



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:29 PM UTC

PDB ID : 8SUG / pdb_00008sug
EMDB ID : EMD-40765
Title : Cryo-EM structure of the wild type *P. aeruginosa* flagellar filament
Authors : Kreutzberger, M.A.; Nedeljkovic, M.; Egelman, E.H.; Sundberg, E.J.
Deposited on : 2023-05-12
Resolution : 4.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

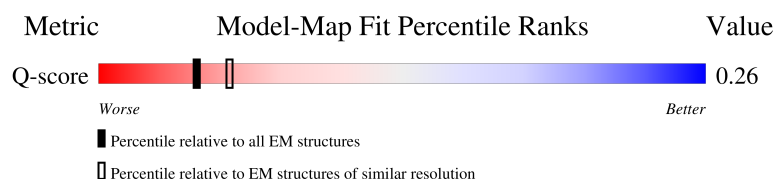
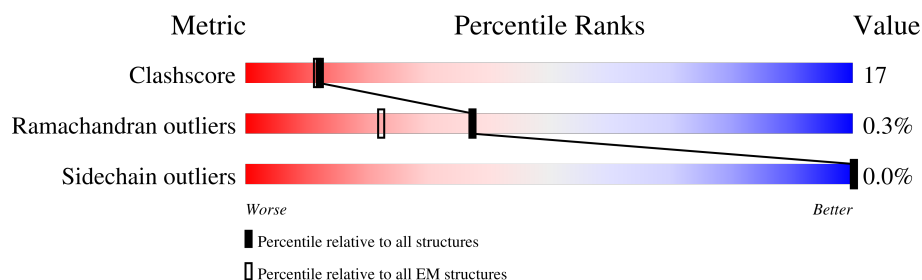
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	484	21% 61% 38%
1	B	484	29% 65% 34%
1	C	484	29% 65% 35%
1	D	484	15% 63% 36%

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Mol	Chain	Length	Quality of chain
1	E	484	15% 67% 33%
1	F	484	20% 68% 32%
1	G	484	14% 66% 33%
1	H	484	9% 64% 35%
1	I	484	13% 62% 37%
1	J	484	15% 65% 34%
1	K	484	10% 63% 37%
1	L	484	11% 66% 33%
1	M	484	15% 67% 33%
1	N	484	9% 63% 37%
1	O	484	10% 69% 30%
1	P	484	11% 68% 32%
1	Q	484	9% 64% 35%
1	R	484	7% 71% 29%
1	S	484	12% 69% 31%
1	T	484	10% 67% 33%
1	U	484	8% 66% 34%
1	V	484	11% 69% 31%
1	W	484	7% 63% 37%
1	X	484	10% 67% 33%
1	Y	484	17% 68% 32%
1	Z	484	10% 66% 34%
1	a	484	11% 61% 38%
1	b	484	14% 64% 36%
1	c	484	14% 64% 35%

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Mol	Chain	Length	Quality of chain
1	d	484	
1	e	484	
1	f	484	
1	g	484	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 113355 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called B-type flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	B	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	C	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	D	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	E	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	F	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	G	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	H	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	I	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	J	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	K	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	L	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	M	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	N	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	O	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	P	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		
1	Q	484	Total	C	N	O	S	1	0
			3435	2072	626	736	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	S	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	T	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	U	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	V	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	W	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	X	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	Y	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	Z	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	a	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	b	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	c	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	d	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	e	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	f	484	Total 3435	C 2072	N 626	O 736	S 1	1	0
1	g	484	Total 3435	C 2072	N 626	O 736	S 1	1	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	ALA	GLY	conflict	UNP P72151
B	420	ALA	GLY	conflict	UNP P72151
C	420	ALA	GLY	conflict	UNP P72151
D	420	ALA	GLY	conflict	UNP P72151
E	420	ALA	GLY	conflict	UNP P72151
F	420	ALA	GLY	conflict	UNP P72151
G	420	ALA	GLY	conflict	UNP P72151

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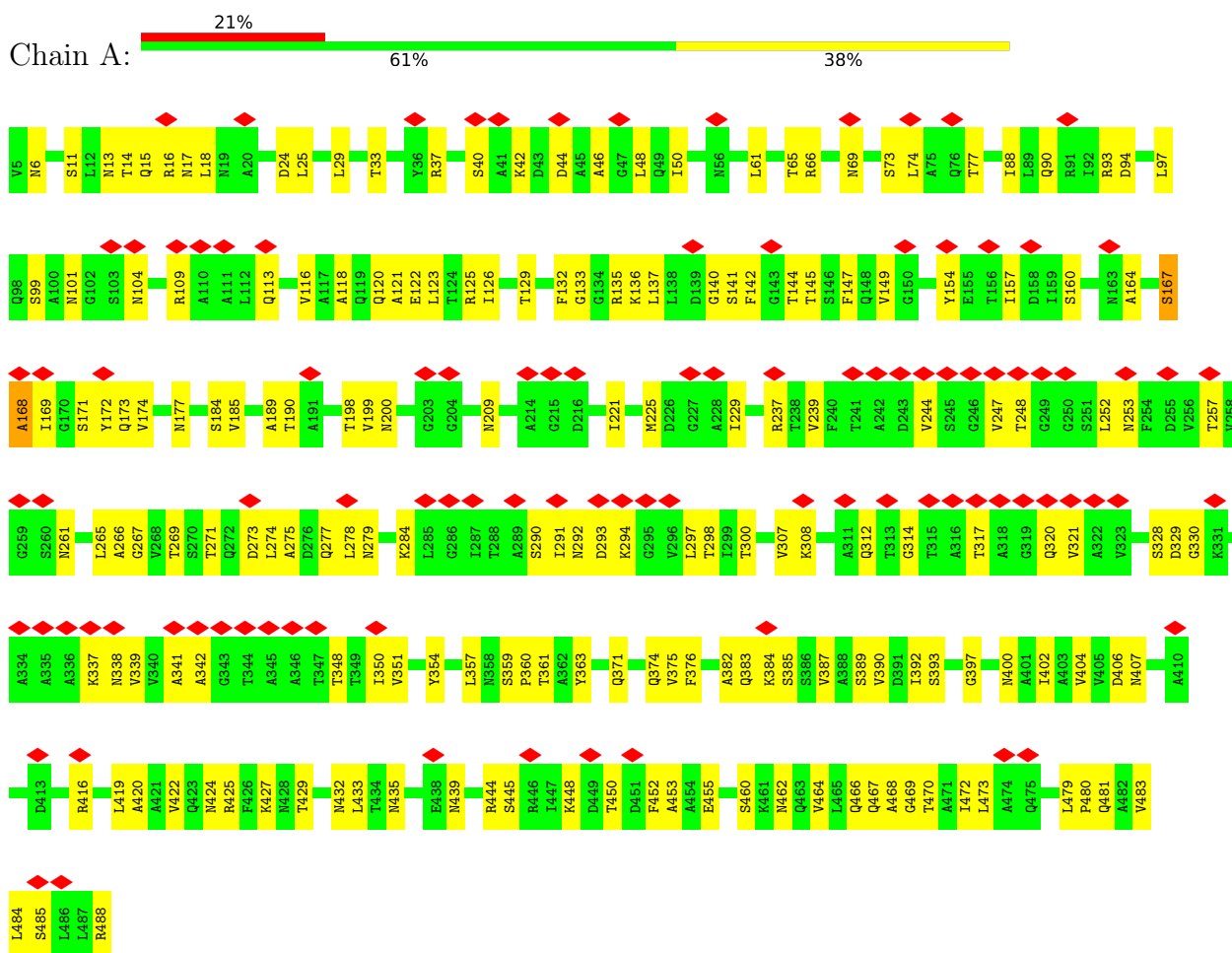
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Chain	Residue	Modelled	Actual	Comment	Reference
H	420	ALA	GLY	conflict	UNP P72151
I	420	ALA	GLY	conflict	UNP P72151
J	420	ALA	GLY	conflict	UNP P72151
K	420	ALA	GLY	conflict	UNP P72151
L	420	ALA	GLY	conflict	UNP P72151
M	420	ALA	GLY	conflict	UNP P72151
N	420	ALA	GLY	conflict	UNP P72151
O	420	ALA	GLY	conflict	UNP P72151
P	420	ALA	GLY	conflict	UNP P72151
Q	420	ALA	GLY	conflict	UNP P72151
R	420	ALA	GLY	conflict	UNP P72151
S	420	ALA	GLY	conflict	UNP P72151
T	420	ALA	GLY	conflict	UNP P72151
U	420	ALA	GLY	conflict	UNP P72151
V	420	ALA	GLY	conflict	UNP P72151
W	420	ALA	GLY	conflict	UNP P72151
X	420	ALA	GLY	conflict	UNP P72151
Y	420	ALA	GLY	conflict	UNP P72151
Z	420	ALA	GLY	conflict	UNP P72151
a	420	ALA	GLY	conflict	UNP P72151
b	420	ALA	GLY	conflict	UNP P72151
c	420	ALA	GLY	conflict	UNP P72151
d	420	ALA	GLY	conflict	UNP P72151
e	420	ALA	GLY	conflict	UNP P72151
f	420	ALA	GLY	conflict	UNP P72151
g	420	ALA	GLY	conflict	UNP P72151

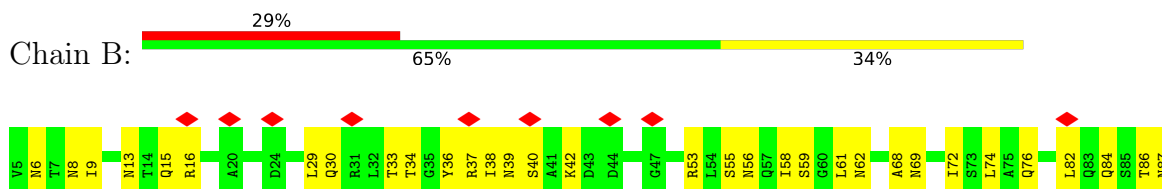
3 Residue-property plots

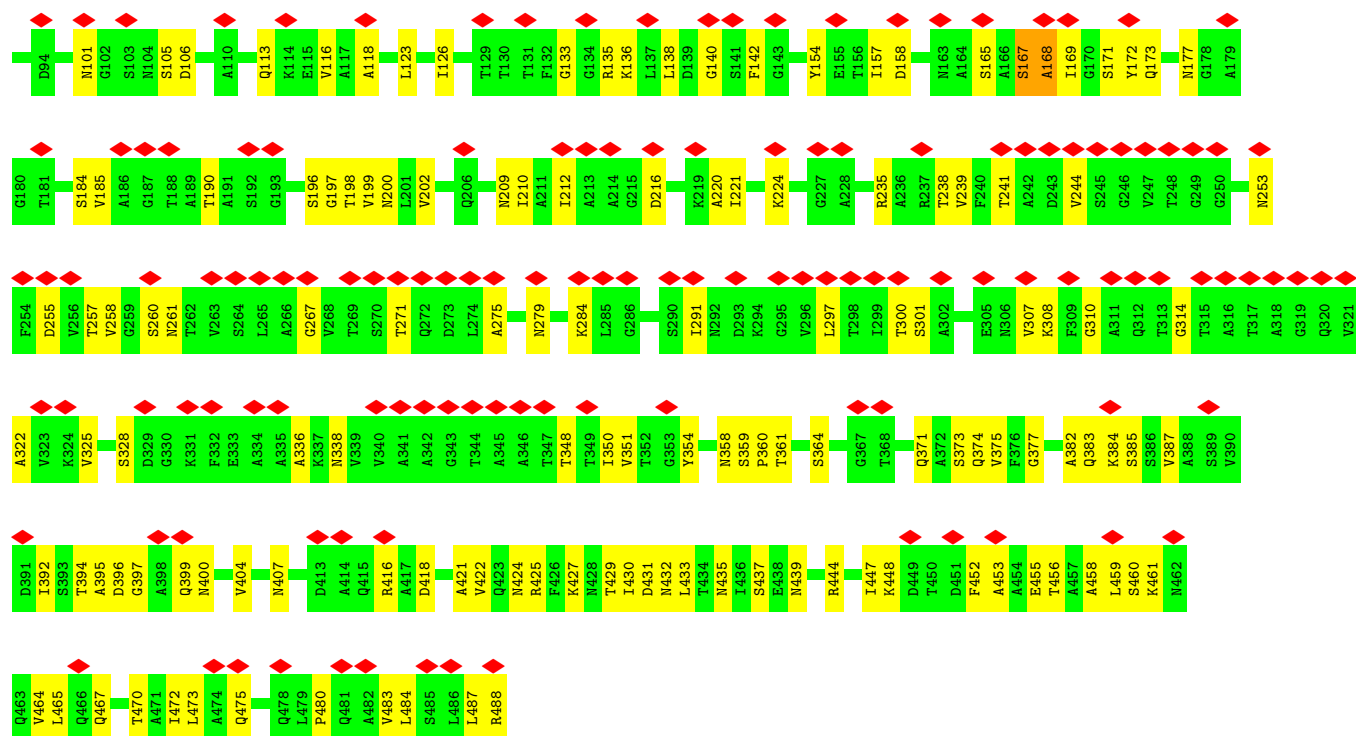
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: B-type flagellin

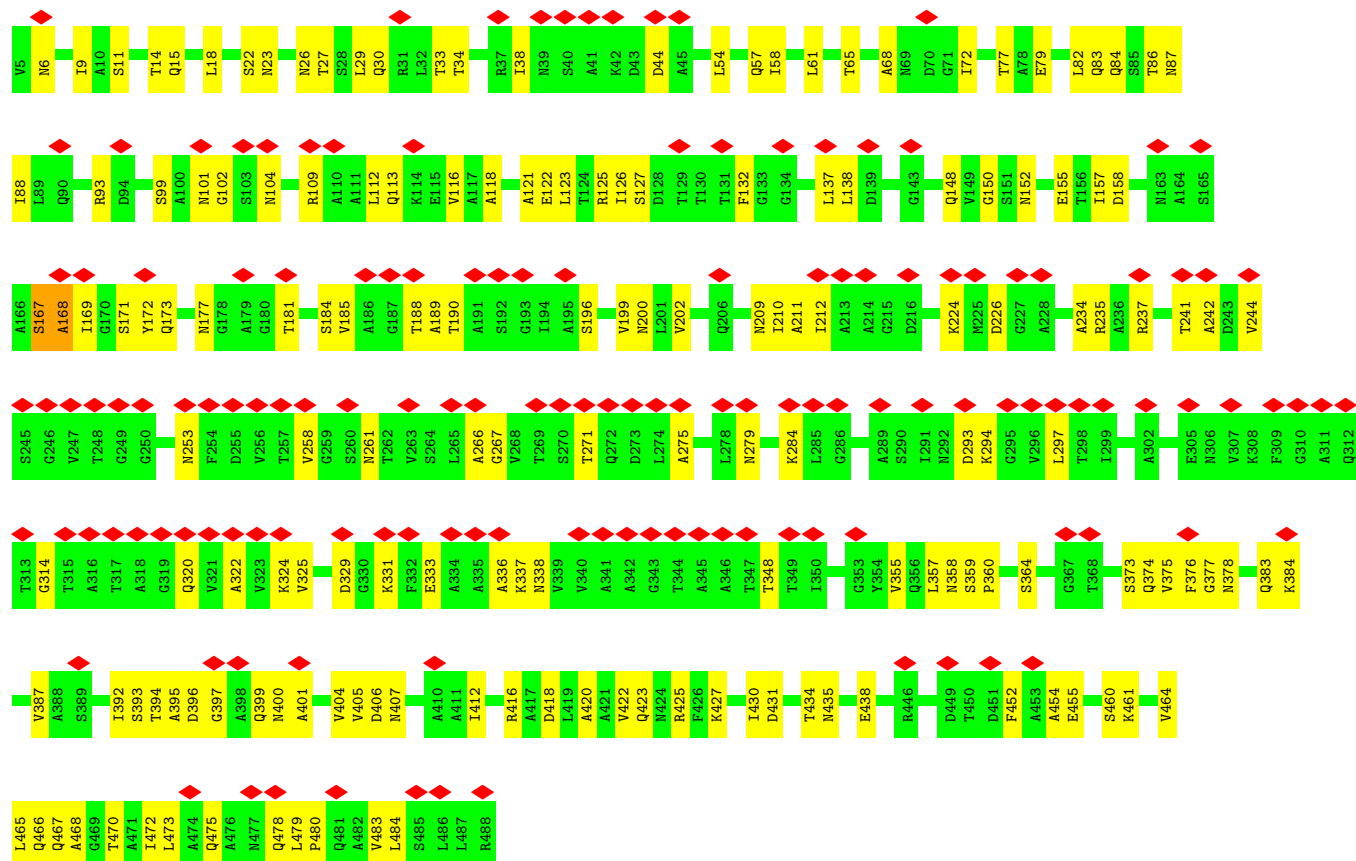


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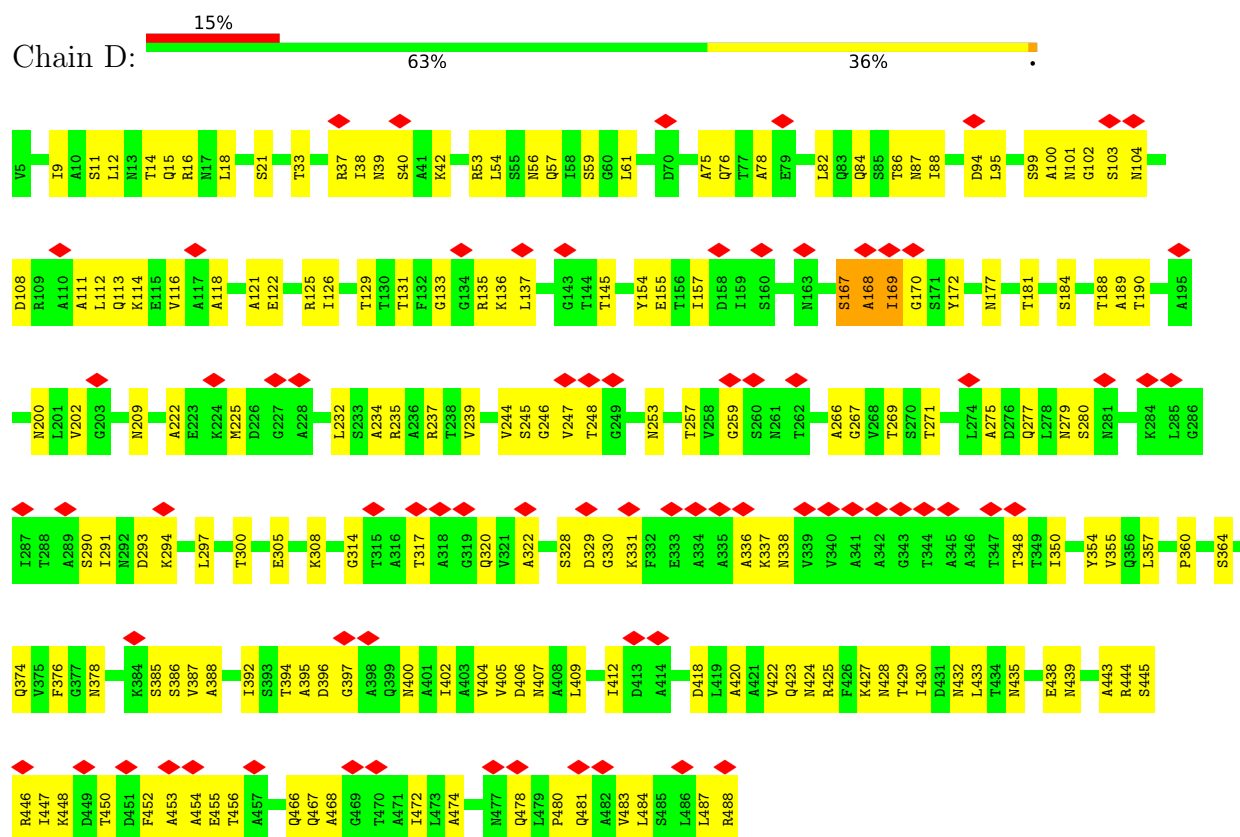




