



wwPDB EM Validation Summary Report ⓘ

Apr 3, 2025 – 02:19 pm BST

PDB ID : 9GNZ / pdb_00009gnz
EMDB ID : EMD-51486
Title : Salmonella cap-filament complex
Authors : Qin, K.; Eikenkel, R.; Erhardt, M.; Bergeron, J.R.C.
Deposited on : 2024-09-04
Resolution : 3.70 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

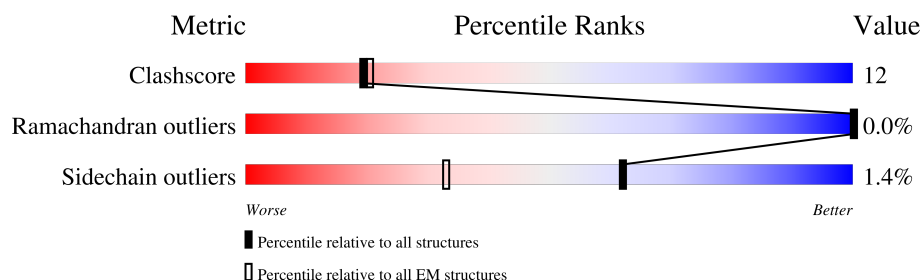
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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	A	495	<div> <div>26%</div> <div>82%</div> <div>17%</div> <div>..</div> </div>
1	B	495	<div> <div>24%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	C	495	<div> <div>24%</div> <div>78%</div> <div>21%</div> <div>..</div> </div>
1	D	495	<div> <div>27%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
1	E	495	<div> <div>16%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
1	F	495	<div> <div>23%</div> <div>75%</div> <div>24%</div> <div></div> </div>
1	G	495	<div> <div>24%</div> <div>80%</div> <div>19%</div> <div>..</div> </div>
1	H	495	<div> <div>25%</div> <div>83%</div> <div>16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	495	
1	J	495	
1	K	495	
1	L	495	
1	M	495	
1	N	495	
1	O	495	
1	P	495	
1	Q	495	
2	R	467	
2	S	467	
2	T	467	
2	U	467	
2	V	467	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 155883 atoms, of which 77572 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Flagellin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	492	Total	C	H	N	O	S	0	0
			7154	2180	3556	635	781	2		
1	B	493	Total	C	H	N	O	S	0	0
			7159	2183	3556	636	782	2		
1	C	492	Total	C	H	N	O	S	0	0
			7137	2181	3537	637	780	2		
1	D	493	Total	C	H	N	O	S	0	0
			7153	2183	3550	636	782	2		
1	E	492	Total	C	H	N	O	S	0	0
			7148	2181	3548	637	780	2		
1	F	493	Total	C	H	N	O	S	0	0
			7154	2186	3545	639	782	2		
1	G	491	Total	C	H	N	O	S	0	0
			7137	2175	3548	633	779	2		
1	H	492	Total	C	H	N	O	S	0	0
			7148	2181	3548	637	780	2		
1	I	491	Total	C	H	N	O	S	0	0
			7137	2175	3548	633	779	2		
1	J	491	Total	C	H	N	O	S	0	0
			7137	2175	3548	633	779	2		
1	K	491	Total	C	H	N	O	S	0	0
			7137	2175	3548	633	779	2		
1	L	491	Total	C	H	N	O	S	0	0
			7137	2175	3548	633	779	2		
1	M	492	Total	C	H	N	O	S	0	0
			7137	2180	3539	635	781	2		
1	N	489	Total	C	H	N	O	S	0	0
			7025	2166	3448	633	776	2		
1	O	493	Total	C	H	N	O	S	0	0
			7137	2186	3528	639	782	2		
1	P	491	Total	C	H	N	O	S	0	0
			7137	2175	3548	633	779	2		
1	Q	490	Total	C	H	N	O	S	0	0
			7110	2170	3528	632	778	2		

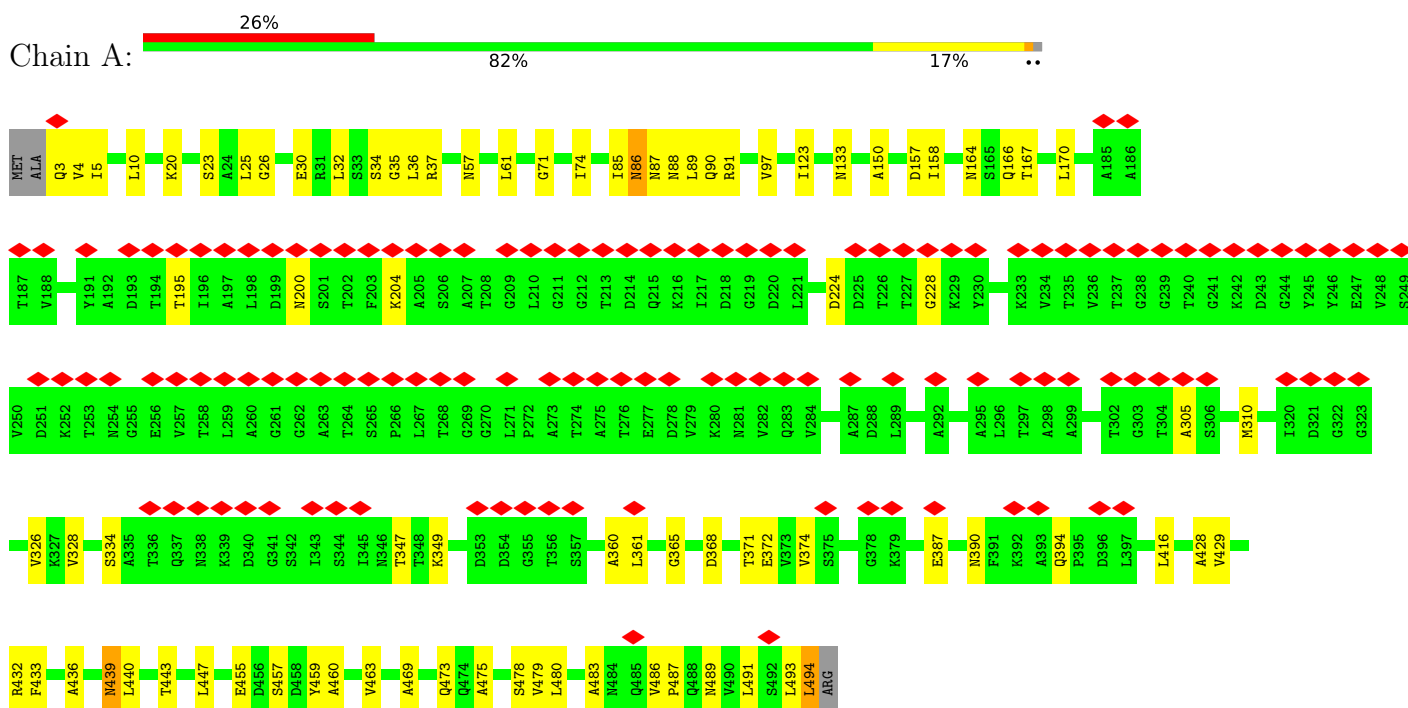
- Molecule 2 is a protein called Flagellar hook-associated protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	R	463	Total	C	H	N	O	S	0	0
			6961	2132	3498	584	740	7		
2	S	467	Total	C	H	N	O	S	0	0
			7008	2149	3516	589	746	8		
2	T	463	Total	C	H	N	O	S	0	0
			6972	2132	3509	584	740	7		
2	U	442	Total	C	H	N	O	S	0	0
			6681	2046	3364	560	705	6		
2	V	463	Total	C	H	N	O	S	0	0
			6977	2132	3514	584	740	7		

3 Residue-property plots

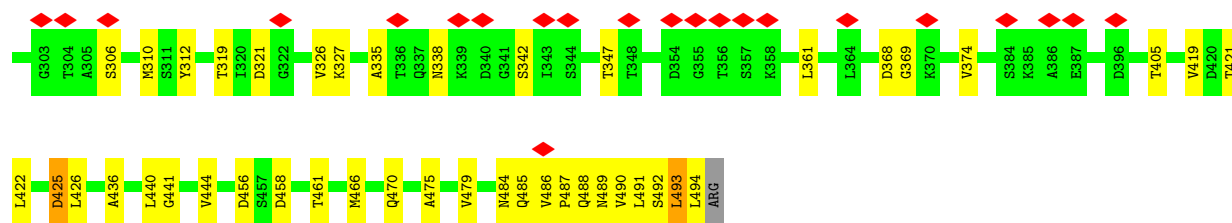
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

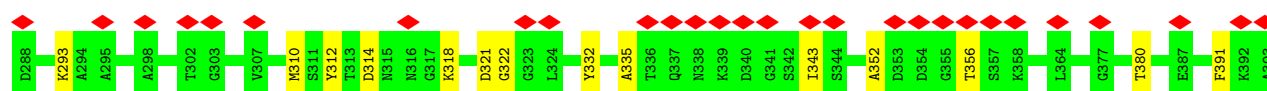
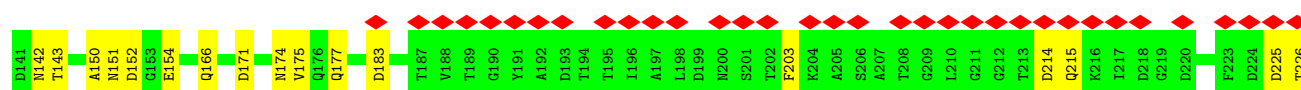
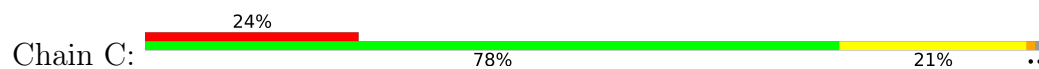


• Molecule 1: Flagellin

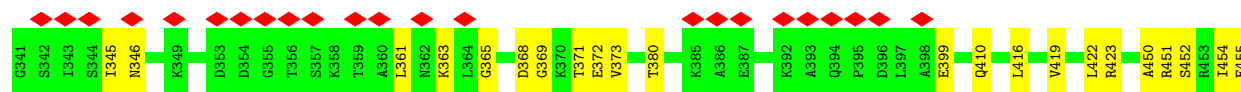
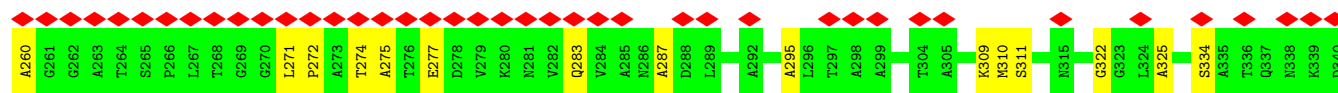
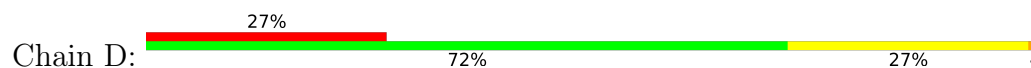


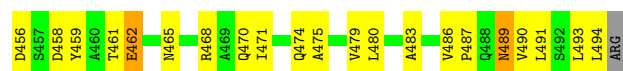


• Molecule 1: Flagellin

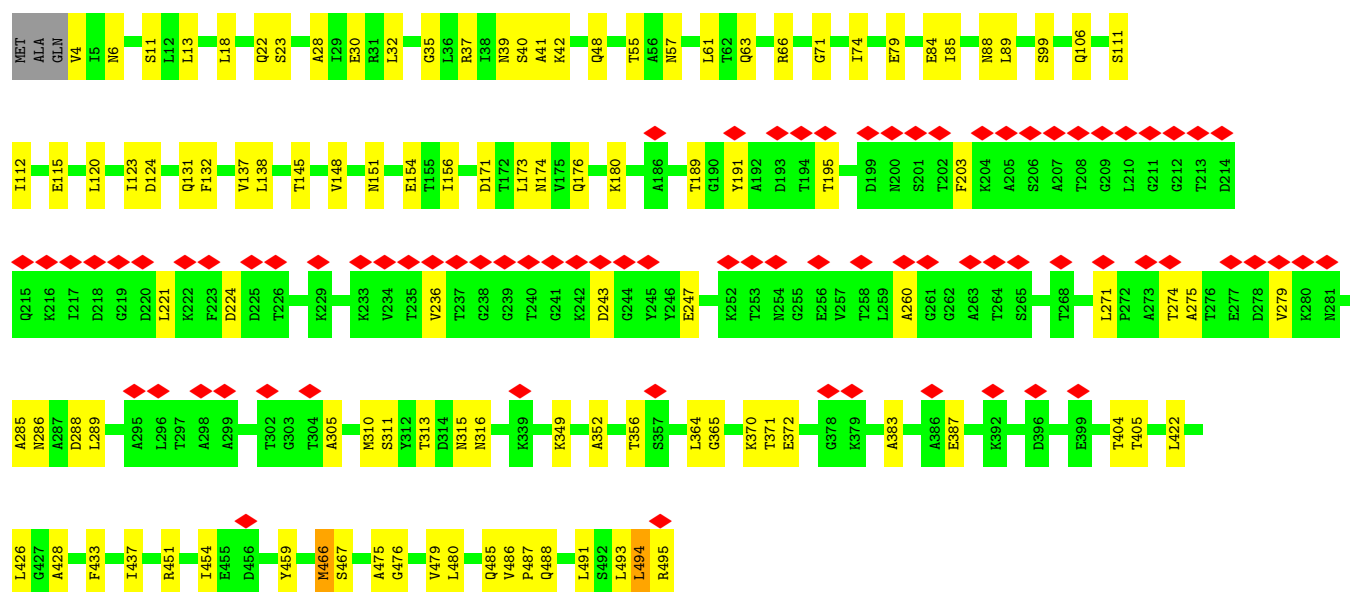
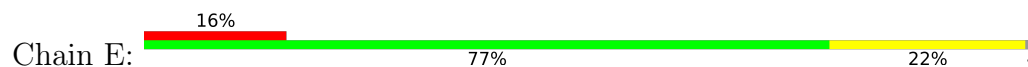


