



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 06:47 PM JST

PDB ID : 9MCG / pdb_00009mcg
EMDB ID : EMD-63802
Title : Structure of the intial complex in filament assembly at 3.31 angstroms resolution, conformation 1.
Authors : Chen, L.X.; Jiang, W.X.; Cheng, X.Q.; Dong, X.; Xing, Q.
Deposited on : 2025-03-17
Resolution : 3.31 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.dev133
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) : 2.50

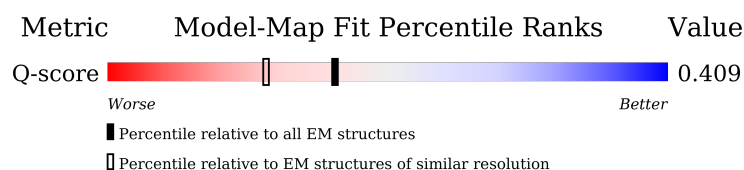
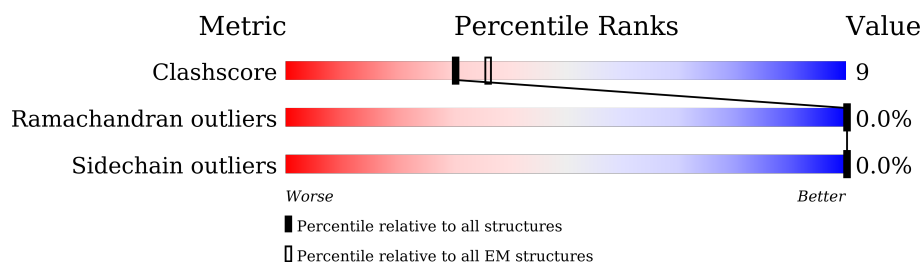
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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	14550 (2.81 - 3.81)

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	AA	467	
1	AB	467	
1	AD	467	
1	AE	467	

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Mol	Chain	Length	Quality of chain
2	AC	467	 8% 80% 16%
3	BA	317	 64% 36%
3	BB	317	 71% 29%
3	BC	317	 77% 23%
3	BD	317	 72% 28%
3	BE	317	 73% 26%
3	BF	317	 75% 25%
3	BG	317	 67% 33%
3	BH	317	 74% 26%
3	BI	317	 78% 22%
3	BJ	317	 75% 25%
3	BK	317	 71% 29%
3	BL	317	 18% 53% 18% 29%
4	CA	553	 75% 25%
4	CB	553	 75% 25%
4	CC	553	 79% 21%
4	CD	553	 77% 23%
4	CE	553	 75% 25%
4	CF	553	 73% 27%
4	CG	553	 71% 29%
4	CH	553	 81% 19%
4	CI	553	 75% 25%
4	CJ	553	 76% 24%
4	CK	553	 74% 26%
5	DA	403	 82% 18%

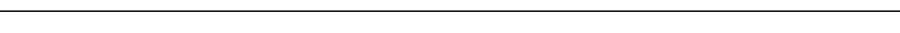
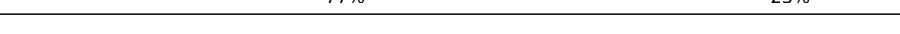
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Mol	Chain	Length	Quality of chain	
5	DB	403		85% 15%
5	DC	403		83% 17%
5	DD	403		84% 16%
5	DE	403		83% 16%
5	DF	403		85% 15%
5	DG	403		83% 16%
5	DH	403		84% 16%
5	DI	403		80% 20%
5	DJ	403		89% 11%
5	DK	403		80% 20%
5	EA	403		84% 16%
5	EB	403		86% 13%
5	EC	403		86% 13%
5	ED	403		85% 15%
5	EE	403		90% 10%
5	EF	403		84% 16%
5	EG	403		86% 14%
5	EH	403		85% 15%
5	EI	403		85% 14%
5	EJ	403		87% 13%
5	EK	403		83% 16%
5	FA	403		86% 14%
5	FB	403		85% 15%
5	FC	403		87% 13%
5	FD	403		79% 21%

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Mol	Chain	Length	Quality of chain
5	FE	403	 83% 17%
5	FF	403	 80% 19%
5	FG	403	 81% 19%
5	FH	403	 82% 18%
5	FI	403	 84% 16%
5	FJ	403	 77% 23%
5	FK	403	 85% 14%
5	GA	403	 86% 14%
5	GB	403	 74% 25%
5	GC	403	 76% 24%
5	GD	403	 74% 26%
5	GE	403	 75% 25%
5	GF	403	 78% 22%
5	GG	403	 78% 21%
5	GH	403	 77% 23%
5	GI	403	 75% 24%
5	GJ	403	 76% 24%
5	GK	403	 84% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 220655 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	316	Total	C	N	O	S	0	0
			2383	1458	416	497	12		
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	316	Total	C	N	O	S	0	0
			2383	1458	416	497	12		
3	BI	317	Total	C	N	O	S	0	0
			2391	1463	417	498	13		
3	BJ	316	Total	C	N	O	S	0	0
			2383	1458	416	497	12		
3	BK	316	Total	C	N	O	S	0	0
			2383	1458	416	497	12		
3	BL	225	Total	C	N	O	S	0	0
			1705	1048	293	356	8		

- 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	552	Total	C	N	O	S	0	0
			4149	2548	725	870	6		
4	CD	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
4	CE	553	Total	C	N	O	S	0	0
			4157	2553	726	871	7		
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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Mol	Chain	Residues	Atoms					AltConf	Trace
5	FA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	FK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
5	GJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

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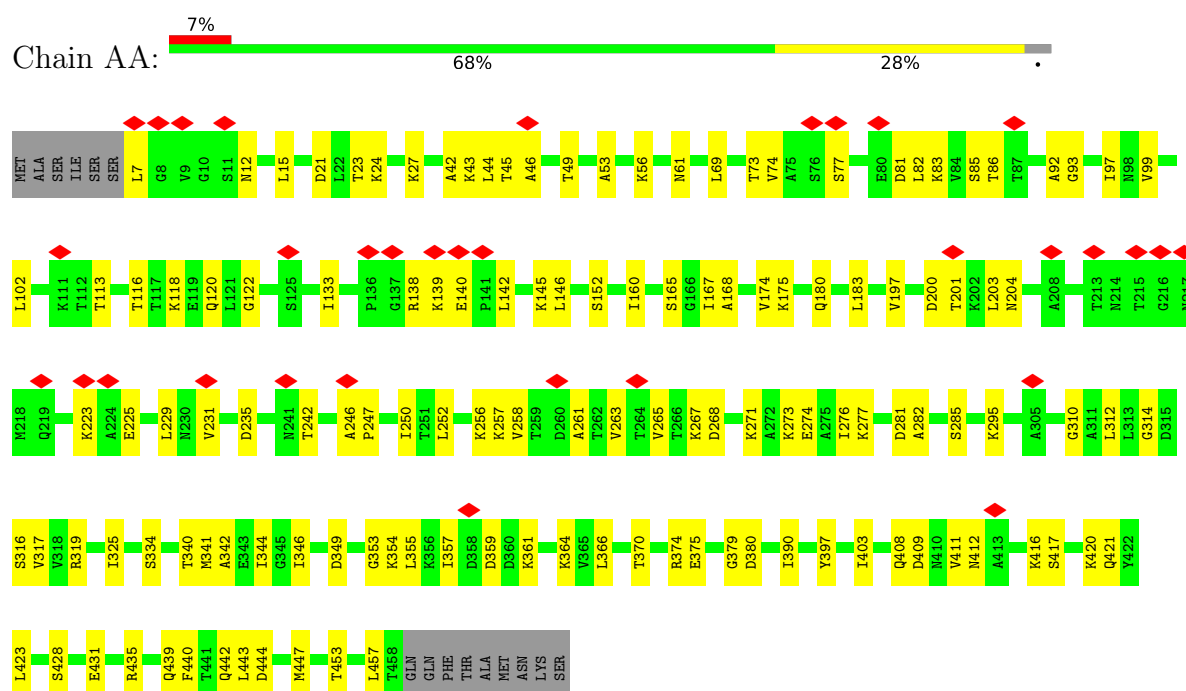
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	GK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

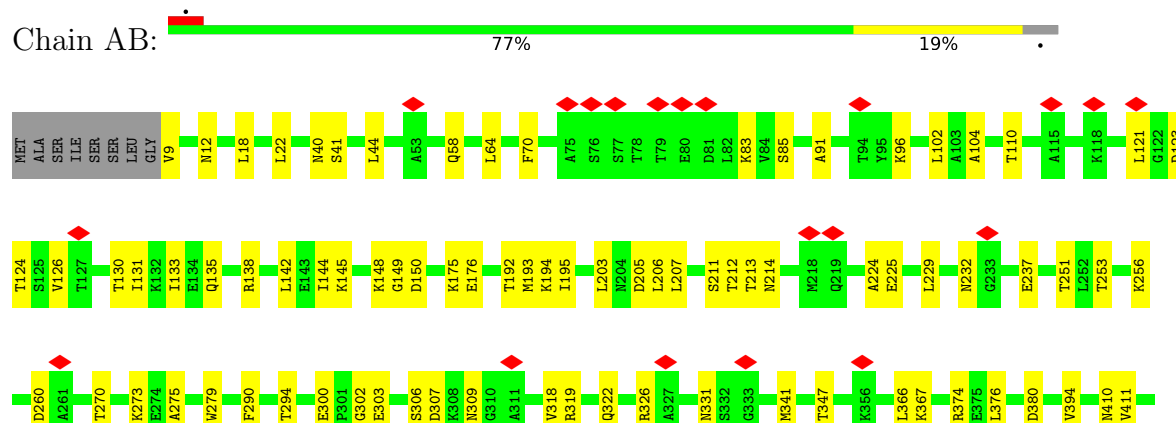
3 Residue-property plots

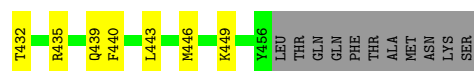
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flagellar hook-associated protein 2

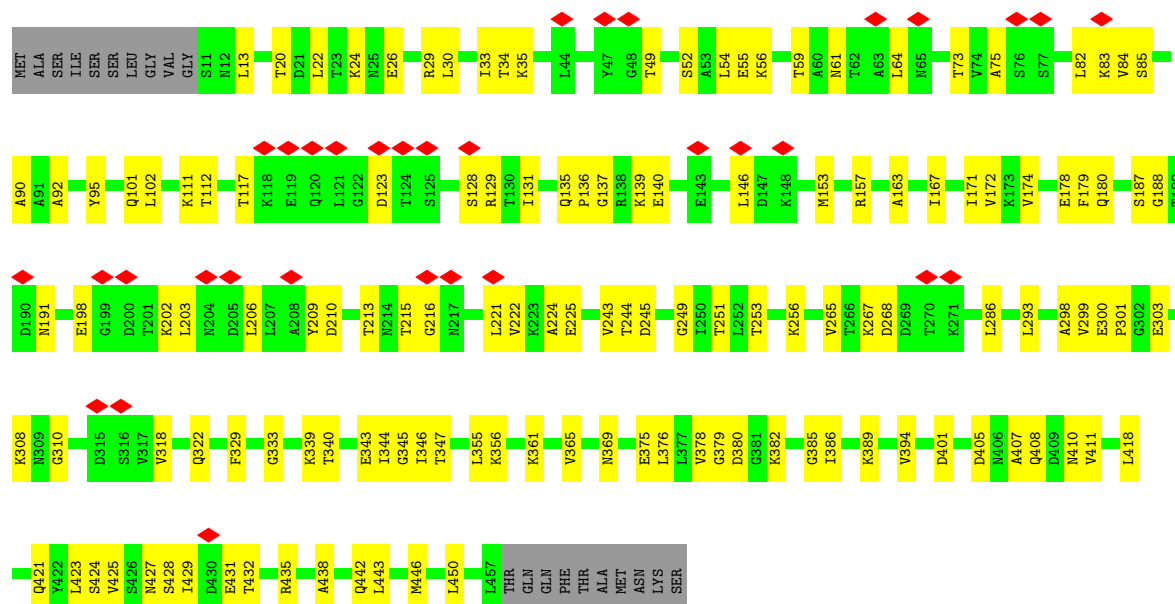


• Molecule 1: Flagellar hook-associated protein 2

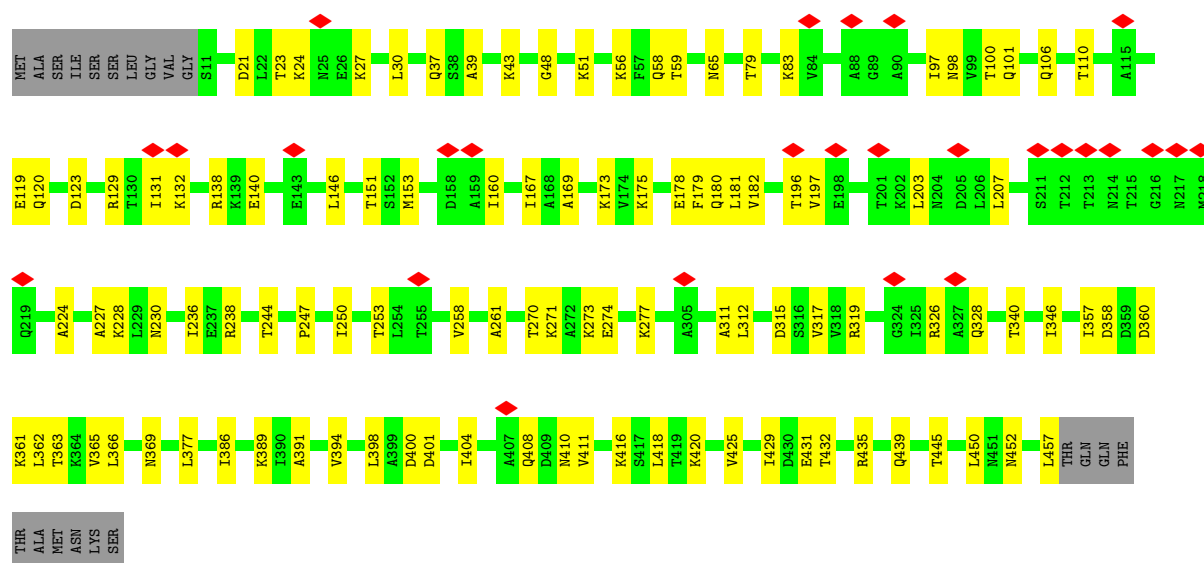
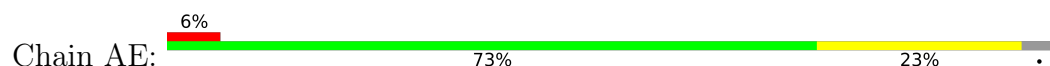




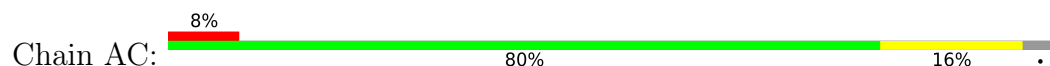
• Molecule 1: Flagellar hook-associated protein 2

