



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 01:57 AM EDT

PDB ID : 5WK5
EMDB ID : EMD-8855
Title : Cryo-EM structure of *P. aeruginosa* flagellar filaments A443V
Authors : Wang, F.; Postel, S.; Sundberg, E.J.; Egelman, E.H.
Deposited on : 2017-07-24
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation 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

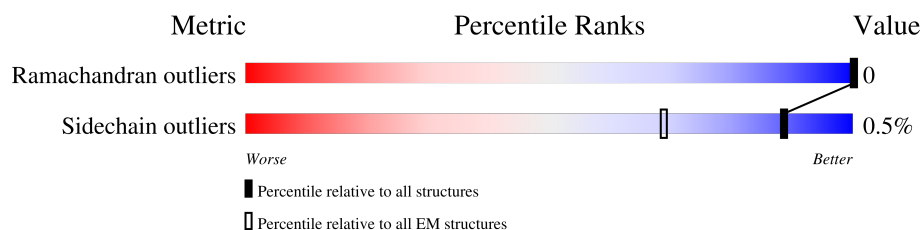
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain	
1	A	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	B	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	C	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	D	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	E	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	F	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	G	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	H	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	I	488	<div><div></div></div> 54%	<div><div></div></div> 45%
1	J	488	<div><div></div></div> 54%	<div><div></div></div> 45%





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Mol	Chain	Length	Quality of chain	
1	K	488		
1	L	488		
1	M	488		
1	N	488		
1	O	488		
1	P	488		
1	Q	488		
1	R	488		
1	S	488		
1	T	488		
1	U	488		
1	V	488		
1	W	488		
1	X	488		
1	Y	488		
1	Z	488		
1	a	488		
1	b	488		
1	c	488		
1	d	488		
1	e	488		
1	f	488		
1	g	488		
1	h	488		
1	i	488		

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Mol	Chain	Length	Quality of chain
1	j	488	
1	k	488	
1	l	488	
1	m	488	
1	n	488	
1	o	488	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 161786 atoms, of which 80606 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 B-type flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	B	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	C	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	D	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	E	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	F	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	G	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	H	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	I	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	J	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	K	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	L	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	M	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	N	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	O	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	P	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	Q	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	S	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	T	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	U	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	V	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	W	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	X	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	Y	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	Z	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	a	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	b	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	c	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	d	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	e	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	f	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	g	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	h	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	i	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	j	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	k	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	l	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	n	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0
1	o	269	Total 3946	C 1188	H 1966	N 371	O 421	0	0

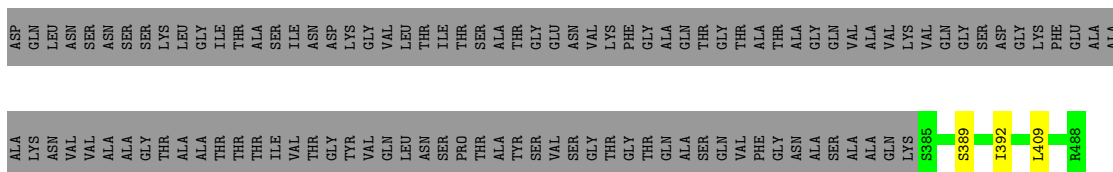
There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	VAL	ALA	engineered mutation	UNP P72151
B	443	VAL	ALA	engineered mutation	UNP P72151
C	443	VAL	ALA	engineered mutation	UNP P72151
D	443	VAL	ALA	engineered mutation	UNP P72151
E	443	VAL	ALA	engineered mutation	UNP P72151
F	443	VAL	ALA	engineered mutation	UNP P72151
G	443	VAL	ALA	engineered mutation	UNP P72151
H	443	VAL	ALA	engineered mutation	UNP P72151
I	443	VAL	ALA	engineered mutation	UNP P72151
J	443	VAL	ALA	engineered mutation	UNP P72151
K	443	VAL	ALA	engineered mutation	UNP P72151
L	443	VAL	ALA	engineered mutation	UNP P72151
M	443	VAL	ALA	engineered mutation	UNP P72151
N	443	VAL	ALA	engineered mutation	UNP P72151
O	443	VAL	ALA	engineered mutation	UNP P72151
P	443	VAL	ALA	engineered mutation	UNP P72151
Q	443	VAL	ALA	engineered mutation	UNP P72151
R	443	VAL	ALA	engineered mutation	UNP P72151
S	443	VAL	ALA	engineered mutation	UNP P72151
T	443	VAL	ALA	engineered mutation	UNP P72151
U	443	VAL	ALA	engineered mutation	UNP P72151
V	443	VAL	ALA	engineered mutation	UNP P72151
W	443	VAL	ALA	engineered mutation	UNP P72151
X	443	VAL	ALA	engineered mutation	UNP P72151
Y	443	VAL	ALA	engineered mutation	UNP P72151
Z	443	VAL	ALA	engineered mutation	UNP P72151
a	443	VAL	ALA	engineered mutation	UNP P72151
b	443	VAL	ALA	engineered mutation	UNP P72151
c	443	VAL	ALA	engineered mutation	UNP P72151
d	443	VAL	ALA	engineered mutation	UNP P72151
e	443	VAL	ALA	engineered mutation	UNP P72151
f	443	VAL	ALA	engineered mutation	UNP P72151

