



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 11:51 PM UTC

PDB ID : 9U7Y / pdb\_00009u7y  
EMDB ID : EMD-63947  
Title : Structure of the tip region of the intial complex in bacterial flagellar filament assembly at 3.68 angstroms resolution, conformation 3.  
Authors : Chen, L.X.; Jiang, W.X.; Cheng, X.Q.; Dong, X.; Xing, Q.  
Deposited on : 2025-03-25  
Resolution : 3.68 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](mailto: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>.

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

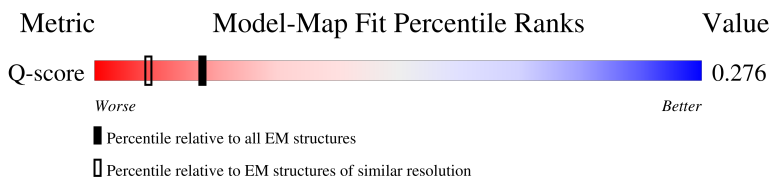
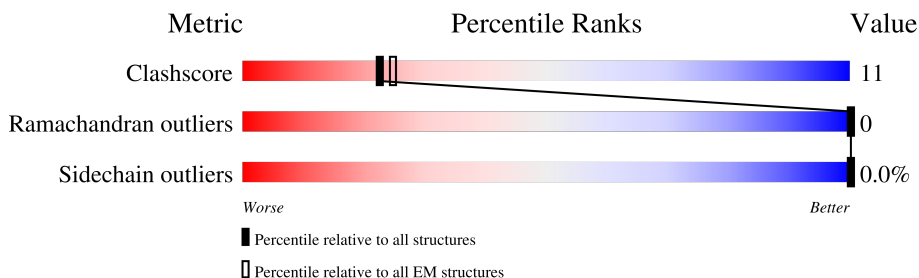
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.68 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.



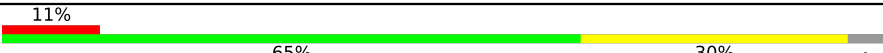

















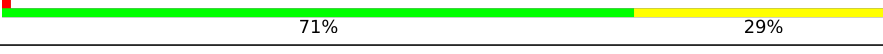

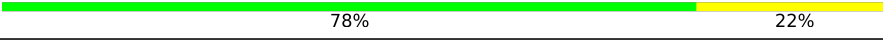




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11376 ( 3.18 - 4.18 )

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  $\geq 3$ , 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	AA	467	
1	AB	467	
1	AD	467	
1	AE	467	












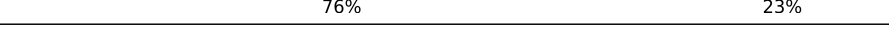







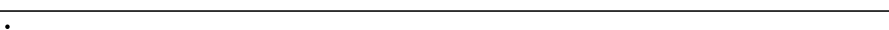

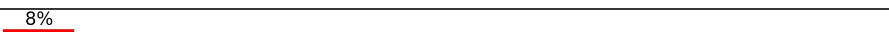
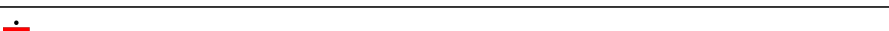


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Mol	Chain	Length	Quality of chain
2	AC	467	
3	BA	317	
3	BB	317	
3	BC	317	
3	BD	317	
3	BE	317	
3	BF	317	
3	BG	317	
3	BH	317	
3	BI	317	
3	BJ	317	
3	BK	317	
4	CA	553	
4	CB	553	
4	CC	553	
4	CD	553	
4	CE	553	
4	CF	553	
4	CG	553	
4	CH	553	
4	CI	553	
4	CJ	553	
4	CK	553	
5	DA	403	
5	DB	403	


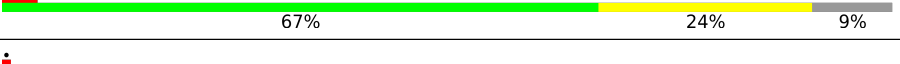
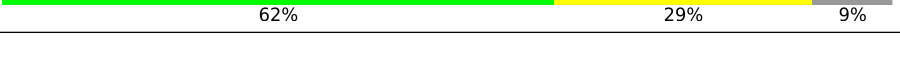
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Mol	Chain	Length	Quality of chain
5	DC	403	
5	DD	403	
5	DE	403	
5	DF	403	
5	DG	403	
5	DH	403	
5	DI	403	
5	DJ	403	
5	DK	403	
5	EA	403	
5	EB	403	
5	EC	403	
5	ED	403	
5	EE	403	
5	EF	403	
5	EG	403	
5	EH	403	
5	EI	403	
5	EJ	403	
5	EK	403	
5	FA	403	
5	FB	403	
5	FC	403	
5	FD	403	
5	FE	403	

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Mol	Chain	Length	Quality of chain
5	FF	403	 5% 60% 22% 13%
5	FG	403	 5% 57% 25% 13%
5	FH	403	 72% 19% 9%
5	FI	403	 61% 26% 13%
5	FJ	403	 5% 67% 24% 4%
5	FK	403	 5% 62% 29% 4%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 181886 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 Flagellar hook-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	452	Total	C	N	O	S	0	0
			3380	2082	570	722	6		
1	AB	448	Total	C	N	O	S	0	0
			3353	2064	566	717	6		
1	AD	447	Total	C	N	O	S	0	0
			3350	2063	565	716	6		
1	AE	447	Total	C	N	O	S	0	0
			3350	2063	565	716	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	447	Total	C	N	O	S	0	0
			3349	2063	565	715	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	47	PHE	TYR	conflict	UNP P16328

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BB	316	Total	C	N	O	S	0	0
			2383	1458	416	497	12		
3	BC	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BD	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BE	316	Total	C	N	O	S	0	0
			2383	1458	416	497	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BF	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BG	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BH	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BI	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BJ	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BK	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		

- Molecule 4 is a protein called Flagellar hook-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CA	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CB	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CC	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CD	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CE	552	Total	C	N	O	S	0	0
			4149	2548	725	870	6		
4	CF	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CG	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CH	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CI	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CJ	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CK	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		

- Molecule 5 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DA	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DB	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DC	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DD	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DE	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DF	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DG	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DH	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DI	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DJ	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	DK	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EA	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EB	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EC	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	ED	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EE	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EF	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EG	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EH	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EI	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EJ	402	Total 2959	C 1820	N 511	O 620	S 8	0	0
5	EK	402	Total 2959	C 1820	N 511	O 620	S 8	0	0

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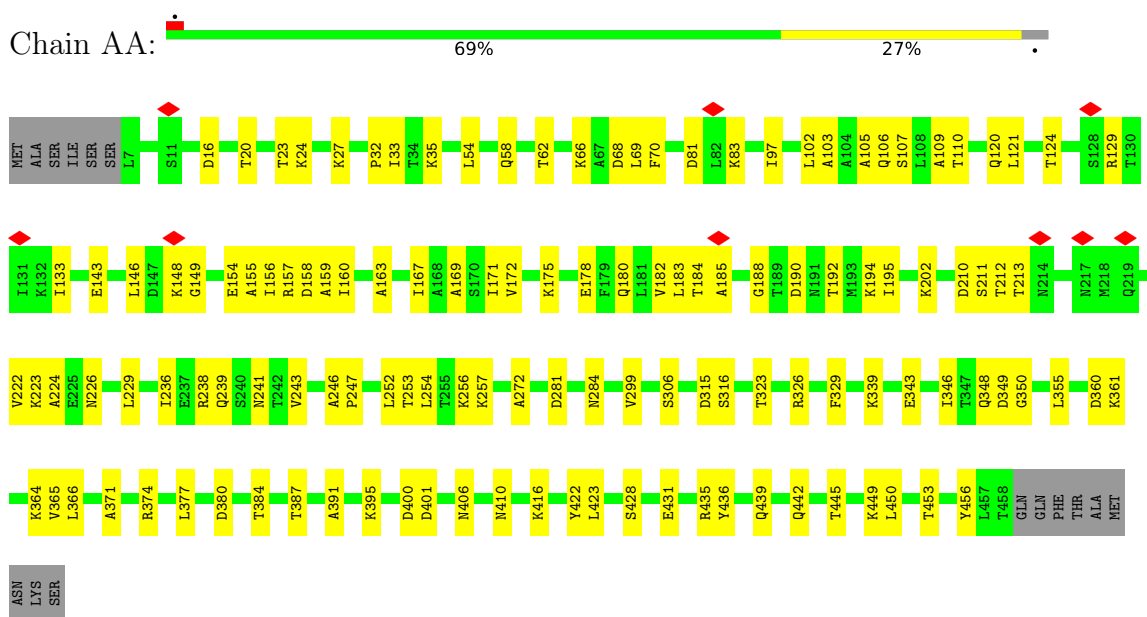
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	FA	347	Total	C	N	O	S	0	0
			2537	1560	435	535	7		
5	FB	345	Total	C	N	O	S	0	0
			2527	1549	434	538	6		
5	FC	330	Total	C	N	O	S	0	0
			2426	1489	416	515	6		
5	FD	330	Total	C	N	O	S	0	0
			2426	1489	416	515	6		
5	FE	366	Total	C	N	O	S	0	0
			2668	1641	457	563	7		
5	FF	330	Total	C	N	O	S	0	0
			2426	1489	416	515	6		
5	FG	330	Total	C	N	O	S	0	0
			2426	1489	416	515	6		
5	FH	366	Total	C	N	O	S	0	0
			2668	1641	457	563	7		
5	FI	352	Total	C	N	O	S	0	0
			2562	1576	440	539	7		
5	FJ	366	Total	C	N	O	S	0	0
			2668	1641	457	563	7		
5	FK	366	Total	C	N	O	S	0	0
			2668	1641	457	563	7		

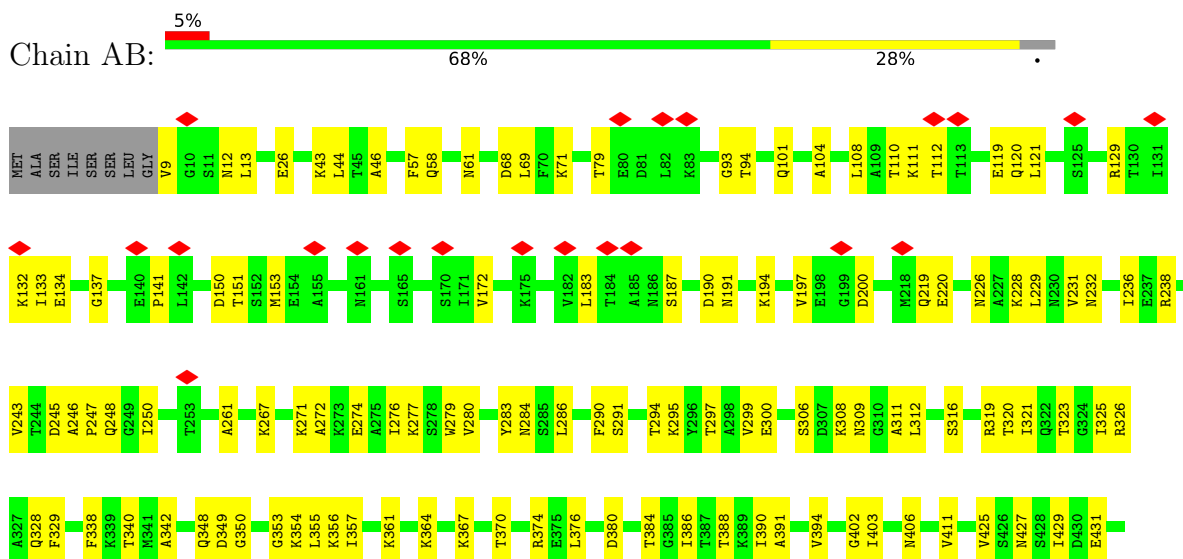
### 3 Residue-property plots [i](#)

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-associated protein 2



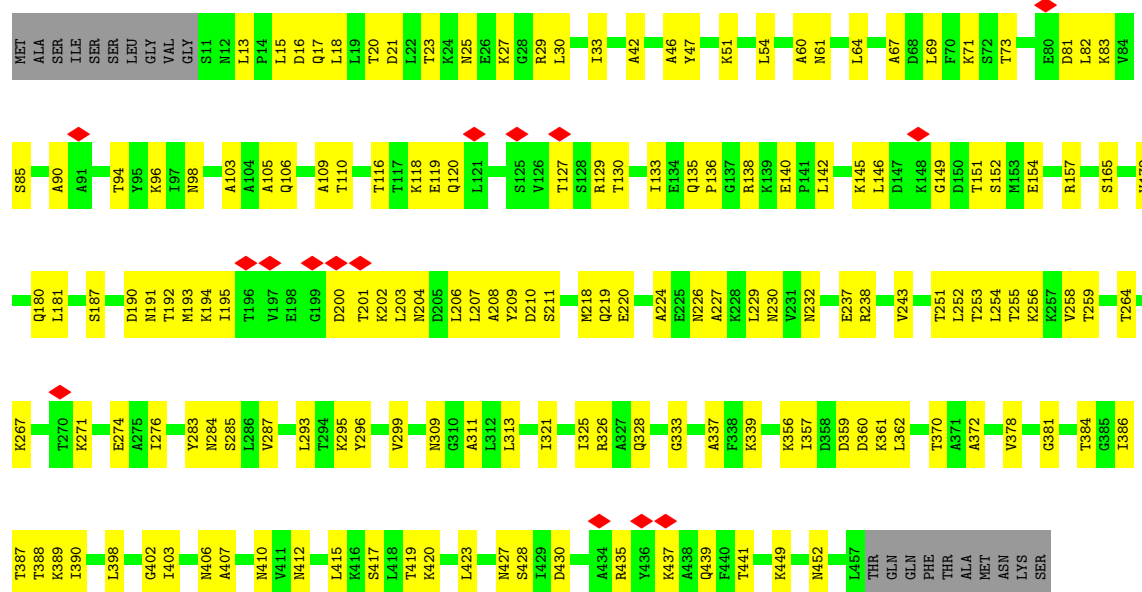
#### • Molecule 1: Flagellar hook-associated protein 2





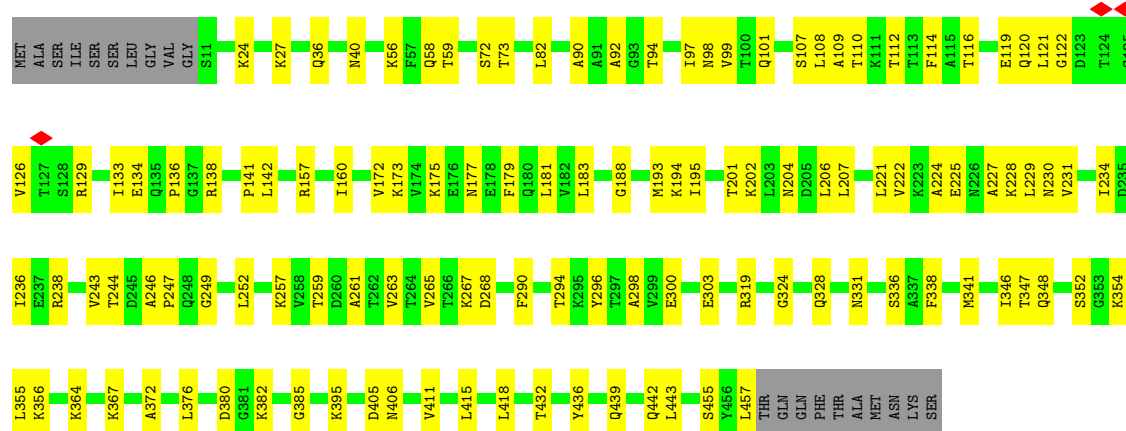
• Molecule 1: Flagellar hook-associated protein 2

Chain AD: 61% 34%



• Molecule 1: Flagellar hook-associated protein 2

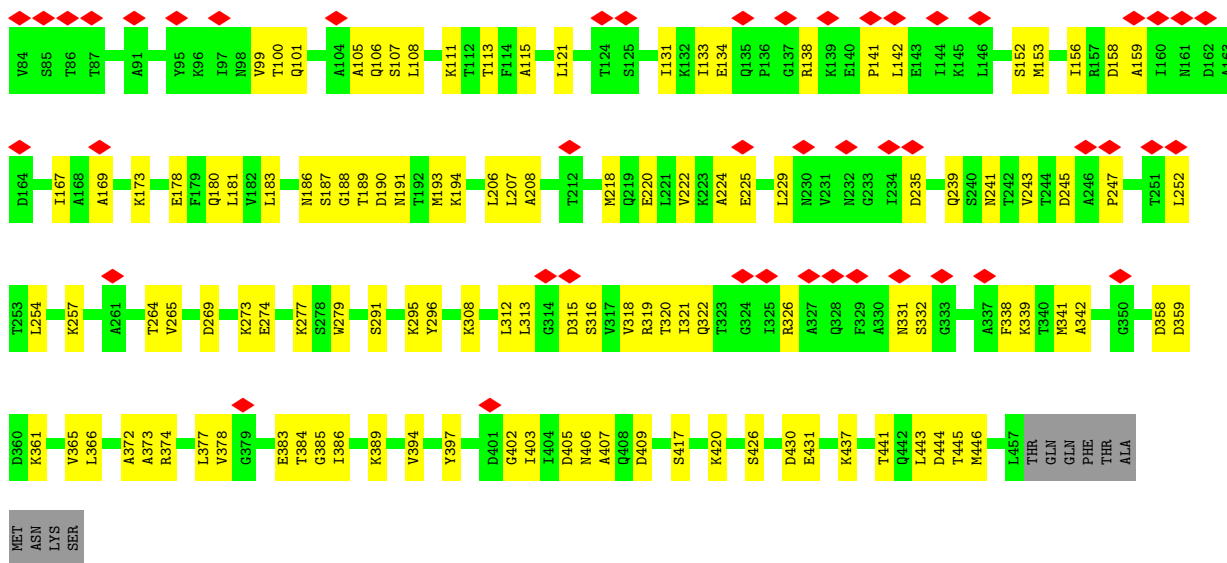
Chain AE: 70% 25%



• Molecule 2: Flagellar hook-associated protein 2

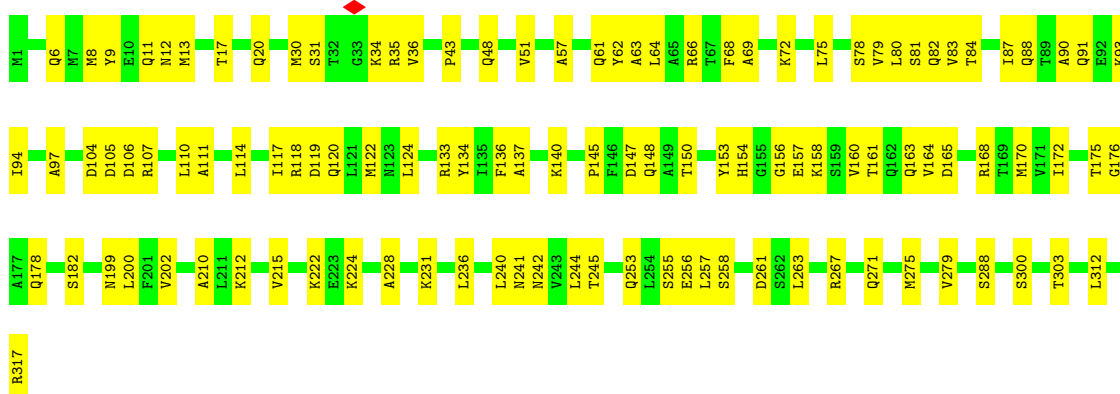
Chain AC: 11% 65% 30%





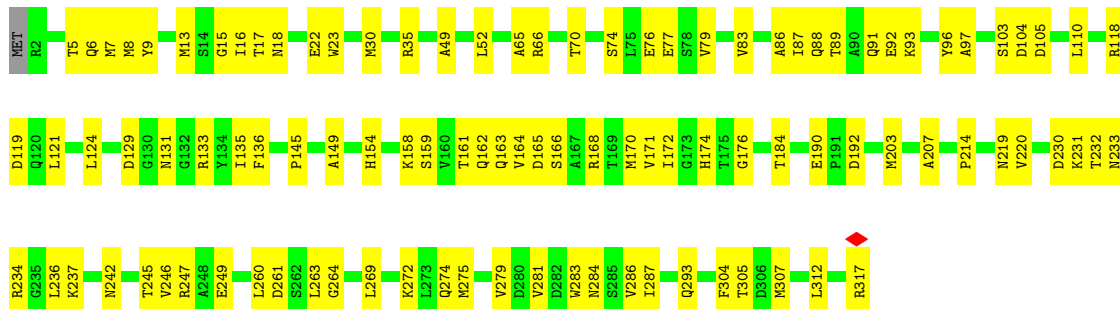
• Molecule 3: Flagellar hook-associated protein 3