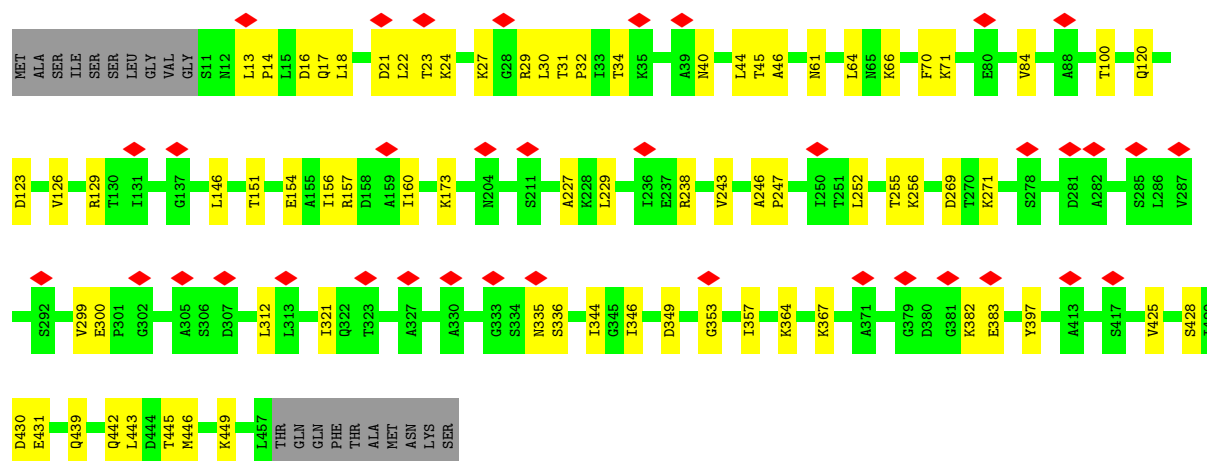


• Molecule 1: Flagellar hook-associated protein 2



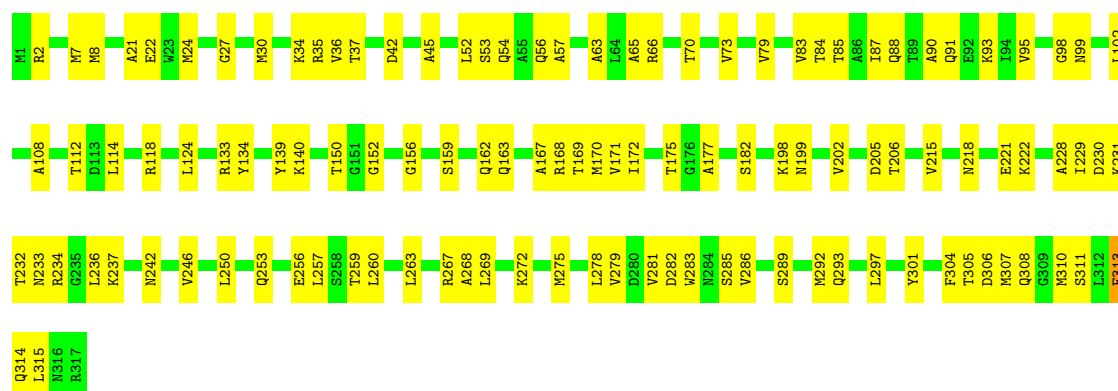
• Molecule 2: Flagellar hook-associated protein 2





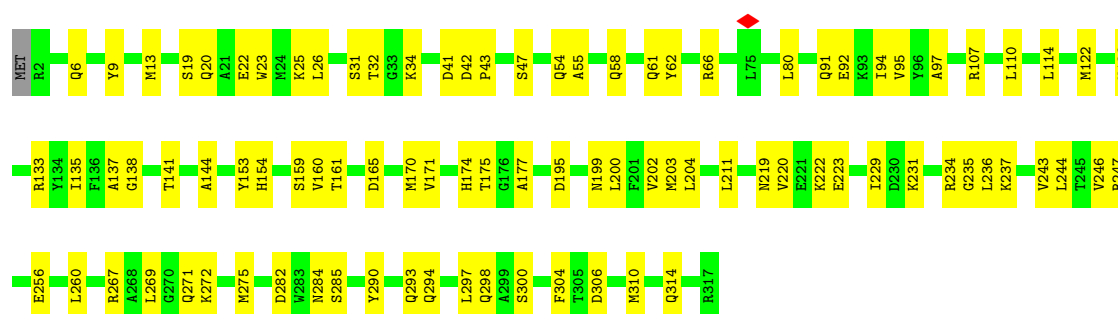
• Molecule 3: Flagellar hook-associated protein 3

Chain BA:



• Molecule 3: Flagellar hook-associated protein 3

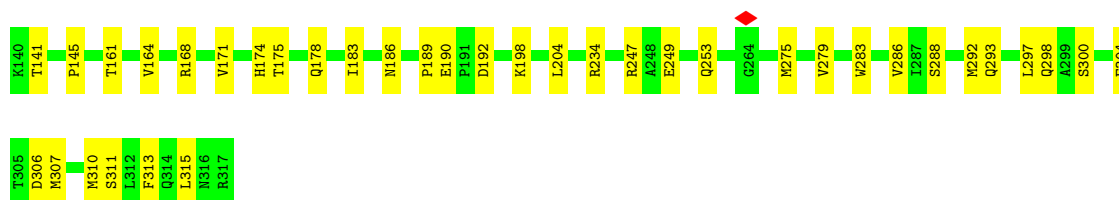
Chain BB:



• Molecule 3: Flagellar hook-associated protein 3

Chain BC:





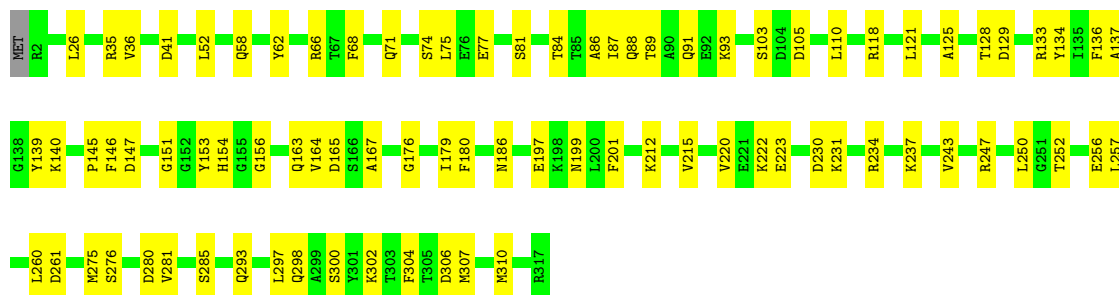
• Molecule 3: Flagellar hook-associated protein 3

Chain BD: 72% 28%



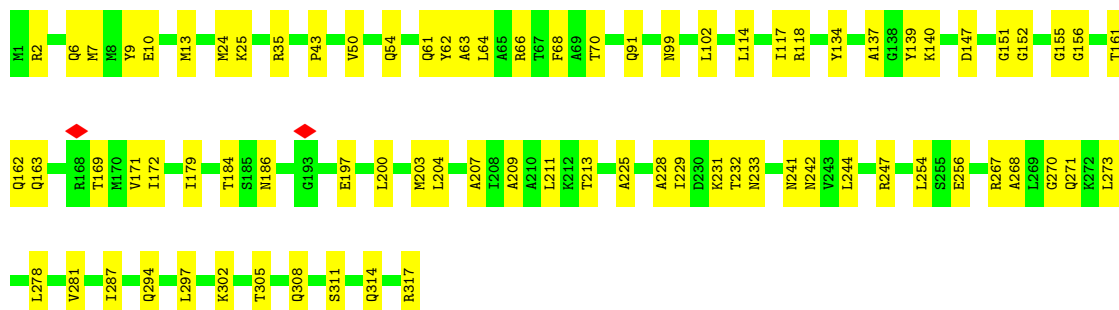
• Molecule 3: Flagellar hook-associated protein 3

Chain BE: 73% 26%



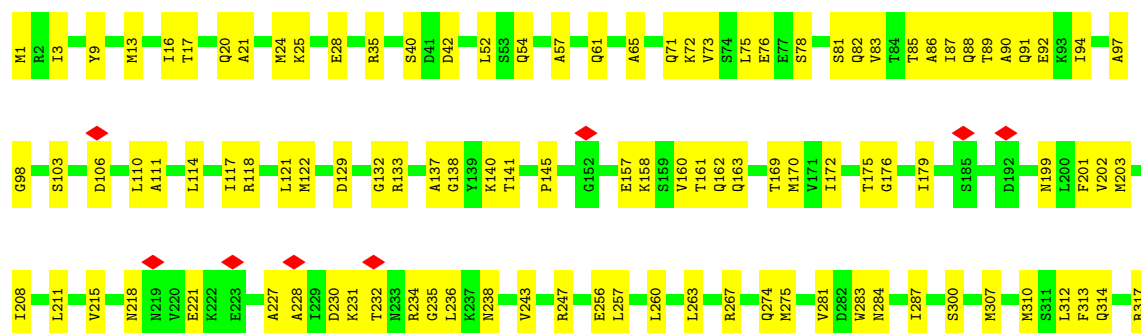
• Molecule 3: Flagellar hook-associated protein 3

Chain BF: 75% 25%



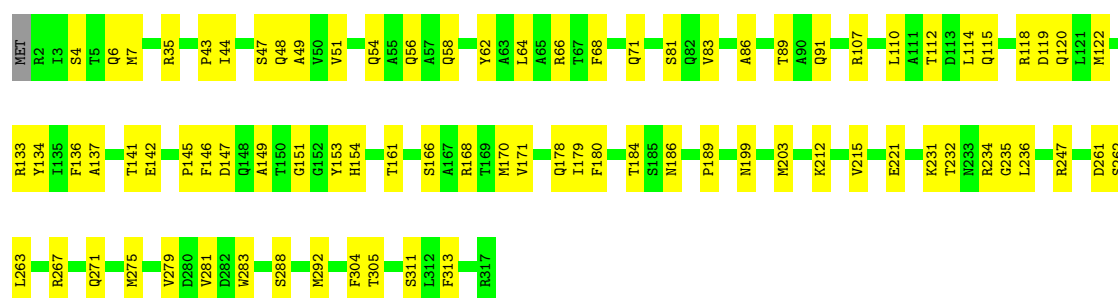
• Molecule 3: Flagellar hook-associated protein 3

Chain BG:  67% 33%



• Molecule 3: Flagellar hook-associated protein 3

Chain BH:  74% 26%



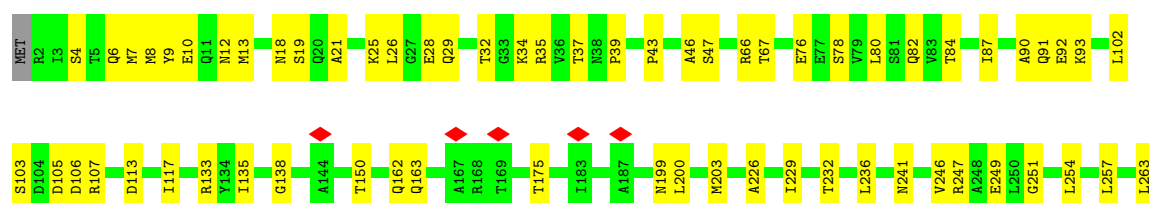
• Molecule 3: Flagellar hook-associated protein 3

Chain BI:  78% 22%



• Molecule 3: Flagellar hook-associated protein 3

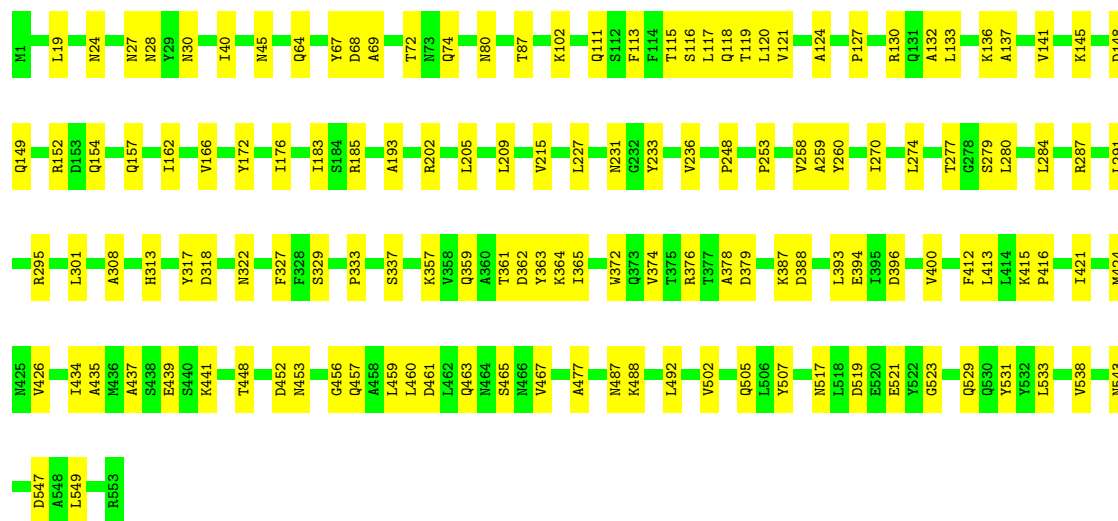
Chain BJ:  75% 25%





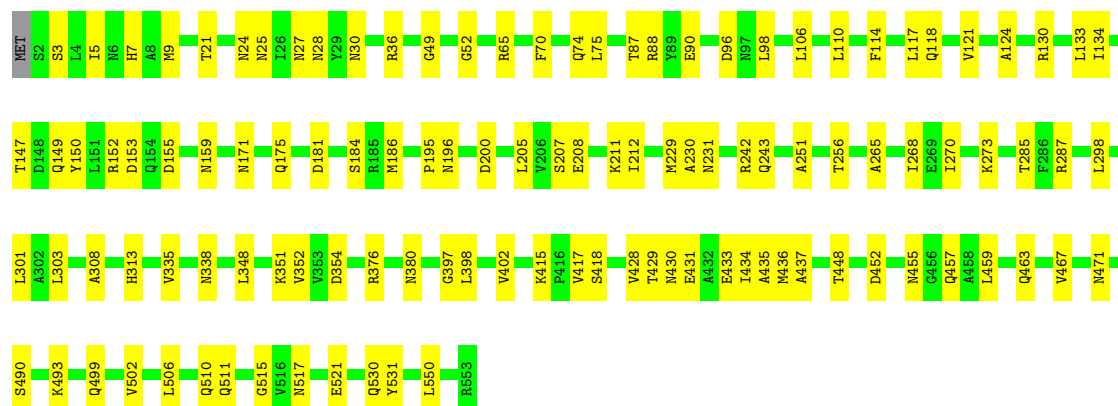
• Molecule 4: Flagellar hook-associated protein 1