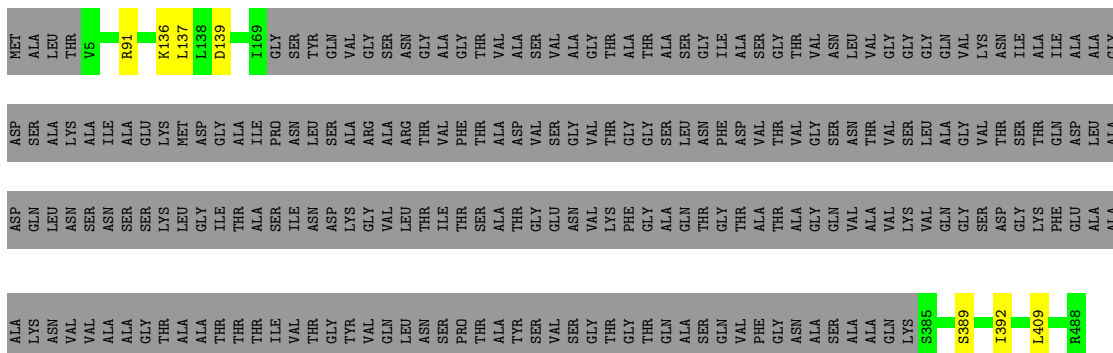
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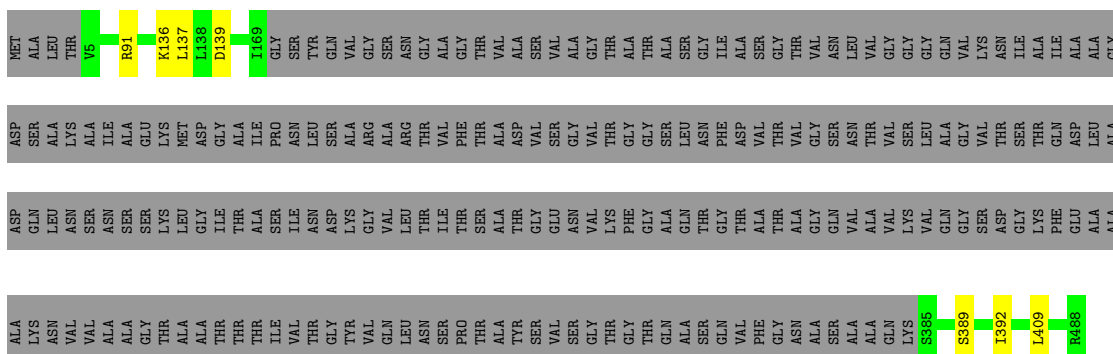
Chain	Residue	Modelled	Actual	Comment	Reference
g	443	VAL	ALA	engineered mutation	UNP P72151
h	443	VAL	ALA	engineered mutation	UNP P72151
i	443	VAL	ALA	engineered mutation	UNP P72151
j	443	VAL	ALA	engineered mutation	UNP P72151
k	443	VAL	ALA	engineered mutation	UNP P72151
l	443	VAL	ALA	engineered mutation	UNP P72151
m	443	VAL	ALA	engineered mutation	UNP P72151
n	443	VAL	ALA	engineered mutation	UNP P72151
o	443	VAL	ALA	engineered mutation	UNP P72151



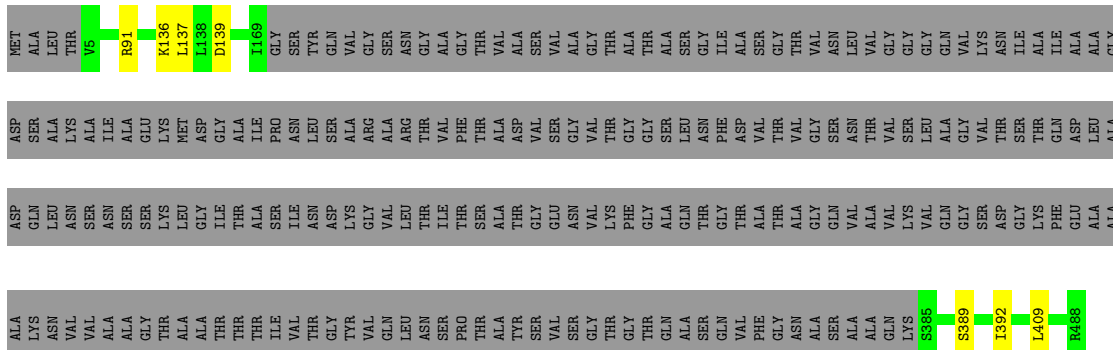
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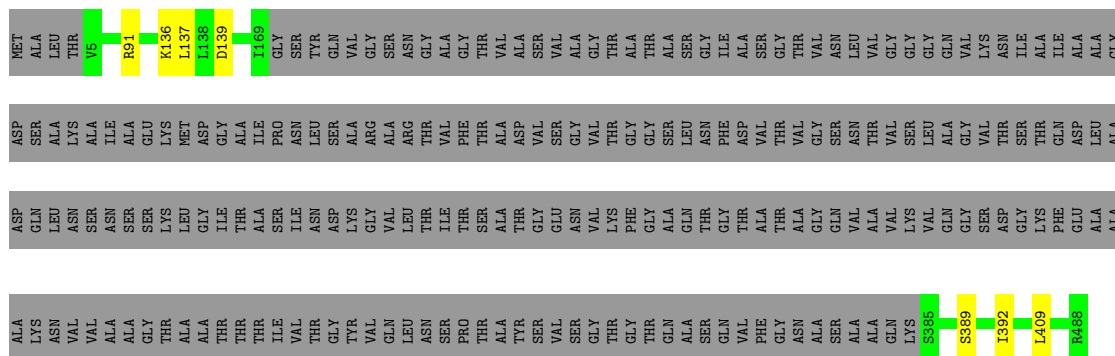