Chain BA: 65% 35%



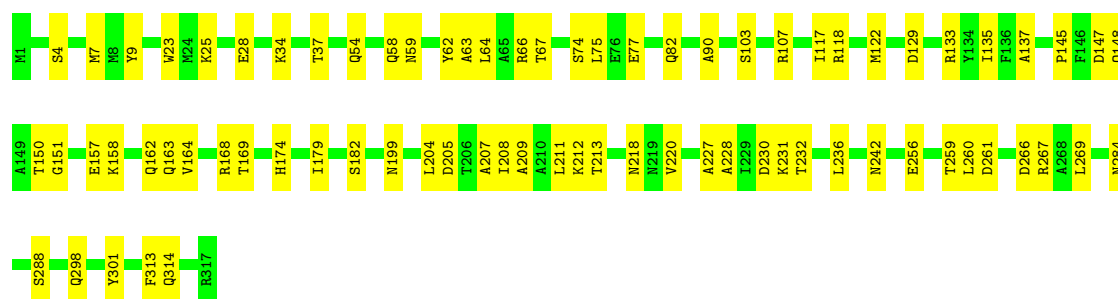
• Molecule 3: Flagellar hook-associated protein 3

Chain BB: 67% 32%



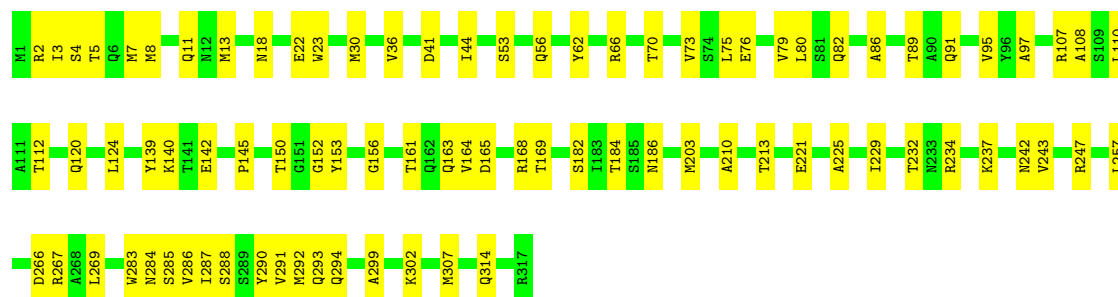
• Molecule 3: Flagellar hook-associated protein 3

Chain BC: 76% 24%



• Molecule 3: Flagellar hook-associated protein 3

Chain BD: 73% 27%



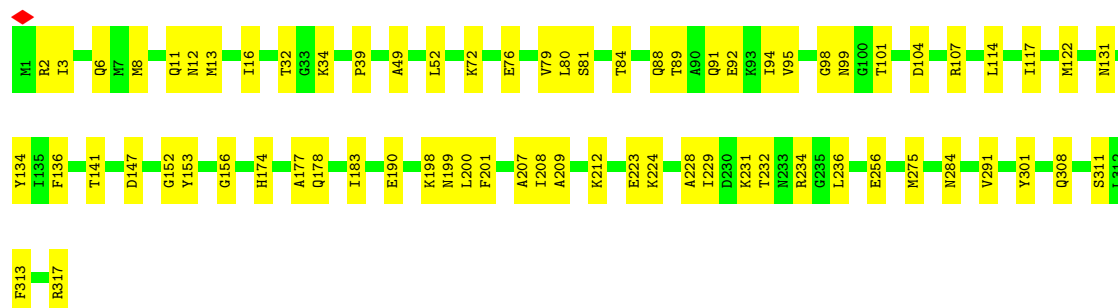
• Molecule 3: Flagellar hook-associated protein 3

Chain BE: 76% 23%

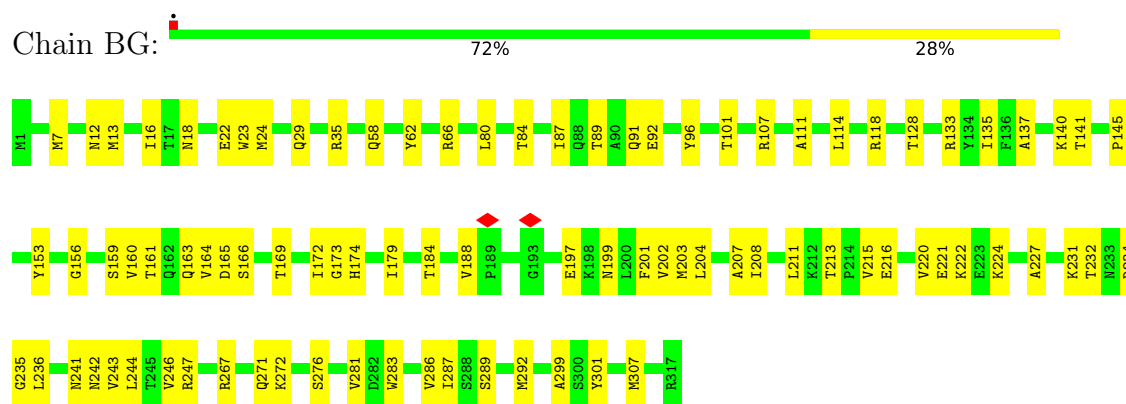


• Molecule 3: Flagellar hook-associated protein 3

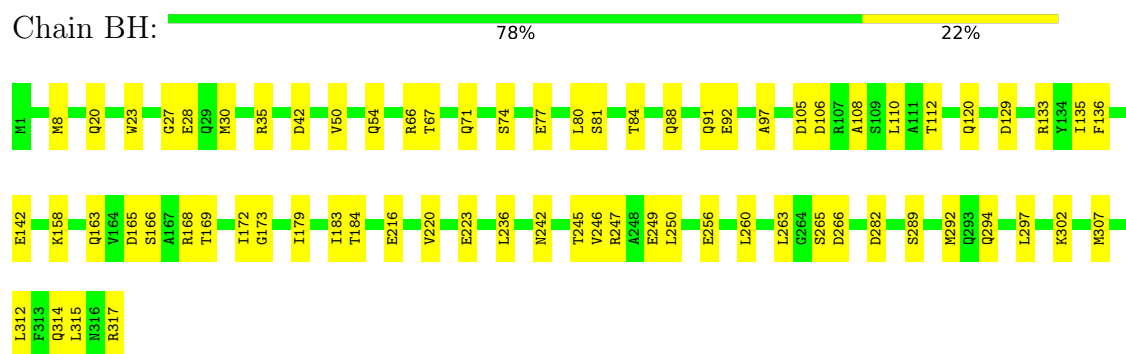
Chain BF: 78% 22%



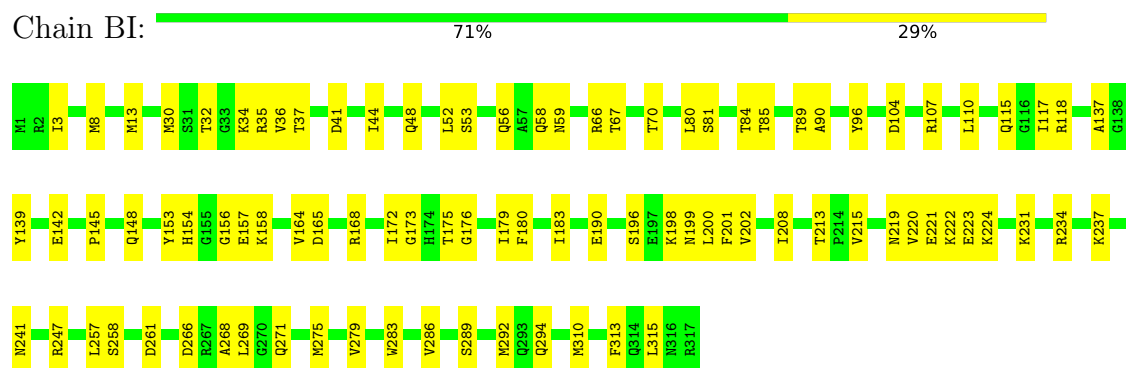
- Molecule 3: Flagellar hook-associated protein 3



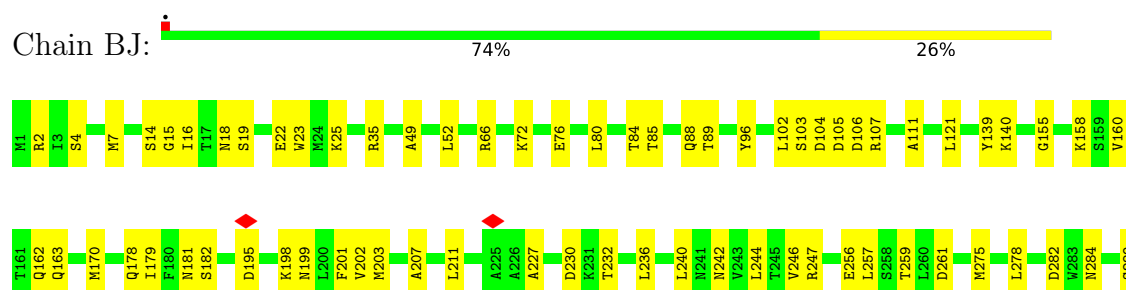
- Molecule 3: Flagellar hook-associated protein 3

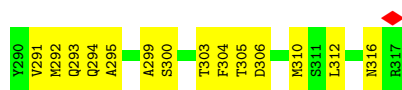


- Molecule 3: Flagellar hook-associated protein 3



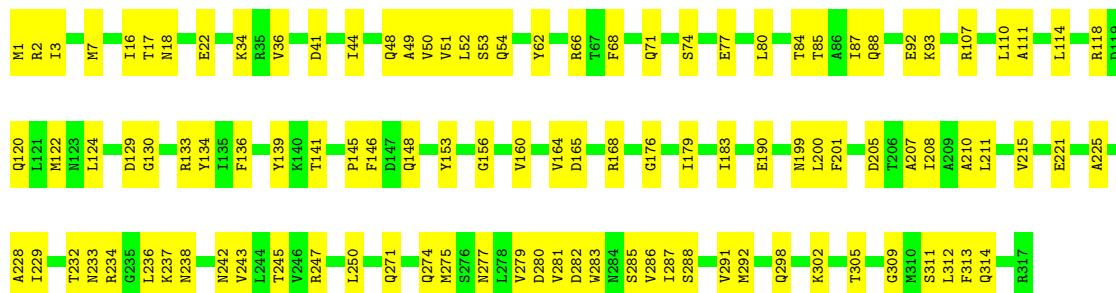
- Molecule 3: Flagellar hook-associated protein 3





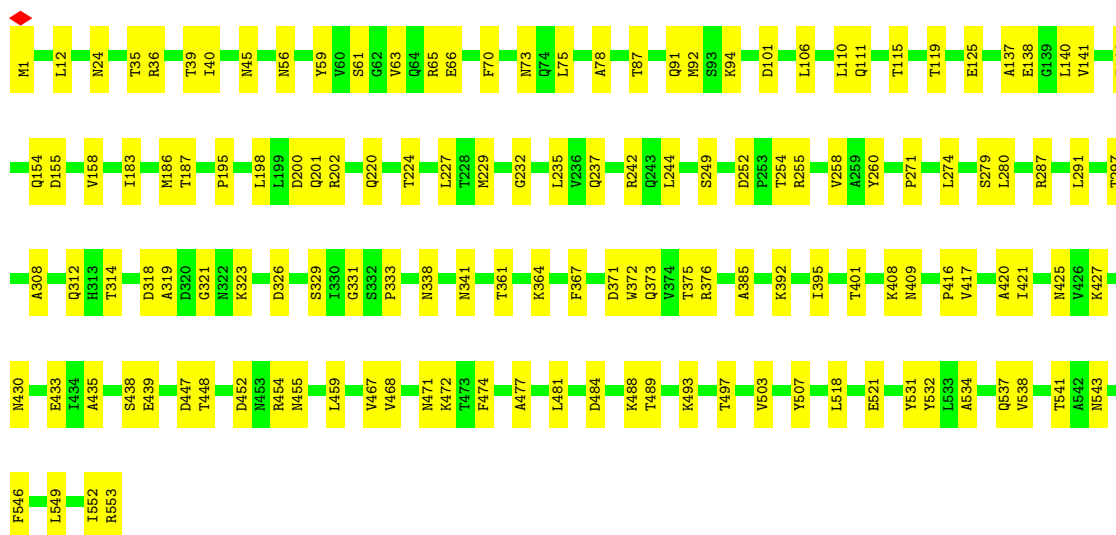
• Molecule 3: Flagellar hook-associated protein 3

Chain BK: 66% 34%



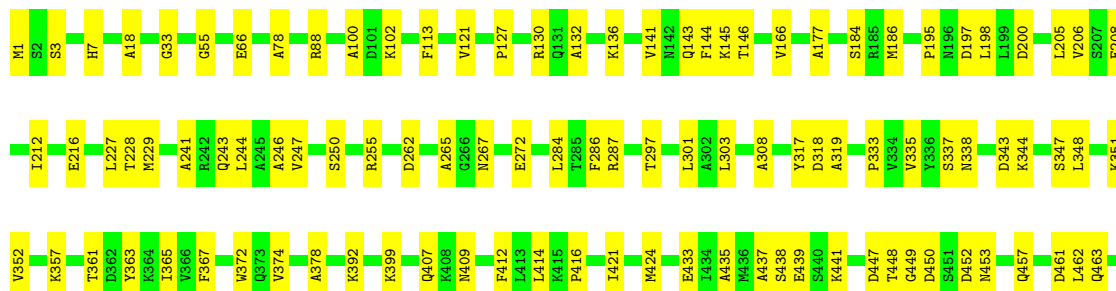
• Molecule 4: Flagellar hook-associated protein 1

Chain CA: 75% 25%



• Molecule 4: Flagellar hook-associated protein 1

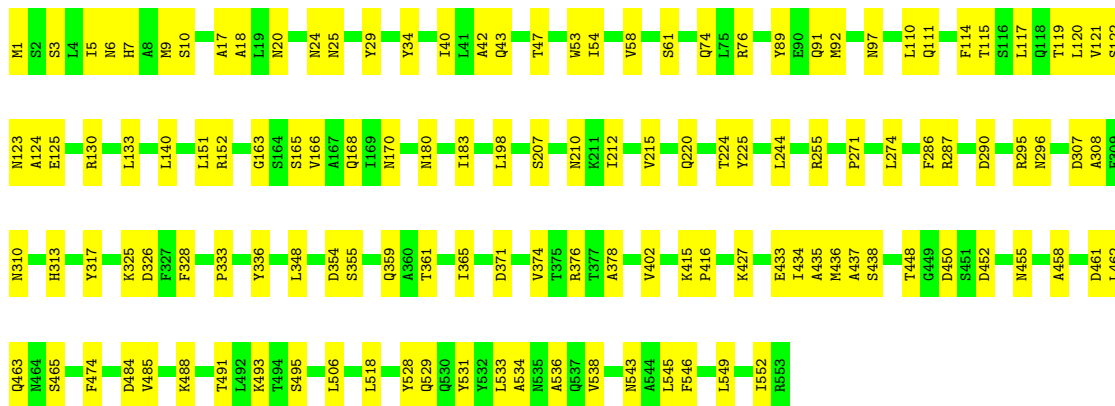
Chain CB: 77% 23%





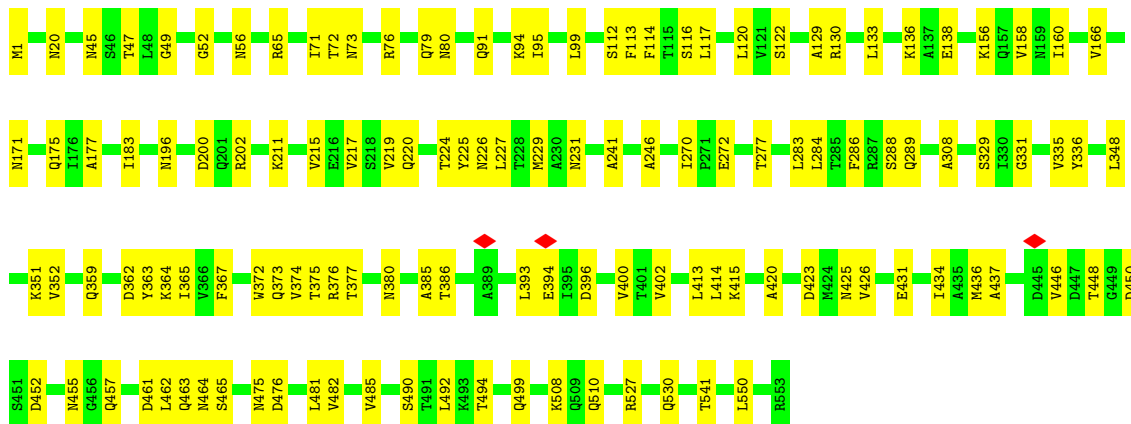
• Molecule 4: Flagellar hook-associated protein 1