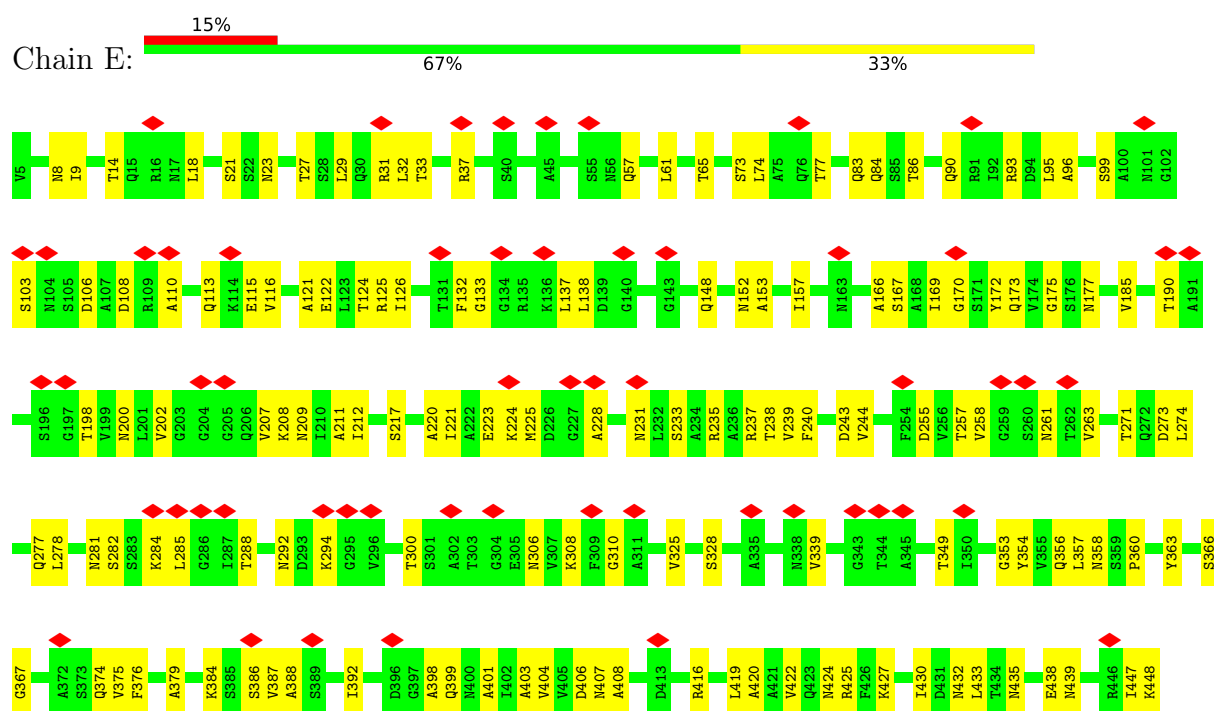
• Molecule 1: B-type flagellin

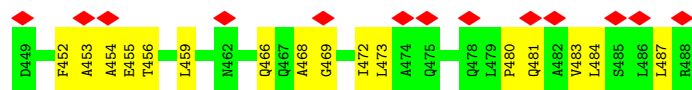


- Molecule 1: B-type flagellin

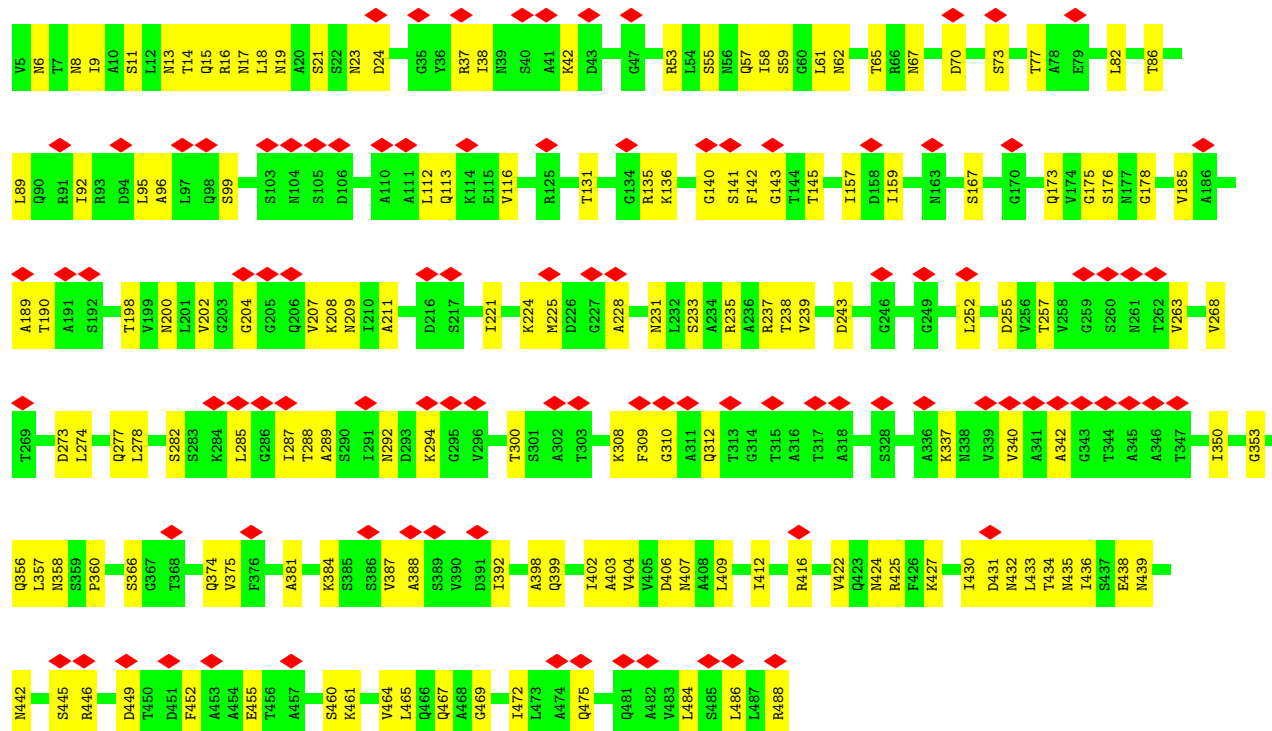


- Molecule 1: B-type flagellin

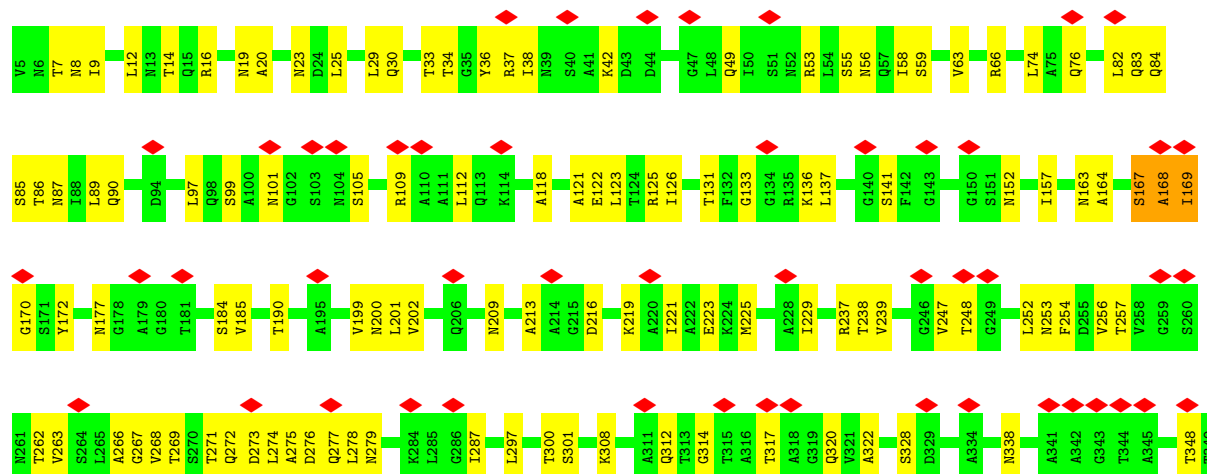


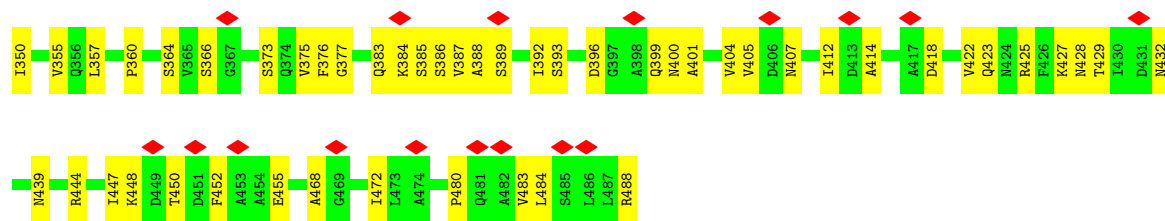


• Molecule 1: B-type flagellin

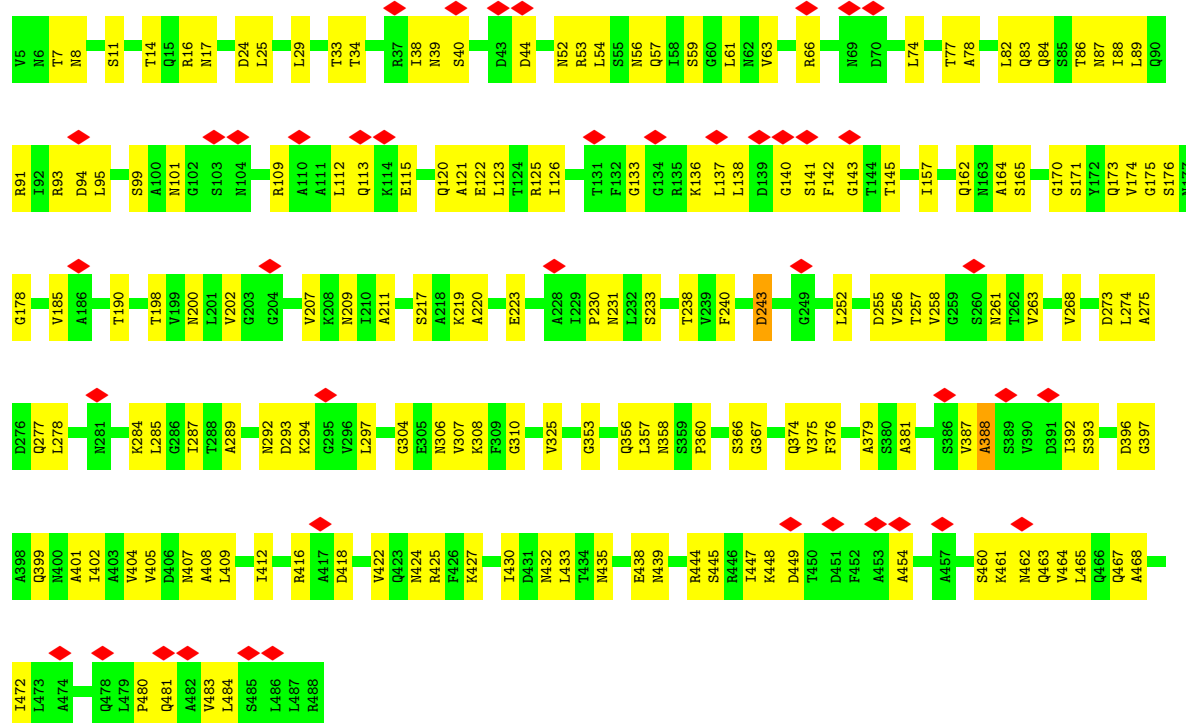


• Molecule 1: B-type flagellin

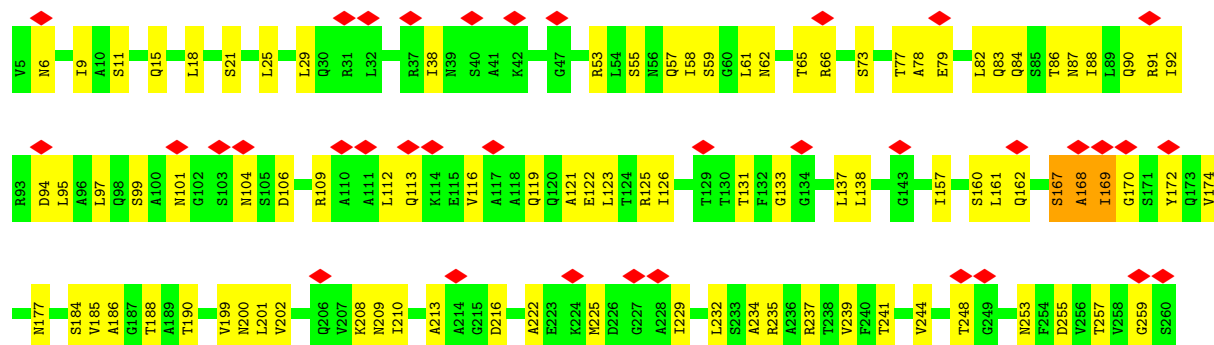


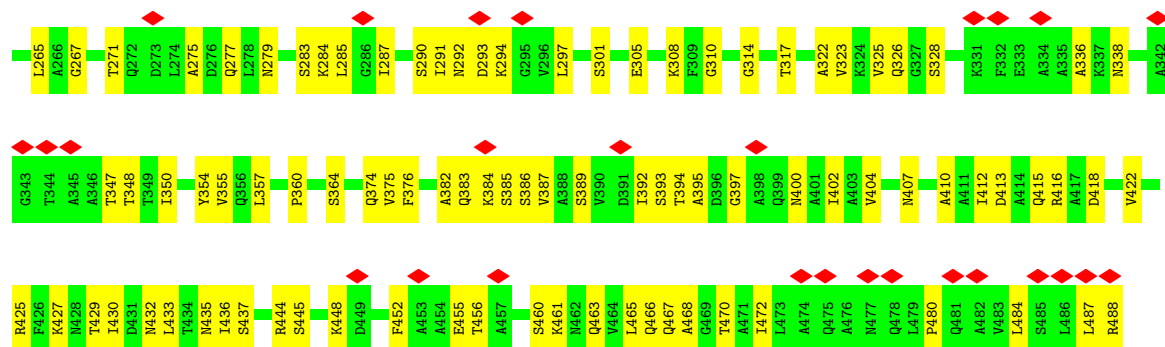


• Molecule 1: B-type flagellin

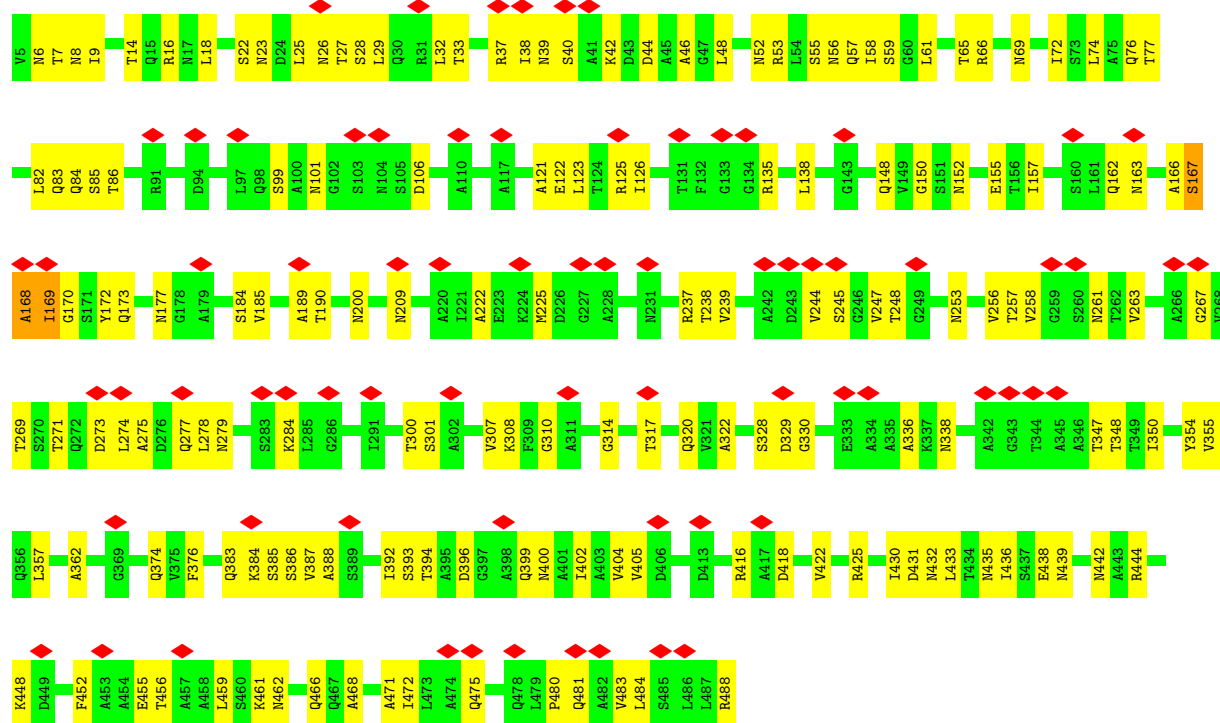


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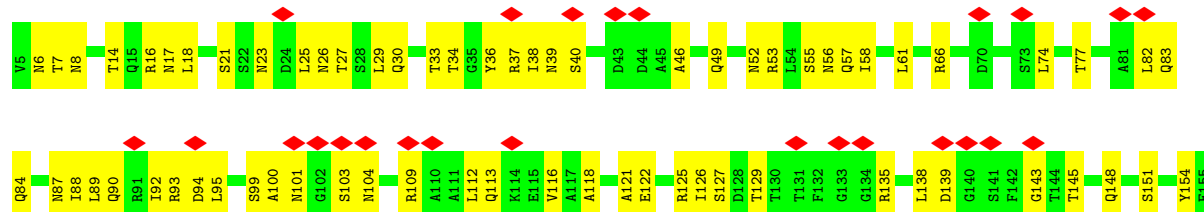