- Molecule 1: B-type flagellin

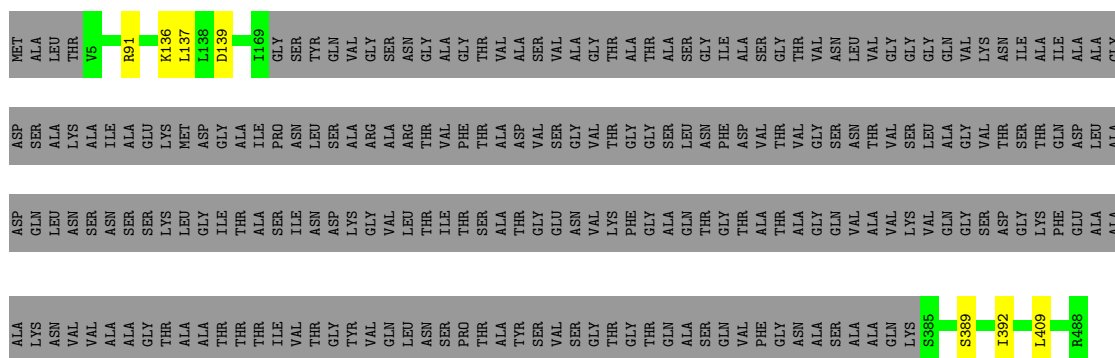


- Molecule 1: B-type flagellin

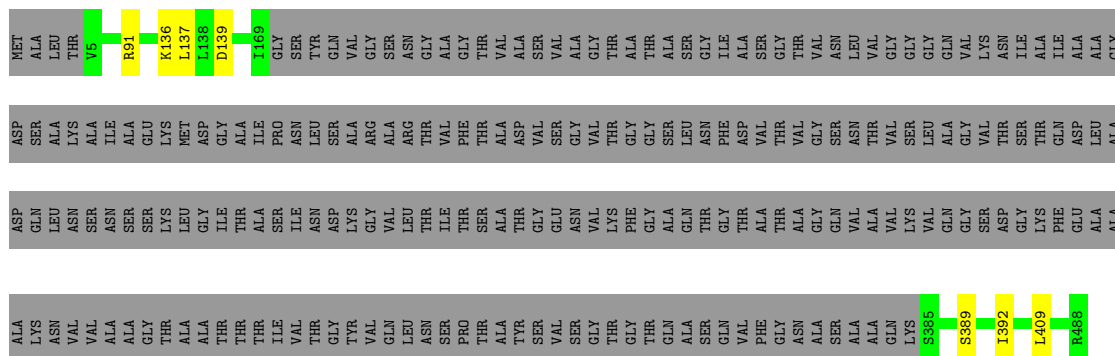




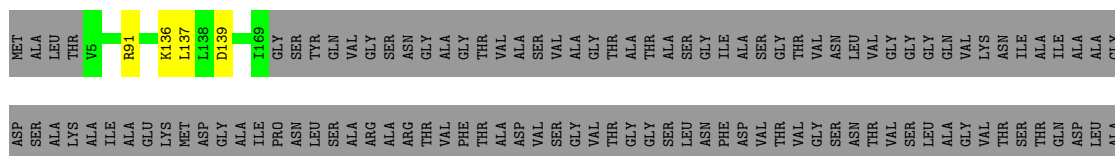
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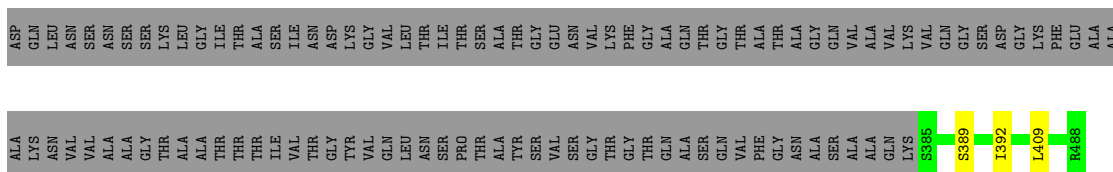


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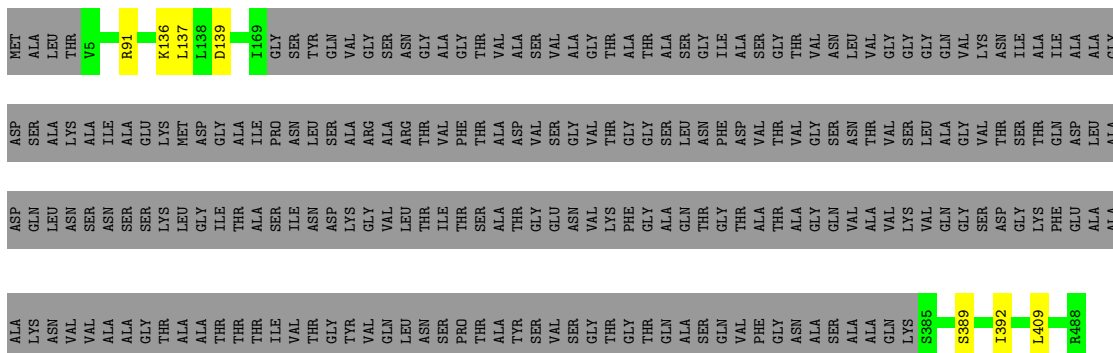


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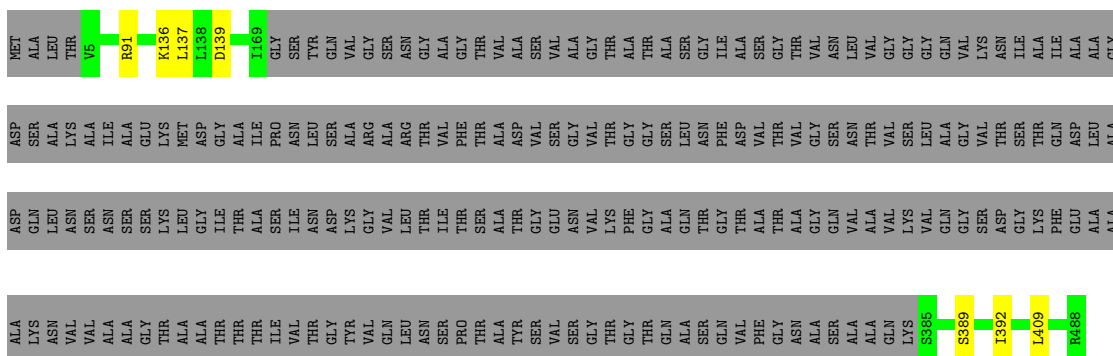




