



wwPDB EM Validation Summary Report ⓘ

Apr 3, 2025 – 02:37 pm BST

PDB ID : 9GO6 / pdb_00009go6
EMDB ID : EMD-51493
Title : Salmonella hook-filament junction complex
Authors : Qin, K.; Eikenkel, R.; Erhardt, E.; Bergeron, J.R.
Deposited on : 2024-09-04
Resolution : 2.90 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:

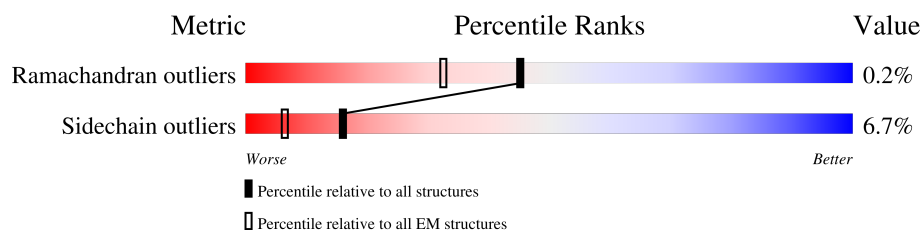
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 2.90 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	207382	16835
Sidechain outliers	206894	16415

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	1	403	<div> <div>46%</div> <div>95%</div> <div>5%</div> </div>
1	2	403	<div> <div>59%</div> <div>95%</div> <div>5%</div> </div>
1	3	403	<div> <div>49%</div> <div>94%</div> <div>6%</div> </div>
1	4	403	<div> <div>64%</div> <div>92%</div> <div>7%</div> </div>
1	5	403	<div> <div>53%</div> <div>94%</div> <div>6%</div> </div>
1	6	403	<div> <div>66%</div> <div>95%</div> <div>5%</div> </div>
1	7	403	<div> <div>57%</div> <div>92%</div> <div>8%</div> </div>
1	8	403	<div> <div>52%</div> <div>94%</div> <div>6%</div> </div>
1	9	403	<div> <div>73%</div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	w	403	58% 93% 7%
1	x	403	59% 94% 6%
1	y	403	52% 96% .
1	z	403	56% 93% 7%
2	A	553	54% 93% 7%
2	B	553	28% 92% 8%
2	C	553	44% 91% 8% .
2	D	553	19% 93% 6%
2	E	553	30% 93% 7% .
2	F	553	22% 93% 7%
2	G	553	26% 94% 6%
2	H	553	35% 95% 5%
2	I	553	31% 92% 8%
2	J	553	35% 91% 8%
2	K	553	28% 92% 7%
3	L	317	. 91% 6% .
3	M	317	9% 89% 9% .
3	N	317	. 92% 6% .
3	O	317	18% 89% 9% .
3	P	317	. 94% . .
3	Q	317	13% 90% 6% .
3	R	317	. 91% 7% .
3	S	317	8% 91% 7% .
3	T	317	. 94% 5% .
3	U	317	6% 93% 6%

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Mol	Chain	Length	Quality of chain
3	V	317	
4	a	495	
4	b	495	
4	c	495	
4	d	495	
4	e	495	
4	f	495	
4	g	495	
4	h	495	
4	i	495	
4	j	495	
4	k	495	
4	l	495	
4	m	495	
4	n	495	
4	o	495	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 324413 atoms, of which 160408 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 Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	2	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	3	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	4	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	5	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	6	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	7	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	8	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	9	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	w	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	x	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	y	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		
1	z	403	Total	C	H	N	O	S	0	0
			5832	1825	2865	512	621	9		

- Molecule 2 is a protein called Flagellar hook-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	552	Total	C	H	N	O	S	0	0
			8201	2547	4056	722	869	7		
2	B	552	Total	C	H	N	O	S	0	0
			8201	2547	4056	722	869	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	550	Total	C	H	N	O	S	0	0
			8184	2542	4048	723	865	6		
2	D	552	Total	C	H	N	O	S	0	0
			8201	2547	4056	722	869	7		
2	E	550	Total	C	H	N	O	S	0	0
			8163	2536	4034	720	867	6		
2	F	551	Total	C	H	N	O	S	0	0
			8182	2542	4045	721	868	6		
2	G	551	Total	C	H	N	O	S	0	0
			8182	2542	4045	721	868	6		
2	H	551	Total	C	H	N	O	S	0	0
			8178	2542	4041	721	868	6		
2	I	552	Total	C	H	N	O	S	0	0
			8201	2547	4056	722	869	7		
2	J	552	Total	C	H	N	O	S	0	0
			8201	2547	4056	722	869	7		
2	K	552	Total	C	H	N	O	S	0	0
			8201	2547	4056	722	869	7		

- Molecule 3 is a protein called Flagellar hook-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	306	Total	C	H	N	O	S	0	0
			4543	1404	2247	398	482	12		
3	M	312	Total	C	H	N	O	S	0	0
			4640	1436	2296	405	491	12		
3	N	313	Total	C	H	N	O	S	0	0
			4666	1443	2309	410	492	12		
3	O	310	Total	C	H	N	O	S	0	0
			4612	1428	2282	403	487	12		
3	P	307	Total	C	H	N	O	S	0	0
			4556	1408	2254	399	484	11		
3	Q	305	Total	C	H	N	O	S	0	0
			4529	1400	2240	397	480	12		
3	R	310	Total	C	H	N	O	S	0	0
			4604	1425	2277	402	488	12		
3	S	312	Total	C	H	N	O	S	0	0
			4653	1439	2303	409	490	12		
3	T	314	Total	C	H	N	O	S	0	0
			4678	1446	2315	411	494	12		
3	U	316	Total	C	H	N	O	S	0	0
			4681	1457	2302	413	496	13		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	V	315	Total	C	H	N	O	S	0	0
			4697	1452	2326	412	495	12		

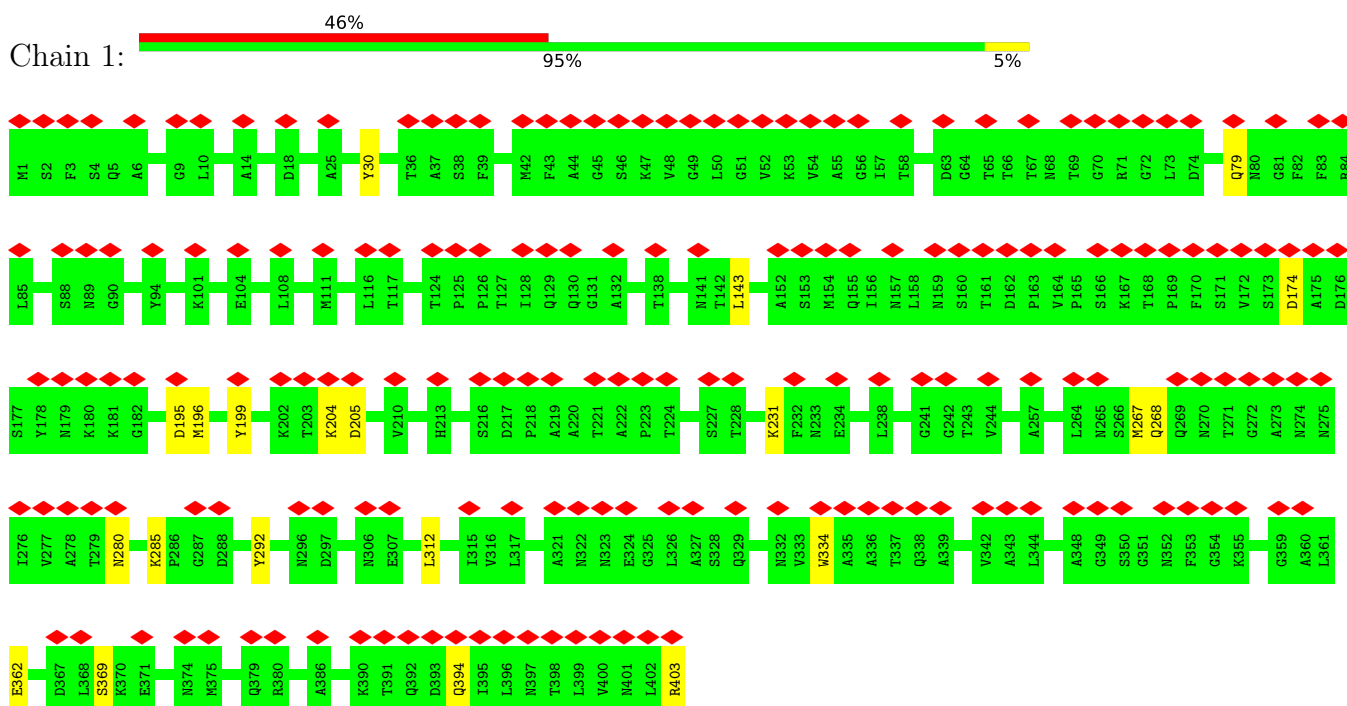
- Molecule 4 is a protein called Flagellin.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	a	494	Total	C	H	N	O	S	0	0
			7189	2189	3574	640	784	2		
4	b	493	Total	C	H	N	O	S	0	0
			7151	2186	3541	639	783	2		
4	c	494	Total	C	H	N	O	S	0	0
			7167	2189	3552	640	784	2		
4	d	494	Total	C	H	N	O	S	0	0
			7189	2189	3574	640	784	2		
4	e	494	Total	C	H	N	O	S	0	0
			7189	2189	3574	640	784	2		
4	f	495	Total	C	H	N	O	S	0	0
			7164	2194	3541	641	785	3		
4	g	493	Total	C	H	N	O	S	0	0
			7179	2186	3569	639	783	2		
4	h	494	Total	C	H	N	O	S	0	0
			7189	2189	3574	640	784	2		
4	i	494	Total	C	H	N	O	S	0	0
			7176	2189	3561	640	784	2		
4	j	493	Total	C	H	N	O	S	0	0
			7179	2186	3569	639	783	2		
4	k	494	Total	C	H	N	O	S	0	0
			7189	2189	3574	640	784	2		
4	l	492	Total	C	H	N	O	S	0	0
			7162	2181	3561	637	781	2		
4	m	492	Total	C	H	N	O	S	0	0
			7162	2181	3561	637	781	2		
4	n	493	Total	C	H	N	O	S	0	0
			7179	2186	3569	639	783	2		
4	o	493	Total	C	H	N	O	S	0	0
			7179	2186	3569	639	783	2		

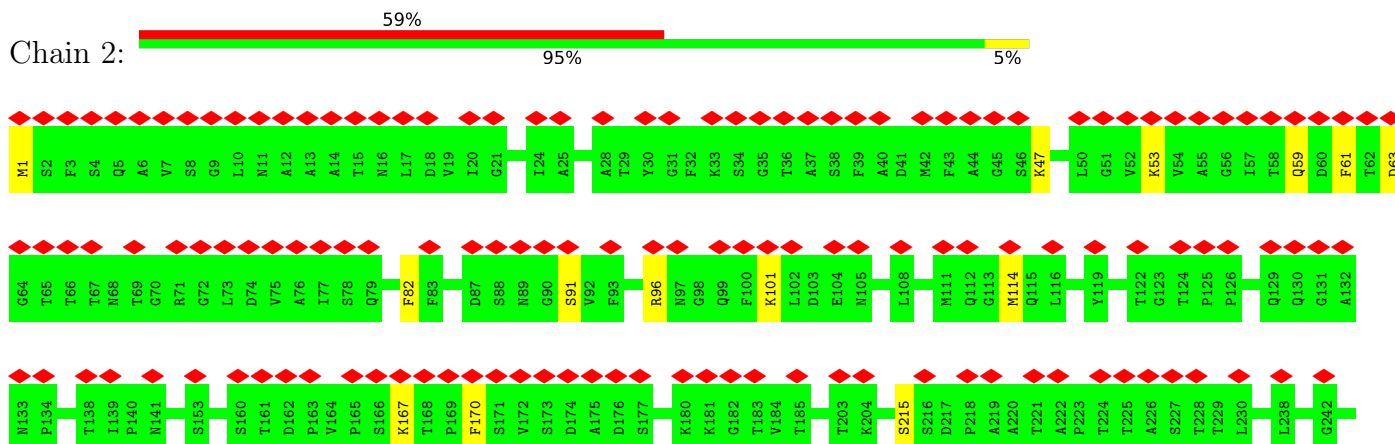
3 Residue-property plots

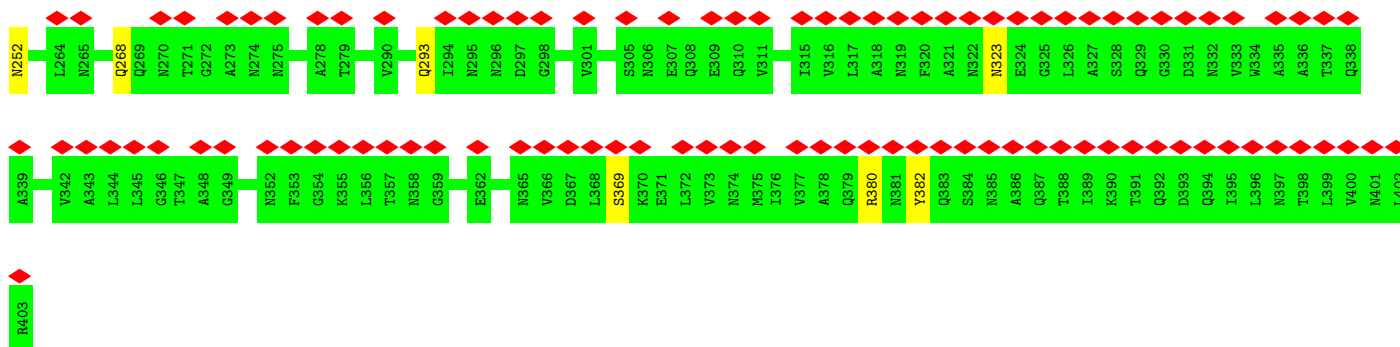
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Flagellar hook protein FlgE



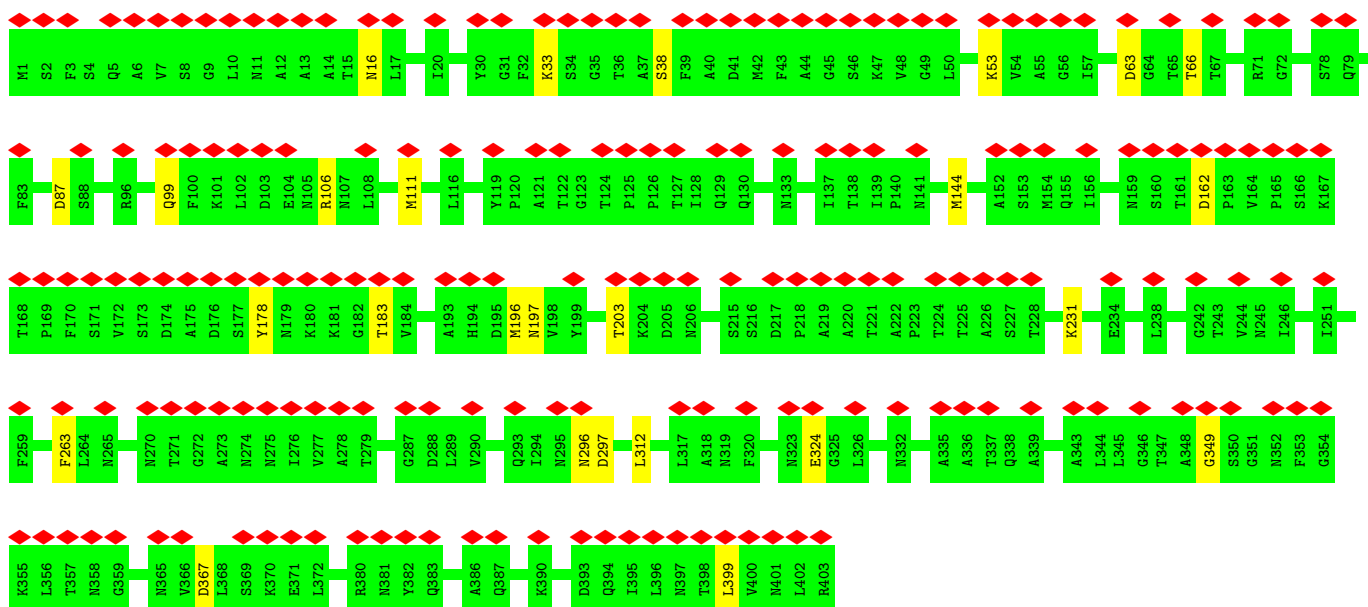
• Molecule 1: Flagellar hook protein FlgE





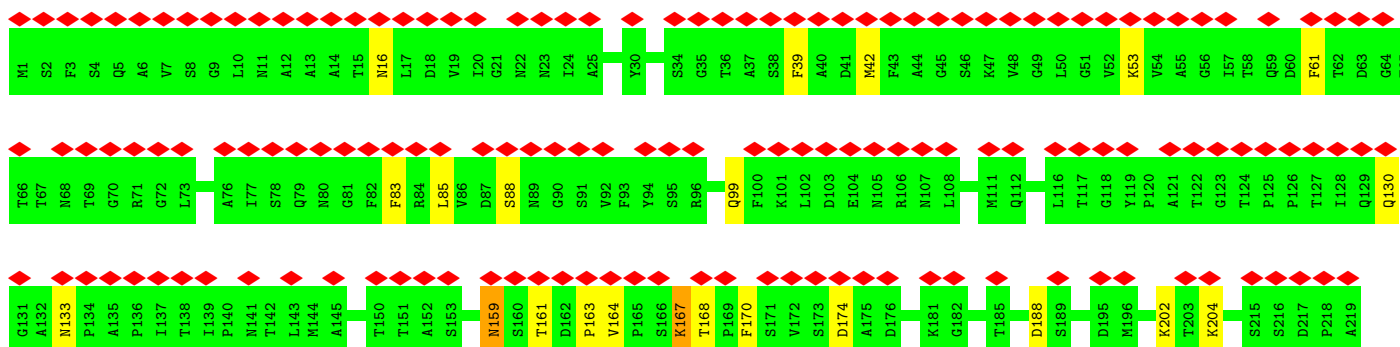
- Molecule 1: Flagellar hook protein FlgE

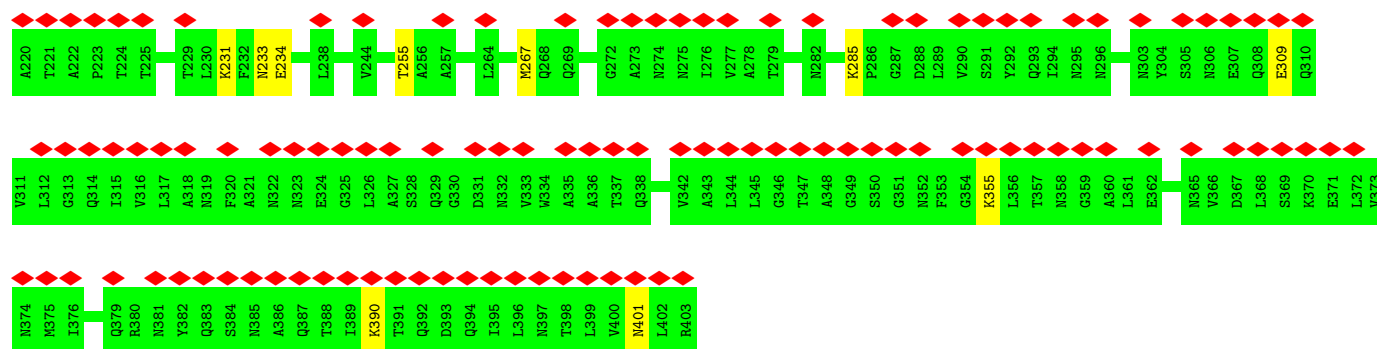
Chain 3: 49% 94% 6%



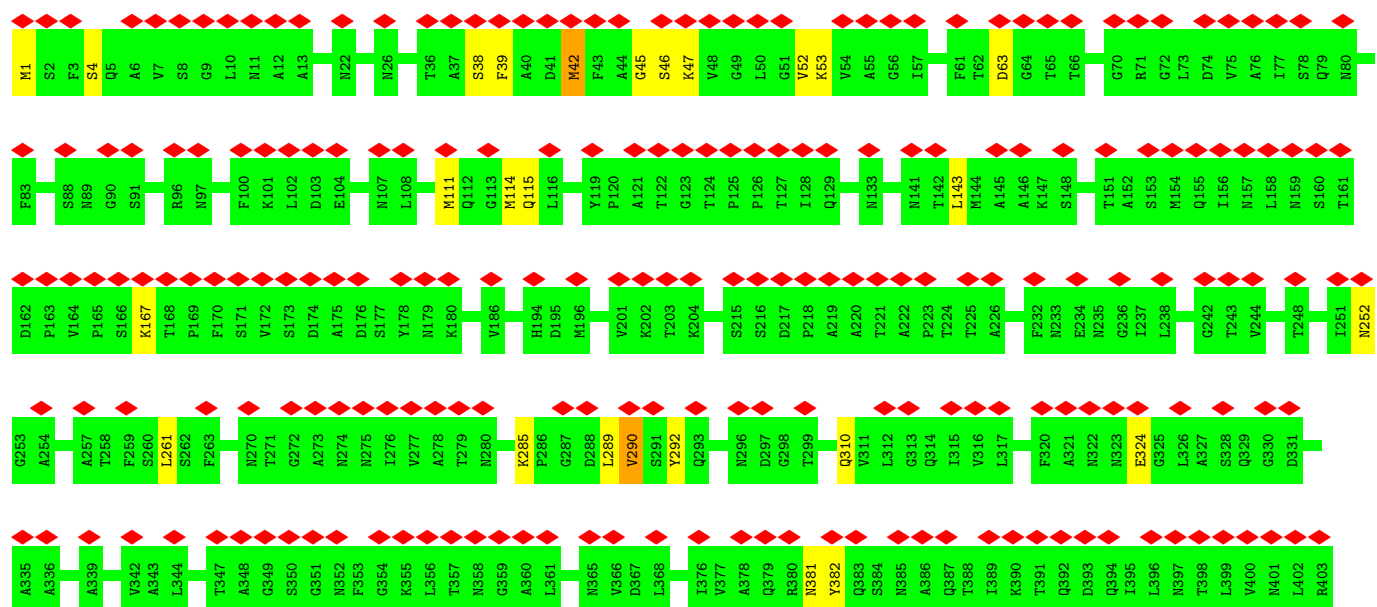
- Molecule 1: Flagellar hook protein FlgE