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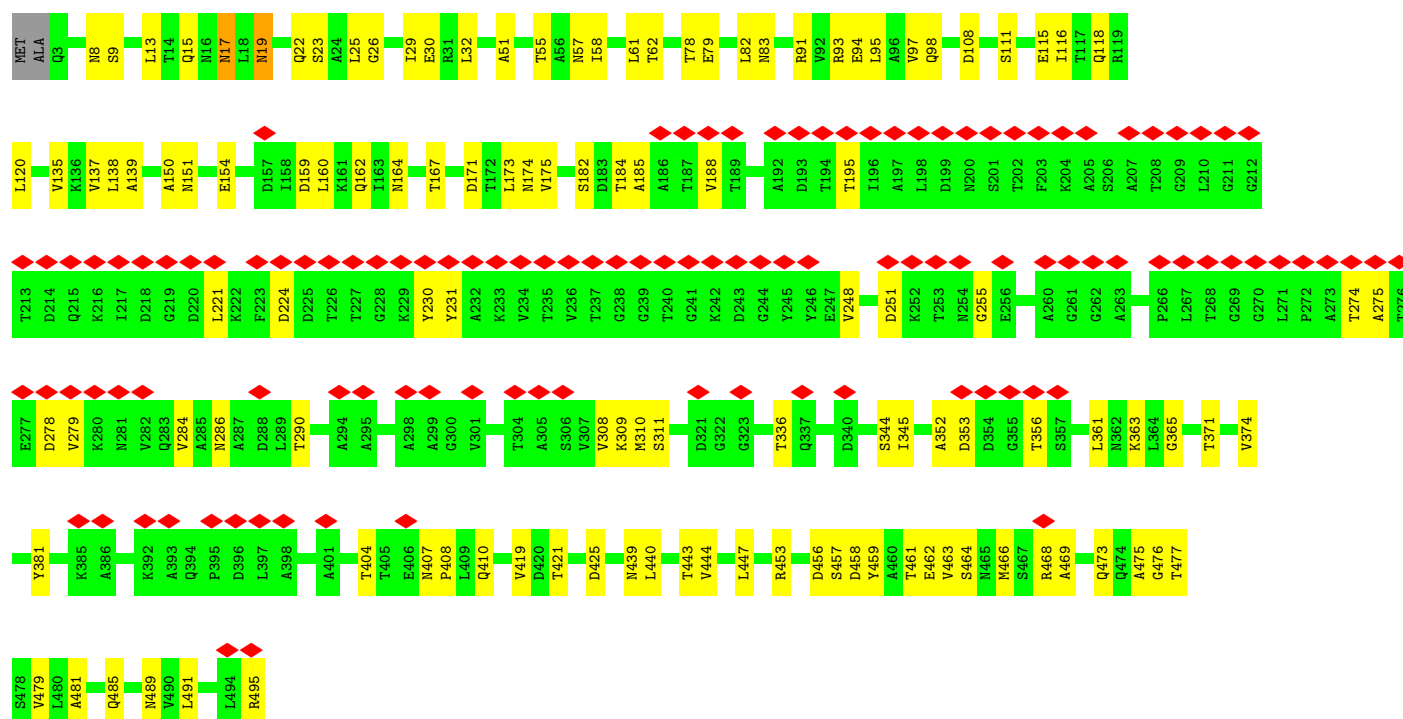
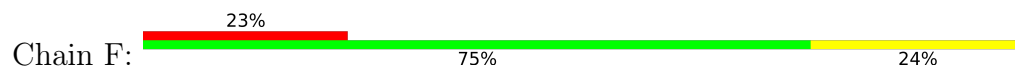