Chain CB: 75% 25%



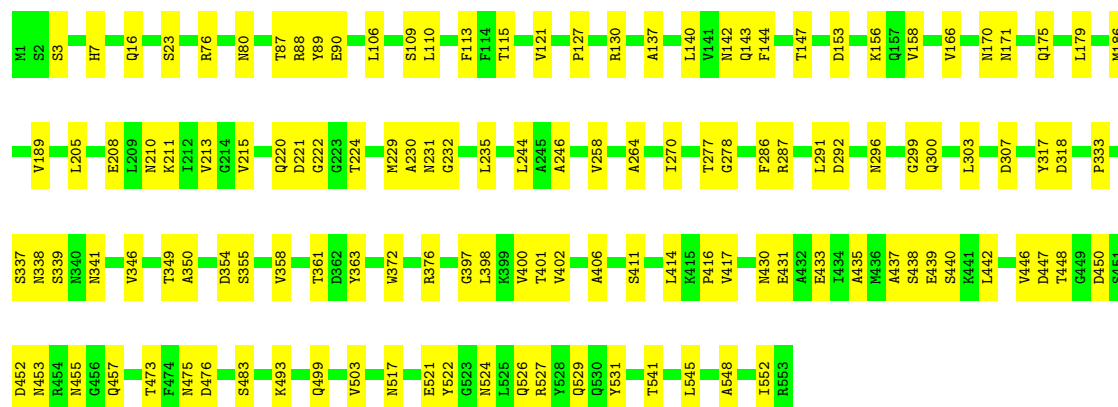
• Molecule 4: Flagellar hook-associated protein 1

Chain CC: 79% 21%

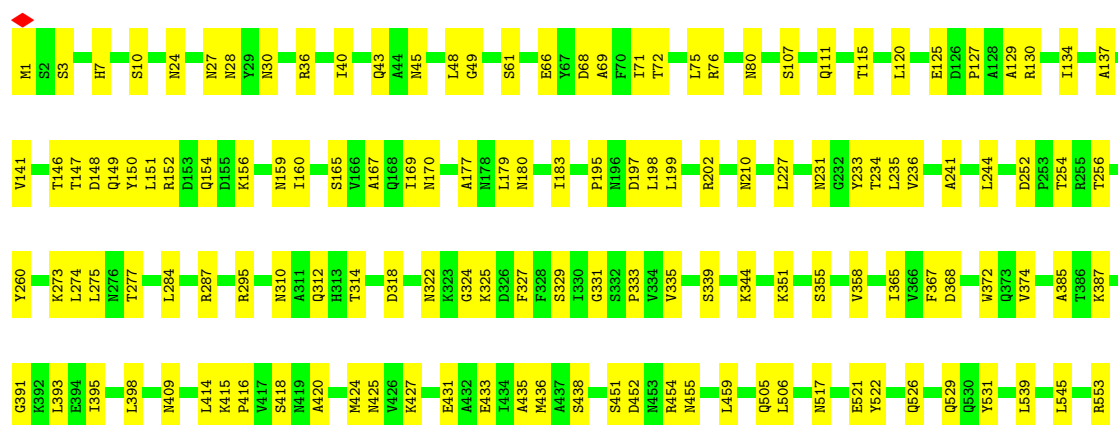
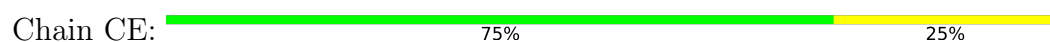


• Molecule 4: Flagellar hook-associated protein 1

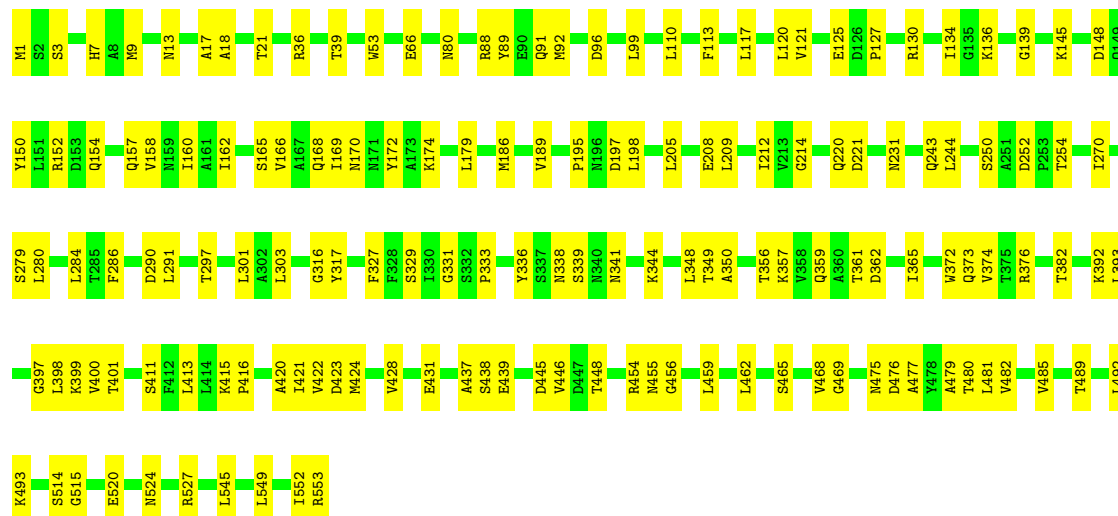
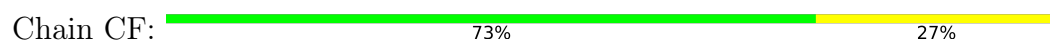
Chain CD: 77% 23%



• Molecule 4: Flagellar hook-associated protein 1

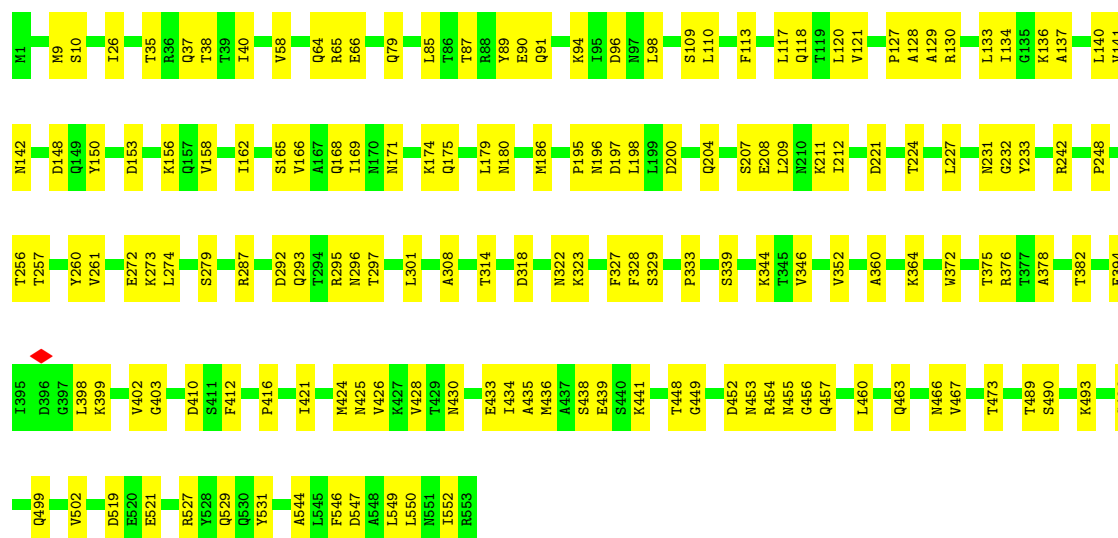


• Molecule 4: Flagellar hook-associated protein 1



• Molecule 4: Flagellar hook-associated protein 1

Chain CG:  71% 29%



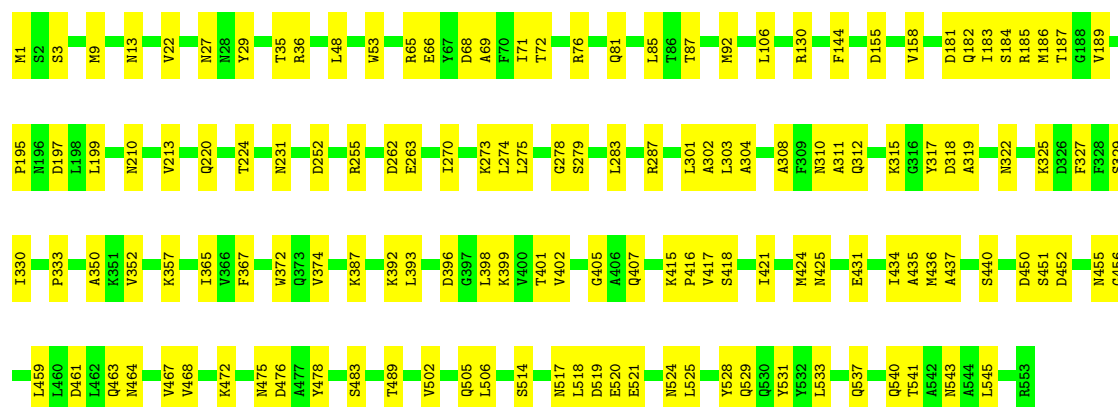
• Molecule 4: Flagellar hook-associated protein 1

Chain CH:  81% 19%

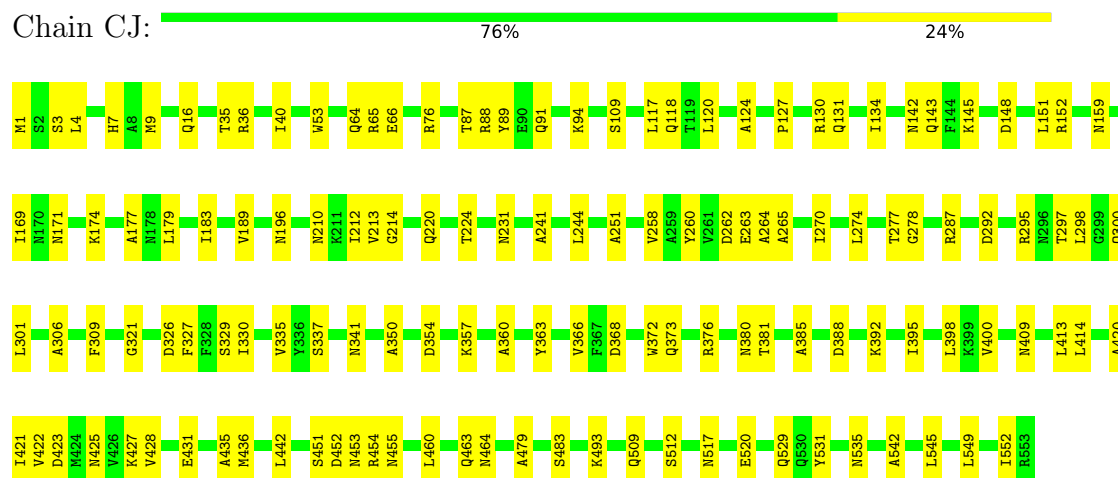


• Molecule 4: Flagellar hook-associated protein 1

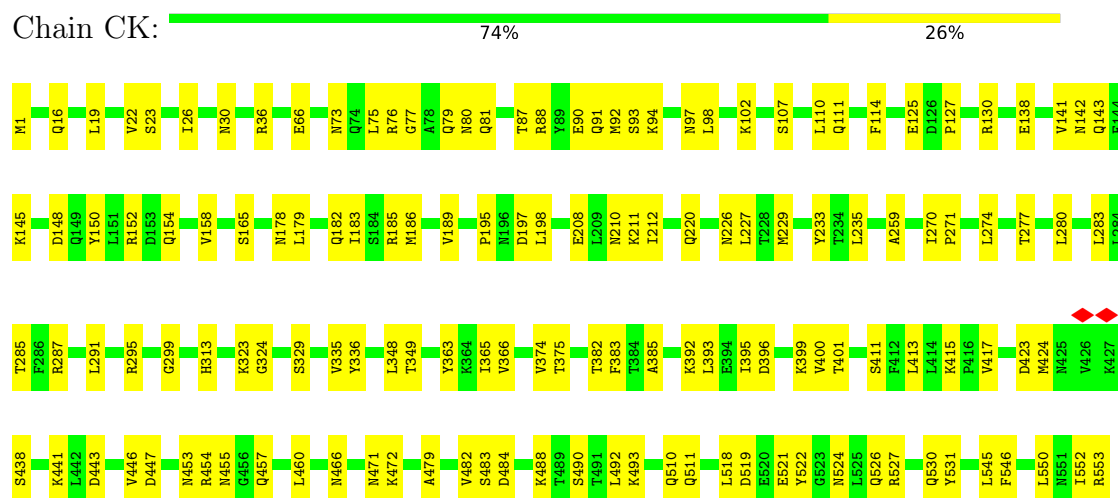
Chain CI:  75% 25%



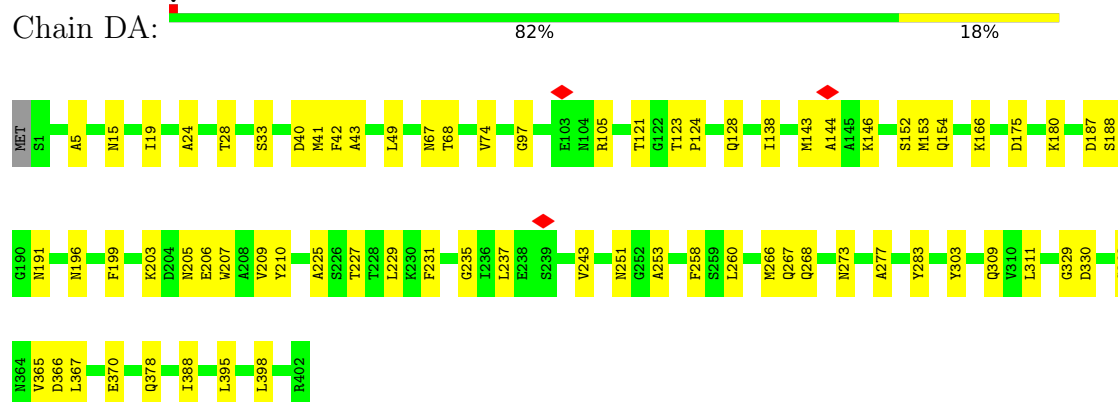
- Molecule 4: Flagellar hook-associated protein 1



- Molecule 4: Flagellar hook-associated protein 1

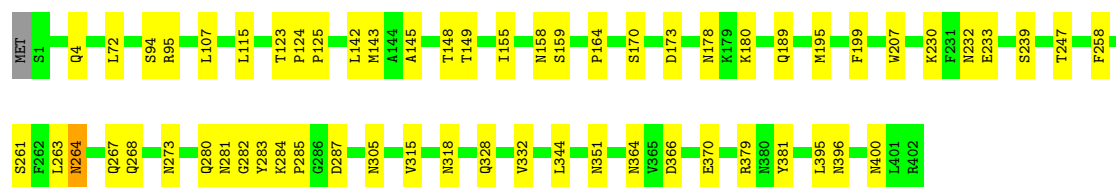


- Molecule 5: Flagellar hook protein FlgE



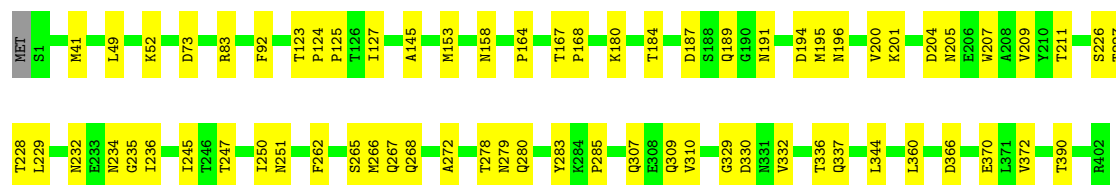
- Molecule 5: Flagellar hook protein FlgE