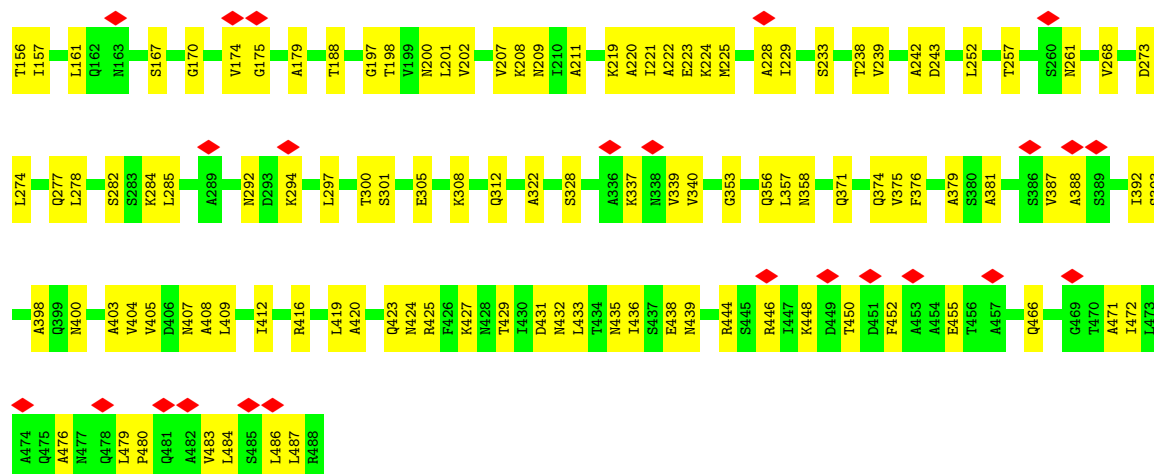


• Molecule 1: B-type flagellin

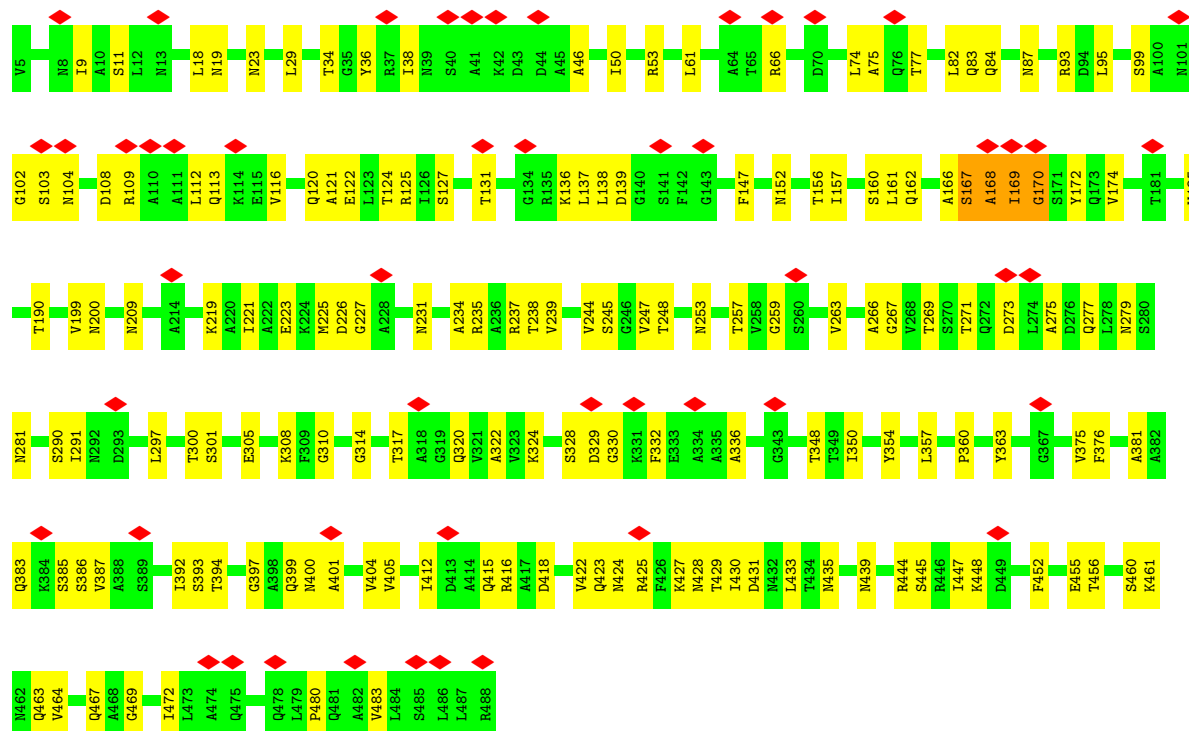


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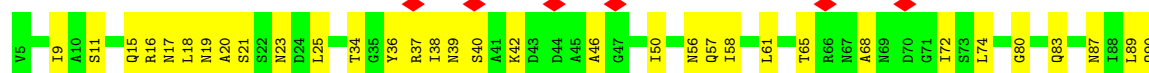


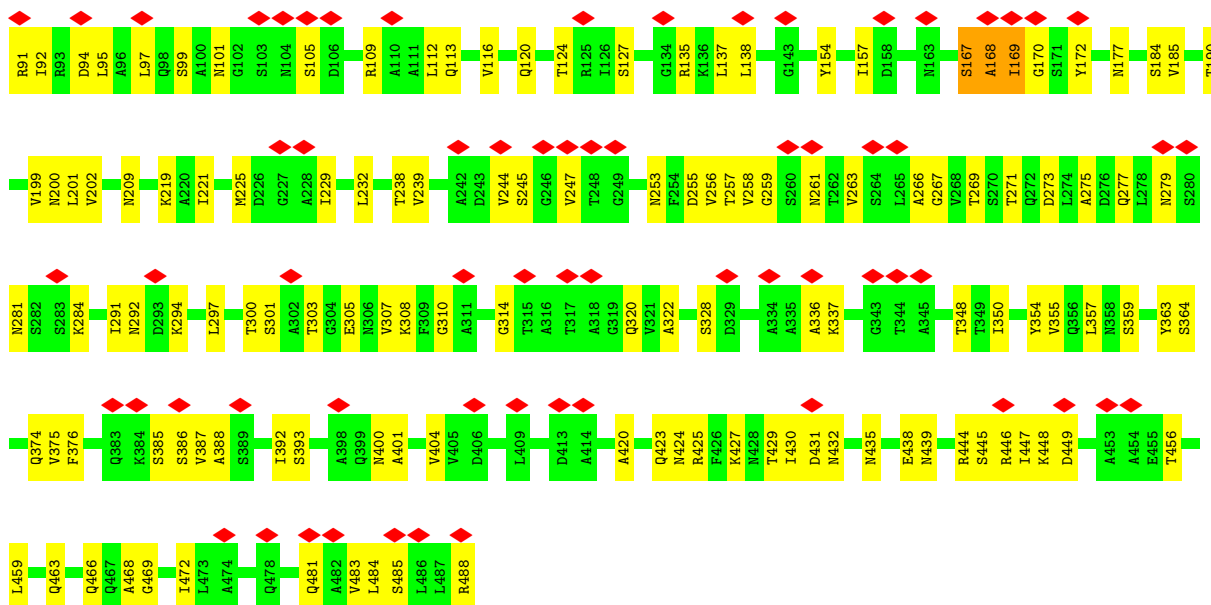


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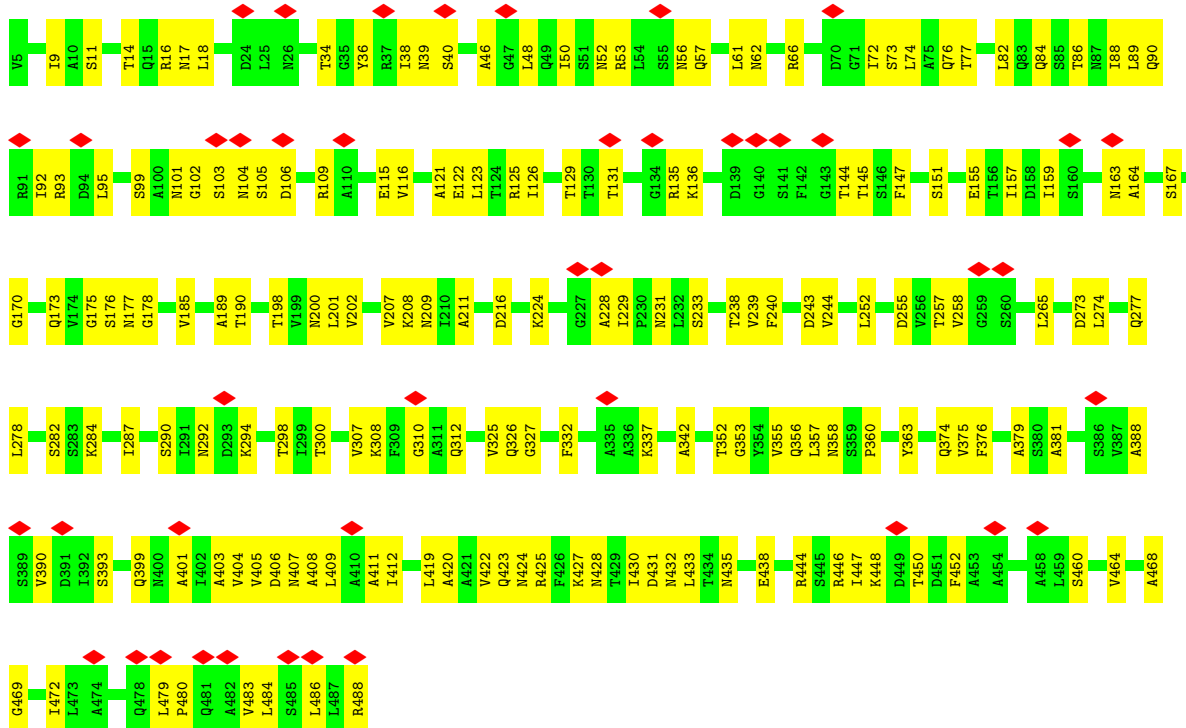


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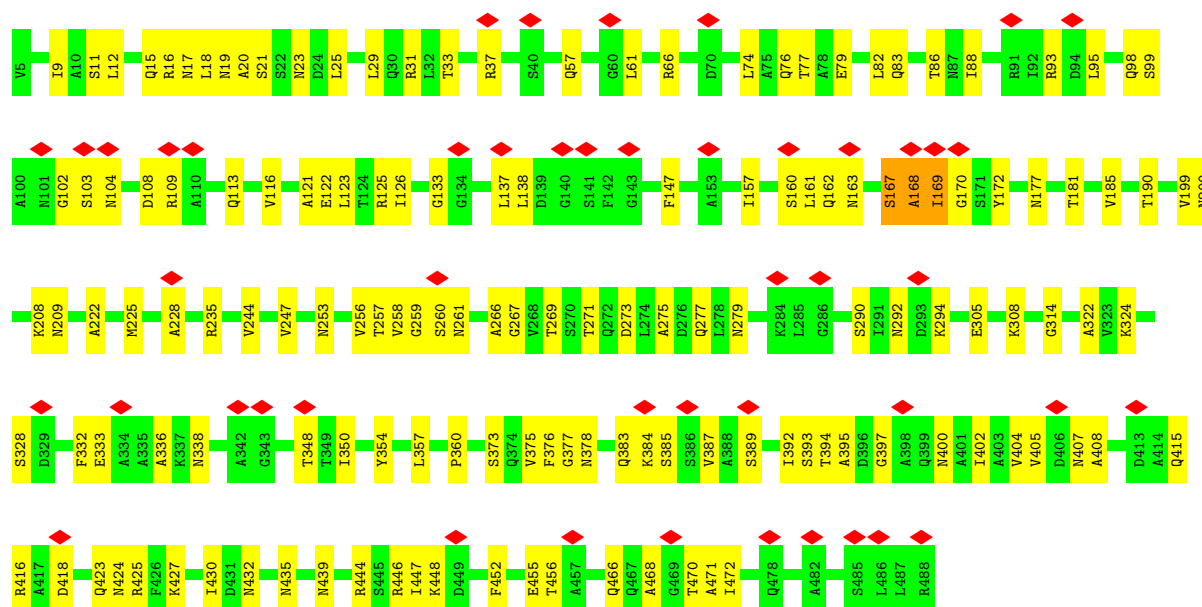


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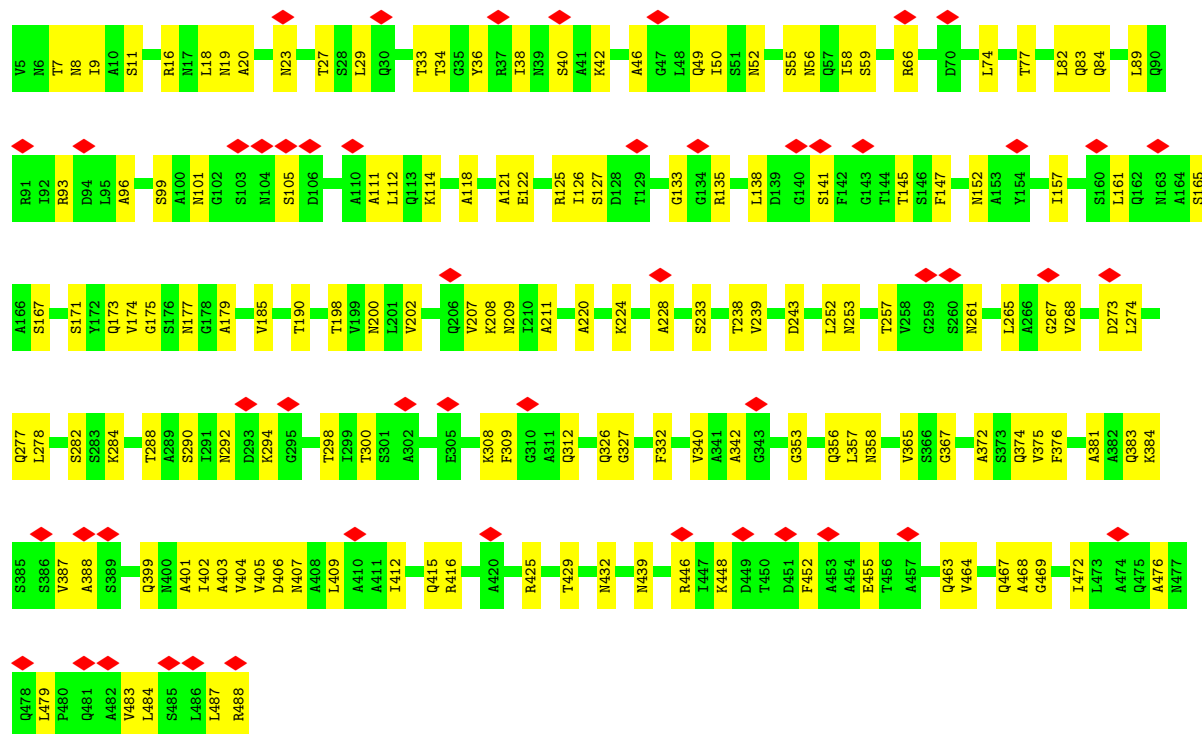


• Molecule 1: B-type flagellin



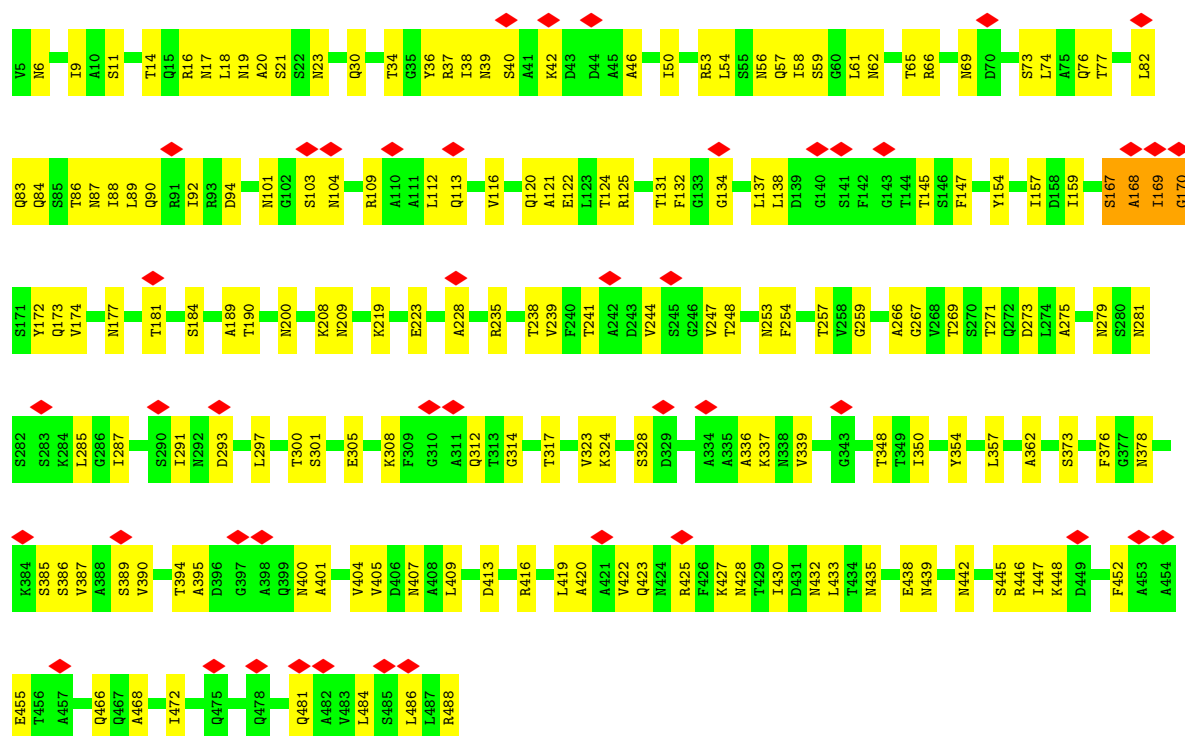


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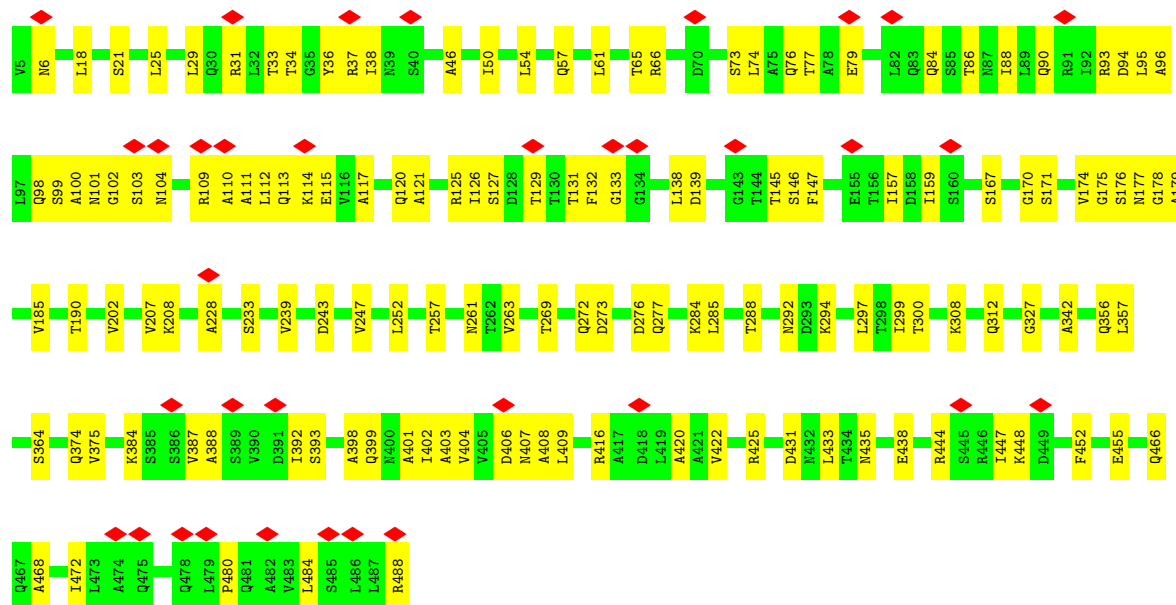