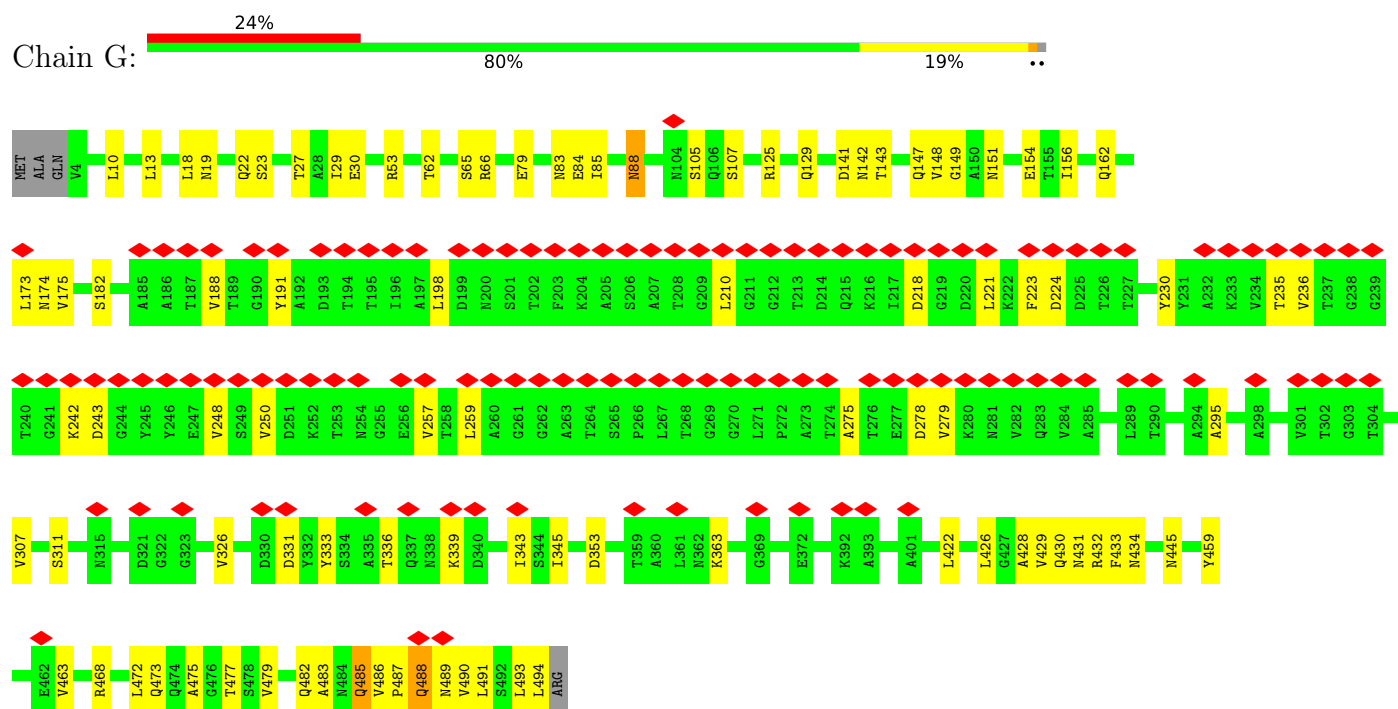
• Molecule 1: Flagellin



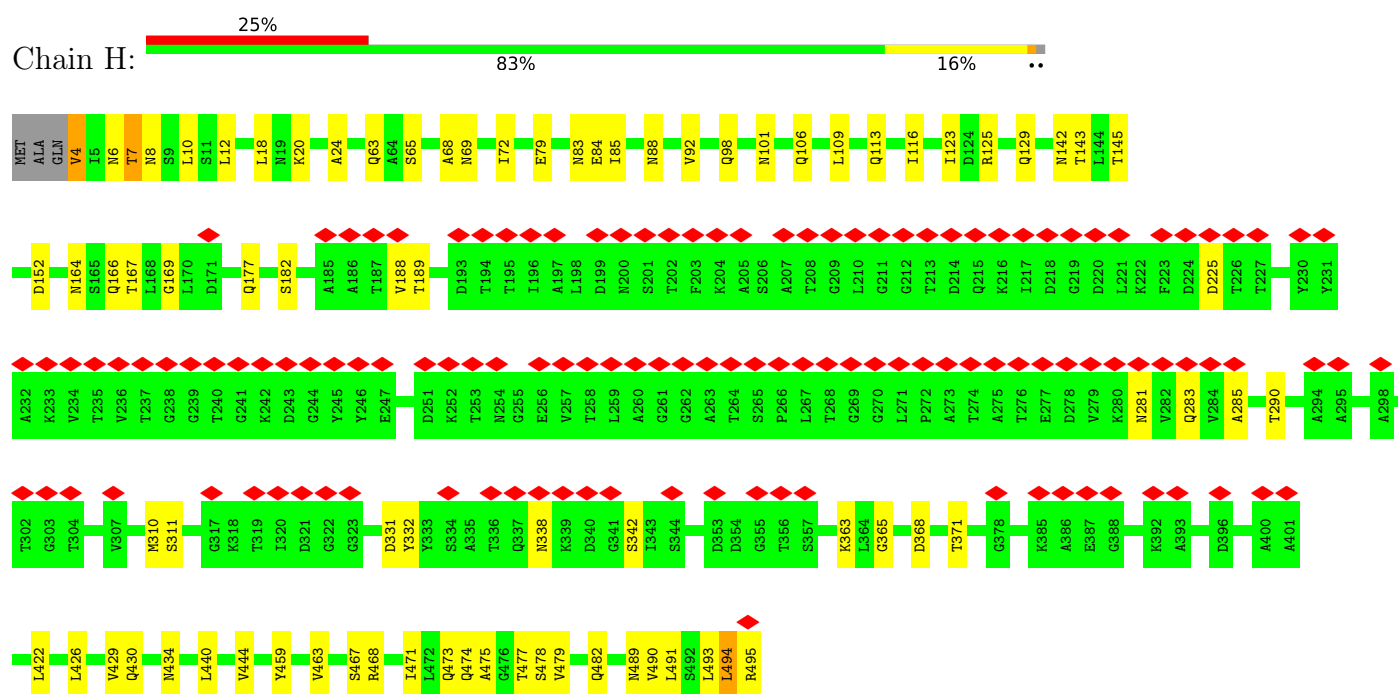
• Molecule 1: Flagellin



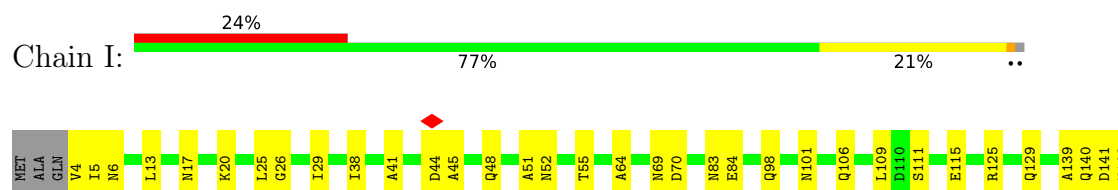
● Molecule 1: Flagellin

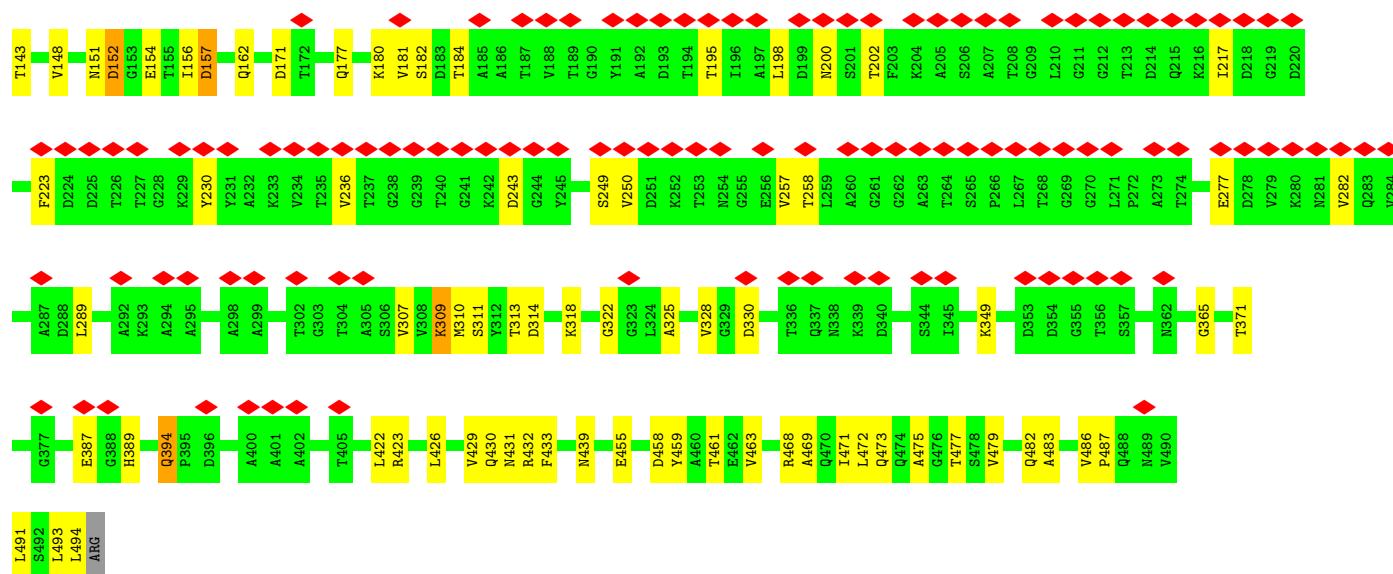


● Molecule 1: Flagellin

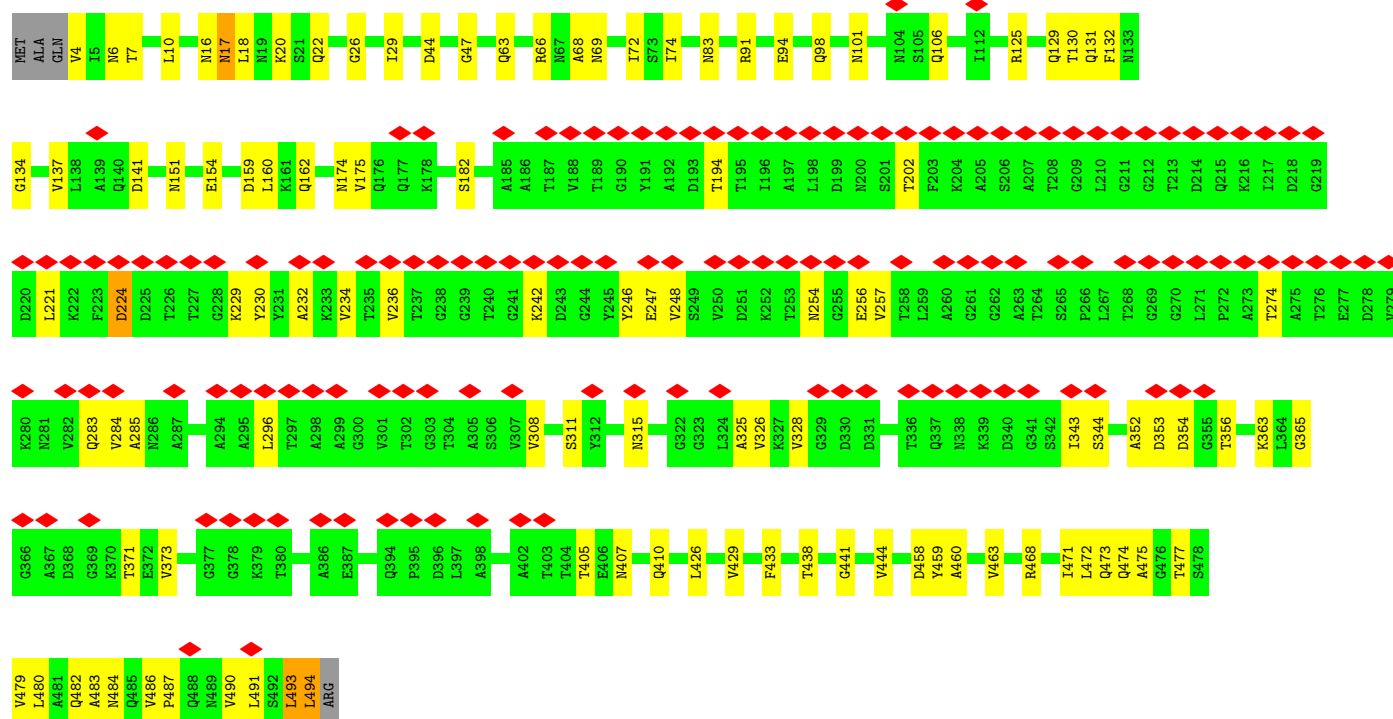
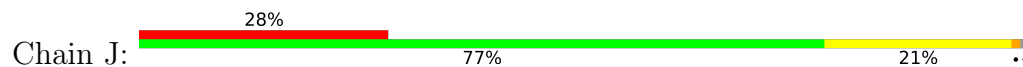


● Molecule 1: Flagellin

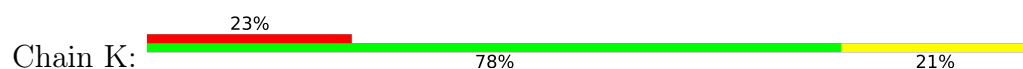


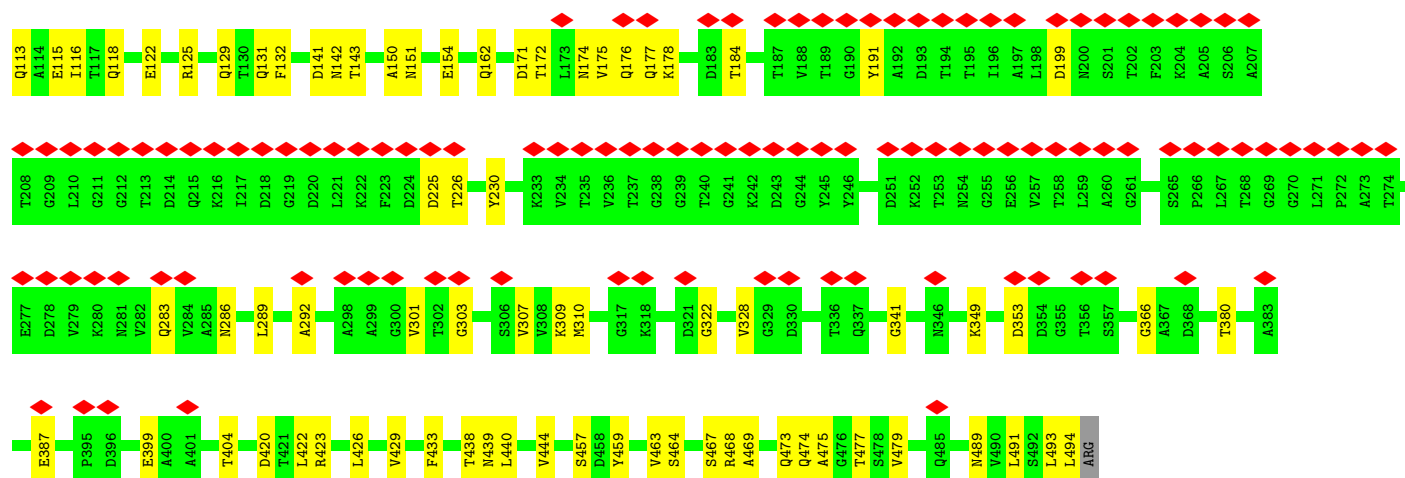


• Molecule 1: Flagellin

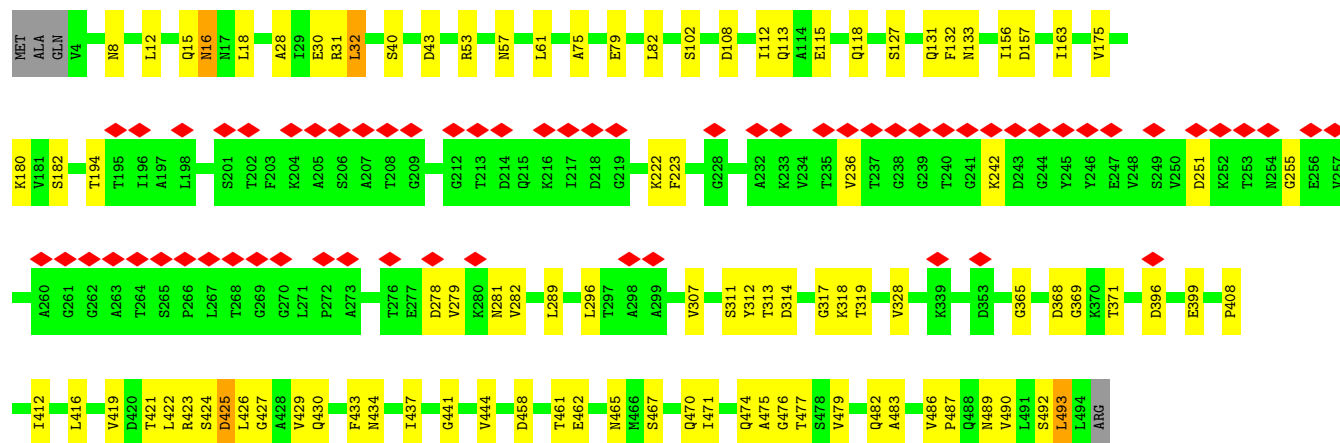
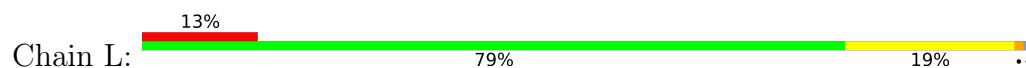


• Molecule 1: Flagellin

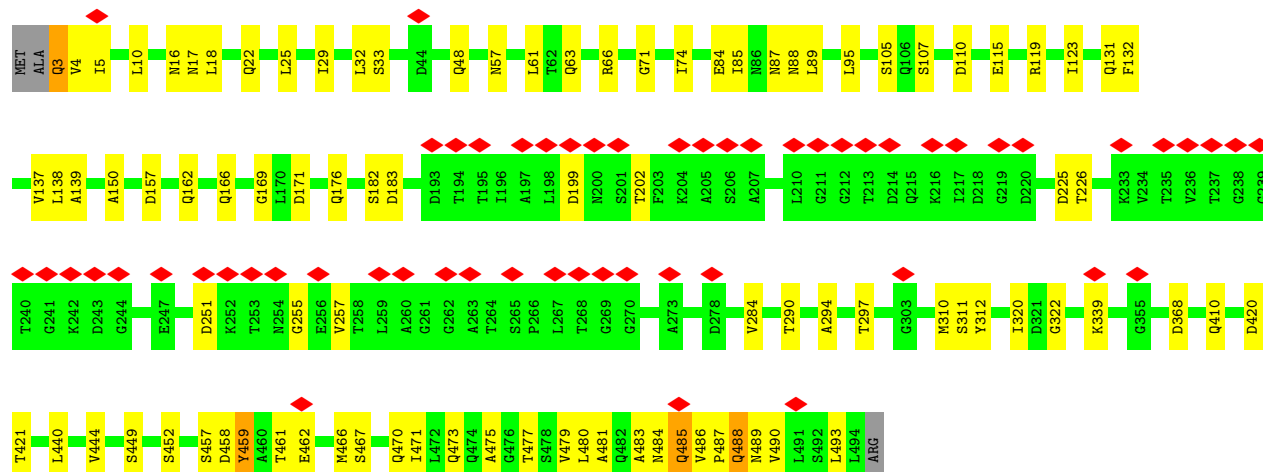
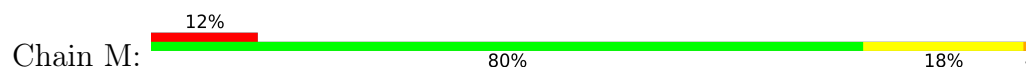




