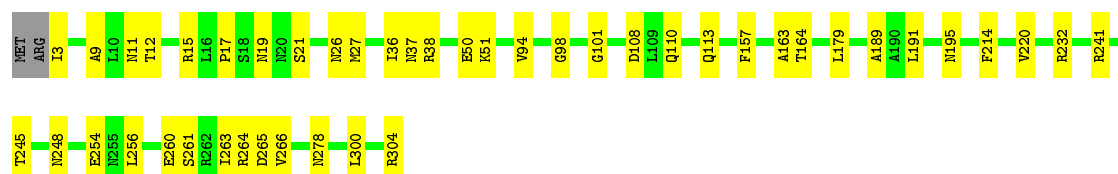
- Molecule 1: Flagellin

Chain M: 85% 14%



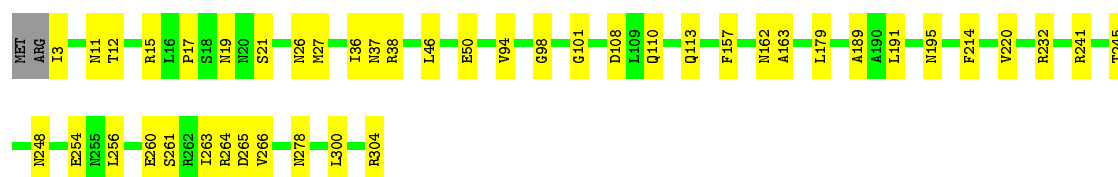
- Molecule 1: Flagellin

Chain N: 85% 15%



- Molecule 1: Flagellin

Chain O: 85% 14%



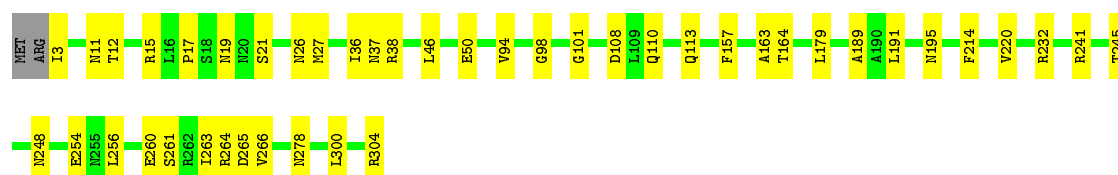
• Molecule 1: Flagellin

Chain P: 86% 14%



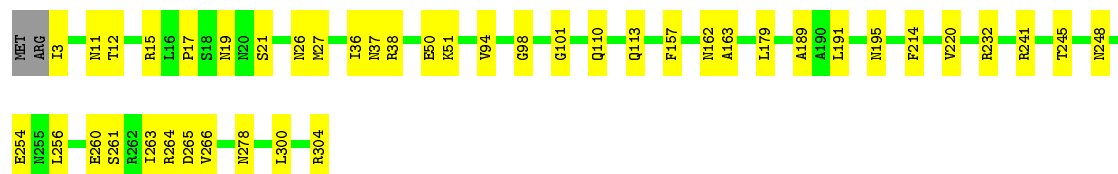
• Molecule 1: Flagellin

Chain Q: 85% 14%



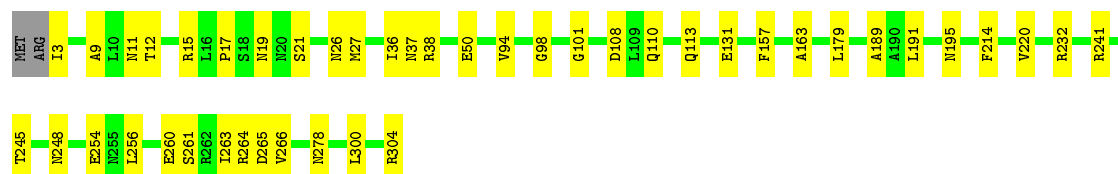
• Molecule 1: Flagellin

Chain R: 85% 14%



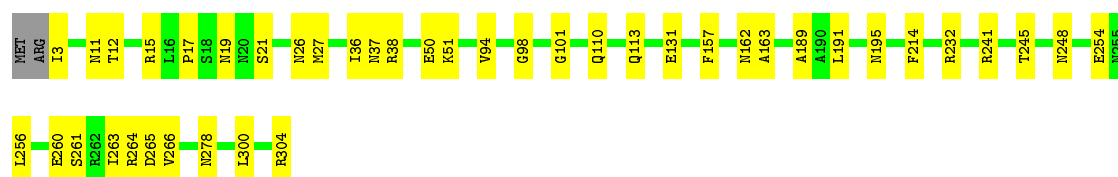
• Molecule 1: Flagellin

Chain S: 85% 14%



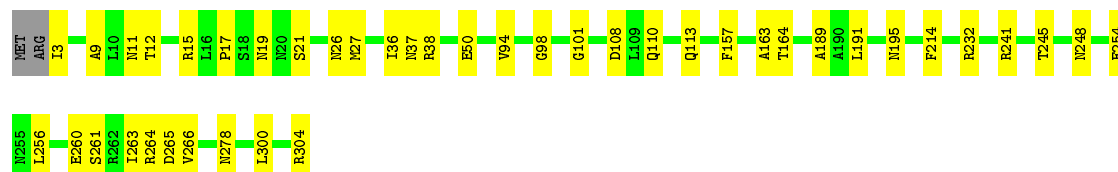
• Molecule 1: Flagellin

Chain T: 86% 14%



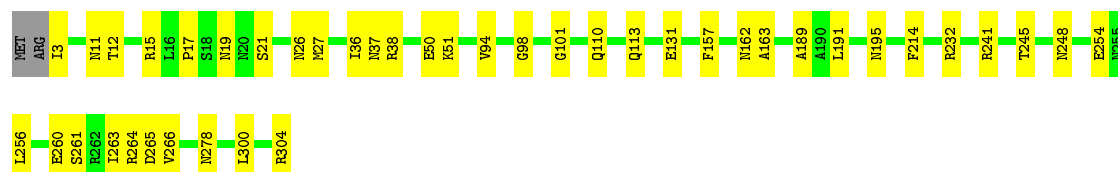
- Molecule 1: Flagellin

Chain U: 86% 14%



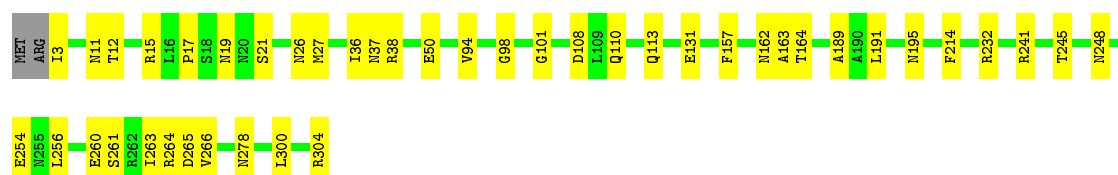
- Molecule 1: Flagellin

Chain V: 86% 14%



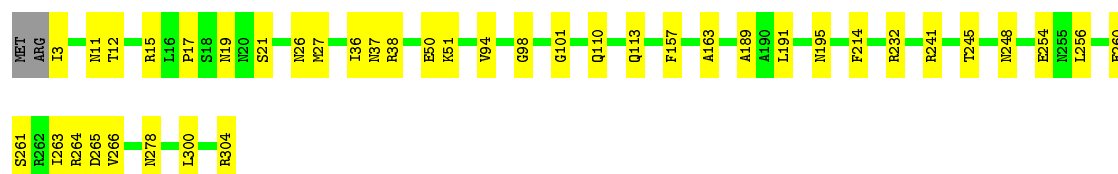
- Molecule 1: Flagellin

Chain W: 85% 14%



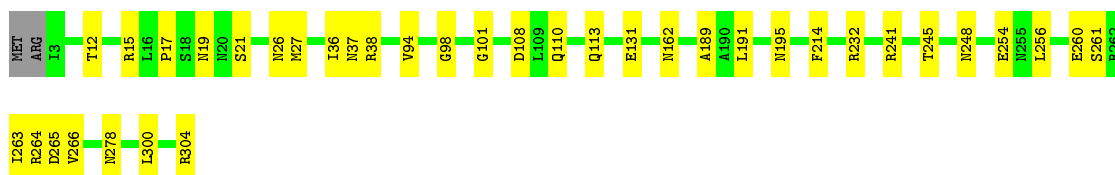
- Molecule 1: Flagellin

Chain X: 86% 13%



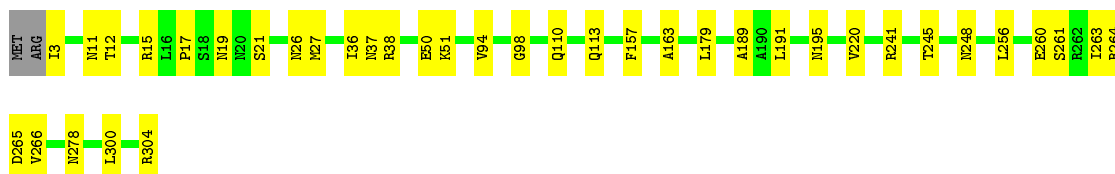
- Molecule 1: Flagellin

Chain Y: 87% 12%



- Molecule 1: Flagellin

Chain Z: 87% 13%



- Molecule 1: Flagellin

Chain a: 99%



- Molecule 1: Flagellin

Chain b: 99%