• Molecule 1: B-type flagellin



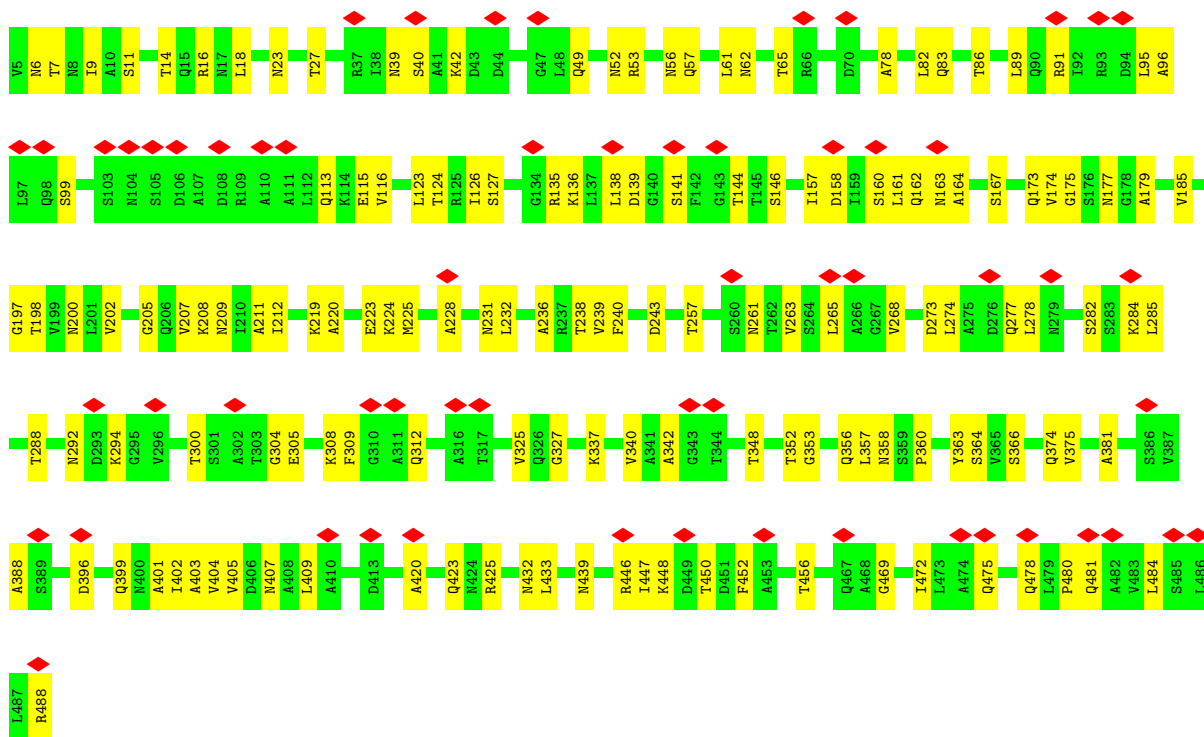


• Molecule 1: B-type flagellin

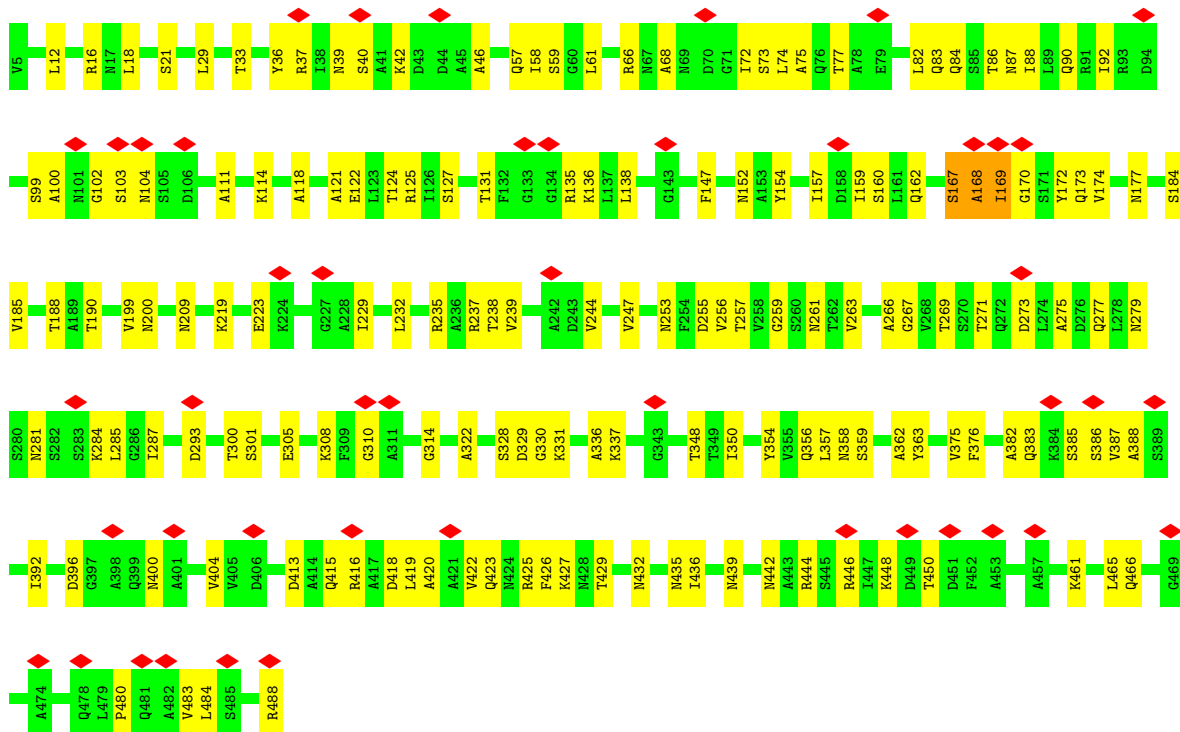


• Molecule 1: B-type flagellin

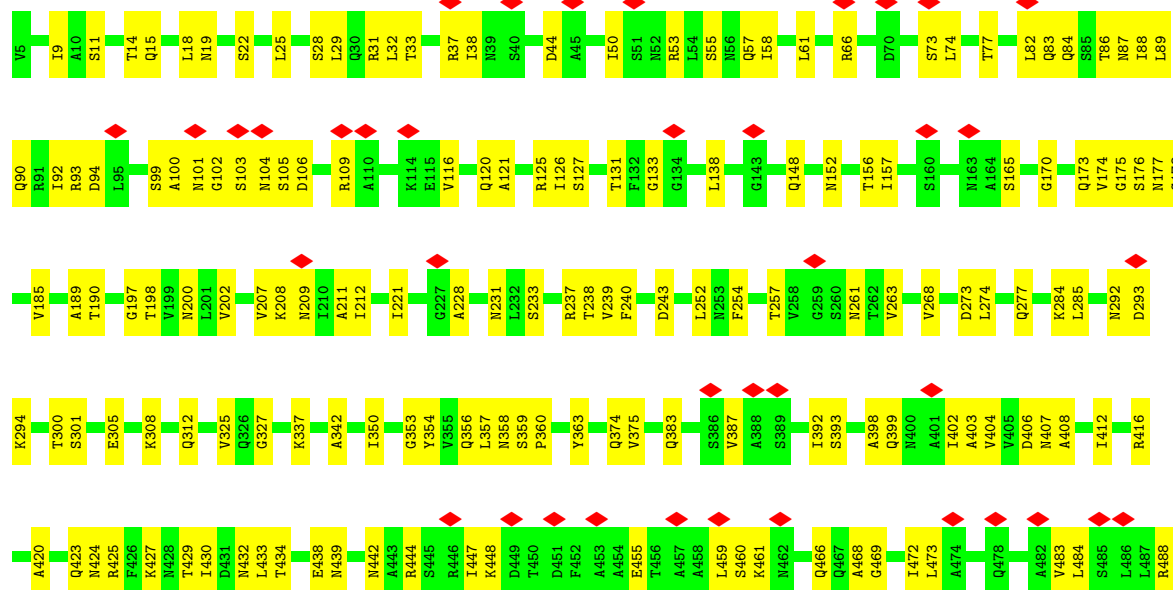




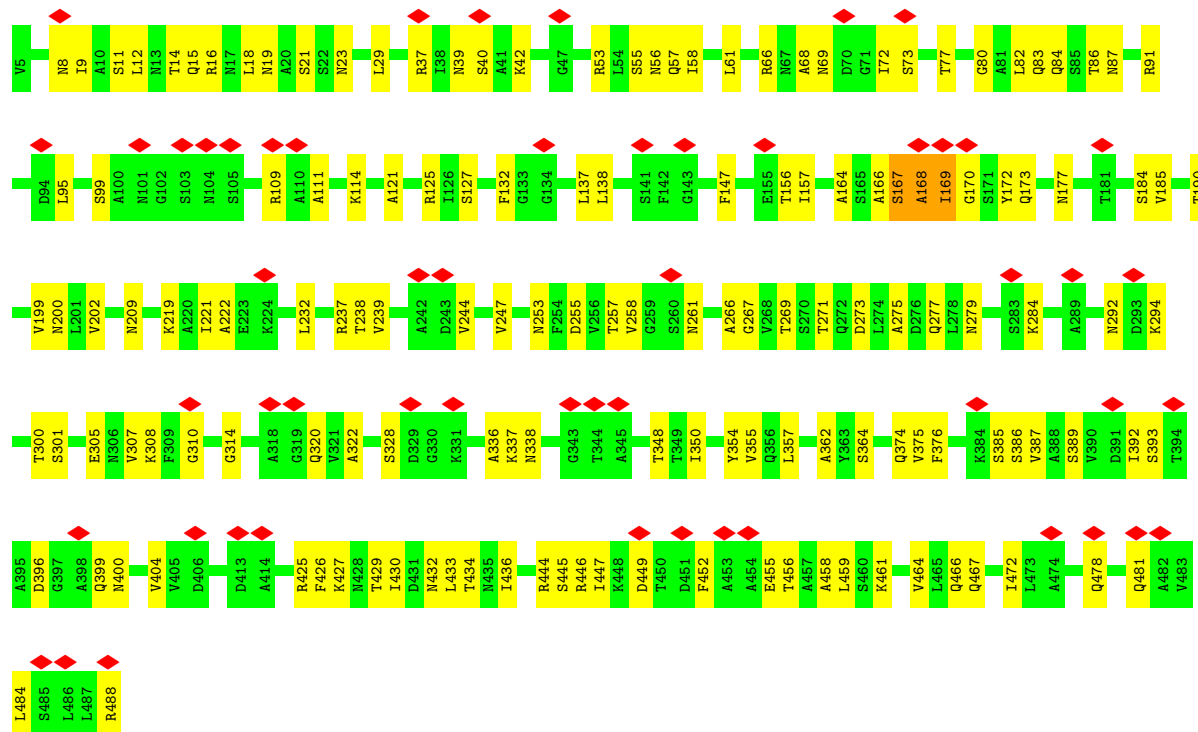
• Molecule 1: B-type flagellin



• Molecule 1: B-type flagellin

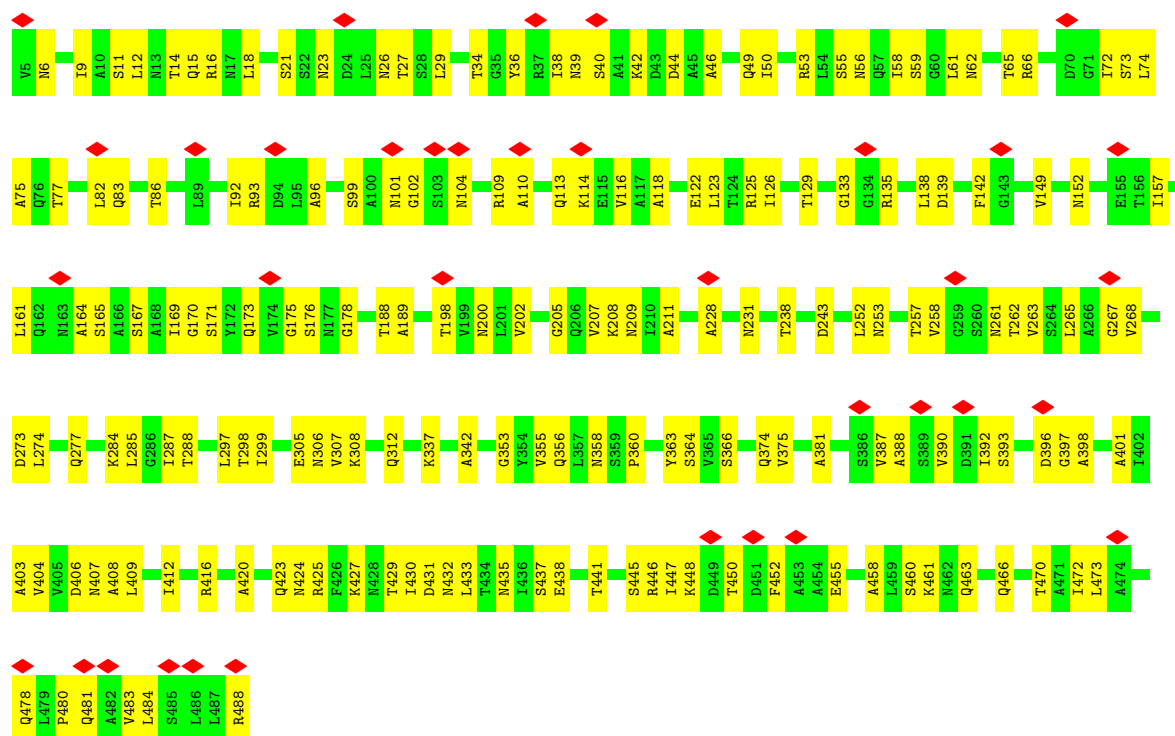


• Molecule 1: B-type flagellin

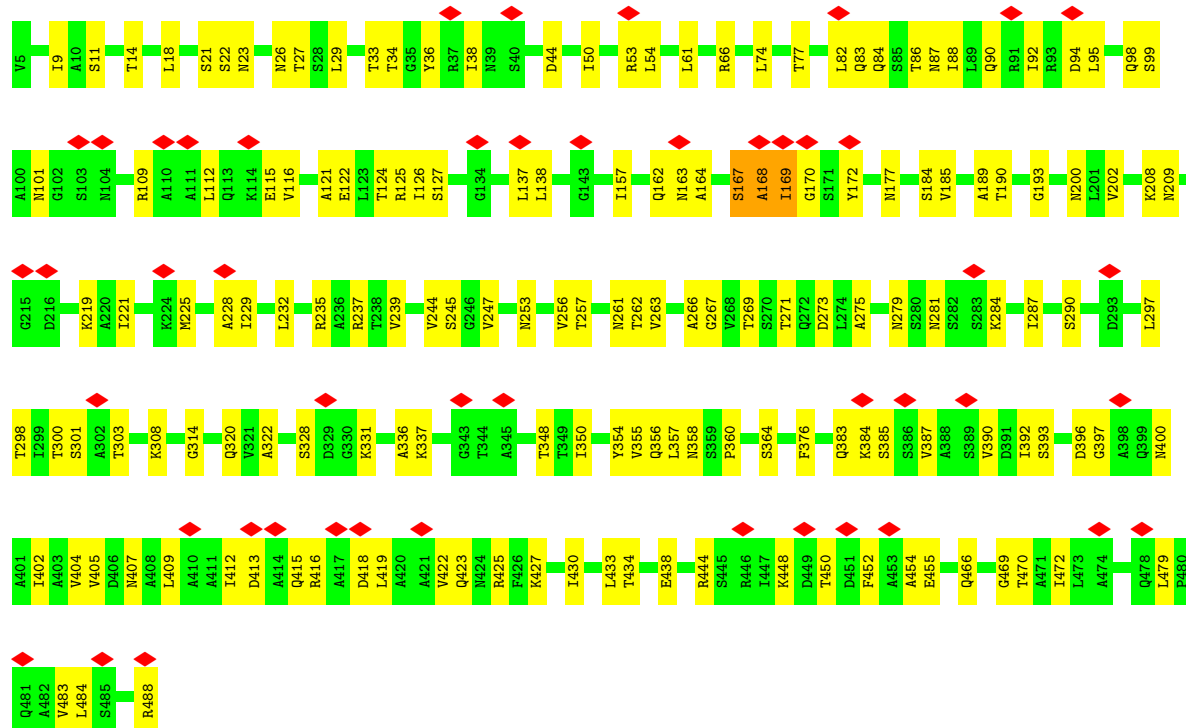


• Molecule 1: B-type flagellin

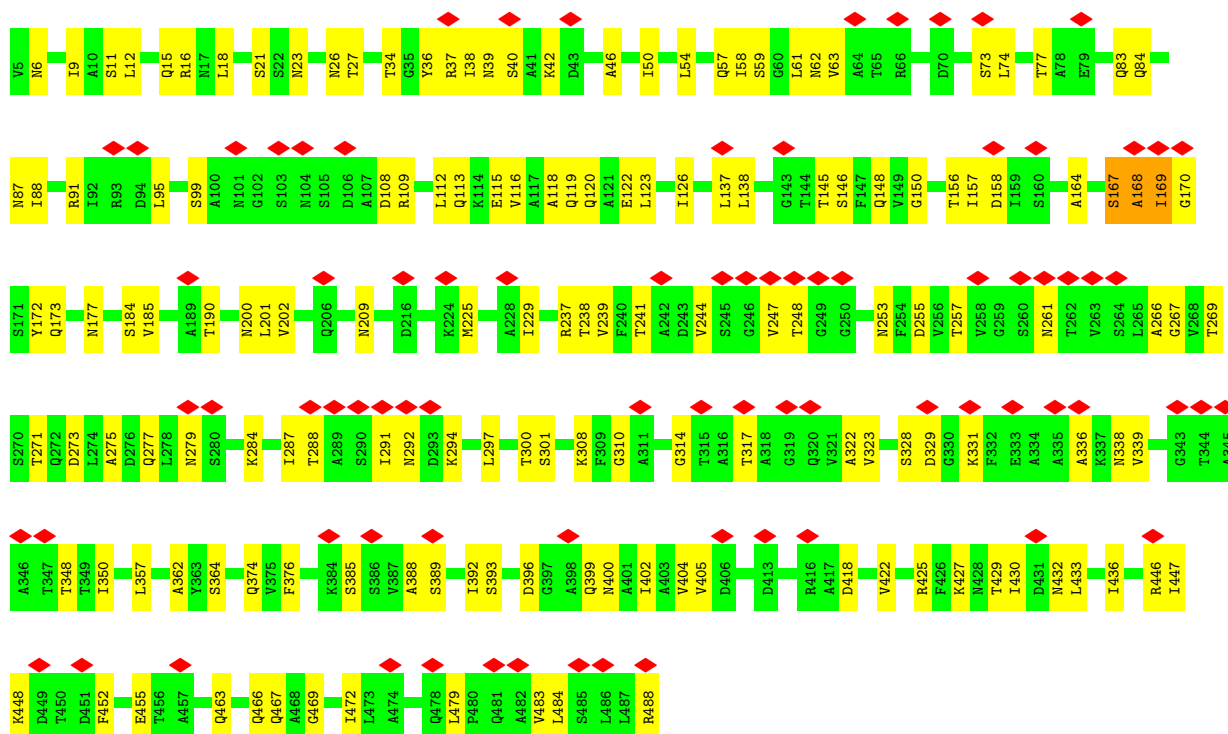




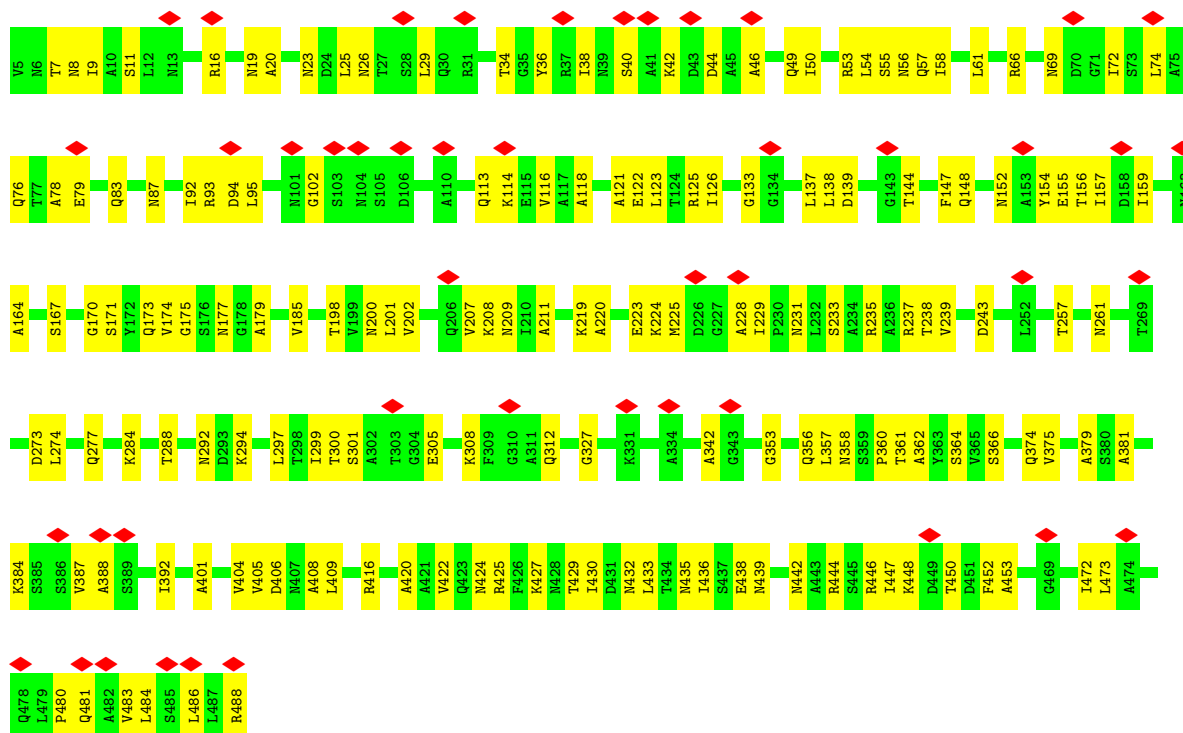
• Molecule 1: B-type flagellin



• Molecule 1: B-type flagellin



• Molecule 1: B-type flagellin



Chain a:

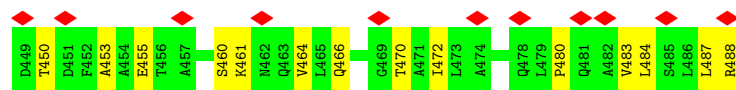
11% 61% 38%

W5, I9, S11, T14, Q15, N17, L18, N19, A20, N23, T27, S28, L29, Q30, R31, T34, G35, Y36, R37, S40, A41, K42, A46, S55, N56, Q57, I58, L61, N69, D70, G71, I72, S73, L74, A75, Q76, T77, A78, E79, L82, Q83, Q84, S85, T86, N87, R91, I92, R93, D94, L95, A96, S99, A100, N101, G102, S103, N104, R109, A110, L111, L112, A118, A121, E122, L123, T124, R125, I126, S127, F132, G133, G134, L137, L138, N152, F147, Q148, I155, E156, T156, I157, S160, A164, S167, A168, I169, G170, S171, Y172, Q173, V174, T181, D185, V185, T188, A189, T190, N200, L201, V202, N209, M225, D226, G227, A228, L229, L232, R235, A236, R237, T238, V239, F240, T241, A242, D243, V244, S245, G246, V247, T248, G249, G250, S251, L252, N253, F254, D255, V256, T257, N261, T262, V263, A266, G267, V268, T269, S270, T271, Q272, D273, L274, A275, D276, Q277, L278, N279, S280, N281, K284, L285, S290, L291, N292, D293, K294, V296, L297, T298, I299, S301, A302, K308, F309, G310, G314, T317, A318, I402, A403, V404, V405, D406, N407, I412, R416, A417, D418, L419, A421, V422, Q423, N424, R425, F426, K427, N428, T429, I430, D431, N432