Chain 4: 64% 92% 7%

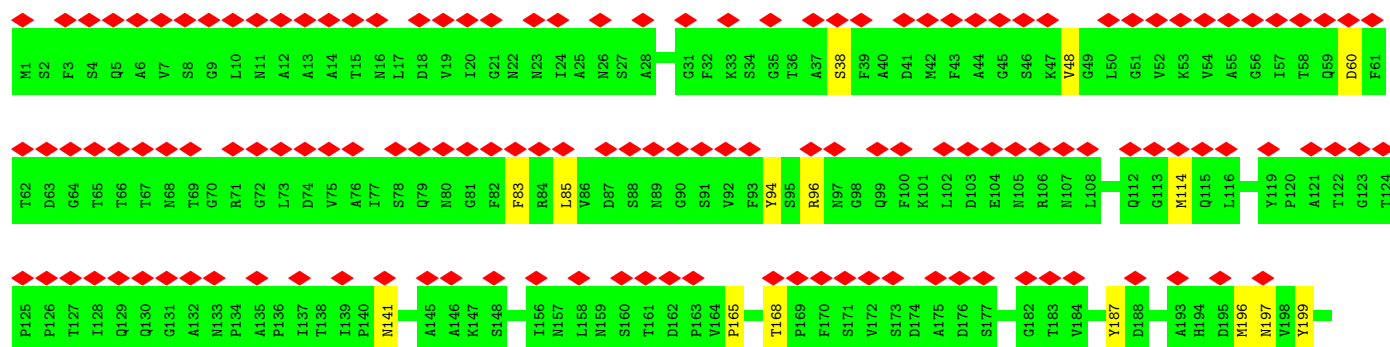


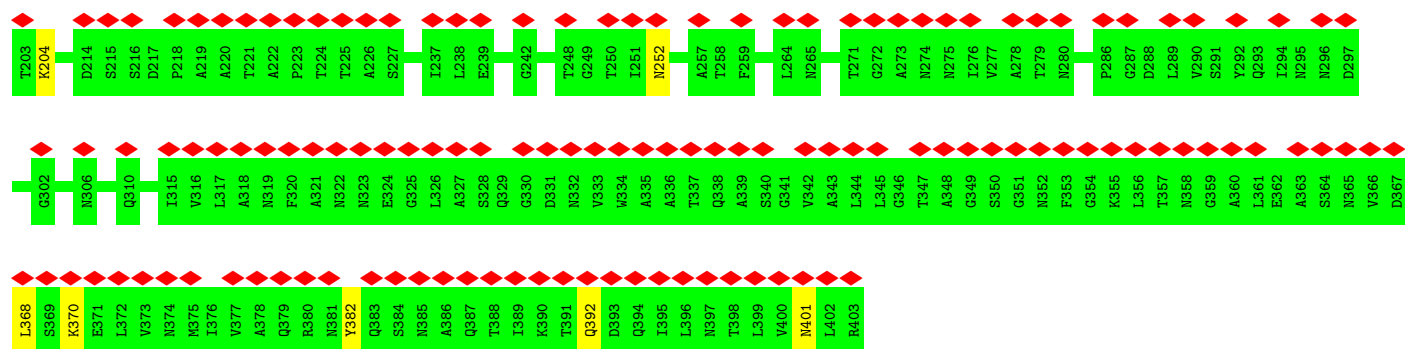


• Molecule 1: Flagellar hook protein FlgE

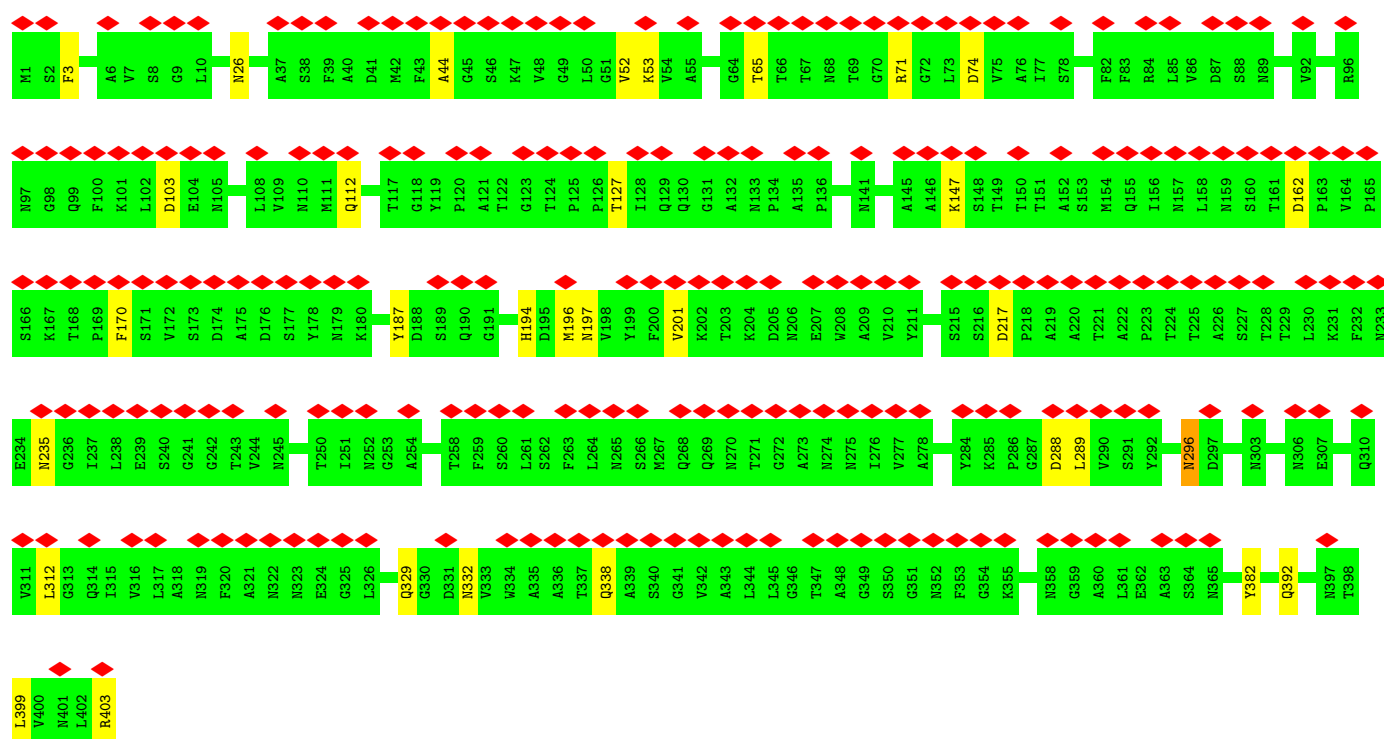
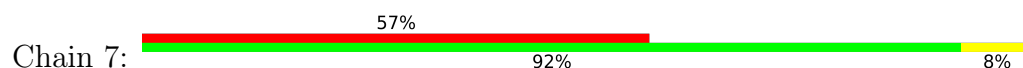


• Molecule 1: Flagellar hook protein FlgE

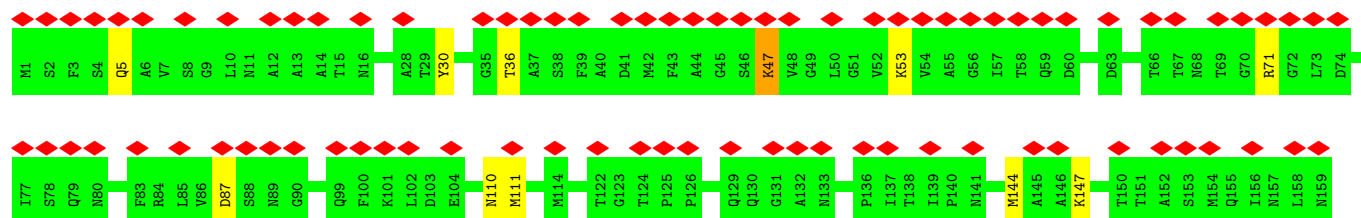


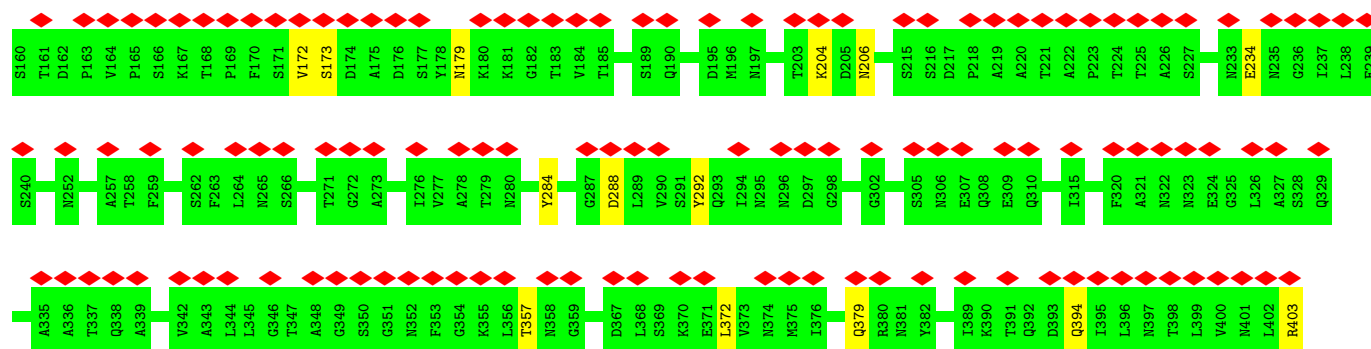


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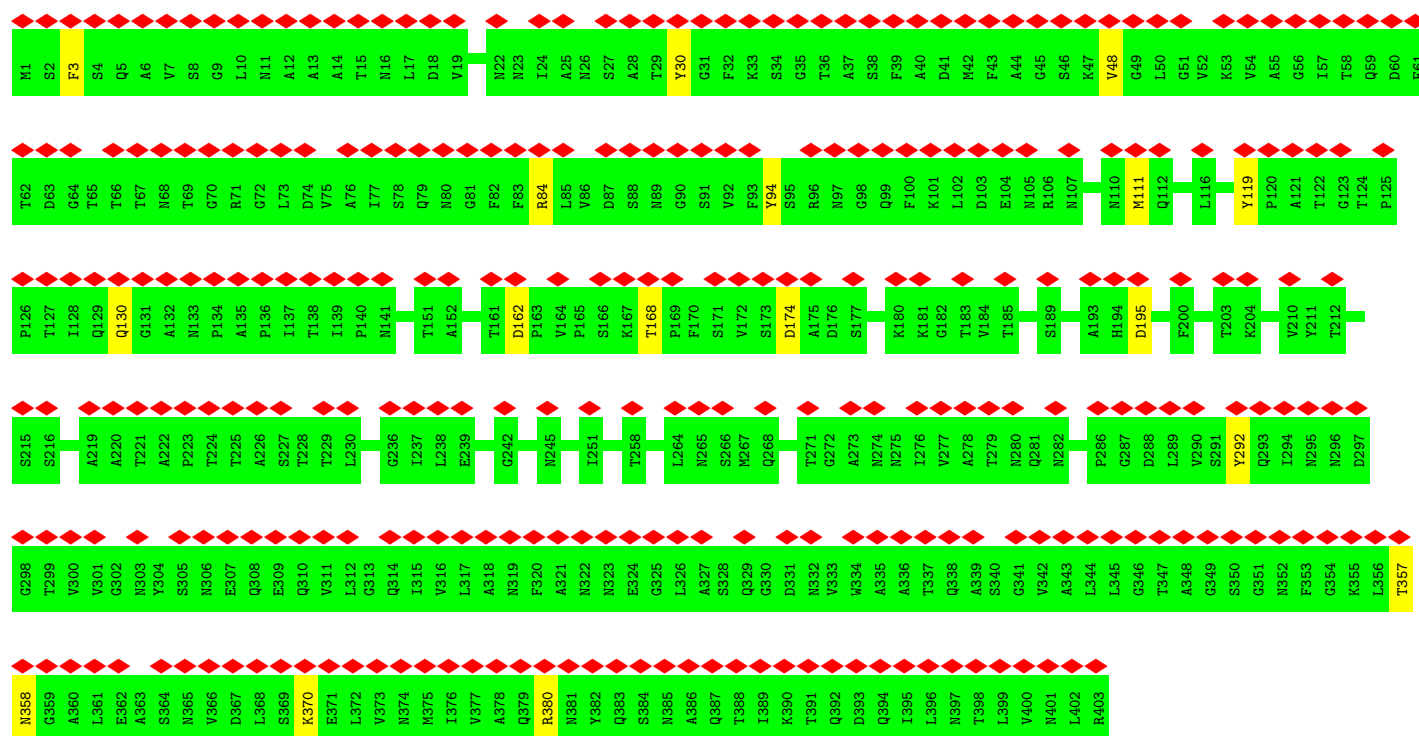
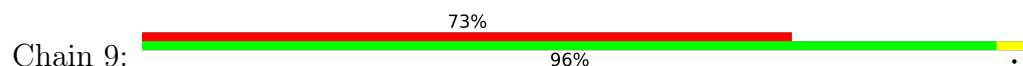