- Molecule 1: Flagellin

Chain c: 99%



- Molecule 1: Flagellin

Chain d: 99%



- Molecule 1: Flagellin

Chain e: 99%



● Molecule 1: Flagellin

Chain f:  99% ..

● Molecule 1: Flagellin

Chain g:  99% ..

● Molecule 1: Flagellin

Chain h:  99% ..

● Molecule 1: Flagellin

Chain i:  99% ..

● Molecule 1: Flagellin

Chain j:  99% ..

● Molecule 1: Flagellin

Chain k:  99% ..

● Molecule 1: Flagellin

Chain l:  99% ..

● Molecule 1: Flagellin

Chain m:  99% ..



- Molecule 1: Flagellin

Chain n:  99% ..



- Molecule 1: Flagellin

Chain o:  99% ..



- Molecule 1: Flagellin

Chain p:  99% ..



- Molecule 1: Flagellin

Chain q:  99% ..



- Molecule 1: Flagellin

Chain r:  99% ..



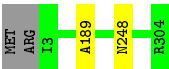
- Molecule 1: Flagellin

Chain s:  99% ..



- Molecule 1: Flagellin

Chain t:  99% ..



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=65.29°, rise=4.68 Å, axial sym=C1	Depositor
Number of segments used	13899	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 ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.41	0/2276	0.61	0/3070
1	B	0.41	0/2276	0.61	0/3070
1	C	0.41	0/2276	0.61	0/3070
1	D	0.41	0/2276	0.61	0/3070
1	E	0.41	0/2276	0.61	0/3070
1	F	0.41	0/2276	0.61	0/3070