Chain DB:  85% 15%



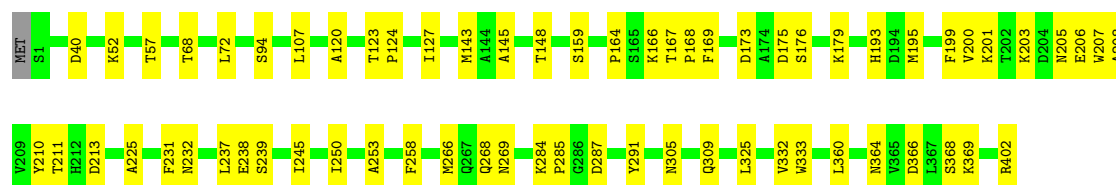
- Molecule 5: Flagellar hook protein FlgE

Chain DC:  83% 17%



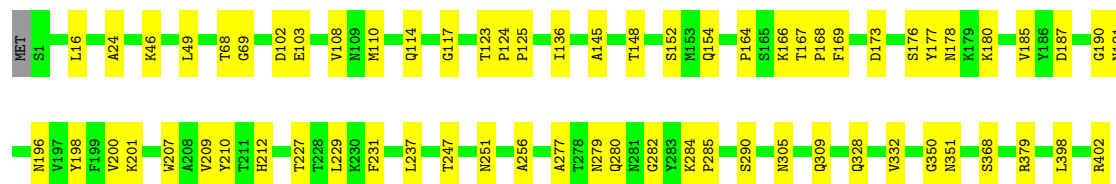
- Molecule 5: Flagellar hook protein FlgE

Chain DD:  84% 16%



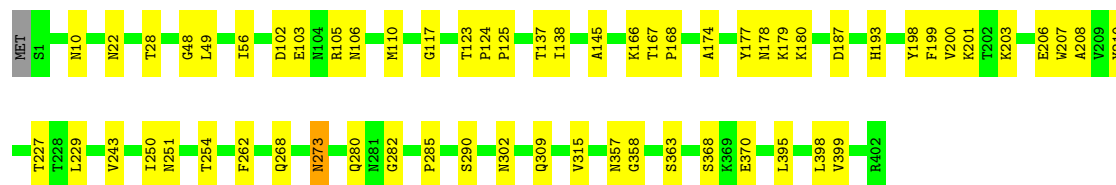
- Molecule 5: Flagellar hook protein FlgE

Chain DE:  83% 16%



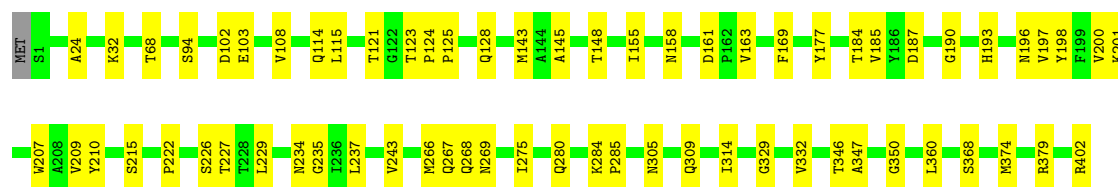
- Molecule 5: Flagellar hook protein FlgE

Chain DF:  85% 15%



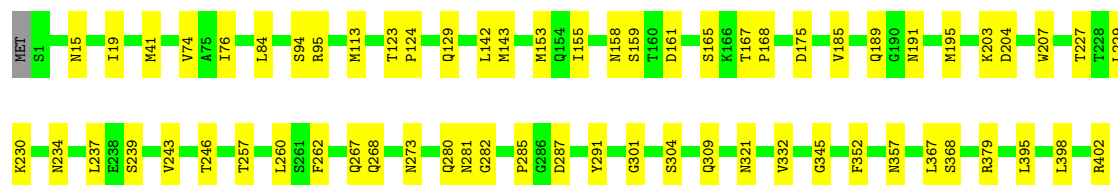
- Molecule 5: Flagellar hook protein FlgE

Chain DG:  83% 16%



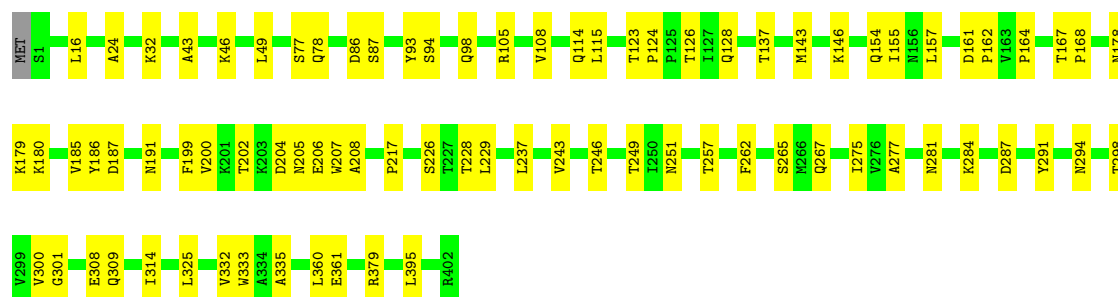
• Molecule 5: Flagellar hook protein FlgE

Chain DH:  84% 16%



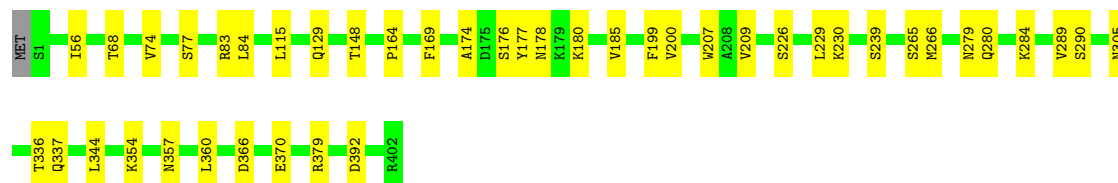
• Molecule 5: Flagellar hook protein FlgE

Chain DI:  80% 20%



• Molecule 5: Flagellar hook protein FlgE

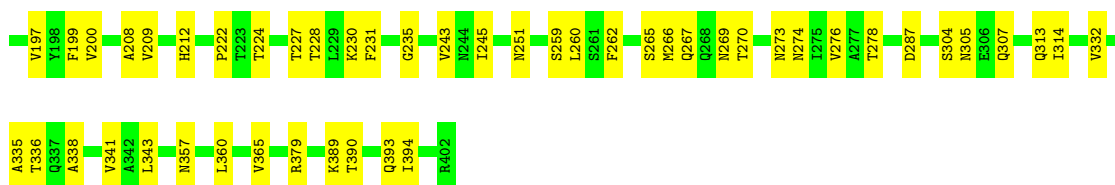
Chain DJ:  89% 11%



• Molecule 5: Flagellar hook protein FlgE

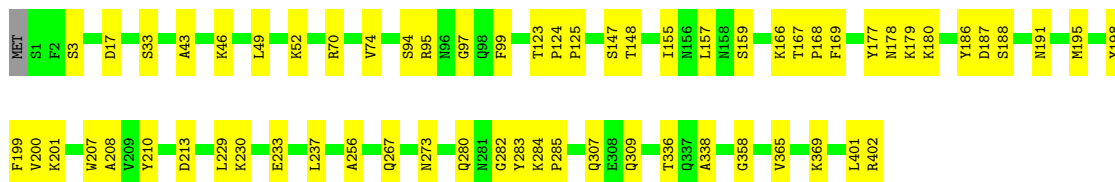
Chain DK:  80% 20%





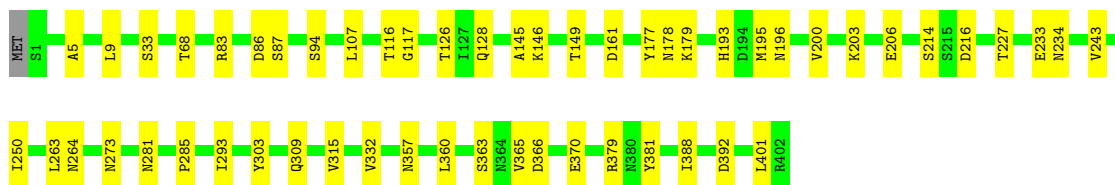
• Molecule 5: Flagellar hook protein FlgE

Chain EA: 84% 16%



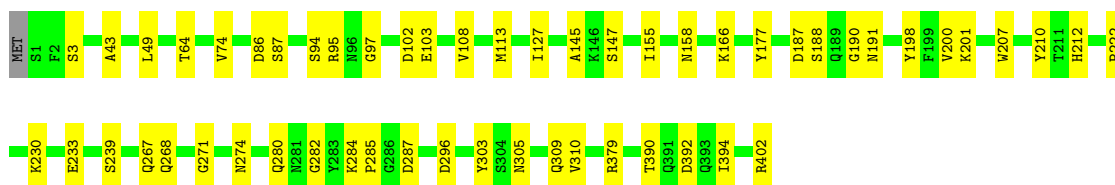
• Molecule 5: Flagellar hook protein FlgE

Chain EB: 86% 13%



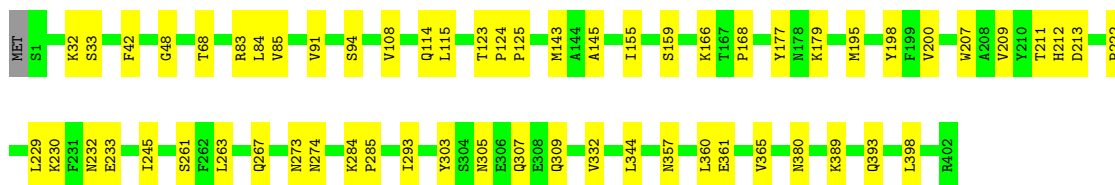
• Molecule 5: Flagellar hook protein FlgE

Chain EC: 86% 13%



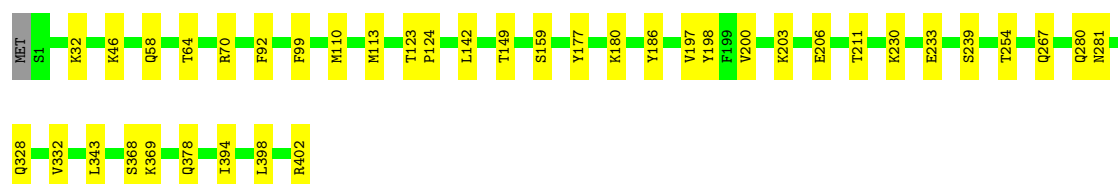
• Molecule 5: Flagellar hook protein FlgE

Chain ED: 85% 15%



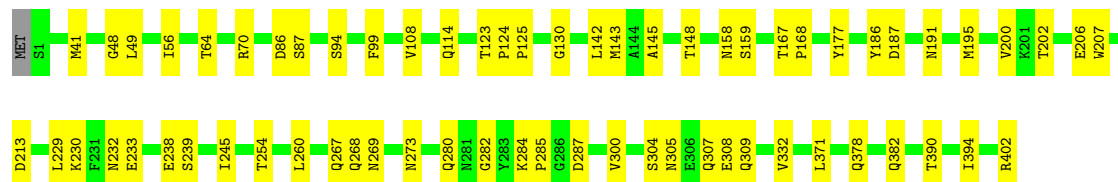
• Molecule 5: Flagellar hook protein FlgE

Chain EE: 90% 10%



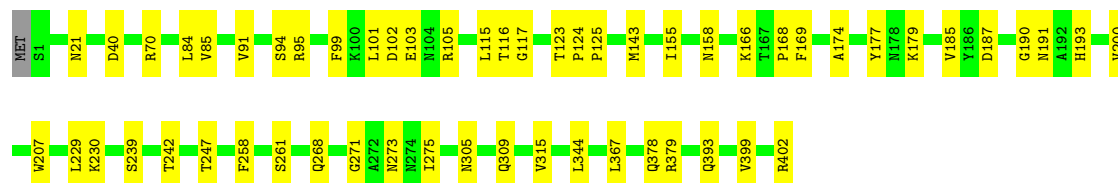
• Molecule 5: Flagellar hook protein FlgE

Chain EF: 84% 16%



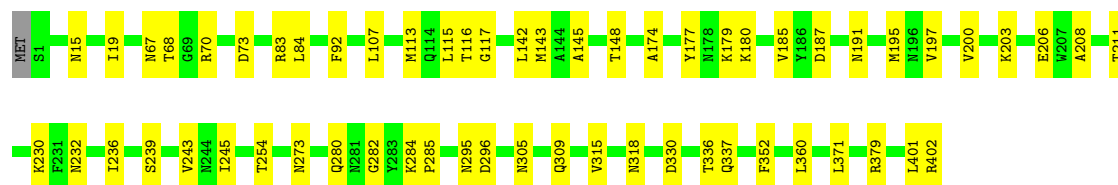
• Molecule 5: Flagellar hook protein FlgE

Chain EG: 86% 14%



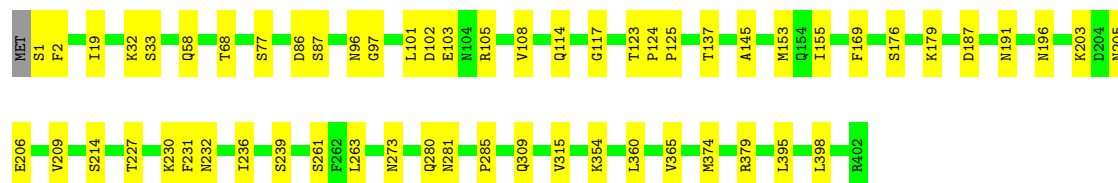
• Molecule 5: Flagellar hook protein FlgE

Chain EH: 85% 15%



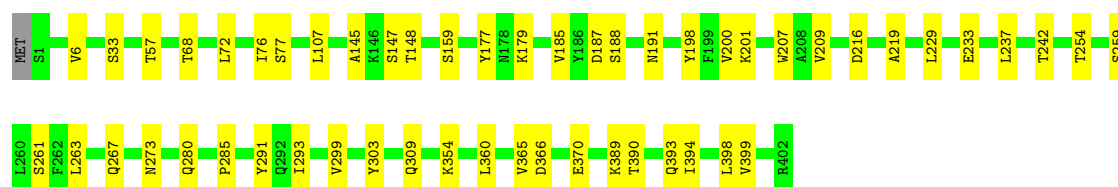
• Molecule 5: Flagellar hook protein FlgE