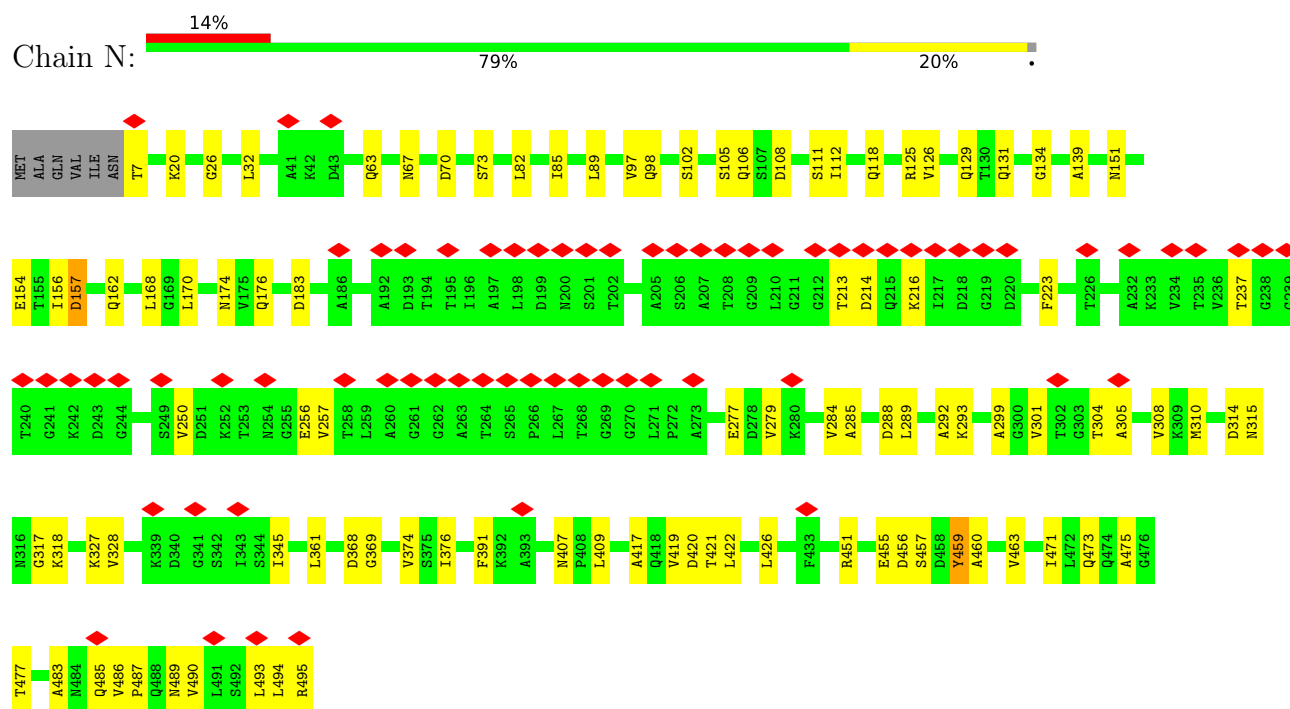
• Molecule 1: Flagellin



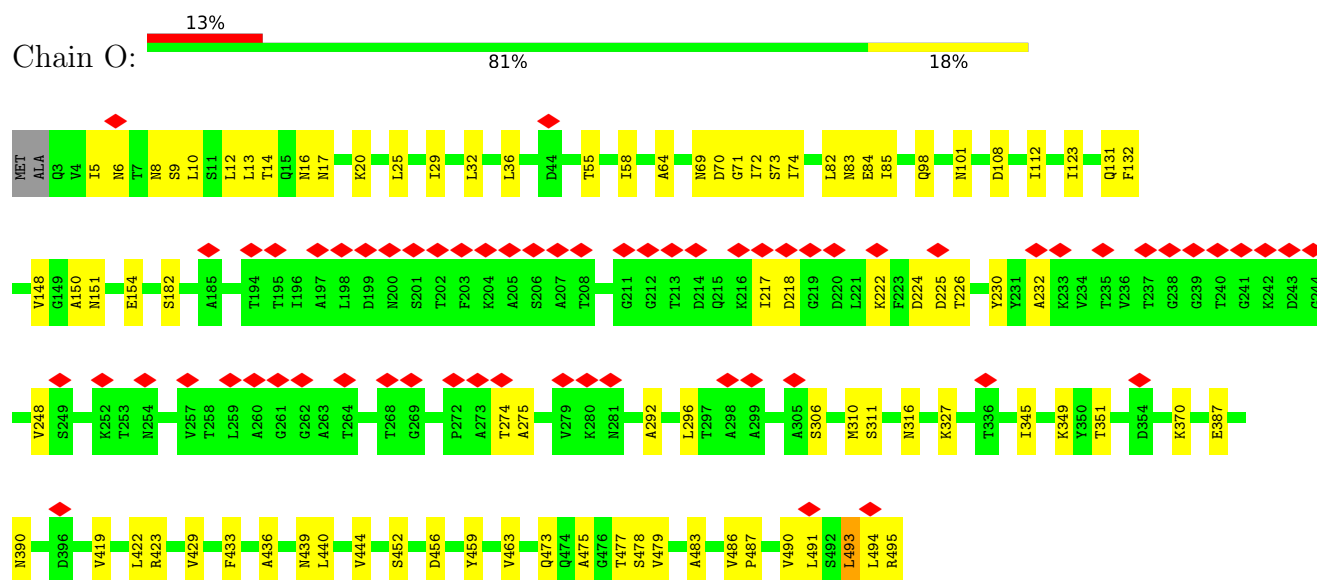
• Molecule 1: Flagellin



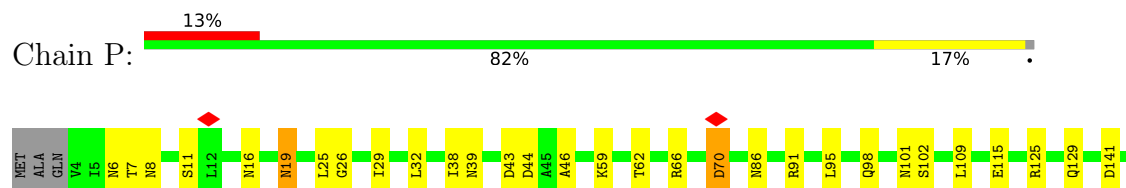
- Molecule 1: Flagellin

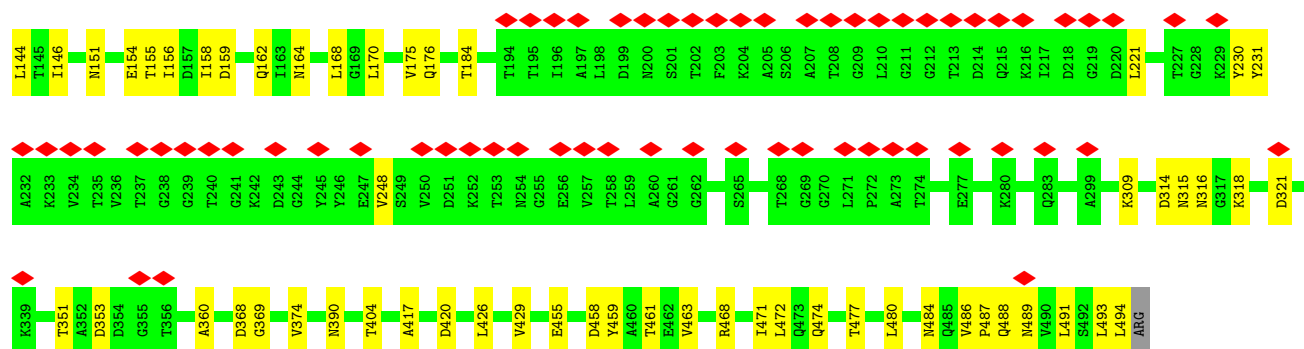


- Molecule 1: Flagellin

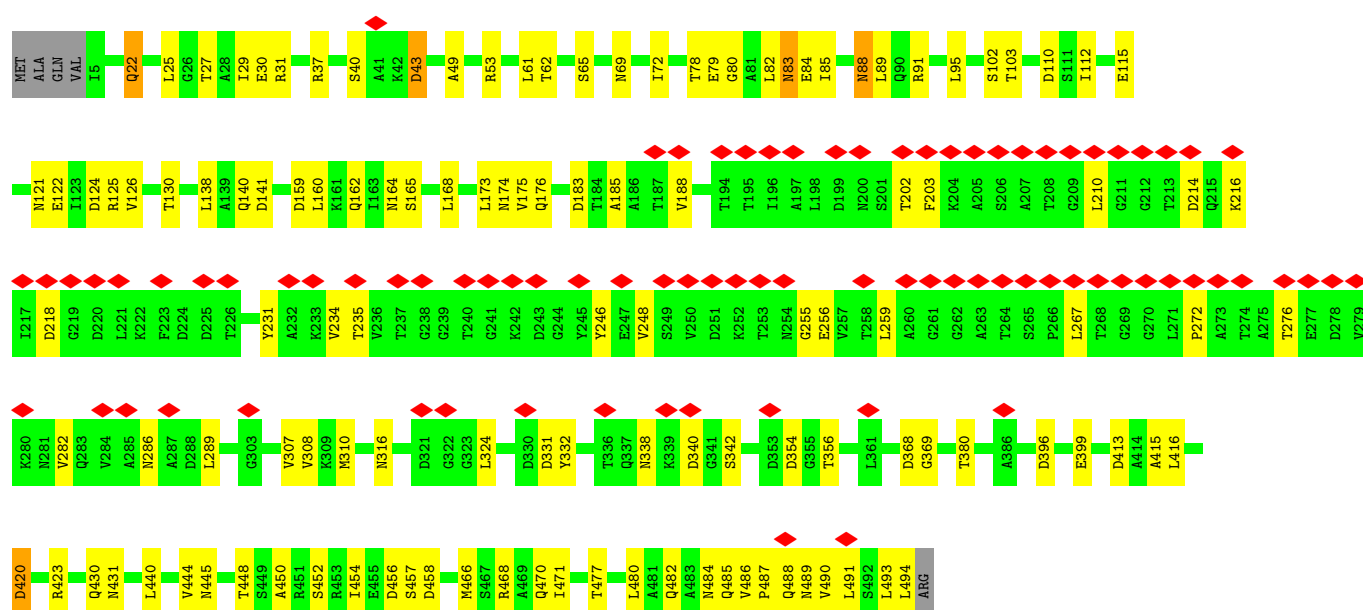
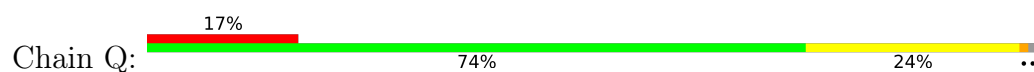


- Molecule 1: Flagellin

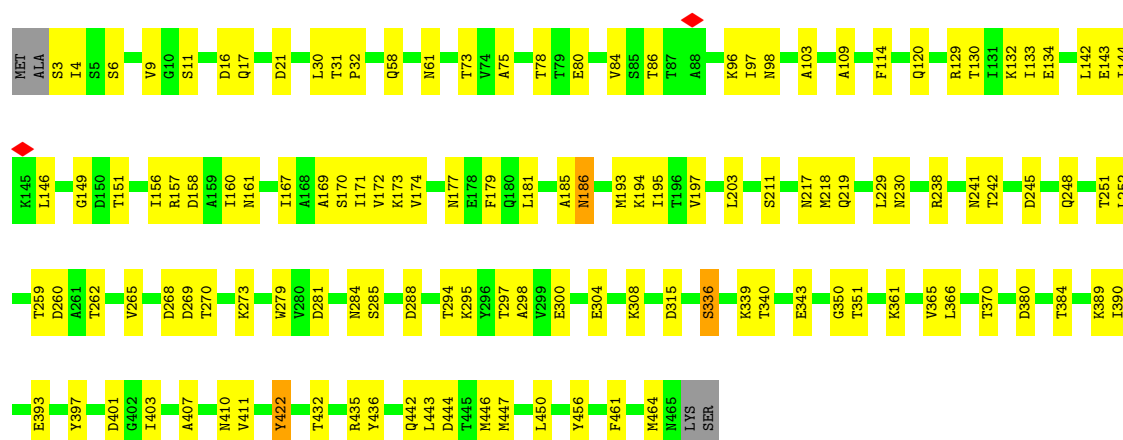




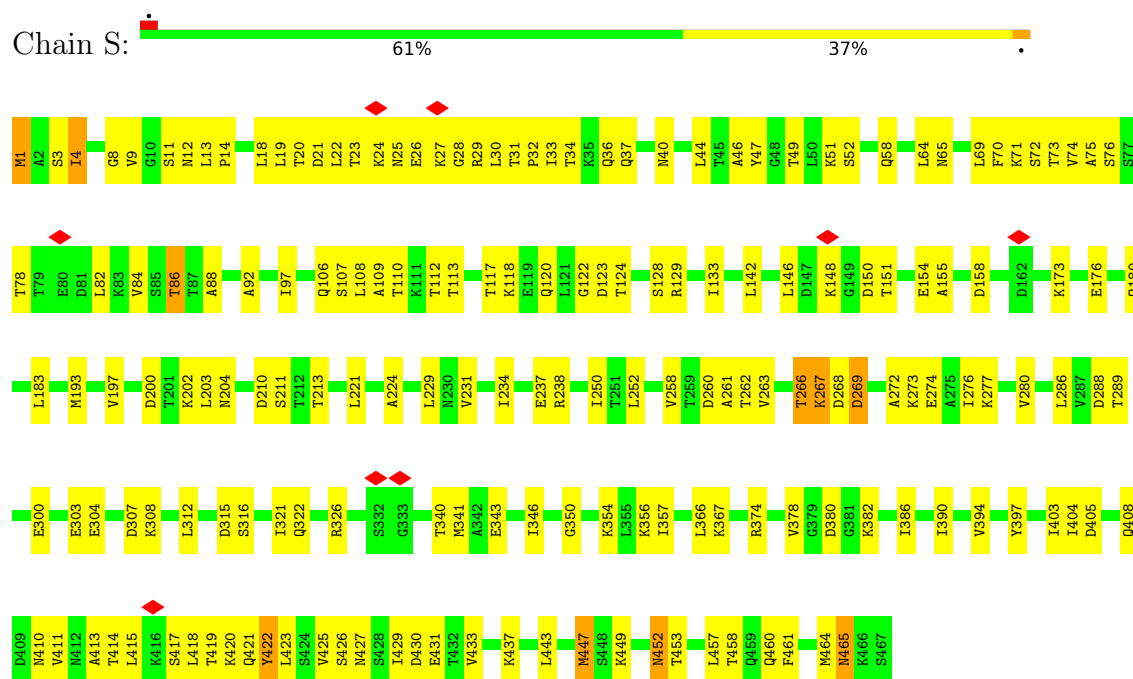
• Molecule 1: Flagellin



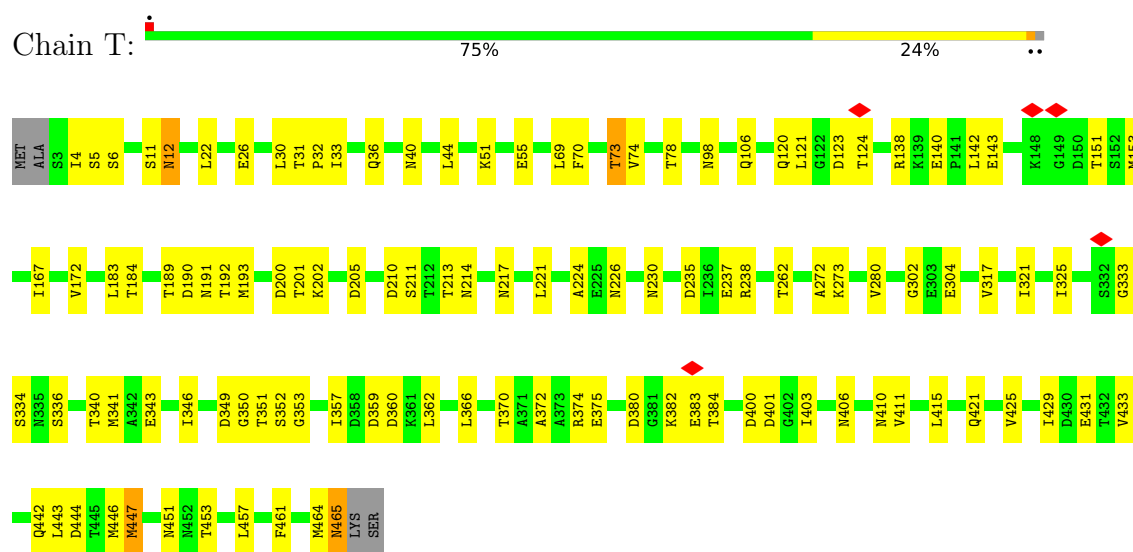
• Molecule 2: Flagellar hook-associated protein 2



