



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 23, 2017 – 11:51 PM EDT

PDB ID : 5WK6  
EMDB ID: : EMD-8856  
Title : Cryo-EM structure of *P. aeruginosa* flagellar filaments G420A  
Authors : Wang, F.; Postel, S.; Sundberg, E.J.; Egelman, E.H.  
Deposited on : unknown  
Resolution : 4.30 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](mailto: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.

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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

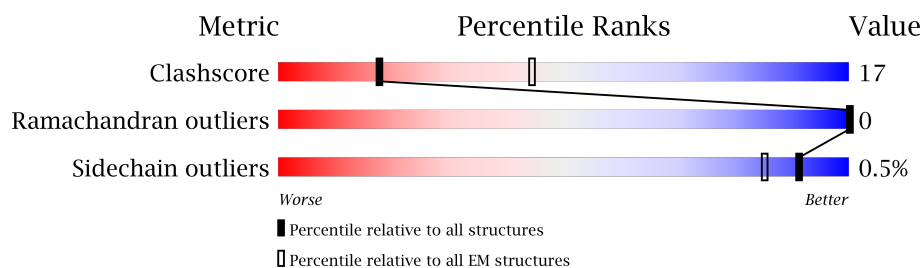
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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.






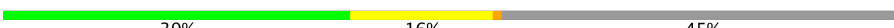
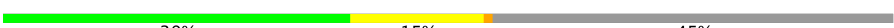
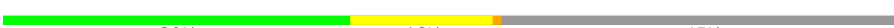







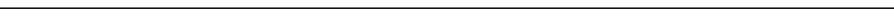

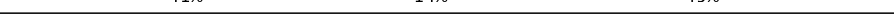
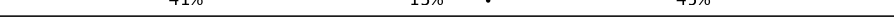
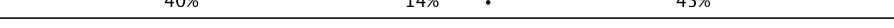







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	488	39% 15% . 45%
1	B	488	39% 15% . 45%
1	C	488	39% 15% . 45%
1	D	488	39% 15% . 45%
1	E	488	39% 15% . 45%
1	F	488	39% 15% . 45%
1	G	488	39% 15% . 45%
1	H	488	39% 15% . 45%
1	I	488	39% 15% . 45%

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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	
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	

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

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 161663 atoms, of which 80524 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 3943	C 1187	H 1964	N 371	O 421	0	0
1	B	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	C	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	D	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	E	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	F	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	G	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	H	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	I	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	J	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	K	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	L	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	M	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	N	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	O	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	P	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	Q	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	S	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	T	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	U	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	V	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	W	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	X	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	Y	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	Z	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	a	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	b	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	c	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	d	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	e	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	f	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	g	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	h	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	i	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	j	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	k	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0
1	l	269	Total 3943	C 1187	H 1964	N 371	O 421	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	269	Total	C	H	N	O	0	0
			3943	1187	1964	371	421		
1	n	269	Total	C	H	N	O	0	0
			3943	1187	1964	371	421		
1	o	269	Total	C	H	N	O	0	0
			3943	1187	1964	371	421		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	ALA	GLY	engineered mutation	UNP P72151
B	420	ALA	GLY	engineered mutation	UNP P72151
C	420	ALA	GLY	engineered mutation	UNP P72151
D	420	ALA	GLY	engineered mutation	UNP P72151
E	420	ALA	GLY	engineered mutation	UNP P72151
F	420	ALA	GLY	engineered mutation	UNP P72151
G	420	ALA	GLY	engineered mutation	UNP P72151
H	420	ALA	GLY	engineered mutation	UNP P72151
I	420	ALA	GLY	engineered mutation	UNP P72151
J	420	ALA	GLY	engineered mutation	UNP P72151
K	420	ALA	GLY	engineered mutation	UNP P72151
L	420	ALA	GLY	engineered mutation	UNP P72151
M	420	ALA	GLY	engineered mutation	UNP P72151
N	420	ALA	GLY	engineered mutation	UNP P72151
O	420	ALA	GLY	engineered mutation	UNP P72151
P	420	ALA	GLY	engineered mutation	UNP P72151
Q	420	ALA	GLY	engineered mutation	UNP P72151
R	420	ALA	GLY	engineered mutation	UNP P72151
S	420	ALA	GLY	engineered mutation	UNP P72151
T	420	ALA	GLY	engineered mutation	UNP P72151
U	420	ALA	GLY	engineered mutation	UNP P72151
V	420	ALA	GLY	engineered mutation	UNP P72151
W	420	ALA	GLY	engineered mutation	UNP P72151
X	420	ALA	GLY	engineered mutation	UNP P72151
Y	420	ALA	GLY	engineered mutation	UNP P72151
Z	420	ALA	GLY	engineered mutation	UNP P72151
a	420	ALA	GLY	engineered mutation	UNP P72151
b	420	ALA	GLY	engineered mutation	UNP P72151
c	420	ALA	GLY	engineered mutation	UNP P72151
d	420	ALA	GLY	engineered mutation	UNP P72151
e	420	ALA	GLY	engineered mutation	UNP P72151
f	420	ALA	GLY	engineered mutation	UNP P72151

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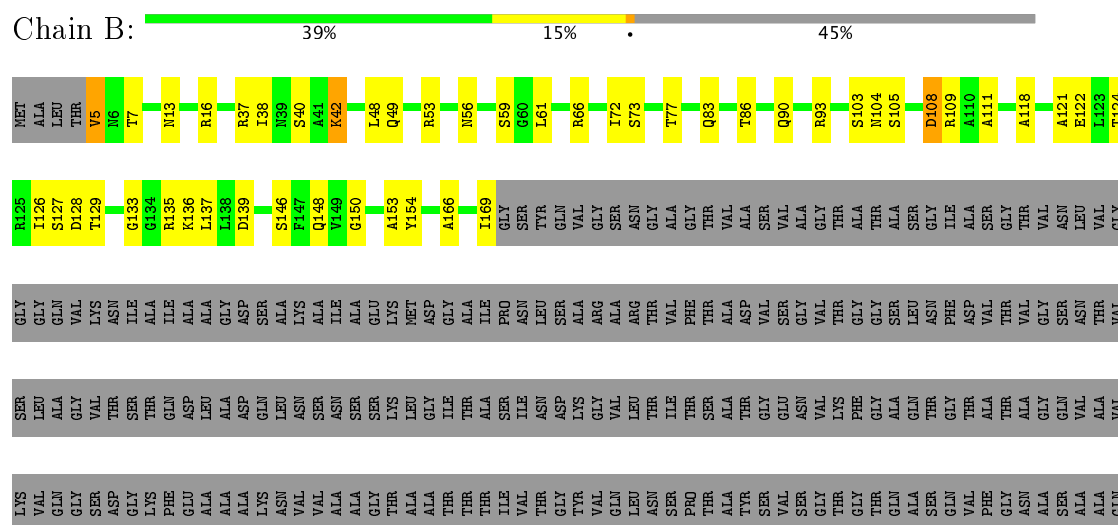
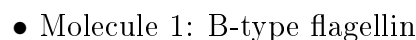
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Chain	Residue	Modelled	Actual	Comment	Reference
g	420	ALA	GLY	engineered mutation	UNP P72151
h	420	ALA	GLY	engineered mutation	UNP P72151
i	420	ALA	GLY	engineered mutation	UNP P72151
j	420	ALA	GLY	engineered mutation	UNP P72151
k	420	ALA	GLY	engineered mutation	UNP P72151
l	420	ALA	GLY	engineered mutation	UNP P72151
m	420	ALA	GLY	engineered mutation	UNP P72151
n	420	ALA	GLY	engineered mutation	UNP P72151
o	420	ALA	GLY	engineered mutation	UNP P72151