Chain EI: 85% 14%

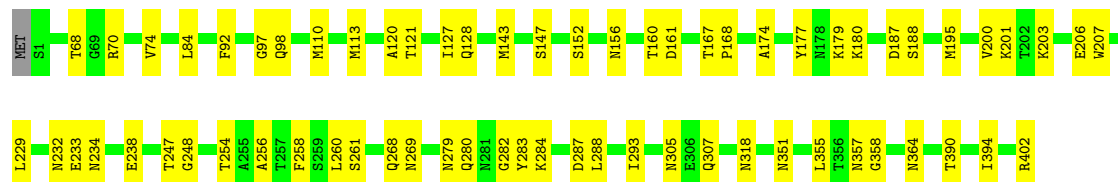
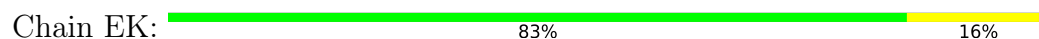


• Molecule 5: Flagellar hook protein FlgE

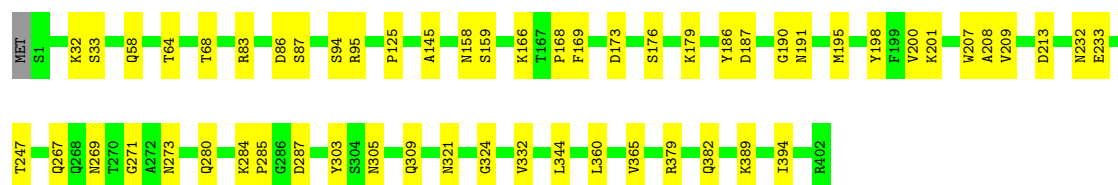
Chain EJ: 87% 13%



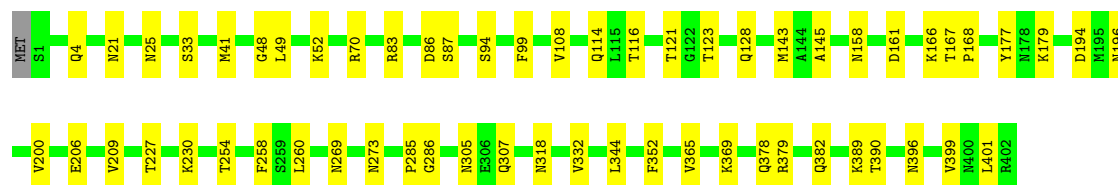
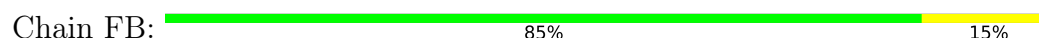
• Molecule 5: Flagellar hook protein FlgE



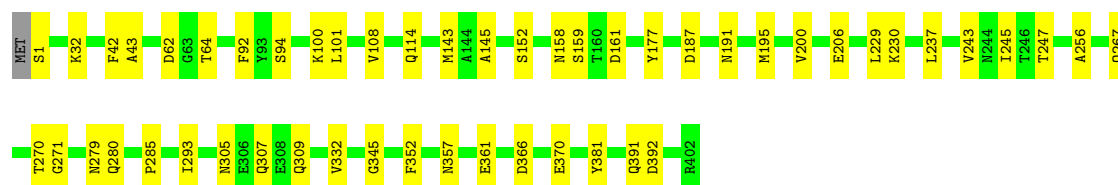
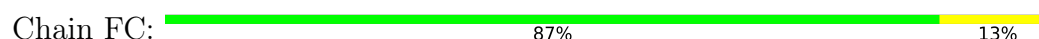
• Molecule 5: Flagellar hook protein FlgE



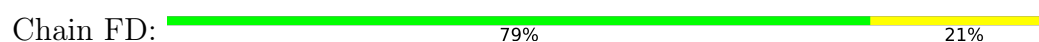
• Molecule 5: Flagellar hook protein FlgE

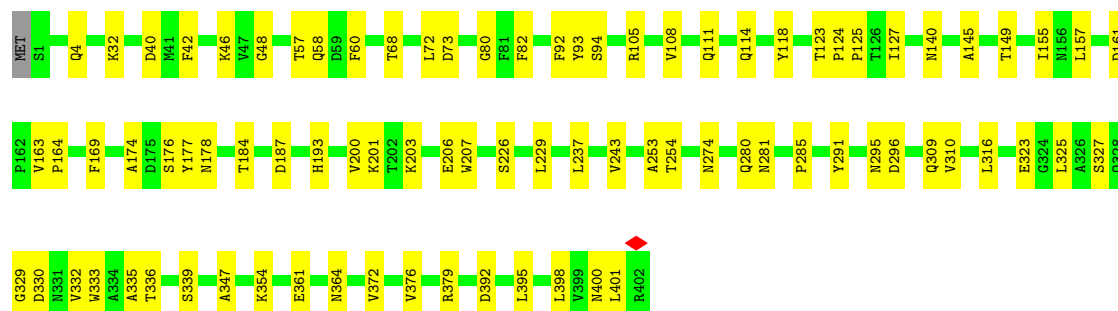


• Molecule 5: Flagellar hook protein FlgE



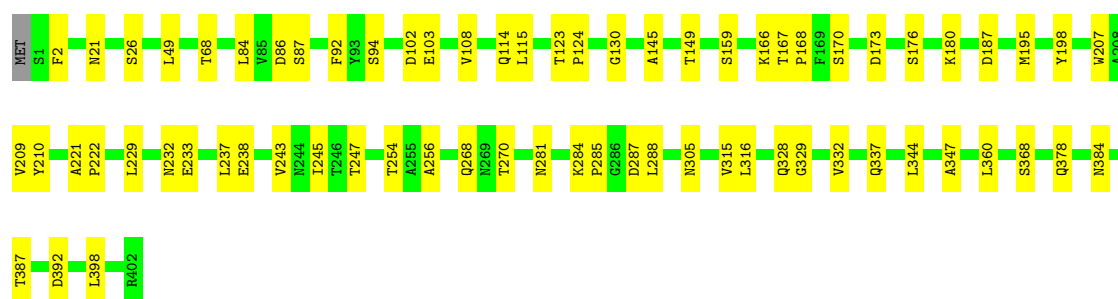
• Molecule 5: Flagellar hook protein FlgE





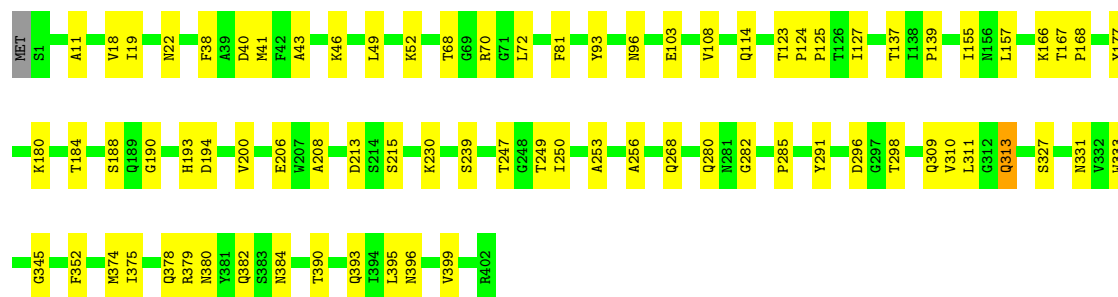
• Molecule 5: Flagellar hook protein FlgE

Chain FE: 83% 17%



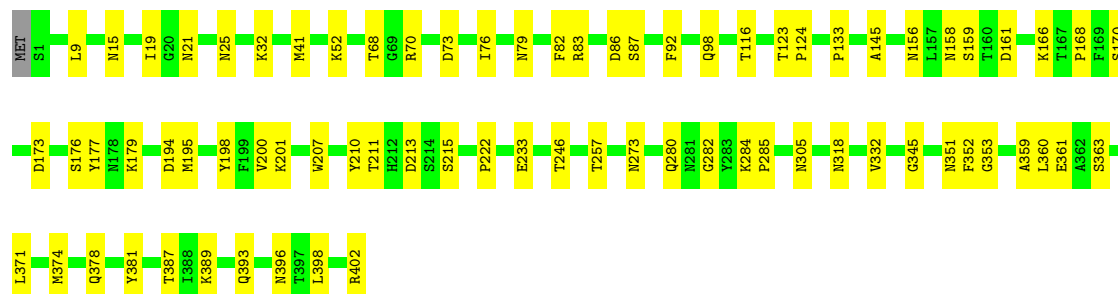
• Molecule 5: Flagellar hook protein FlgE

Chain FF: 80% 19%

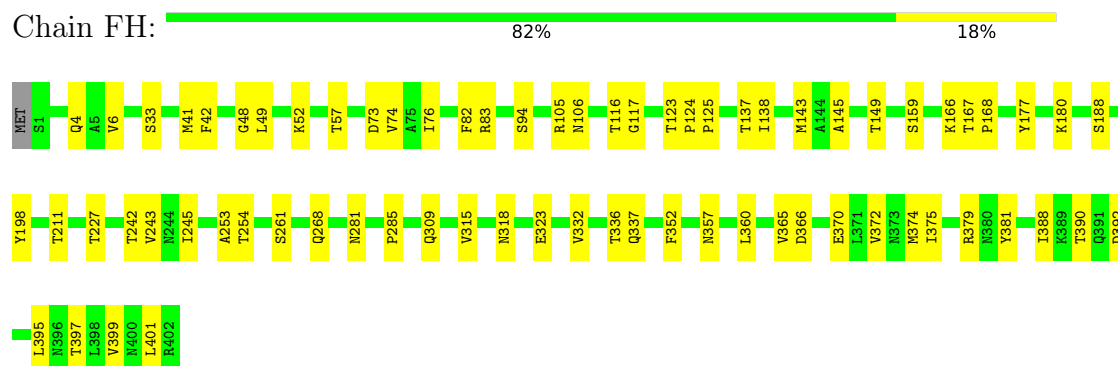


• Molecule 5: Flagellar hook protein FlgE

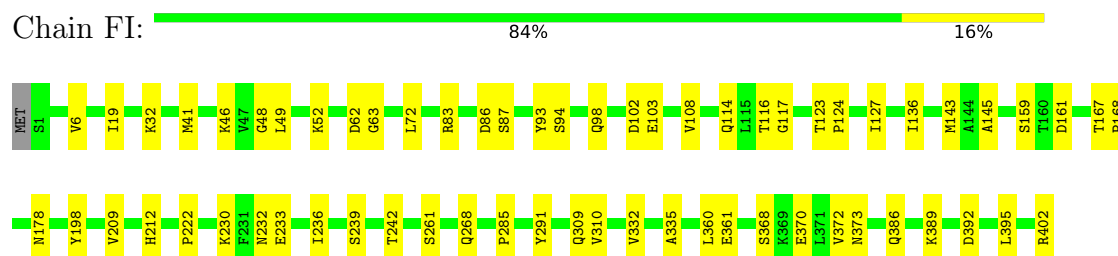
Chain FG: 81% 19%



- Molecule 5: Flagellar hook protein FlgE



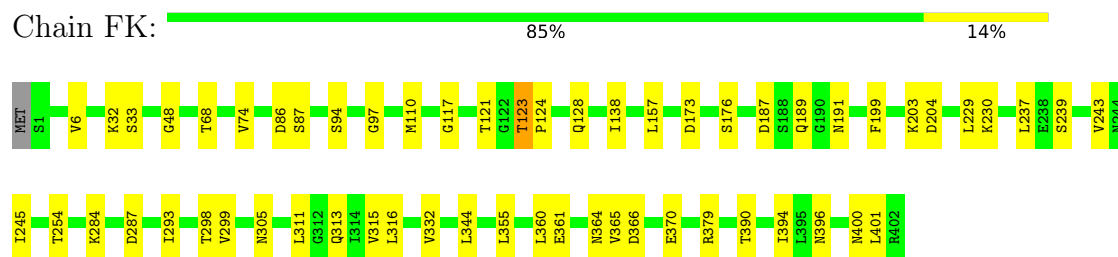
- Molecule 5: Flagellar hook protein FlgE



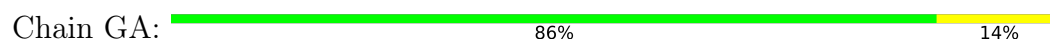
- Molecule 5: Flagellar hook protein FlgE

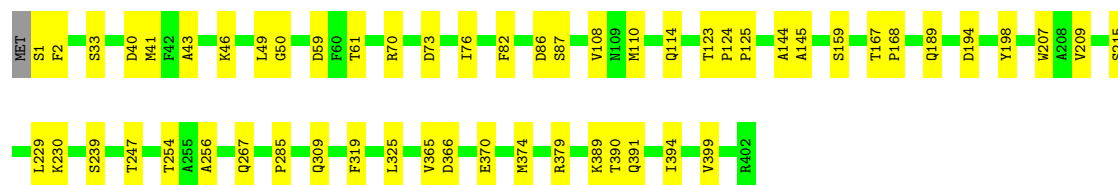


- Molecule 5: Flagellar hook protein FlgE



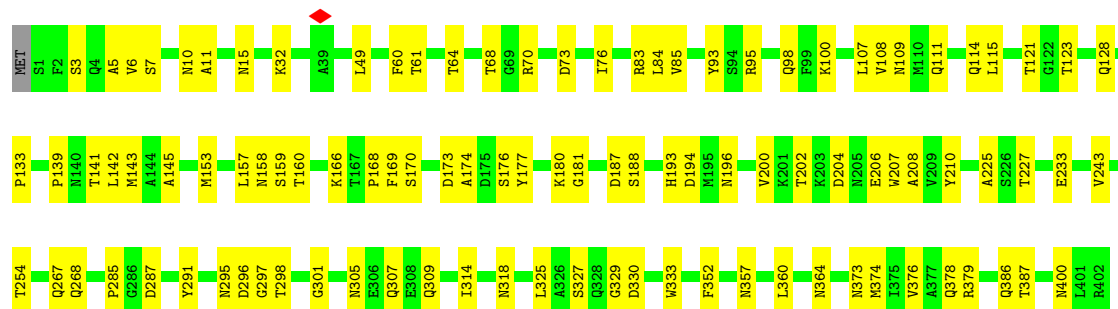
- Molecule 5: Flagellar hook protein FlgE





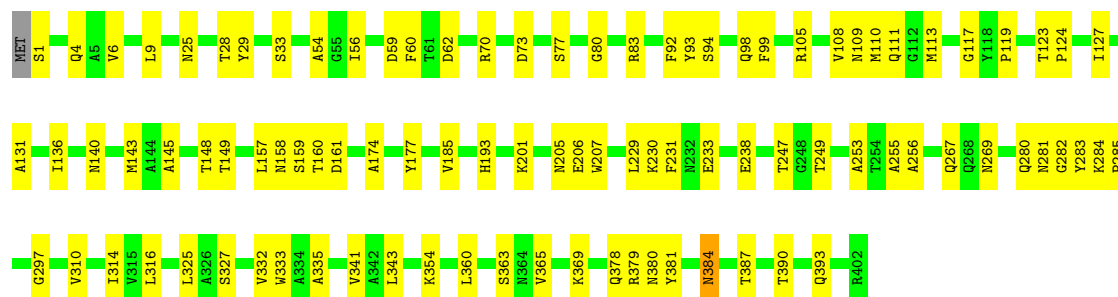
• Molecule 5: Flagellar hook protein FlgE

Chain GB:



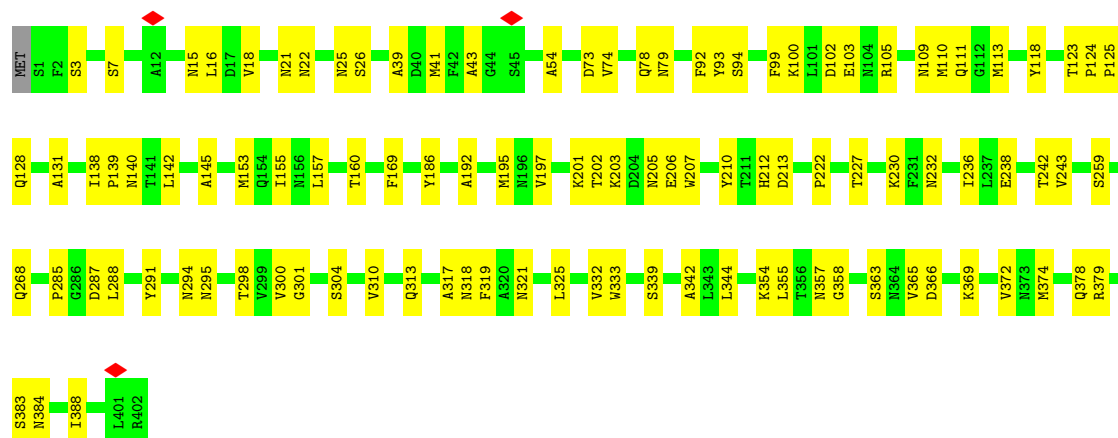
• Molecule 5: Flagellar hook protein FlgE

Chain GC:

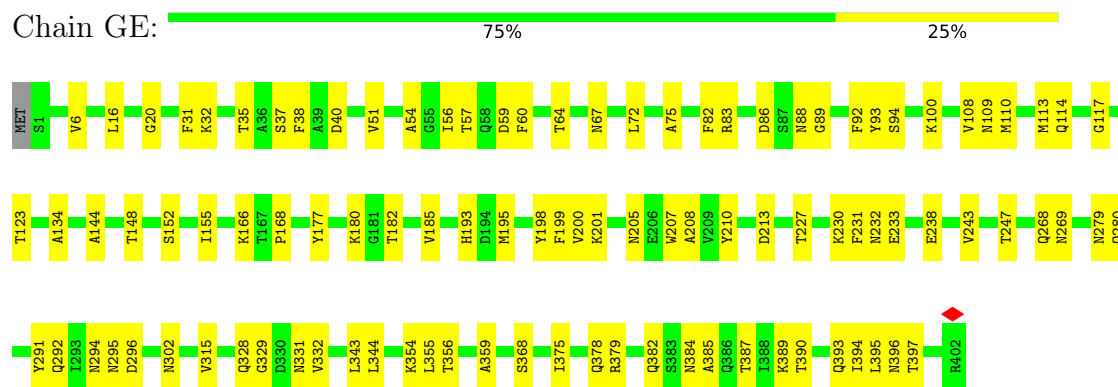


• Molecule 5: Flagellar hook protein FlgE

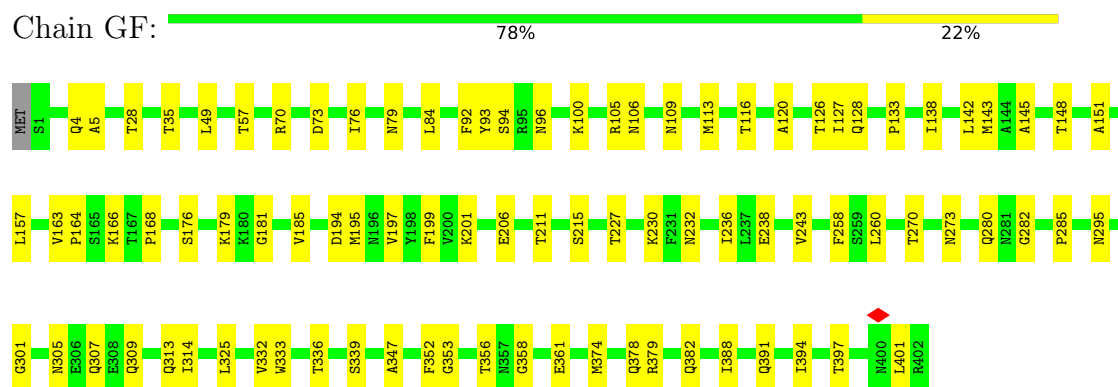
Chain GD:



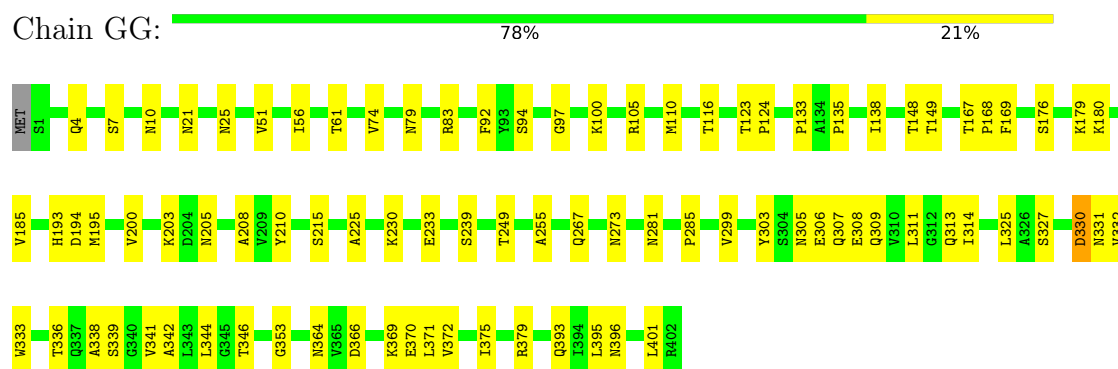
- Molecule 5: Flagellar hook protein FlgE



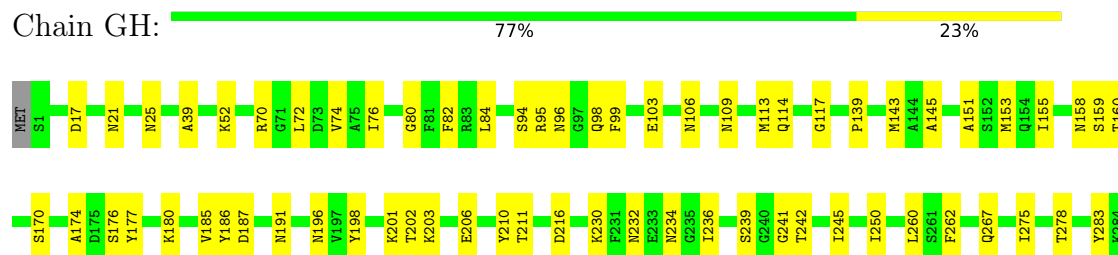
- Molecule 5: Flagellar hook protein FlgE



- Molecule 5: Flagellar hook protein FlgE



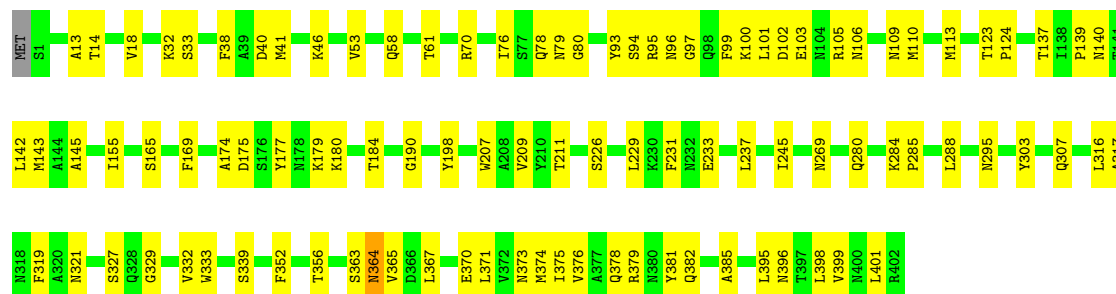
- Molecule 5: Flagellar hook protein FlgE





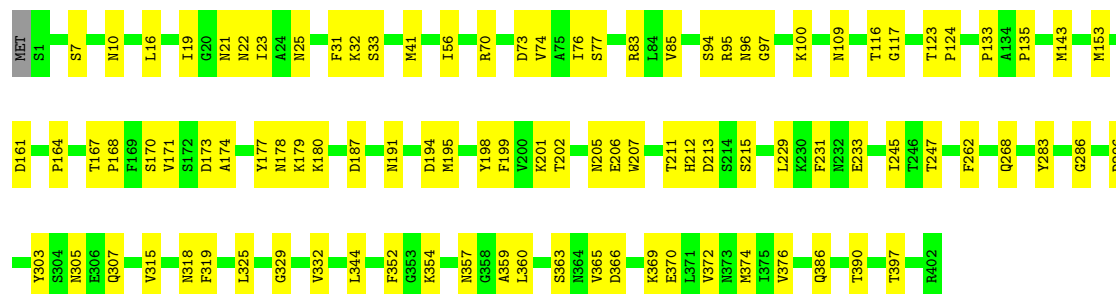
• Molecule 5: Flagellar hook protein FlgE

Chain GI: 75% 24%



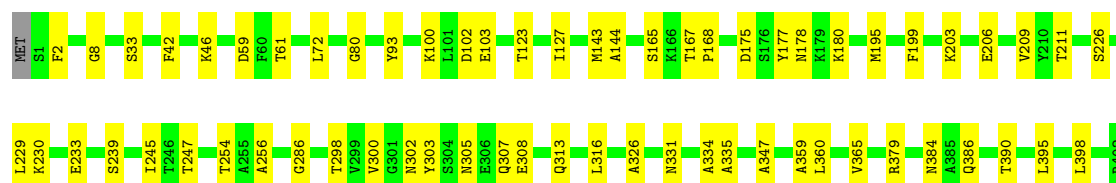
• Molecule 5: Flagellar hook protein FlgE

Chain GJ: 76% 24%



• Molecule 5: Flagellar hook protein FlgE

Chain GK: 84% 16%



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	0.853	Depositor
Minimum map value	-0.456	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	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 [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	AA	0.12	0/3404	0.30	0/4609
1	AB	0.10	0/3377	0.27	0/4572
1	AD	0.11	0/3374	0.31	0/4568
1	AE	0.10	0/3374	0.27	0/4568
2	AC	0.12	0/3373	0.33	0/4566
3	BA	0.17	0/2417	0.39	0/3268
3	BB	0.14	0/2409	0.34	0/3258
3	BC	0.13	0/2409	0.29	0/3258
3	BD	0.13	0/2417	0.32	0/3268
3	BE	0.13	0/2409	0.31	0/3258
3	BF	0.13	0/2417	0.33	0/3268
3	BG	0.12	0/2417	0.29	0/3268
3	BH	0.14	0/2409	0.34	0/3258
3	BI	0.14	0/2417	0.34	0/3268
3	BJ	0.13	0/2409	0.29	0/3258
3	BK	0.12	0/2409	0.28	0/3258
3	BL	0.11	0/1717	0.32	0/2314
4	CA	0.16	0/4203	0.32	0/5706
4	CB	0.16	0/4203	0.31	0/5706
4	CC	0.15	0/4195	0.31	0/5696
4	CD	0.14	0/4203	0.29	0/5706
4	CE	0.16	0/4203	0.32	0/5706
4	CF	0.16	0/4203	0.32	0/5706
4	CG	0.14	0/4203	0.32	0/5706
4	CH	0.16	0/4203	0.28	0/5706
4	CI	0.16	0/4203	0.32	0/5706
4	CJ	0.15	0/4203	0.34	0/5706
4	CK	0.15	0/4203	0.32	0/5706
5	DA	0.17	0/3003	0.33	0/4090
5	DB	0.19	0/3003	0.33	0/4090
5	DC	0.20	0/3003	0.36	0/4090
5	DD	0.20	0/3003	0.30	0/4090
5	DE	0.18	0/3003	0.30	0/4090
5	DF	0.19	0/3003	0.32	0/4090

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	DG	0.16	0/3003	0.32	0/4090
5	DH	0.20	0/3003	0.33	0/4090
5	DI	0.17	0/3003	0.32	0/4090
5	DJ	0.18	0/3003	0.31	0/4090
5	DK	0.17	0/3003	0.32	0/4090
5	EA	0.21	0/3003	0.32	0/4090
5	EB	0.21	0/3003	0.31	0/4090
5	EC	0.21	0/3003	0.31	0/4090
5	ED	0.21	0/3003	0.29	0/4090
5	EE	0.21	0/3003	0.31	0/4090
5	EF	0.20	0/3003	0.29	0/4090
5	EG	0.20	0/3003	0.32	0/4090
5	EH	0.19	0/3003	0.32	0/4090
5	EI	0.19	0/3003	0.30	0/4090
5	EJ	0.21	0/3003	0.34	0/4090
5	EK	0.21	0/3003	0.33	0/4090
5	FA	0.21	0/3003	0.32	0/4090
5	FB	0.19	0/3003	0.30	0/4090
5	FC	0.19	0/3003	0.30	0/4090
5	FD	0.16	0/3003	0.34	0/4090
5	FE	0.18	0/3003	0.35	0/4090
5	FF	0.14	0/3003	0.30	0/4090
5	FG	0.17	0/3003	0.31	0/4090
5	FH	0.15	0/3003	0.32	0/4090
5	FI	0.17	0/3003	0.32	0/4090
5	FJ	0.17	0/3003	0.32	0/4090
5	FK	0.20	0/3003	0.28	0/4090
5	GA	0.18	0/3003	0.35	0/4090
5	GB	0.13	0/3003	0.29	0/4090
5	GC	0.15	0/3003	0.32	0/4090
5	GD	0.12	0/3003	0.31	0/4090
5	GE	0.12	0/3003	0.29	0/4090
5	GF	0.11	0/3003	0.29	0/4090
5	GG	0.13	0/3003	0.35	1/4090 (0.0%)
5	GH	0.11	0/3003	0.30	0/4090
5	GI	0.13	0/3003	0.31	0/4090
5	GJ	0.12	0/3003	0.29	0/4090
5	GK	0.15	0/3003	0.33	0/4090
All	All	0.16	0/223515	0.31	1/303801 (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
3	BA	0	1
5	FB	0	1
5	FK	0	1
5	GB	0	1
5	GE	0	1
5	GK	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	GG	330	ASP	CB-CA-C	-5.01	110.77	116.54