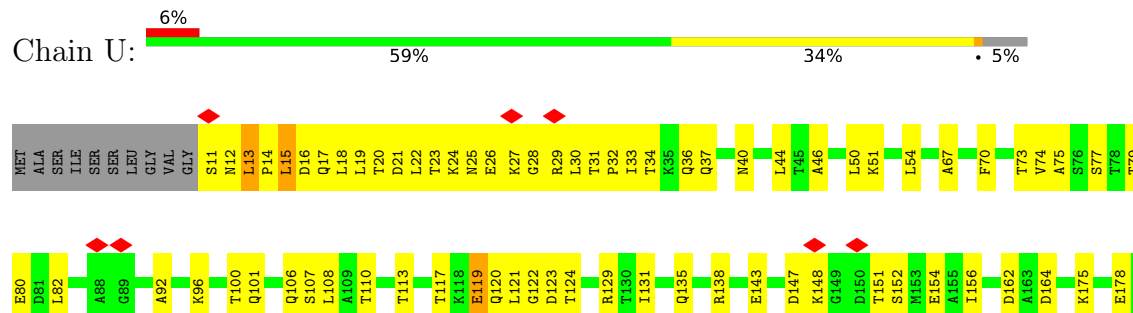
- Molecule 2: Flagellar hook-associated protein 2

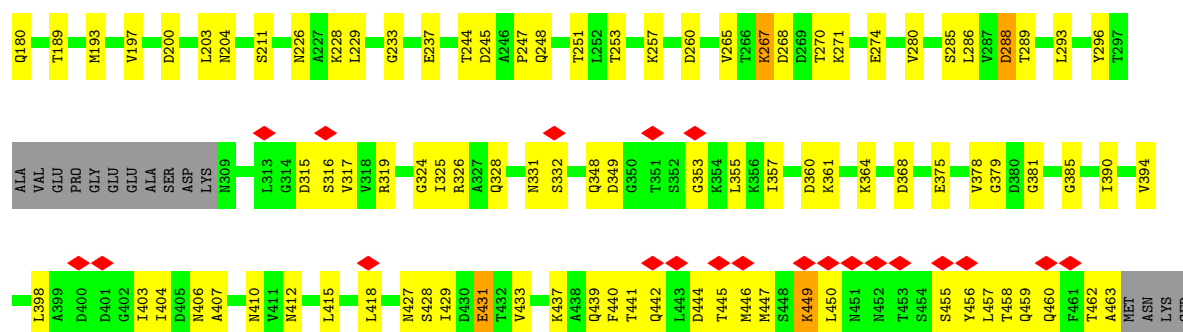


- Molecule 2: Flagellar hook-associated protein 2



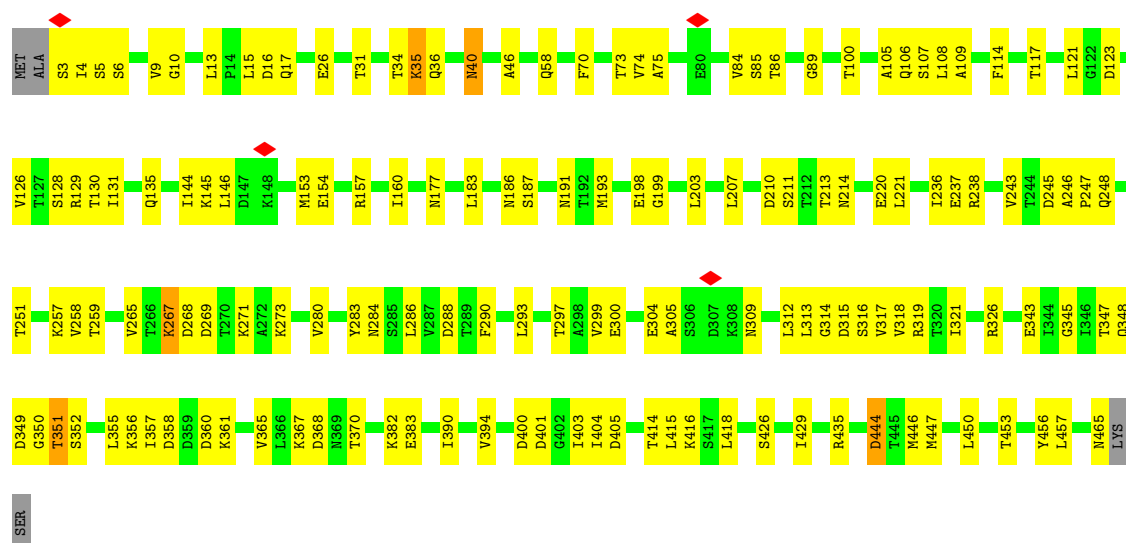
- Molecule 2: Flagellar hook-associated protein 2





• Molecule 2: Flagellar hook-associated protein 2

Chain V: 67% 31%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15225	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	0.664	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.16	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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/3621	0.49	0/4917
1	B	0.27	0/3626	0.51	1/4924 (0.0%)
1	C	0.27	0/3623	0.49	0/4919
1	D	0.28	1/3626 (0.0%)	0.50	0/4924
1	E	0.28	0/3623	0.52	2/4919 (0.0%)
1	F	0.27	0/3632	0.49	0/4931
1	G	0.26	0/3612	0.49	0/4905
1	H	0.31	1/3623 (0.0%)	0.49	0/4919
1	I	0.31	0/3612	0.50	0/4905
1	J	0.26	0/3612	0.48	0/4905
1	K	0.26	0/3612	0.48	0/4905
1	L	0.27	0/3612	0.50	0/4905
1	M	0.27	0/3621	0.49	0/4917
1	N	0.29	0/3600	0.50	0/4887
1	O	0.27	0/3632	0.49	0/4931
1	P	0.27	0/3612	0.49	0/4905
1	Q	0.26	0/3605	0.50	0/4895
2	R	0.27	0/3488	0.48	0/4722
2	S	0.32	0/3517	0.54	0/4758
2	T	0.28	0/3488	0.48	0/4722
2	U	0.39	1/3339 (0.0%)	0.58	4/4518 (0.1%)
2	V	0.27	0/3488	0.51	0/4722
All	All	0.28	3/78824 (0.0%)	0.50	7/106955 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	119	GLU	CG-CD	-13.19	1.32	1.51
1	H	4	VAL	CB-CG2	-8.88	1.34	1.52
1	D	462	GLU	CG-CD	-5.39	1.43	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	LEU	CB-CG-CD2	8.56	125.54	111.00
1	E	494	LEU	CB-CG-CD2	6.66	122.32	111.00
2	U	13	LEU	CB-CG-CD2	6.46	121.98	111.00
2	U	15	LEU	CA-CB-CG	5.71	128.43	115.30
2	U	119	GLU	CG-CD-OE1	-5.69	106.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3598	3556	3555	80	0
1	B	3603	3556	3560	97	0
1	C	3600	3537	3560	100	0
1	D	3603	3550	3560	119	0
1	E	3600	3548	3560	108	0
1	F	3609	3545	3568	97	0
1	G	3589	3548	3547	88	0
1	H	3600	3548	3560	81	0
1	I	3589	3548	3547	99	0
1	J	3589	3548	3547	87	0
1	K	3589	3548	3547	78	0
1	L	3589	3548	3547	95	0
1	M	3598	3539	3555	73	0
1	N	3577	3448	3534	94	0
1	O	3609	3528	3568	73	0
1	P	3589	3548	3547	70	0
1	Q	3582	3528	3538	101	0
2	R	3463	3498	3513	94	0
2	S	3492	3516	3548	183	0
2	T	3463	3509	3513	84	0
2	U	3317	3364	3371	156	0
2	V	3463	3514	3513	119	0
All	All	78311	77572	77858	1934	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 12.

The worst 5 of 1934 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:C:79:GLU:OE1	1:C:83:ASN:ND2	1.82	1.13
1:G:486:VAL:HG11	1:L:470:GLN:HE22	1.25	1.01
1:M:3:GLN:HG2	1:M:4:VAL:H	1.25	0.99
2:U:119:GLU:OE1	2:U:121:LEU:HD23	1.64	0.98
1:A:34:SER:O	2:V:4:ILE:N	1.97	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/495 (99%)	484 (99%)	6 (1%)	0	100	100
1	B	491/495 (99%)	479 (98%)	12 (2%)	0	100	100
1	C	490/495 (99%)	462 (94%)	28 (6%)	0	100	100
1	D	491/495 (99%)	483 (98%)	8 (2%)	0	100	100
1	E	490/495 (99%)	466 (95%)	24 (5%)	0	100	100
1	F	491/495 (99%)	470 (96%)	21 (4%)	0	100	100
1	G	489/495 (99%)	478 (98%)	11 (2%)	0	100	100
1	H	490/495 (99%)	476 (97%)	13 (3%)	1 (0%)	44	72
1	I	489/495 (99%)	471 (96%)	18 (4%)	0	100	100
1	J	489/495 (99%)	479 (98%)	10 (2%)	0	100	100
1	K	489/495 (99%)	479 (98%)	10 (2%)	0	100	100
1	L	489/495 (99%)	474 (97%)	15 (3%)	0	100	100
1	M	490/495 (99%)	470 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	487/495 (98%)	476 (98%)	11 (2%)	0	100	100
1	O	491/495 (99%)	479 (98%)	12 (2%)	0	100	100
1	P	489/495 (99%)	479 (98%)	10 (2%)	0	100	100
1	Q	488/495 (99%)	466 (96%)	22 (4%)	0	100	100
2	R	461/467 (99%)	435 (94%)	26 (6%)	0	100	100
2	S	465/467 (100%)	436 (94%)	28 (6%)	1 (0%)	44	72
2	T	461/467 (99%)	446 (97%)	15 (3%)	0	100	100
2	U	438/467 (94%)	425 (97%)	13 (3%)	0	100	100
2	V	461/467 (99%)	432 (94%)	27 (6%)	2 (0%)	30	62
All	All	10609/10750 (99%)	10245 (97%)	360 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	7	THR
2	V	351	THR
2	S	4	ILE
2	V	267	LYS

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	389/391 (100%)	385 (99%)	4 (1%)	73	82
1	B	389/391 (100%)	381 (98%)	8 (2%)	48	67
1	C	389/391 (100%)	383 (98%)	6 (2%)	60	75
1	D	389/391 (100%)	385 (99%)	4 (1%)	73	82
1	E	389/391 (100%)	386 (99%)	3 (1%)	79	85
1	F	390/391 (100%)	385 (99%)	5 (1%)	65	77
1	G	388/391 (99%)	384 (99%)	4 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	389/391 (100%)	386 (99%)	3 (1%)	79	85
1	I	388/391 (99%)	381 (98%)	7 (2%)	54	71
1	J	388/391 (99%)	384 (99%)	4 (1%)	73	82
1	K	388/391 (99%)	385 (99%)	3 (1%)	79	85
1	L	388/391 (99%)	382 (98%)	6 (2%)	60	75
1	M	389/391 (100%)	381 (98%)	8 (2%)	48	67
1	N	386/391 (99%)	383 (99%)	3 (1%)	79	85
1	O	390/391 (100%)	388 (100%)	2 (0%)	86	92
1	P	388/391 (99%)	384 (99%)	4 (1%)	73	82
1	Q	387/391 (99%)	379 (98%)	8 (2%)	48	67
2	R	388/391 (99%)	380 (98%)	8 (2%)	48	67
2	S	391/391 (100%)	379 (97%)	12 (3%)	35	57
2	T	388/391 (99%)	382 (98%)	6 (2%)	60	75
2	U	372/391 (95%)	367 (99%)	5 (1%)	65	77
2	V	388/391 (99%)	382 (98%)	6 (2%)	60	75
All	All	8531/8602 (99%)	8412 (99%)	119 (1%)	62	76

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLN
2	U	288	ASP
1	P	70	ASP
2	U	267	LYS
2	V	465	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	470	GLN
2	V	226	ASN
1	M	488	GLN
2	U	37	GLN
1	M	485	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

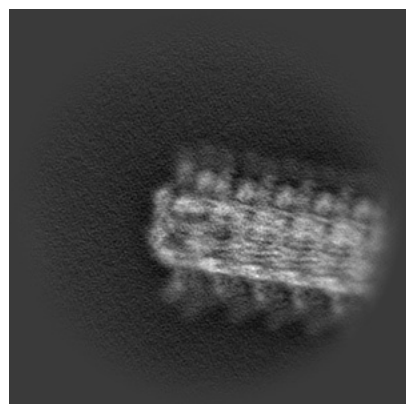
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51486. These allow visual inspection of the internal detail of the map and identification of artifacts.