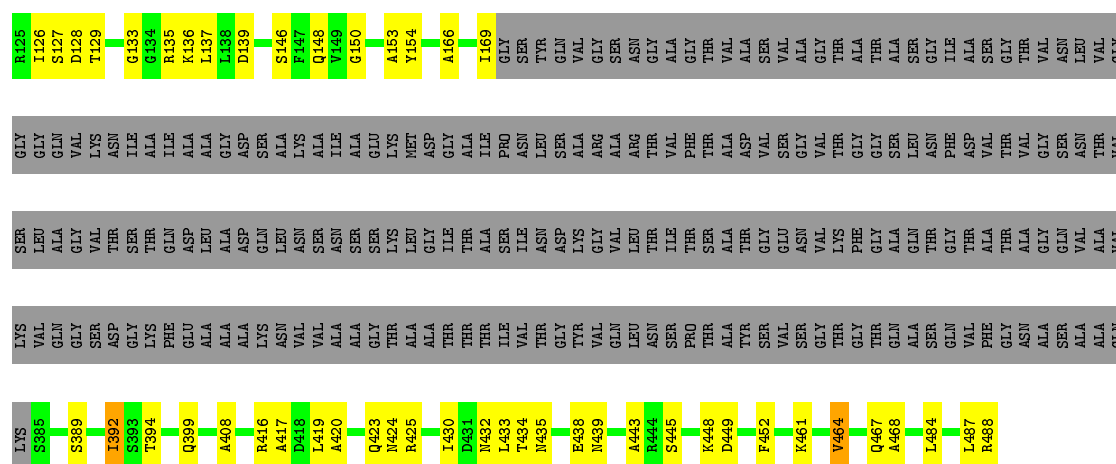




- Molecule 1: B-type flagellin

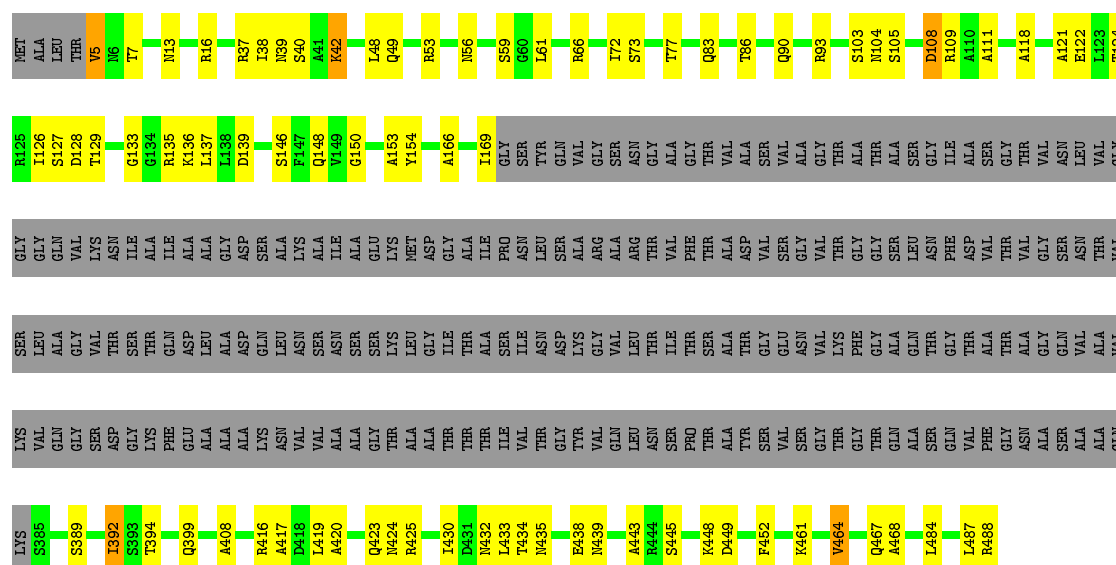






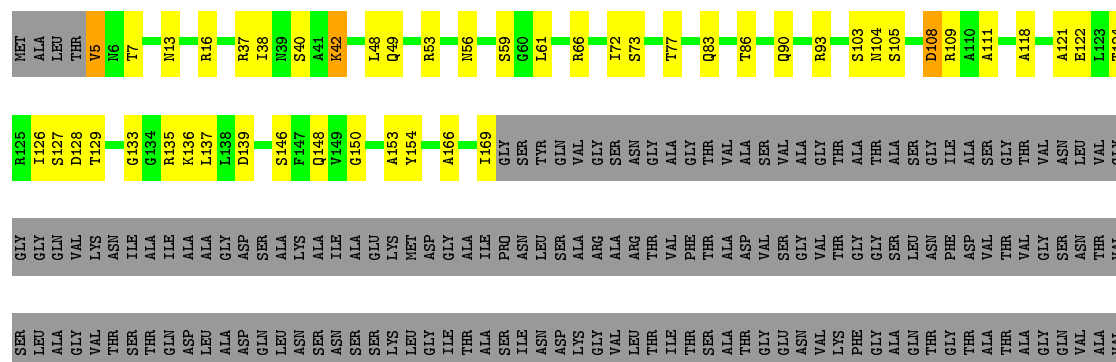
• Molecule 1: B-type flagellin

Chain F: 39% 15% 45%



• Molecule 1: B-type flagellin

Chain G: 39% 15% 45%



LYS	VAL	GLN	GLY	SER	ASP	GLY	LYS	PHE	GLU	ALA	ALA	LYS	LYS	VAL	VAL	ALA	ALA	GLY	THR	ALA	ALA	ALA	THR	THR	THR	THR	THR	VAL	GLN	LEU	ASN	SER	PRO	THR	ALA	TYR	SER	VAL	SER	GLY	THR	GLY	THR	GLN	GLN	VAL	PHE	GLY	ASN	SER	ALA	ALA	GLN
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LYS	S385	S389	I392	S393	T394	Q399	A408	R416	A417	D418	L419	A420	Q423	M424	R425	I430	D431	M432	L433	T434	M435	E438	M439	A443	R444	S445	K448	D449	F452	K461	V464	Q467	A468	L484	L487	R488
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• Molecule 1: B-type flagellin



MET	ALA	LEU	THR	V5	R6	T7	M13	R16	R37	I38	R39	S40	A41	K42	L48	Q49	R53	M56	S59	G60	L61	R66	I72	S73	T77	Q83	T86	Q90	R93	S103	M104	S105	D108	R109	A110	A111	A118	A121	E122	I123	T124
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R125	I126	S127	T129	G133	G134	R136	K137	L138	D139	S146	F147	Q148	V149	G150	A153	Y154	A166	I169	GLY	SER	TYR	GLN	VAL	GLY	ASN	GLY	THR	THR	VAL	SER	VAL	GLY	THR	GLY	ALA	THR	THR	ASN	LEU	VAL	THR	GLY
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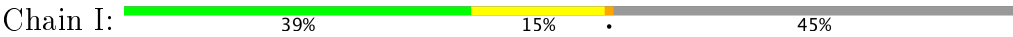
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SER	LEU	ALA	GLY	VAL	THR	SER	THR	GLN	ASP	ALA	ASP	GLN	LEU	ASN	SER	ALA	SER	LYS	LEU	ILE	ASP	LYS	ARG	GLY	VAL	LEU	THR	THR	ILE	THR	ASN	THR	THR	ALA	THR	GLY	ASN	VAL	LYS	PHE	GLY	THR	GLN	ALA	SER	LEU	THR	GLY	THR	ALA	GLN	VAL	VAL
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LYS	VAL	GLN	GLY	SER	ASP	GLY	LYS	PHE	GLU	ALA	ALA	LYS	LYS	VAL	VAL	ALA	GLY	THR	THR	ILE	VAL	GLY	TYR	VAL	GLN	LEU	ASN	SER	PRO	THR	ALA	TYR	SER	VAL	SER	GLY	THR	GLY	THR	GLN	GLN	VAL	PHE	GLY	GLY	ASN	ALA	SER	ALA	ALA	GLN
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LYS	S385	S389	I392	S393	T394	Q399	A408	R416	A417	D418	L419	A420	Q423	M424	R425	I430	D431	M432	L433	T434	M435	E438	M439	A443	R444	S445	K448	D449	F452	K461	V464	Q467	A468	L484	L487	R488
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• Molecule 1: B-type flagellin



MET	ALA	LEU	THR	V5	R6	T7	M13	R16	R37	I38	R39	S40	A41	K42	L48	Q49	R53	M56	S59	G60	L61	R66	I72	S73	T77	Q83	T86	Q90	R93	S103	M104	S105	D108	R109	A110	A111	A118	A121	E122	I123	T124
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R125	I126	S127	T129	G133	G134	R136	K137	L138	D139	S146	F147	Q148	V149	G150	A153	Y154	A166	I169	GLY	SER	TYR	GLN	VAL	GLY	ASN	GLY	THR	THR	VAL	SER	VAL	GLY	THR	GLY	ALA	THR	THR	ASN	LEU	VAL	THR	GLY	VAL	VAL	ASN	LEU	VAL	THR	GLY
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GLY	GLY	GLN	VAL	LYS	ASN	ILE	ALA	ALA	GLY	SER	SER	LYS	ASN	ILE	ALA	GLU	LYS	LEU	MET	ASP	GLY	ILE	THR	ALA	ILE	PRO	ASN	ARG	THR	THR	GLY	ASN	VAL	PHE	THR	ALA	ASP	VAL	GLY	ASN	VAL	LYS	PHE	GLY	THR	GLN	ALA	SER	LEU	THR	GLY	THR	ALA	GLN	VAL	VAL
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SER	LEU	ALA	GLY	VAL	THR	SER	THR	GLN	ASP	ALA	ASP	GLN	LEU	ASN	SER	ALA	SER	LYS	LEU	ILE	ASP	LYS	ARG	GLY	VAL	LEU	THR	THR	ILE	THR	ASN	THR	THR	ALA	THR	GLY	ASN	VAL	LYS	PHE	GLY	THR	GLN	ALA	SER	LEU	THR	GLY	THR	ALA	GLN	VAL	VAL
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LYS	VAL	GLN	GLY	SER	ASP	GLY	LYS	PHE	GLU	ALA	ALA	LYS	LYS	VAL	VAL	ALA	GLY	THR	THR	ILE	VAL	GLY	TYR	VAL	GLN	LEU	ASN	SER	PRO	THR	ALA	TYR	SER	VAL	SER	GLY	THR	GLY	THR	GLN	GLN	VAL	PHE	GLY	GLY	ASN	ALA	SER	ALA	ALA	GLN
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LYS	S385	S389	I392	S393	T394	Q399	A408	R416	A417	D418	L419	A420	Q423	M424	R425	I430	D431	M432	L433	T434	M435	E438	M439	A443	R444	S445	K448	D449	F452	K461	V464	Q467	A468	L484	L487	R488
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• Molecule 1: B-type flagellin



MET	ALA	LEU	THR	V5	N6	I7	M13	R16	R37	I38	I39	S40	A41	K42	L48	R53	N56	S59	G60	L61	R66	I72	S73	T77	Q83	T86	Q90	R93	S103	M104	S105	D108	R109	A110	A111	A118	A121	E122	L123	T124	R125						
I126	S127	D128	T129	G133	G134	R135	K136	L137	L138	D139	S146	F147	Q148	V149	G150	A153	Y154	A166	I169	GLY	SER	TYR	GLN	VAL	GLY	ARG	ALA	SER	ASN	GLY	ALA	SER	LEU	ASN	GLY	ILE	ALA	SER	THR	GLY	VAL	ASN	LEU	VAL	GLY	GLY	
GLY	GLN	VAL	LYS	ASN	ILE	ALA	ILE	ALA	GLY	ASP	SER	ALA	LYS	ILE	ALA	GLY	ASP	GLY	ILE	ALA	PRO	ASN	LEU	SER	GLN	VAL	ARG	ALA	SER	ASN	GLY	THR	LEU	ASN	GLY	PHE	THR	ALA	VAL	ASP	VAL	THR	GLY	GLY	GLY	GLY	
LEU	ALA	GLY	VAL	THR	SER	THR	GLN	ALA	ALA	ASP	GLN	LEU	ASN	ALA	SER	GLY	LYS	LEU	ALA	ILE	SER	ILE	ASN	LEU	THR	ILE	VAL	THR	PHE	THR	ALA	THR	GLY	ASN	PHE	THR	ALA	VAL	THR	GLY	GLN	VAL	ASN	THR	VAL	VAL	LYS
VAL	GLN	GLY	SER	ASP	GLY	LYS	PHE	ALA	ALA	ALA	LYS	ASN	VAL	VAL	ALA	GLY	THR	ALA	ILE	SER	VAL	THR	ASN	GLY	TYR	VAL	GLN	THR	TYR	SER	VAL	GLY	THR	LYS	PHE	GLY	THR	GLN	ALA	GLN	SER	THR	GLY	VAL	GLN	LYS	
S385	S389	I392	S393	T394	Q399	A408	R416	A417	D418	L419	A420	Q423	M424	R425	I430	D431	L433	T434	M435	E438	M439	A443	R444	S445	K448	D449	F452	K461	V464	Q467	A468	L484	L487	R488													