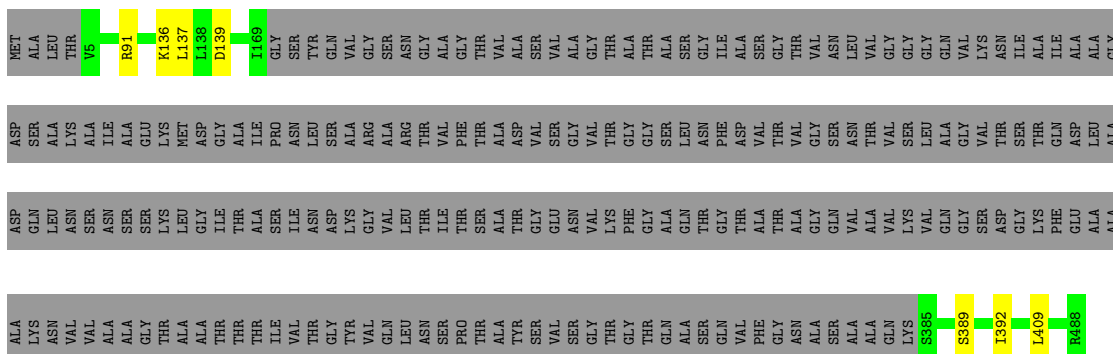
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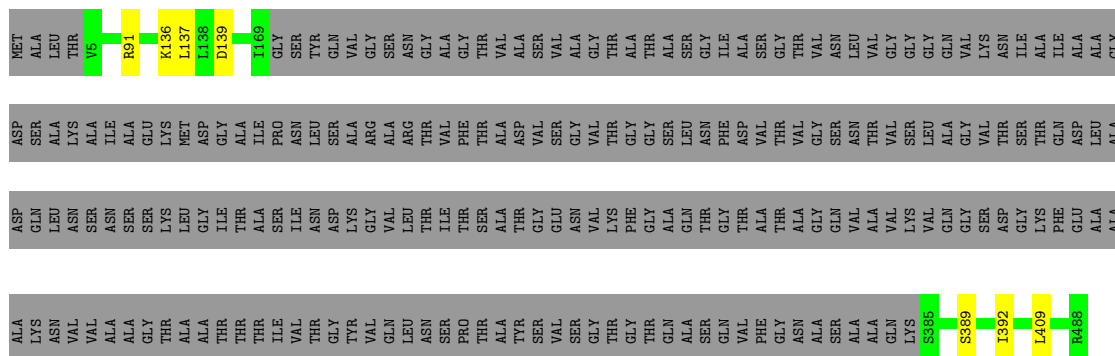


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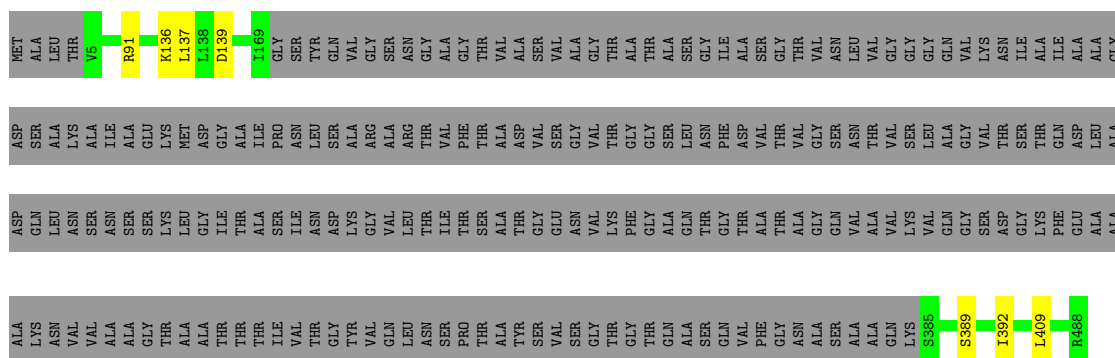


- Molecule 1: B-type flagellin

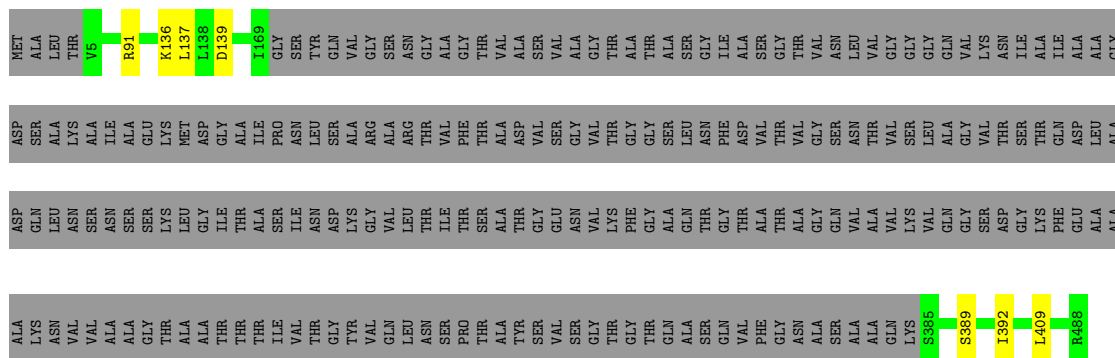




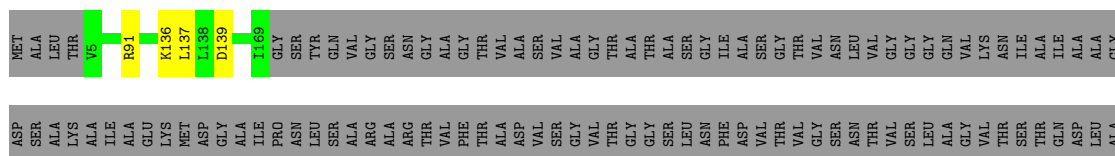
- Molecule 1: B-type flagellin



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ASP	GLN	LEU	ASN	THR	SER	ASN	SER	SER	LYS	LEU	ALA	GLY	THR	ILE	THR	ALA	SER	GLY	ASP
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ALA	LYS	ASN	VAL	VAL	ALA	ALA	GLY	ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 1: B-type flagellin