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	BA	313	PHE	Peptide
5	FB	123	THR	Peptide
5	FK	123	THR	Peptide
5	GB	123	THR	Peptide
5	GE	123	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3380	0	3435	92	0
1	AB	3353	0	3403	61	0
1	AD	3350	0	3402	106	0
1	AE	3350	0	3402	73	0
2	AC	3349	0	3402	48	0
3	BA	2391	0	2350	97	0
3	BB	2383	0	2338	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BC	2383	0	2338	50	0
3	BD	2391	0	2350	65	0
3	BE	2383	0	2338	58	0
3	BF	2391	0	2350	56	0
3	BG	2391	0	2350	78	0
3	BH	2383	0	2338	62	0
3	BI	2391	0	2350	54	0
3	BJ	2383	0	2338	62	0
3	BK	2383	0	2338	63	0
3	BL	1705	0	1685	45	0
4	CA	4157	0	4071	110	0
4	CB	4157	0	4071	101	0
4	CC	4149	0	4059	80	0
4	CD	4157	0	4071	90	0
4	CE	4157	0	4071	92	0
4	CF	4157	0	4071	110	0
4	CG	4157	0	4071	121	0
4	CH	4157	0	4071	70	0
4	CI	4157	0	4071	101	0
4	CJ	4157	0	4071	97	0
4	CK	4157	0	4071	110	0
5	DA	2959	0	2855	55	0
5	DB	2959	0	2855	47	0
5	DC	2959	0	2855	43	0
5	DD	2959	0	2855	47	0
5	DE	2959	0	2855	46	0
5	DF	2959	0	2855	44	0
5	DG	2959	0	2855	48	0
5	DH	2959	0	2855	41	0
5	DI	2959	0	2855	51	0
5	DJ	2959	0	2855	30	0
5	DK	2959	0	2855	55	0
5	EA	2959	0	2855	44	0
5	EB	2959	0	2855	36	0
5	EC	2959	0	2855	41	0
5	ED	2959	0	2855	35	0
5	EE	2959	0	2855	29	0
5	EF	2959	0	2855	42	0
5	EG	2959	0	2855	37	0
5	EH	2959	0	2855	39	0
5	EI	2959	0	2855	32	0
5	EJ	2959	0	2855	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	EK	2959	0	2855	42	0
5	FA	2959	0	2855	43	0
5	FB	2959	0	2855	39	0
5	FC	2959	0	2855	36	0
5	FD	2959	0	2855	59	0
5	FE	2959	0	2855	47	0
5	FF	2959	0	2855	62	0
5	FG	2959	0	2855	44	0
5	FH	2959	0	2855	49	0
5	FI	2959	0	2855	41	0
5	FJ	2959	0	2855	60	0
5	FK	2959	0	2855	40	0
5	GA	2959	0	2855	36	0
5	GB	2959	0	2855	71	0
5	GC	2959	0	2855	69	0
5	GD	2959	0	2855	72	0
5	GE	2959	0	2855	74	0
5	GF	2959	0	2855	56	0
5	GG	2959	0	2855	59	0
5	GH	2959	0	2855	60	0
5	GI	2959	0	2855	66	0
5	GJ	2959	0	2855	66	0
5	GK	2959	0	2855	43	0
All	All	220655	0	214896	3897	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 9.

The worst 5 of 3897 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)
4:CF:365:ILE:O	4:CF:411:SER:HA	1.58	1.01
3:BA:8:MET:HB3	3:BA:307:MET:HE1	1.50	0.92
5:DJ:148:THR:HG21	5:DJ:185:VAL:HB	1.56	0.87
3:BK:55:ALA:HB3	3:BK:271:GLN:HE22	1.40	0.86
3:BA:8:MET:HE1	4:CJ:16:GLN:HG2	1.59	0.85

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	450/467 (96%)	432 (96%)	18 (4%)	0	100	100
1	AB	446/467 (96%)	426 (96%)	20 (4%)	0	100	100
1	AD	445/467 (95%)	426 (96%)	19 (4%)	0	100	100
1	AE	445/467 (95%)	428 (96%)	17 (4%)	0	100	100
2	AC	445/467 (95%)	425 (96%)	20 (4%)	0	100	100
3	BA	315/317 (99%)	307 (98%)	8 (2%)	0	100	100
3	BB	314/317 (99%)	305 (97%)	9 (3%)	0	100	100
3	BC	314/317 (99%)	305 (97%)	9 (3%)	0	100	100
3	BD	315/317 (99%)	307 (98%)	8 (2%)	0	100	100
3	BE	314/317 (99%)	304 (97%)	10 (3%)	0	100	100
3	BF	315/317 (99%)	306 (97%)	9 (3%)	0	100	100
3	BG	315/317 (99%)	306 (97%)	9 (3%)	0	100	100
3	BH	314/317 (99%)	308 (98%)	6 (2%)	0	100	100
3	BI	315/317 (99%)	305 (97%)	10 (3%)	0	100	100
3	BJ	314/317 (99%)	302 (96%)	12 (4%)	0	100	100
3	BK	314/317 (99%)	308 (98%)	6 (2%)	0	100	100
3	BL	215/317 (68%)	206 (96%)	9 (4%)	0	100	100
4	CA	551/553 (100%)	536 (97%)	15 (3%)	0	100	100
4	CB	551/553 (100%)	542 (98%)	9 (2%)	0	100	100
4	CC	550/553 (100%)	536 (98%)	14 (2%)	0	100	100
4	CD	551/553 (100%)	544 (99%)	7 (1%)	0	100	100
4	CE	551/553 (100%)	543 (98%)	8 (2%)	0	100	100
4	CF	551/553 (100%)	543 (98%)	8 (2%)	0	100	100
4	CG	551/553 (100%)	538 (98%)	13 (2%)	0	100	100
4	CH	551/553 (100%)	541 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CI	551/553 (100%)	539 (98%)	12 (2%)	0	100	100
4	CJ	551/553 (100%)	544 (99%)	7 (1%)	0	100	100
4	CK	551/553 (100%)	536 (97%)	15 (3%)	0	100	100
5	DA	400/403 (99%)	380 (95%)	20 (5%)	0	100	100
5	DB	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	DC	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	DD	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
5	DE	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	DF	400/403 (99%)	390 (98%)	10 (2%)	0	100	100
5	DG	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	DH	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
5	DI	400/403 (99%)	381 (95%)	19 (5%)	0	100	100
5	DJ	400/403 (99%)	383 (96%)	17 (4%)	0	100	100
5	DK	400/403 (99%)	381 (95%)	19 (5%)	0	100	100
5	EA	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	EB	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
5	EC	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	ED	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	EE	400/403 (99%)	386 (96%)	14 (4%)	0	100	100
5	EF	400/403 (99%)	373 (93%)	27 (7%)	0	100	100
5	EG	400/403 (99%)	386 (96%)	14 (4%)	0	100	100
5	EH	400/403 (99%)	389 (97%)	11 (3%)	0	100	100
5	EI	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
5	EJ	400/403 (99%)	389 (97%)	11 (3%)	0	100	100
5	EK	400/403 (99%)	392 (98%)	8 (2%)	0	100	100
5	FA	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	FB	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
5	FC	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
5	FD	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	FE	400/403 (99%)	382 (96%)	18 (4%)	0	100	100
5	FF	400/403 (99%)	376 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	FG	400/403 (99%)	382 (96%)	18 (4%)	0	100	100
5	FH	400/403 (99%)	390 (98%)	10 (2%)	0	100	100
5	FI	400/403 (99%)	390 (98%)	10 (2%)	0	100	100
5	FJ	400/403 (99%)	378 (94%)	22 (6%)	0	100	100
5	FK	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	GA	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	GB	400/403 (99%)	382 (96%)	18 (4%)	0	100	100
5	GC	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
5	GD	400/403 (99%)	383 (96%)	17 (4%)	0	100	100
5	GE	400/403 (99%)	376 (94%)	24 (6%)	0	100	100
5	GF	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
5	GG	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
5	GH	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
5	GI	400/403 (99%)	385 (96%)	14 (4%)	1 (0%)	36	66
5	GJ	400/403 (99%)	383 (96%)	17 (4%)	0	100	100
5	GK	400/403 (99%)	391 (98%)	9 (2%)	0	100	100
All	All	29565/29954 (99%)	28583 (97%)	981 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	GI	364	ASN

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	375 (100%)	0	100	100
3	BA	261/261 (100%)	261 (100%)	0	100	100
3	BB	260/261 (100%)	260 (100%)	0	100	100
3	BC	260/261 (100%)	260 (100%)	0	100	100
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	260/261 (100%)	260 (100%)	0	100	100
3	BI	261/261 (100%)	261 (100%)	0	100	100
3	BJ	260/261 (100%)	260 (100%)	0	100	100
3	BK	260/261 (100%)	260 (100%)	0	100	100
3	BL	188/261 (72%)	188 (100%)	0	100	100
4	CA	453/453 (100%)	453 (100%)	0	100	100
4	CB	453/453 (100%)	452 (100%)	1 (0%)	87	87
4	CC	452/453 (100%)	452 (100%)	0	100	100
4	CD	453/453 (100%)	453 (100%)	0	100	100
4	CE	453/453 (100%)	452 (100%)	1 (0%)	87	87
4	CF	453/453 (100%)	453 (100%)	0	100	100
4	CG	453/453 (100%)	452 (100%)	1 (0%)	87	87
4	CH	453/453 (100%)	453 (100%)	0	100	100
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%)	321 (100%)	1 (0%)	86	85
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%)	321 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	DF	322/323 (100%)	321 (100%)	1 (0%)	86	85
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%)	322 (100%)	0	100	100
5	DK	322/323 (100%)	322 (100%)	0	100	100
5	EA	322/323 (100%)	322 (100%)	0	100	100
5	EB	322/323 (100%)	322 (100%)	0	100	100
5	EC	322/323 (100%)	322 (100%)	0	100	100
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	322/323 (100%)	322 (100%)	0	100	100
5	FB	322/323 (100%)	322 (100%)	0	100	100
5	FC	322/323 (100%)	322 (100%)	0	100	100
5	FD	322/323 (100%)	322 (100%)	0	100	100
5	FE	322/323 (100%)	322 (100%)	0	100	100
5	FF	322/323 (100%)	321 (100%)	1 (0%)	86	85
5	FG	322/323 (100%)	322 (100%)	0	100	100
5	FH	322/323 (100%)	322 (100%)	0	100	100
5	FI	322/323 (100%)	322 (100%)	0	100	100
5	FJ	322/323 (100%)	322 (100%)	0	100	100
5	FK	322/323 (100%)	322 (100%)	0	100	100
5	GA	322/323 (100%)	322 (100%)	0	100	100
5	GB	322/323 (100%)	322 (100%)	0	100	100
5	GC	322/323 (100%)	321 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	GD	322/323 (100%)	322 (100%)	0	100	100
5	GE	322/323 (100%)	322 (100%)	0	100	100
5	GF	322/323 (100%)	322 (100%)	0	100	100
5	GG	322/323 (100%)	321 (100%)	1 (0%)	86	85
5	GH	322/323 (100%)	322 (100%)	0	100	100
5	GI	322/323 (100%)	322 (100%)	0	100	100
5	GJ	322/323 (100%)	322 (100%)	0	100	100
5	GK	322/323 (100%)	321 (100%)	1 (0%)	86	85
All	All	24081/24282 (99%)	24071 (100%)	10 (0%)	100	100

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	GC	384	ASN
5	GG	10	ASN
5	GK	331	ASN
5	DB	264	ASN
5	DE	212	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 381 such sidechains are listed below:

Mol	Chain	Res	Type
5	EB	212	HIS
5	FB	128	GLN
5	EC	132	ASN
5	EG	393	GLN
5	FF	191	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

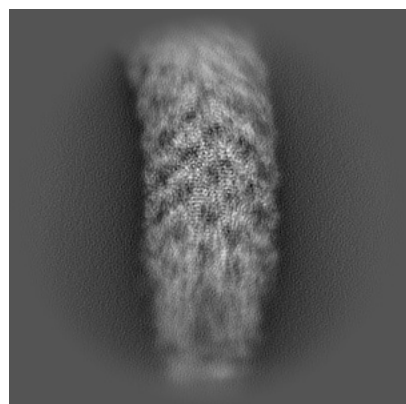
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63802. These allow visual inspection of the internal detail of the map and identification of artifacts.

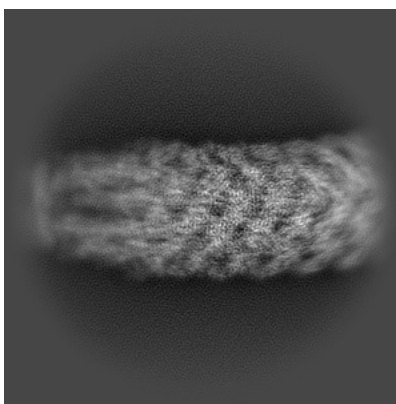
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

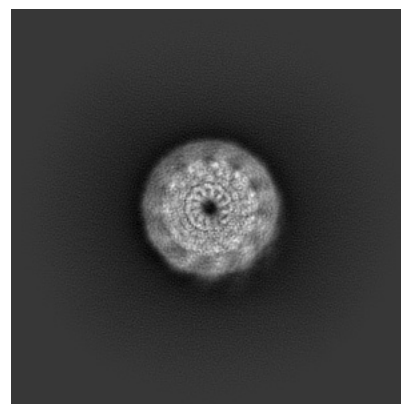
6.1.1 Primary map



X

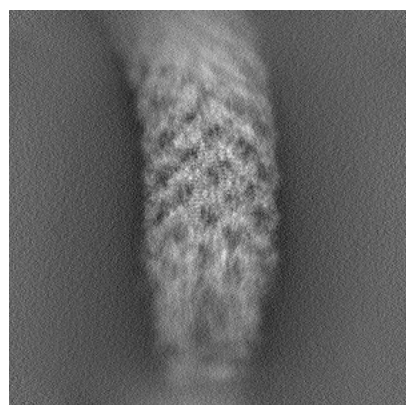


Y

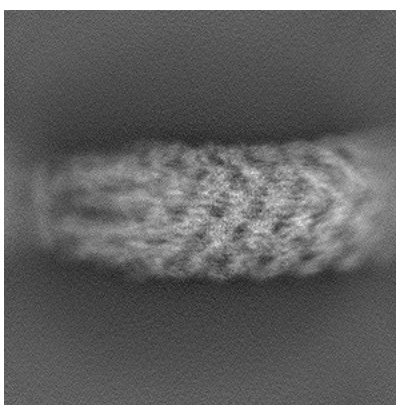


Z

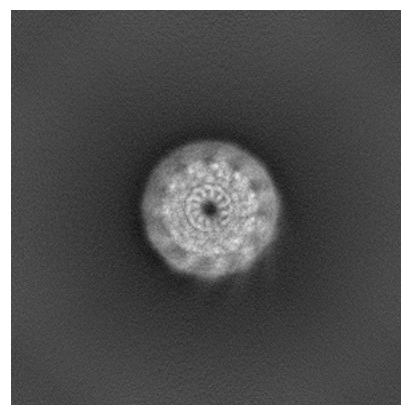
6.1.2 Raw map



X



Y

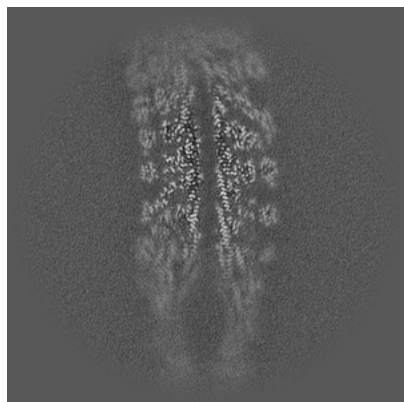


Z

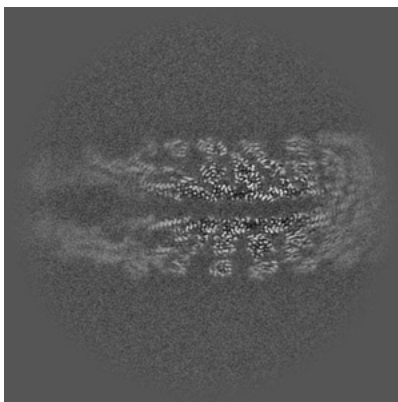
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