• Molecule 1: B-type flagellin

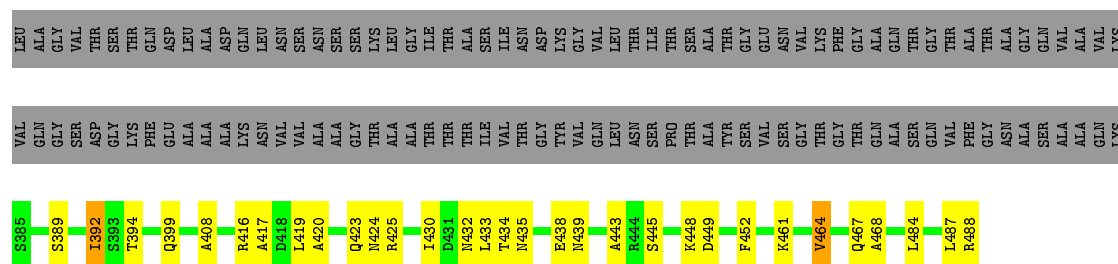
Chain K:  39% 15% 45%

MET	ALA	LEU	THR	V5	N6	T7	M13	R16	R37	I38	N39	S40	A41	K42	L48	Q49	R53	N56	S59	G60	L61	R66	I72	S73	T77	Q83	T86	Q90	R93	S103	M104	S105	D108	R109	A110	A111	A118	A121	E122	L123	T124				
R125	I126	S127	D128	T129	G133	G134	R135	K136	L137	L138	D139	S146	F147	Q148	V149	G150	A153	Y154	A166	I169	GLY	SER	TYR	GLN	VAL	GLY	ARG	ALA	SER	ASN	GLY	THR	LEU	ASN	GLY	ILE	ALA	SER	THR	GLY	VAL	ASN	LEU	VAL	GLY
GLY	GLN	GLN	VAL	LYS	ASN	ILE	ALA	ALA	GLY	GLY	ASP	SER	LYS	ALA	ILE	ALA	GLY	ASP	GLY	ALA	ILE	ALA	ARG	ALA	ARG	ALA	THR	THR	VAL	PHE	GLY	THR	THR	ASN	GLY	PHE	ASP	THR	VAL	VAL	THR	GLY	ASN	THR	VAL
SER	LEU	ALA	GLY	VAL	THR	SER	THR	GLN	ASP	ALA	GLN	LEU	ASN	VAL	SER	SER	LEU	ILE	GLY	ALA	THR	ALA	GLY	LEU	THR	ILE	VAL	THR	ALA	THR	LYS	PHE	GLY	GLY	THR	GLY	THR	ALA	VAL	THR	GLY	GLN	VAL	VAL	
LYS	VAL	GLN	SER	ASP	GLY	LYS	PHE	ALA	ALA	ALA	LYS	ASN	VAL	VAL	ALA	GLY	THR	ALA	ILE	SER	VAL	THR	ASN	GLY	TYR	VAL	GLN	THR	TYR	SER	VAL	GLY	THR	LYS	PHE	GLY	THR	GLN	ALA	GLN	SER	THR	GLY	GLN	
LYS	S385	S389	I392	S393	T394	Q399	A408	R416	A417	D418	L419	A420	Q423	M424	R425	I430	D431	L433	T434	M435	E438	N439	A443	K448	D449	F452	K461	V464	Q467	A468	L484	L487	R488												

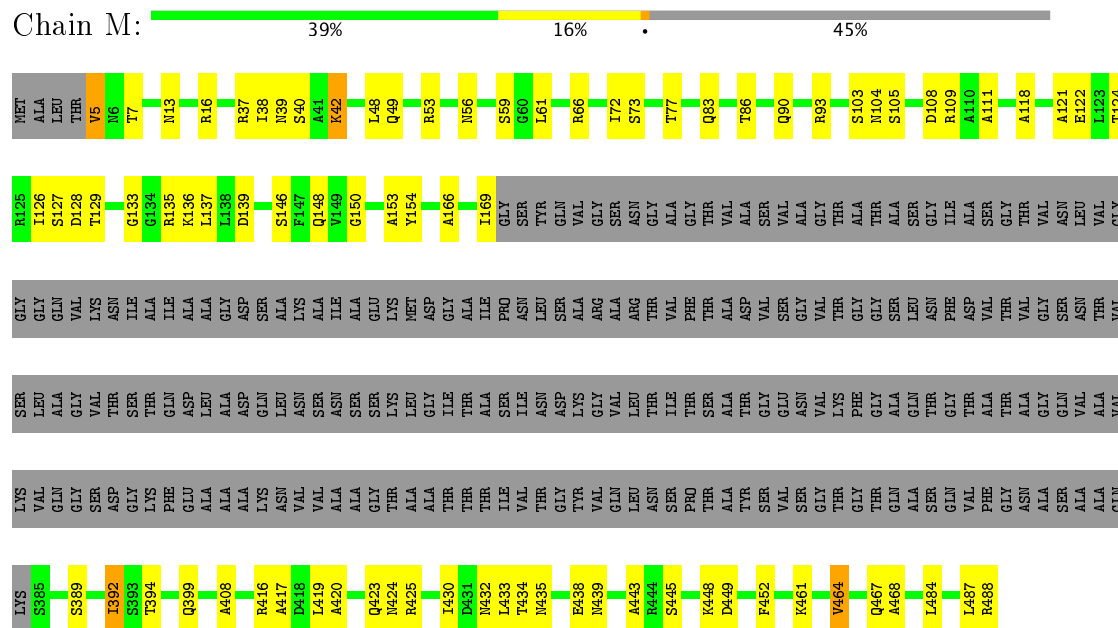
• Molecule 1: B-type flagellin

Chain L:  39% 15% 45%

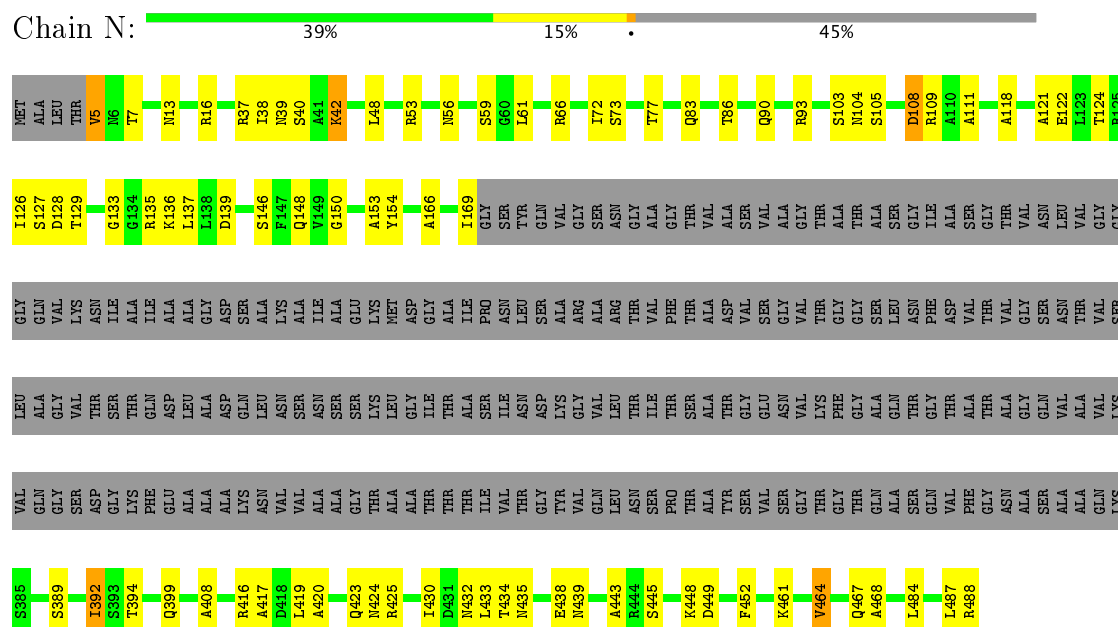
MET	ALA	LEU	THR	V6	N6	I7	M13	R16	R37	I38	I39	S40	A41	K42	L48	R53	N56	S59	G60	L61	R66	I72	S73	T77	Q83	T86	Q90	R93	S103	M104	S105	D108	R109	A110	A111	A118	A121	E122	L123	T124	R125							
I126	S127	D128	T129	G133	G134	R135	K136	L137	L138	D139	S146	F147	Q148	V149	G150	A153	Y154	A166	I169	GLY	SER	TYR	GLN	VAL	GLY	ARG	ALA	SER	ASN	GLY	THR	LEU	ASN	GLY	ILE	ALA	SER	THR	GLY	VAL	ASN	LEU	VAL	GLY	GLY			
GLY	GLN	VAL	LYS	ASN	ILE	ALA	ILE	ALA	GLY	ASP	SER	ALA	LYS	ILE	ALA	GLU	LYS	ASP	GLY	ILE	ALA	PRO	ASN	LEU	SER	GLN	VAL	ARG	ALA	SER	ASN	GLY	THR	LEU	ASN	GLY	PHE	THR	ALA	VAL	THR	GLY	GLN	VAL	ASN	THR	VAL	SER
LEU	ALA	GLY	VAL	THR	SER	THR	GLN	ASP	ALA	GLN	LEU	ASN	VAL	VAL	ALA	SER	SER	LEU	ILE	GLY	ALA	ILE	SER	ILE	ASN	LEU	THR	ILE	VAL	THR	ALA	THR	LYS	PHE	GLY	THR	ALA	VAL	THR	GLY	GLN	VAL	ASN	THR	VAL	GLN		
LYS	S385	S389	I392	S393	T394	Q399	A408	R416	A417	D418	L419	A420	Q423	M424	R425	I430	D431	L433	T434	M435	E438	M439	A443	K448	D449	F452	K461	V464	Q467	A468	L484	L487	R488															