MET	ALA	THR	V5	R91	K136	L137	L138	D139	I169	GLY	TYR	GLN	VAL	GLY	VAL	GLN	VAL	GLY	ASP
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ASP	SER	ALA	LYS	ILE	ALA	GLY	THR	ALA	ILE	PRO	ASN	LEU	SER	ALA	ARG	VAL	ARG	THR	THR
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ASP	GLN	LEU	ASN	SER	ASN	SER	LYS	ILE	ALA	SER	ILE	ASN	ASP	GLN	VAL	VAL	THR	THR	SER
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ALA	LYS	ASN	VAL	VAL	ALA	ALA	GLY	THR	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 1: B-type flagellin



MET	ALA	THR	V5	R91	K136	L137	L138	D139	I169	GLY	SER	GLN	VAL	GLY	VAL	GLN	VAL	GLY	ASP
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ASP	SER	ALA	LYS	ILE	ALA	GLY	THR	ALA	ILE	PRO	ASN	LEU	SER	ALA	ARG	VAL	ARG	THR	THR
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ASP	GLN	LEU	ASN	SER	ASN	SER	LYS	ILE	ALA	SER	ILE	ASN	ASP	GLN	VAL	VAL	THR	THR	SER
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ALA	LYS	ASN	VAL	VAL	ALA	ALA	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 1: B-type flagellin

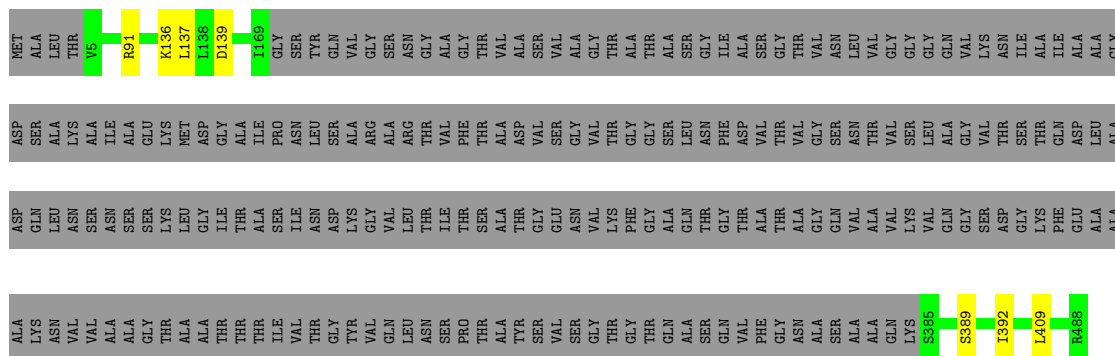


MET	ALA	THR	V5	R91	K136	L137	L138	D139	I169	GLY	TYR	GLN	VAL	GLY	VAL	GLN	VAL	GLY	ASP
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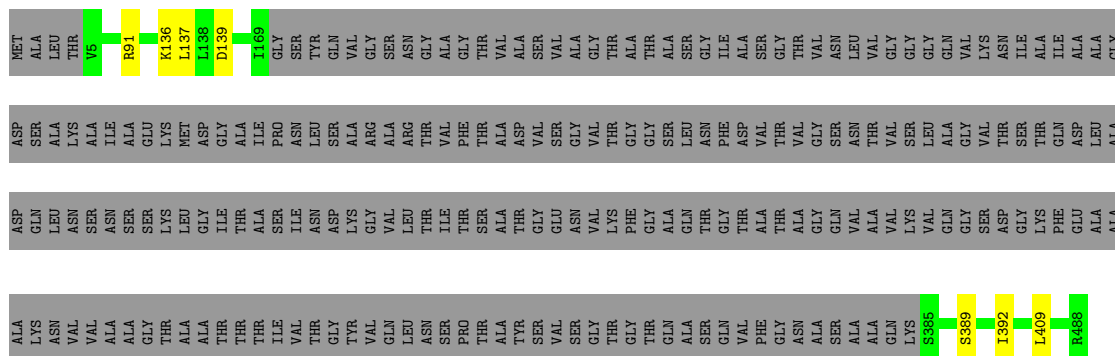
ASP	SER	ALA	LYS	ILE	ALA	GLY	THR	ALA	ILE	PRO	ASN	LEU	SER	ALA	ARG	VAL	ARG	THR	THR
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ASP	GLN	LEU	ASN	SER	ASN	SER	LYS	ILE	ALA	SER	ILE	ASN	ASP	GLN	VAL	VAL	THR	THR	SER
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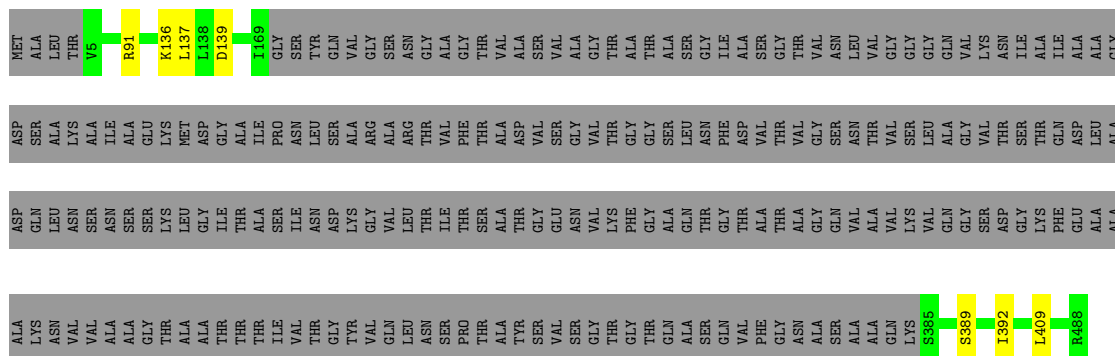
ALA	LYS	ASN	VAL	VAL	ALA	ALA	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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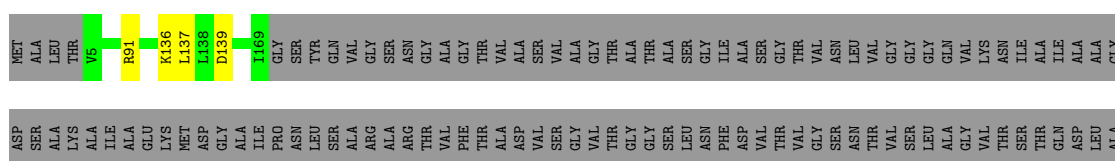
- Molecule 1: B-type flagellin