Chain CC: 77% 23%



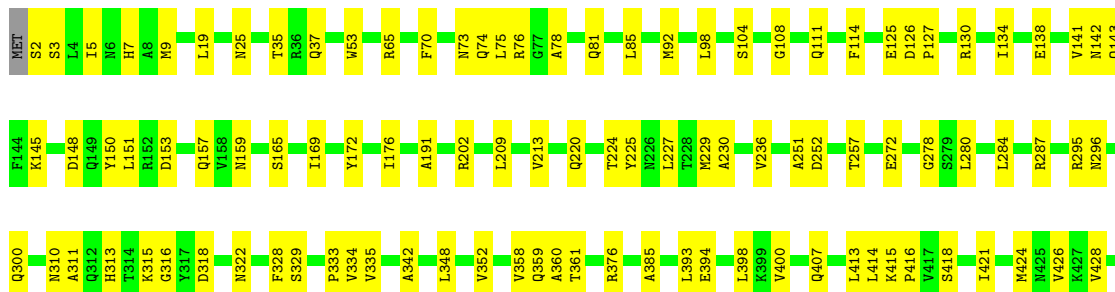
• Molecule 4: Flagellar hook-associated protein 1

Chain CD: 77% 23%



• Molecule 4: Flagellar hook-associated protein 1

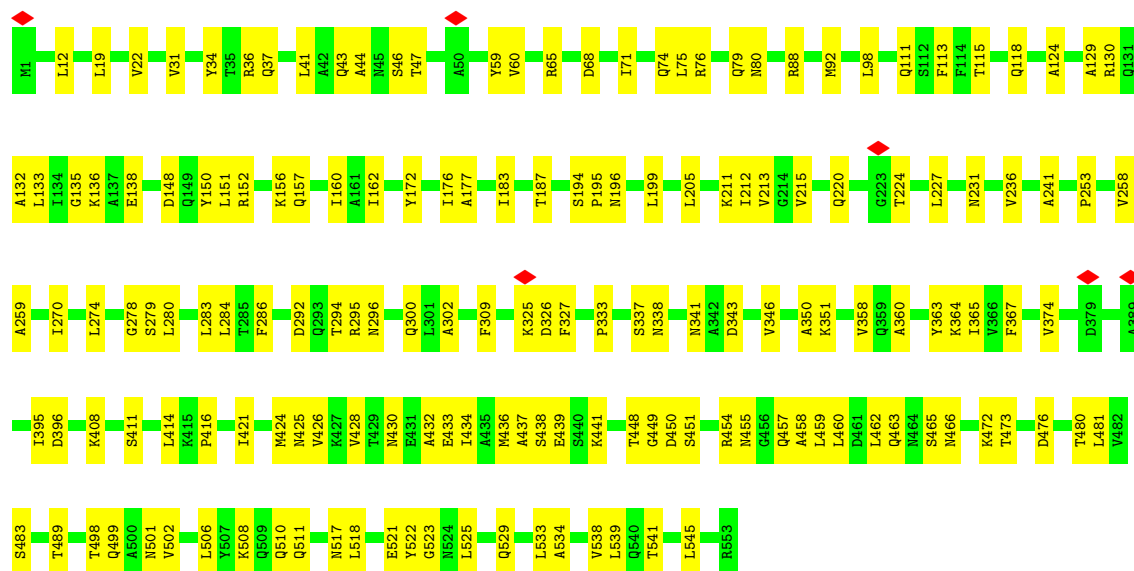
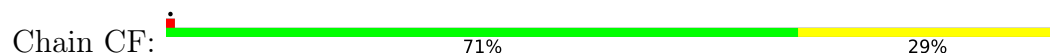
Chain CE: 77% 23%



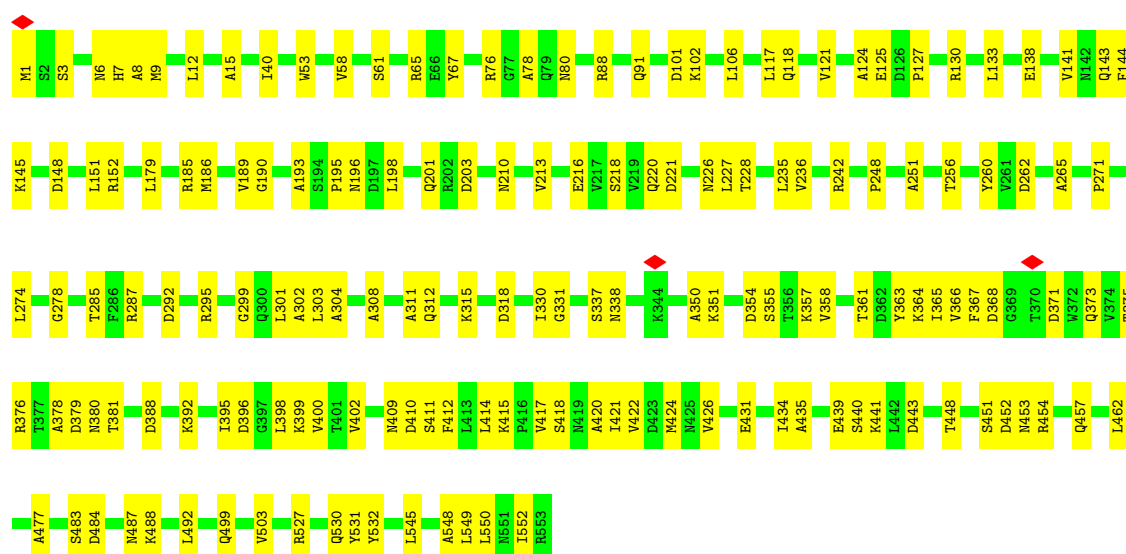




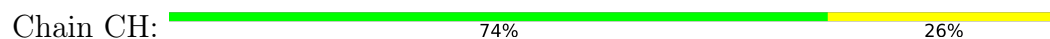
• Molecule 4: Flagellar hook-associated protein 1

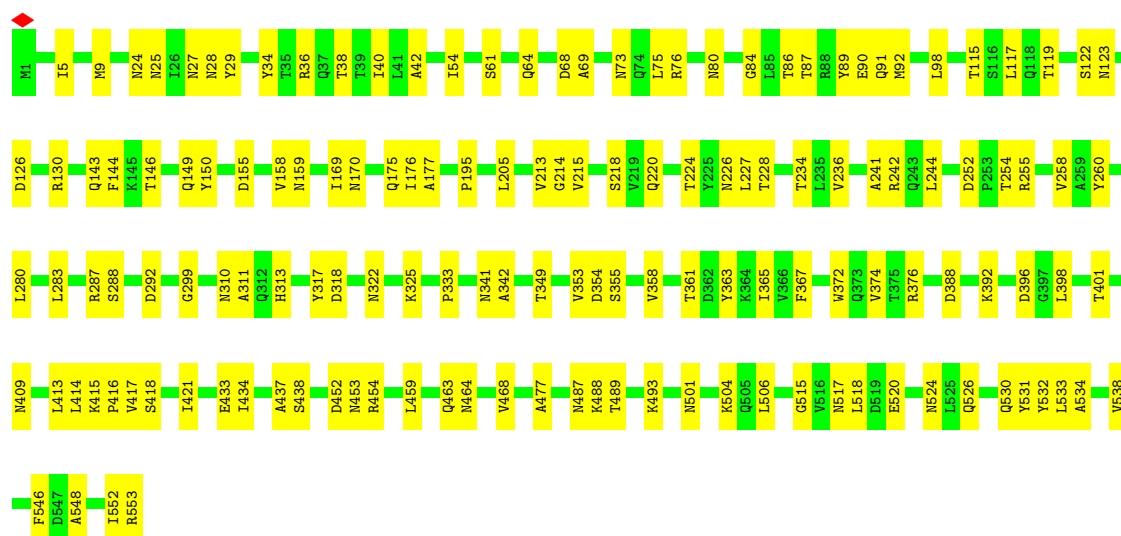


• Molecule 4: Flagellar hook-associated protein 1



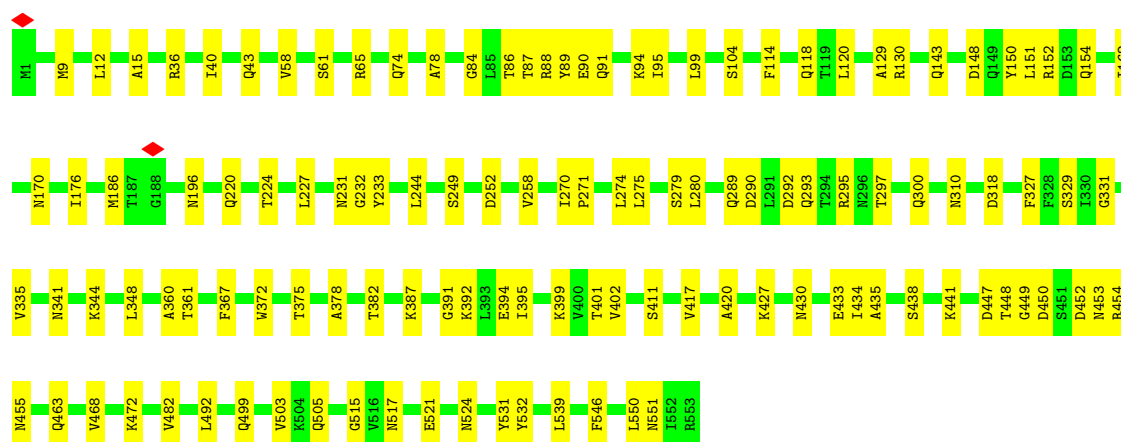
• Molecule 4: Flagellar hook-associated protein 1





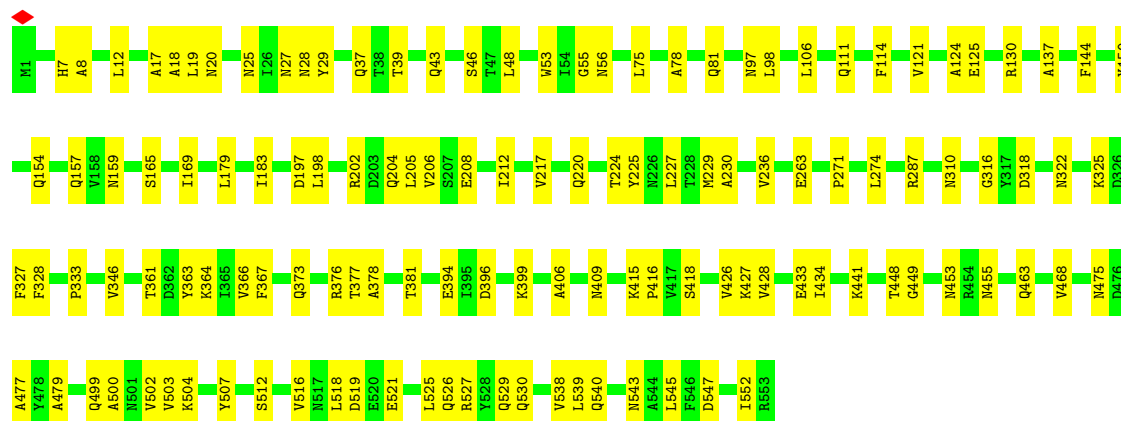
• Molecule 4: Flagellar hook-associated protein 1

Chain CI: 78% 22%

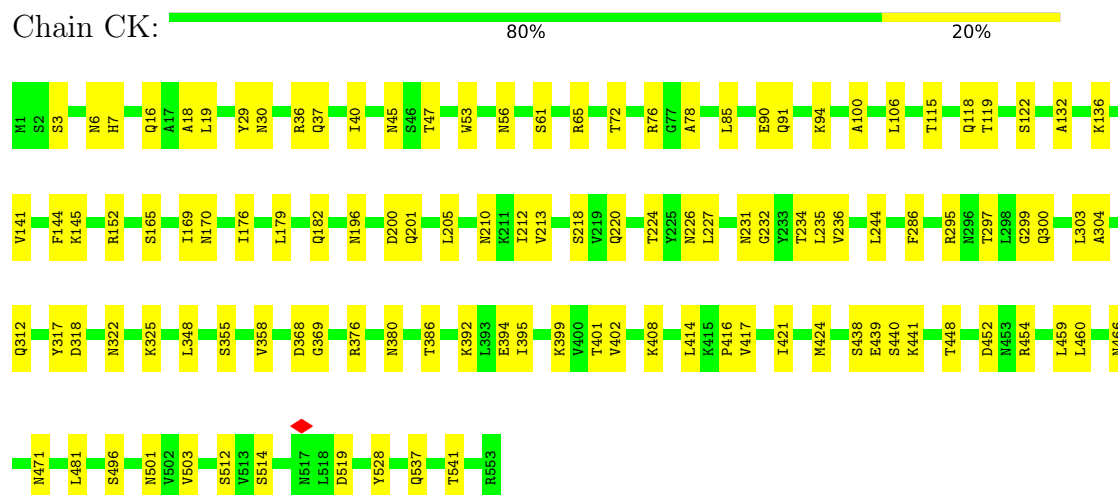


• Molecule 4: Flagellar hook-associated protein 1

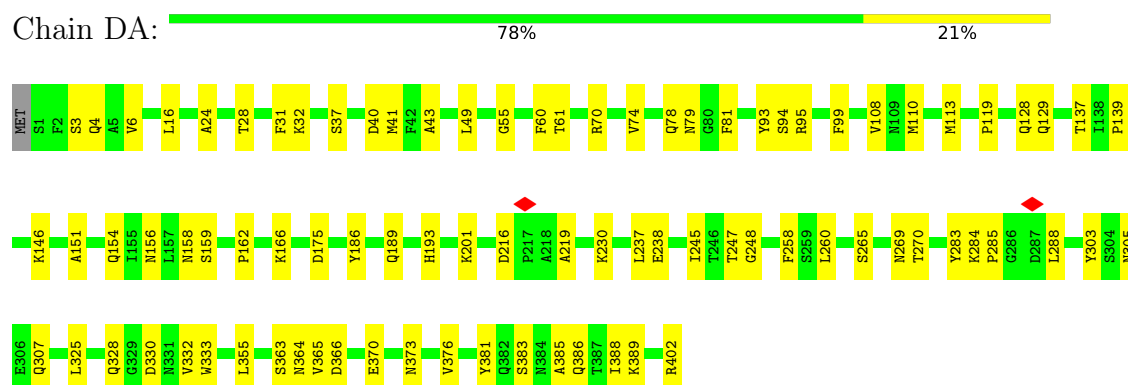
Chain CJ: 77% 23%



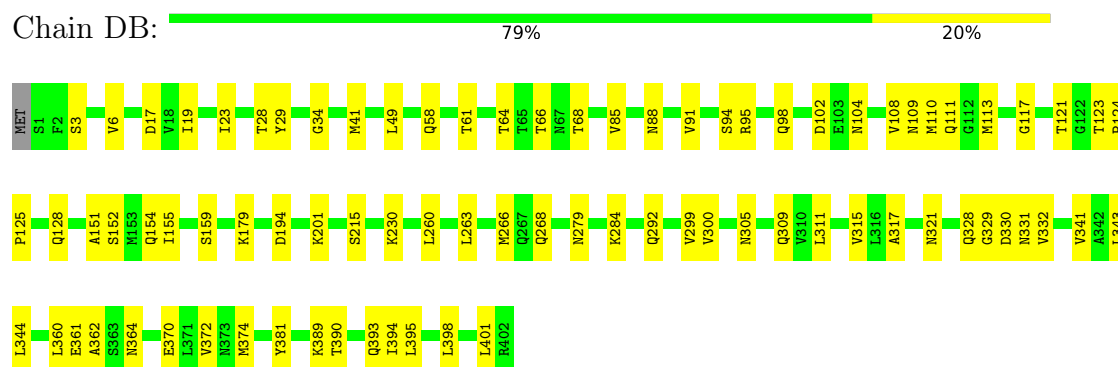
- Molecule 4: Flagellar hook-associated protein 1



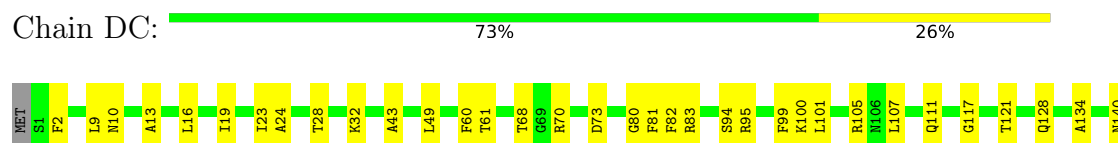
- Molecule 5: Flagellar hook protein FlgE

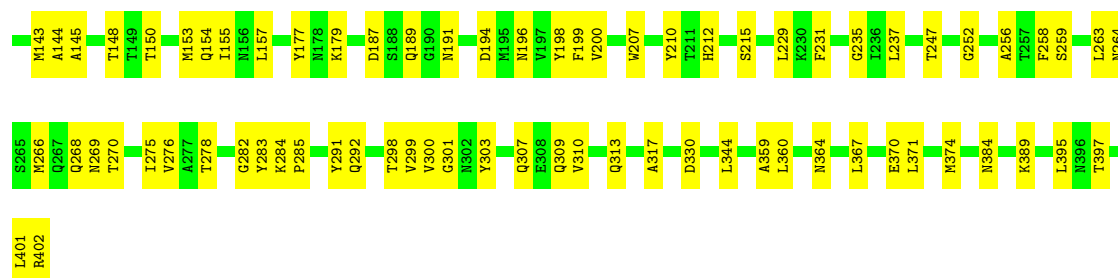


- Molecule 5: Flagellar hook protein FlgE



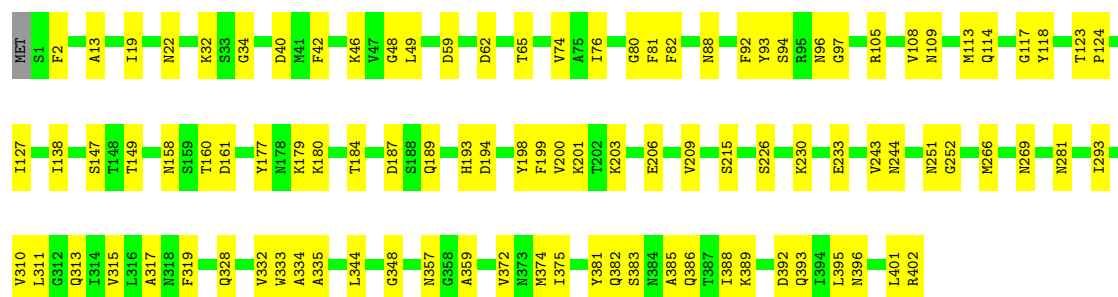
- Molecule 5: Flagellar hook protein FlgE





• Molecule 5: Flagellar hook protein FlgE

Chain DD:   75% 25%



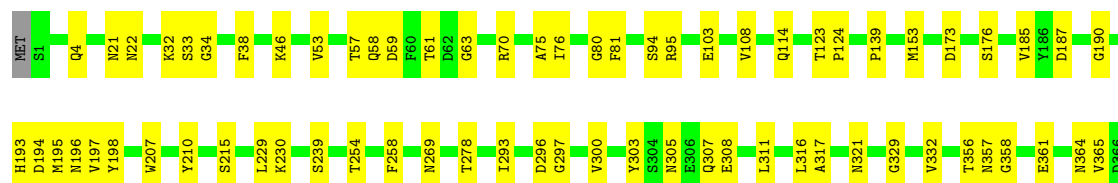
• Molecule 5: Flagellar hook protein FlgE