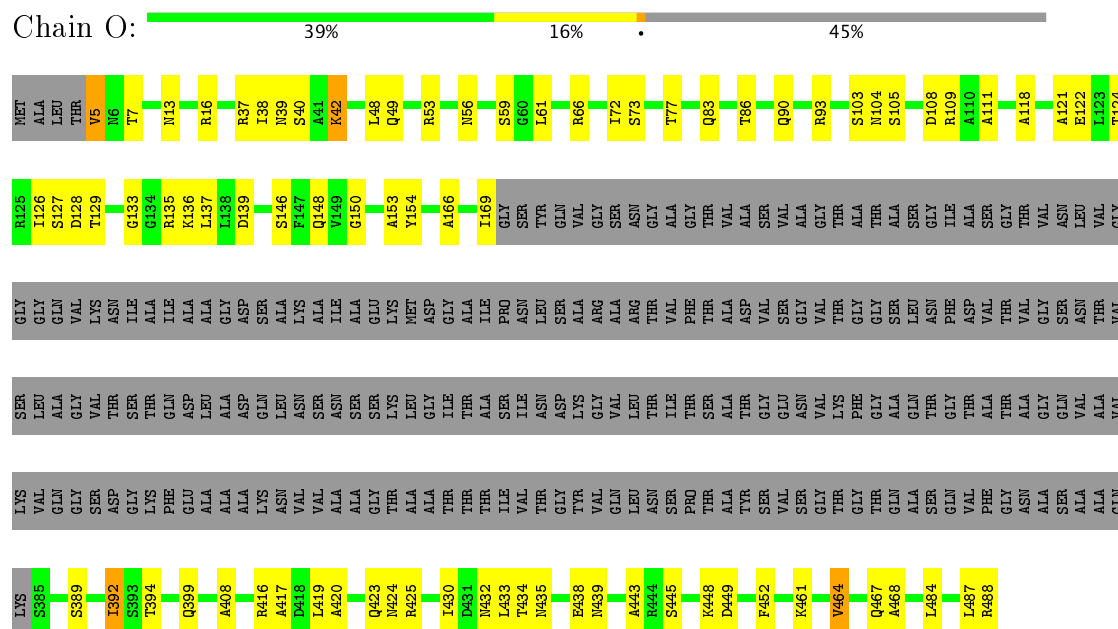
• Molecule 1: B-type flagellin



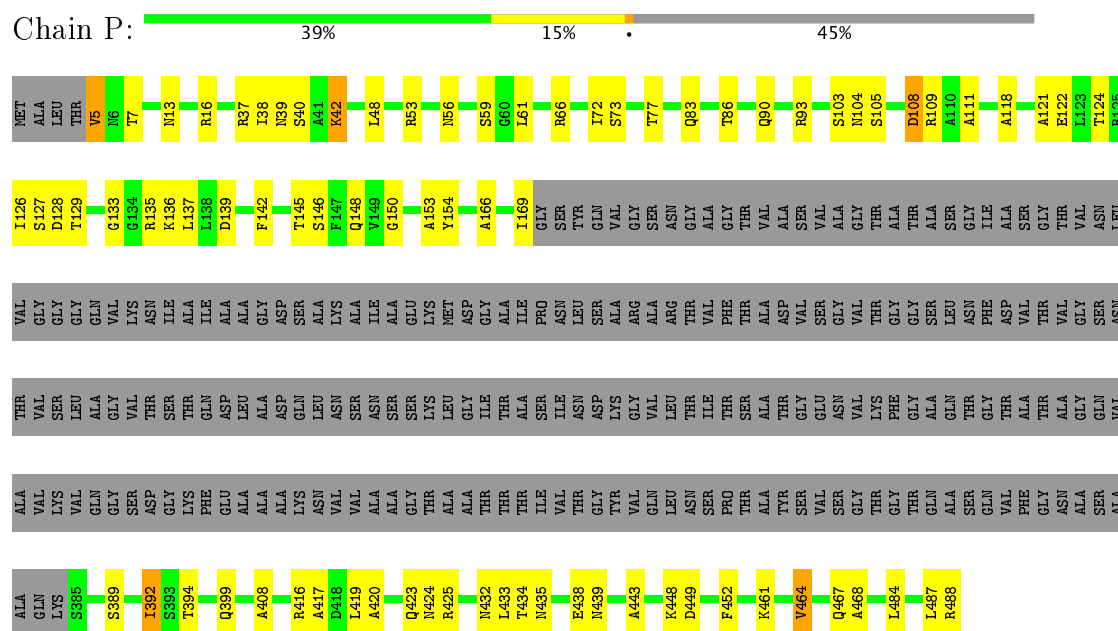
• Molecule 1: B-type flagellin



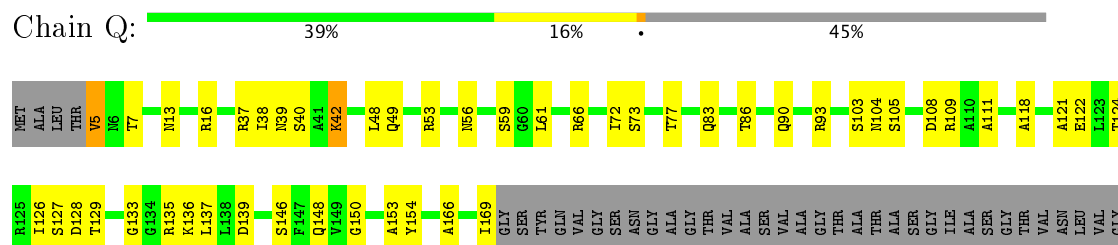
- Molecule 1: B-type flagellin

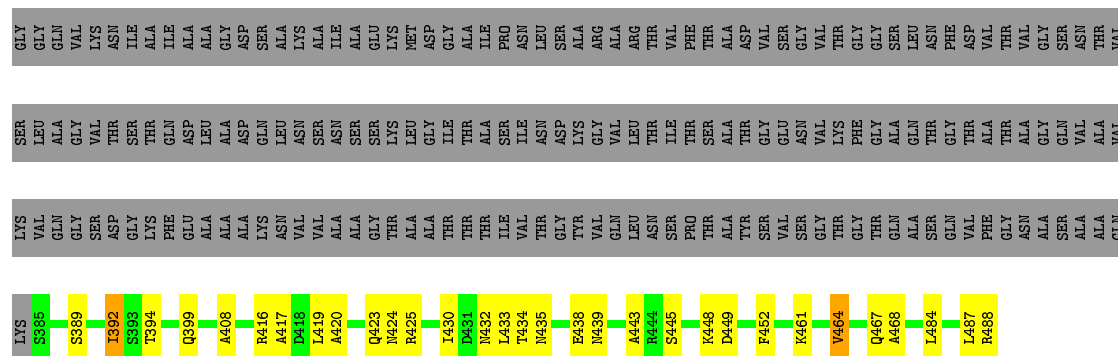


- Molecule 1: B-type flagellin

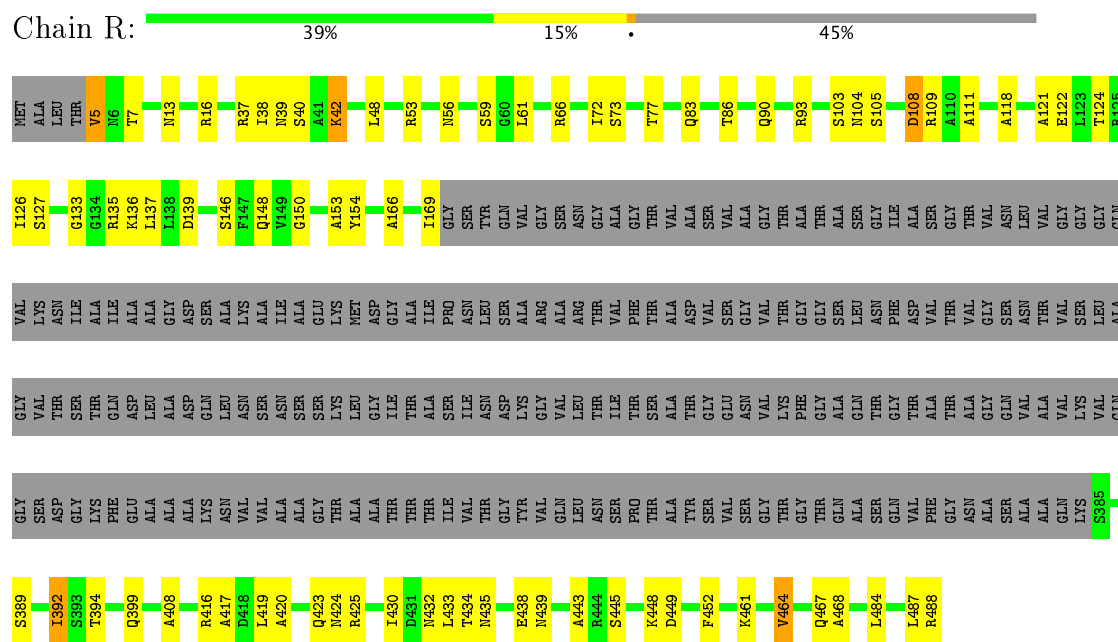


- Molecule 1: B-type flagellin

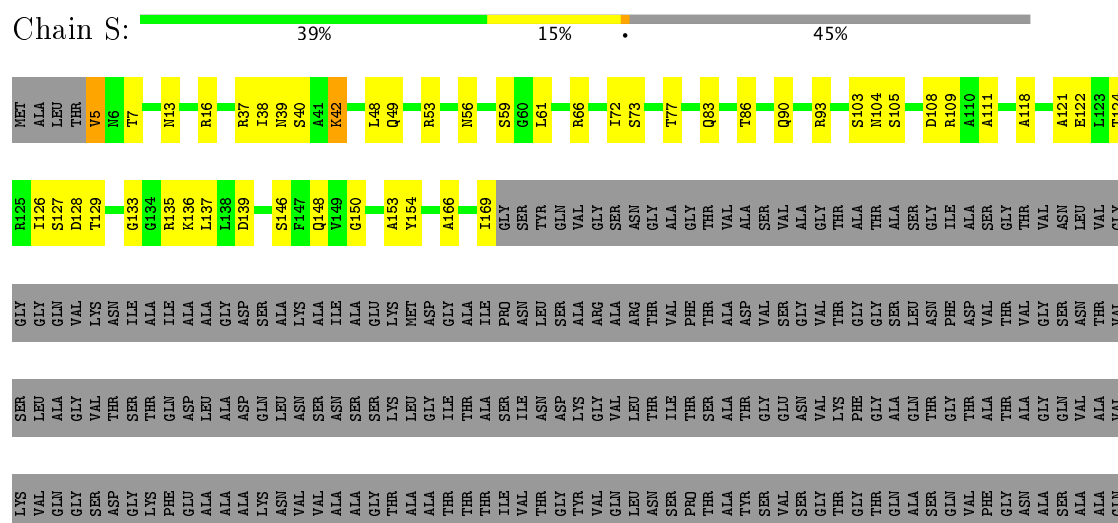




### • Molecule 1: B-type flagellin



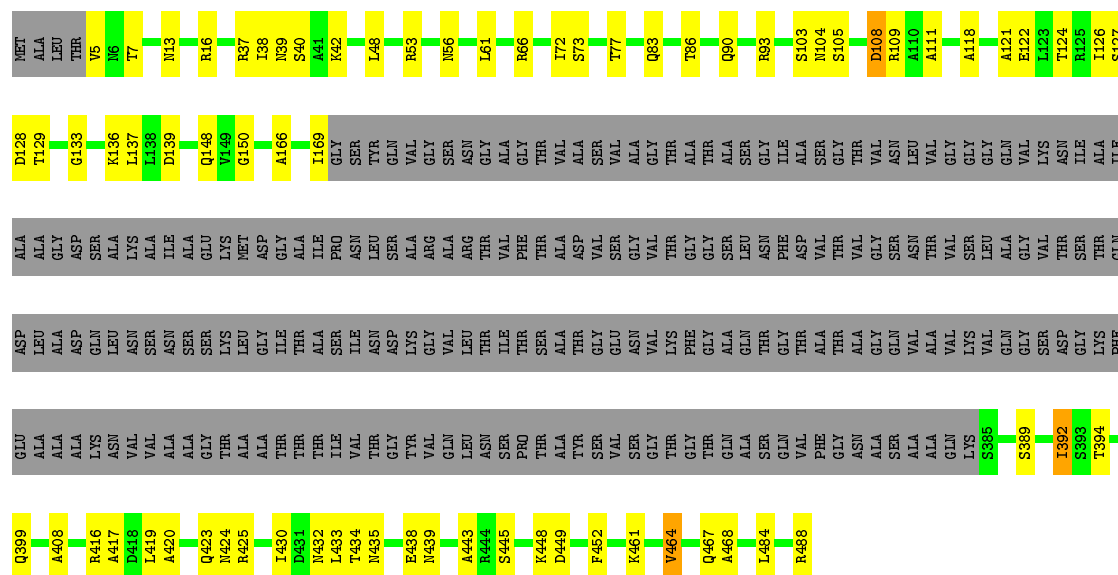
### • Molecule 1: B-type flagellin



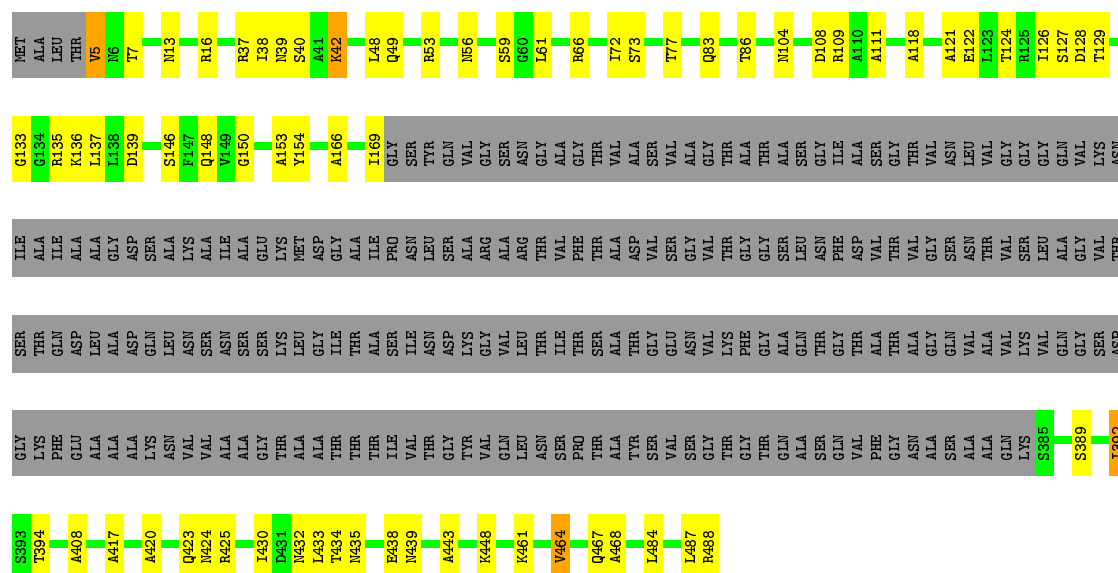




• Molecule 1: B-type flagellin

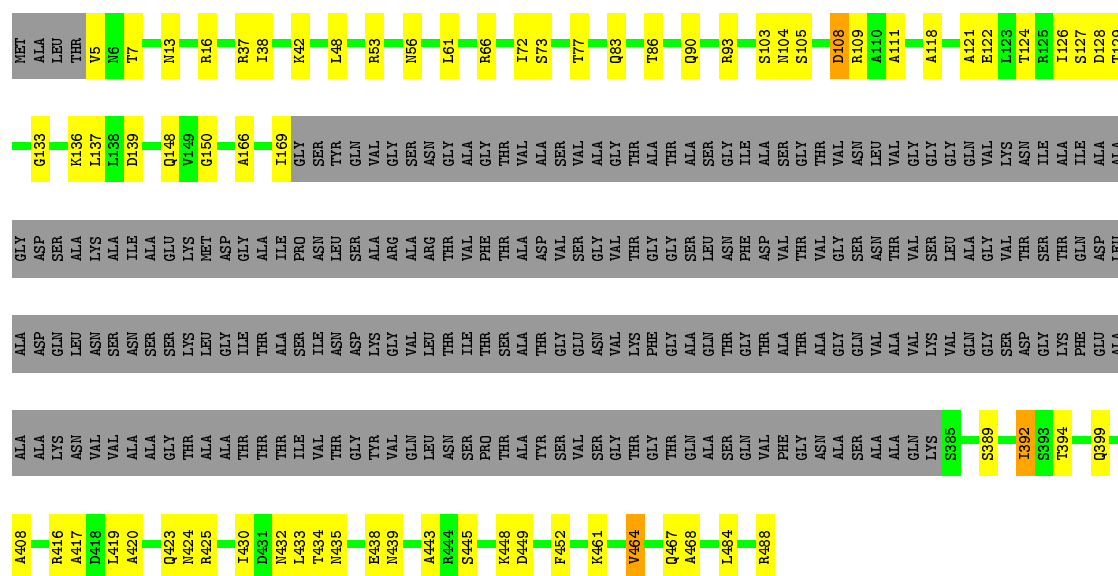


• Molecule 1: B-type flagellin

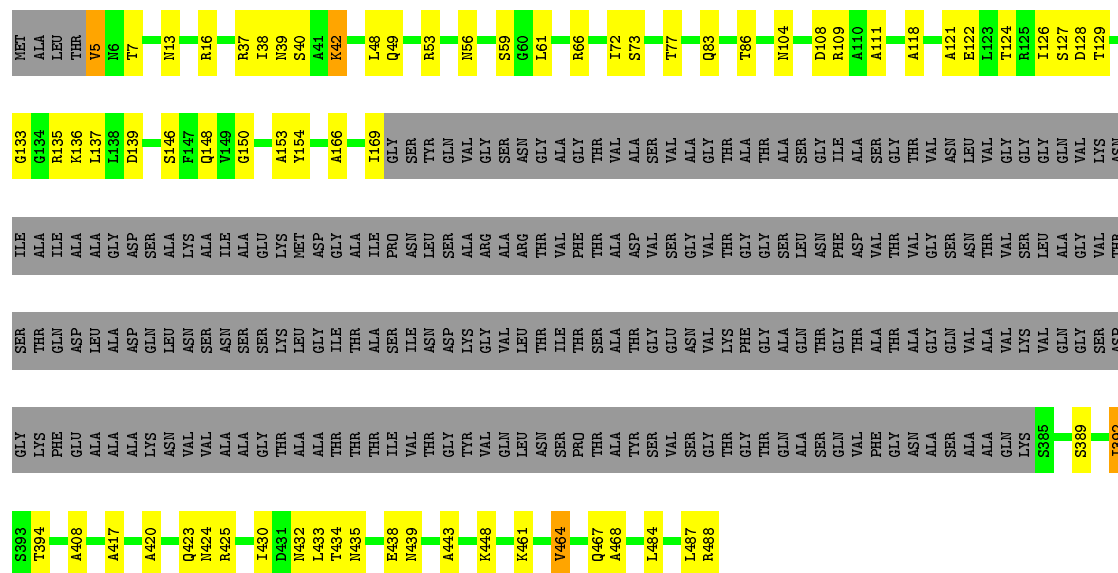


• Molecule 1: B-type flagellin

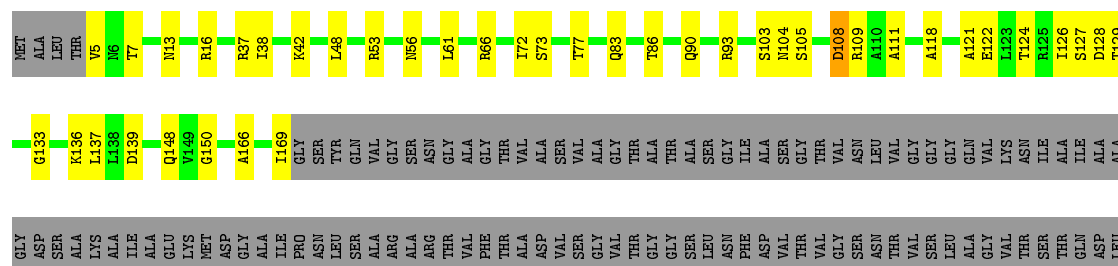


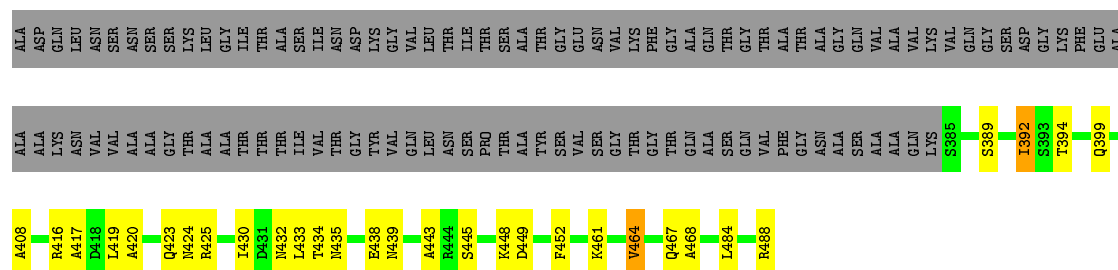


- Molecule 1: B-type flagellin



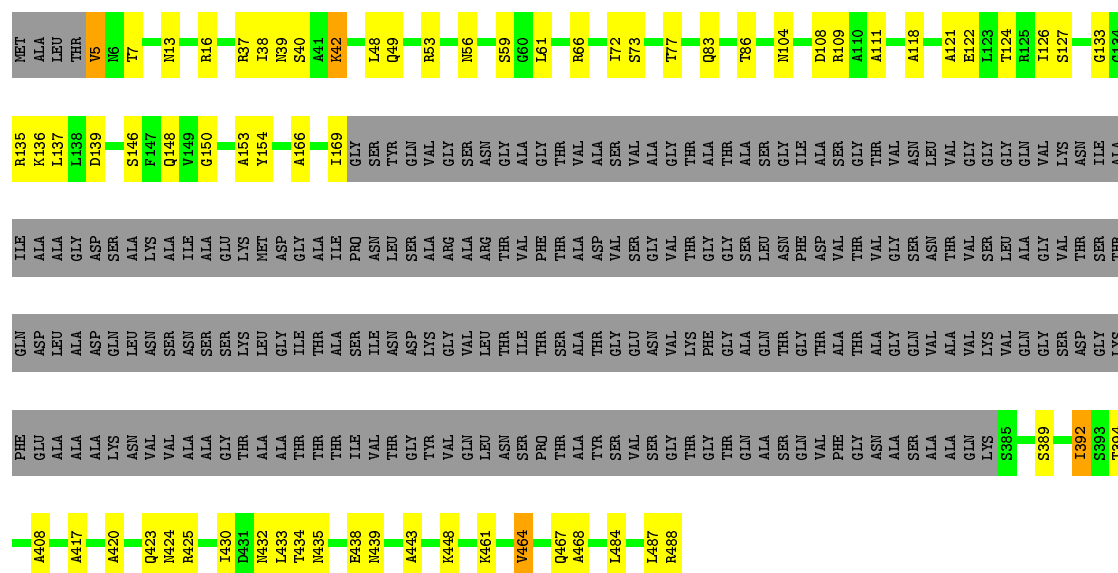
- Molecule 1: B-type flagellin





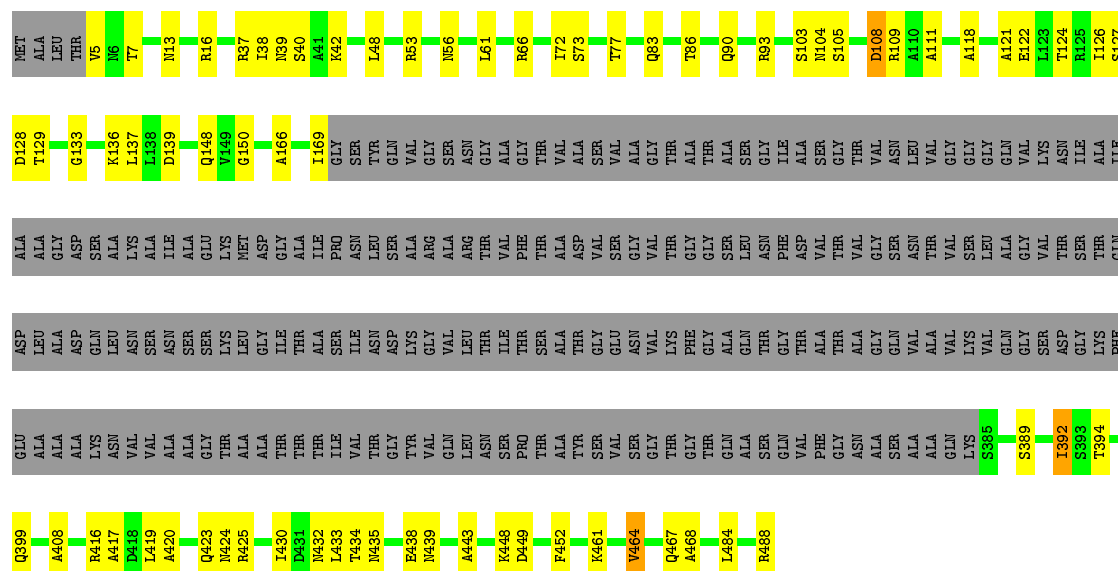
- Molecule 1: B-type flagellin

Chain Y:  41% 13% 45%

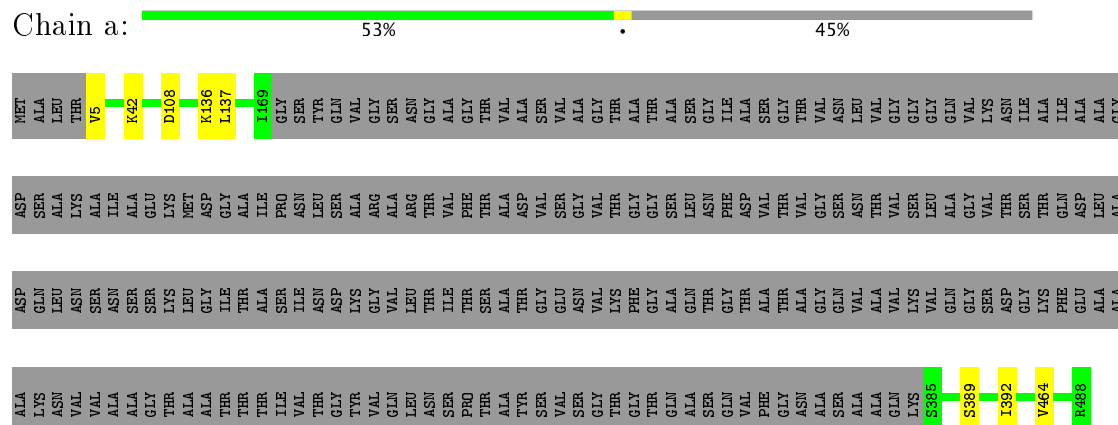


- Molecule 1: B-type flagellin

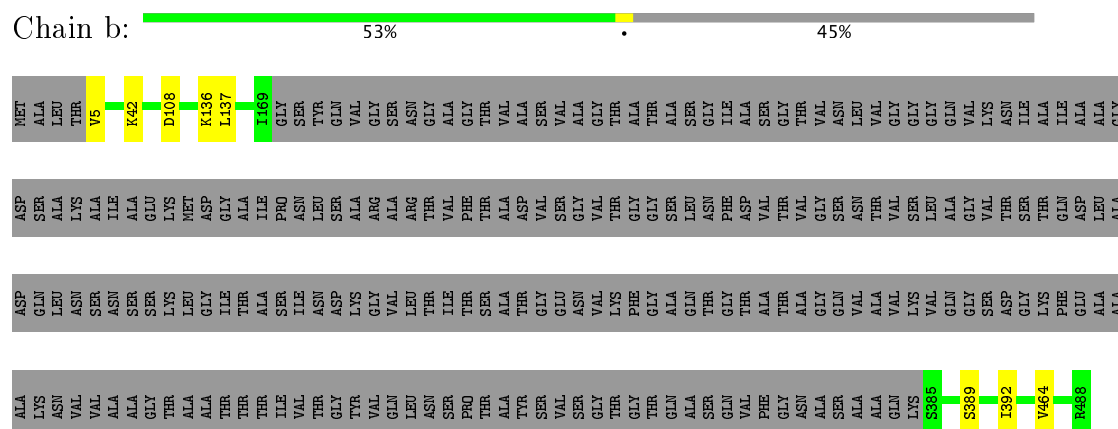
Chain Z:  40% 14% . 45%



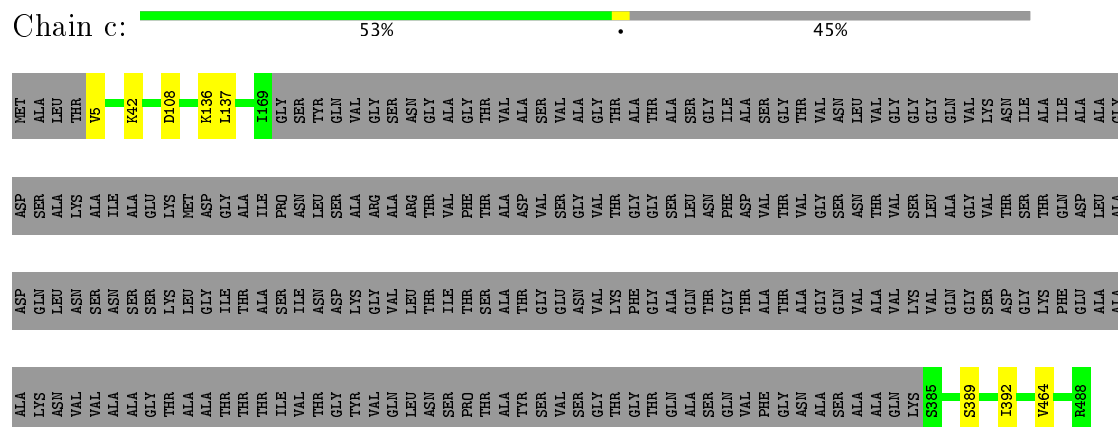
- Molecule 1: B-type flagellin



- Molecule 1: B-type flagellin

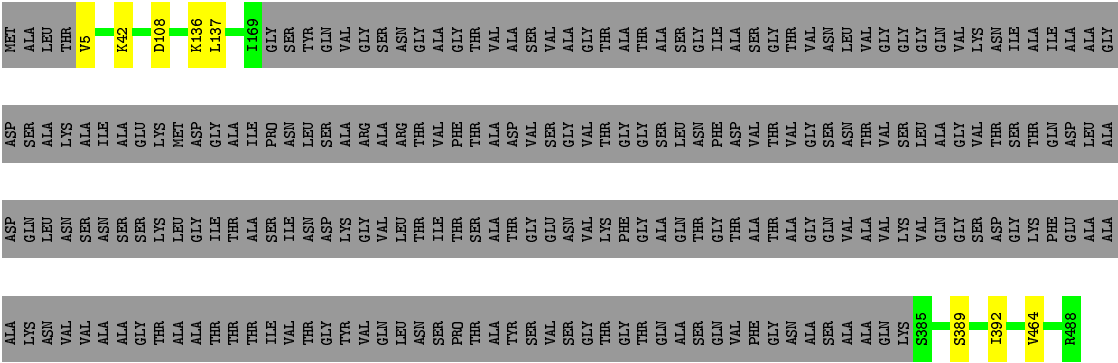


- Molecule 1: B-type flagellin

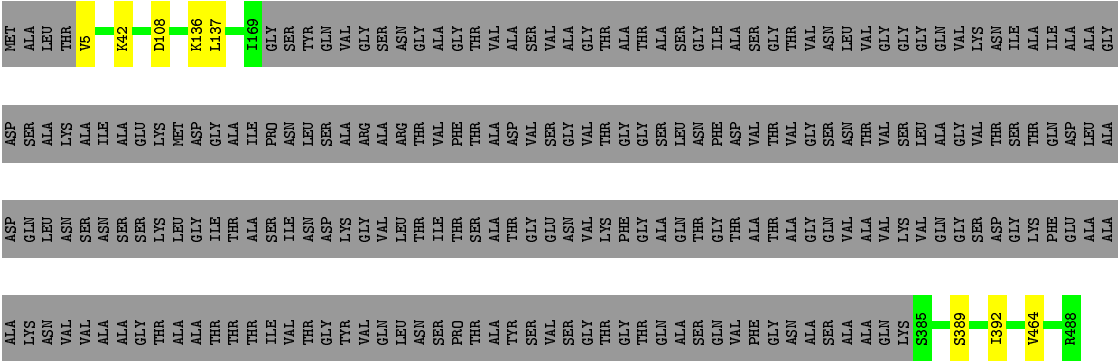


- Molecule 1: B-type flagellin

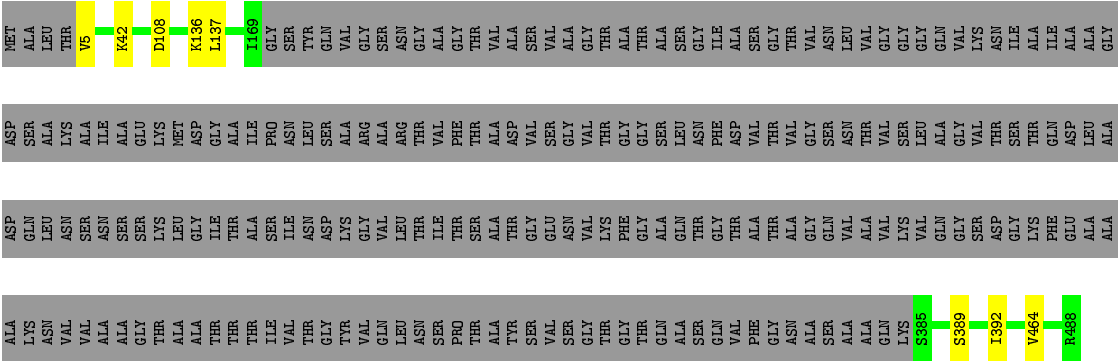




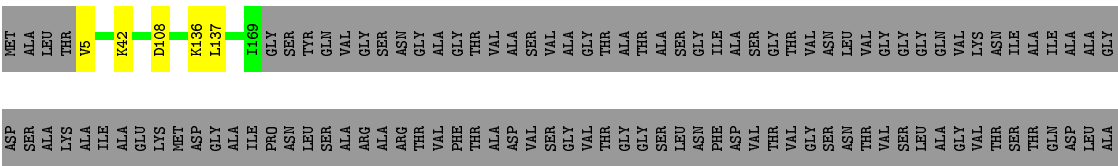
• Molecule 1: B-type flagellin

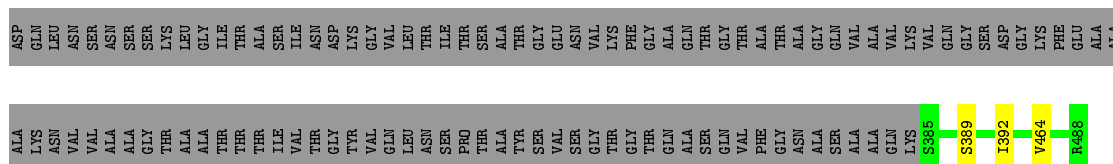


• Molecule 1: B-type flagellin



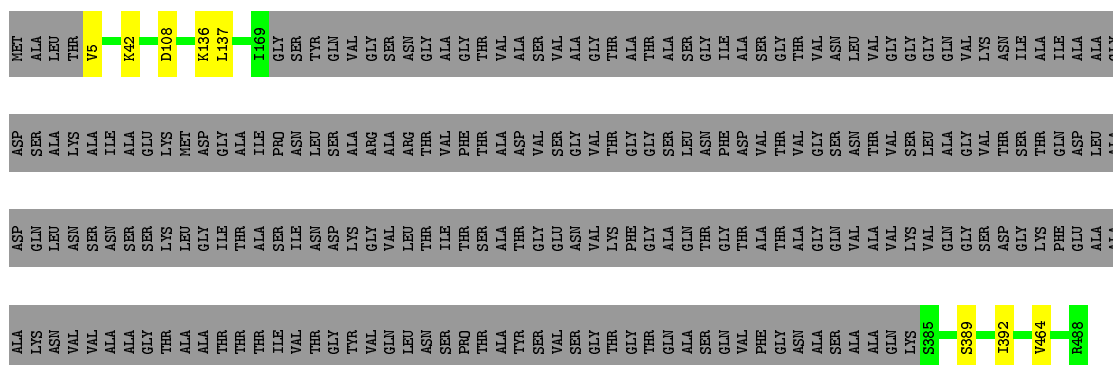
• Molecule 1: B-type flagellin





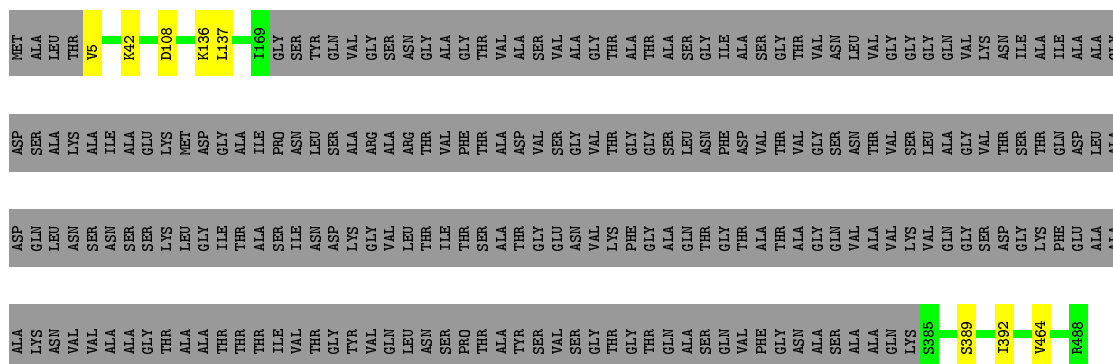
- Molecule 1: B-type flagellin

Chain h:  53% . 45%



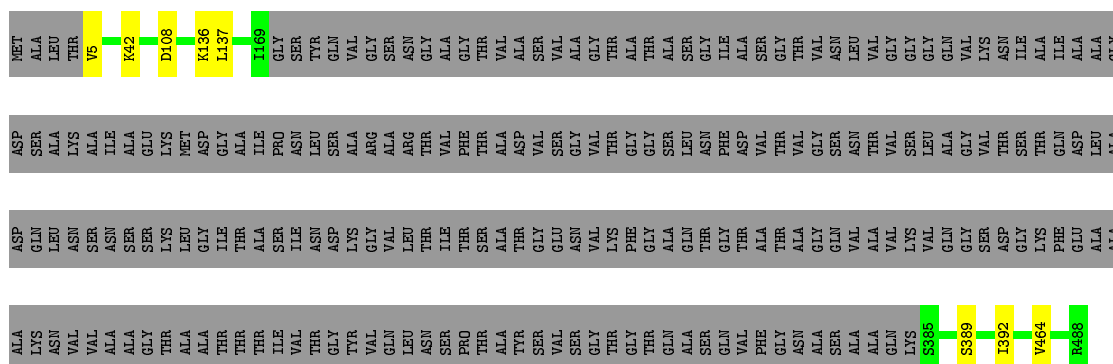
- Molecule 1: B-type flagellin

Chain i:  53% . 45%



- Molecule 1: B-type flagellin

Chain j:  53% . 45%



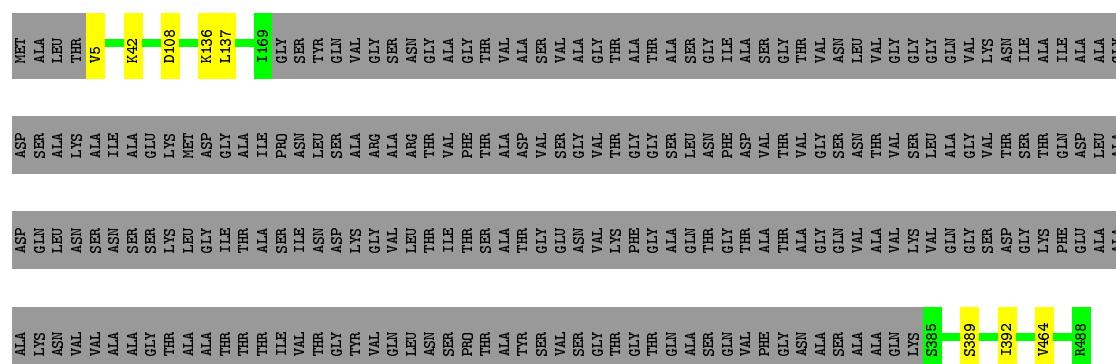
- Molecule 1: B-type flagellin

Chain k:  53% . 45%



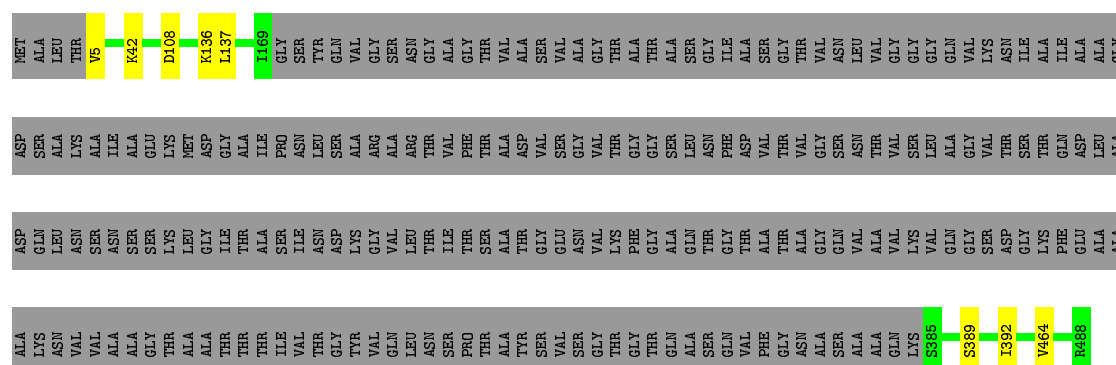
- Molecule 1: B-type flagellin

Chain 1:  53% . 45%



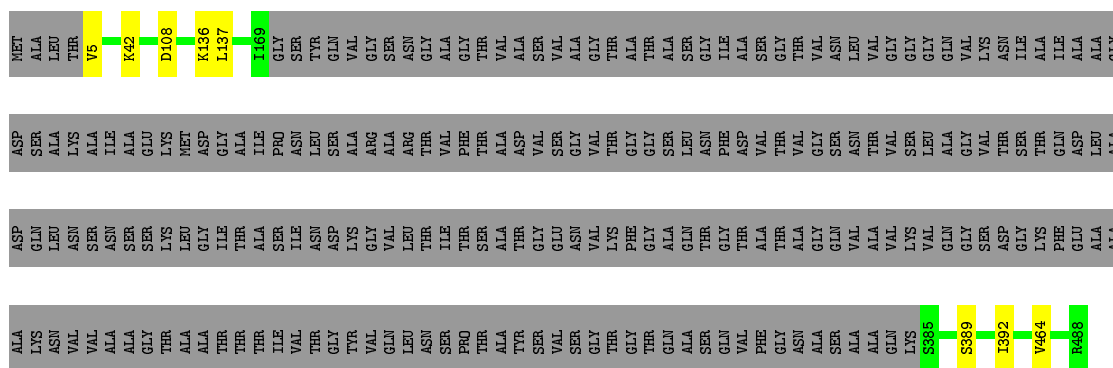
- Molecule 1: B-type flagellin

Chain m:  53% 45%

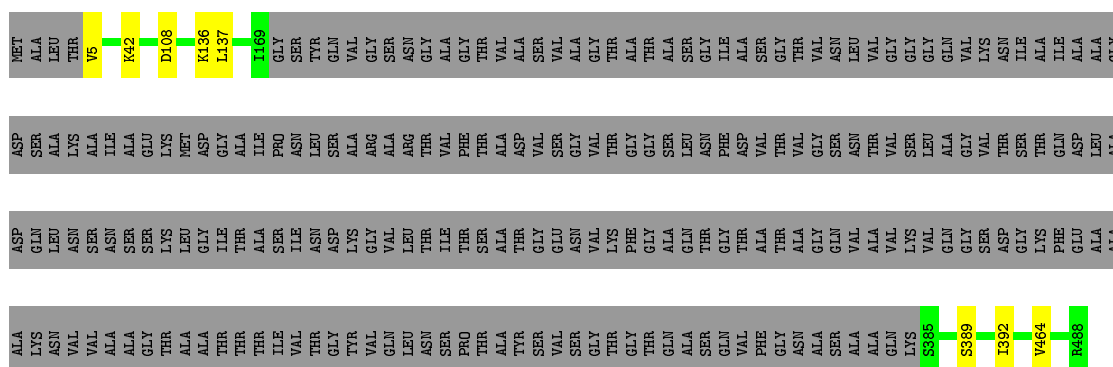


- Molecule 1: B-type flagellin

Chain n:  53% . 45%



- Molecule 1: B-type flagellin





## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=65.27°, rise=4.73 Å, axial sym=C1	Depositor