- Molecule 1: B-type flagellin



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ALA	LYS	ASN	VAL	VAL	ALA	ALA	GLY	THR	ALA	ALA	THR	THR	THR	ILE	VAL	THR	GLY	TVR	VAL	GLN	LEU	ASN	SER	PRO	THR	ALA	TYR	SER	VAL	SER	GLY	THR	GLY	THR	GLN	PHE	GLN	VAL	ASN	SER	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY
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● Molecule 1: B-type flagellin



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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=65.75°, rise=4.61 Å, axial sym=C1	Depositor
Number of segments used	102119	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	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/1986	0.68	3/2693 (0.1%)
1	B	0.42	0/1986	0.68	3/2693 (0.1%)
1	C	0.42	0/1986	0.68	3/2693 (0.1%)
1	D	0.42	0/1986	0.68	3/2693 (0.1%)
1	E	0.42	0/1986	0.68	3/2693 (0.1%)
1	F	0.42	0/1986	0.68	3/2693 (0.1%)
1	G	0.42	0/1986	0.68	3/2693 (0.1%)
1	H	0.42	0/1986	0.68	3/2693 (0.1%)
1	I	0.42	0/1986	0.68	3/2693 (0.1%)
1	J	0.42	0/1986	0.68	3/2693 (0.1%)
1	K	0.42	0/1986	0.68	3/2693 (0.1%)
1	L	0.42	0/1986	0.68	3/2693 (0.1%)
1	M	0.42	0/1986	0.68	3/2693 (0.1%)
1	N	0.42	0/1986	0.68	3/2693 (0.1%)
1	O	0.42	0/1986	0.68	3/2693 (0.1%)
1	P	0.42	0/1986	0.68	3/2693 (0.1%)
1	Q	0.42	0/1986	0.68	3/2693 (0.1%)
1	R	0.42	0/1986	0.68	3/2693 (0.1%)
1	S	0.42	0/1986	0.68	3/2693 (0.1%)
1	T	0.42	0/1986	0.68	3/2693 (0.1%)
1	U	0.42	0/1986	0.68	3/2693 (0.1%)
1	V	0.42	0/1986	0.68	3/2693 (0.1%)
1	W	0.42	0/1986	0.68	3/2693 (0.1%)
1	X	0.42	0/1986	0.68	3/2693 (0.1%)
1	Y	0.42	0/1986	0.68	3/2693 (0.1%)
1	Z	0.42	0/1986	0.68	3/2693 (0.1%)
1	a	0.42	0/1986	0.68	3/2693 (0.1%)
1	b	0.42	0/1986	0.68	3/2693 (0.1%)
1	c	0.42	0/1986	0.68	3/2693 (0.1%)
1	d	0.42	0/1986	0.68	3/2693 (0.1%)
1	e	0.42	0/1986	0.68	3/2693 (0.1%)
1	f	0.42	0/1986	0.68	3/2693 (0.1%)
1	g	0.42	0/1986	0.68	3/2693 (0.1%)
1	h	0.42	0/1986	0.68	3/2693 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.42	0/1986	0.68	3/2693 (0.1%)
1	j	0.42	0/1986	0.68	3/2693 (0.1%)
1	k	0.42	0/1986	0.68	3/2693 (0.1%)
1	l	0.42	0/1986	0.68	3/2693 (0.1%)
1	m	0.42	0/1986	0.68	3/2693 (0.1%)
1	n	0.42	0/1986	0.68	3/2693 (0.1%)
1	o	0.42	0/1986	0.68	3/2693 (0.1%)
All	All	0.42	0/81426	0.68	123/110413 (0.1%)

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
1	Q	0	3
1	R	0	3
1	S	0	3
1	T	0	3
1	U	0	3
1	V	0	3
1	W	0	3
1	X	0	3
1	Y	0	3
1	Z	0	3
1	a	0	3

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Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	3
1	c	0	3
1	d	0	3
1	e	0	3
1	f	0	3
1	g	0	3
1	h	0	3
1	i	0	3
1	j	0	3
1	k	0	3
1	l	0	3
1	m	0	3
1	n	0	3
1	o	0	3
All	All	0	123