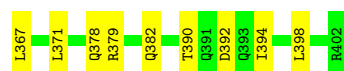
Chain DE:   74% 26%



• Molecule 5: Flagellar hook protein FlgE

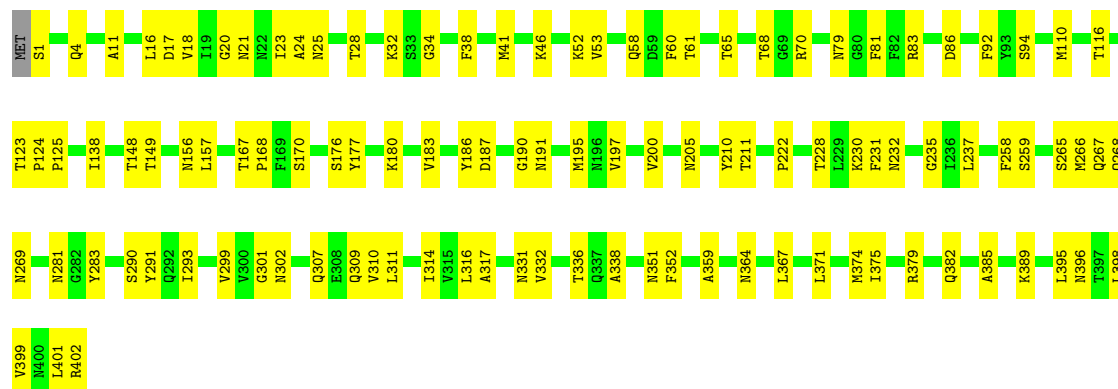
Chain DF:   80% 19%





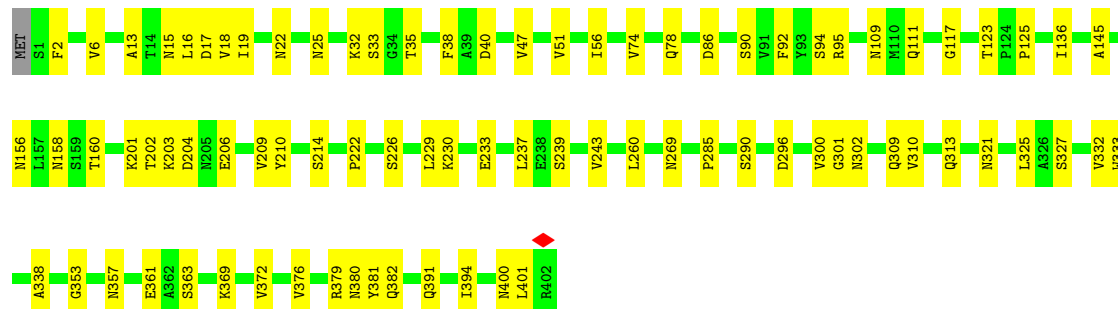
• Molecule 5: Flagellar hook protein FlgE

Chain DG: 73% 27%



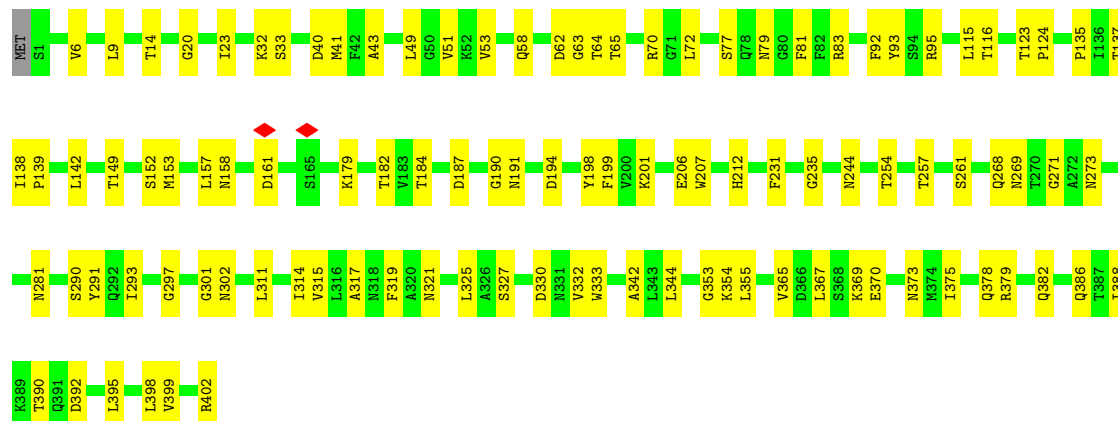
• Molecule 5: Flagellar hook protein FlgE

Chain DH: 79% 21%

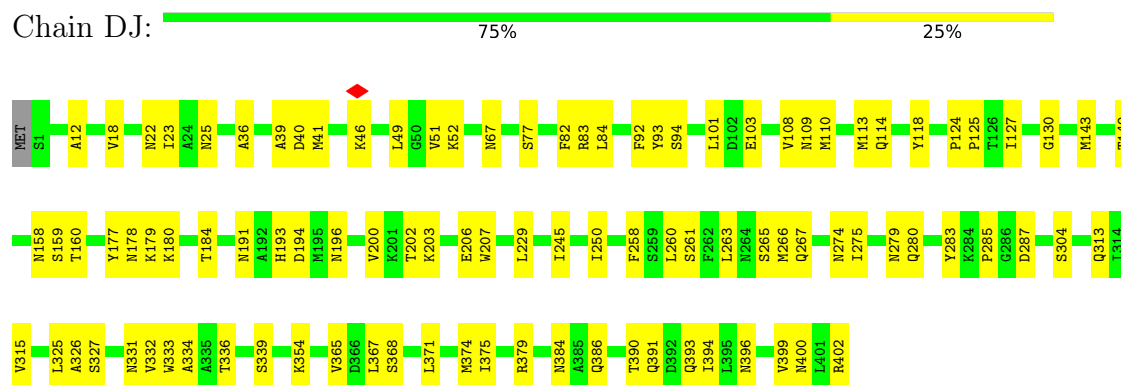


• Molecule 5: Flagellar hook protein FlgE

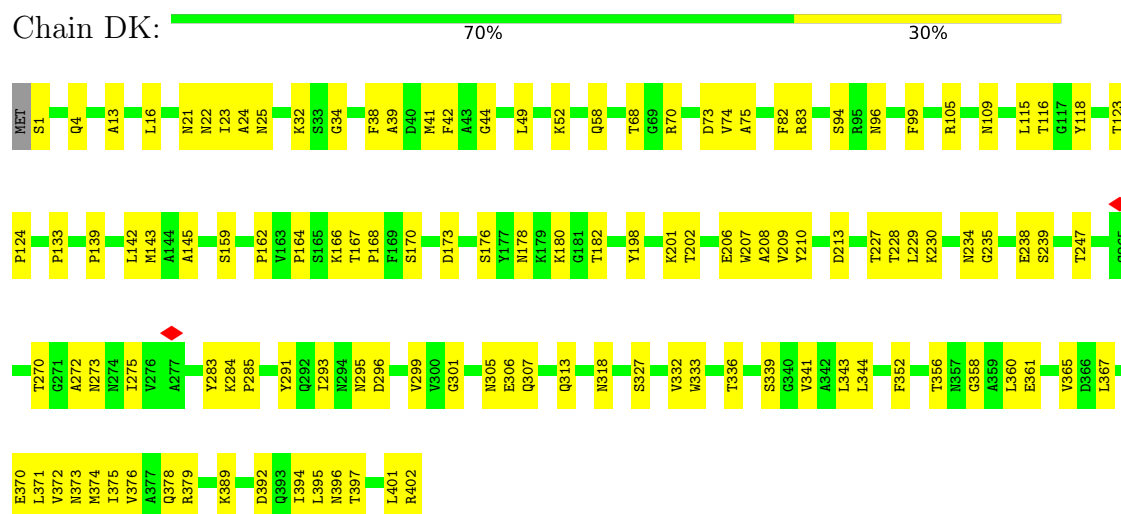
Chain DI: 73% 26%



- Molecule 5: Flagellar hook protein FlgE



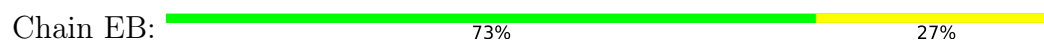
- Molecule 5: Flagellar hook protein FlgE

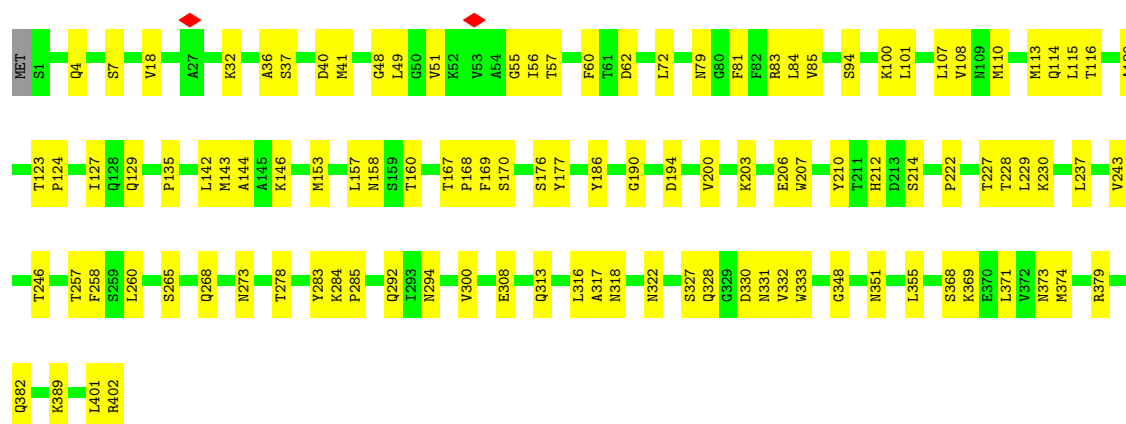


- Molecule 5: Flagellar hook protein FlgE



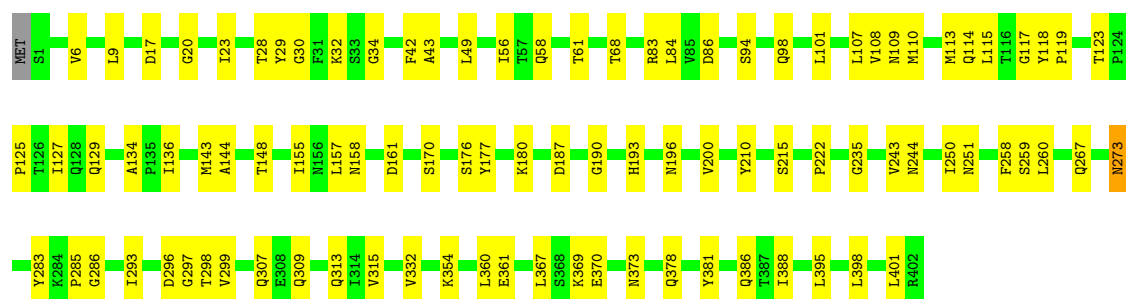
- Molecule 5: Flagellar hook protein FlgE





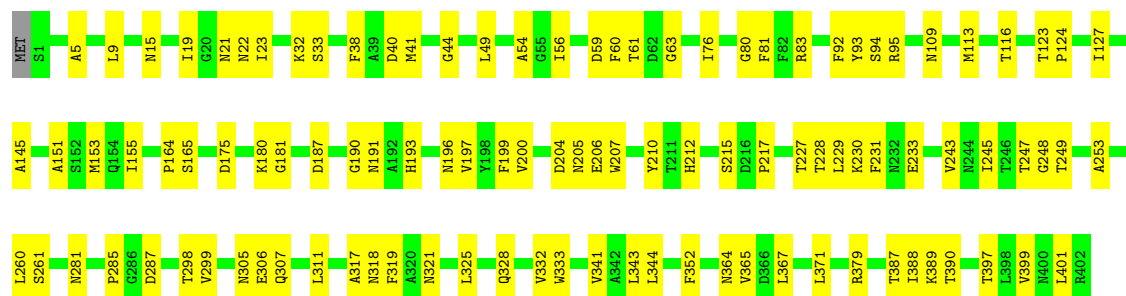
• Molecule 5: Flagellar hook protein FlgE

Chain EC:   76% 23%



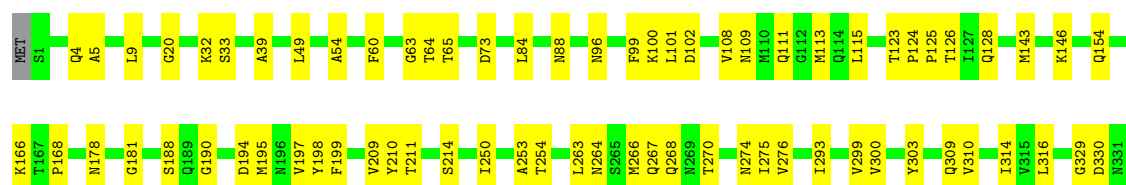
• Molecule 5: Flagellar hook protein FlgE

Chain ED:   73% 26%



• Molecule 5: Flagellar hook protein FlgE

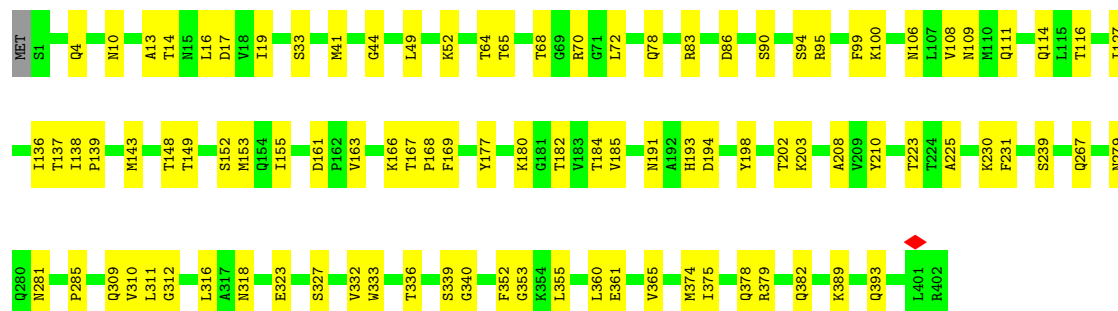
Chain EE:   77% 23%





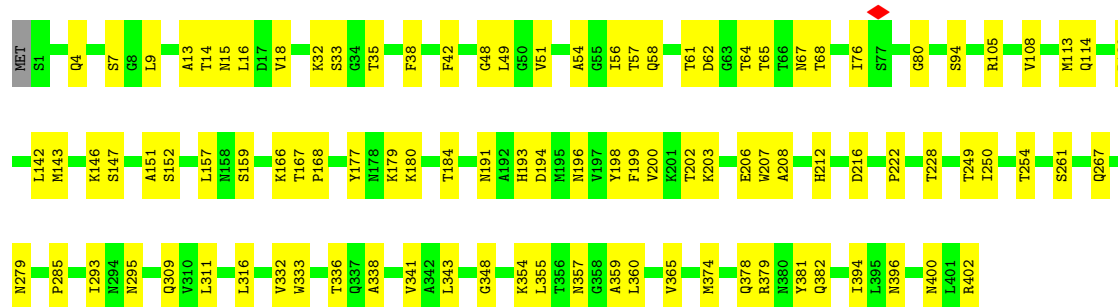
• Molecule 5: Flagellar hook protein FlgE

Chain EF: 76% 24%



• Molecule 5: Flagellar hook protein FlgE

Chain EG: 75% 25%



• Molecule 5: Flagellar hook protein FlgE

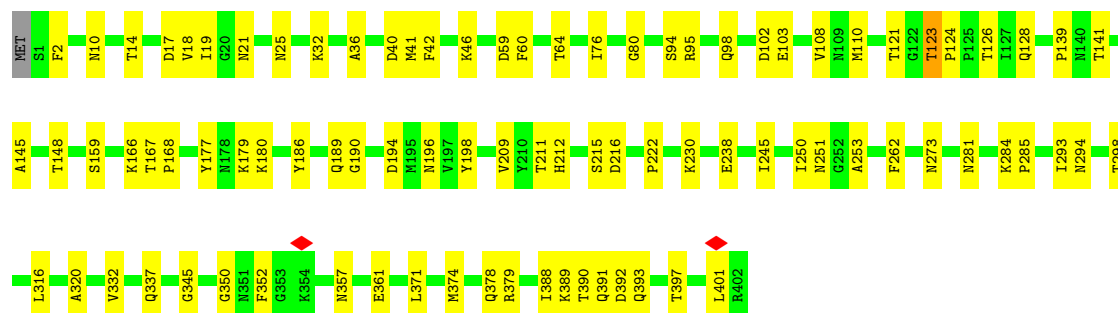
Chain EH: 77% 22%



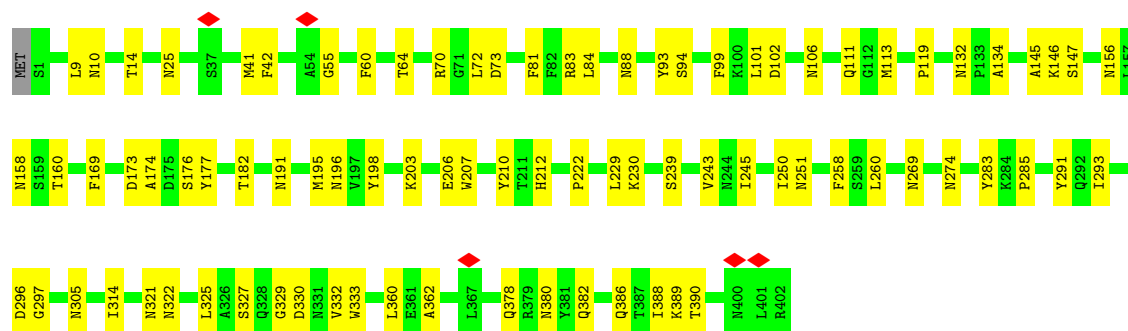
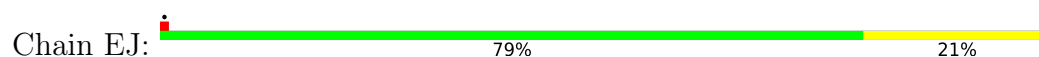
• Molecule 5: Flagellar hook protein FlgE