, V355, Q356, L357, P360, S364, V365, S366, Q374, V375, F376, G377, N378, Q383, K384, S385, S386, V387, A388, S389, T392, S393, T394, A395, D396, G397, A398, Q399, N400, A401, A402, A403, V404, V405, D406, N407, I412, R416, A417, D418, L419, A421, V422, Q423, N424, R425, F426, K427, N428, T429, I430, D431, N432, L433, T434, N435, I436, N439, R444, S445, R446, I447, K448, D449, T450, D451, F452, A453, A454, E455, S460, K461, N462, Q463, V464, A468, G469, I472, L473, A474, Q478, L479, P480, Q481, A482, V483, L484, S485, L486, L487, R488, V354, Y354

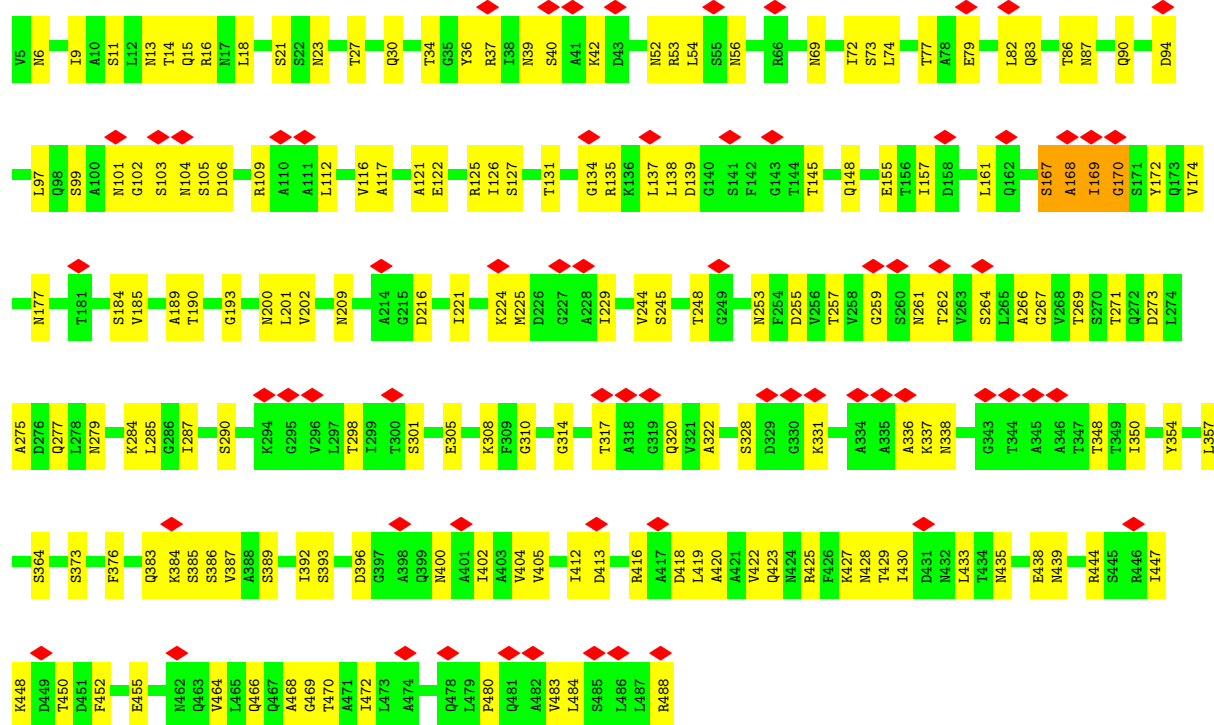
Chain b:

14% 64% 36%

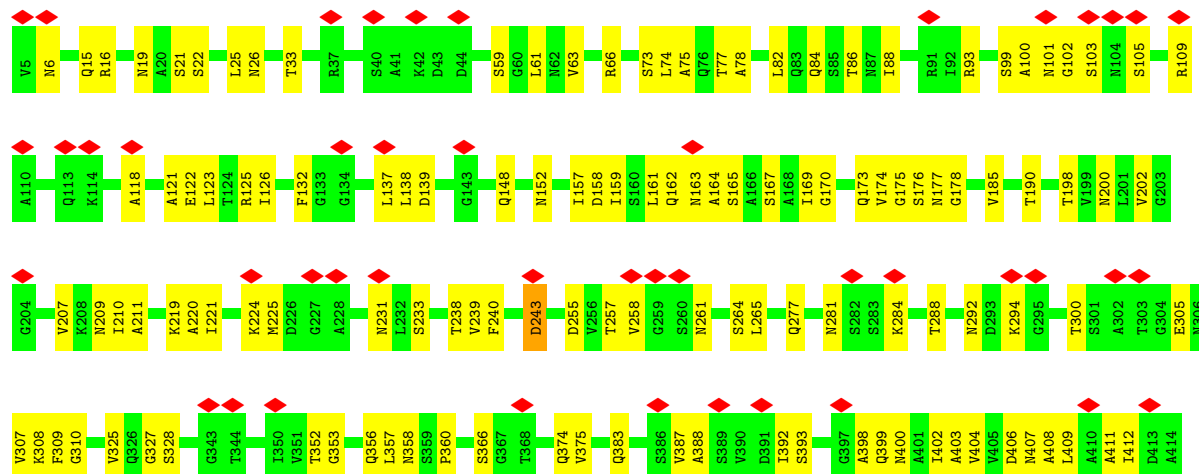
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I9
A10
S11
L12
M13
T14
Q15
R16
N17
L18
M19
A20
S21
Q22
N23
N26
L29
Q30
T34
G35
V36
R37
L38
N39
S40
A41
K42
D43
D44
A45
A46
Q49
R53
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A96
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G102
S103
M104
S105
D106
A110
A111
L112
Q113
K114
E115
V116
A117
A118
Q119
Q120
A121
E122
R126
T129
T130
T131
F132
G133
G134
R135
K136
L137
L138
D139
G143
T144
T145
L157
S160
A164
S167
S171
Y172
Q173
V174
G175
S176
M177
V185
A186
G187
T190
G197
T198
V199
M200
L201
T202
G203
G204
G205
Q206
V207
K208
A211
T212
G215
D216
K219
A220
K224
G227
A228
N231
L232
S233
T238
A242
D243
L252
N253
T257
V258
G259
S260
N261
L265
A266
G267
V268
T269
D273
L274
Q277
L278
N279
S280
N281
K284
L285
G286
T287
T288
A289
N292
D293
K294
L297
S301
A302
E305
N306
V307
K308
P309
G310
A311
Q312
Q316
T317
G327
K331
V340
G343
T344
G353
Q356
L357
N358
P360
Y363
S366
G367
Q374
V375
A381
S386
V387
A388
S389
V390
D391
I392
Q399
M400
A401
I402
A403
V404
V405
D406
N407
A410
A411
I412
D413
R416
A417
D418
L419
A420
A421
V422
Q423
N424
R425
F426
K427
N428
T429
I430
D431
N432
M439
R444
S445
R446
I447
K448