• Molecule 1: Flagellar hook protein FlgE

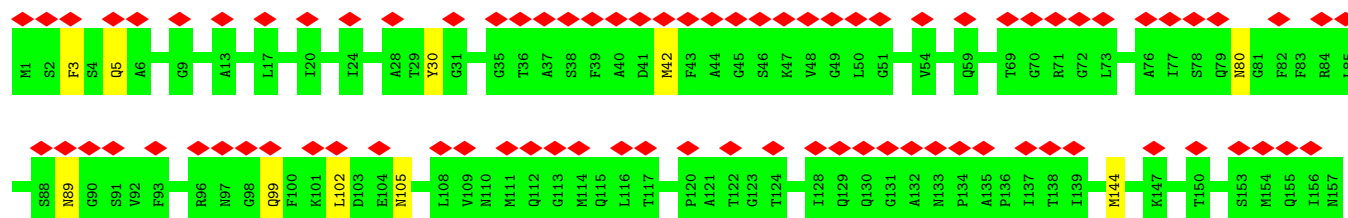


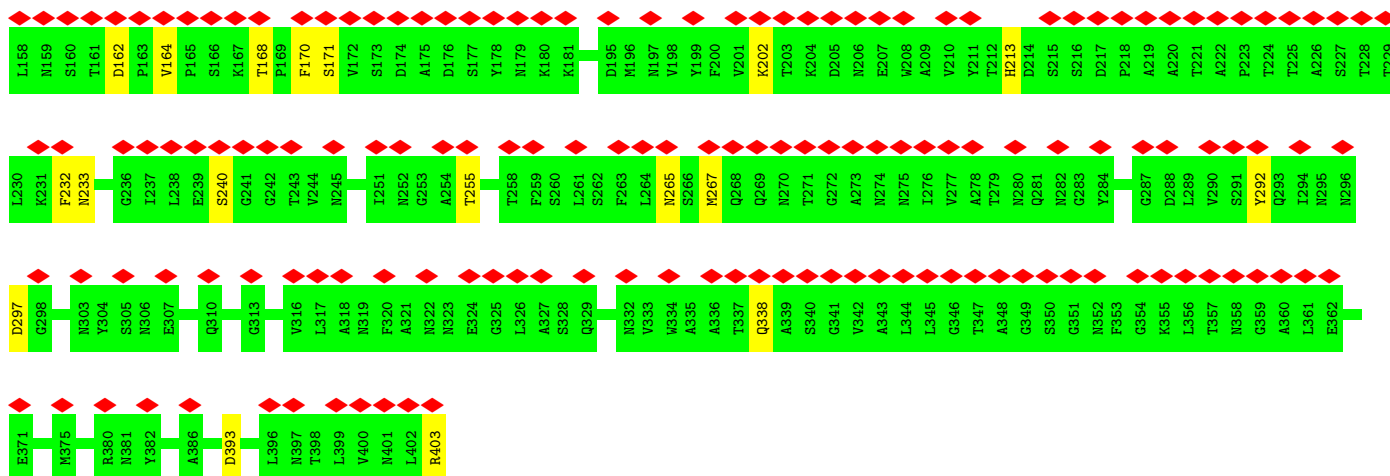


• Molecule 1: Flagellar hook protein FlgE

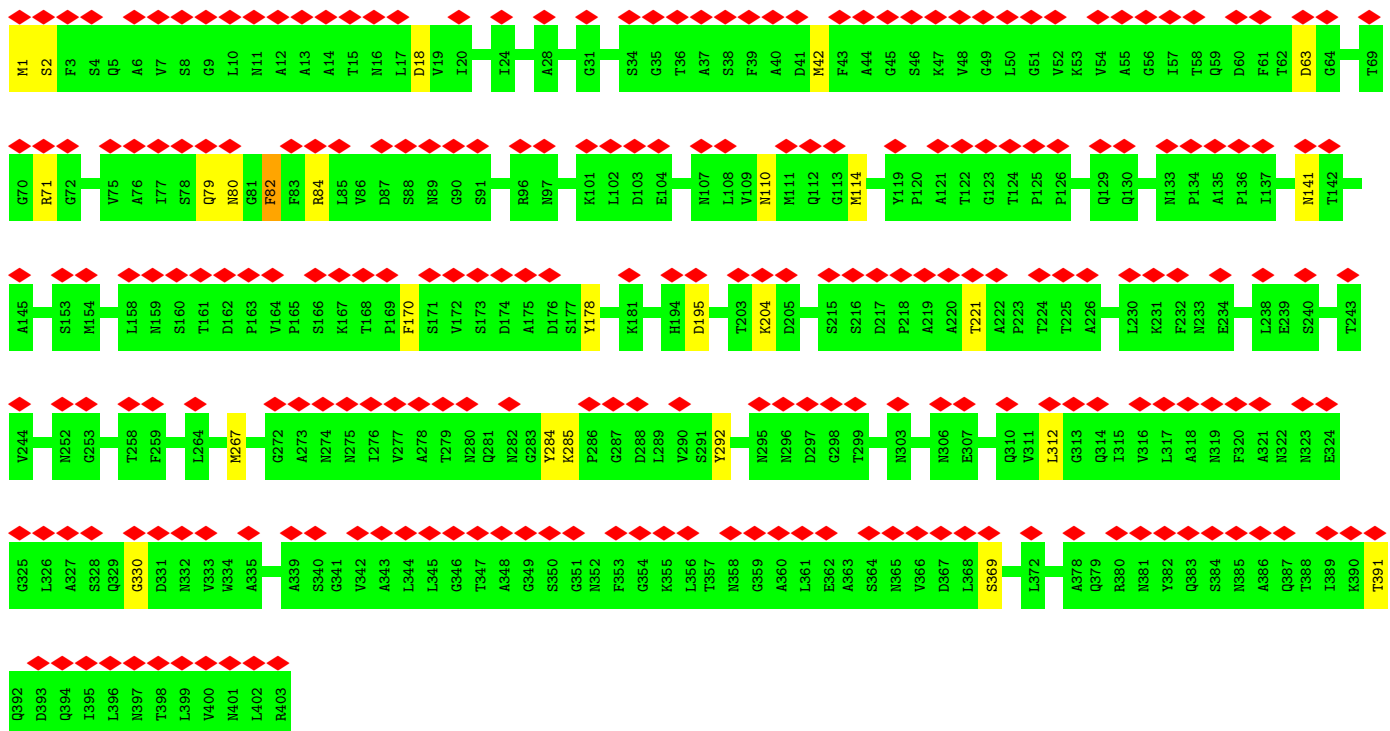


• Molecule 1: Flagellar hook protein FlgE

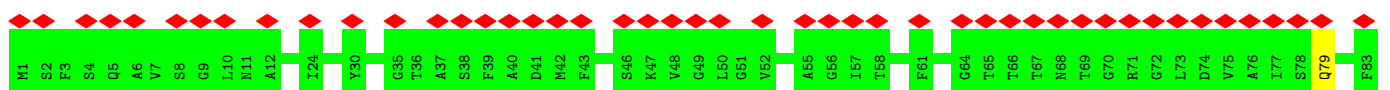


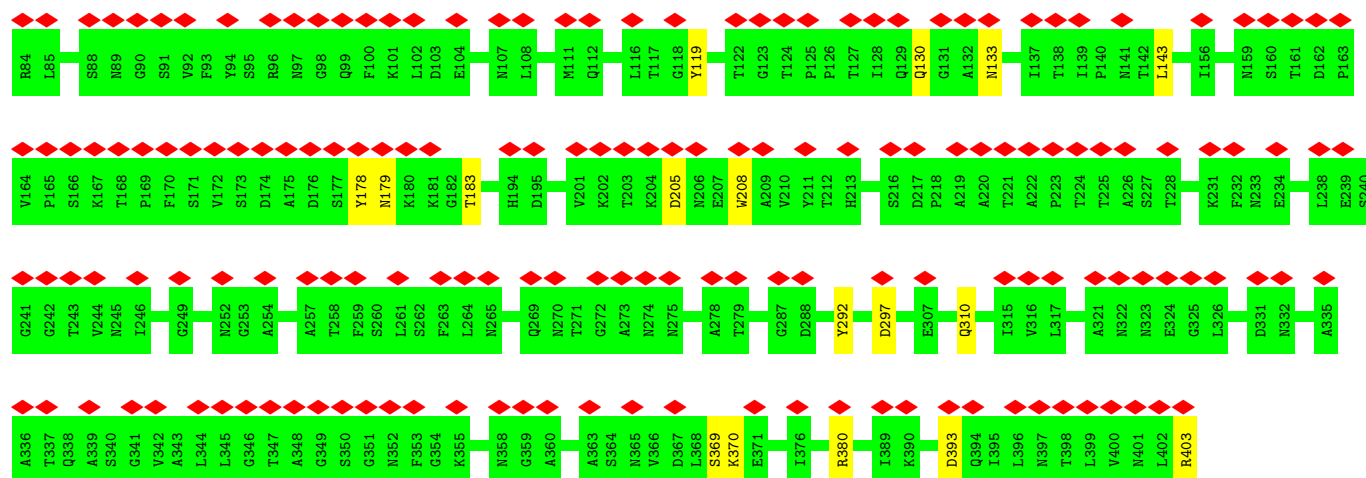


• Molecule 1: Flagellar hook protein FlgE

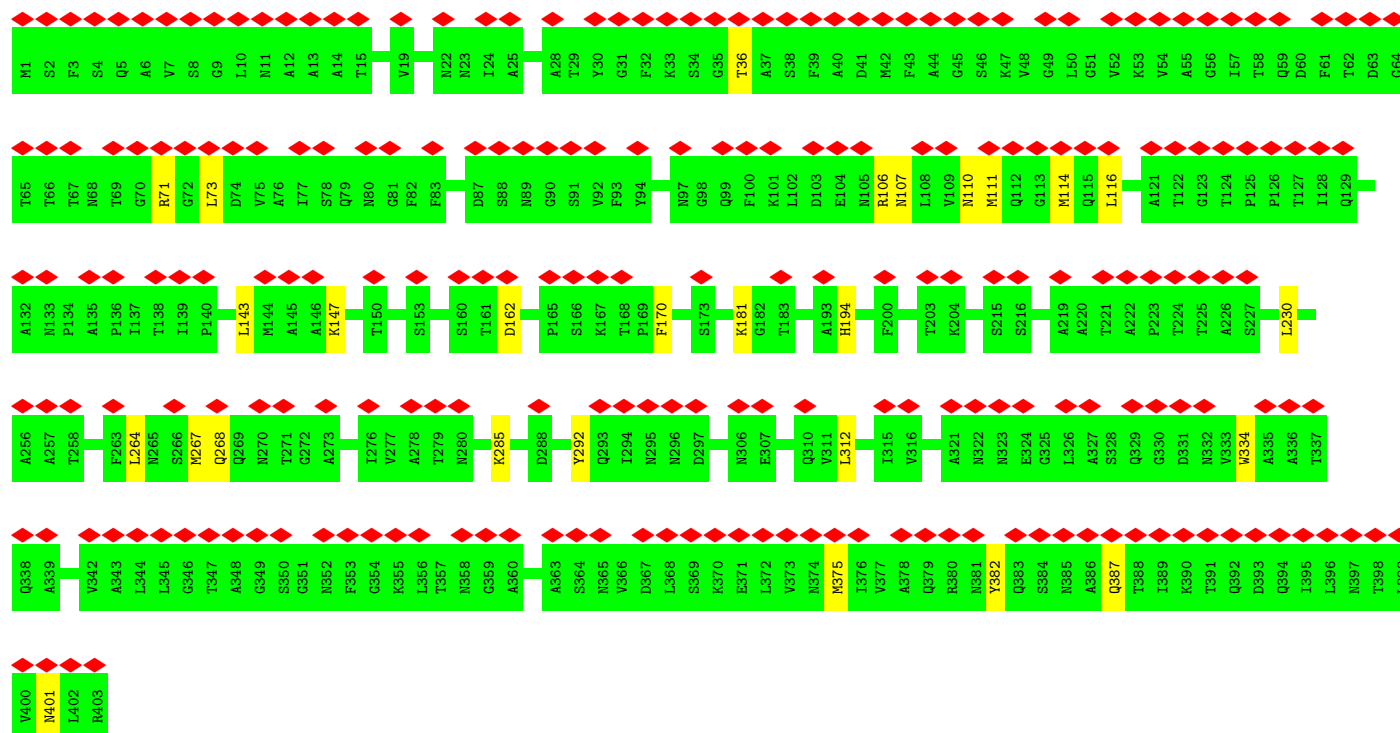
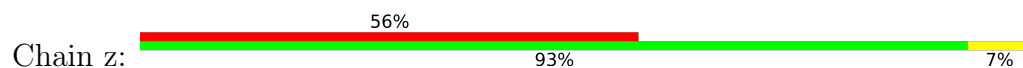


• Molecule 1: Flagellar hook protein FlgE

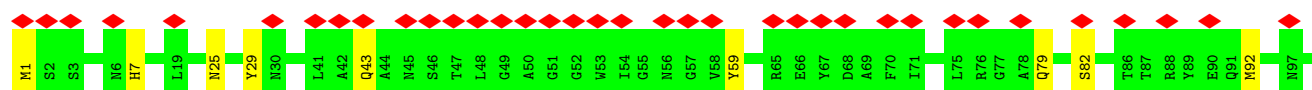


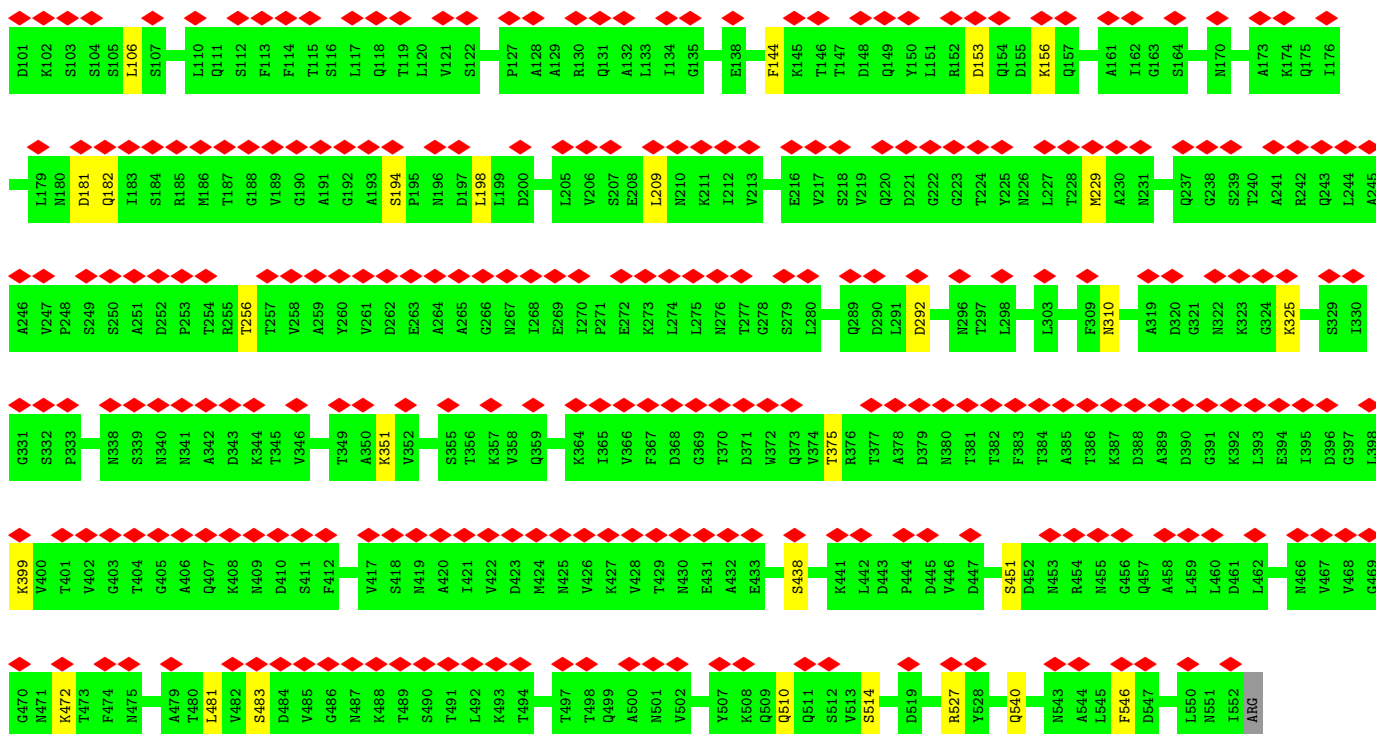


• Molecule 1: Flagellar hook protein FlgE

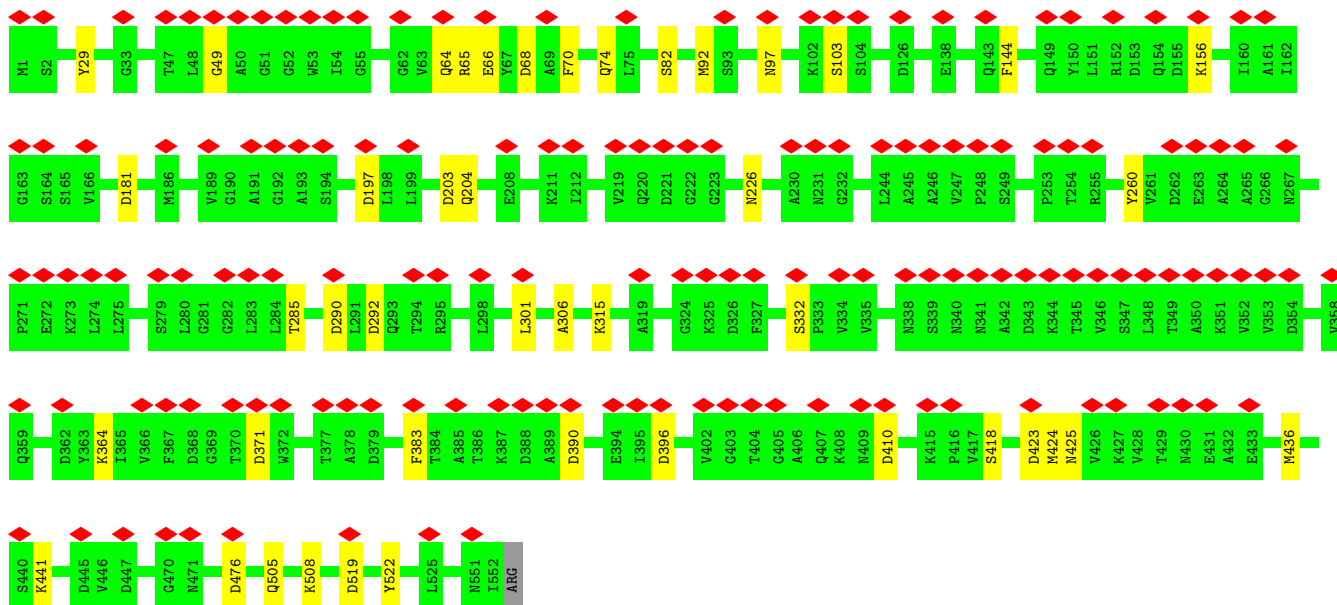
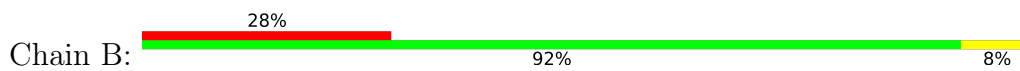


• Molecule 2: Flagellar hook-associated protein 1

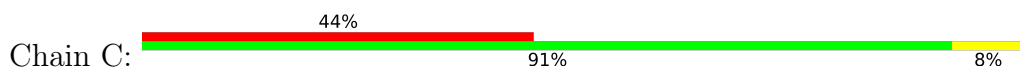


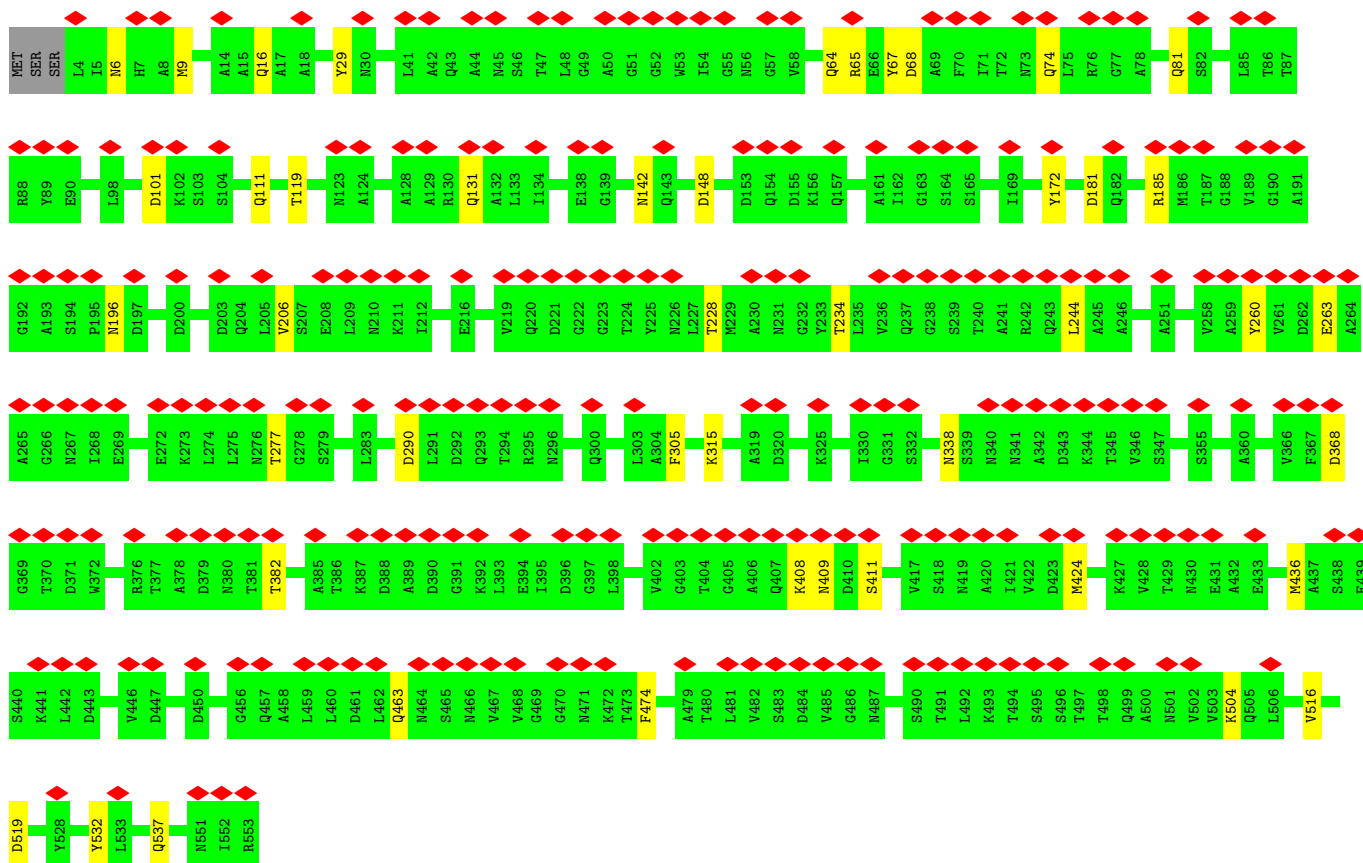


• Molecule 2: Flagellar hook-associated protein 1

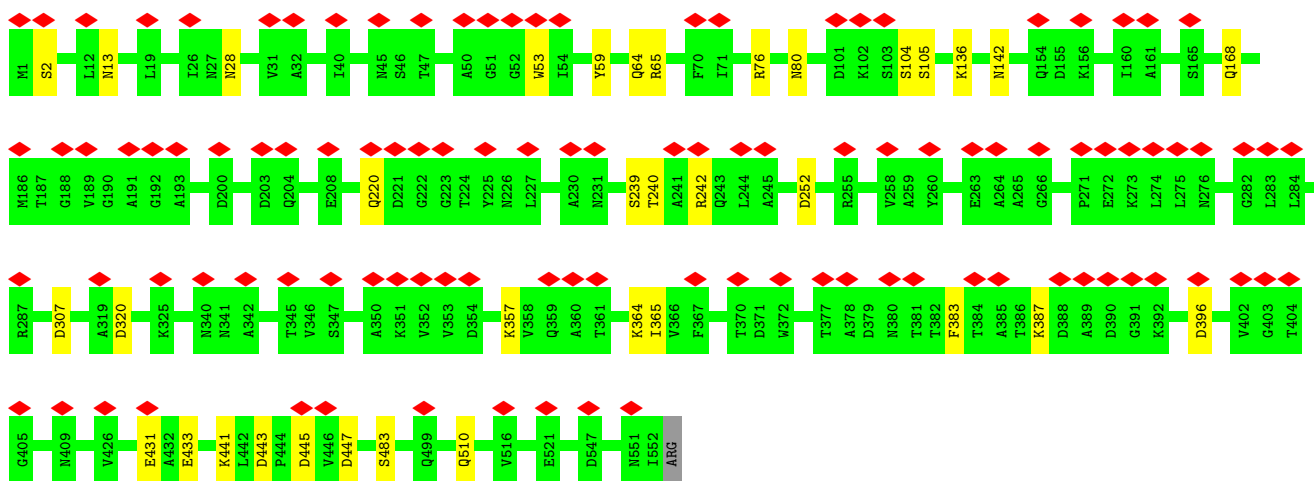
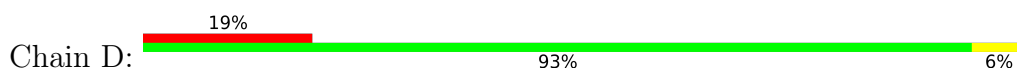


• Molecule 2: Flagellar hook-associated protein 1

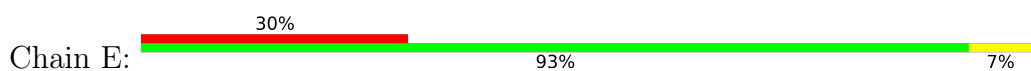


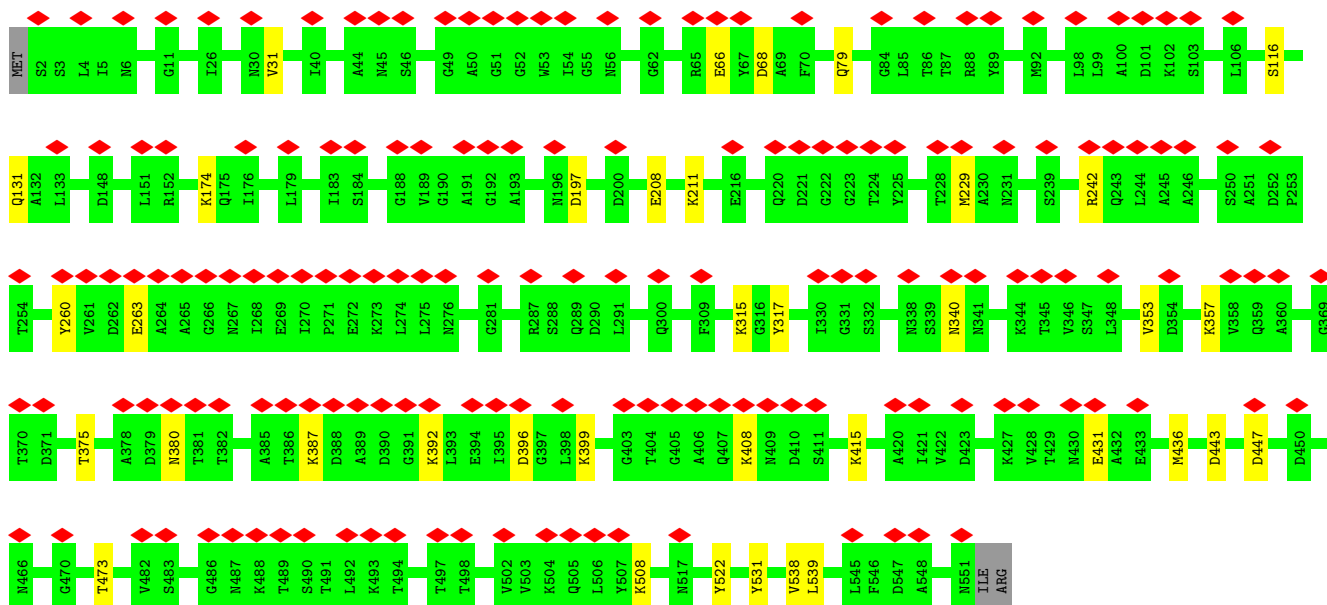


• Molecule 2: Flagellar hook-associated protein 1



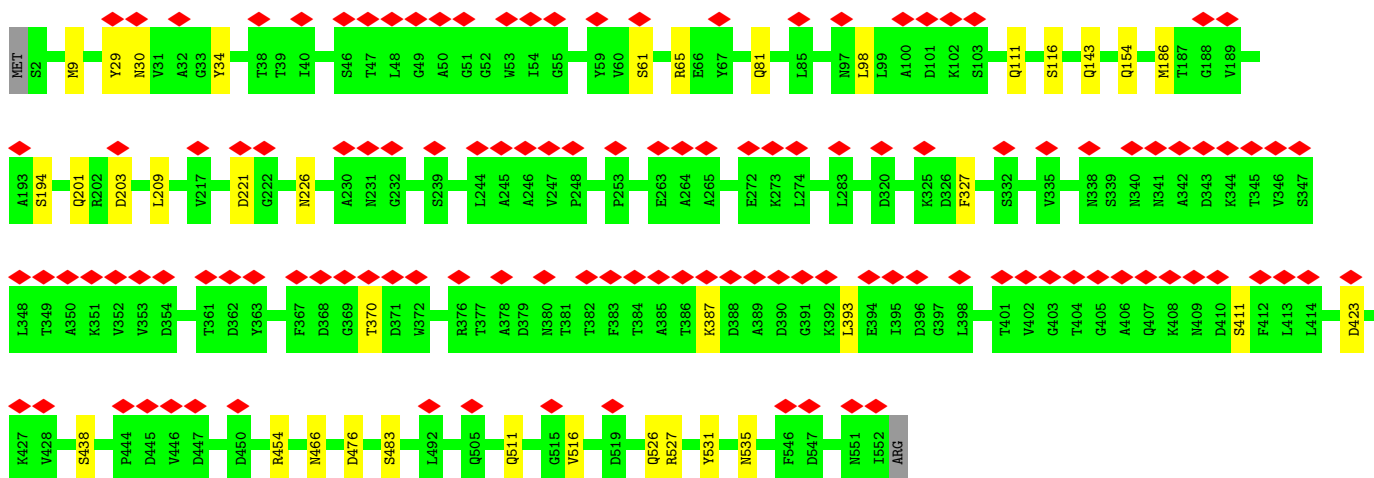
• Molecule 2: Flagellar hook-associated protein 1