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	409	LEU	CA-CB-CG	6.21	129.58	115.30
1	j	409	LEU	CA-CB-CG	6.21	129.57	115.30
1	X	409	LEU	CA-CB-CG	6.20	129.57	115.30
1	N	409	LEU	CA-CB-CG	6.20	129.56	115.30
1	S	409	LEU	CA-CB-CG	6.20	129.56	115.30
1	h	91	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	g	409	LEU	CA-CB-CG	6.20	129.55	115.30
1	o	409	LEU	CA-CB-CG	6.20	129.55	115.30
1	e	409	LEU	CA-CB-CG	6.19	129.55	115.30
1	M	409	LEU	CA-CB-CG	6.19	129.54	115.30
1	K	409	LEU	CA-CB-CG	6.19	129.54	115.30
1	O	409	LEU	CA-CB-CG	6.19	129.54	115.30
1	Q	409	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	409	LEU	CA-CB-CG	6.19	129.53	115.30
1	c	409	LEU	CA-CB-CG	6.19	129.53	115.30
1	i	409	LEU	CA-CB-CG	6.19	129.53	115.30
1	J	409	LEU	CA-CB-CG	6.18	129.52	115.30
1	k	91	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	V	409	LEU	CA-CB-CG	6.18	129.52	115.30
1	h	409	LEU	CA-CB-CG	6.18	129.52	115.30
1	R	409	LEU	CA-CB-CG	6.18	129.52	115.30
1	P	409	LEU	CA-CB-CG	6.18	129.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	k	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	B	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	C	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	G	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	T	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	W	409	LEU	CA-CB-CG	6.18	129.50	115.30
1	n	409	LEU	CA-CB-CG	6.18	129.51	115.30
1	H	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	I	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	L	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	U	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	Z	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	f	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	l	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	D	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	a	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	m	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	F	409	LEU	CA-CB-CG	6.17	129.49	115.30
1	Y	409	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	409	LEU	CA-CB-CG	6.17	129.49	115.30
1	S	91	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	f	91	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	P	91	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	V	91	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	g	91	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	c	91	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	j	91	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	91	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	E	91	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	N	91	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	U	91	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	91	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	l	91	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	Q	91	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	J	91	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	H	91	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	Y	91	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	L	91	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	e	91	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	n	91	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	W	91	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	91	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	K	91	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	G	91	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	T	91	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	O	91	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	i	91	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	o	91	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	d	91	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	a	91	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	91	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	Z	91	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	91	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	F	91	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	X	91	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	R	91	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	M	91	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	m	91	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	b	91	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	R	139	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	k	139	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	Q	139	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	g	139	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	P	139	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	N	139	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	c	139	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	E	139	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	Y	139	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	F	139	ASP	CB-CG-OD1	-5.32	113.52	118.30
1	U	139	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	V	139	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	S	139	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	o	139	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	K	139	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	M	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	X	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	I	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	d	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	e	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	n	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	J	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	W	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	b	139	ASP	CB-CG-OD1	-5.29	113.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	139	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	D	139	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	Z	139	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	G	139	ASP	CB-CG-OD1	-5.27	113.55	118.30
1	m	139	ASP	CB-CG-OD1	-5.27	113.55	118.30
1	T	139	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	139	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	B	139	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	H	139	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	C	139	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	a	139	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	i	139	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	L	139	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	l	139	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	O	139	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	f	139	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	h	139	ASP	CB-CG-OD1	-5.22	113.60	118.30

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	LEU	Peptide
1	A	389	SER	Peptide
1	A	392	ILE	Peptide
1	B	137	LEU	Peptide
1	B	389	SER	Peptide
1	B	392	ILE	Peptide
1	C	137	LEU	Peptide
1	C	389	SER	Peptide
1	C	392	ILE	Peptide
1	D	137	LEU	Peptide
1	D	389	SER	Peptide
1	D	392	ILE	Peptide
1	E	137	LEU	Peptide
1	E	389	SER	Peptide
1	E	392	ILE	Peptide
1	F	137	LEU	Peptide
1	F	389	SER	Peptide
1	F	392	ILE	Peptide
1	G	137	LEU	Peptide
1	G	389	SER	Peptide

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Mol	Chain	Res	Type	Group
1	G	392	ILE	Peptide
1	H	137	LEU	Peptide
1	H	389	SER	Peptide
1	H	392	ILE	Peptide
1	I	137	LEU	Peptide
1	I	389	SER	Peptide
1	I	392	ILE	Peptide
1	J	137	LEU	Peptide
1	J	389	SER	Peptide
1	J	392	ILE	Peptide
1	K	137	LEU	Peptide
1	K	389	SER	Peptide
1	K	392	ILE	Peptide
1	L	137	LEU	Peptide
1	L	389	SER	Peptide
1	L	392	ILE	Peptide
1	M	137	LEU	Peptide
1	M	389	SER	Peptide
1	M	392	ILE	Peptide
1	N	137	LEU	Peptide
1	N	389	SER	Peptide
1	N	392	ILE	Peptide
1	O	137	LEU	Peptide
1	O	389	SER	Peptide
1	O	392	ILE	Peptide
1	P	137	LEU	Peptide
1	P	389	SER	Peptide
1	P	392	ILE	Peptide
1	Q	137	LEU	Peptide
1	Q	389	SER	Peptide
1	Q	392	ILE	Peptide
1	R	137	LEU	Peptide
1	R	389	SER	Peptide
1	R	392	ILE	Peptide
1	S	137	LEU	Peptide
1	S	389	SER	Peptide
1	S	392	ILE	Peptide
1	T	137	LEU	Peptide
1	T	389	SER	Peptide
1	T	392	ILE	Peptide
1	U	137	LEU	Peptide
1	U	389	SER	Peptide