Chain EI: 78% 22%

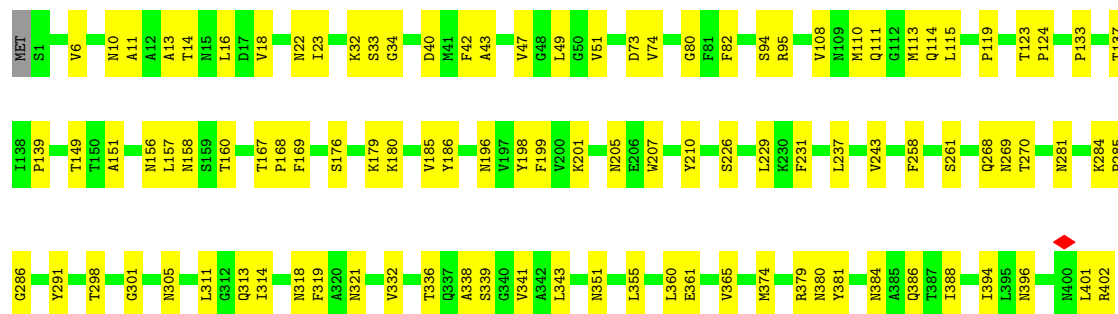




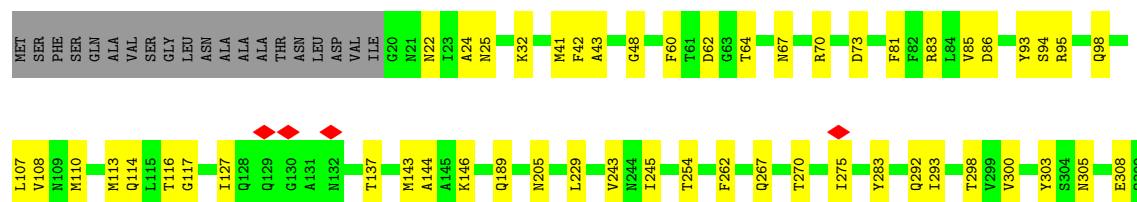
• Molecule 5: Flagellar hook protein FlgE



• Molecule 5: Flagellar hook protein FlgE

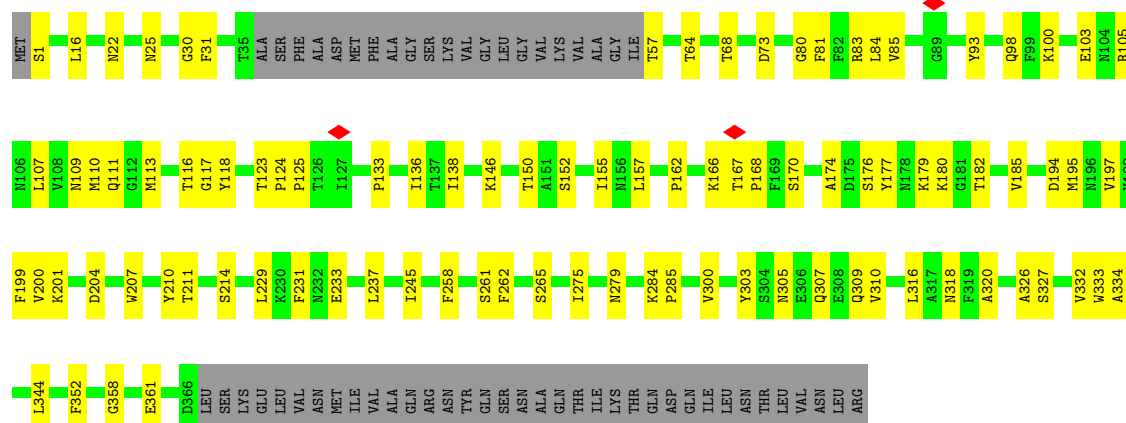


• Molecule 5: Flagellar hook protein FlgE

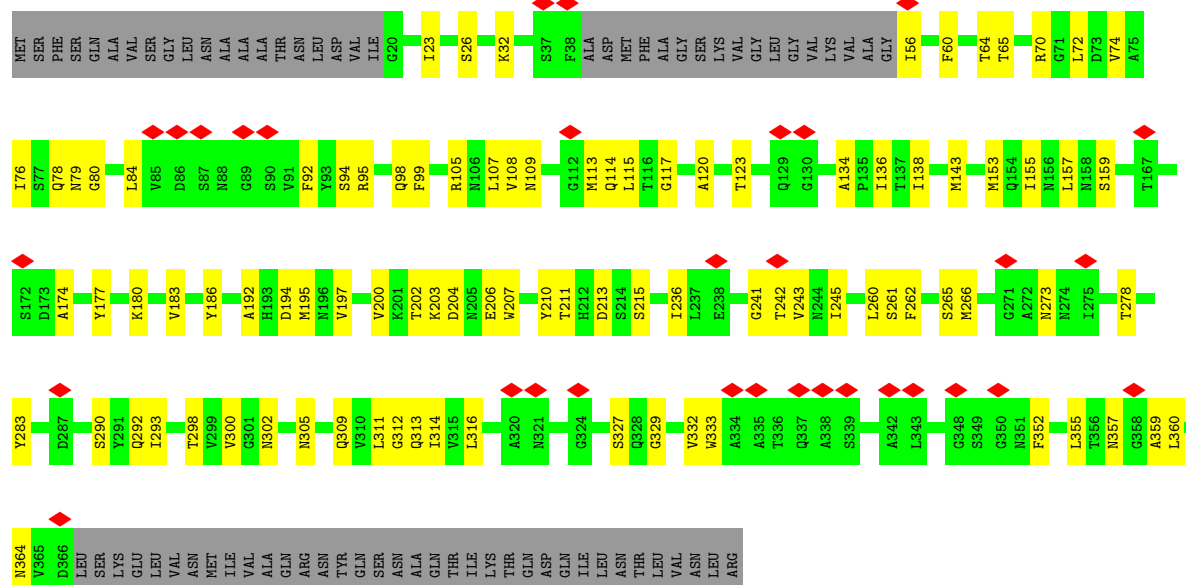




• Molecule 5: Flagellar hook protein FlgE



• Molecule 5: Flagellar hook protein FlgE

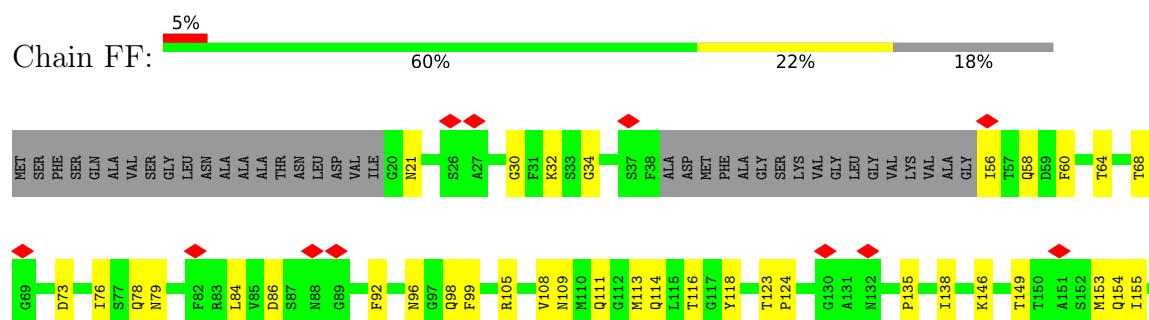


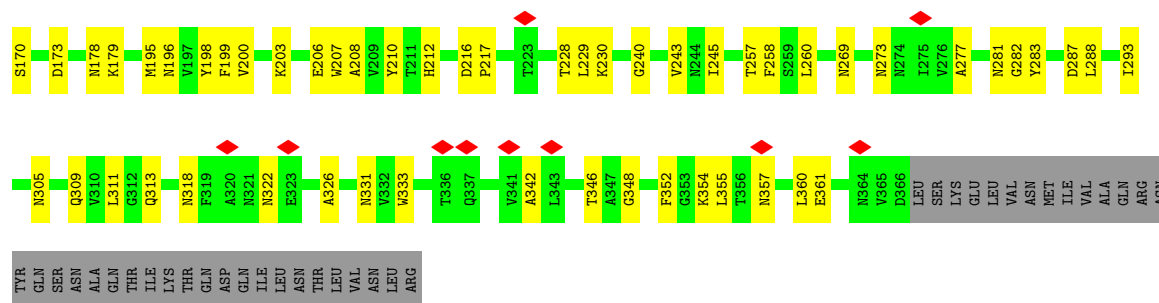
• Molecule 5: Flagellar hook protein FlgE



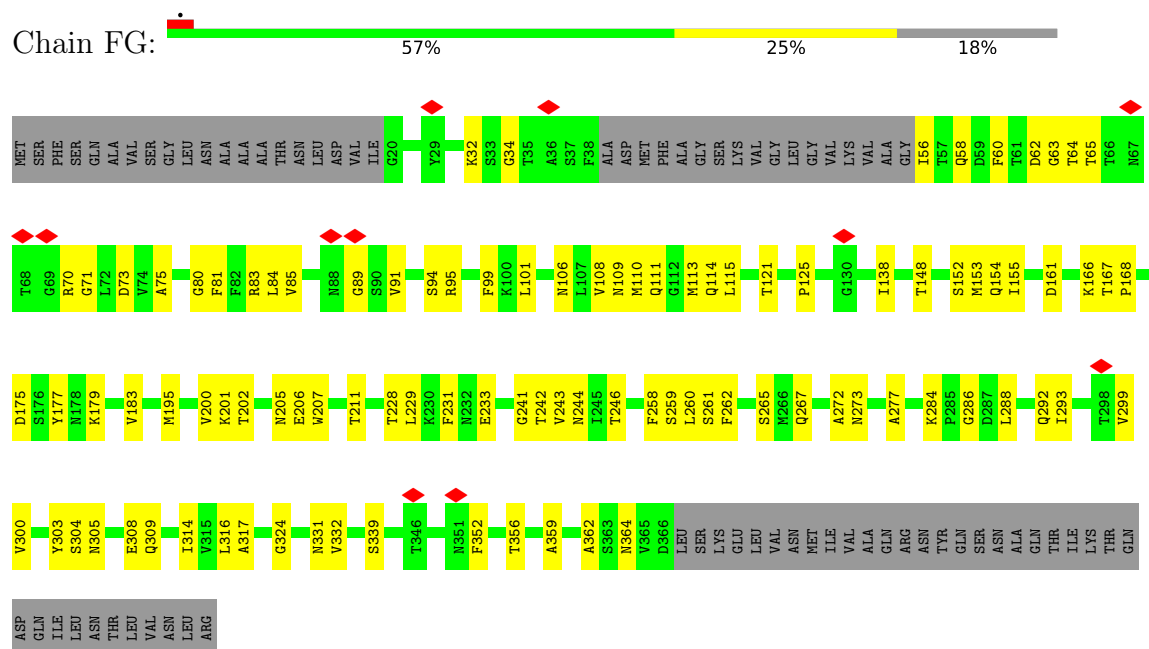
- Molecule 5: Flagellar hook protein FlgE

- Molecule 5: Flagellar hook protein FlgE

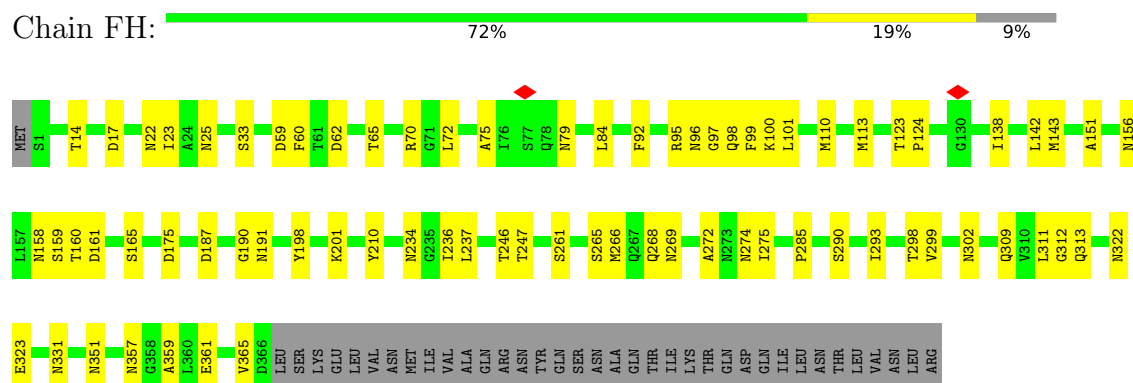




- Molecule 5: Flagellar hook protein FlgE

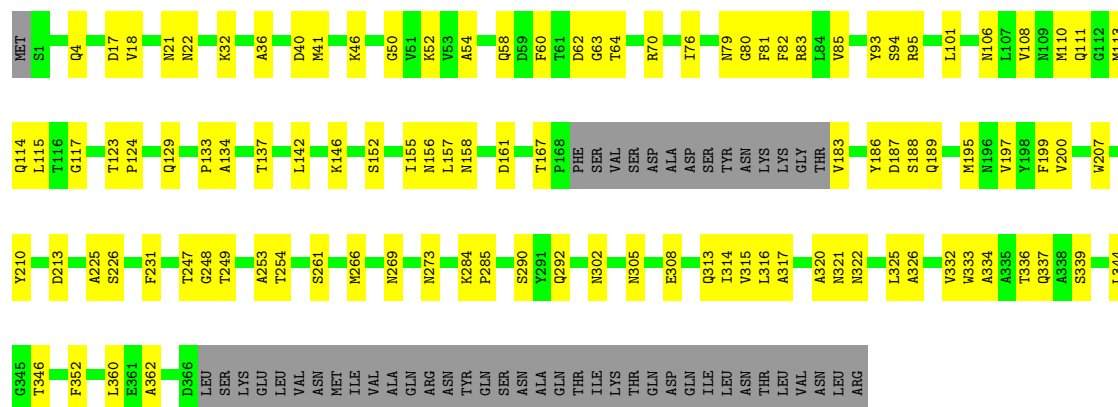


- Molecule 5: Flagellar hook protein FlgE



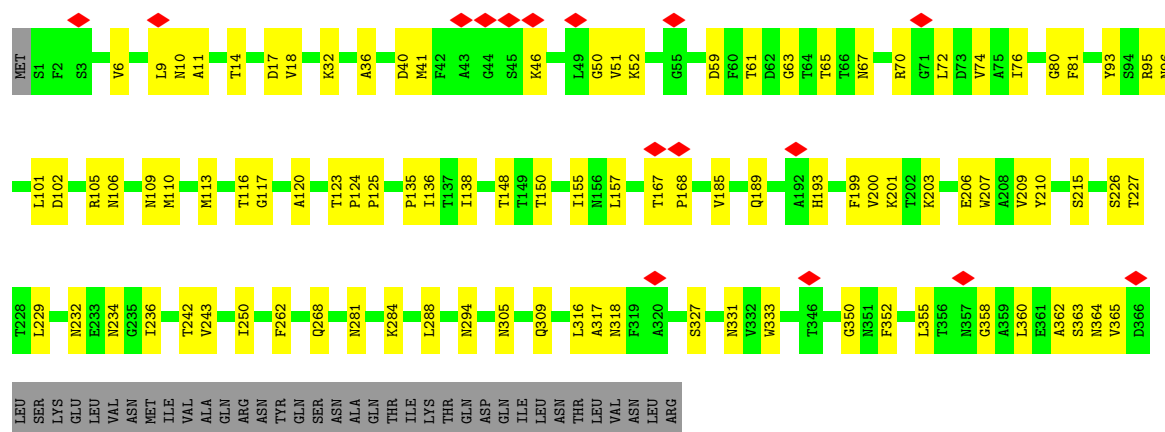
- Molecule 5: Flagellar hook protein FlgE





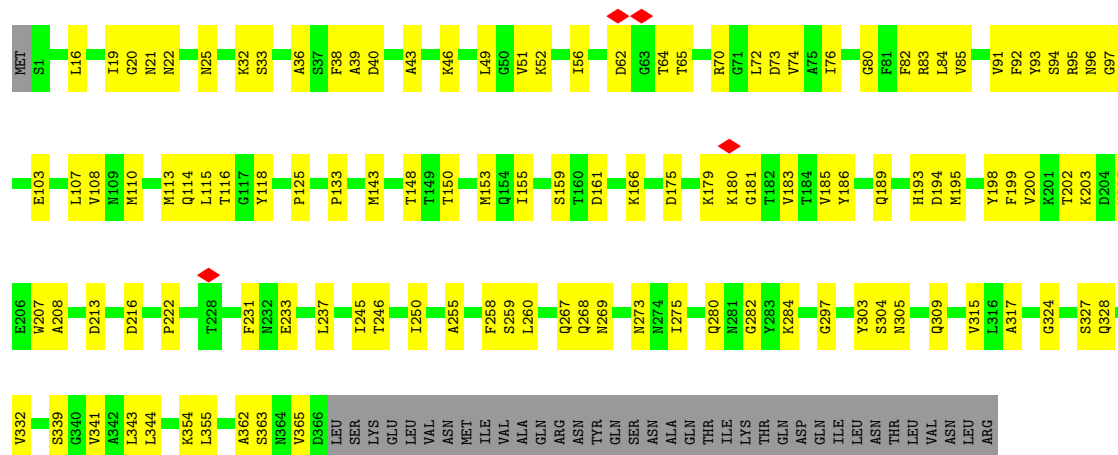
• Molecule 5: Flagellar hook protein FlgE

Chain FJ: 67% 24% 9%



• Molecule 5: Flagellar hook protein FlgE

Chain FK: 62% 29% 9%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.543	Depositor
Minimum map value	-0.315	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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	AA	0.13	0/3404	0.31	0/4609
1	AB	0.13	0/3377	0.30	0/4572
1	AD	0.13	0/3374	0.35	0/4568
1	AE	0.11	0/3374	0.28	0/4568
2	AC	0.12	0/3373	0.34	0/4566
3	BA	0.15	0/2417	0.36	0/3268
3	BB	0.16	0/2409	0.38	0/3258
3	BC	0.14	0/2417	0.31	0/3268
3	BD	0.16	0/2417	0.33	0/3268
3	BE	0.17	0/2409	0.35	0/3258
3	BF	0.16	0/2417	0.34	0/3268
3	BG	0.15	0/2417	0.34	0/3268
3	BH	0.17	0/2417	0.36	0/3268
3	BI	0.15	0/2417	0.32	0/3268
3	BJ	0.15	0/2417	0.33	0/3268
3	BK	0.16	0/2417	0.39	0/3268
4	CA	0.13	0/4203	0.31	0/5706
4	CB	0.13	0/4203	0.27	0/5706
4	CC	0.12	0/4203	0.29	0/5706
4	CD	0.14	0/4203	0.31	0/5706
4	CE	0.13	0/4195	0.30	0/5696
4	CF	0.12	0/4203	0.30	0/5706
4	CG	0.14	0/4203	0.30	0/5706
4	CH	0.13	0/4203	0.32	0/5706
4	CI	0.13	0/4203	0.30	0/5706
4	CJ	0.12	0/4203	0.27	0/5706
4	CK	0.13	0/4203	0.28	0/5706
5	DA	0.11	0/3003	0.29	0/4090
5	DB	0.12	0/3003	0.33	0/4090
5	DC	0.11	0/3003	0.31	0/4090
5	DD	0.11	0/3003	0.32	0/4090
5	DE	0.10	0/3003	0.27	0/4090
5	DF	0.09	0/3003	0.26	0/4090
5	DG	0.09	0/3003	0.26	0/4090