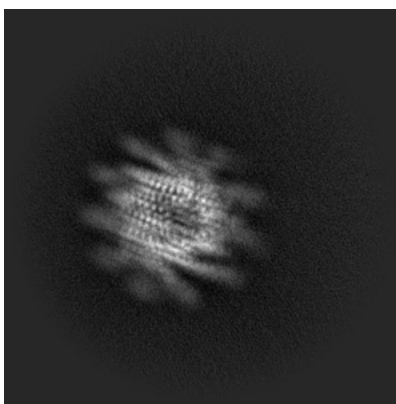
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

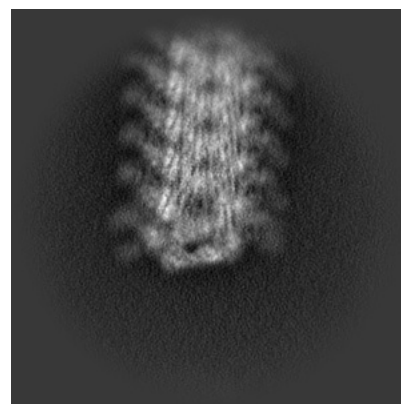
6.1.1 Primary map



X

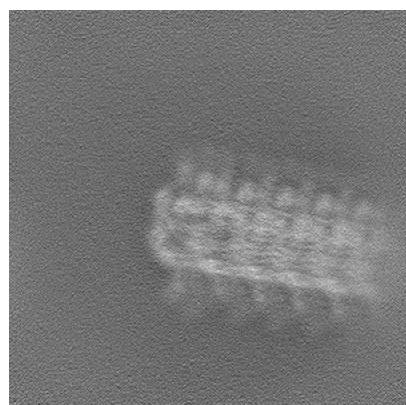


Y

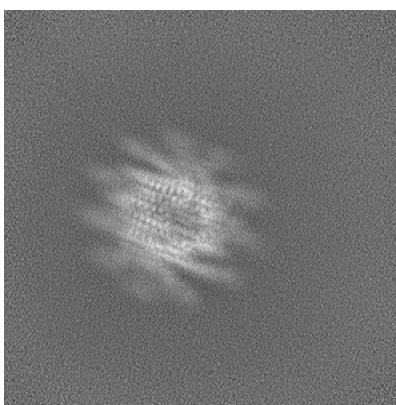


Z

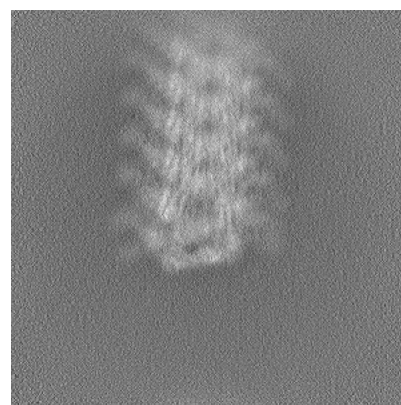
6.1.2 Raw map



X



Y

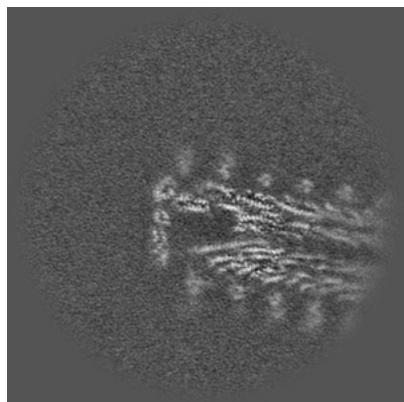


Z

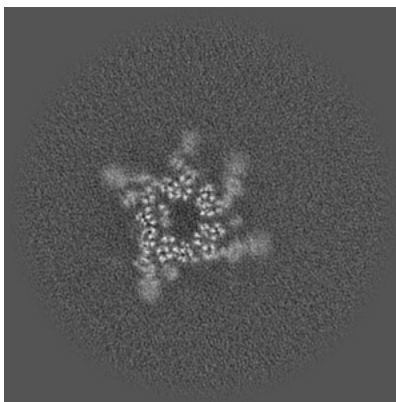
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

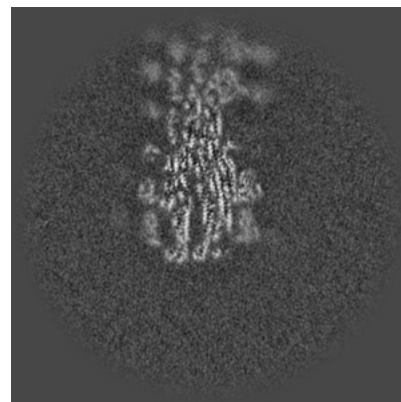
6.2.1 Primary map



X Index: 250

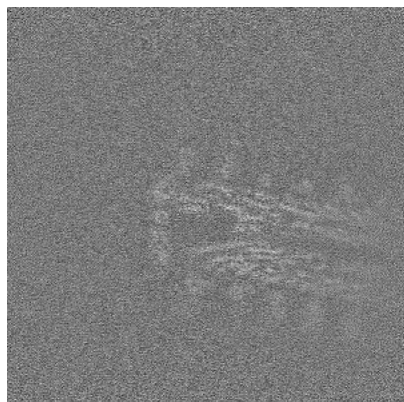


Y Index: 250

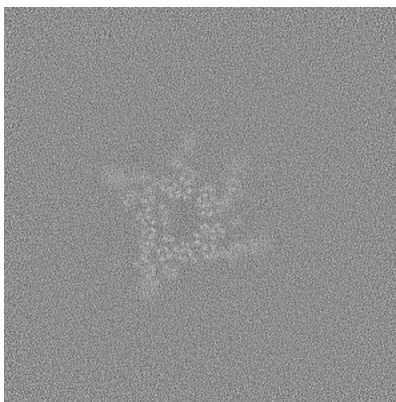


Z Index: 250

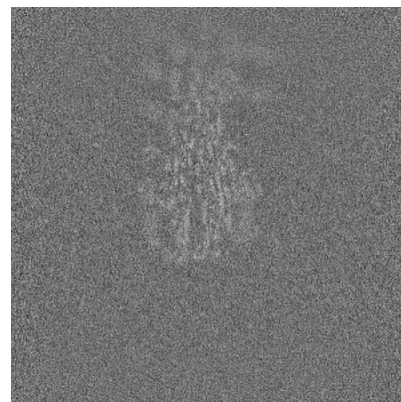
6.2.2 Raw map



X Index: 250



Y Index: 250

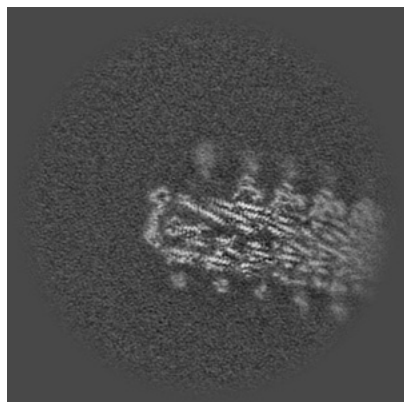


Z Index: 250

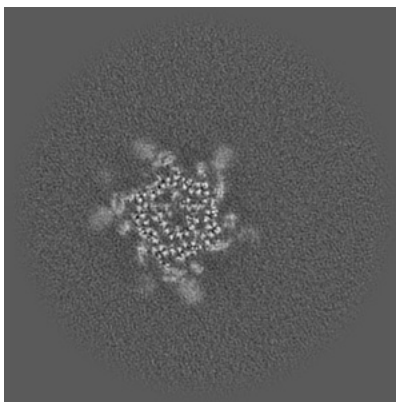
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

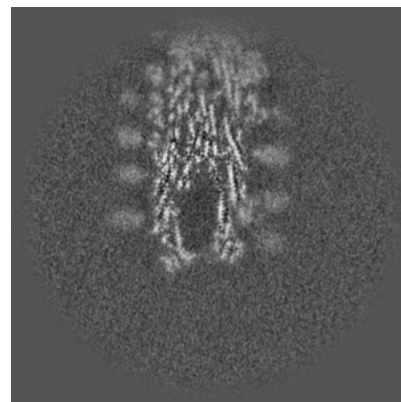
6.3.1 Primary map



X Index: 205

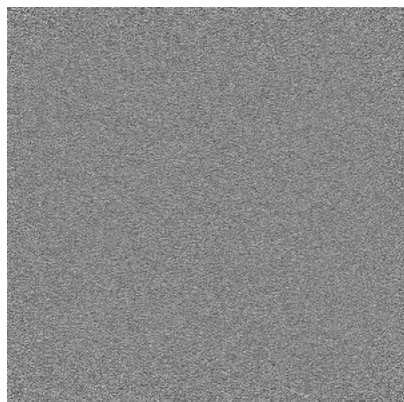


Y Index: 290

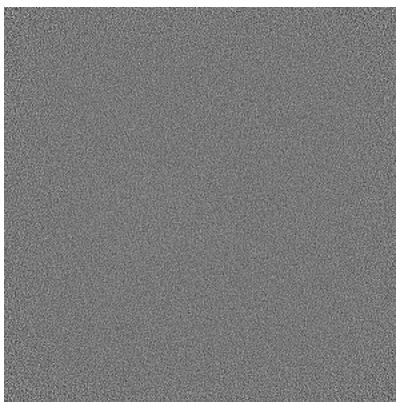


Z Index: 226

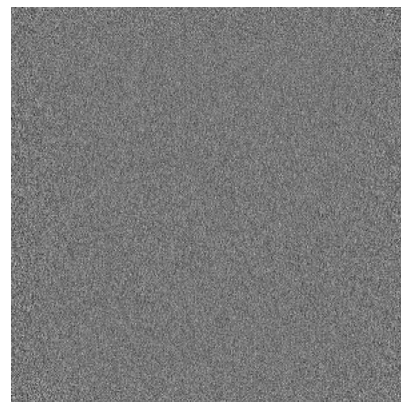
6.3.2 Raw map



X Index: 0



Y Index: 0

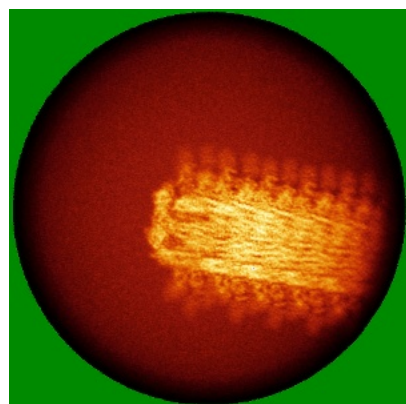


Z Index: 0

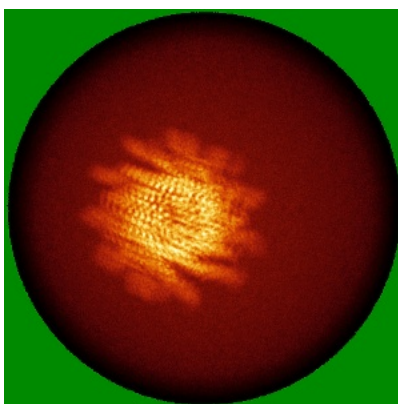
The images above show the largest variance slices of the map in three orthogonal directions.

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

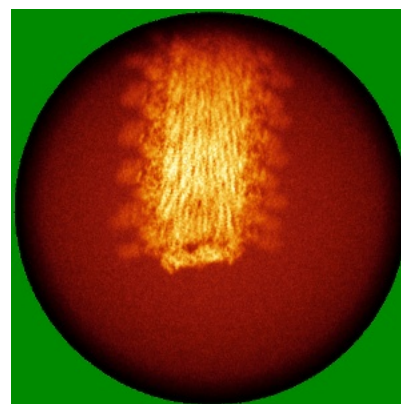
6.4.1 Primary map



X

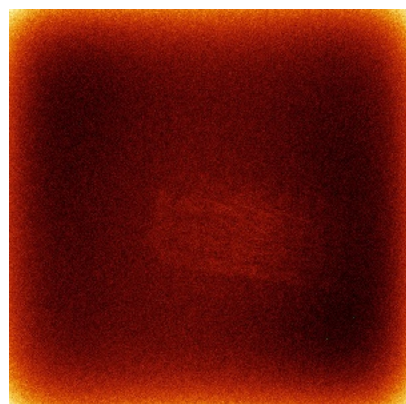


Y

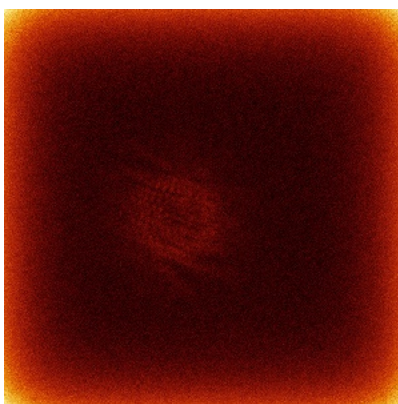


Z

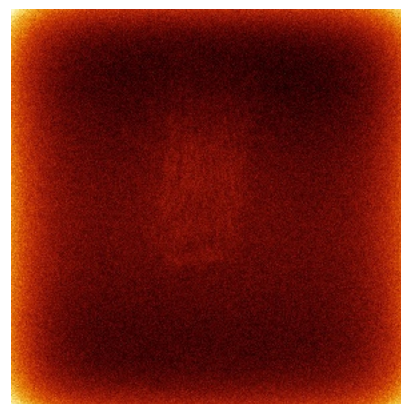
6.4.2 Raw map



X



Y

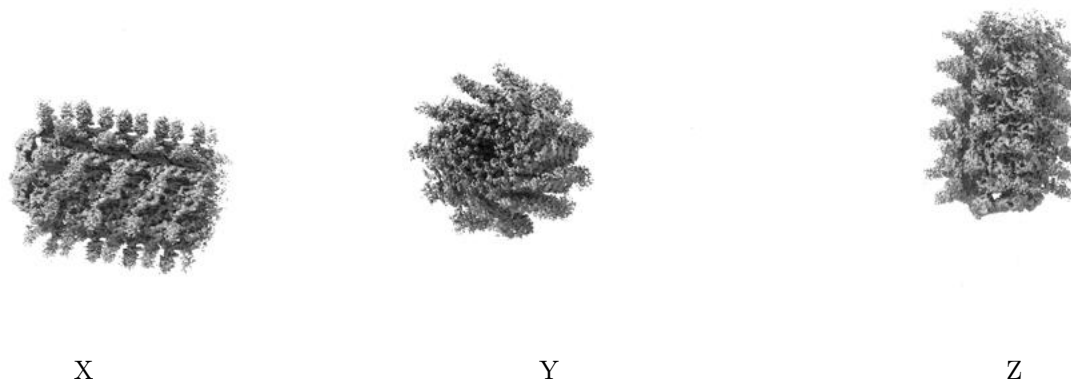


Z

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.