Number of segments used	17450	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 ( $e^-/\text{\AA}^2$ )	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	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	B	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	C	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	D	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	E	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	F	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	G	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	H	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	I	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	J	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	K	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	L	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	M	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	N	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	O	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	P	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	Q	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	R	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	S	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	T	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	U	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	V	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	W	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	X	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	Y	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	Z	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	a	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	b	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	c	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	d	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	e	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	f	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	g	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	h	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	i	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	j	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	k	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	l	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	m	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	n	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
1	o	0.57	2/1985 (0.1%)	0.73	1/2692 (0.0%)
All	All	0.57	82/81385 (0.1%)	0.73	41/110372 (0.0%)

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	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4
1	H	0	4
1	I	0	4
1	J	0	4
1	K	0	4
1	L	0	4
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	4
1	Q	0	4
1	R	0	4
1	S	0	4
1	T	0	4
1	U	0	4
1	V	0	4
1	W	0	4
1	X	0	4
1	Y	0	4
1	Z	0	4
1	a	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	4
1	c	0	4
1	d	0	4
1	e	0	4
1	f	0	4
1	g	0	4
1	h	0	4
1	i	0	4
1	j	0	4
1	k	0	4
1	l	0	4
1	m	0	4
1	n	0	4
1	o	0	4
All	All	0	164

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	464	VAL	CB-CG1	-6.67	1.38	1.52
1	U	464	VAL	CB-CG1	-6.67	1.38	1.52
1	h	464	VAL	CB-CG1	-6.67	1.38	1.52
1	m	464	VAL	CB-CG1	-6.67	1.38	1.52
1	L	464	VAL	CB-CG1	-6.67	1.38	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	42	LYS	CD-CE-NZ	-5.48	99.10	111.70
1	f	42	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	h	42	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	i	42	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	B	42	LYS	CD-CE-NZ	-5.47	99.12	111.70

There are no chirality outliers.

5 of 164 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ASP	Peptide
1	A	137	LEU	Peptide
1	A	389	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	392	ILE	Peptide
1	B	108	ASP	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	1979	1964	1964	206	0
1	B	1979	1964	1964	209	0
1	C	1979	1964	1964	205	0
1	D	1979	1964	1964	207	0
1	E	1979	1964	1964	204	0
1	F	1979	1964	1964	210	0
1	G	1979	1964	1964	204	0
1	H	1979	1964	1964	210	0
1	I	1979	1964	1964	205	0
1	J	1979	1964	1964	204	0
1	K	1979	1964	1964	188	0
1	L	1979	1964	1964	188	0
1	M	1979	1964	1964	181	0
1	N	1979	1964	1964	185	0
1	O	1979	1964	1964	188	0
1	P	1979	1964	1964	145	0
1	Q	1979	1964	1964	149	0
1	R	1979	1964	1964	146	0
1	S	1979	1964	1964	150	0
1	T	1979	1964	1964	116	0
1	U	1979	1964	1964	119	0
1	V	1979	1964	1964	114	0
1	W	1979	1964	1964	117	0
1	X	1979	1964	1964	115	0
1	Y	1979	1964	1964	117	0
1	Z	1979	1964	1964	114	0
1	a	1979	1964	1964	0	0
1	b	1979	1964	1964	0	0
1	c	1979	1964	1964	0	0
1	d	1979	1964	1964	0	0
1	e	1979	1964	1964	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	1979	1964	1964	0	0
1	g	1979	1964	1964	0	0
1	h	1979	1964	1964	0	0
1	i	1979	1964	1964	0	0
1	j	1979	1964	1964	0	0
1	k	1979	1964	1964	0	0
1	l	1979	1964	1964	0	0
1	m	1979	1964	1964	0	0
1	n	1979	1964	1964	0	0
1	o	1979	1964	1964	0	0
All	All	81139	80524	80524	2731	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 17.

The worst 5 of 2731 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:R:38:ILE:HD11	1:R:48:LEU:HB2	1.36	1.08
1:K:38:ILE:HD11	1:K:48:LEU:HB2	1.36	1.07
1:M:38:ILE:HD11	1:M:48:LEU:HB2	1.36	1.07