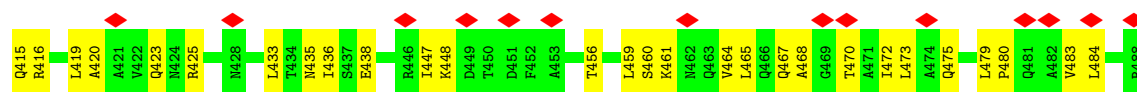


• Molecule 1: B-type flagellin

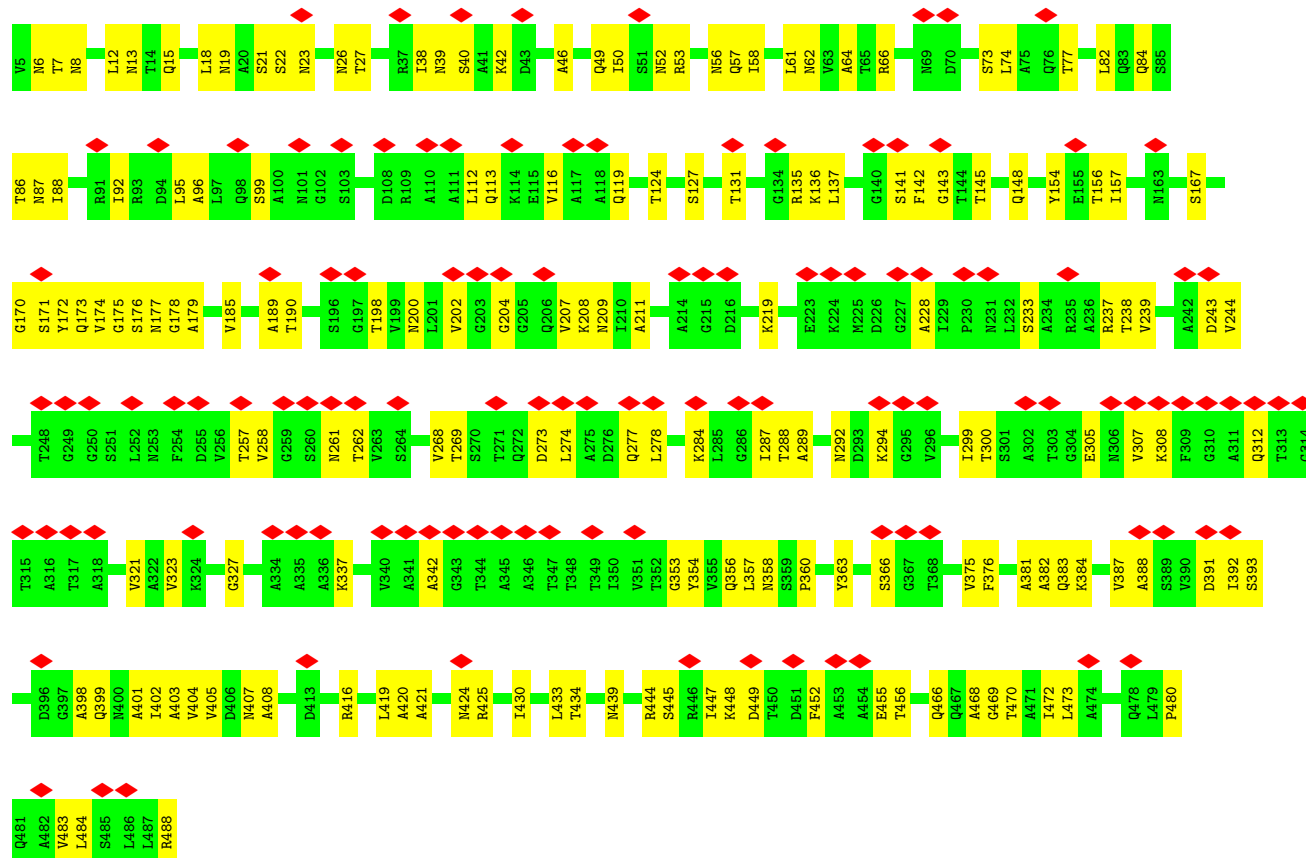


• Molecule 1: B-type flagellin

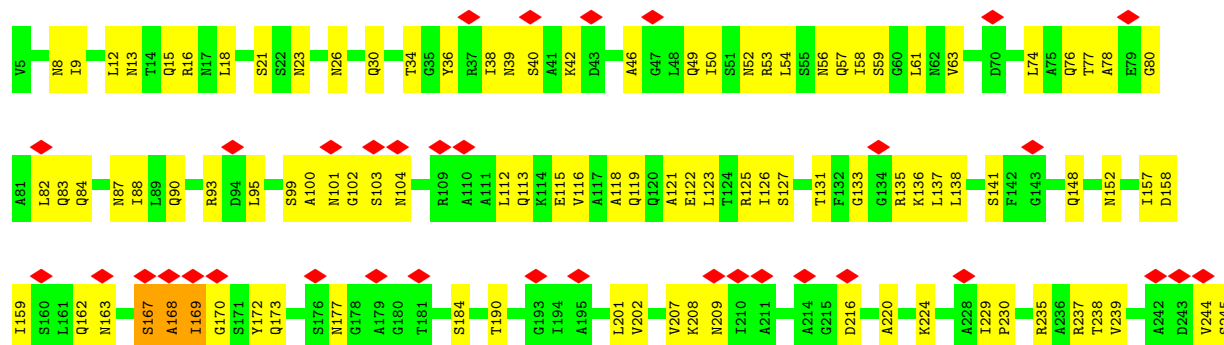


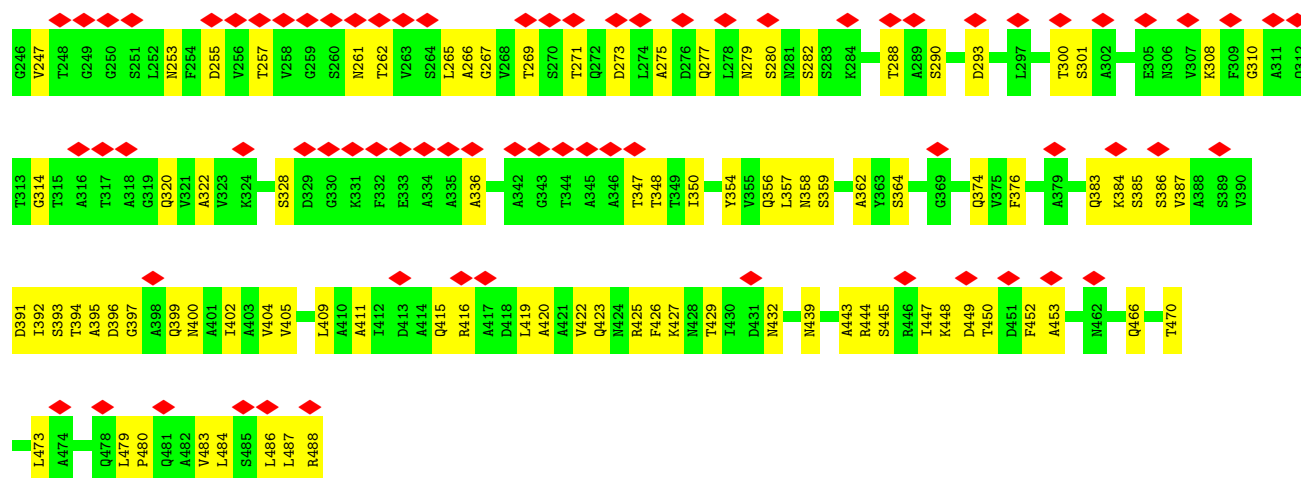


• Molecule 1: B-type flagellin

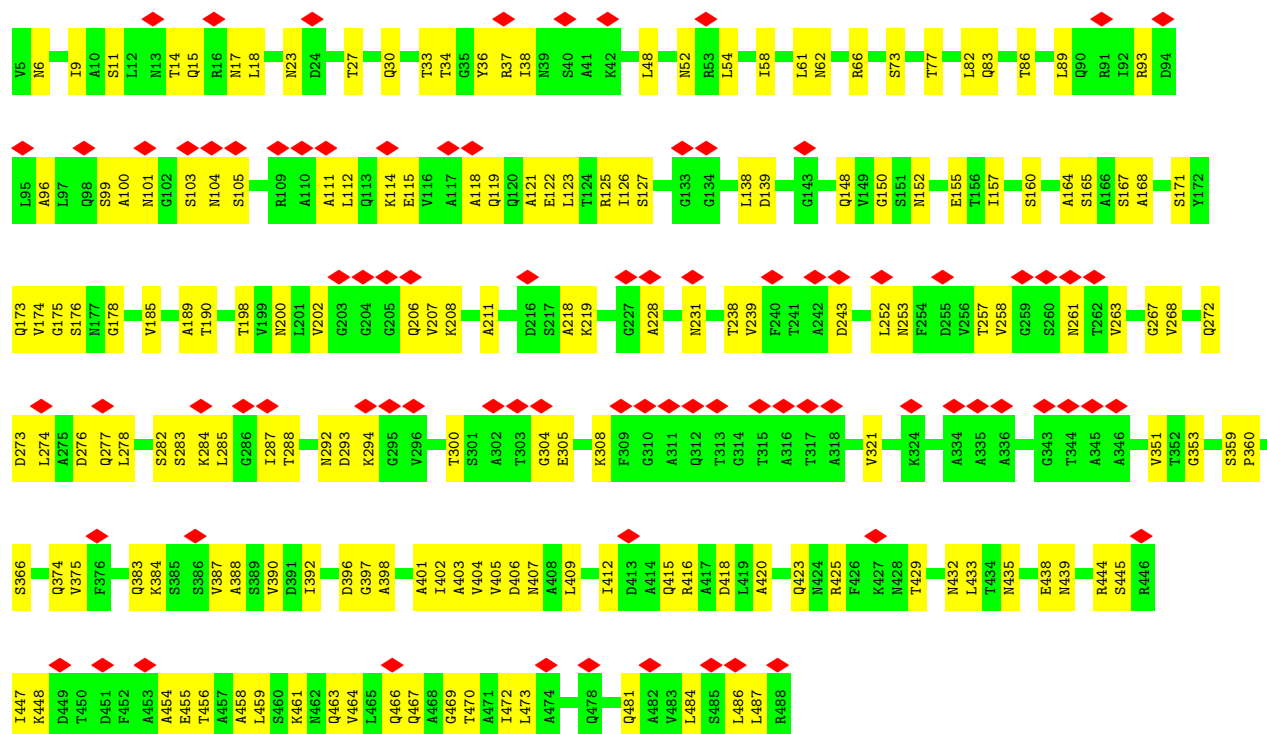


• Molecule 1: B-type flagellin





• Molecule 1: B-type flagellin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.379	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3455	0.49	0/4695
1	B	0.15	0/3455	0.49	0/4695
1	C	0.15	0/3455	0.47	0/4695
1	D	0.16	0/3455	0.48	0/4695
1	E	0.15	0/3455	0.48	1/4695 (0.0%)
1	F	0.15	0/3455	0.49	1/4695 (0.0%)
1	G	0.15	0/3455	0.47	0/4695
1	H	0.15	0/3455	0.48	1/4695 (0.0%)
1	I	0.16	0/3455	0.49	0/4695
1	J	0.15	0/3455	0.47	0/4695
1	K	0.15	0/3455	0.49	1/4695 (0.0%)
1	L	0.15	0/3455	0.47	0/4695
1	M	0.15	0/3455	0.47	0/4695
1	N	0.14	0/3455	0.49	1/4695 (0.0%)
1	O	0.15	0/3455	0.47	0/4695
1	P	0.15	0/3455	0.48	1/4695 (0.0%)
1	Q	0.16	0/3455	0.48	0/4695
1	R	0.14	0/3455	0.47	1/4695 (0.0%)
1	S	0.14	0/3455	0.48	1/4695 (0.0%)
1	T	0.15	0/3455	0.47	0/4695
1	U	0.14	0/3455	0.47	0/4695
1	V	0.16	0/3455	0.47	0/4695
1	W	0.15	0/3455	0.49	1/4695 (0.0%)
1	X	0.15	0/3455	0.47	0/4695
1	Y	0.16	0/3455	0.49	0/4695
1	Z	0.15	0/3455	0.48	1/4695 (0.0%)
1	a	0.16	0/3455	0.48	0/4695
1	b	0.15	0/3455	0.48	1/4695 (0.0%)
1	c	0.16	0/3455	0.48	0/4695
1	d	0.14	0/3455	0.48	1/4695 (0.0%)
1	e	0.14	0/3455	0.47	1/4695 (0.0%)
1	f	0.16	0/3455	0.49	0/4695
1	g	0.15	0/3455	0.49	1/4695 (0.0%)
All	All	0.15	0/114015	0.48	14/154935 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	388	ALA	N-CA-C	-6.24	106.89	114.75
1	K	388	ALA	N-CA-C	-6.05	106.88	114.56
1	F	388	ALA	N-CA-C	-5.94	107.26	114.75
1	W	388	ALA	N-CA-C	-5.92	107.28	114.75
1	H	388	ALA	N-CA-C	-5.90	107.32	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3435	0	3417	160	0
1	B	3435	0	3417	143	0
1	C	3435	0	3417	123	0
1	D	3435	0	3417	168	0
1	E	3435	0	3417	123	0
1	F	3435	0	3417	112	0
1	G	3435	0	3417	137	0
1	H	3435	0	3417	144	0
1	I	3435	0	3417	146	0
1	J	3435	0	3417	145	0
1	K	3435	0	3417	144	0
1	L	3435	0	3417	135	0
1	M	3435	0	3417	125	0
1	N	3435	0	3417	141	0
1	O	3435	0	3417	129	0
1	P	3435	0	3417	123	0
1	Q	3435	0	3417	151	0
1	R	3435	0	3417	102	0
1	S	3435	0	3417	103	0
1	T	3435	0	3417	136	0
1	U	3435	0	3417	134	0
1	V	3435	0	3417	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	3435	0	3417	156	0
1	X	3435	0	3417	133	0
1	Y	3435	0	3417	116	0
1	Z	3435	0	3417	142	0
1	a	3435	0	3417	157	0
1	b	3435	0	3417	127	0
1	c	3435	0	3417	144	0
1	d	3435	0	3417	115	0
1	e	3435	0	3417	129	0
1	f	3435	0	3417	161	0
1	g	3435	0	3417	140	0
All	All	113355	0	112761	3856	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 3856 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:W:205:GLY:H	1:X:281:ASN:HD22	1.25	0.82
1:A:171:SER:HB3	1:A:387:VAL:HB	1.59	0.82
1:U:61:LEU:HD22	1:U:433:LEU:HD11	1.62	0.81
1:H:157:ILE:HD12	1:H:425:ARG:HE	1.46	0.81
1:D:157:ILE:HD12	1:D:425:ARG:HE	1.47	0.80

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	483/484 (100%)	430 (89%)	51 (11%)	2 (0%)	30 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	483/484 (100%)	442 (92%)	39 (8%)	2 (0%)	30	66
1	C	483/484 (100%)	439 (91%)	42 (9%)	2 (0%)	30	66
1	D	483/484 (100%)	440 (91%)	40 (8%)	3 (1%)	21	58
1	E	483/484 (100%)	445 (92%)	38 (8%)	0	100	100
1	F	483/484 (100%)	447 (92%)	36 (8%)	0	100	100
1	G	483/484 (100%)	439 (91%)	41 (8%)	3 (1%)	21	58
1	H	483/484 (100%)	440 (91%)	43 (9%)	0	100	100
1	I	483/484 (100%)	439 (91%)	41 (8%)	3 (1%)	21	58
1	J	483/484 (100%)	433 (90%)	47 (10%)	3 (1%)	21	58
1	K	483/484 (100%)	449 (93%)	34 (7%)	0	100	100
1	L	483/484 (100%)	435 (90%)	44 (9%)	4 (1%)	16	52
1	M	483/484 (100%)	438 (91%)	42 (9%)	3 (1%)	21	58
1	N	483/484 (100%)	444 (92%)	39 (8%)	0	100	100
1	O	483/484 (100%)	444 (92%)	36 (8%)	3 (1%)	21	58
1	P	483/484 (100%)	447 (92%)	36 (8%)	0	100	100
1	Q	483/484 (100%)	434 (90%)	45 (9%)	4 (1%)	16	52
1	R	483/484 (100%)	447 (92%)	36 (8%)	0	100	100
1	S	483/484 (100%)	452 (94%)	31 (6%)	0	100	100
1	T	483/484 (100%)	437 (90%)	43 (9%)	3 (1%)	21	58
1	U	483/484 (100%)	446 (92%)	37 (8%)	0	100	100
1	V	483/484 (100%)	438 (91%)	42 (9%)	3 (1%)	21	58
1	W	483/484 (100%)	440 (91%)	43 (9%)	0	100	100
1	X	483/484 (100%)	440 (91%)	40 (8%)	3 (1%)	21	58
1	Y	483/484 (100%)	441 (91%)	39 (8%)	3 (1%)	21	58
1	Z	483/484 (100%)	445 (92%)	38 (8%)	0	100	100
1	a	483/484 (100%)	439 (91%)	40 (8%)	4 (1%)	16	52
1	b	483/484 (100%)	444 (92%)	39 (8%)	0	100	100
1	c	483/484 (100%)	439 (91%)	40 (8%)	4 (1%)	16	52
1	d	483/484 (100%)	443 (92%)	40 (8%)	0	100	100
1	e	483/484 (100%)	441 (91%)	42 (9%)	0	100	100
1	f	483/484 (100%)	435 (90%)	45 (9%)	3 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	483/484 (100%)	440 (91%)	43 (9%)	0	100	100
All	All	15939/15972 (100%)	14552 (91%)	1332 (8%)	55 (0%)	37	71

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	168	ALA
1	A	168	ALA
1	B	168	ALA
1	C	168	ALA
1	D	168	ALA

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	361/360 (100%)	361 (100%)	0	100	100
1	B	361/360 (100%)	361 (100%)	0	100	100
1	C	361/360 (100%)	361 (100%)	0	100	100
1	D	361/360 (100%)	361 (100%)	0	100	100
1	E	361/360 (100%)	361 (100%)	0	100	100
1	F	361/360 (100%)	361 (100%)	0	100	100
1	G	361/360 (100%)	361 (100%)	0	100	100
1	H	361/360 (100%)	359 (99%)	2 (1%)	78	80
1	I	361/360 (100%)	361 (100%)	0	100	100
1	J	361/360 (100%)	361 (100%)	0	100	100
1	K	361/360 (100%)	361 (100%)	0	100	100
1	L	361/360 (100%)	361 (100%)	0	100	100
1	M	361/360 (100%)	361 (100%)	0	100	100
1	N	361/360 (100%)	361 (100%)	0	100	100
1	O	361/360 (100%)	361 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	361/360 (100%)	361 (100%)	0	100	100
1	Q	361/360 (100%)	361 (100%)	0	100	100
1	R	361/360 (100%)	361 (100%)	0	100	100
1	S	361/360 (100%)	361 (100%)	0	100	100
1	T	361/360 (100%)	361 (100%)	0	100	100
1	U	361/360 (100%)	361 (100%)	0	100	100
1	V	361/360 (100%)	361 (100%)	0	100	100
1	W	361/360 (100%)	361 (100%)	0	100	100
1	X	361/360 (100%)	361 (100%)	0	100	100
1	Y	361/360 (100%)	361 (100%)	0	100	100
1	Z	361/360 (100%)	361 (100%)	0	100	100
1	a	361/360 (100%)	361 (100%)	0	100	100
1	b	361/360 (100%)	361 (100%)	0	100	100
1	c	361/360 (100%)	361 (100%)	0	100	100
1	d	361/360 (100%)	359 (99%)	2 (1%)	78	80
1	e	361/360 (100%)	361 (100%)	0	100	100
1	f	361/360 (100%)	361 (100%)	0	100	100
1	g	361/360 (100%)	361 (100%)	0	100	100
All	All	11913/11880 (100%)	11909 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	243[A]	ASP
1	H	243[B]	ASP
1	d	243[A]	ASP
1	d	243[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 423 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	432	ASN
1	V	481	GLN
1	f	253	ASN
1	R	200	ASN

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Mol	Chain	Res	Type
1	T	442	ASN

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 oligosaccharides 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.

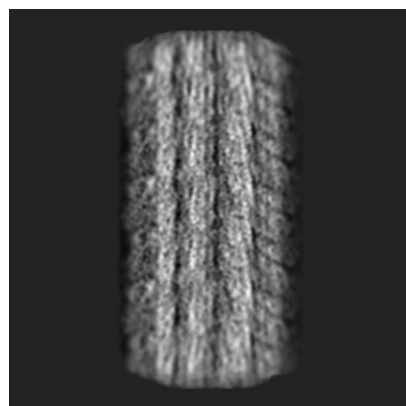
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40765. These allow visual inspection of the internal detail of the map and identification of artifacts.