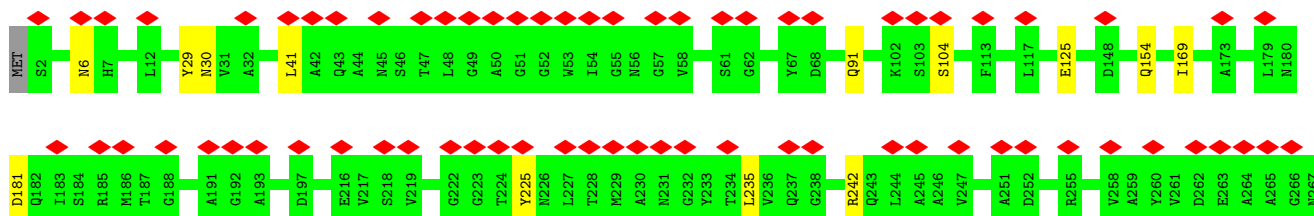
• Molecule 2: Flagellar hook-associated protein 1

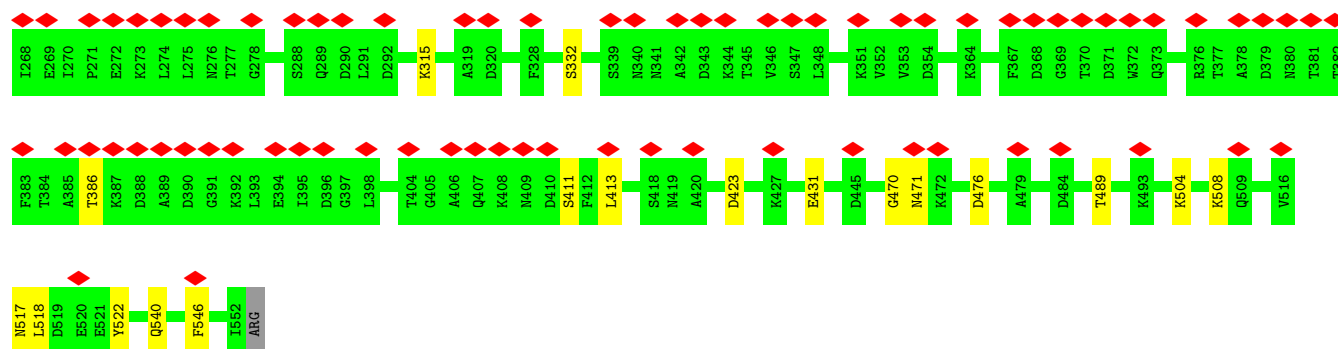
Chain F: 22% 93% 7%



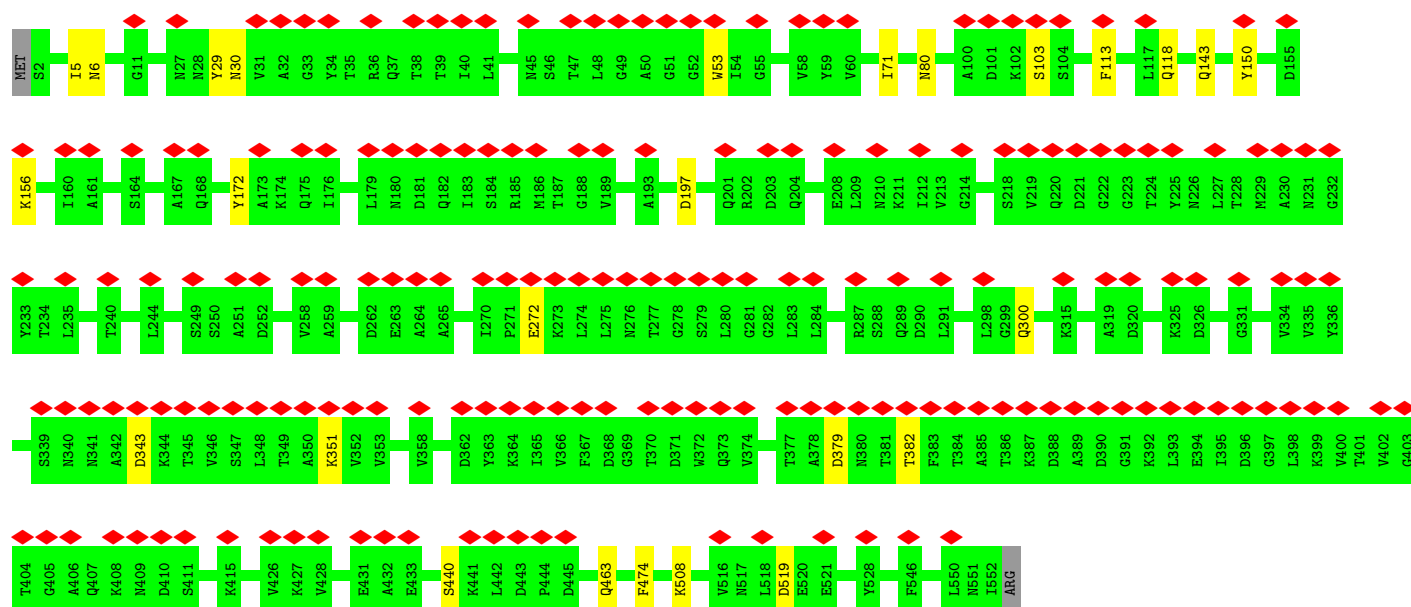
• Molecule 2: Flagellar hook-associated protein 1

Chain G: 26% 94% 6%

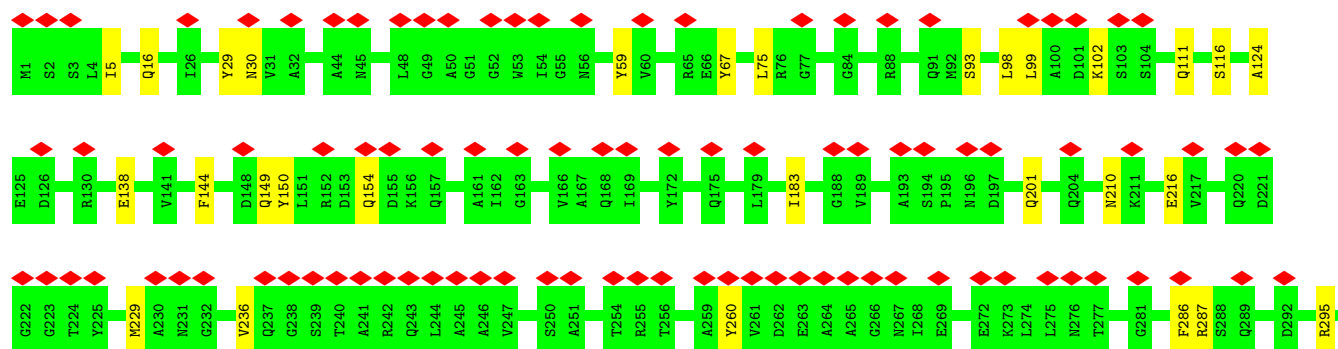
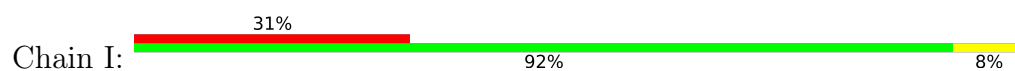


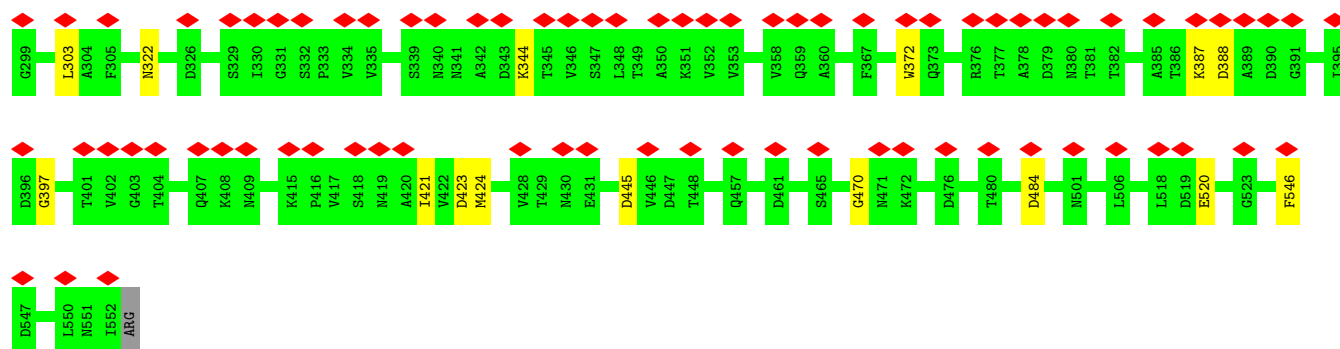


• Molecule 2: Flagellar hook-associated protein 1

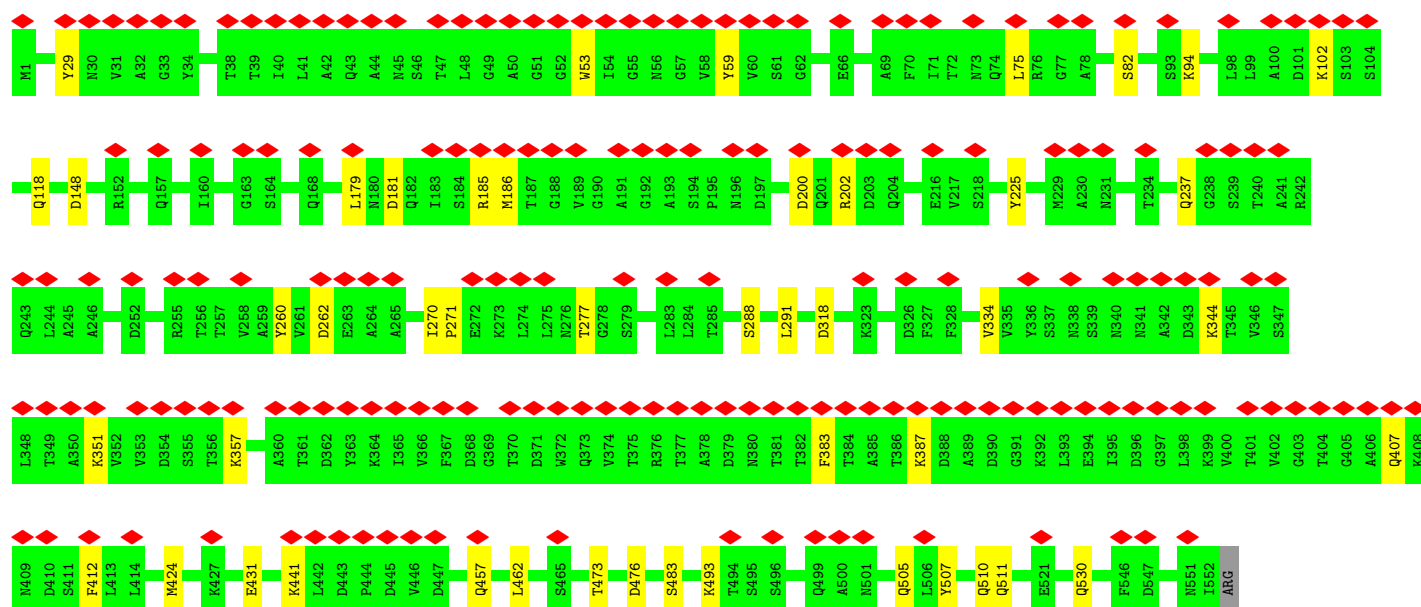
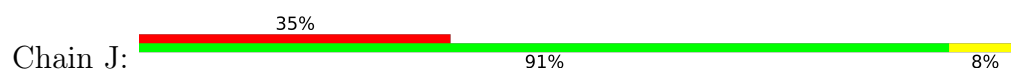


• Molecule 2: Flagellar hook-associated protein 1

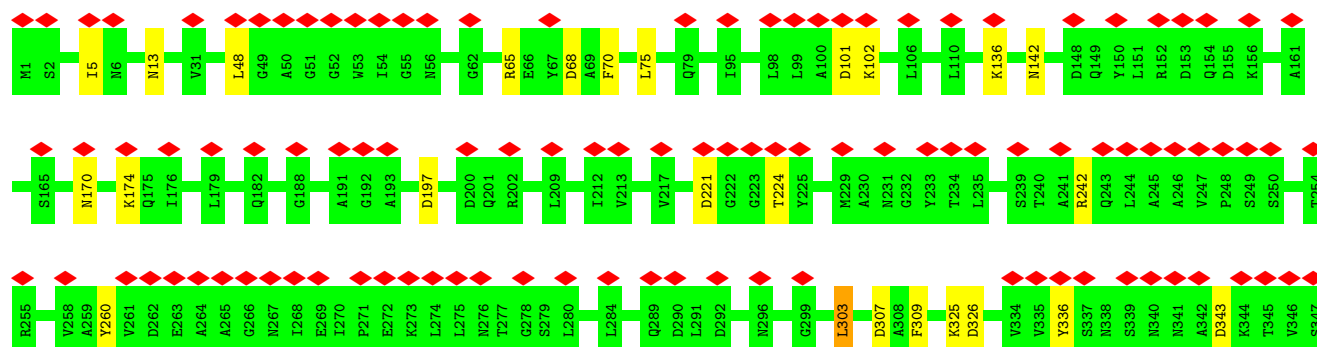


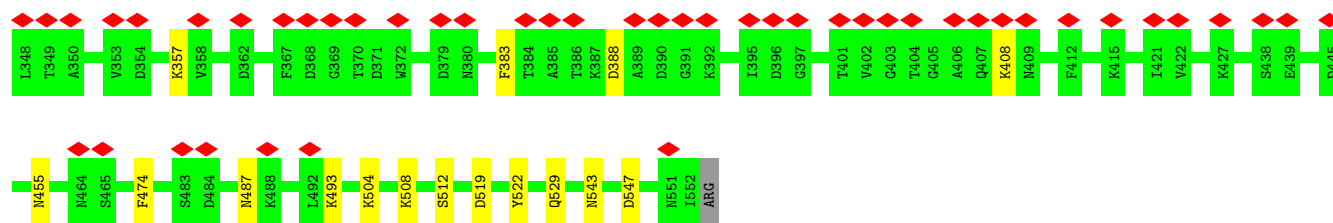


• Molecule 2: Flagellar hook-associated protein 1



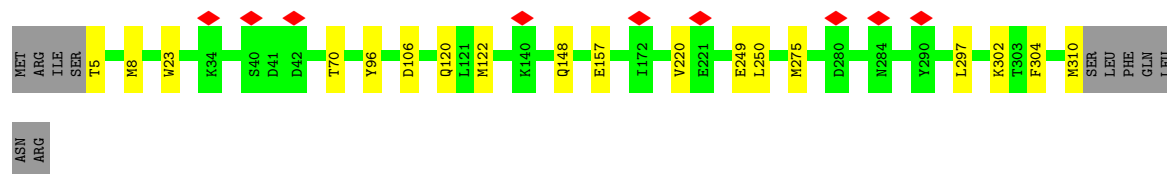
• Molecule 2: Flagellar hook-associated protein 1





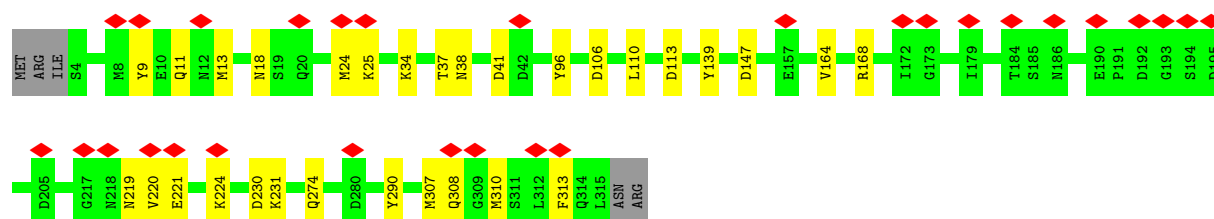
• Molecule 3: Flagellar hook-associated protein

Chain L: 91% 6%



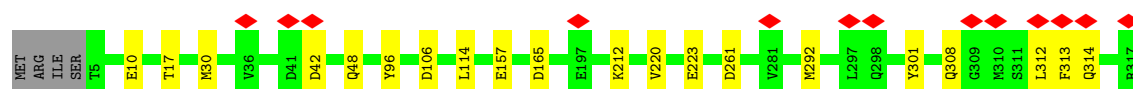
• Molecule 3: Flagellar hook-associated protein

Chain M: 9% 89% 9%



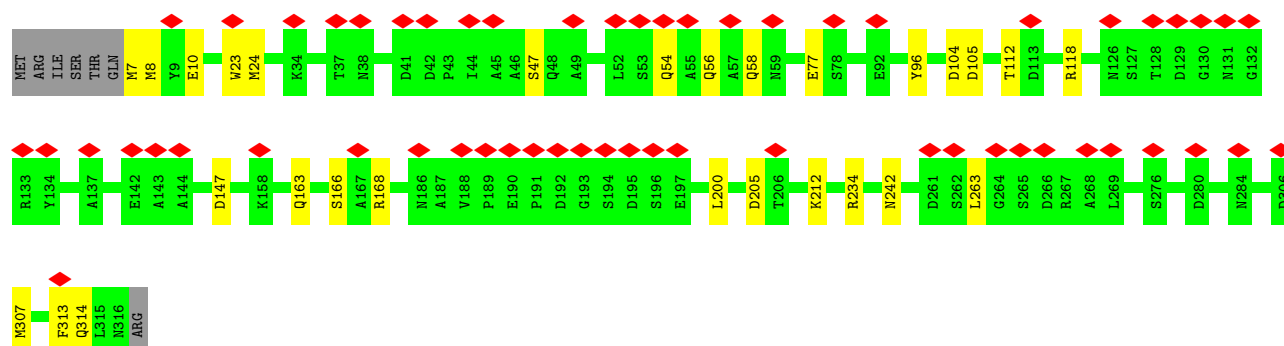
• Molecule 3: Flagellar hook-associated protein

Chain N: 92% 6%



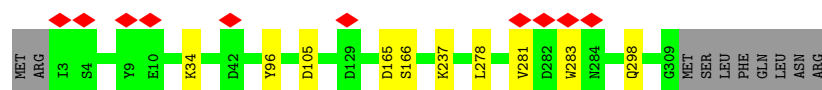
• Molecule 3: Flagellar hook-associated protein

Chain O: 18% 89% 9%




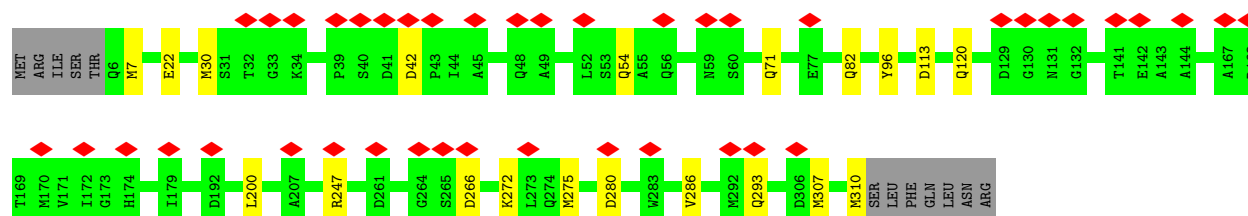
- Molecule 3: Flagellar hook-associated protein

Chain P:  94% . .



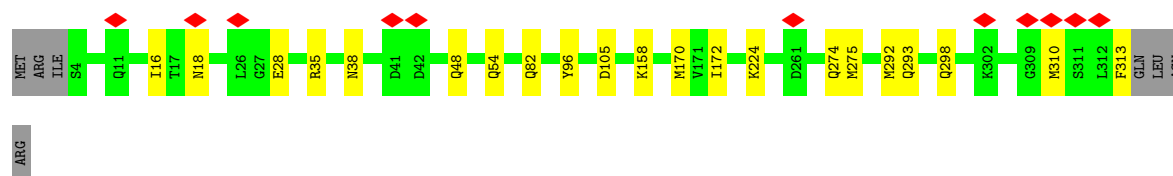
- Molecule 3: Flagellar hook-associated protein

Chain Q:  13% 90% 6% .