1:N:38:ILE:HD11	1:N:48:LEU:HB2	1.36	1.07
1:E:38:ILE:HD11	1:E:48:LEU:HB2	1.36	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	246 (93%)	19 (7%)	0	100	100
1	B	265/488 (54%)	246 (93%)	19 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	D	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	E	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	F	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	G	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	H	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	I	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	J	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	K	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	L	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	M	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	N	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	O	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	P	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	Q	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	R	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	S	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	T	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	U	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	V	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	W	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	X	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	Y	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	Z	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	a	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	b	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	c	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	d	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	e	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	f	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	g	265/488 (54%)	246 (93%)	19 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	i	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	j	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	k	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	l	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	m	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	n	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
1	o	265/488 (54%)	246 (93%)	19 (7%)	0	100	100
All	All	10865/20008 (54%)	10086 (93%)	779 (7%)	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	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	B	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	C	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	D	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	E	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	F	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	G	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	H	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	I	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	J	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	K	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	L	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	M	211/363 (58%)	210 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	O	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	P	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	Q	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	R	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	S	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	T	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	U	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	V	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	W	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	X	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	Y	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	Z	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	a	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	b	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	c	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	d	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	e	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	f	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	g	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	h	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	i	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	j	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	k	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	l	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	m	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	n	211/363 (58%)	210 (100%)	1 (0%)	91	95
1	o	211/363 (58%)	210 (100%)	1 (0%)	91	95
All	All	8651/14883 (58%)	8610 (100%)	41 (0%)	91	95

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	136	LYS
1	W	136	LYS
1	I	136	LYS
1	T	136	LYS
1	U	136	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 229 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	83	GLN
1	W	424	ASN
1	I	148	GLN
1	S	432	ASN
1	U	148	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.