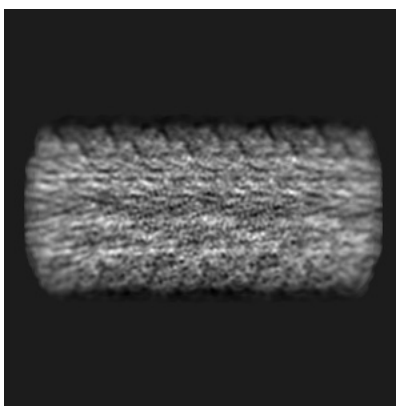
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

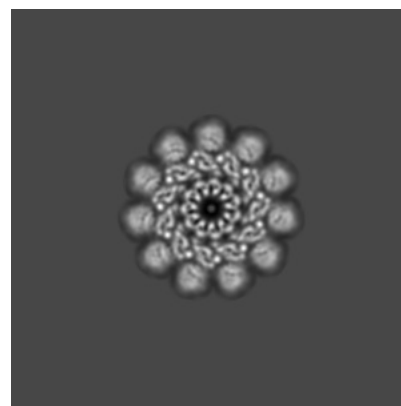
6.1.1 Primary map



X

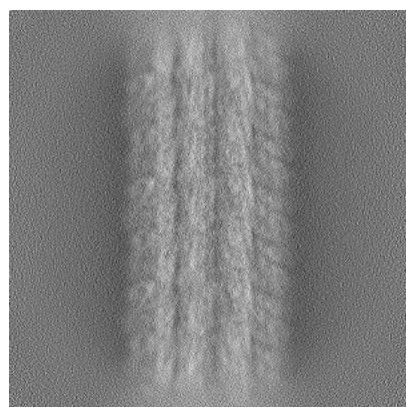


Y

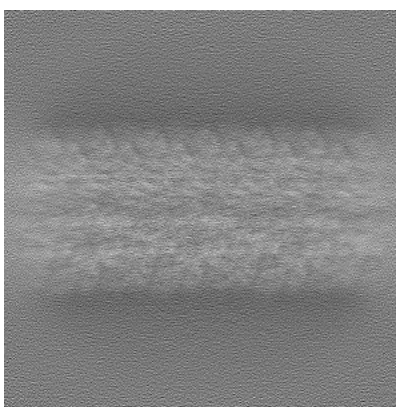


Z

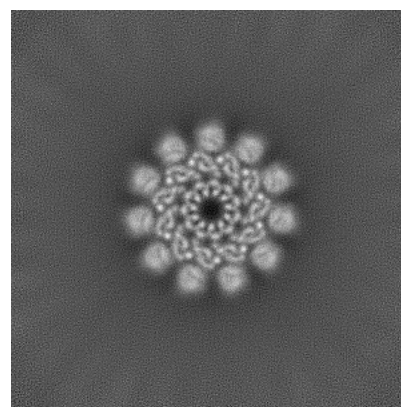
6.1.2 Raw map



X



Y

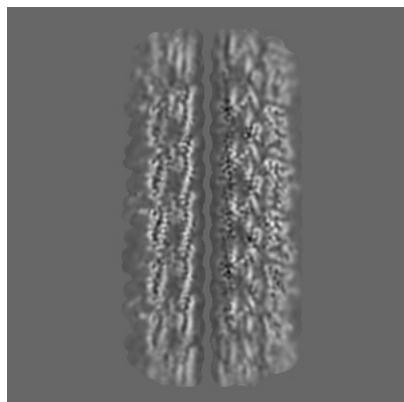


Z

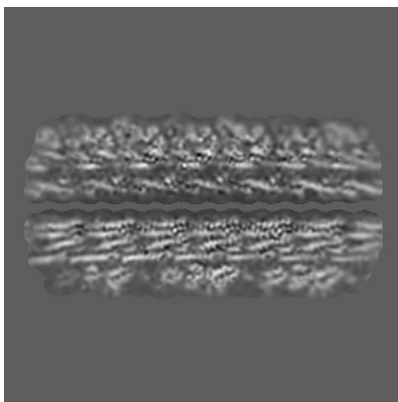
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

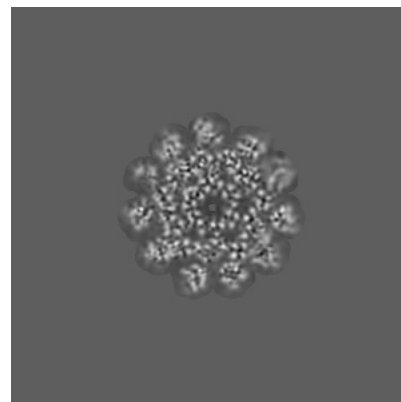
6.2.1 Primary map



X Index: 216

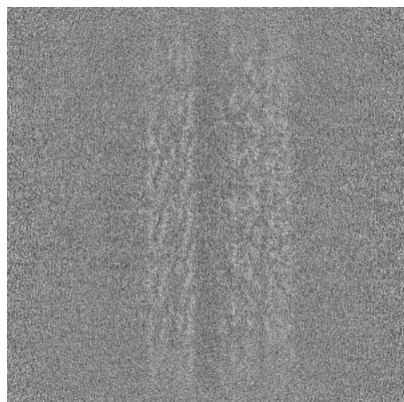


Y Index: 216

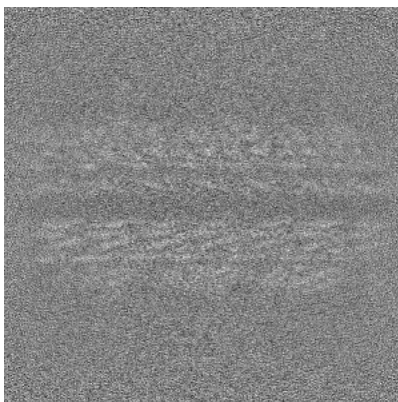


Z Index: 216

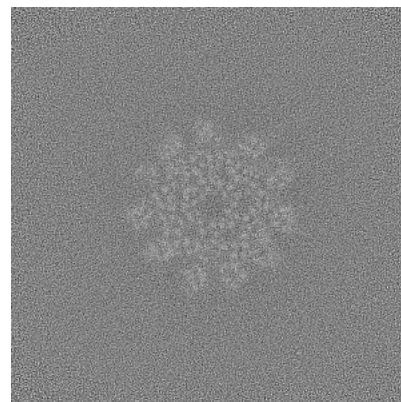
6.2.2 Raw map



X Index: 216



Y Index: 216

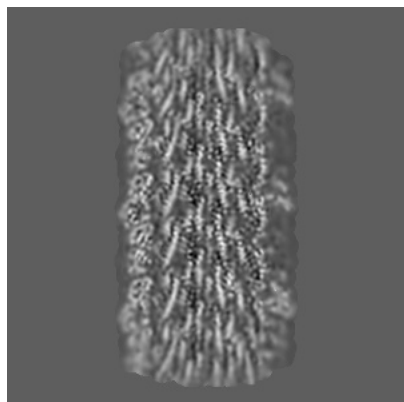


Z Index: 216

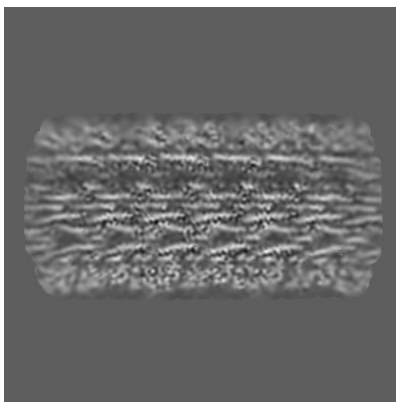
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

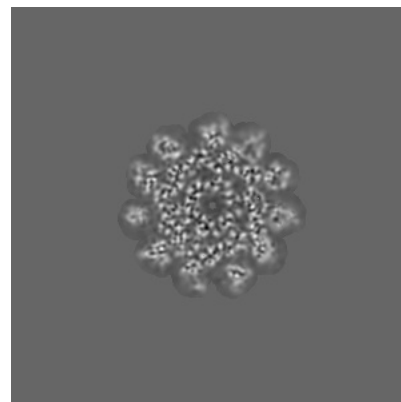
6.3.1 Primary map



X Index: 200

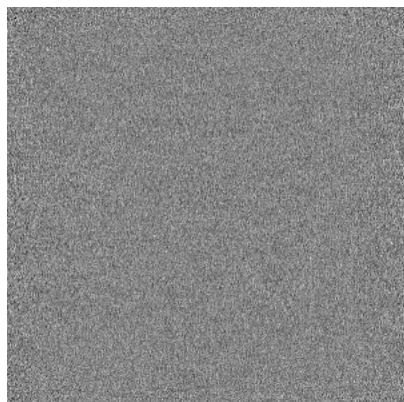


Y Index: 199

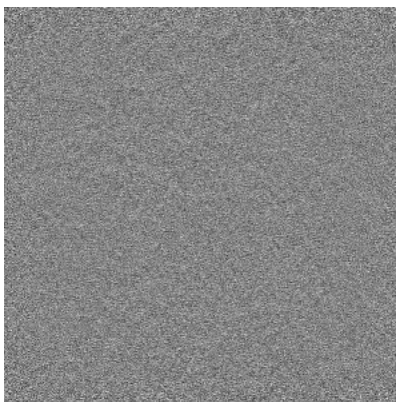


Z Index: 195

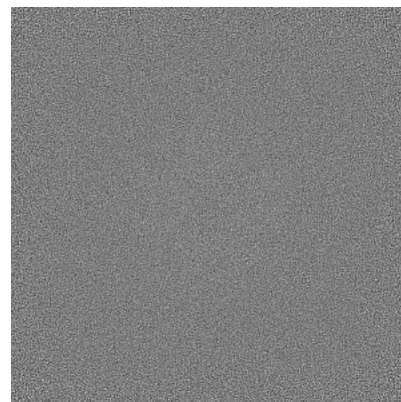
6.3.2 Raw map



X Index: 0



Y Index: 0

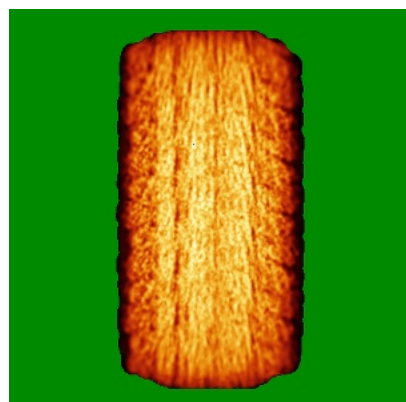


Z Index: 0

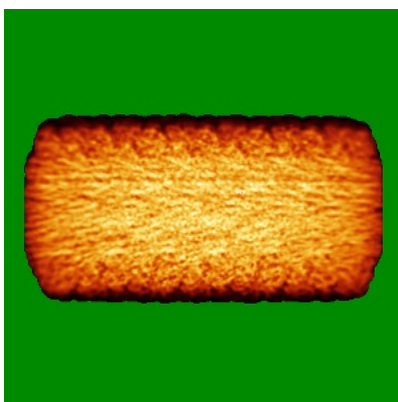
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

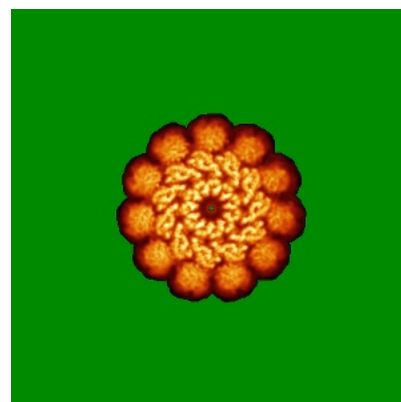
6.4.1 Primary map



X

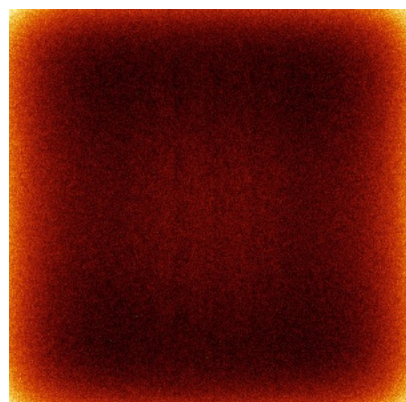


Y

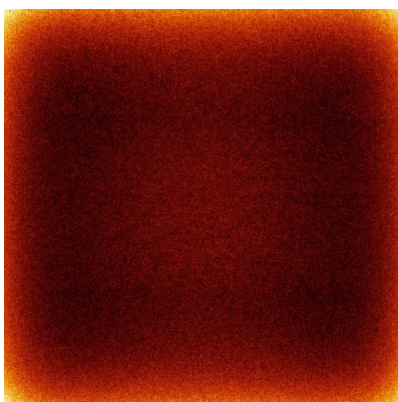


Z

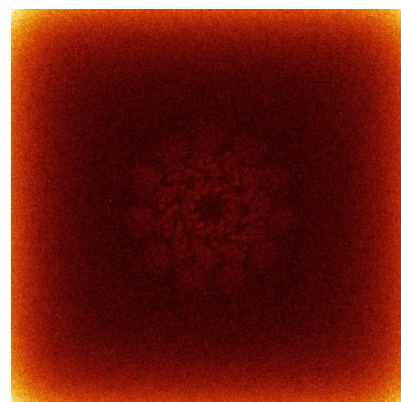
6.4.2 Raw map



X



Y



Z

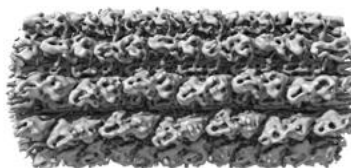
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



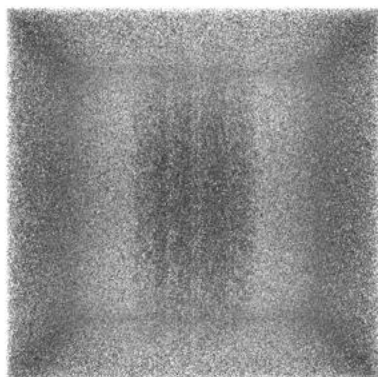
Y



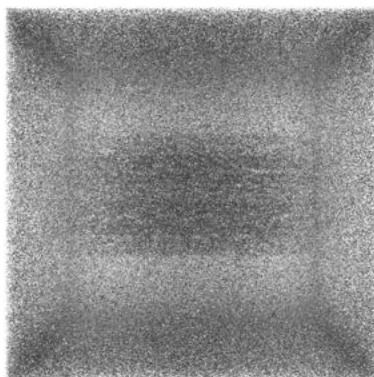
Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

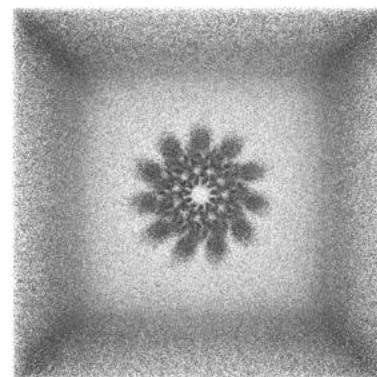
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

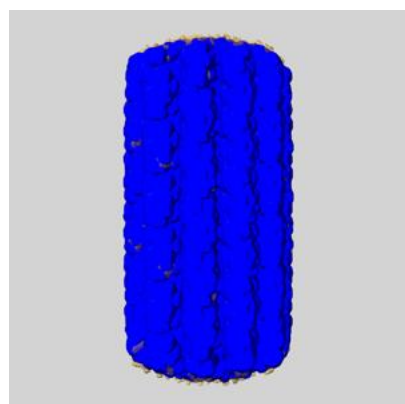
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

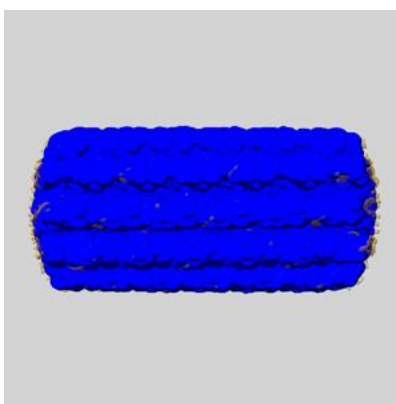
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

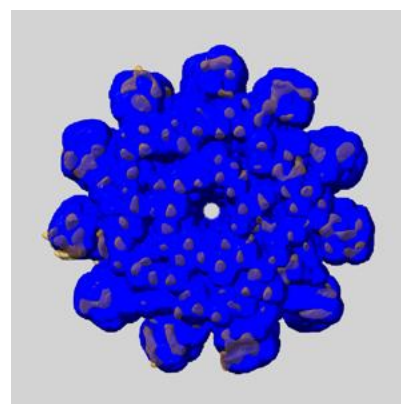
6.6.1 emd_40765_msk_1.map [i](#)



X



Y

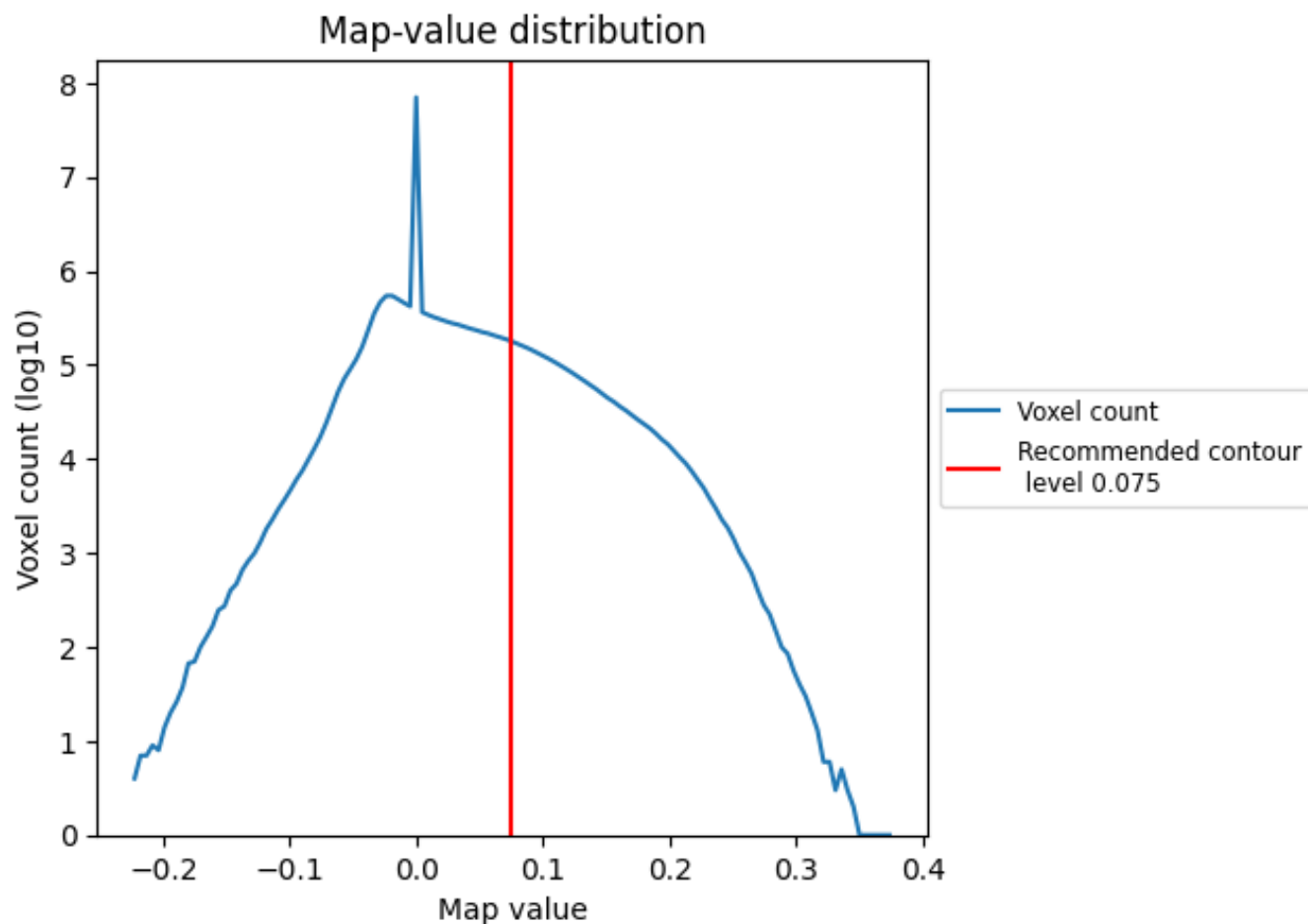


Z

7 Map analysis [i](#)

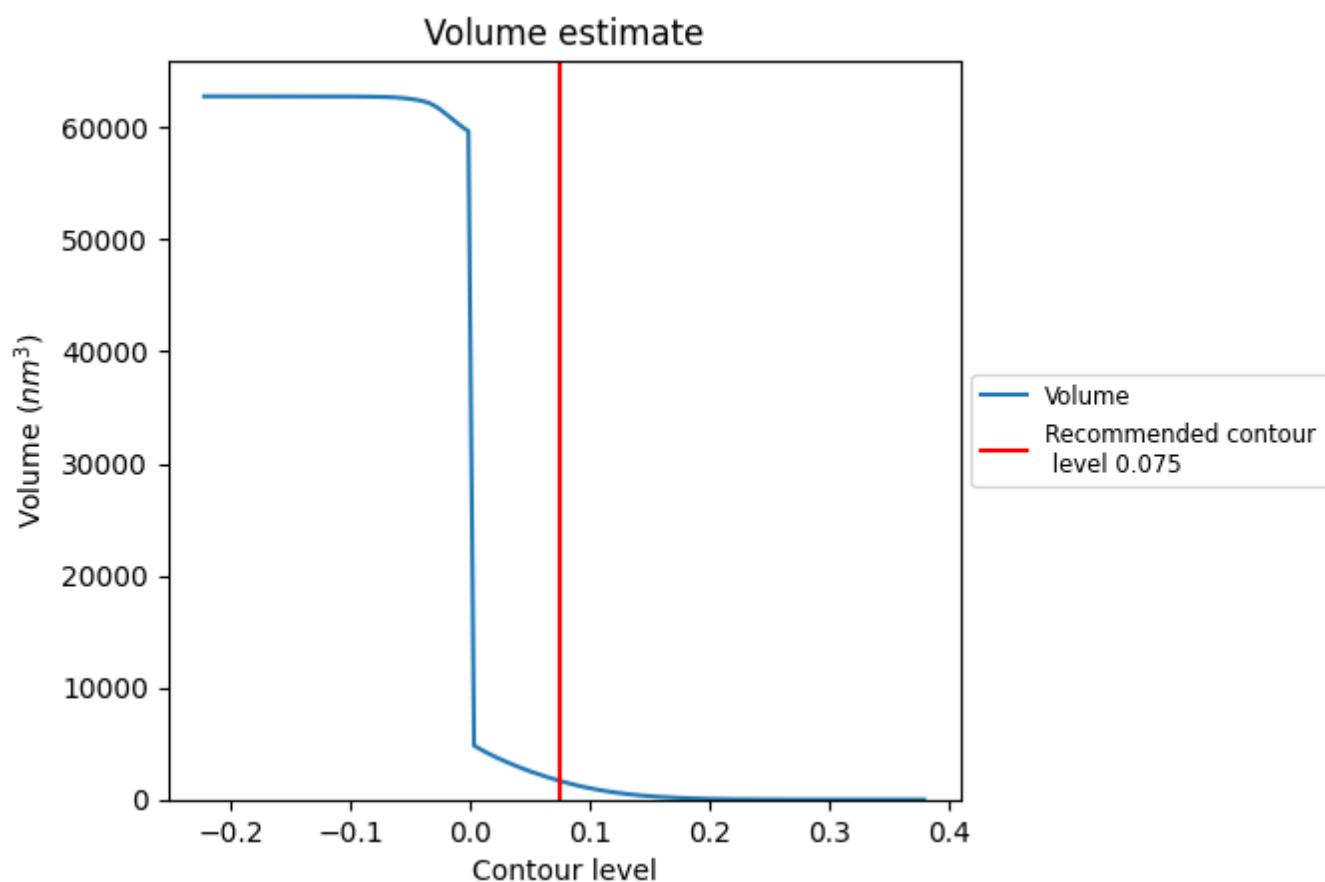
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