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	DH	0.09	0/3003	0.26	0/4090
5	DI	0.10	0/3003	0.29	0/4090
5	DJ	0.10	0/3003	0.31	2/4090 (0.0%)
5	DK	0.11	0/3003	0.29	0/4090
5	EA	0.09	0/3003	0.27	0/4090
5	EB	0.10	0/3003	0.27	0/4090
5	EC	0.11	0/3003	0.27	0/4090
5	ED	0.10	0/3003	0.28	0/4090
5	EE	0.11	0/3003	0.28	0/4090
5	EF	0.09	0/3003	0.27	0/4090
5	EG	0.10	0/3003	0.27	0/4090
5	EH	0.10	0/3003	0.28	0/4090
5	EI	0.09	0/3003	0.26	0/4090
5	EJ	0.10	0/3003	0.27	0/4090
5	EK	0.10	0/3003	0.27	0/4090
5	FA	0.10	0/2579	0.30	0/3515
5	FB	0.10	0/2567	0.29	0/3502
5	FC	0.09	0/2466	0.27	0/3363
5	FD	0.10	0/2466	0.28	0/3363
5	FE	0.10	0/2711	0.28	0/3696
5	FF	0.10	0/2466	0.28	0/3363
5	FG	0.10	0/2466	0.28	0/3363
5	FH	0.10	0/2711	0.30	0/3696
5	FI	0.11	0/2602	0.30	0/3548
5	FJ	0.10	0/2711	0.27	0/3696
5	FK	0.10	0/2711	0.28	0/3696
All	All	0.12	0/184220	0.30	2/250348 (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
5	DH	0	1
5	EI	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	DJ	283	TYR	CA-C-N	5.05	128.63	121.61
5	DJ	283	TYR	C-N-CA	5.05	128.63	121.61

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	DH	123	THR	Peptide
5	EI	123	THR	Peptide

## 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	AA	3380	0	3435	99	0
1	AB	3353	0	3403	109	0
1	AD	3350	0	3402	113	0
1	AE	3350	0	3402	80	0
2	AC	3349	0	3402	106	0
3	BA	2391	0	2350	94	0
3	BB	2383	0	2338	83	0
3	BC	2391	0	2350	56	0
3	BD	2391	0	2350	72	0
3	BE	2383	0	2338	62	0
3	BF	2391	0	2350	53	0
3	BG	2391	0	2350	64	0
3	BH	2391	0	2350	53	0
3	BI	2391	0	2350	70	0
3	BJ	2391	0	2350	71	0
3	BK	2391	0	2350	79	0
4	CA	4157	0	4071	95	0
4	CB	4157	0	4071	85	0
4	CC	4157	0	4071	88	0
4	CD	4157	0	4071	98	0
4	CE	4149	0	4059	86	0
4	CF	4157	0	4071	124	0
4	CG	4157	0	4071	121	0
4	CH	4157	0	4071	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CI	4157	0	4071	82	0
4	CJ	4157	0	4071	92	0
4	CK	4157	0	4071	75	0
5	DA	2959	0	2855	56	0
5	DB	2959	0	2855	64	0
5	DC	2959	0	2855	73	0
5	DD	2959	0	2855	68	0
5	DE	2959	0	2855	76	0
5	DF	2959	0	2855	58	0
5	DG	2959	0	2855	73	0
5	DH	2959	0	2855	56	0
5	DI	2959	0	2855	76	0
5	DJ	2959	0	2855	69	0
5	DK	2959	0	2855	88	0
5	EA	2959	0	2855	70	0
5	EB	2959	0	2855	80	0
5	EC	2959	0	2855	69	0
5	ED	2959	0	2855	72	0
5	EE	2959	0	2855	76	0
5	EF	2959	0	2855	65	0
5	EG	2959	0	2855	65	0
5	EH	2959	0	2855	63	0
5	EI	2959	0	2855	61	0
5	EJ	2959	0	2855	56	0
5	EK	2959	0	2855	70	0
5	FA	2537	0	2417	44	0
5	FB	2527	0	2400	61	0
5	FC	2426	0	2298	57	0
5	FD	2426	0	2298	69	0
5	FE	2668	0	2549	79	0
5	FF	2426	0	2298	66	0
5	FG	2426	0	2298	64	0
5	FH	2668	0	2549	51	0
5	FI	2562	0	2451	73	0
5	FJ	2668	0	2549	67	0
5	FK	2668	0	2549	85	0
All	All	181886	0	177105	4050	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 11.

The worst 5 of 4050 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)
3:BB:91:GLN:HE21	3:BB:237:LYS:HE3	1.29	0.98
1:AD:25:ASN:HB3	1:AD:29:ARG:HH12	1.27	0.96
4:CJ:545:LEU:HD11	5:DI:378:GLN:HB2	1.50	0.92
3:BD:299:ALA:HB1	3:BE:30:MET:HE3	1.55	0.87
3:BI:30:MET:HE3	3:BJ:299:ALA:HB1	1.55	0.86

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	AA	450/467 (96%)	435 (97%)	15 (3%)	0	100	100
1	AB	446/467 (96%)	429 (96%)	17 (4%)	0	100	100
1	AD	445/467 (95%)	424 (95%)	21 (5%)	0	100	100
1	AE	445/467 (95%)	434 (98%)	11 (2%)	0	100	100
2	AC	445/467 (95%)	421 (95%)	24 (5%)	0	100	100
3	BA	315/317 (99%)	308 (98%)	7 (2%)	0	100	100
3	BB	314/317 (99%)	309 (98%)	5 (2%)	0	100	100
3	BC	315/317 (99%)	309 (98%)	6 (2%)	0	100	100
3	BD	315/317 (99%)	307 (98%)	8 (2%)	0	100	100
3	BE	314/317 (99%)	310 (99%)	4 (1%)	0	100	100
3	BF	315/317 (99%)	306 (97%)	9 (3%)	0	100	100
3	BG	315/317 (99%)	304 (96%)	11 (4%)	0	100	100
3	BH	315/317 (99%)	307 (98%)	8 (2%)	0	100	100
3	BI	315/317 (99%)	306 (97%)	9 (3%)	0	100	100
3	BJ	315/317 (99%)	311 (99%)	4 (1%)	0	100	100
3	BK	315/317 (99%)	304 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CA	551/553 (100%)	543 (98%)	8 (2%)	0	100	100
4	CB	551/553 (100%)	542 (98%)	9 (2%)	0	100	100
4	CC	551/553 (100%)	543 (98%)	8 (2%)	0	100	100
4	CD	551/553 (100%)	543 (98%)	8 (2%)	0	100	100
4	CE	550/553 (100%)	541 (98%)	9 (2%)	0	100	100
4	CF	551/553 (100%)	541 (98%)	10 (2%)	0	100	100
4	CG	551/553 (100%)	546 (99%)	5 (1%)	0	100	100
4	CH	551/553 (100%)	545 (99%)	6 (1%)	0	100	100
4	CI	551/553 (100%)	540 (98%)	11 (2%)	0	100	100
4	CJ	551/553 (100%)	544 (99%)	7 (1%)	0	100	100
4	CK	551/553 (100%)	541 (98%)	10 (2%)	0	100	100
5	DA	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
5	DB	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	DC	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	DD	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	DE	400/403 (99%)	390 (98%)	10 (2%)	0	100	100
5	DF	400/403 (99%)	393 (98%)	7 (2%)	0	100	100
5	DG	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	DH	400/403 (99%)	389 (97%)	11 (3%)	0	100	100
5	DI	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	DJ	400/403 (99%)	386 (96%)	14 (4%)	0	100	100
5	DK	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	EA	400/403 (99%)	394 (98%)	6 (2%)	0	100	100
5	EB	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	EC	400/403 (99%)	393 (98%)	7 (2%)	0	100	100
5	ED	400/403 (99%)	394 (98%)	6 (2%)	0	100	100
5	EE	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	EF	400/403 (99%)	389 (97%)	11 (3%)	0	100	100
5	EG	400/403 (99%)	393 (98%)	7 (2%)	0	100	100
5	EH	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	EI	400/403 (99%)	391 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	EJ	400/403 (99%)	394 (98%)	6 (2%)	0	100	100
5	EK	400/403 (99%)	389 (97%)	11 (3%)	0	100	100
5	FA	345/403 (86%)	332 (96%)	13 (4%)	0	100	100
5	FB	341/403 (85%)	326 (96%)	15 (4%)	0	100	100
5	FC	326/403 (81%)	317 (97%)	9 (3%)	0	100	100
5	FD	326/403 (81%)	317 (97%)	9 (3%)	0	100	100
5	FE	364/403 (90%)	359 (99%)	5 (1%)	0	100	100
5	FF	326/403 (81%)	321 (98%)	5 (2%)	0	100	100
5	FG	326/403 (81%)	313 (96%)	13 (4%)	0	100	100
5	FH	364/403 (90%)	351 (96%)	13 (4%)	0	100	100
5	FI	348/403 (86%)	337 (97%)	11 (3%)	0	100	100
5	FJ	364/403 (90%)	356 (98%)	8 (2%)	0	100	100
5	FK	364/403 (90%)	350 (96%)	14 (4%)	0	100	100
All	All	24348/25204 (97%)	23764 (98%)	584 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	378/391 (97%)	378 (100%)	0	100	100
1	AB	375/391 (96%)	375 (100%)	0	100	100
1	AD	375/391 (96%)	375 (100%)	0	100	100
1	AE	375/391 (96%)	375 (100%)	0	100	100
2	AC	375/391 (96%)	374 (100%)	1 (0%)	86	83
3	BA	261/261 (100%)	261 (100%)	0	100	100
3	BB	260/261 (100%)	260 (100%)	0	100	100
3	BC	261/261 (100%)	261 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BD	261/261 (100%)	261 (100%)	0	100	100
3	BE	260/261 (100%)	260 (100%)	0	100	100
3	BF	261/261 (100%)	261 (100%)	0	100	100
3	BG	261/261 (100%)	261 (100%)	0	100	100
3	BH	261/261 (100%)	261 (100%)	0	100	100
3	BI	261/261 (100%)	261 (100%)	0	100	100
3	BJ	261/261 (100%)	261 (100%)	0	100	100
3	BK	261/261 (100%)	261 (100%)	0	100	100
4	CA	453/453 (100%)	452 (100%)	1 (0%)	87	86
4	CB	453/453 (100%)	453 (100%)	0	100	100
4	CC	453/453 (100%)	453 (100%)	0	100	100
4	CD	453/453 (100%)	453 (100%)	0	100	100
4	CE	452/453 (100%)	452 (100%)	0	100	100
4	CF	453/453 (100%)	453 (100%)	0	100	100
4	CG	453/453 (100%)	453 (100%)	0	100	100
4	CH	453/453 (100%)	452 (100%)	1 (0%)	87	86
4	CI	453/453 (100%)	453 (100%)	0	100	100
4	CJ	453/453 (100%)	453 (100%)	0	100	100
4	CK	453/453 (100%)	453 (100%)	0	100	100
5	DA	322/323 (100%)	322 (100%)	0	100	100
5	DB	322/323 (100%)	322 (100%)	0	100	100
5	DC	322/323 (100%)	322 (100%)	0	100	100
5	DD	322/323 (100%)	322 (100%)	0	100	100
5	DE	322/323 (100%)	322 (100%)	0	100	100
5	DF	322/323 (100%)	322 (100%)	0	100	100
5	DG	322/323 (100%)	322 (100%)	0	100	100
5	DH	322/323 (100%)	322 (100%)	0	100	100
5	DI	322/323 (100%)	322 (100%)	0	100	100
5	DJ	322/323 (100%)	321 (100%)	1 (0%)	86	83
5	DK	322/323 (100%)	322 (100%)	0	100	100
5	EA	322/323 (100%)	322 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	EB	322/323 (100%)	322 (100%)	0	100	100
5	EC	322/323 (100%)	321 (100%)	1 (0%)	86	83
5	ED	322/323 (100%)	322 (100%)	0	100	100
5	EE	322/323 (100%)	322 (100%)	0	100	100
5	EF	322/323 (100%)	322 (100%)	0	100	100
5	EG	322/323 (100%)	322 (100%)	0	100	100
5	EH	322/323 (100%)	322 (100%)	0	100	100
5	EI	322/323 (100%)	322 (100%)	0	100	100
5	EJ	322/323 (100%)	322 (100%)	0	100	100
5	EK	322/323 (100%)	322 (100%)	0	100	100
5	FA	274/323 (85%)	274 (100%)	0	100	100
5	FB	275/323 (85%)	275 (100%)	0	100	100
5	FC	264/323 (82%)	264 (100%)	0	100	100
5	FD	264/323 (82%)	264 (100%)	0	100	100
5	FE	288/323 (89%)	288 (100%)	0	100	100
5	FF	264/323 (82%)	264 (100%)	0	100	100
5	FG	264/323 (82%)	264 (100%)	0	100	100
5	FH	288/323 (89%)	288 (100%)	0	100	100
5	FI	276/323 (85%)	276 (100%)	0	100	100
5	FJ	288/323 (89%)	288 (100%)	0	100	100
5	FK	288/323 (89%)	288 (100%)	0	100	100
All	All	19846/20468 (97%)	19841 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AC	180	GLN
4	CA	24	ASN
4	CH	149	GLN
5	DJ	196	ASN
5	EC	273	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 329 such sidechains are listed below:

Mol	Chain	Res	Type
5	EE	154	GLN
5	FE	15	ASN
5	EG	58	GLN
5	EJ	267	GLN
5	FG	111	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.



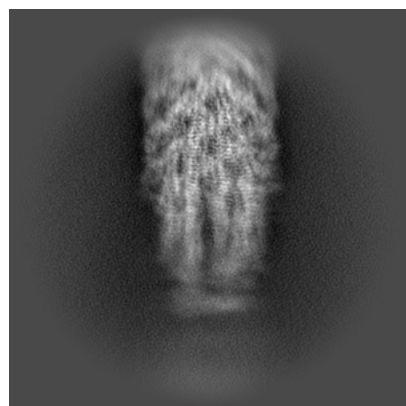
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63947. These allow visual inspection of the internal detail of the map and identification of artifacts.

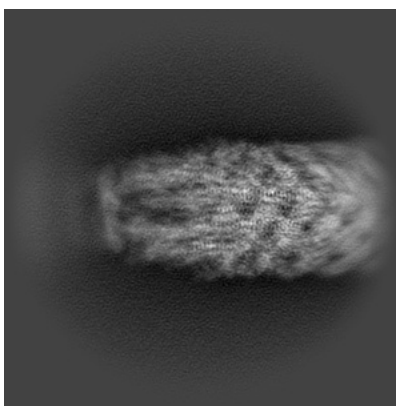
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

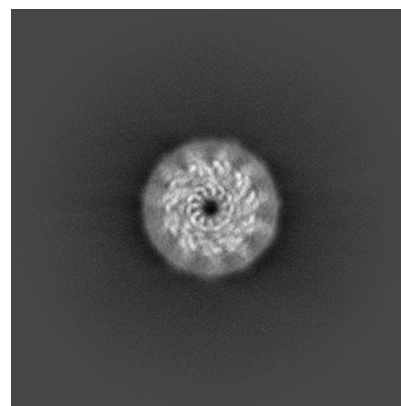
#### 6.1.1 Primary map



X

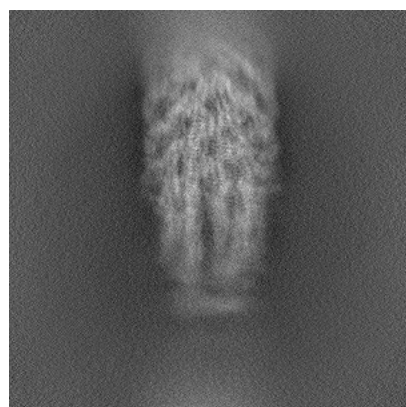


Y

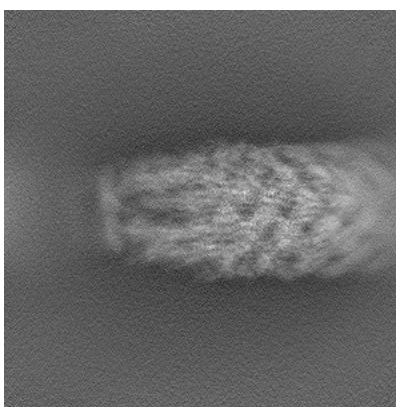


Z

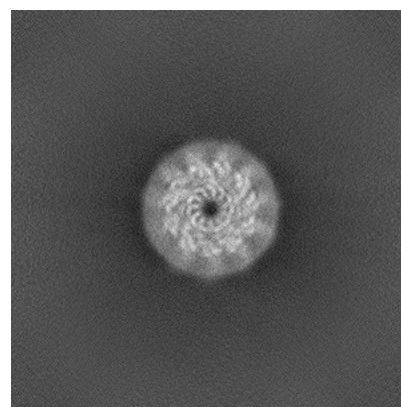
#### 6.1.2 Raw map



X



Y

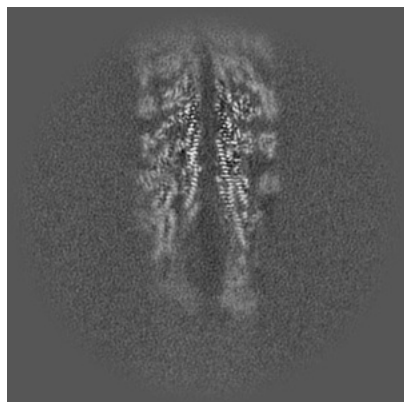


Z

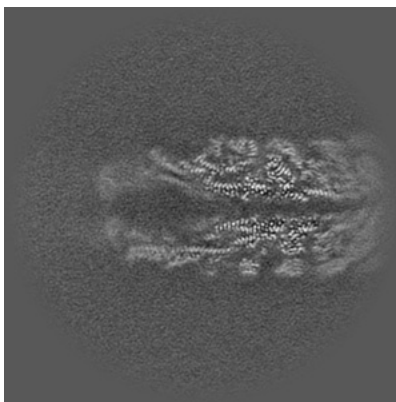
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