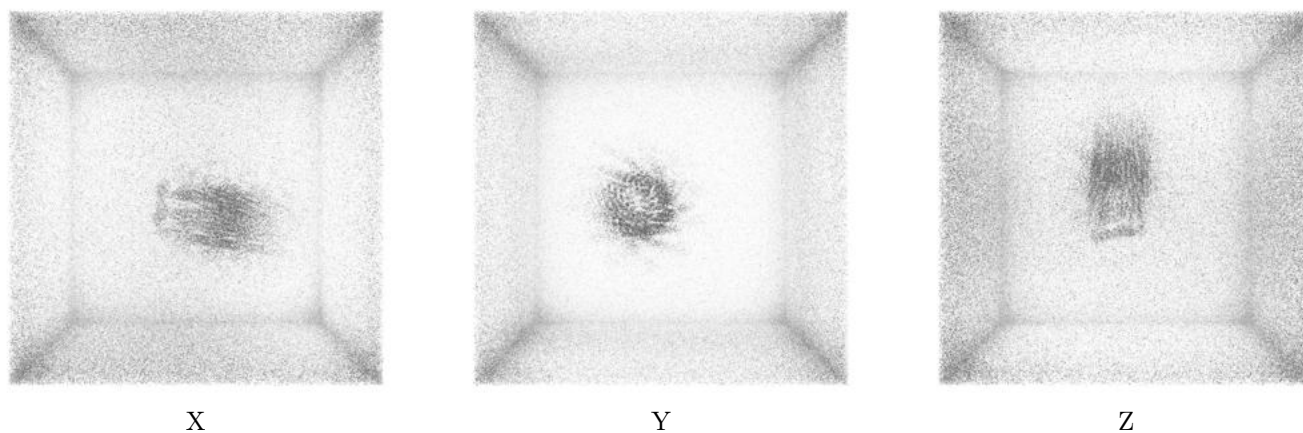
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

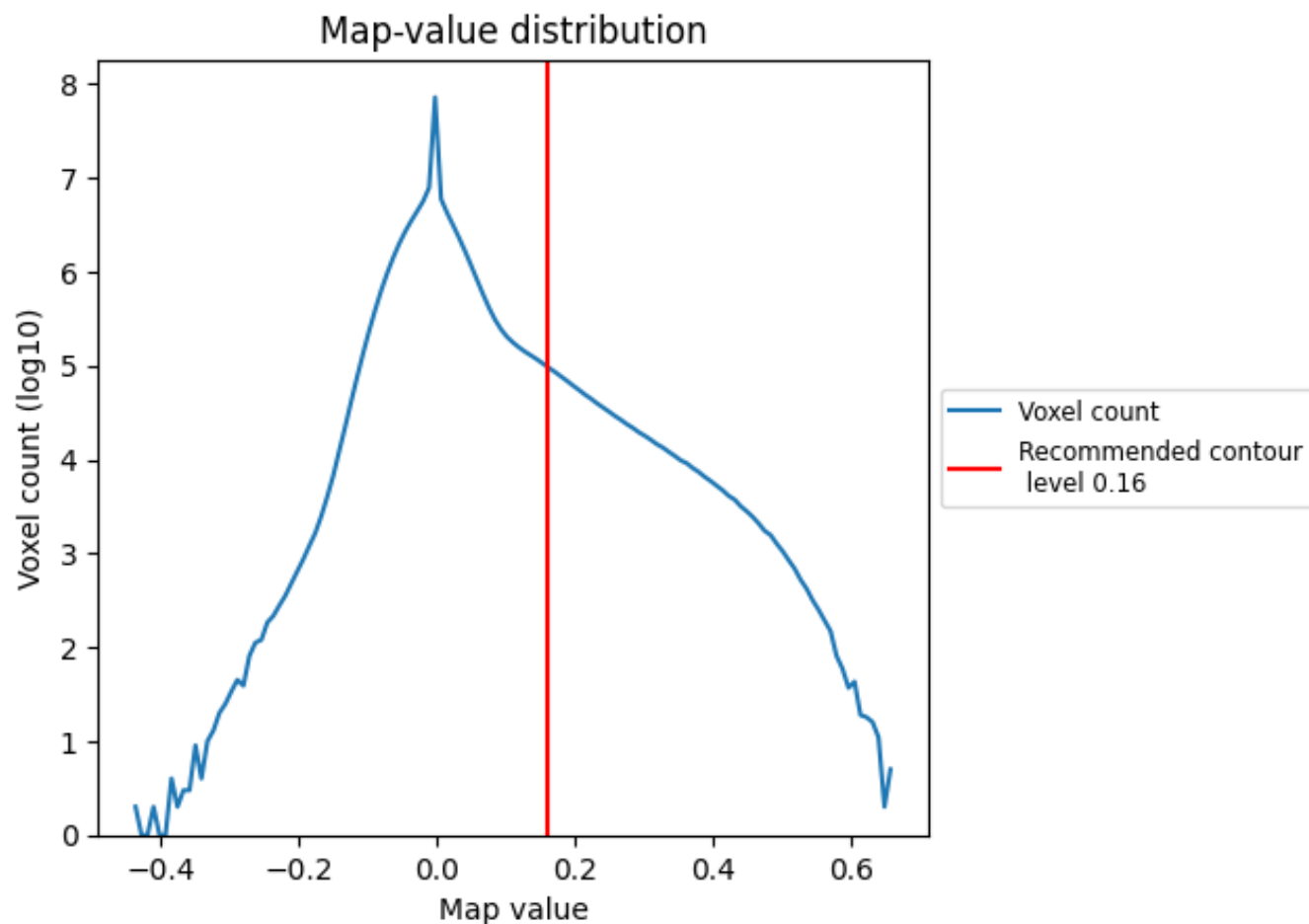
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

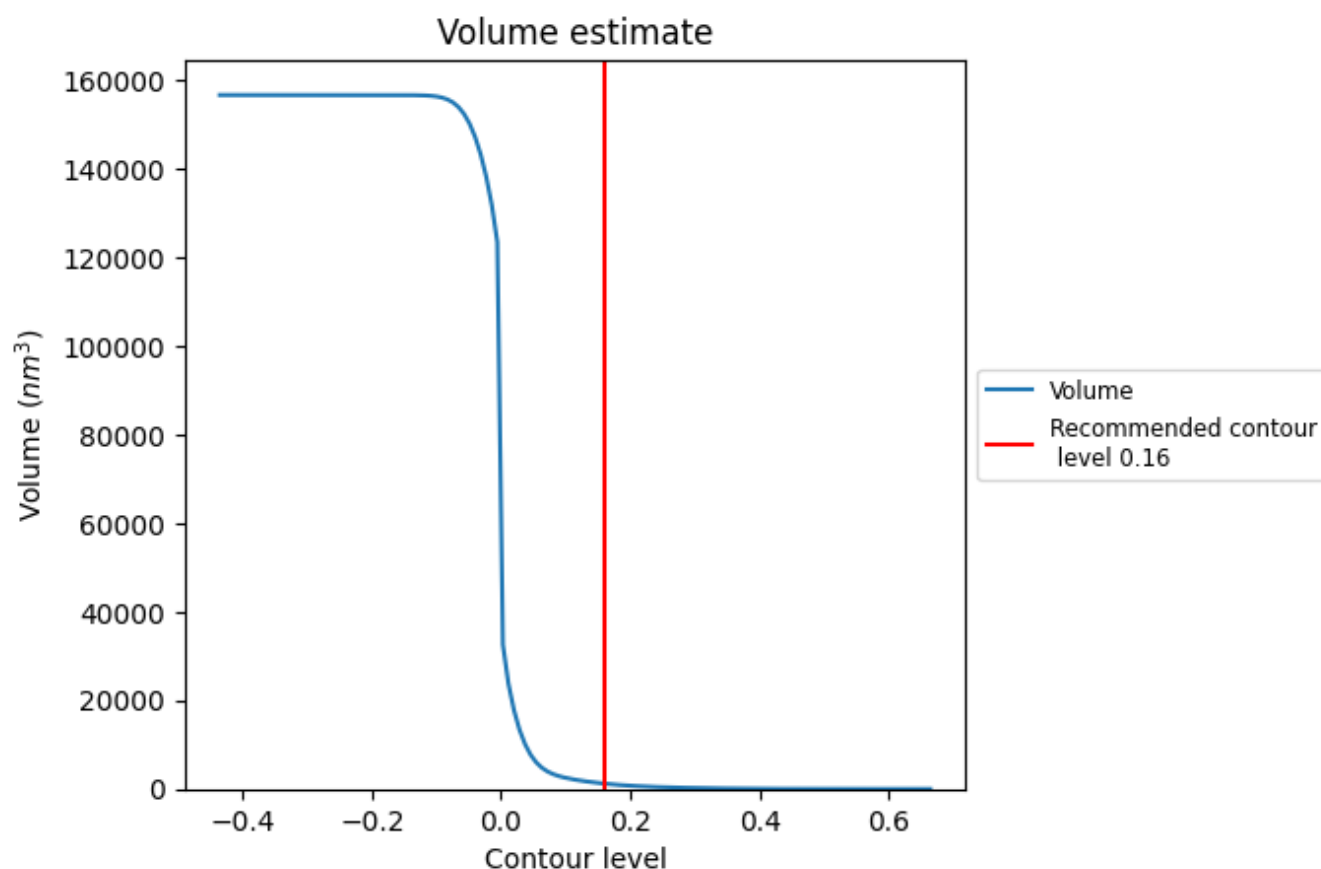
This section contains the results of statistical analysis of the map.

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.

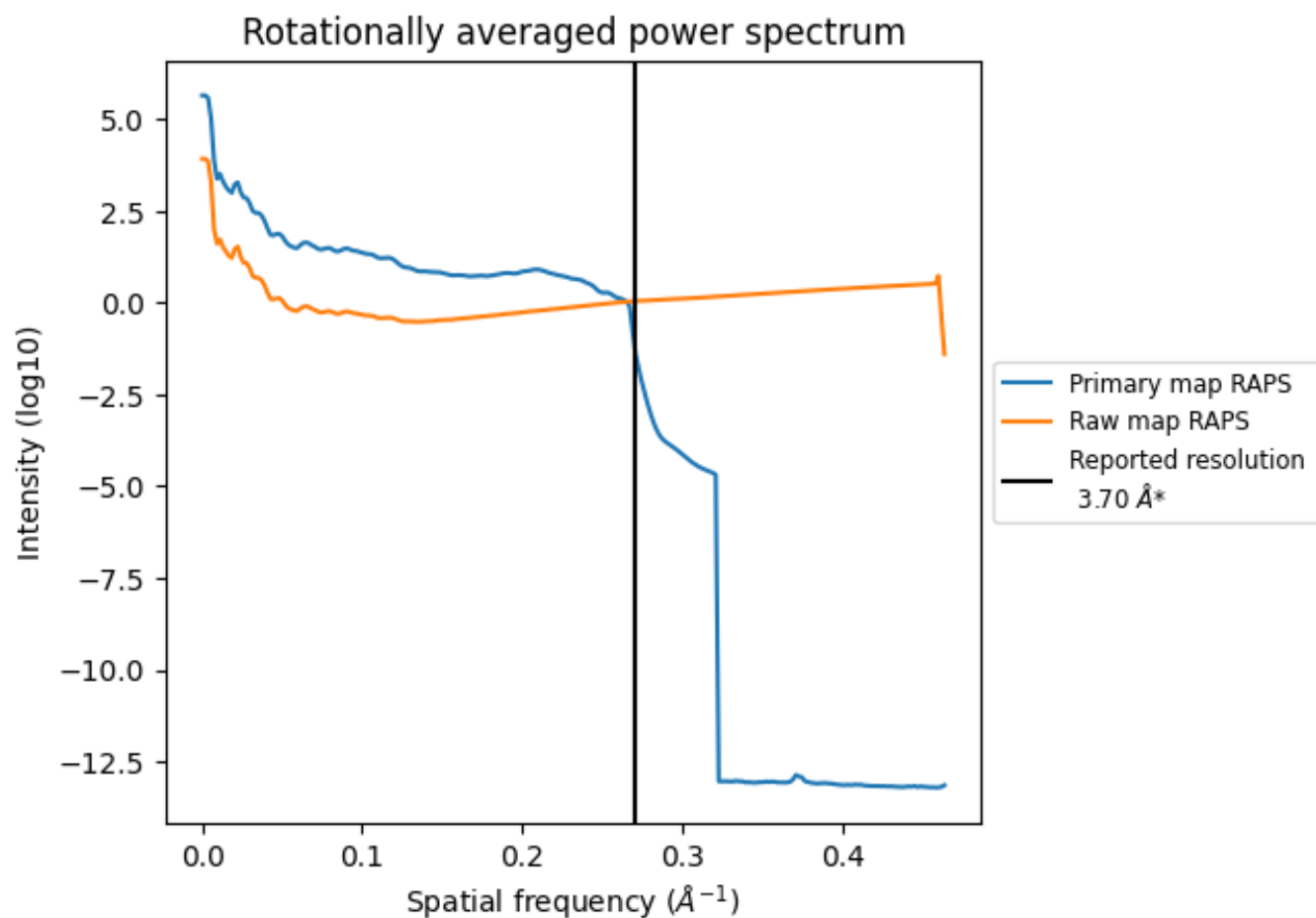
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1206 nm³; this corresponds to an approximate mass of 1090 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 ⓘ