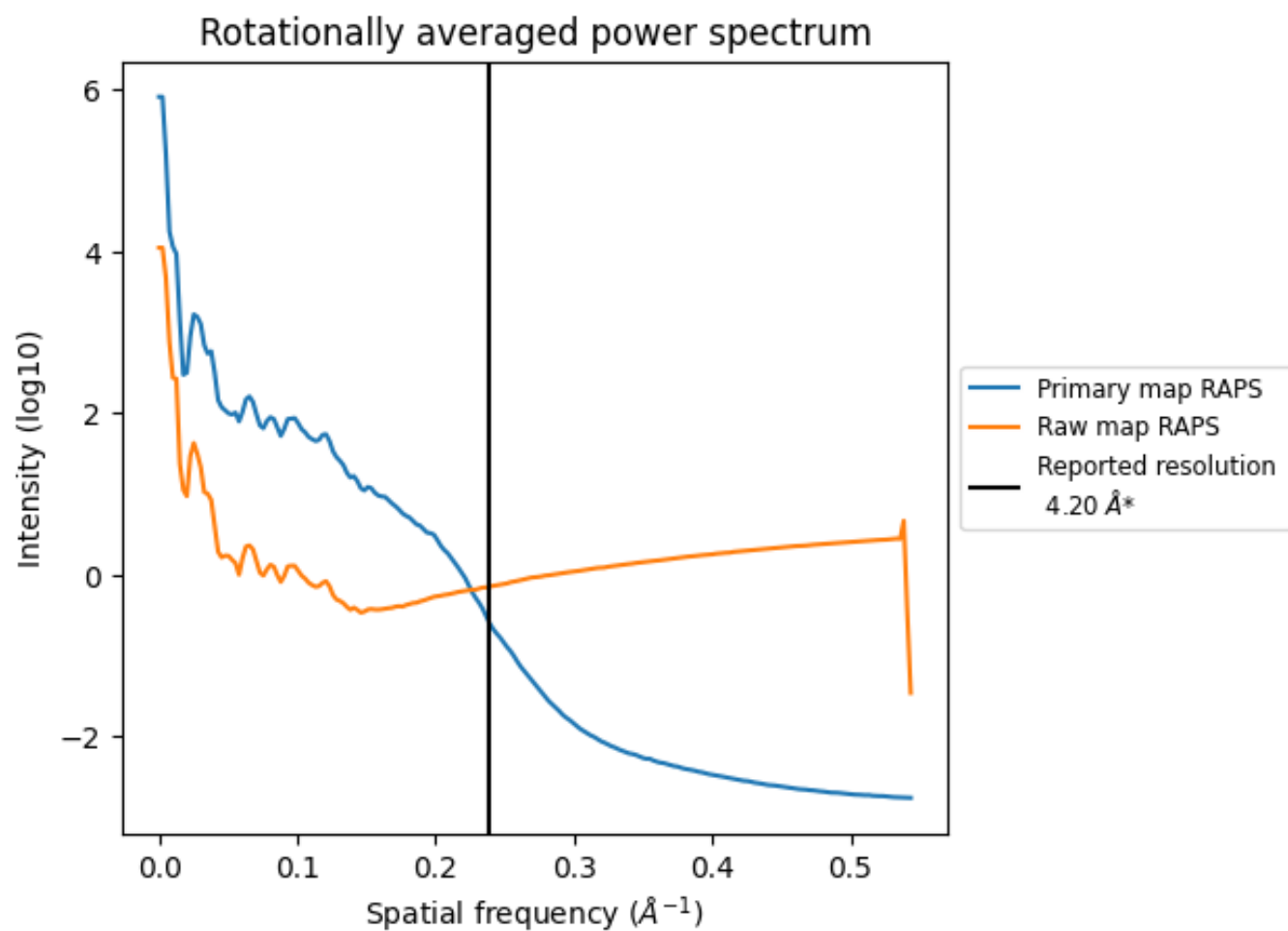
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1651 nm³; this corresponds to an approximate mass of 1491 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

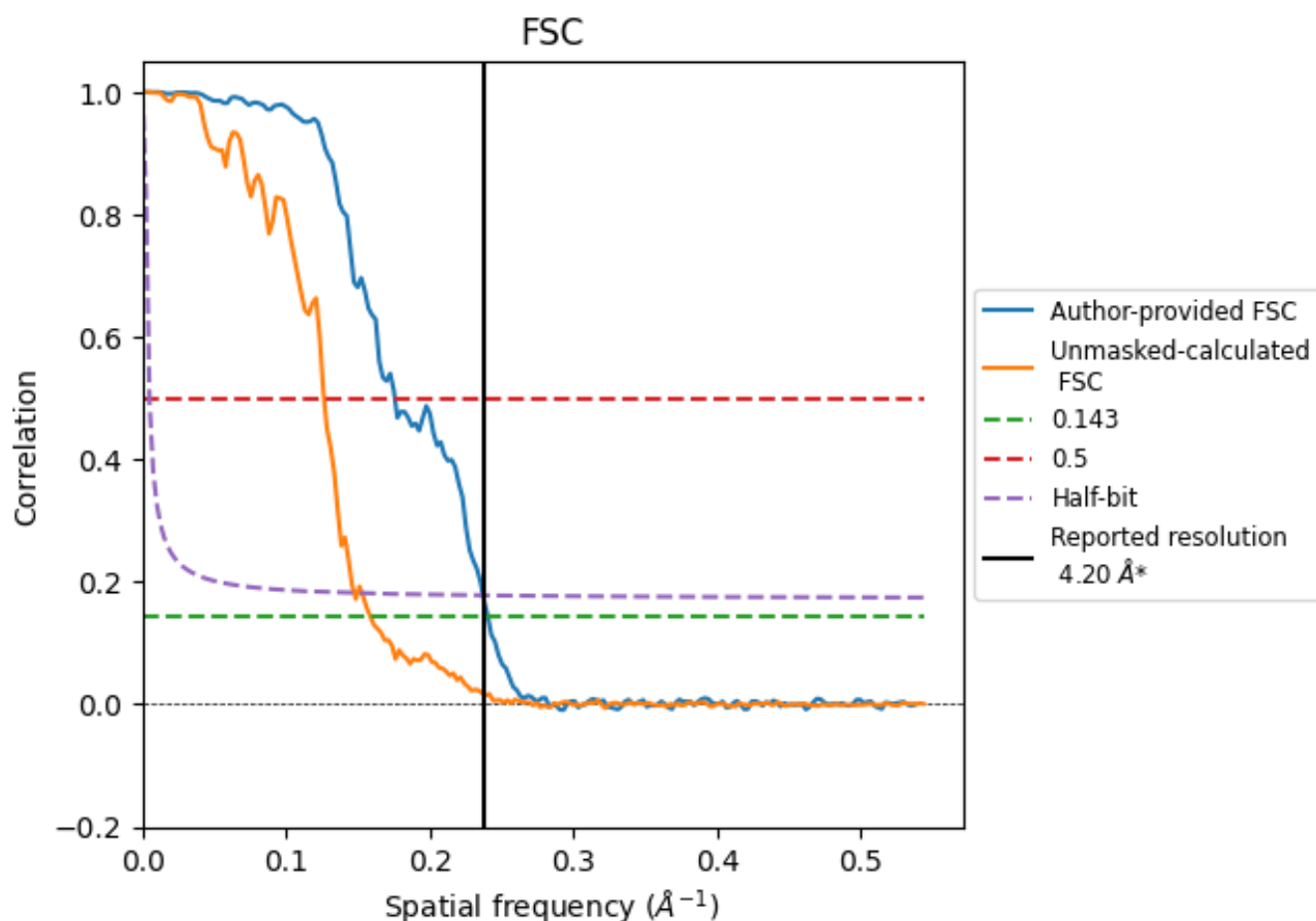


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	5.69	4.22
Unmasked-calculated*	6.30	7.91	6.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.30 differs from the reported value 4.2 by more than 10 %

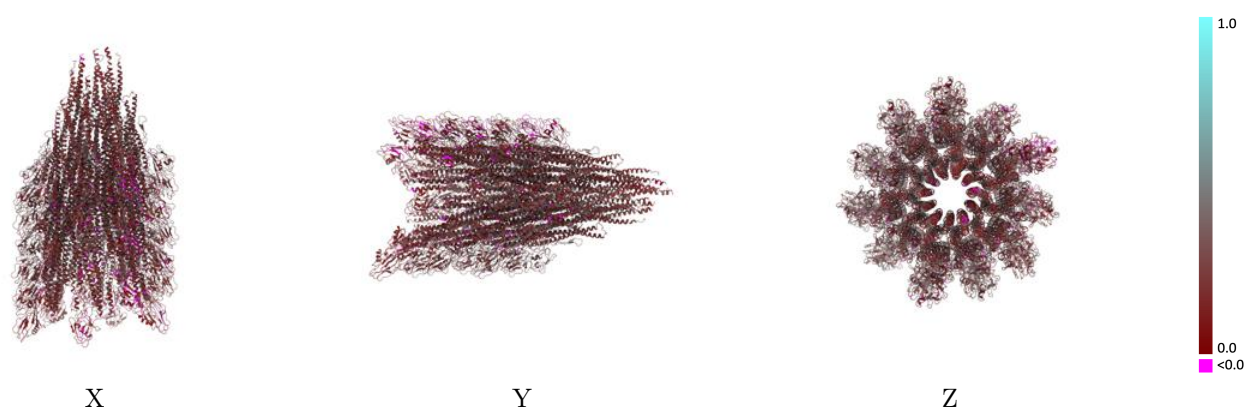
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40765 and PDB model 8SUG. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

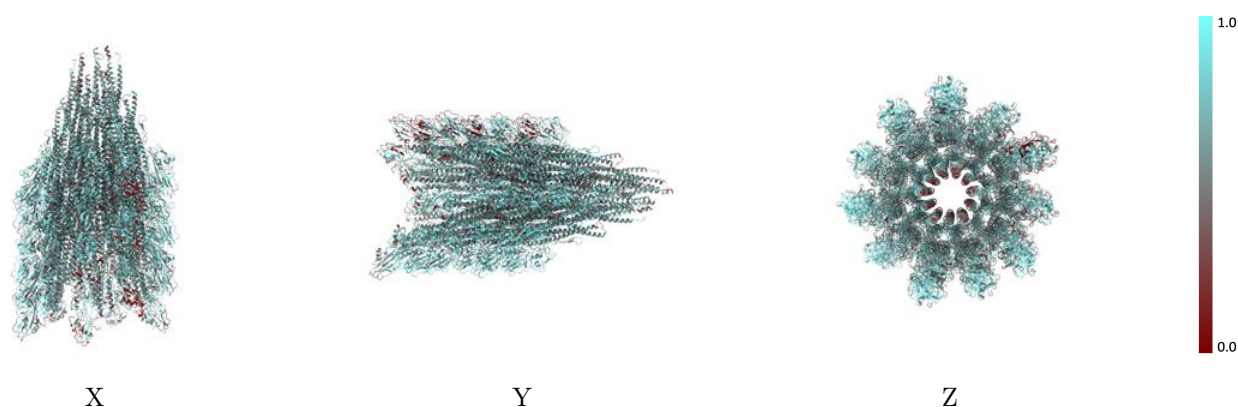
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



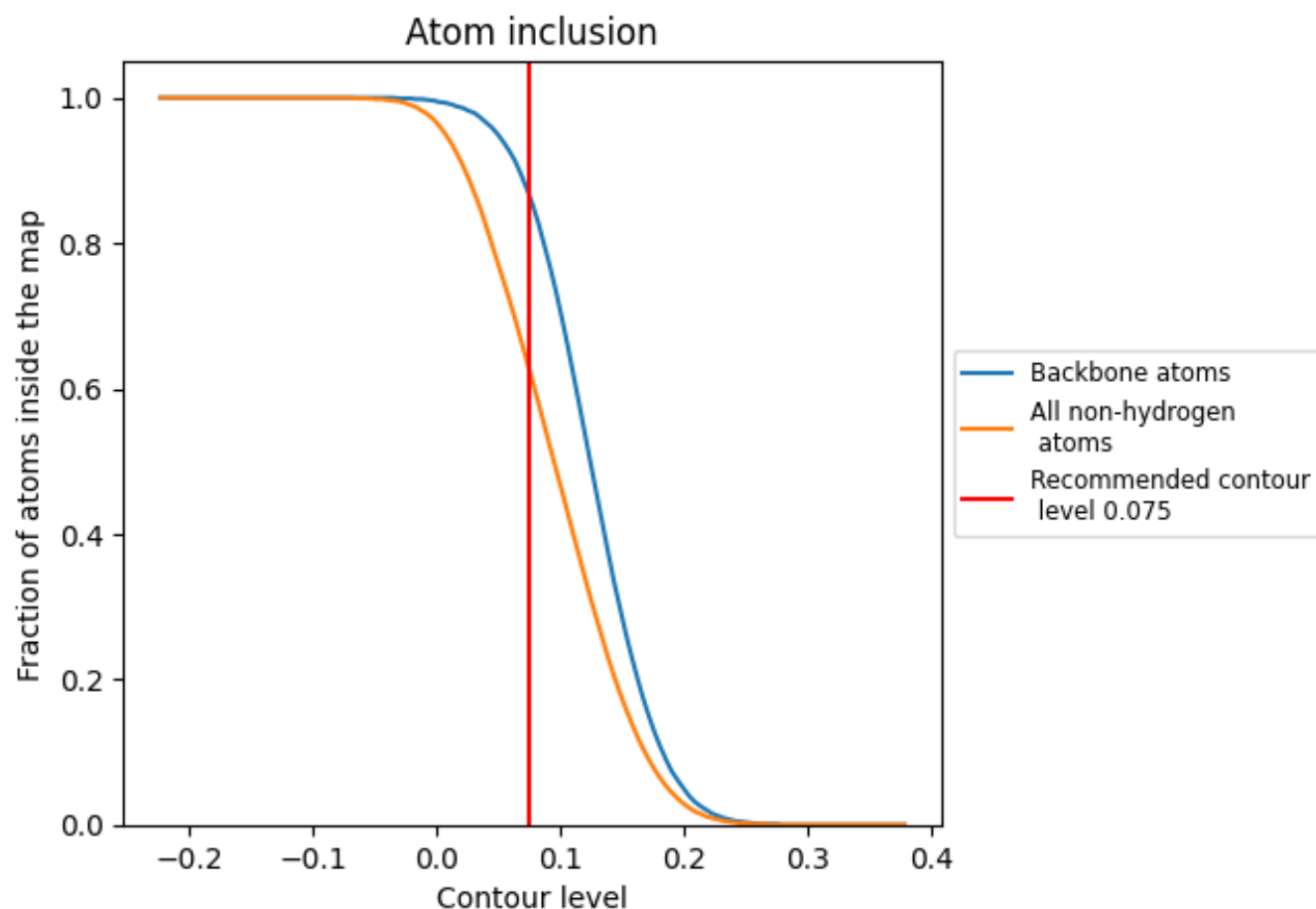
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6290	 0.2600
A	 0.5890	 0.2300
B	 0.5360	 0.2140
C	 0.5380	 0.2090
D	 0.6320	 0.2640
E	 0.6280	 0.2570
F	 0.5820	 0.2240
G	 0.6330	 0.2690
H	 0.6670	 0.2820
I	 0.6320	 0.2640
J	 0.6190	 0.2490
K	 0.6580	 0.2770
L	 0.6630	 0.2840
M	 0.6050	 0.2400
N	 0.6650	 0.2810
O	 0.6630	 0.2760
P	 0.6500	 0.2690
Q	 0.6630	 0.2840
R	 0.6790	 0.2950
S	 0.6240	 0.2530
T	 0.6630	 0.2750
U	 0.6770	 0.2880
V	 0.6360	 0.2580
W	 0.6710	 0.2900
X	 0.6440	 0.2680
Y	 0.5980	 0.2380
Z	 0.6500	 0.2760
a	 0.6390	 0.2720
b	 0.6270	 0.2490
c	 0.6280	 0.2590
d	 0.6330	 0.2620
e	 0.5630	 0.2190
f	 0.5860	 0.2400
g	 0.6180	 0.2550