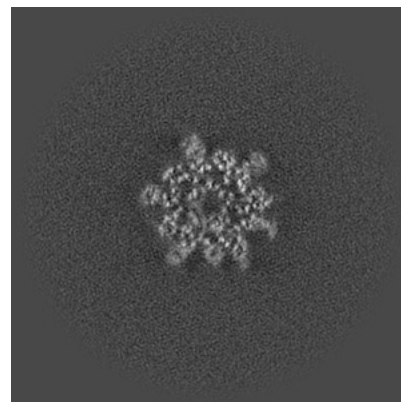
### 6.2.1 Primary map



X Index: 300

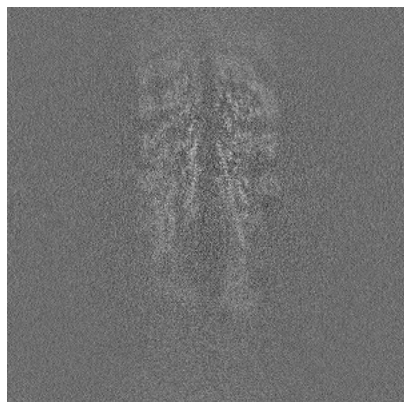


Y Index: 300

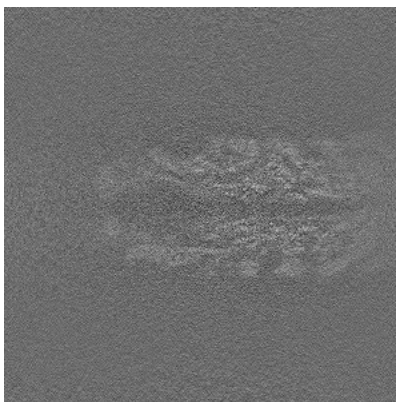


Z Index: 300

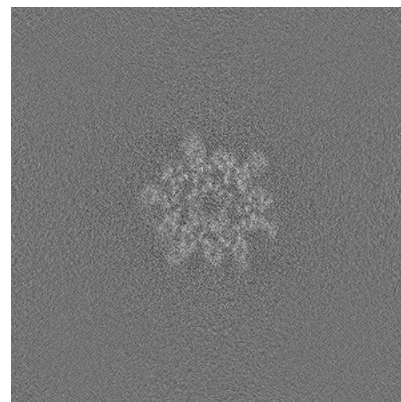
### 6.2.2 Raw map



X Index: 300



Y Index: 300

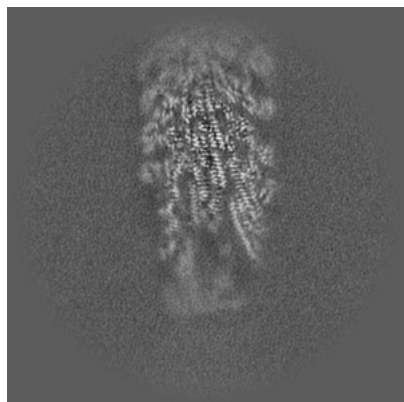


Z Index: 300

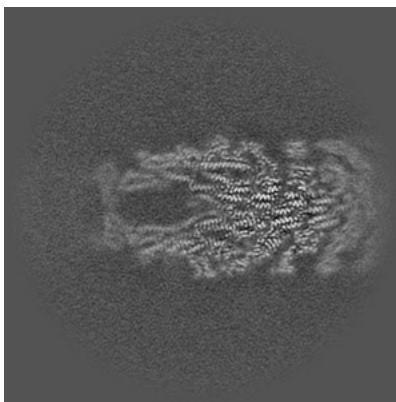
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

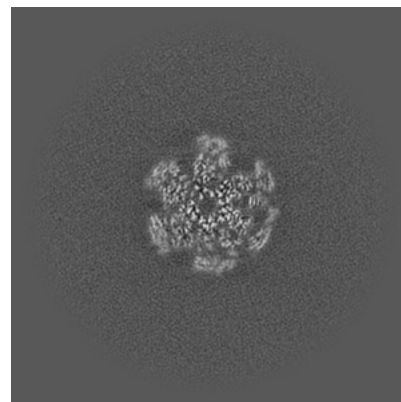
### 6.3.1 Primary map



X Index: 325

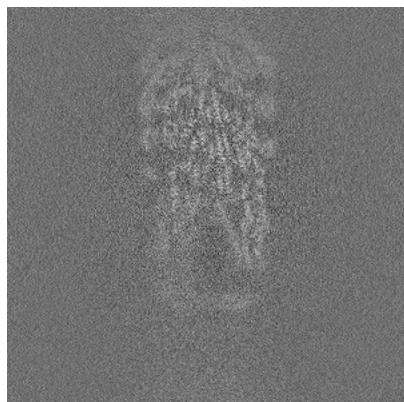


Y Index: 319

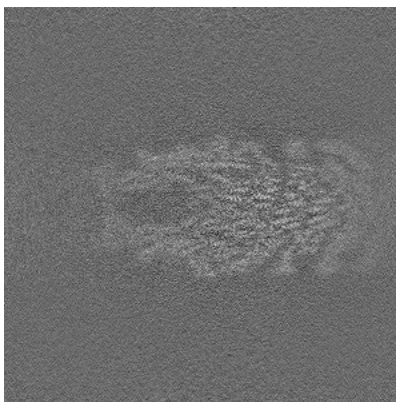


Z Index: 392

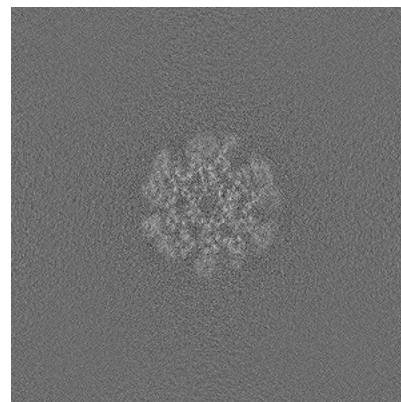
### 6.3.2 Raw map



X Index: 315



Y Index: 319



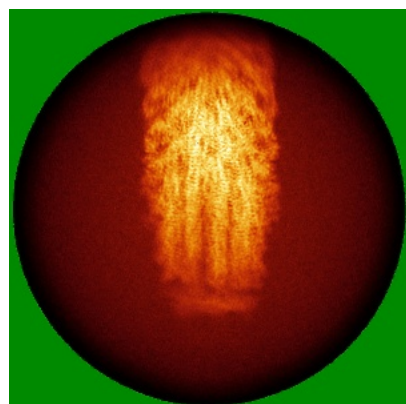
Z Index: 335

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

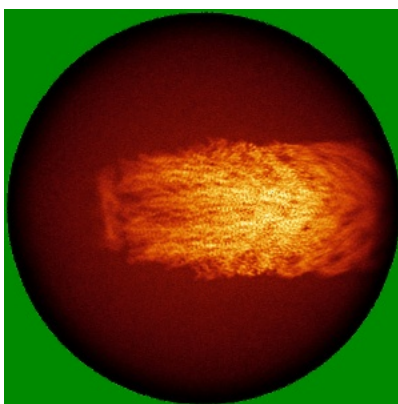


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

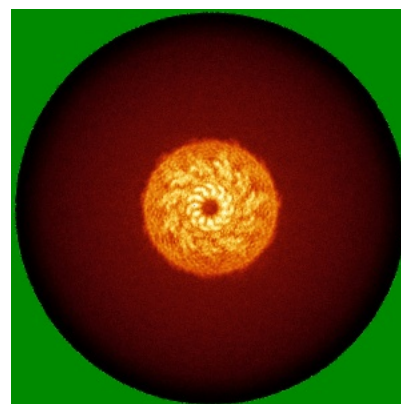
### 6.4.1 Primary map



X

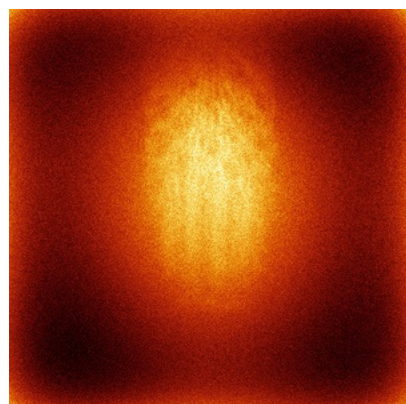


Y

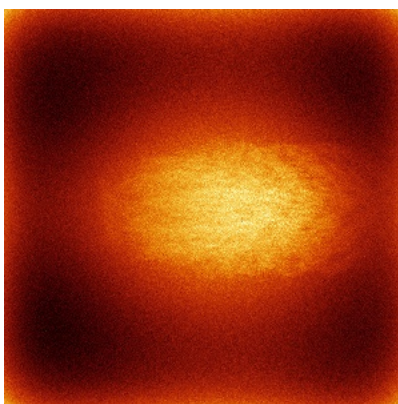


Z

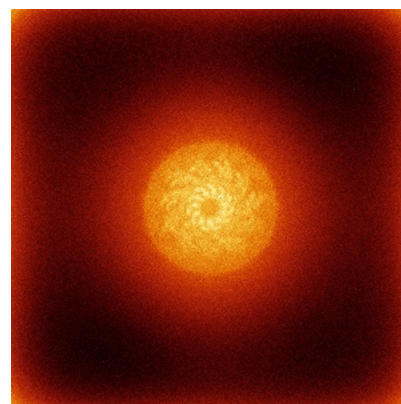
### 6.4.2 Raw map



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



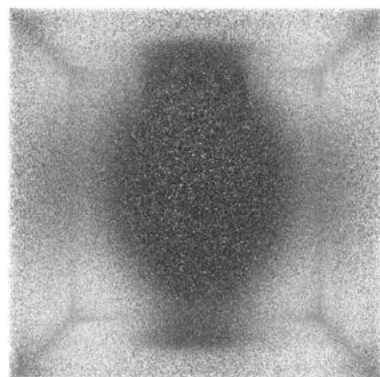
Y



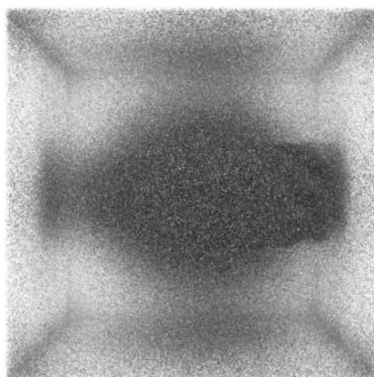
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

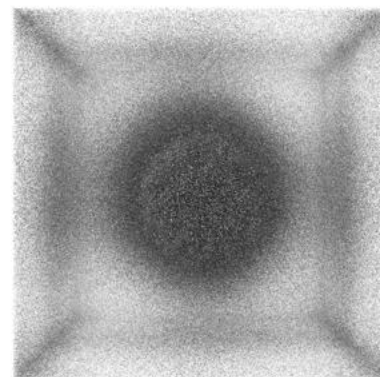
### 6.5.2 Raw map



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

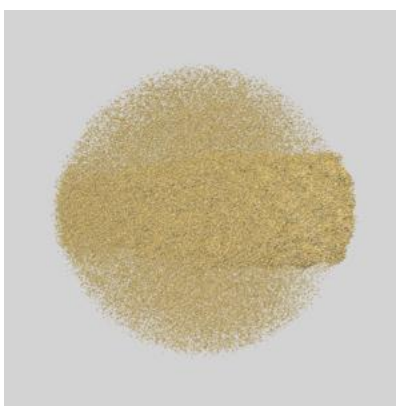
A mask typically either:

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

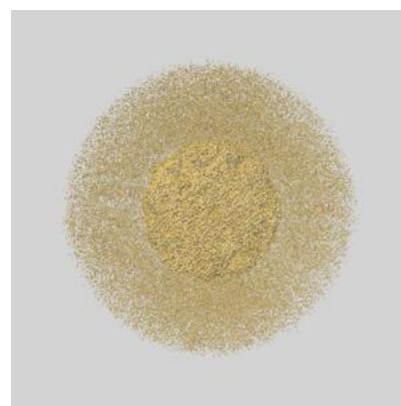
### 6.6.1 emd\_63947\_msk\_1.map [i](#)



X



Y

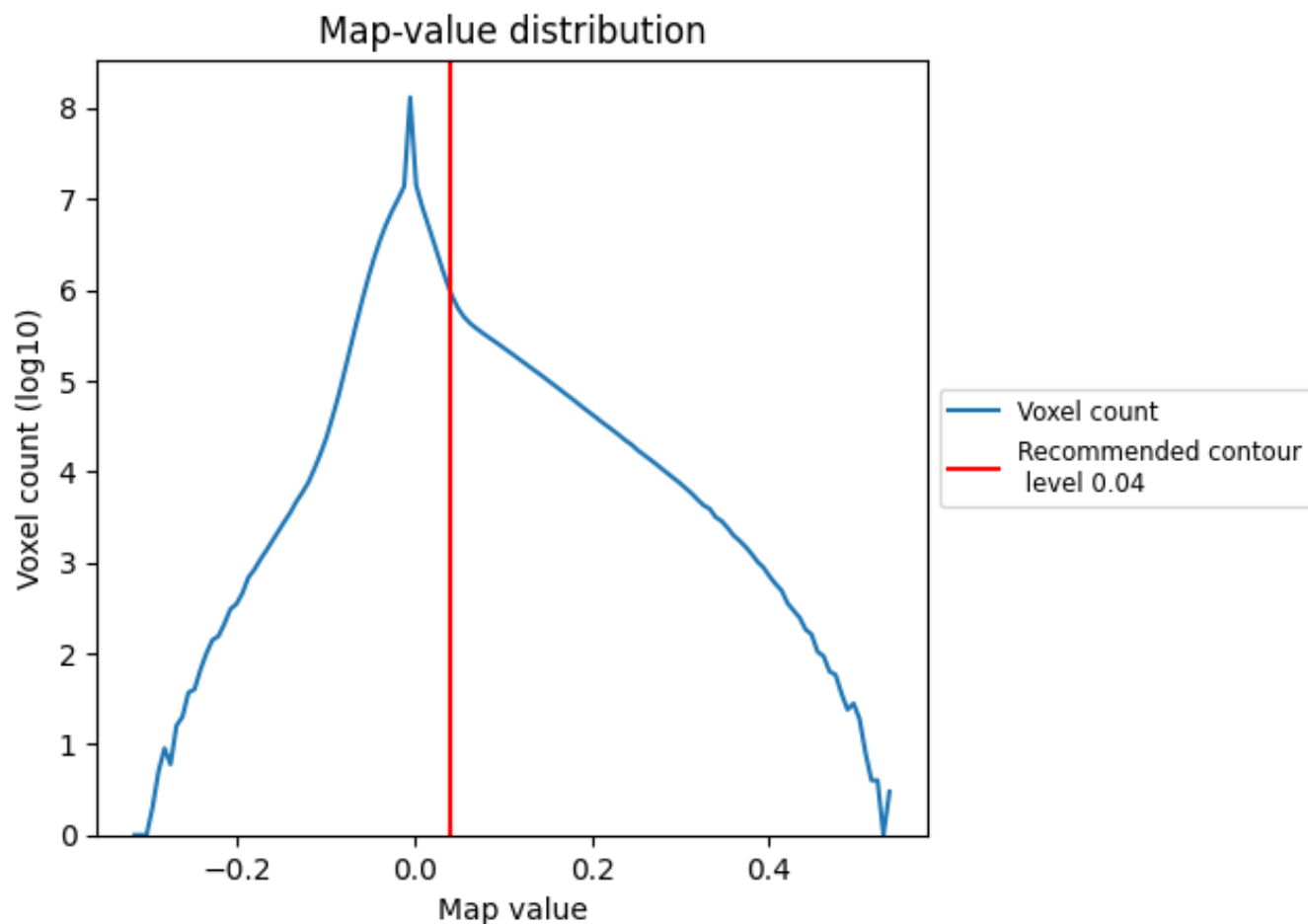


Z

## 7 Map analysis [i](#)

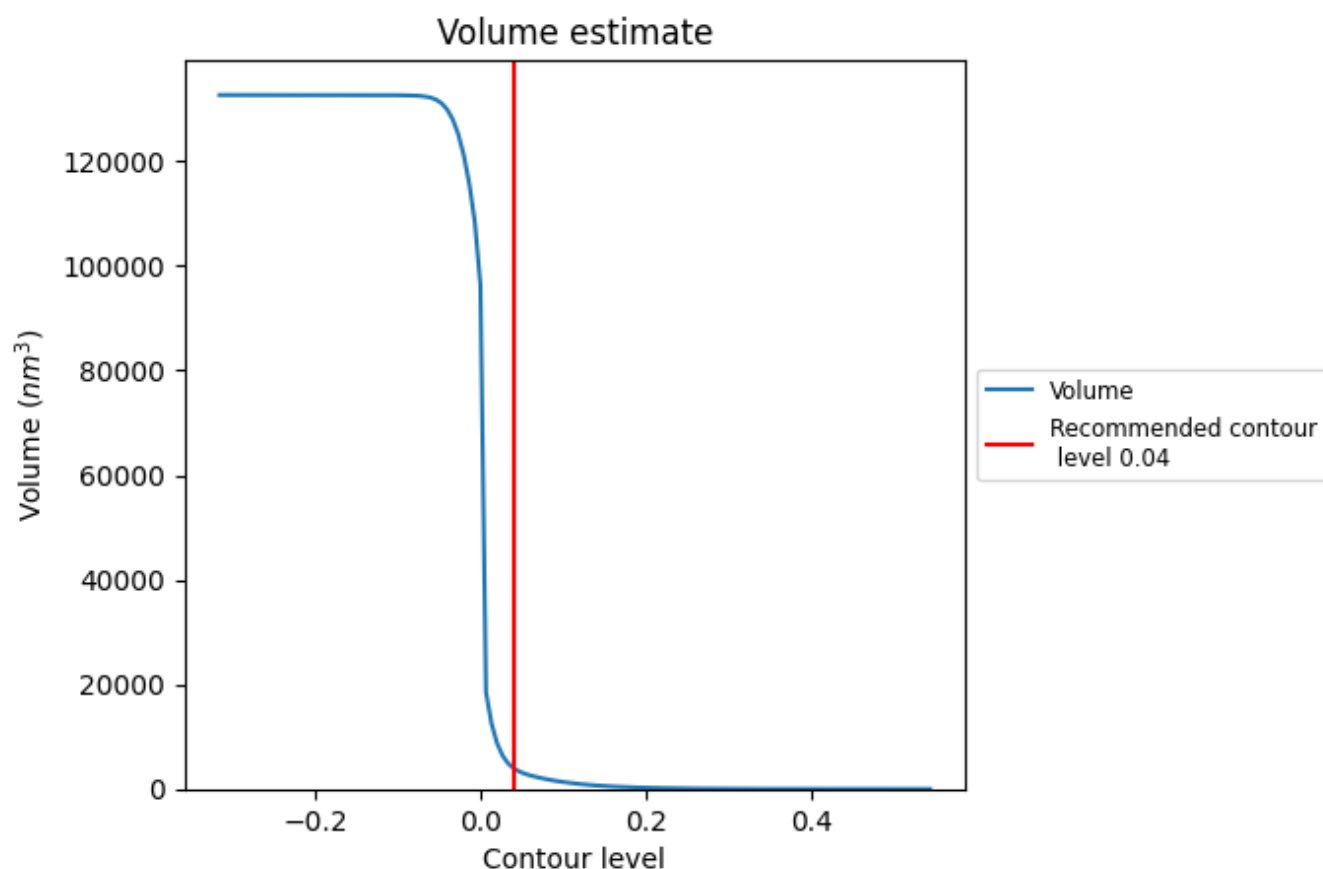
This section contains the results of statistical analysis of the map.