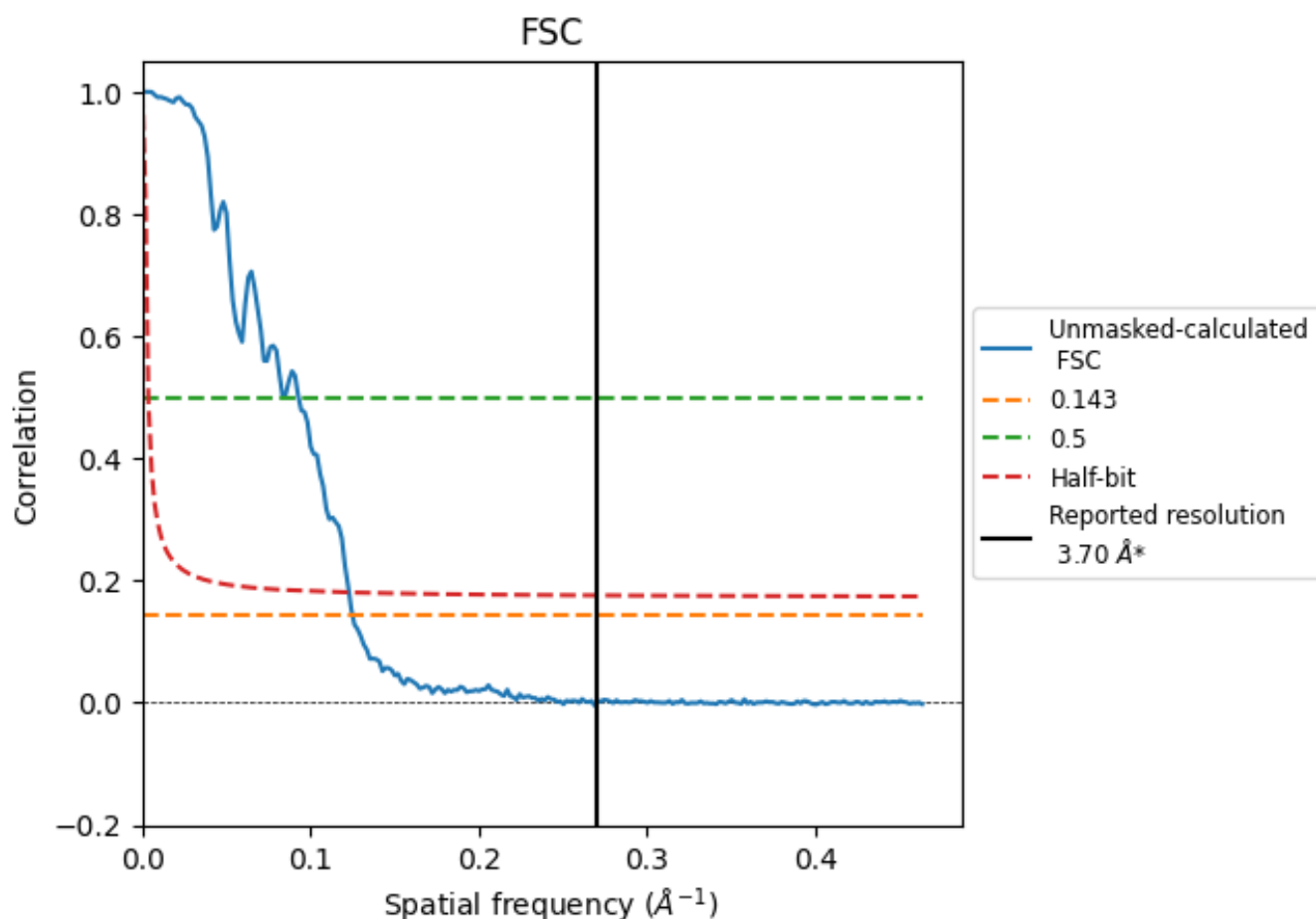


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

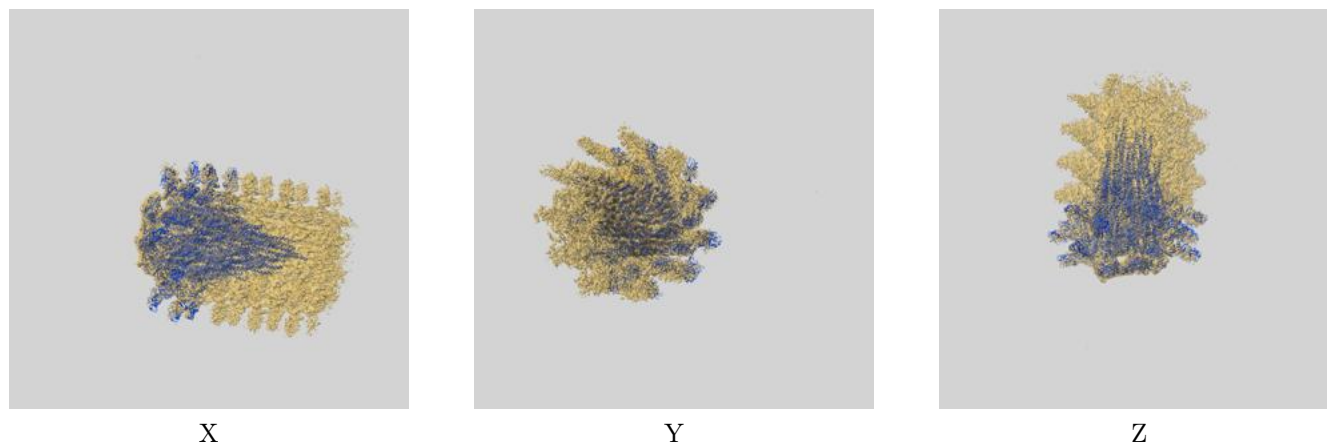
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.99	10.76	8.13

*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 7.99 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

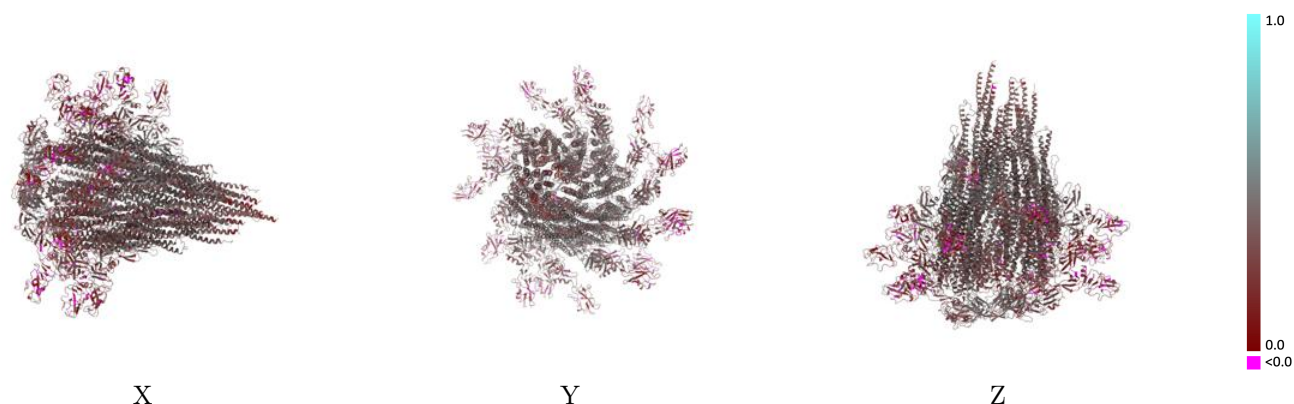
This section contains information regarding the fit between EMDB map EMD-51486 and PDB model 9GNZ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



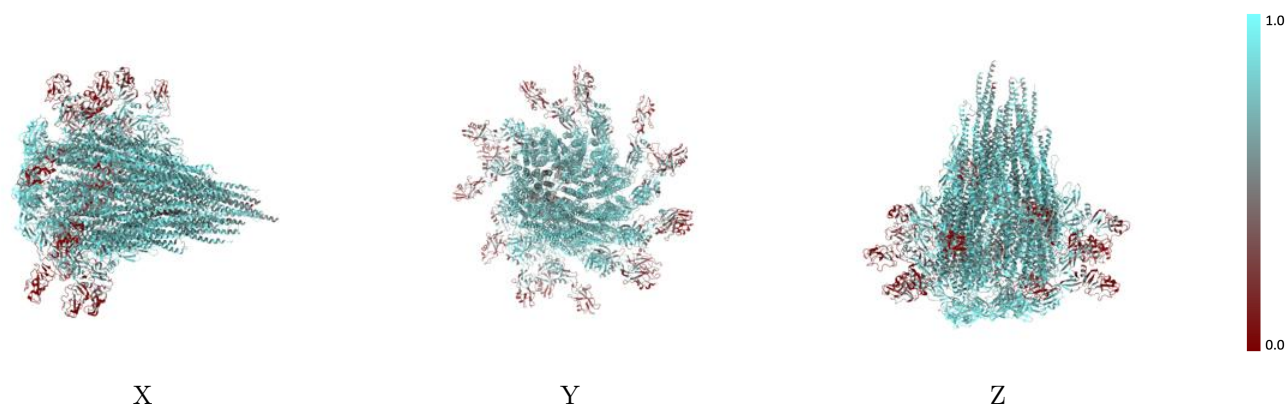
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



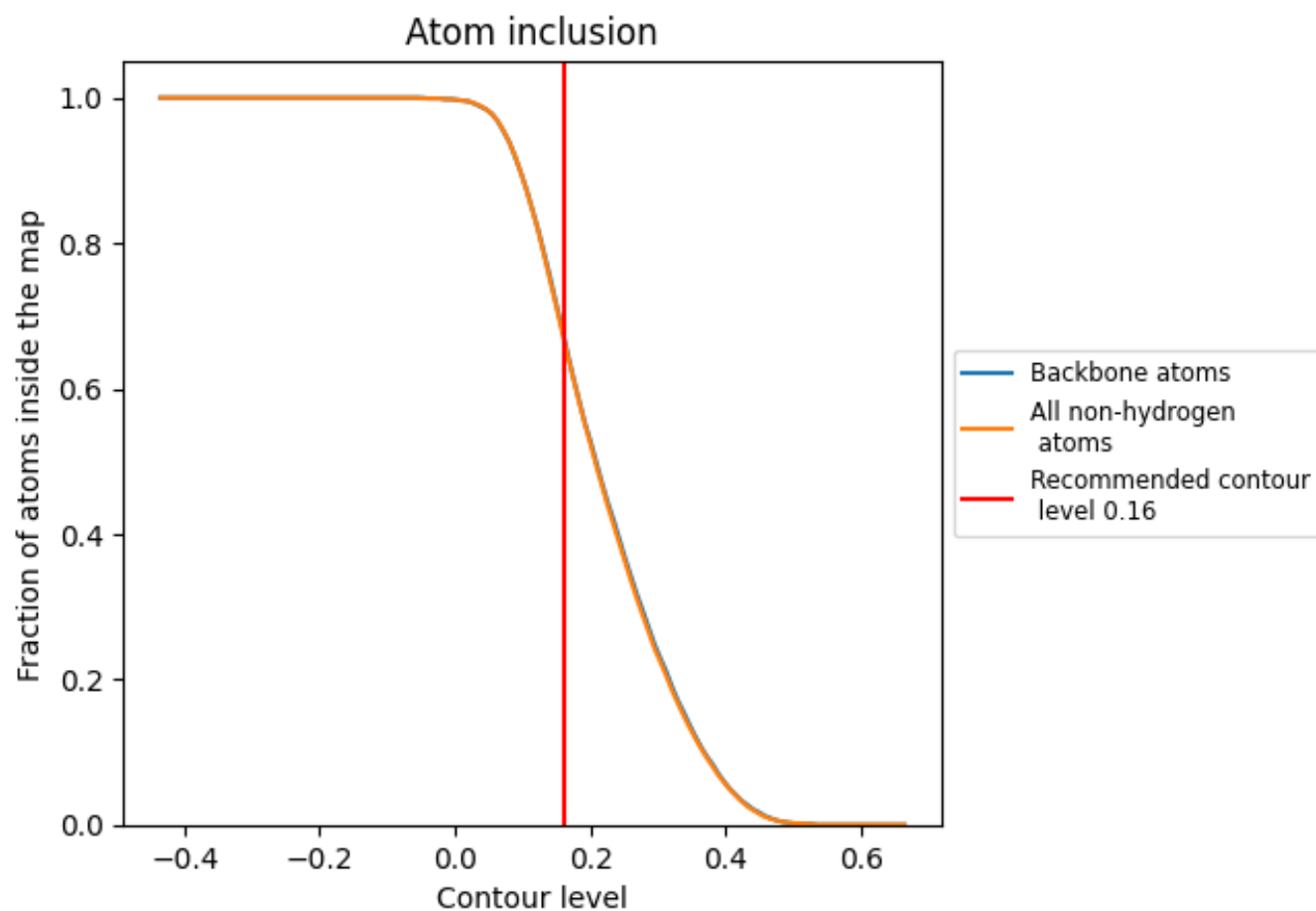
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6720	 0.3360
A	 0.6120	 0.2940
B	 0.6280	 0.3190
C	 0.6240	 0.3210
D	 0.5860	 0.2920
E	 0.6710	 0.3220
F	 0.6180	 0.2980
G	 0.6060	 0.3230
H	 0.6070	 0.3190
I	 0.6070	 0.3120
J	 0.5740	 0.3090
K	 0.6200	 0.3170
L	 0.7090	 0.3490
M	 0.7020	 0.3550
N	 0.6890	 0.3620
O	 0.7050	 0.3560
P	 0.7070	 0.3600
Q	 0.6630	 0.3300
R	 0.8080	 0.3900
S	 0.7970	 0.3730
T	 0.7940	 0.3860
U	 0.7350	 0.3290
V	 0.8030	 0.3730