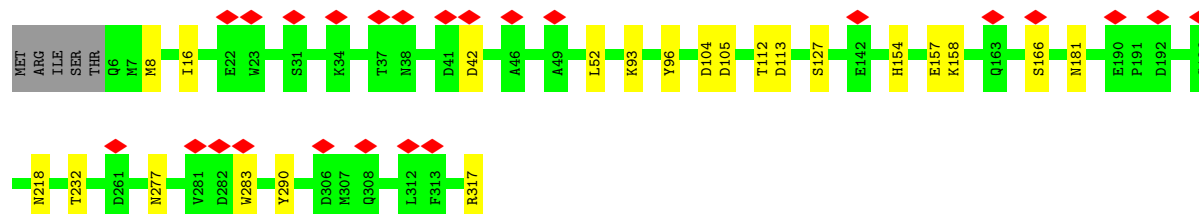
- Molecule 3: Flagellar hook-associated protein

Chain R:  91% 7% .



- Molecule 3: Flagellar hook-associated protein

Chain S:  8% 91% 7% .

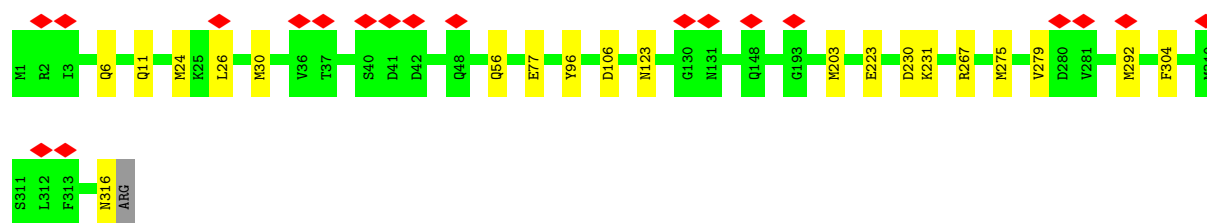
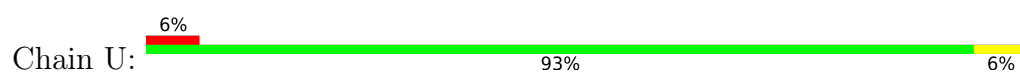


- Molecule 3: Flagellar hook-associated protein

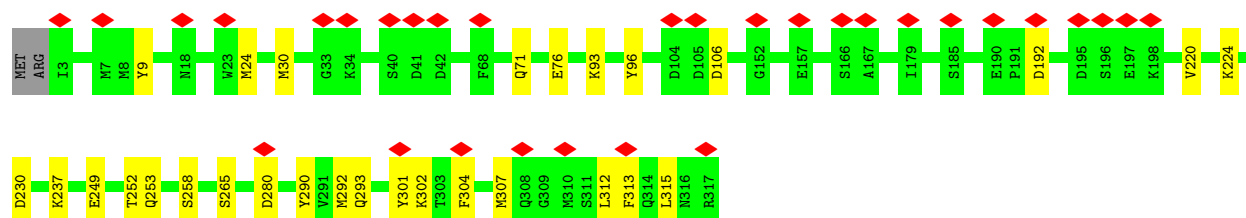
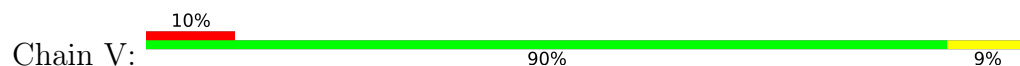
Chain T:  94% 5% .



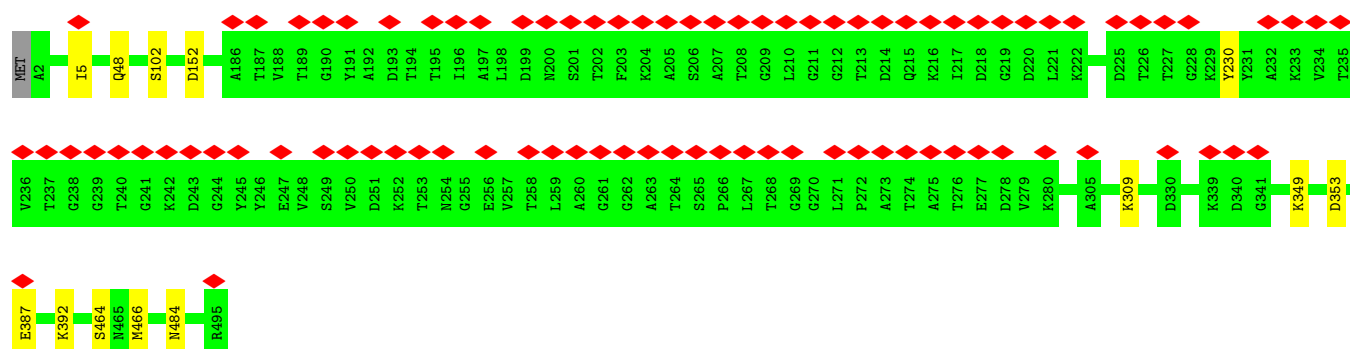
- Molecule 3: Flagellar hook-associated protein



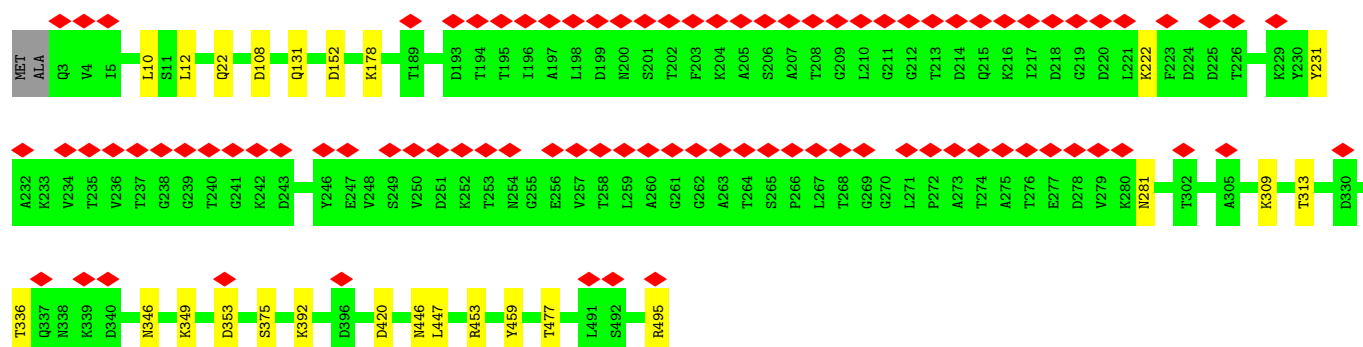
• Molecule 3: Flagellar hook-associated protein



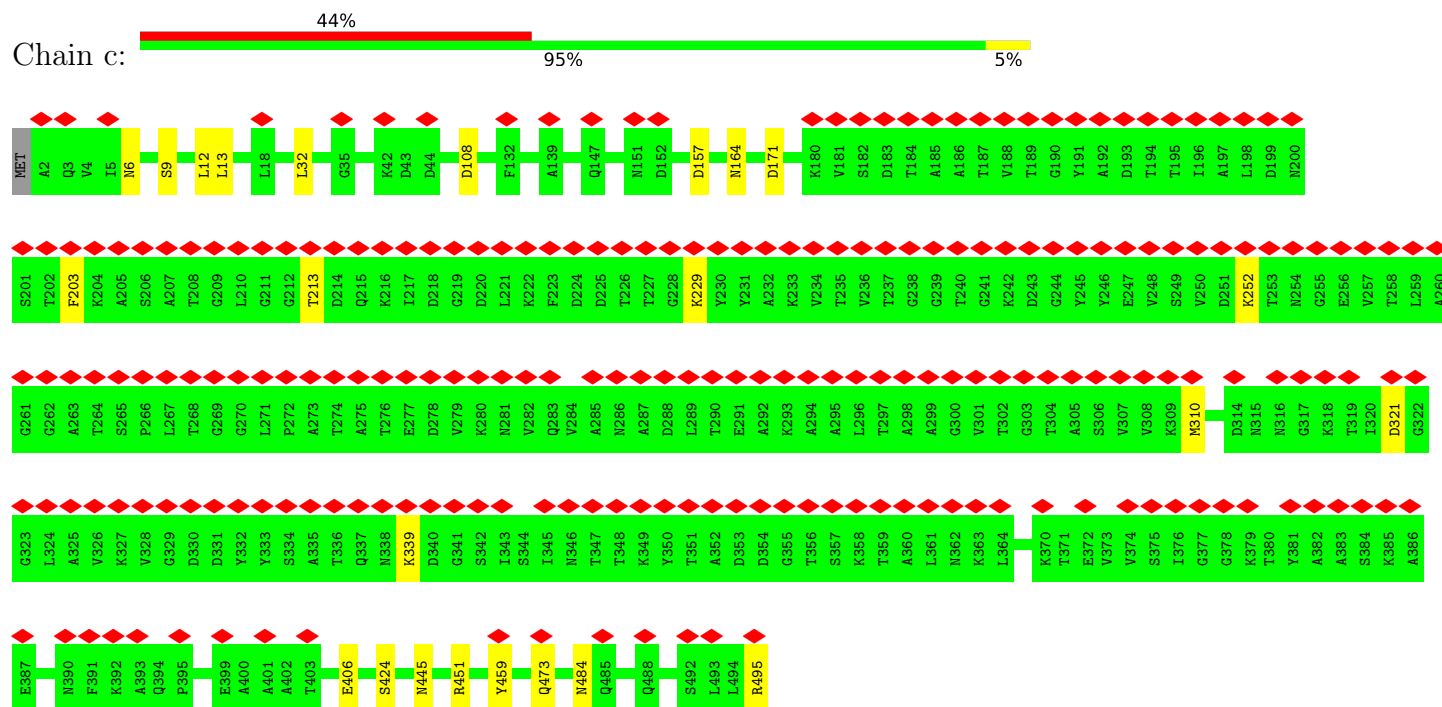
• Molecule 4: Flagellin



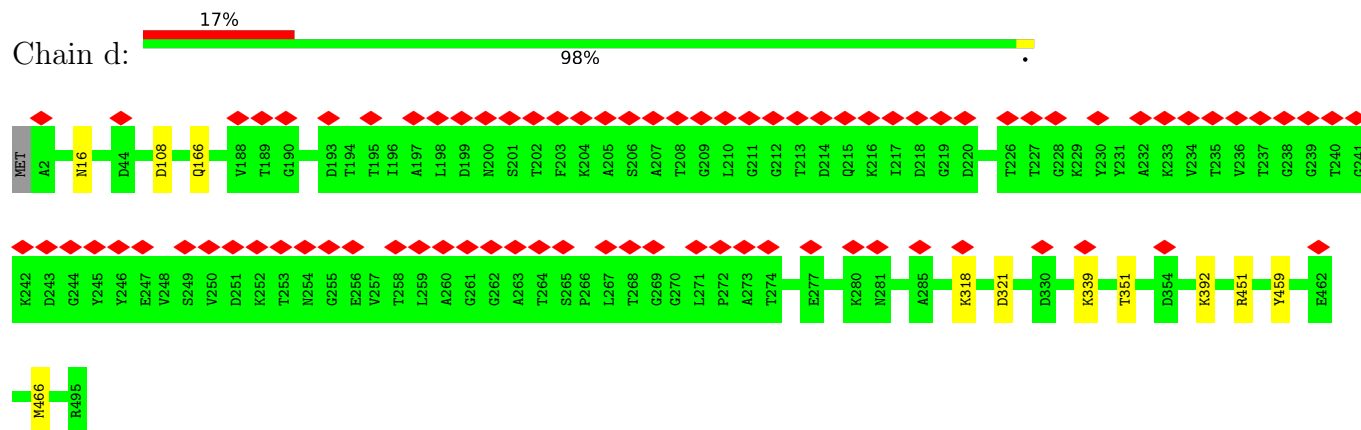
• Molecule 4: Flagellin



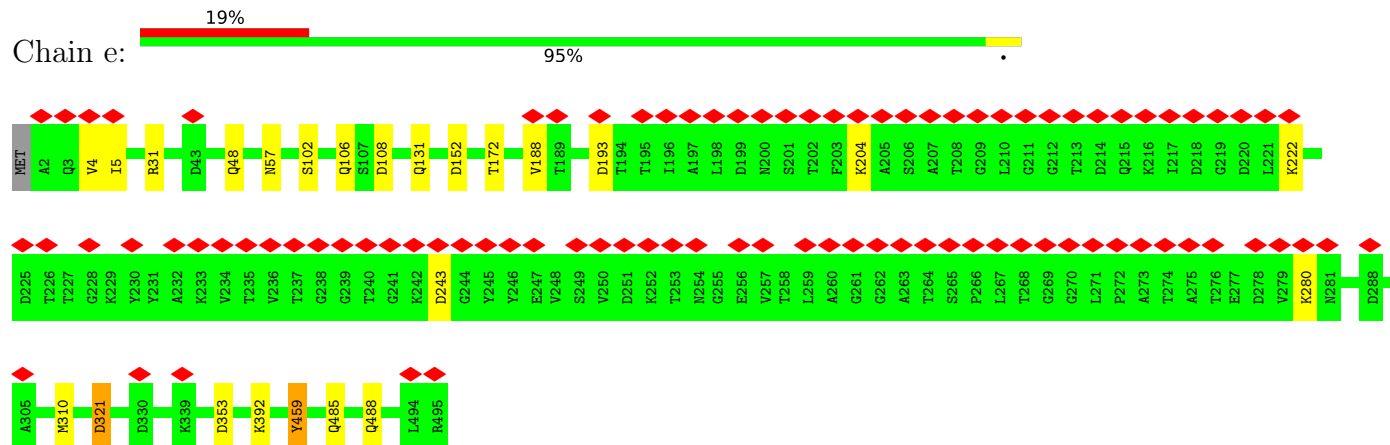
Chain c:



Chain d:

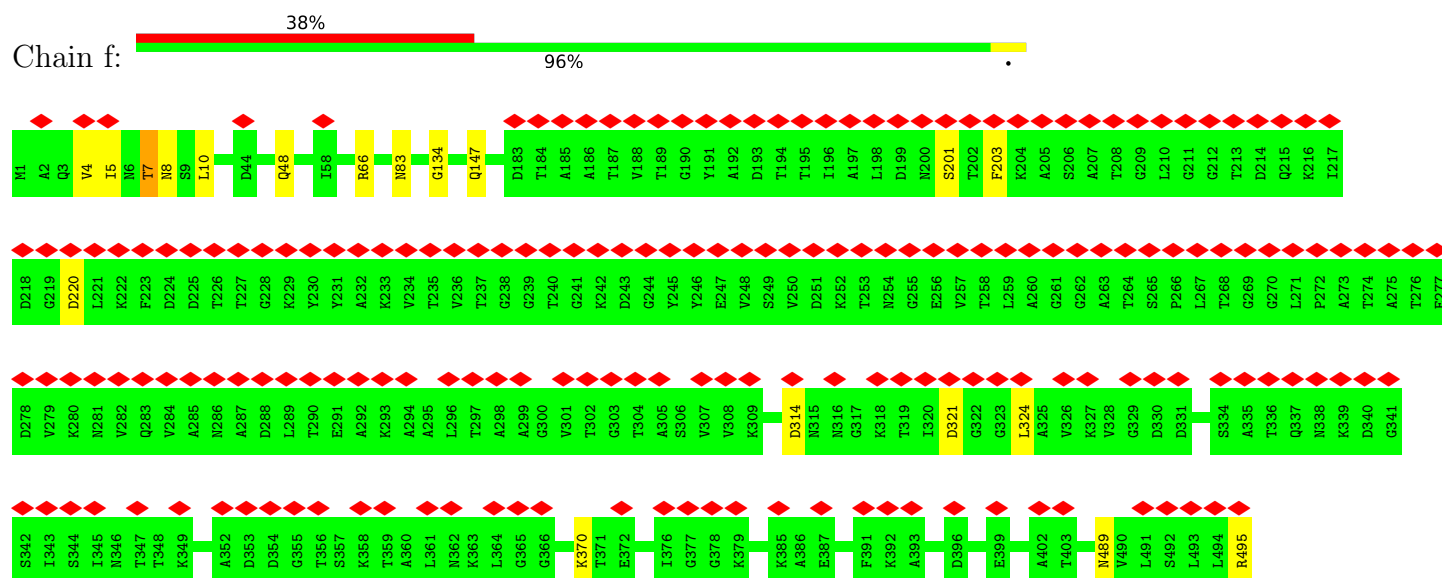


Chain e:



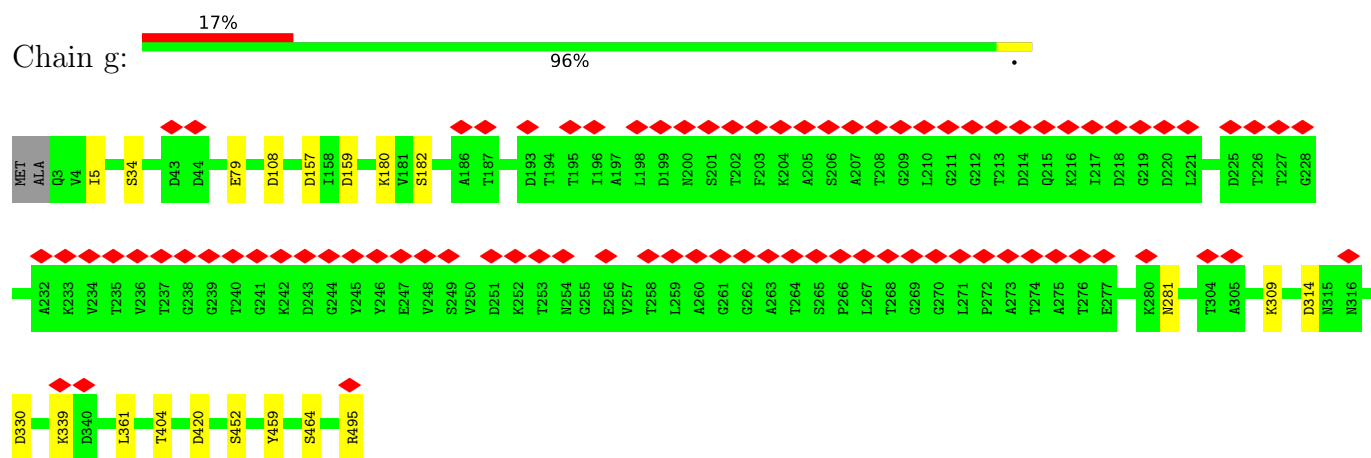
- Molecule 4: Flagellin

Chain f:



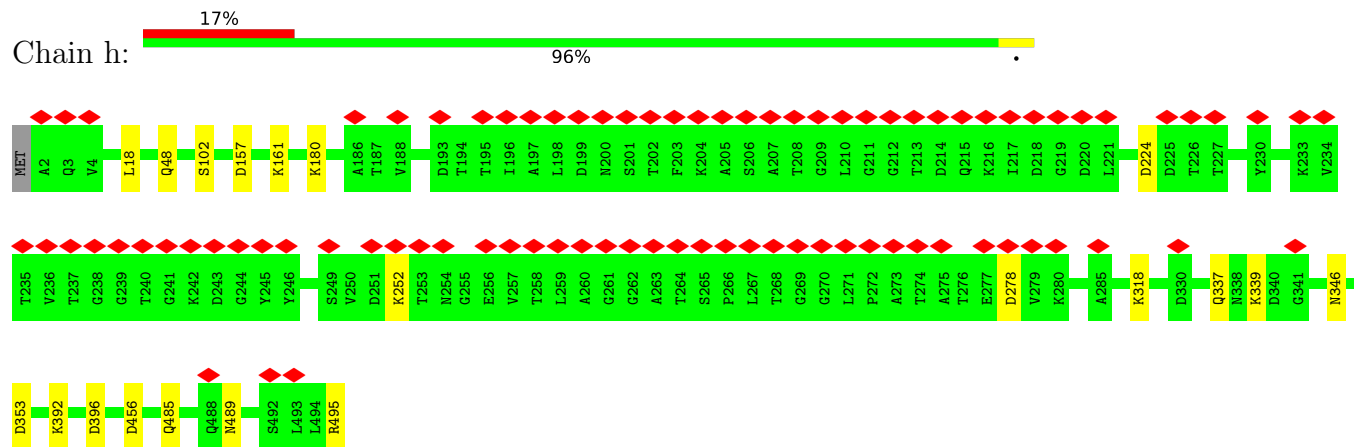
- Molecule 4: Flagellin

Chain g:

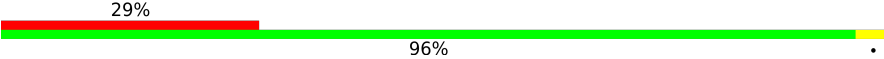


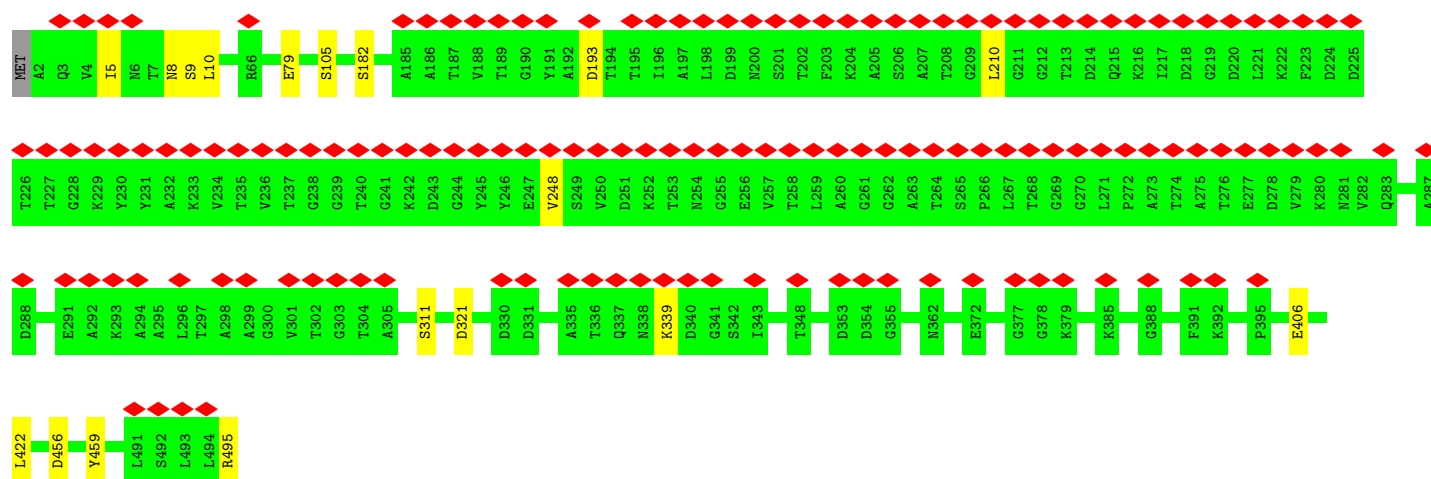
- Molecule 4: Flagellin

Chain h:



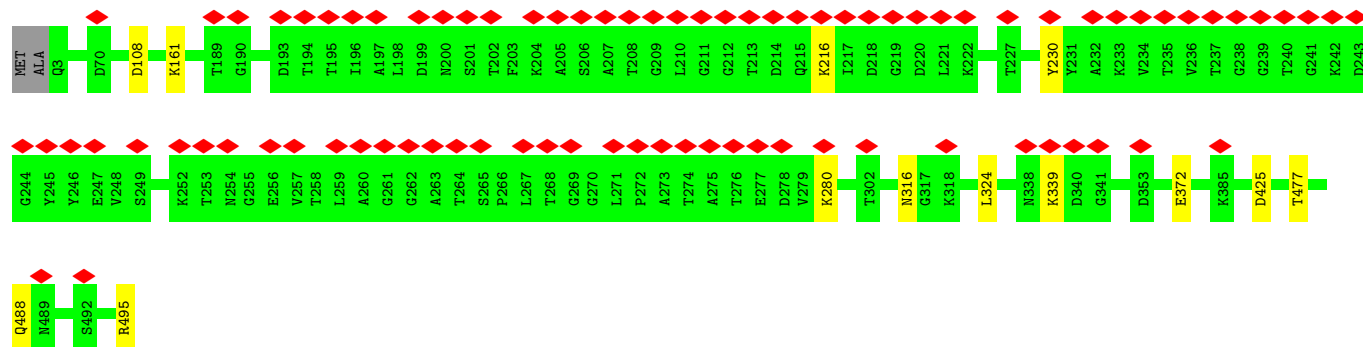
- Molecule 4: Flagellin

Chain i: 



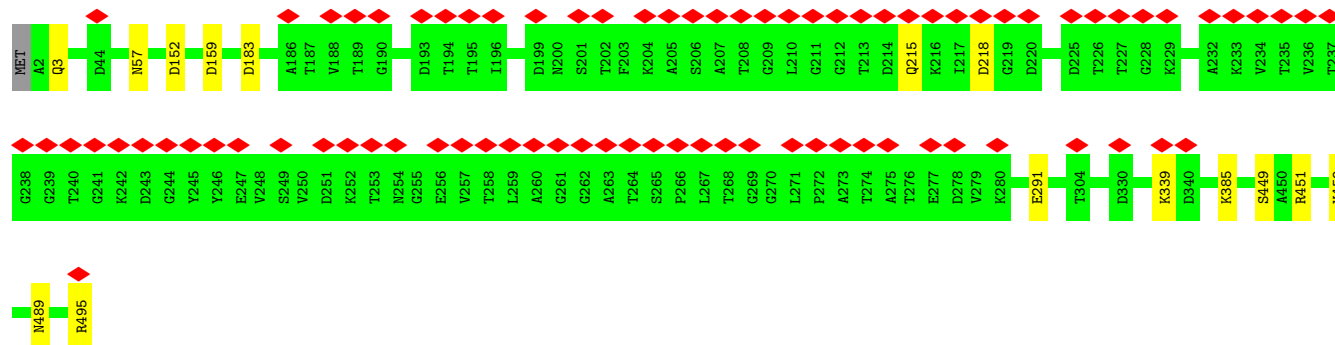
• Molecule 4: Flagellin

Chain j: 



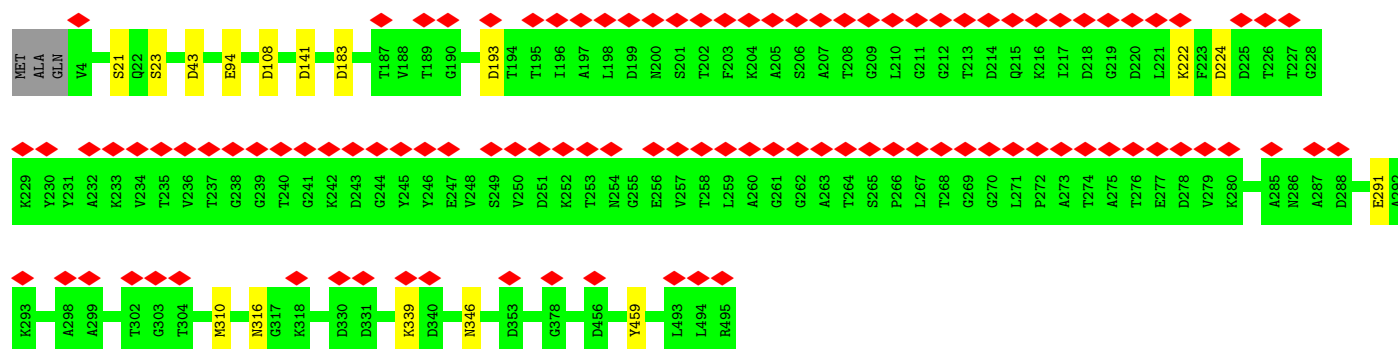
• Molecule 4: Flagellin

Chain k: 

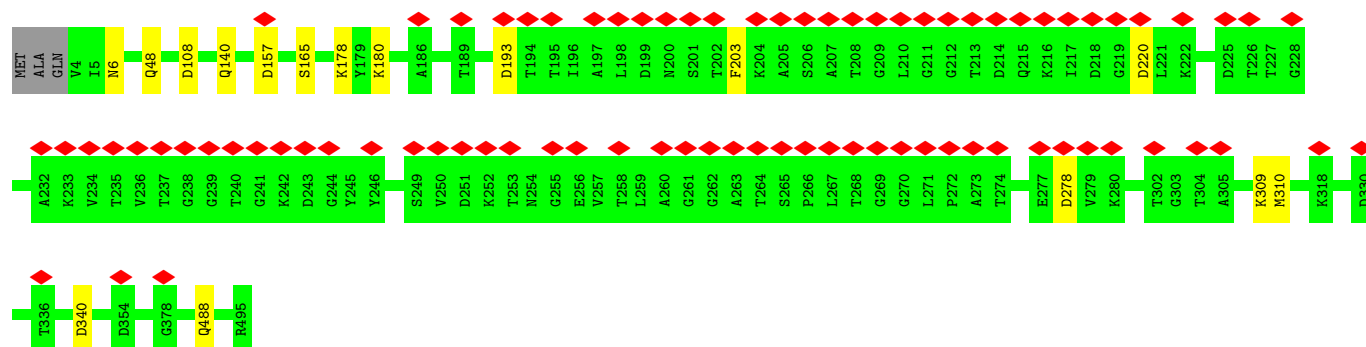


• Molecule 4: Flagellin

Chain l: 



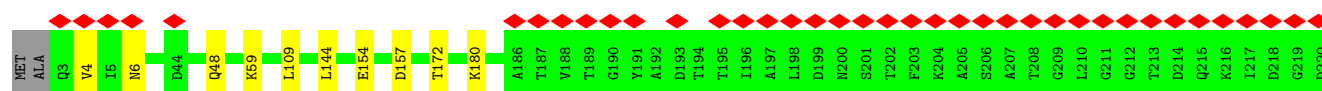
• Molecule 4: Flagellin

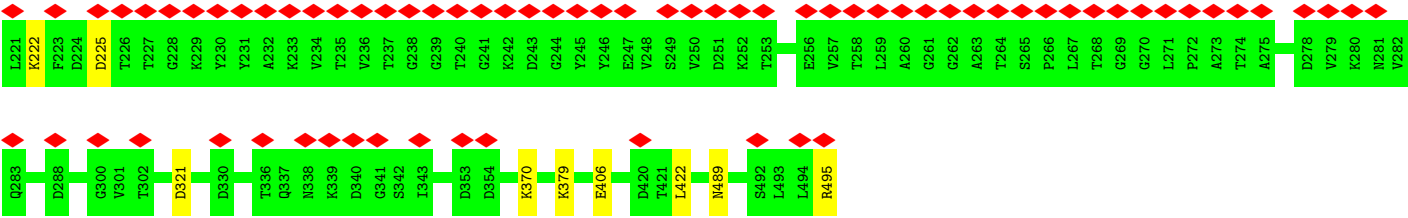


• Molecule 4: Flagellin



• Molecule 4: Flagellin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.721	Depositor
Minimum map value	-0.376	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	539.0, 539.0, 539.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.078, 1.078, 1.078	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	1	0.30	0/3011	0.53	0/4100
1	2	0.29	0/3011	0.53	0/4100
1	3	0.29	0/3011	0.53	0/4100
1	4	0.31	0/3011	0.56	1/4100 (0.0%)
1	5	0.31	0/3011	0.56	2/4100 (0.0%)
1	6	0.30	0/3011	0.54	0/4100
1	7	0.31	0/3011	0.60	1/4100 (0.0%)
1	8	0.29	0/3011	0.55	0/4100
1	9	0.27	0/3011	0.53	0/4100
1	w	0.34	0/3011	0.60	1/4100 (0.0%)
1	x	0.30	0/3011	0.54	0/4100
1	y	0.31	0/3011	0.53	0/4100
1	z	0.33	0/3011	0.57	1/4100 (0.0%)
2	A	0.32	0/4191	0.54	0/5692
2	B	0.32	0/4191	0.54	0/5692
2	C	0.32	1/4182 (0.0%)	0.57	0/5680
2	D	0.31	0/4191	0.53	1/5692 (0.0%)
2	E	0.33	0/4175	0.54	0/5671
2	F	0.29	0/4183	0.54	0/5682
2	G	0.31	0/4183	0.55	0/5682
2	H	0.33	0/4183	0.53	0/5682
2	I	0.32	0/4191	0.56	0/5692
2	J	0.32	1/4191 (0.0%)	0.57	2/5692 (0.0%)
2	K	0.32	0/4191	0.56	0/5692
3	L	0.31	0/2321	0.53	0/3142
3	M	0.33	0/2370	0.55	1/3208 (0.0%)
3	N	0.33	0/2383	0.53	0/3225
3	O	0.33	0/2356	0.54	0/3189
3	P	0.34	0/2327	0.53	0/3151
3	Q	0.33	0/2314	0.55	0/3132
3	R	0.32	0/2353	0.51	0/3185
3	S	0.33	0/2376	0.56	0/3215
3	T	0.33	0/2389	0.53	0/3233
3	U	0.33	0/2405	0.53	0/3254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	V	0.37	0/2397	0.58	0/3244
4	a	0.30	0/3638	0.51	0/4938
4	b	0.32	0/3633	0.53	0/4931
4	c	0.33	1/3638 (0.0%)	0.55	0/4938
4	d	0.30	0/3638	0.54	0/4938
4	e	0.30	0/3638	0.54	2/4938 (0.0%)
4	f	0.31	0/3646	0.55	2/4948 (0.0%)
4	g	0.29	0/3633	0.51	0/4931
4	h	0.30	0/3638	0.52	0/4938
4	i	0.32	0/3638	0.54	0/4938
4	j	0.29	0/3633	0.52	0/4931
4	k	0.29	0/3638	0.51	0/4938
4	l	0.30	0/3624	0.52	0/4919
4	m	0.31	0/3624	0.52	0/4919
4	n	0.31	0/3633	0.52	0/4931
4	o	0.29	0/3633	0.52	0/4931
All	All	0.31	3/165711 (0.0%)	0.54	14/225034 (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	6	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	516	VAL	CB-CG2	-5.82	1.40	1.52
4	c	6	ASN	C-N	-5.48	1.21	1.34
2	J	237	GLN	CD-NE2	-5.04	1.20	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	4	VAL	N-CA-C	-6.20	94.27	111.00
1	5	45	GLY	N-CA-C	-6.17	97.69	113.10
2	J	271	PRO	N-CA-C	6.06	127.86	112.10
1	4	159	ASN	N-CA-C	-5.95	94.93	111.00
1	w	144	MET	CG-SD-CE	5.67	109.28	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	6	168	THR	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	1	401/403 (100%)	377 (94%)	24 (6%)	0	100	100
1	2	401/403 (100%)	360 (90%)	41 (10%)	0	100	100
1	3	401/403 (100%)	365 (91%)	35 (9%)	1 (0%)	44	73
1	4	401/403 (100%)	356 (89%)	42 (10%)	3 (1%)	19	49
1	5	401/403 (100%)	354 (88%)	45 (11%)	2 (0%)	25	56
1	6	401/403 (100%)	364 (91%)	35 (9%)	2 (0%)	25	56
1	7	401/403 (100%)	355 (88%)	44 (11%)	2 (0%)	25	56
1	8	401/403 (100%)	372 (93%)	28 (7%)	1 (0%)	44	73
1	9	401/403 (100%)	371 (92%)	30 (8%)	0	100	100
1	w	401/403 (100%)	355 (88%)	45 (11%)	1 (0%)	44	73
1	x	401/403 (100%)	365 (91%)	32 (8%)	4 (1%)	13	40
1	y	401/403 (100%)	374 (93%)	27 (7%)	0	100	100
1	z	401/403 (100%)	361 (90%)	40 (10%)	0	100	100
2	A	550/553 (100%)	520 (94%)	30 (6%)	0	100	100
2	B	550/553 (100%)	514 (94%)	34 (6%)	2 (0%)	30	60
2	C	548/553 (99%)	512 (93%)	34 (6%)	2 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	550/553 (100%)	502 (91%)	47 (8%)	1 (0%)	44	73
2	E	548/553 (99%)	500 (91%)	46 (8%)	2 (0%)	30	60
2	F	549/553 (99%)	524 (95%)	25 (5%)	0	100	100
2	G	549/553 (99%)	502 (91%)	45 (8%)	2 (0%)	30	60
2	H	549/553 (99%)	509 (93%)	40 (7%)	0	100	100
2	I	550/553 (100%)	494 (90%)	52 (10%)	4 (1%)	19	49
2	J	550/553 (100%)	506 (92%)	43 (8%)	1 (0%)	44	73
2	K	550/553 (100%)	514 (94%)	34 (6%)	2 (0%)	30	60
3	L	304/317 (96%)	286 (94%)	17 (6%)	1 (0%)	37	66
3	M	310/317 (98%)	296 (96%)	14 (4%)	0	100	100
3	N	311/317 (98%)	291 (94%)	19 (6%)	1 (0%)	37	66
3	O	308/317 (97%)	295 (96%)	13 (4%)	0	100	100
3	P	305/317 (96%)	294 (96%)	10 (3%)	1 (0%)	37	66
3	Q	303/317 (96%)	286 (94%)	17 (6%)	0	100	100
3	R	308/317 (97%)	291 (94%)	17 (6%)	0	100	100
3	S	310/317 (98%)	298 (96%)	11 (4%)	1 (0%)	37	66
3	T	312/317 (98%)	304 (97%)	8 (3%)	0	100	100
3	U	314/317 (99%)	298 (95%)	16 (5%)	0	100	100
3	V	313/317 (99%)	295 (94%)	17 (5%)	1 (0%)	37	66
4	a	492/495 (99%)	475 (96%)	17 (4%)	0	100	100
4	b	491/495 (99%)	480 (98%)	11 (2%)	0	100	100
4	c	492/495 (99%)	475 (96%)	17 (4%)	0	100	100
4	d	492/495 (99%)	473 (96%)	19 (4%)	0	100	100
4	e	492/495 (99%)	480 (98%)	10 (2%)	2 (0%)	30	60
4	f	493/495 (100%)	478 (97%)	13 (3%)	2 (0%)	30	60
4	g	491/495 (99%)	475 (97%)	16 (3%)	0	100	100
4	h	492/495 (99%)	480 (98%)	12 (2%)	0	100	100
4	i	492/495 (99%)	478 (97%)	13 (3%)	1 (0%)	44	73
4	j	491/495 (99%)	472 (96%)	19 (4%)	0	100	100
4	k	492/495 (99%)	476 (97%)	16 (3%)	0	100	100
4	l	490/495 (99%)	469 (96%)	20 (4%)	1 (0%)	44	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	m	490/495 (99%)	480 (98%)	10 (2%)	0	100	100
4	n	491/495 (99%)	472 (96%)	19 (4%)	0	100	100
4	o	491/495 (99%)	472 (96%)	18 (4%)	1 (0%)	44	73
All	All	22026/22234 (99%)	20695 (94%)	1287 (6%)	44 (0%)	45	73

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	7	44	ALA
2	J	29	TYR
3	N	220	VAL
3	S	127	SER
4	e	5	ILE

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	1	323/323 (100%)	302 (94%)	21 (6%)	14	40
1	2	323/323 (100%)	302 (94%)	21 (6%)	14	40
1	3	323/323 (100%)	298 (92%)	25 (8%)	10	31
1	4	323/323 (100%)	293 (91%)	30 (9%)	7	23
1	5	323/323 (100%)	299 (93%)	24 (7%)	11	34
1	6	323/323 (100%)	304 (94%)	19 (6%)	16	45
1	7	323/323 (100%)	293 (91%)	30 (9%)	7	23
1	8	323/323 (100%)	298 (92%)	25 (8%)	10	31
1	9	323/323 (100%)	306 (95%)	17 (5%)	19	49
1	w	323/323 (100%)	297 (92%)	26 (8%)	10	30
1	x	323/323 (100%)	300 (93%)	23 (7%)	12	36
1	y	323/323 (100%)	305 (94%)	18 (6%)	17	47
1	z	323/323 (100%)	297 (92%)	26 (8%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	452/453 (100%)	416 (92%)	36 (8%)	10	30
2	B	452/453 (100%)	410 (91%)	42 (9%)	7	23
2	C	450/453 (99%)	408 (91%)	42 (9%)	7	23
2	D	452/453 (100%)	419 (93%)	33 (7%)	11	34
2	E	450/453 (99%)	415 (92%)	35 (8%)	10	31
2	F	451/453 (100%)	415 (92%)	36 (8%)	10	30
2	G	451/453 (100%)	422 (94%)	29 (6%)	14	41
2	H	451/453 (100%)	425 (94%)	26 (6%)	17	46
2	I	452/453 (100%)	412 (91%)	40 (9%)	8	26
2	J	452/453 (100%)	409 (90%)	43 (10%)	7	22
2	K	452/453 (100%)	412 (91%)	40 (9%)	8	26
3	L	250/261 (96%)	233 (93%)	17 (7%)	13	38
3	M	256/261 (98%)	227 (89%)	29 (11%)	4	15
3	N	257/261 (98%)	238 (93%)	19 (7%)	11	34
3	O	254/261 (97%)	226 (89%)	28 (11%)	5	16
3	P	251/261 (96%)	242 (96%)	9 (4%)	30	65
3	Q	249/261 (95%)	229 (92%)	20 (8%)	10	30
3	R	254/261 (97%)	233 (92%)	21 (8%)	9	28
3	S	256/261 (98%)	235 (92%)	21 (8%)	9	29
3	T	258/261 (99%)	241 (93%)	17 (7%)	14	39
3	U	260/261 (100%)	240 (92%)	20 (8%)	10	31
3	V	259/261 (99%)	231 (89%)	28 (11%)	5	17
4	a	390/391 (100%)	377 (97%)	13 (3%)	33	68
4	b	390/391 (100%)	365 (94%)	25 (6%)	14	41
4	c	390/391 (100%)	367 (94%)	23 (6%)	16	45
4	d	390/391 (100%)	379 (97%)	11 (3%)	38	73
4	e	390/391 (100%)	368 (94%)	22 (6%)	17	47
4	f	391/391 (100%)	375 (96%)	16 (4%)	26	60
4	g	390/391 (100%)	370 (95%)	20 (5%)	20	51
4	h	390/391 (100%)	370 (95%)	20 (5%)	20	51
4	i	390/391 (100%)	373 (96%)	17 (4%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	390/391 (100%)	377 (97%)	13 (3%)	33	68
4	k	390/391 (100%)	375 (96%)	15 (4%)	28	63
4	l	389/391 (100%)	374 (96%)	15 (4%)	27	62
4	m	389/391 (100%)	373 (96%)	16 (4%)	26	60
4	n	390/391 (100%)	378 (97%)	12 (3%)	35	70
4	o	390/391 (100%)	372 (95%)	18 (5%)	23	55
All	All	17817/17918 (99%)	16625 (93%)	1192 (7%)	16	39

5 of 1192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	e	204	LYS
1	x	369	SER
4	g	5	ILE
4	e	193	ASP
4	l	94	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	277	ASN
3	U	11	GLN
1	y	23	ASN
3	P	274	GLN
3	S	11	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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.