### 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](#)

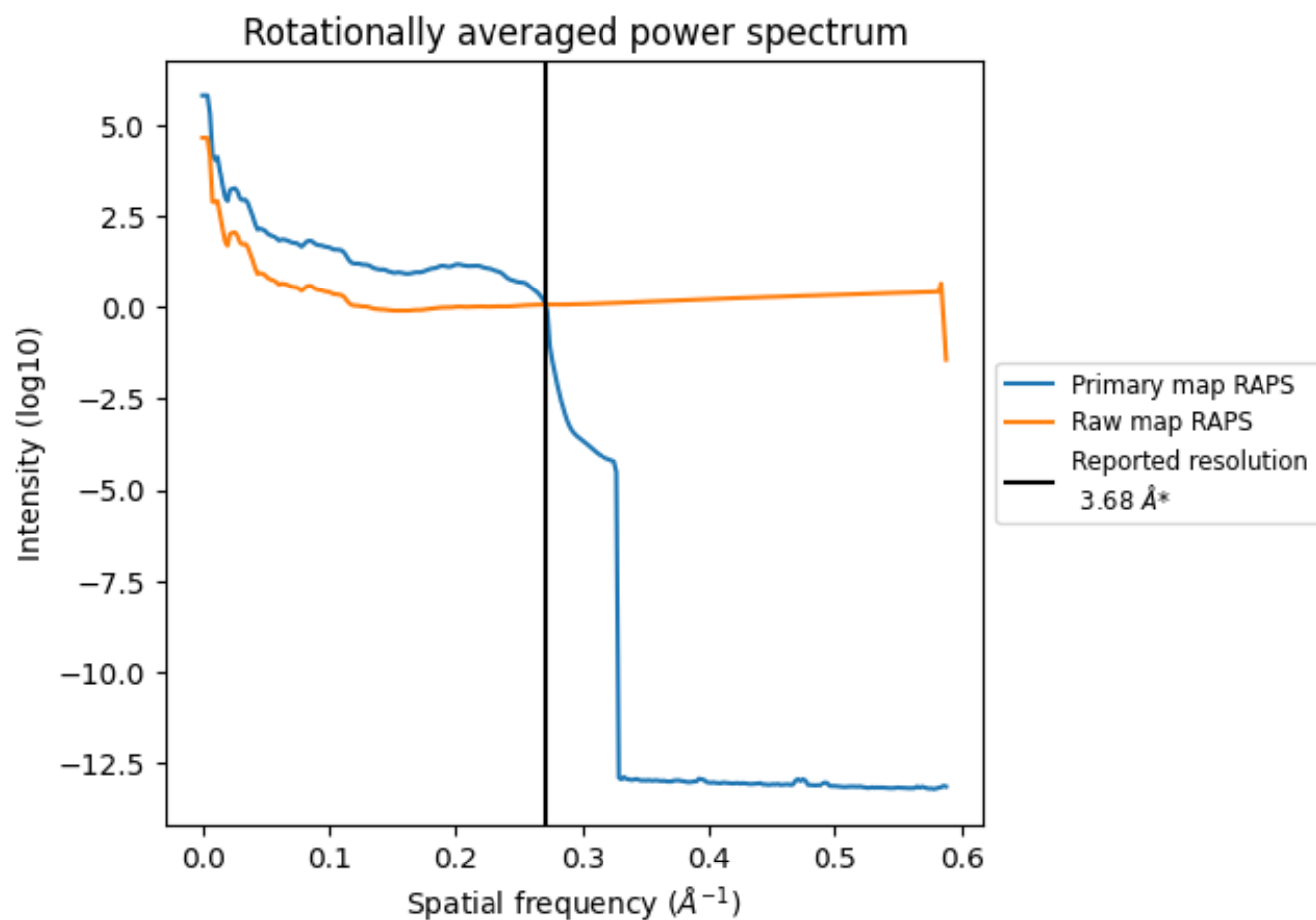


The volume at the recommended contour level is 3933  $\text{nm}^3$ ; this corresponds to an approximate mass of 3553 kDa.

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 ⓘ

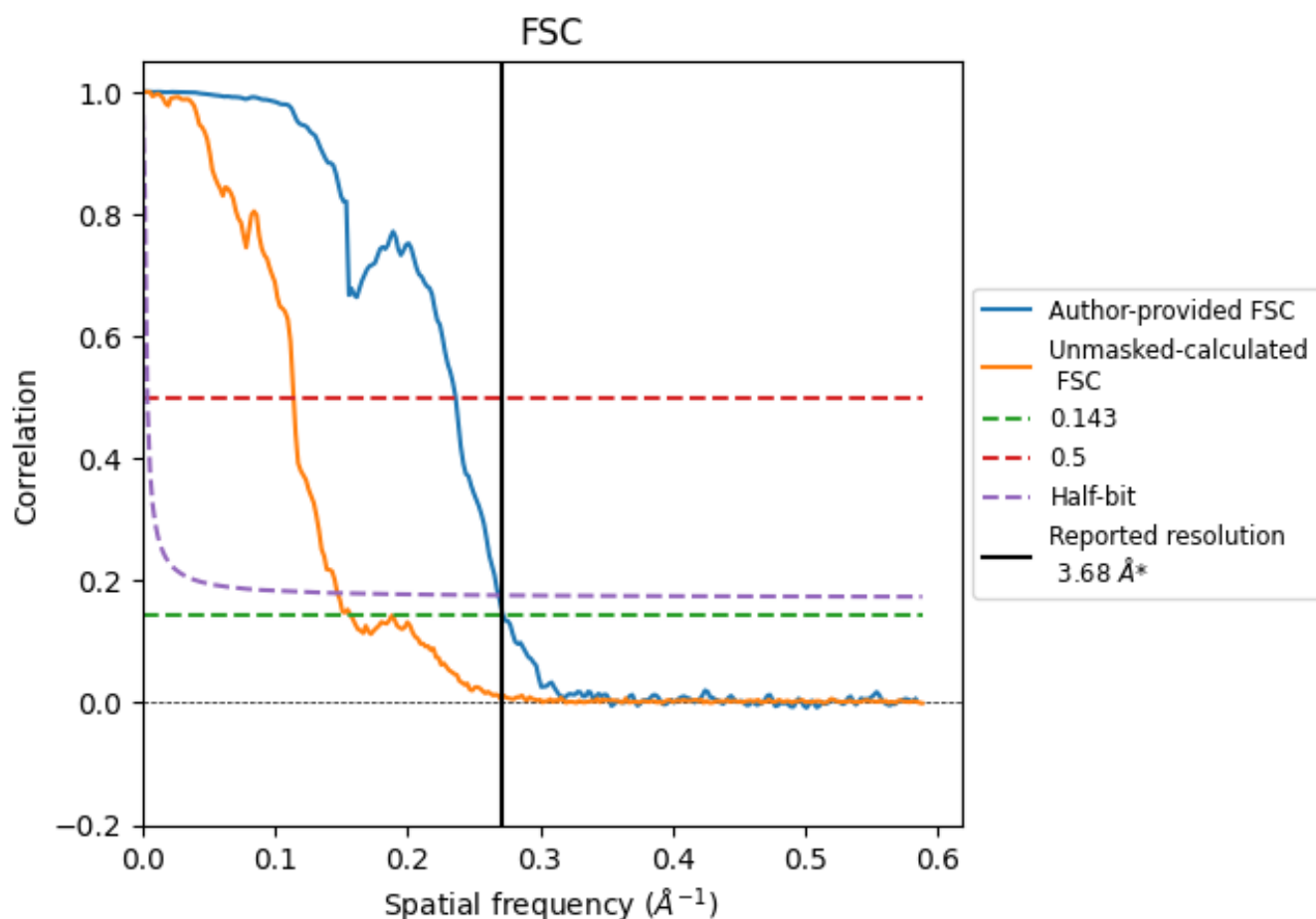


\*Reported resolution corresponds to spatial frequency of 0.272 Å<sup>-1</sup>

## 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 0.272 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

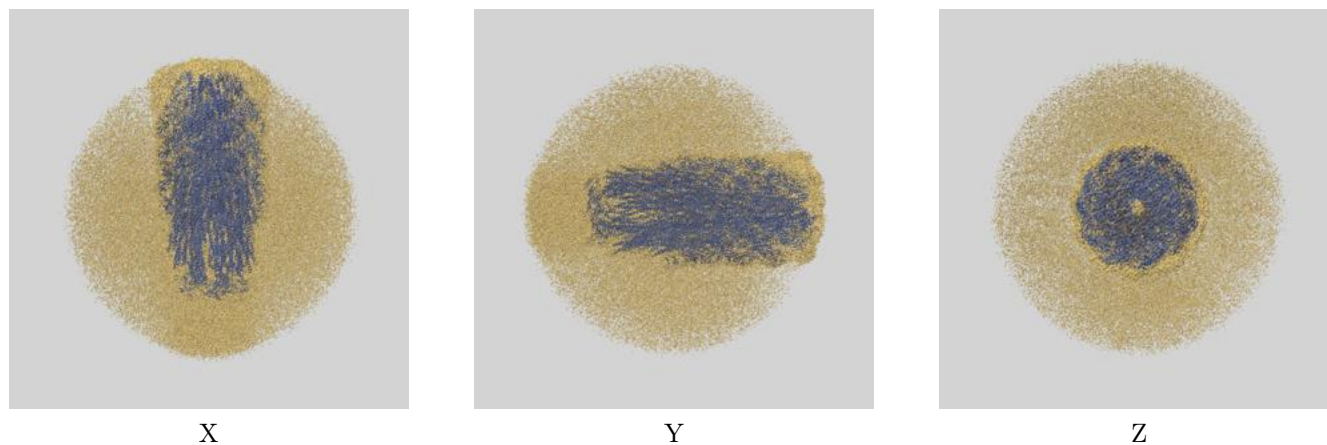
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.23	3.72
Unmasked-calculated*	6.36	8.76	6.80

\*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 6.36 differs from the reported value 3.68 by more than 10 %

## 9 Map-model fit [i](#)

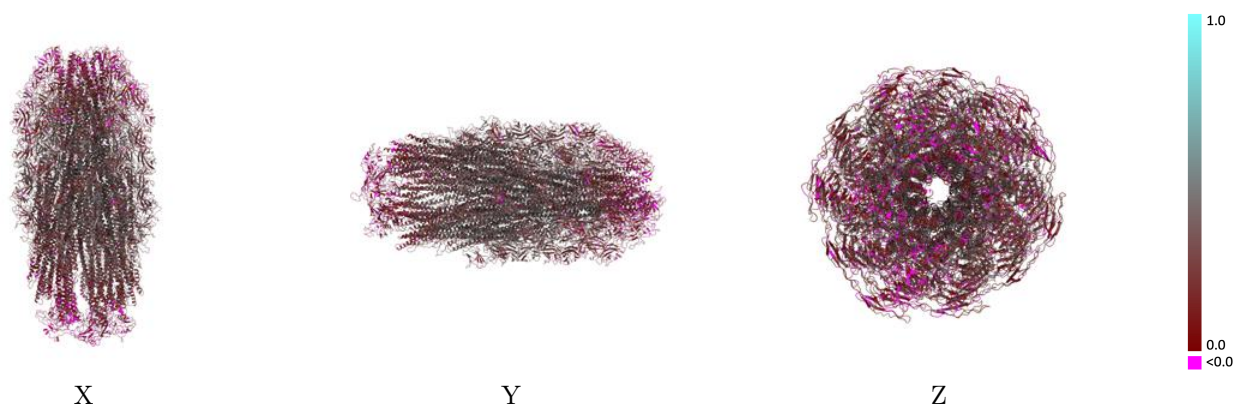
This section contains information regarding the fit between EMDB map EMD-63947 and PDB model 9U7Y. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

### 9.1 Map-model overlay [i](#)



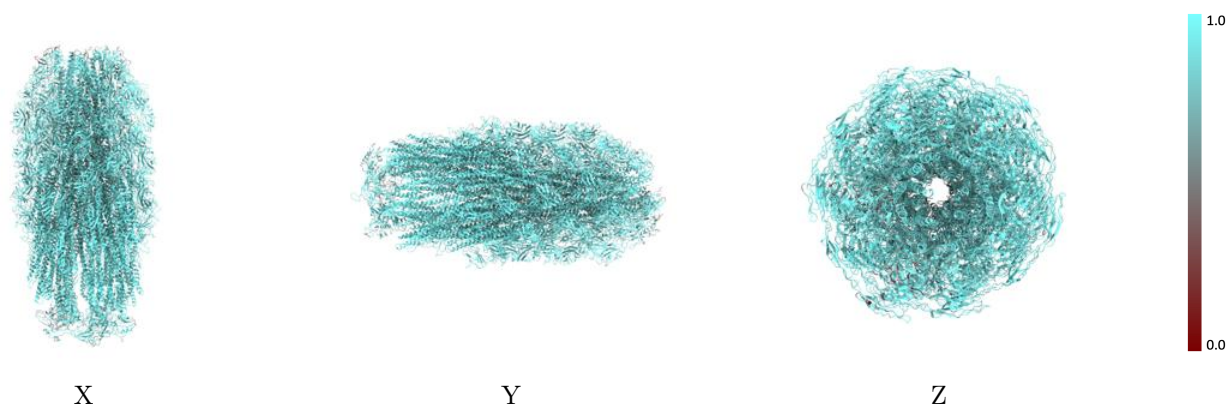
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



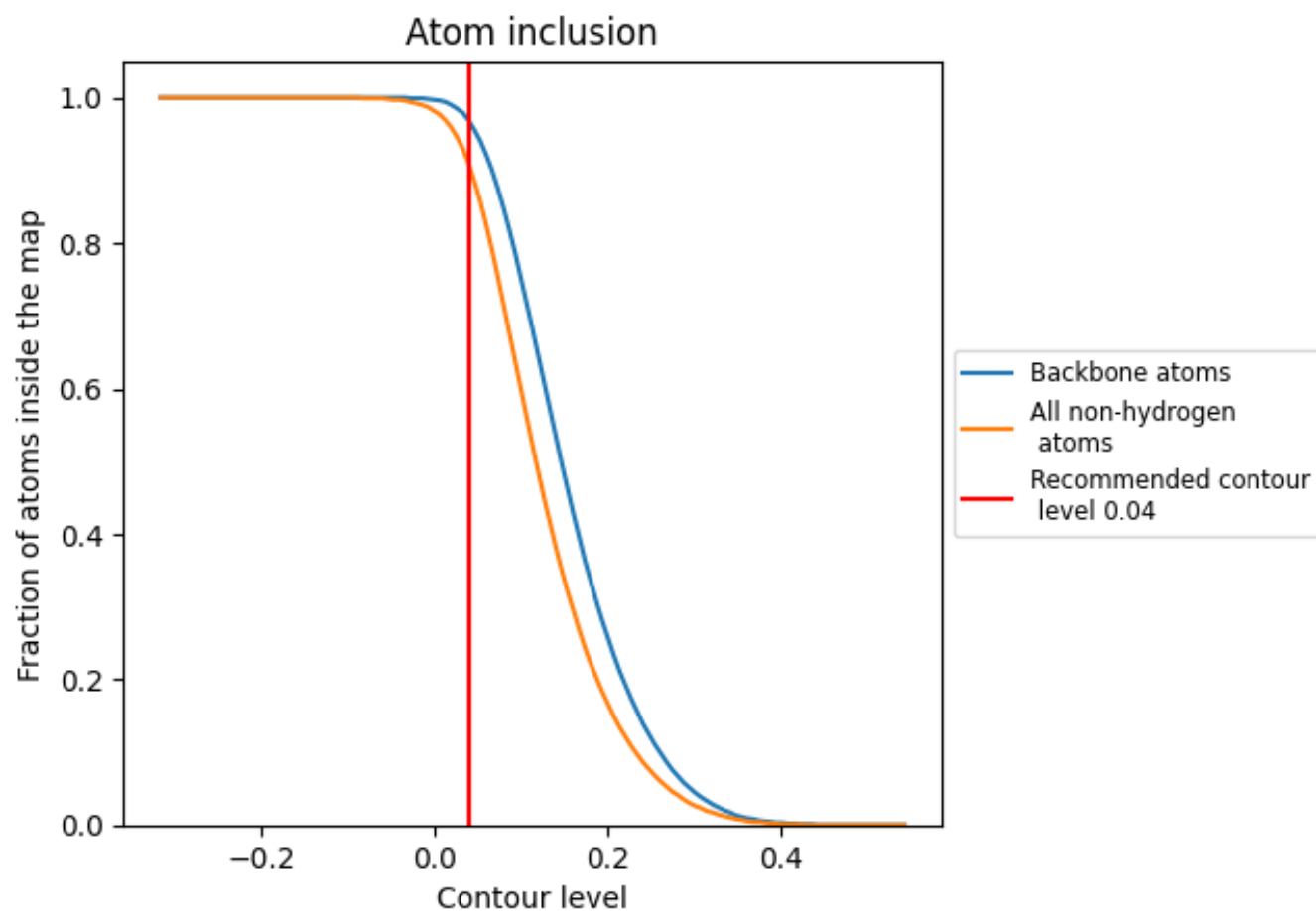
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.2760
AA	0.8750	0.1930
AB	0.8560	0.1760
AC	0.7490	0.1160
AD	0.8690	0.1480
AE	0.9060	0.1940
BA	0.9190	0.2450
BB	0.9360	0.2670
BC	0.9290	0.3030
BD	0.9580	0.3140
BE	0.9510	0.3450
BF	0.9390	0.3080
BG	0.8970	0.2310
BH	0.9400	0.3370
BI	0.9440	0.3250
BJ	0.9280	0.2850
BK	0.9470	0.2840
CA	0.9440	0.3670
CB	0.9450	0.3540
CC	0.9350	0.3630
CD	0.9260	0.3230
CE	0.9390	0.3390
CF	0.8980	0.3030
CG	0.9340	0.3070
CH	0.9290	0.3510
CI	0.9320	0.3560
CJ	0.9390	0.3840
CK	0.9490	0.3620
DA	0.8780	0.3060
DB	0.9190	0.3450
DC	0.9010	0.3300
DD	0.9140	0.3400
DE	0.9070	0.3280
DF	0.9140	0.3450
DG	0.9130	0.3420



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
DH	 0.9220	 0.3560
DI	 0.8870	 0.3200
DJ	 0.9080	 0.3430
DK	 0.9020	 0.3160
EA	 0.8990	 0.2640
EB	 0.9120	 0.2060
EC	 0.9170	 0.3100
ED	 0.9210	 0.2990
EE	 0.8990	 0.3000
EF	 0.9310	 0.2410
EG	 0.9240	 0.3010
EH	 0.9150	 0.2160
EI	 0.9000	 0.2700
EJ	 0.9000	 0.2160
EK	 0.9180	 0.3090
FA	 0.8930	 0.1750
FB	 0.8990	 0.2220
FC	 0.8000	 0.1030
FD	 0.8820	 0.1210
FE	 0.8760	 0.1470
FF	 0.8350	 0.1180
FG	 0.9000	 0.1140
FH	 0.9170	 0.1760
FI	 0.9350	 0.1640
FJ	 0.8510	 0.1550
FK	 0.9180	 0.1800