1	G	0.41	0/2276	0.61	0/3070
1	H	0.41	0/2276	0.61	0/3070
1	I	0.41	0/2276	0.61	0/3070
1	J	0.41	0/2276	0.61	0/3070
1	K	0.41	0/2276	0.61	0/3070
1	L	0.41	0/2276	0.61	0/3070
1	M	0.41	0/2276	0.61	0/3070
1	N	0.41	0/2276	0.61	0/3070
1	O	0.41	0/2276	0.61	0/3070
1	P	0.41	0/2276	0.61	0/3070
1	Q	0.41	0/2276	0.61	0/3070
1	R	0.41	0/2276	0.61	0/3070
1	S	0.41	0/2276	0.61	0/3070
1	T	0.41	0/2276	0.61	0/3070
1	U	0.41	0/2276	0.61	0/3070
1	V	0.41	0/2276	0.61	0/3070
1	W	0.41	0/2276	0.61	0/3070
1	X	0.41	0/2276	0.61	0/3070
1	Y	0.41	0/2276	0.61	0/3070
1	Z	0.41	0/2276	0.61	0/3070
1	a	0.41	0/2276	0.61	0/3070
1	b	0.41	0/2276	0.61	0/3070
1	c	0.41	0/2276	0.61	0/3070
1	d	0.41	0/2276	0.61	0/3070
1	e	0.41	0/2276	0.61	0/3070
1	f	0.41	0/2276	0.61	0/3070
1	g	0.41	0/2276	0.61	0/3070
1	h	0.41	0/2276	0.61	0/3070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	i	0.41	0/2276	0.61	0/3070
1	j	0.41	0/2276	0.61	0/3070
1	k	0.41	0/2276	0.61	0/3070
1	l	0.41	0/2276	0.61	0/3070
1	m	0.41	0/2276	0.61	0/3070
1	n	0.41	0/2276	0.61	0/3070
1	o	0.41	0/2276	0.61	0/3070
1	p	0.41	0/2276	0.61	0/3070
1	q	0.41	0/2276	0.61	0/3070
1	r	0.41	0/2276	0.61	0/3070
1	s	0.41	0/2276	0.61	0/3070
1	t	0.41	0/2276	0.61	0/3070
All	All	0.41	0/104696	0.61	0/141220