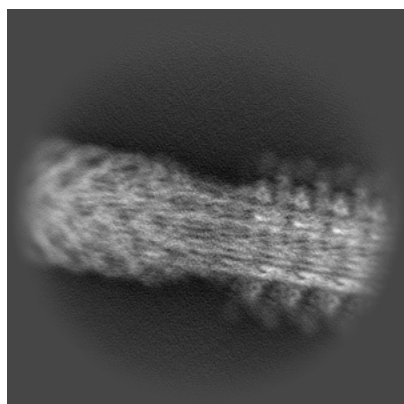
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51493. These allow visual inspection of the internal detail of the map and identification of artifacts.

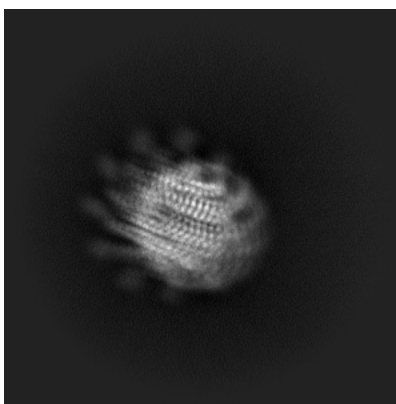
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

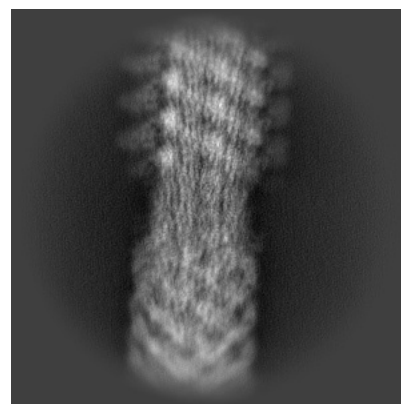
6.1.1 Primary map



X

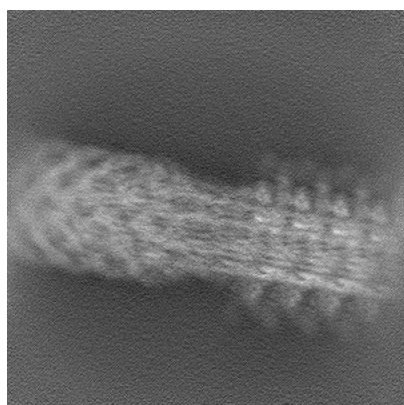


Y

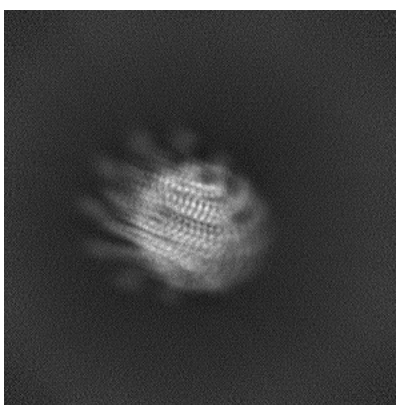


Z

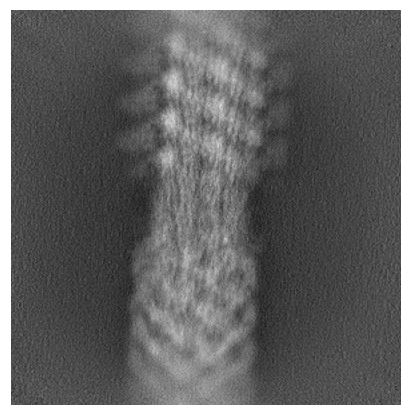
6.1.2 Raw map



X



Y

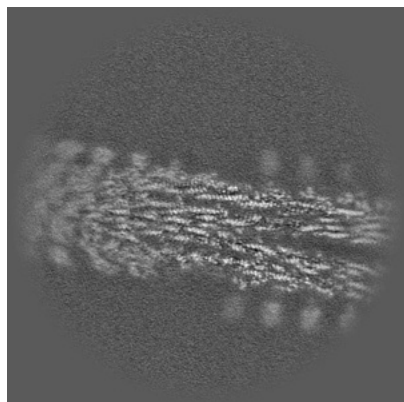


Z

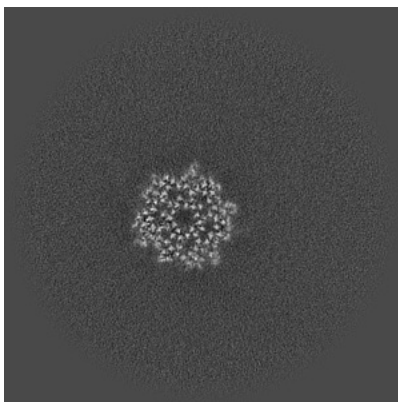
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

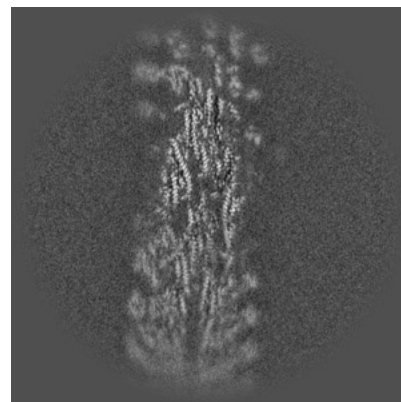
6.2.1 Primary map



X Index: 250

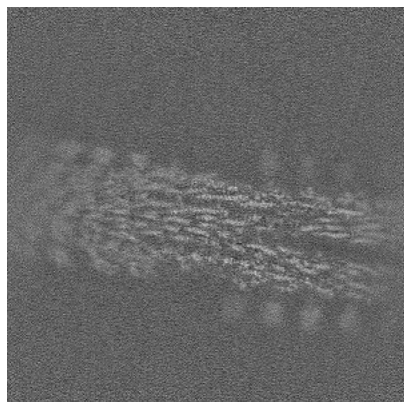


Y Index: 250

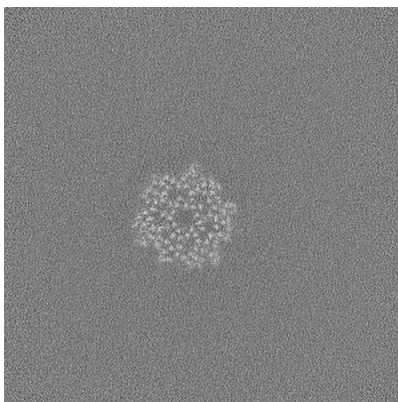


Z Index: 250

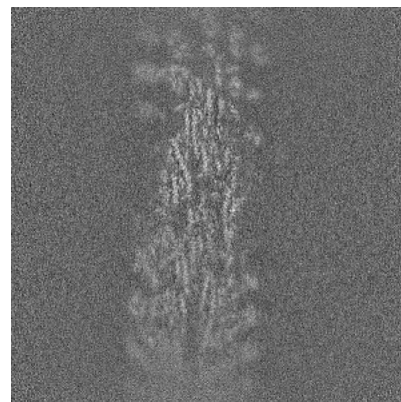
6.2.2 Raw map



X Index: 250



Y Index: 250

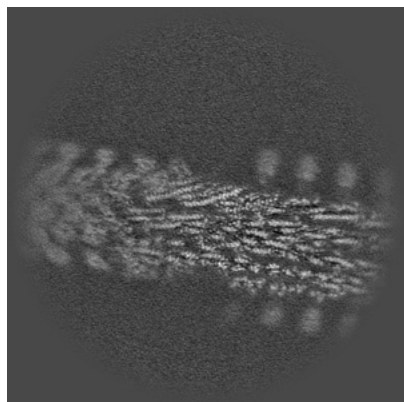


Z Index: 250

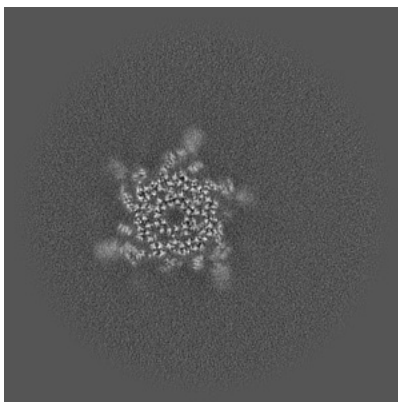
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

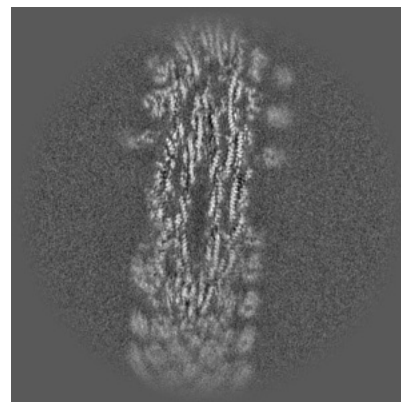
6.3.1 Primary map



X Index: 257

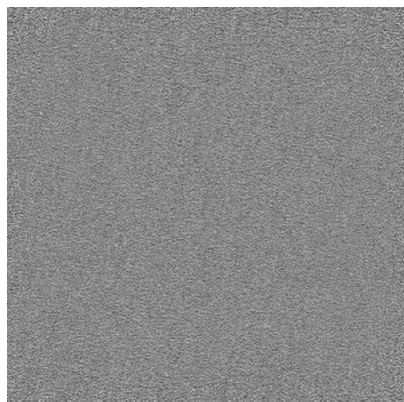


Y Index: 314

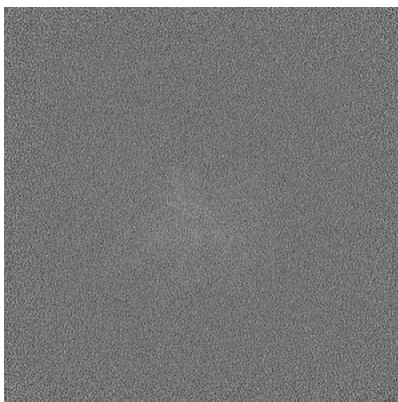


Z Index: 227

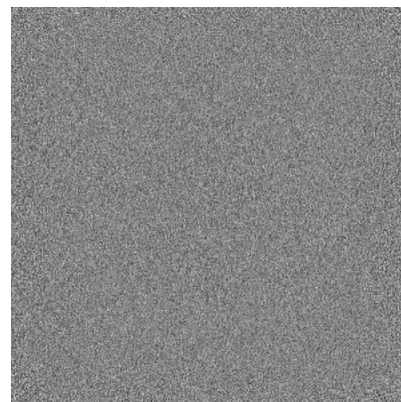
6.3.2 Raw map



X Index: 0



Y Index: 0

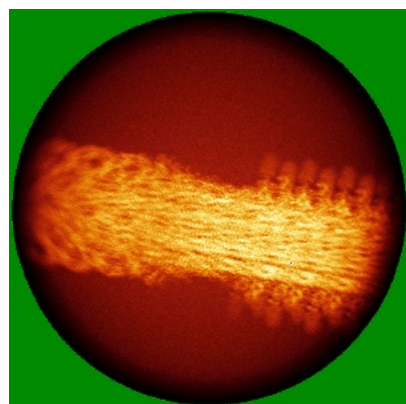


Z Index: 0

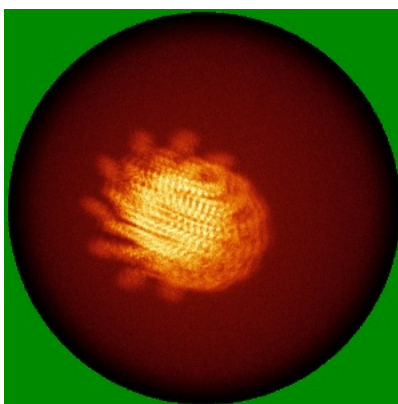
The images above show the largest variance slices of the map in three orthogonal directions.

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

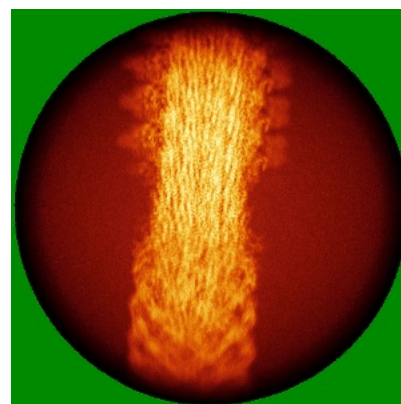
6.4.1 Primary map



X

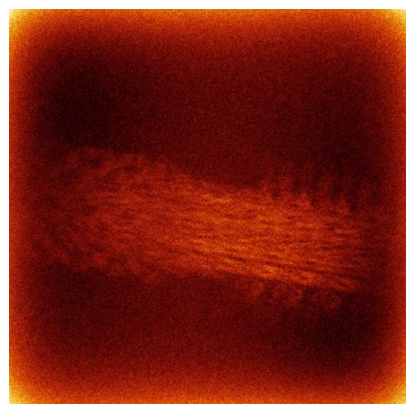


Y

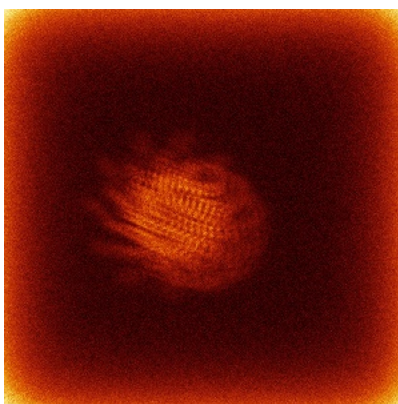


Z

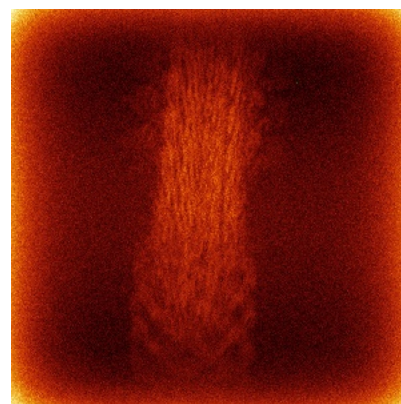
6.4.2 Raw map



X



Y

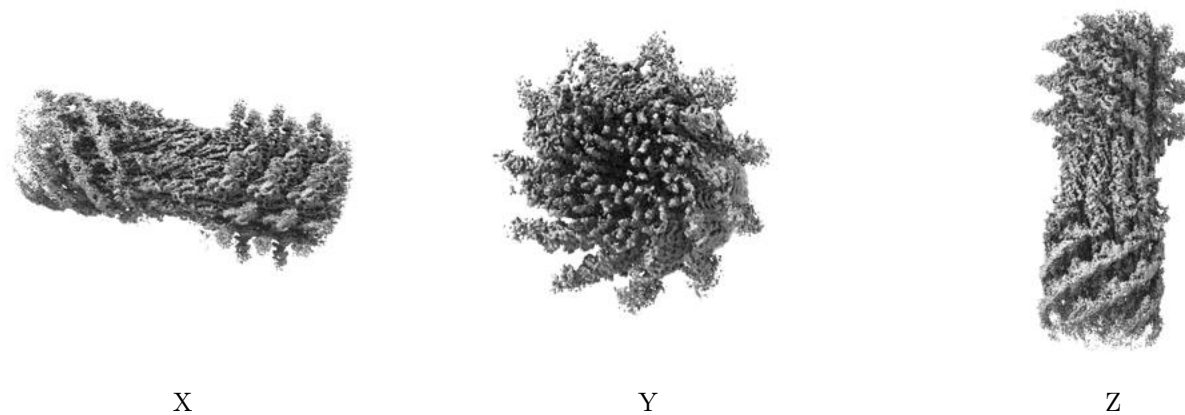


Z

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.

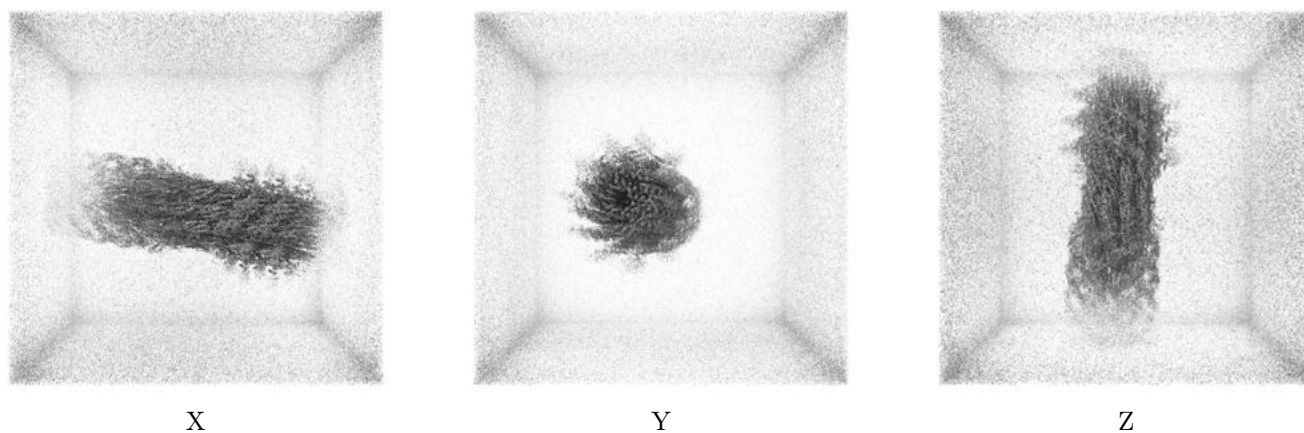
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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



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.

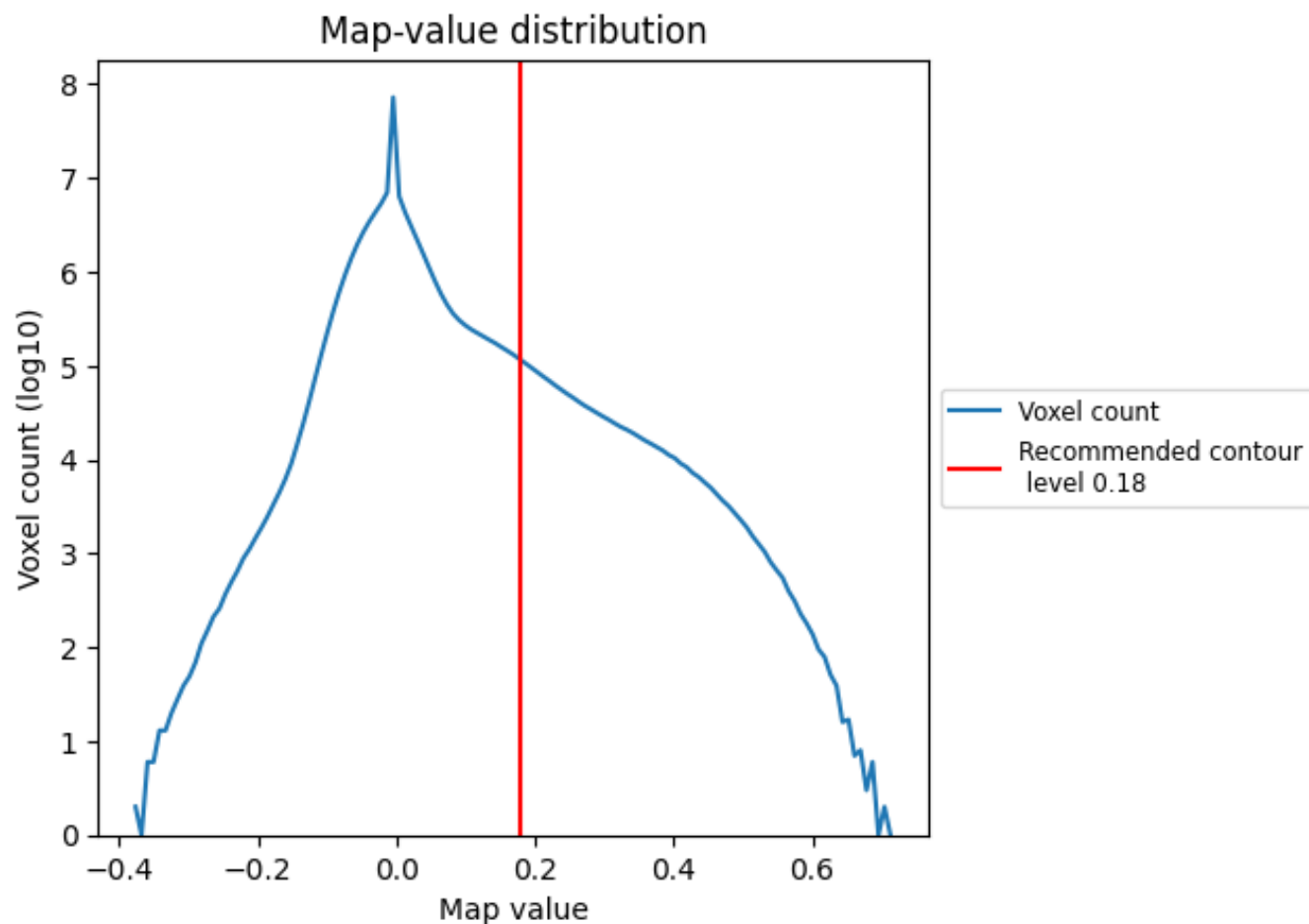
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

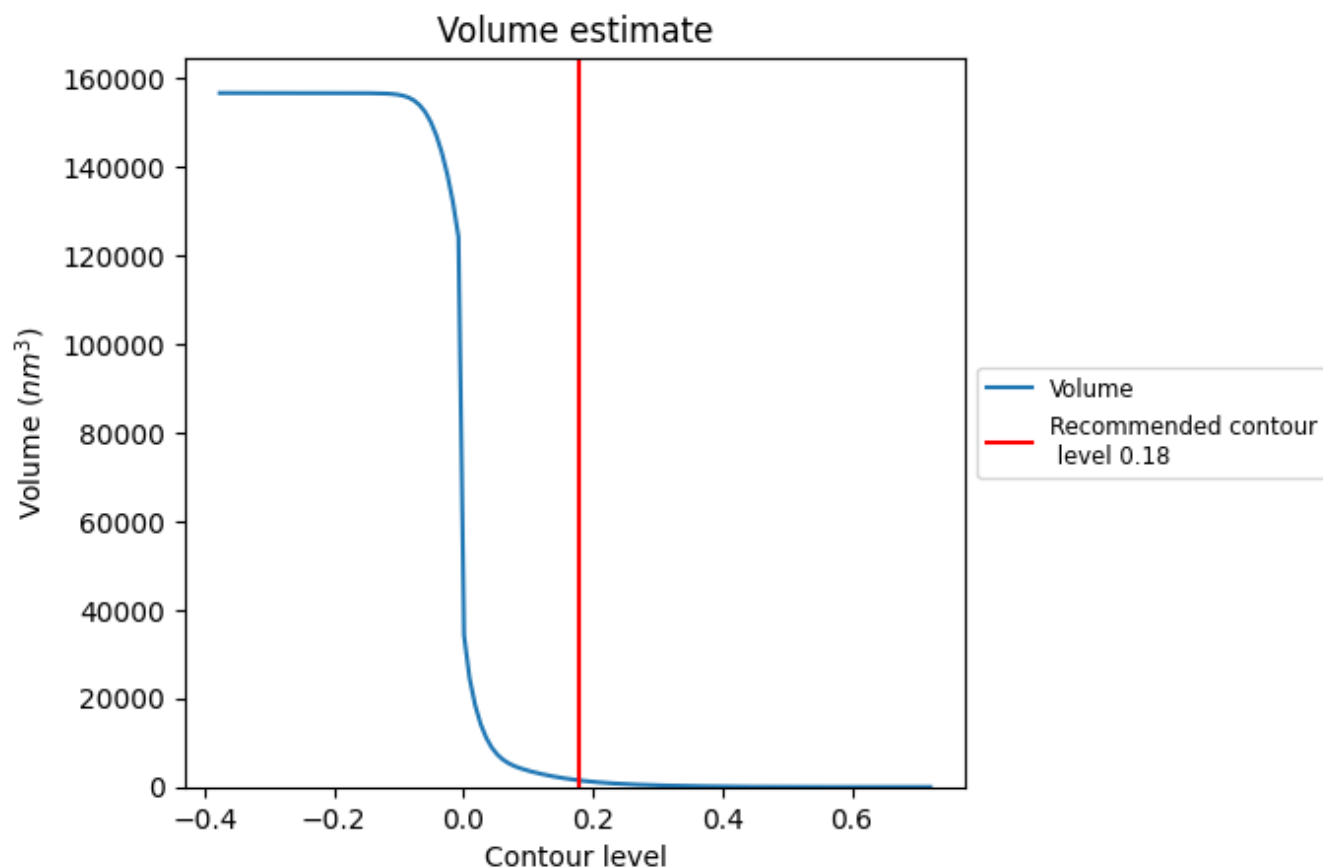
This section contains the results of statistical analysis of the map.