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Mol	Chain	Res	Type	Group
1	U	392	ILE	Peptide
1	V	137	LEU	Peptide
1	V	389	SER	Peptide
1	V	392	ILE	Peptide
1	W	137	LEU	Peptide
1	W	389	SER	Peptide
1	W	392	ILE	Peptide
1	X	137	LEU	Peptide
1	X	389	SER	Peptide
1	X	392	ILE	Peptide
1	Y	137	LEU	Peptide
1	Y	389	SER	Peptide
1	Y	392	ILE	Peptide
1	Z	137	LEU	Peptide
1	Z	389	SER	Peptide
1	Z	392	ILE	Peptide
1	a	137	LEU	Peptide
1	a	389	SER	Peptide
1	a	392	ILE	Peptide
1	b	137	LEU	Peptide
1	b	389	SER	Peptide
1	b	392	ILE	Peptide
1	c	137	LEU	Peptide
1	c	389	SER	Peptide
1	c	392	ILE	Peptide
1	d	137	LEU	Peptide
1	d	389	SER	Peptide
1	d	392	ILE	Peptide
1	e	137	LEU	Peptide
1	e	389	SER	Peptide
1	e	392	ILE	Peptide
1	f	137	LEU	Peptide
1	f	389	SER	Peptide
1	f	392	ILE	Peptide
1	g	137	LEU	Peptide
1	g	389	SER	Peptide
1	g	392	ILE	Peptide
1	h	137	LEU	Peptide
1	h	389	SER	Peptide
1	h	392	ILE	Peptide
1	i	137	LEU	Peptide
1	i	389	SER	Peptide

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Mol	Chain	Res	Type	Group
1	i	392	ILE	Peptide
1	j	137	LEU	Peptide
1	j	389	SER	Peptide
1	j	392	ILE	Peptide
1	k	137	LEU	Peptide
1	k	389	SER	Peptide
1	k	392	ILE	Peptide
1	l	137	LEU	Peptide
1	l	389	SER	Peptide
1	l	392	ILE	Peptide
1	m	137	LEU	Peptide
1	m	389	SER	Peptide
1	m	392	ILE	Peptide
1	n	137	LEU	Peptide
1	n	389	SER	Peptide
1	n	392	ILE	Peptide
1	o	137	LEU	Peptide
1	o	389	SER	Peptide
1	o	392	ILE	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	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	B	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	C	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	D	265/488 (54%)	239 (90%)	26 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	F	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	G	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	H	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	I	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	J	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	K	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	L	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	M	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	N	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	O	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	P	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	Q	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	R	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	S	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	T	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	U	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	V	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	W	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	X	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	Y	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	Z	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	a	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	b	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	c	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	d	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	e	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	f	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	g	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	h	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	i	265/488 (54%)	239 (90%)	26 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	k	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	l	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	m	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	n	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
1	o	265/488 (54%)	239 (90%)	26 (10%)	0	100	100
All	All	10865/20008 (54%)	9799 (90%)	1066 (10%)	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	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	B	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	C	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	D	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	E	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	F	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	G	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	H	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	I	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	J	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	K	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	L	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	M	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	N	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	O	212/364 (58%)	211 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	Q	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	R	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	S	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	T	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	U	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	V	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	W	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	X	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	Y	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	Z	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	a	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	b	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	c	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	d	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	e	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	f	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	g	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	h	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	i	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	j	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	k	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	l	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	m	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	n	212/364 (58%)	211 (100%)	1 (0%)	88	93
1	o	212/364 (58%)	211 (100%)	1 (0%)	88	93
All	All	8692/14924 (58%)	8651 (100%)	41 (0%)	89	93

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	B	136	LYS

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Mol	Chain	Res	Type
1	C	136	LYS
1	D	136	LYS
1	E	136	LYS
1	F	136	LYS
1	G	136	LYS
1	H	136	LYS
1	I	136	LYS
1	J	136	LYS
1	K	136	LYS
1	L	136	LYS
1	M	136	LYS
1	N	136	LYS
1	O	136	LYS
1	P	136	LYS
1	Q	136	LYS
1	R	136	LYS
1	S	136	LYS
1	T	136	LYS
1	U	136	LYS
1	V	136	LYS
1	W	136	LYS
1	X	136	LYS
1	Y	136	LYS
1	Z	136	LYS
1	a	136	LYS
1	b	136	LYS
1	c	136	LYS
1	d	136	LYS
1	e	136	LYS
1	f	136	LYS
1	g	136	LYS
1	h	136	LYS
1	i	136	LYS
1	j	136	LYS
1	k	136	LYS
1	l	136	LYS
1	m	136	LYS
1	n	136	LYS
1	o	136	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	15	GLN
1	B	6	ASN
1	B	15	GLN
1	C	6	ASN
1	C	15	GLN
1	D	6	ASN
1	D	15	GLN
1	E	6	ASN
1	E	15	GLN
1	F	6	ASN
1	F	15	GLN
1	G	6	ASN
1	G	15	GLN
1	G	39	ASN
1	H	6	ASN
1	H	15	GLN
1	I	6	ASN
1	I	15	GLN
1	J	6	ASN
1	J	15	GLN
1	K	6	ASN
1	K	15	GLN
1	L	6	ASN
1	L	15	GLN
1	M	6	ASN
1	M	15	GLN
1	N	6	ASN
1	N	15	GLN
1	O	6	ASN
1	O	15	GLN
1	P	6	ASN
1	P	15	GLN
1	Q	6	ASN
1	Q	15	GLN
1	R	6	ASN
1	R	15	GLN
1	S	6	ASN
1	S	15	GLN
1	T	6	ASN
1	T	15	GLN
1	U	15	GLN
1	V	6	ASN

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Mol	Chain	Res	Type
1	V	15	GLN
1	W	15	GLN
1	X	6	ASN
1	X	15	GLN
1	Y	15	GLN
1	Y	39	ASN
1	Z	6	ASN
1	Z	15	GLN
1	a	15	GLN
1	b	6	ASN
1	b	15	GLN
1	c	15	GLN
1	c	39	ASN
1	d	6	ASN
1	d	15	GLN
1	f	6	ASN
1	f	15	GLN
1	f	466	GLN
1	g	439	ASN
1	h	6	ASN
1	h	15	GLN
1	h	466	GLN
1	i	439	ASN
1	j	6	ASN
1	k	439	ASN
1	l	6	ASN
1	l	466	GLN
1	n	6	ASN
1	n	15	GLN
1	n	466	GLN
1	o	439	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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-8855. 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

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

9 Map-model fit ⓘ

This section was not generated.