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	1
1	k	0	1
1	l	0	1
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
All	All	0	46

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	ALA	Peptide
1	B	189	ALA	Peptide
1	C	189	ALA	Peptide
1	D	189	ALA	Peptide
1	E	189	ALA	Peptide

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	2264	2252	2251	37	0
1	B	2264	2252	2251	36	0
1	C	2264	2252	2251	39	0
1	D	2264	2252	2251	39	0
1	E	2264	2252	2251	37	0
1	F	2264	2252	2251	39	0
1	G	2264	2252	2251	40	0
1	H	2264	2252	2251	38	0
1	I	2264	2252	2251	40	0
1	J	2264	2252	2251	39	0
1	K	2264	2252	2251	36	0
1	L	2264	2252	2251	38	0
1	M	2264	2252	2251	37	0
1	N	2264	2252	2251	37	0
1	O	2264	2252	2251	36	0
1	P	2264	2252	2251	35	0
1	Q	2264	2252	2251	37	0
1	R	2264	2252	2251	35	0
1	S	2264	2252	2251	37	0
1	T	2264	2252	2251	35	0
1	U	2264	2252	2251	29	0
1	V	2264	2252	2251	29	0
1	W	2264	2252	2251	30	0
1	X	2264	2252	2251	27	0
1	Y	2264	2252	2251	24	0
1	Z	2264	2252	2251	24	0
1	a	2264	2252	2251	0	0
1	b	2264	2252	2251	0	0
1	c	2264	2252	2251	0	0
1	d	2264	2252	2251	0	0
1	e	2264	2252	2251	0	0
1	f	2264	2252	2251	0	0
1	g	2264	2252	2251	0	0
1	h	2264	2252	2251	0	0
1	i	2264	2252	2251	0	0
1	j	2264	2252	2251	0	0
1	k	2264	2252	2251	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	l	2264	2252	2251	0	0
1	m	2264	2252	2251	0	0
1	n	2264	2252	2251	0	0
1	o	2264	2252	2251	0	0
1	p	2264	2252	2251	0	0
1	q	2264	2252	2251	0	0
1	r	2264	2252	2251	0	0
1	s	2264	2252	2251	0	0
1	t	2264	2252	2251	0	0
All	All	104144	103592	103546	653	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 3.

The worst 5 of 653 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:J:241:ARG:O	1:J:245:THR:OG1	2.02	0.78
1:Y:241:ARG:O	1:Y:245:THR:OG1	2.01	0.78
1:M:241:ARG:O	1:M:245:THR:OG1	2.02	0.78
1:Q:241:ARG:O	1:Q:245:THR:OG1	2.01	0.76
1:C:241:ARG:O	1:C:245:THR:OG1	2.02	0.76

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	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	B	300/304 (99%)	262 (87%)	38 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	D	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	E	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	F	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	G	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	H	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	I	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	J	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	K	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	L	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	M	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	N	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	O	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	P	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	Q	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	R	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	S	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	T	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	U	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	V	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	W	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	X	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	Y	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	Z	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	a	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	b	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	c	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	d	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	e	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	f	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	g	300/304 (99%)	262 (87%)	38 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	i	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	j	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	k	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	l	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	m	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	n	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	o	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	p	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	q	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	r	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	s	300/304 (99%)	262 (87%)	38 (13%)	0	100	100
1	t	300/304 (99%)	261 (87%)	39 (13%)	0	100	100
All	All	13800/13984 (99%)	12051 (87%)	1749 (13%)	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	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	B	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	C	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	D	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	E	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	F	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	G	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	H	244/246 (99%)	243 (100%)	1 (0%)	93	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	J	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	K	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	L	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	M	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	N	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	O	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	P	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	Q	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	R	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	S	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	T	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	U	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	V	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	W	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	X	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	Y	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	Z	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	a	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	b	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	c	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	d	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	e	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	f	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	g	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	h	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	i	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	j	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	k	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	l	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	m	244/246 (99%)	243 (100%)	1 (0%)	93	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	n	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	o	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	p	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	q	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	r	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	s	244/246 (99%)	243 (100%)	1 (0%)	93	95
1	t	244/246 (99%)	243 (100%)	1 (0%)	93	95
All	All	11224/11316 (99%)	11178 (100%)	46 (0%)	93	95

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	248	ASN
1	Z	248	ASN
1	q	248	ASN
1	V	248	ASN
1	X	248	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	295	GLN
1	Y	24	GLN
1	q	24	GLN
1	U	247	ASN
1	W	24	GLN

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](#)

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.