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.

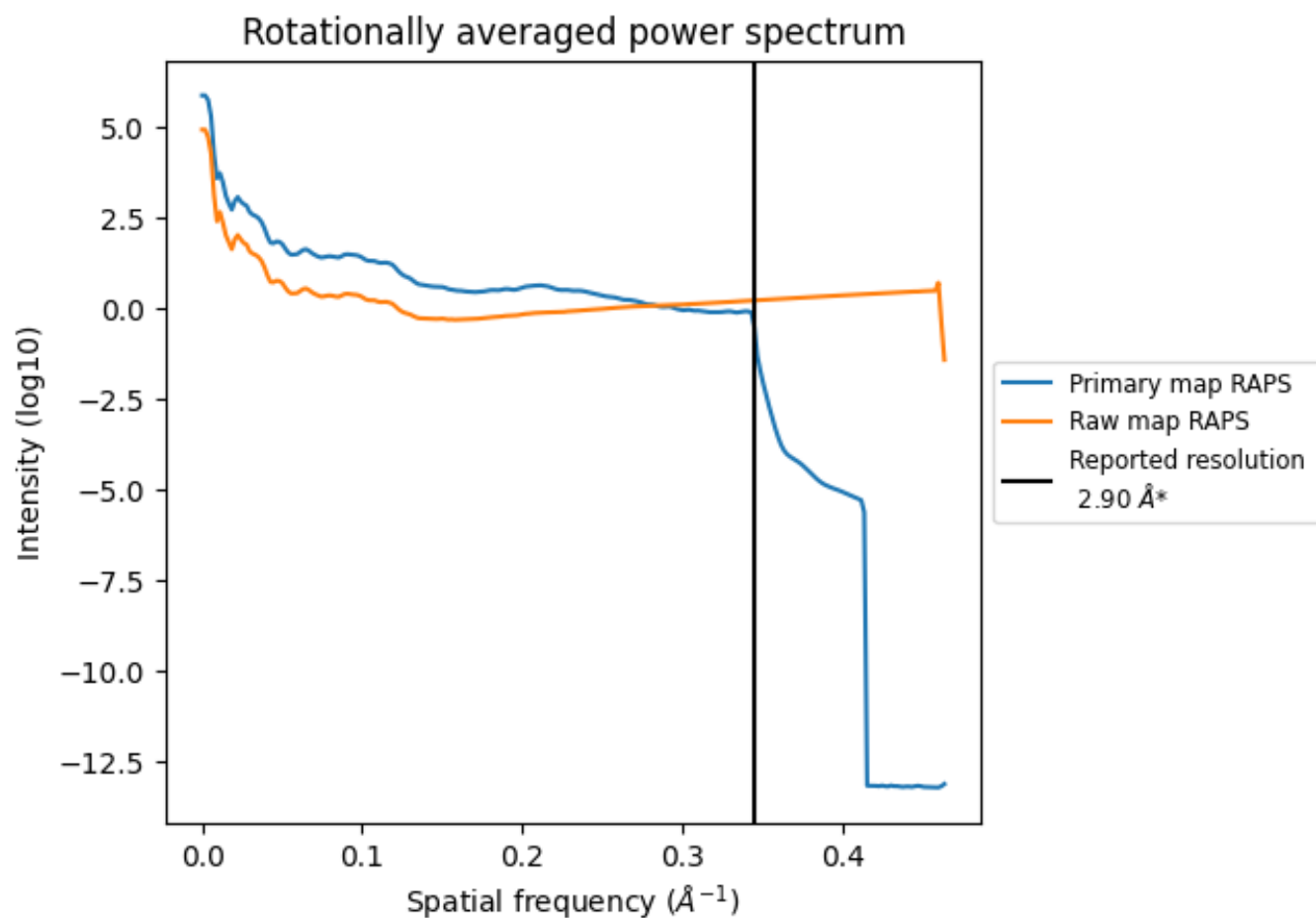
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1471 nm³; this corresponds to an approximate mass of 1329 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 ⓘ

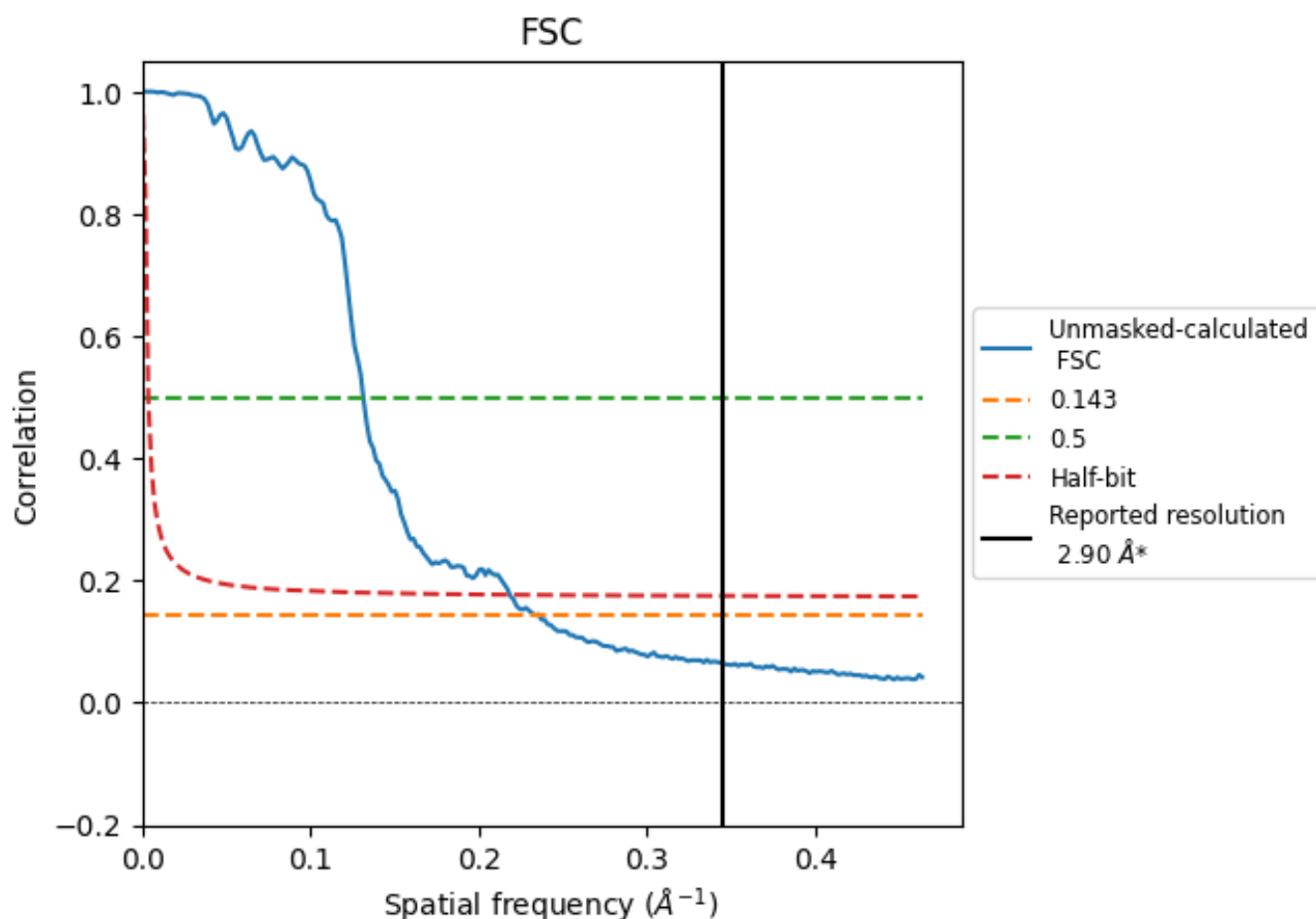


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

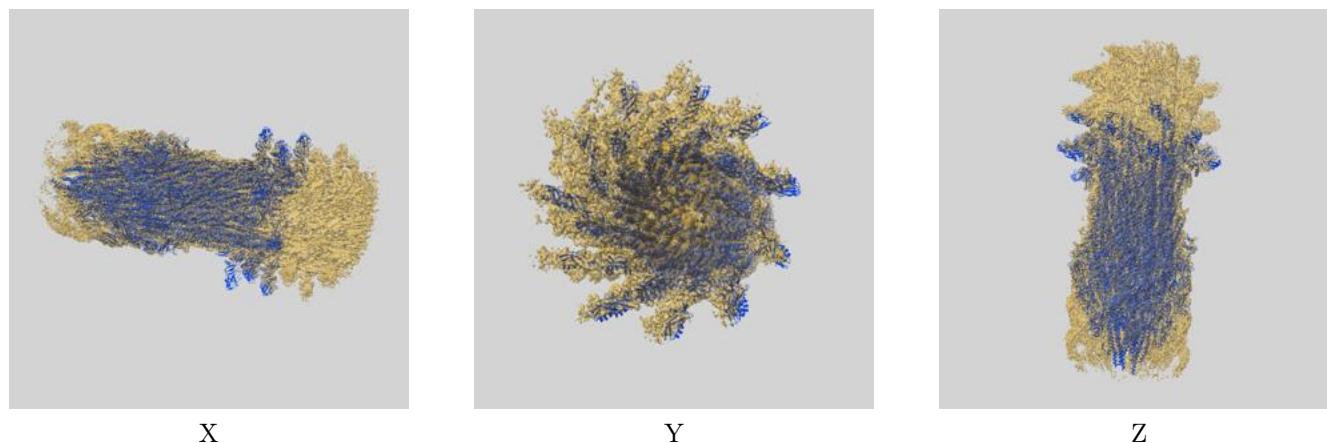
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	7.60	4.57

*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 4.28 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

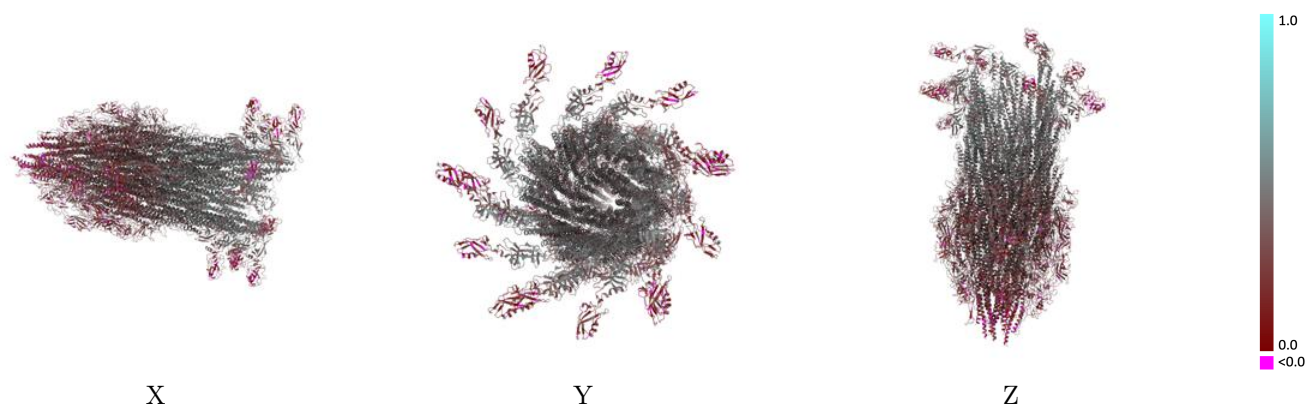
This section contains information regarding the fit between EMDB map EMD-51493 and PDB model 9GO6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



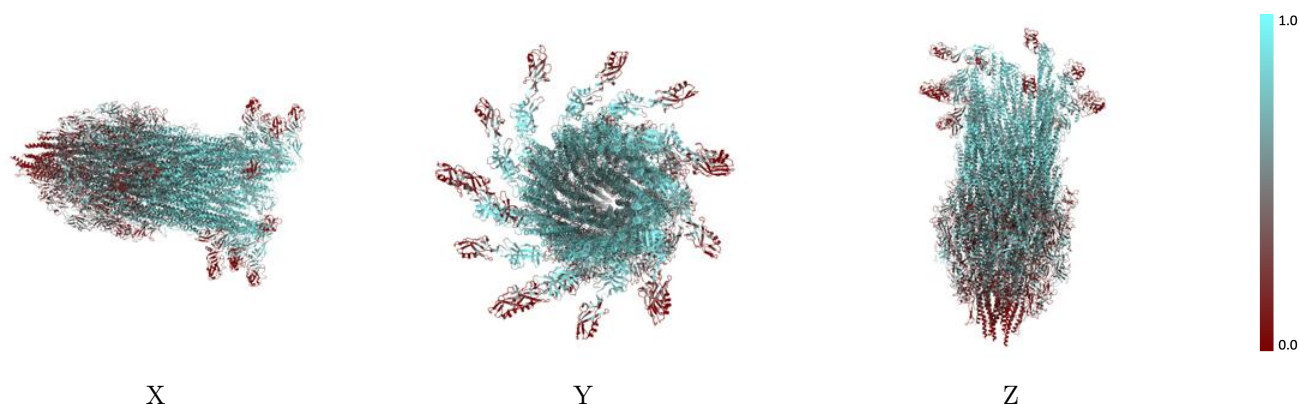
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



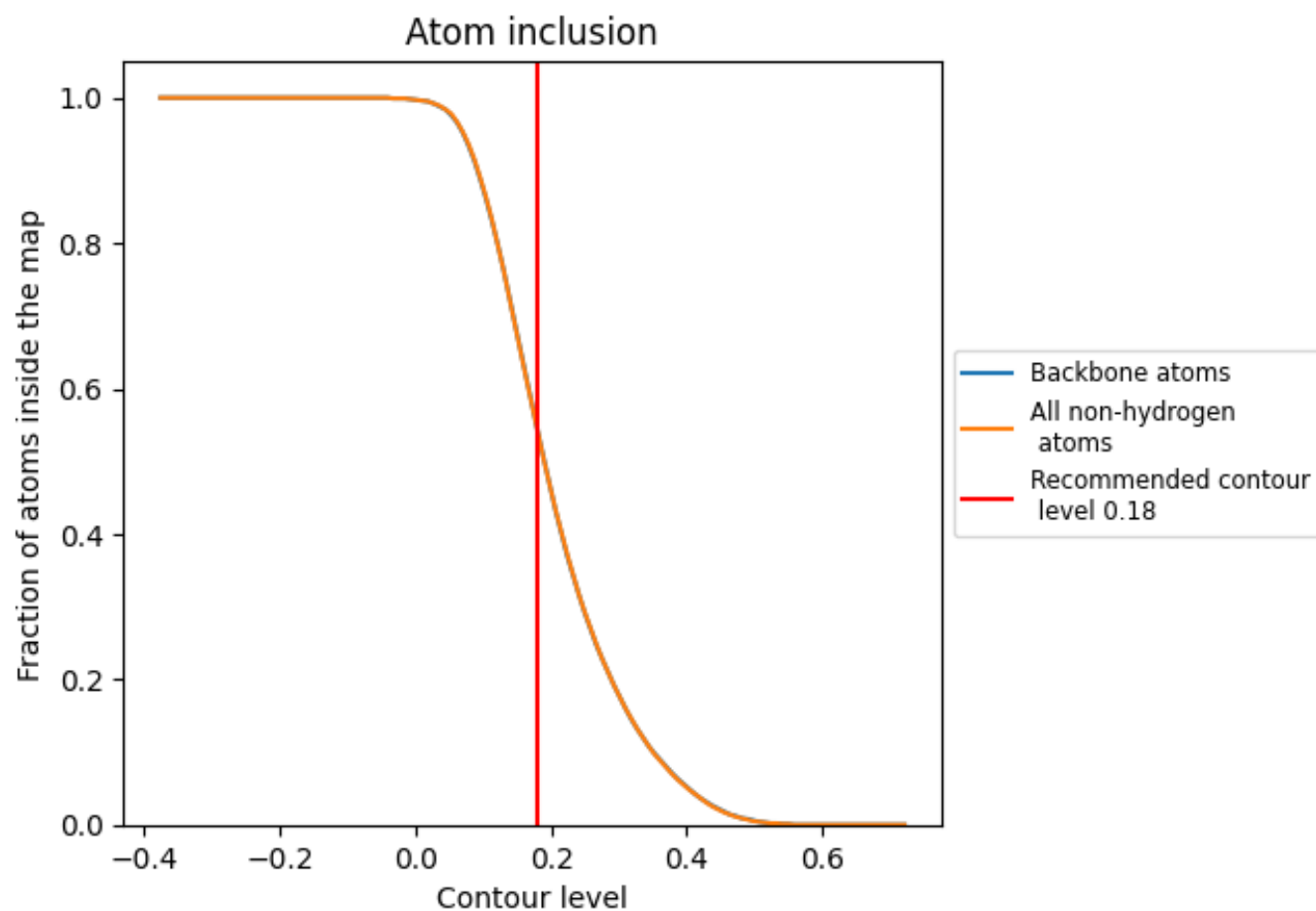
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5420	 0.3490
1	 0.4310	 0.3030
2	 0.3670	 0.2460
3	 0.4200	 0.2880
4	 0.3200	 0.2300
5	 0.3850	 0.2650
6	 0.3070	 0.2320
7	 0.3430	 0.2750
8	 0.3900	 0.2620
9	 0.2720	 0.1930
A	 0.3700	 0.2830
B	 0.5380	 0.3250
C	 0.4460	 0.3070
D	 0.5890	 0.3610
E	 0.5320	 0.3380
F	 0.5780	 0.3610
G	 0.5480	 0.3300
H	 0.5130	 0.3390
I	 0.5090	 0.2960
J	 0.5010	 0.3390
K	 0.5500	 0.3070
L	 0.7320	 0.4140
M	 0.6990	 0.4170
N	 0.7400	 0.4280
O	 0.6230	 0.3320
P	 0.7510	 0.4370
Q	 0.6500	 0.3850
R	 0.7420	 0.4440
S	 0.6870	 0.3980
T	 0.7360	 0.4380
U	 0.7080	 0.4060
V	 0.6950	 0.4200
a	 0.6620	 0.4100
b	 0.6530	 0.4190
c	 0.4440	 0.3590



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Chain	Atom inclusion	Q-score
d	 0.6640	 0.4080
e	 0.6630	 0.4160
f	 0.4980	 0.3840
g	 0.6610	 0.4060
h	 0.6550	 0.4180
i	 0.5580	 0.3960
j	 0.6710	 0.4060
k	 0.6730	 0.4130
l	 0.6180	 0.3960
m	 0.6680	 0.4020
n	 0.6710	 0.4120
o	 0.6350	 0.4050
w	 0.3450	 0.2620
x	 0.3550	 0.2420
y	 0.3890	 0.3100
z	 0.3660	 0.2350