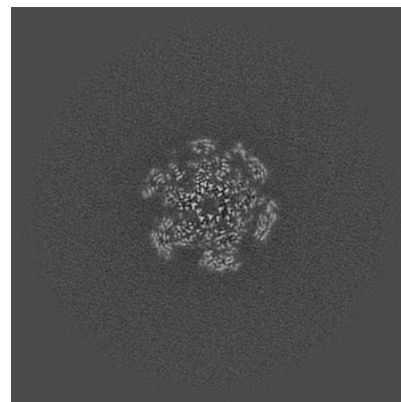
6.2.1 Primary map



X Index: 300

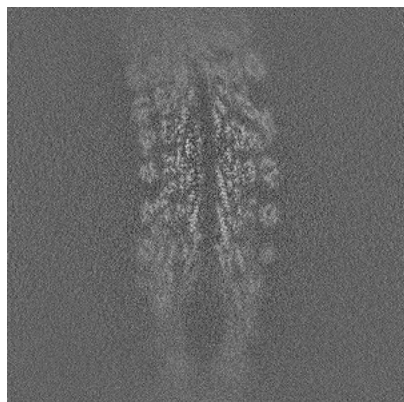


Y Index: 300

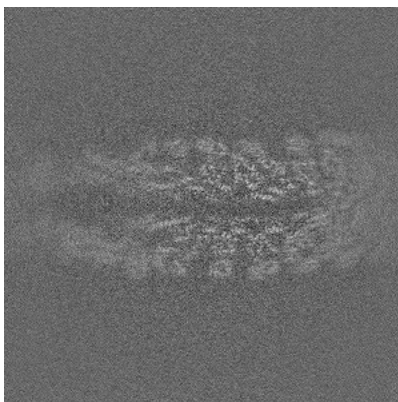


Z Index: 300

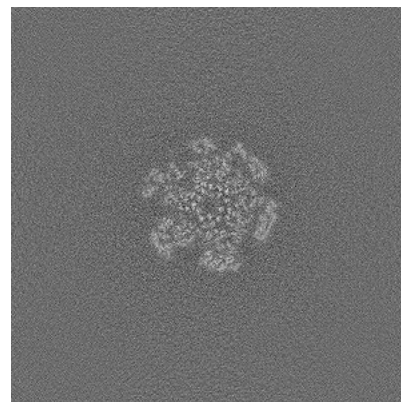
6.2.2 Raw map



X Index: 300



Y Index: 300

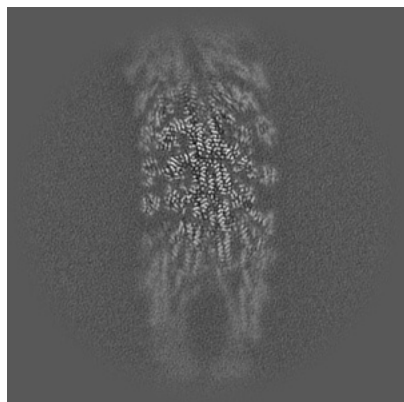


Z Index: 300

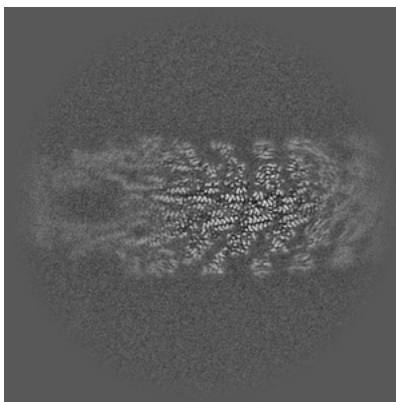
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

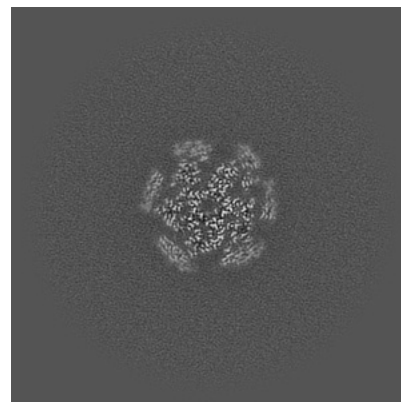
6.3.1 Primary map



X Index: 314

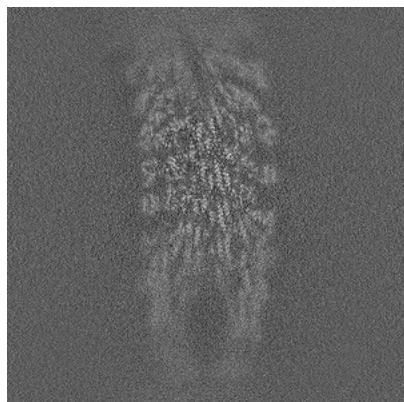


Y Index: 318

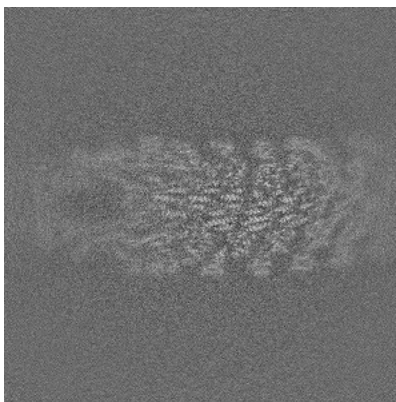


Z Index: 374

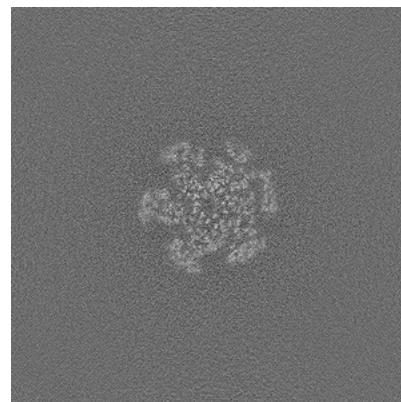
6.3.2 Raw map



X Index: 313



Y Index: 319

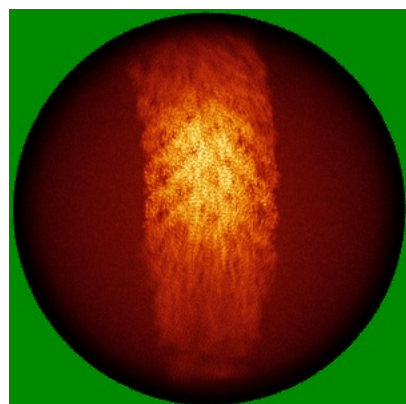


Z Index: 325

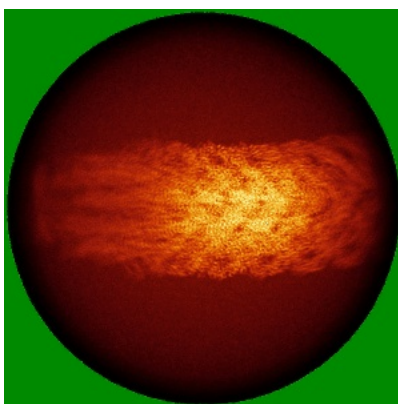
The images above show the largest variance slices of the map in three orthogonal directions.

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

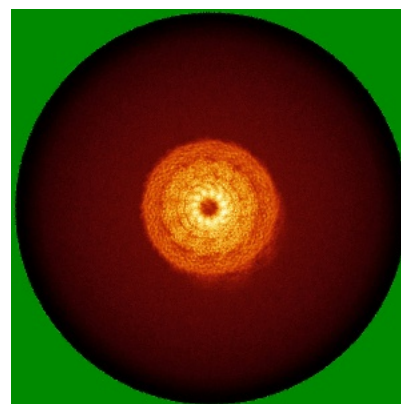
6.4.1 Primary map



X

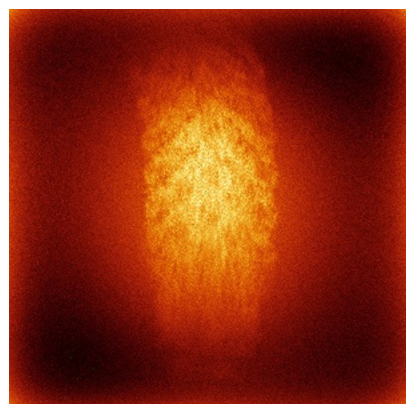


Y

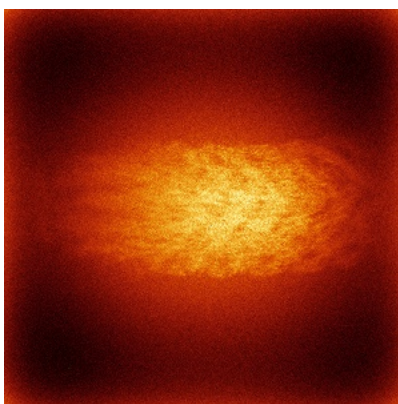


Z

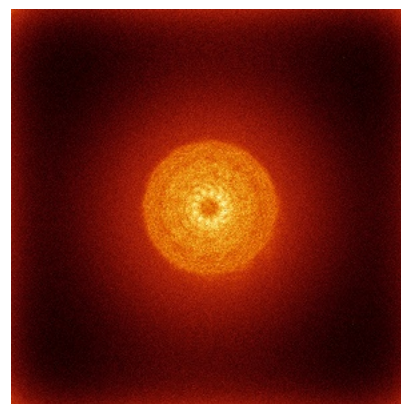
6.4.2 Raw map



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



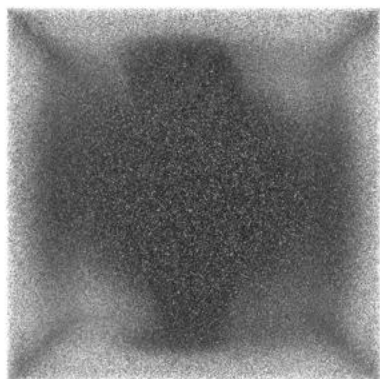
Y



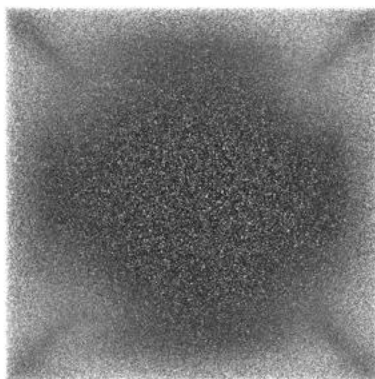
Z

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.

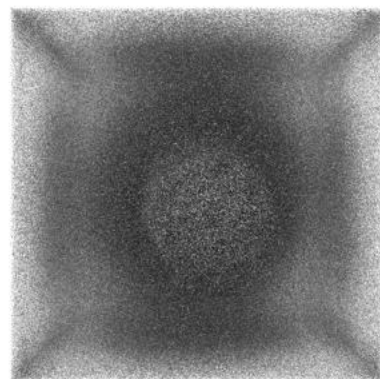
6.5.2 Raw map



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_63802_msk_1.map [i](#)



X



Y

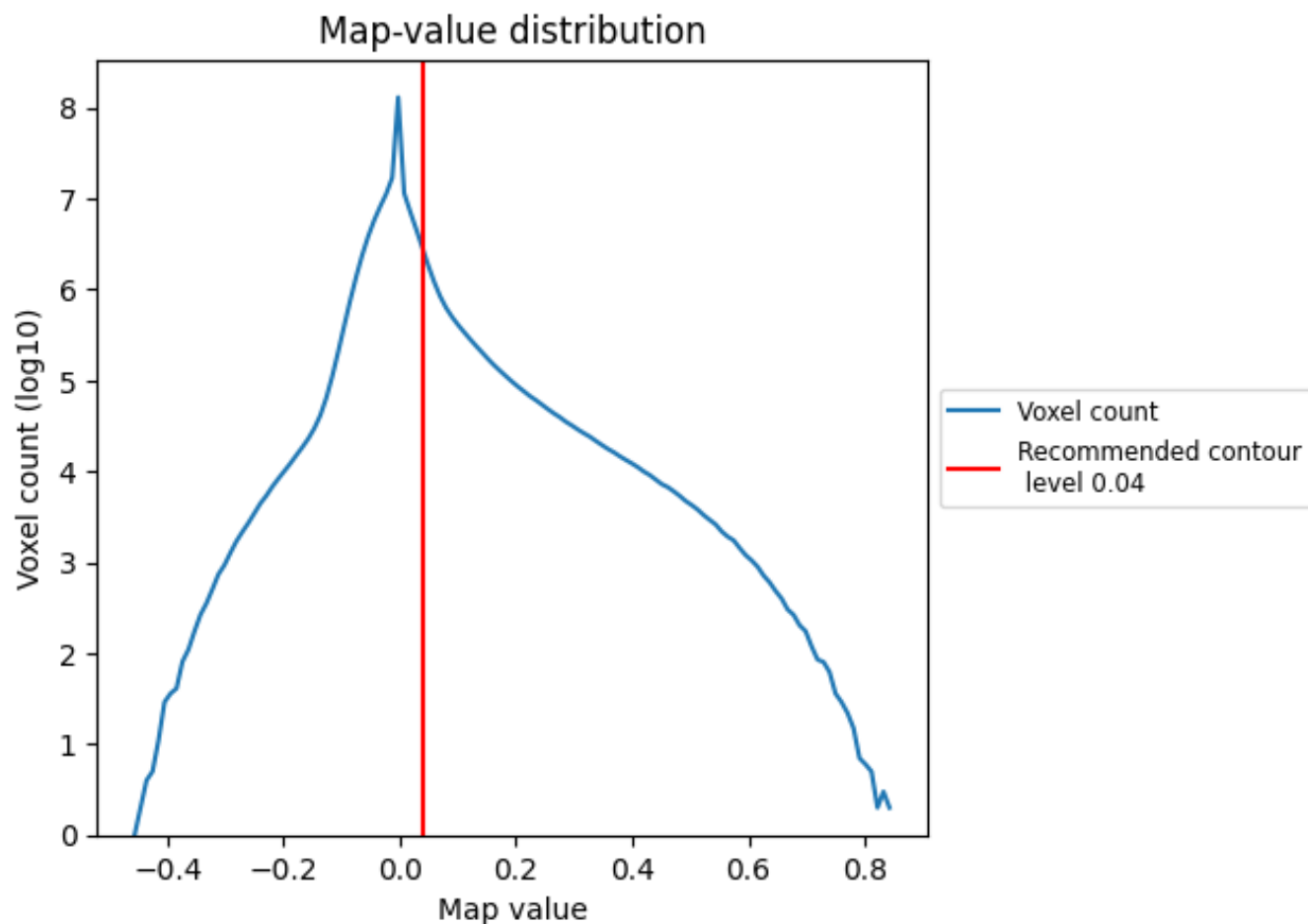


Z

7 Map analysis [i](#)

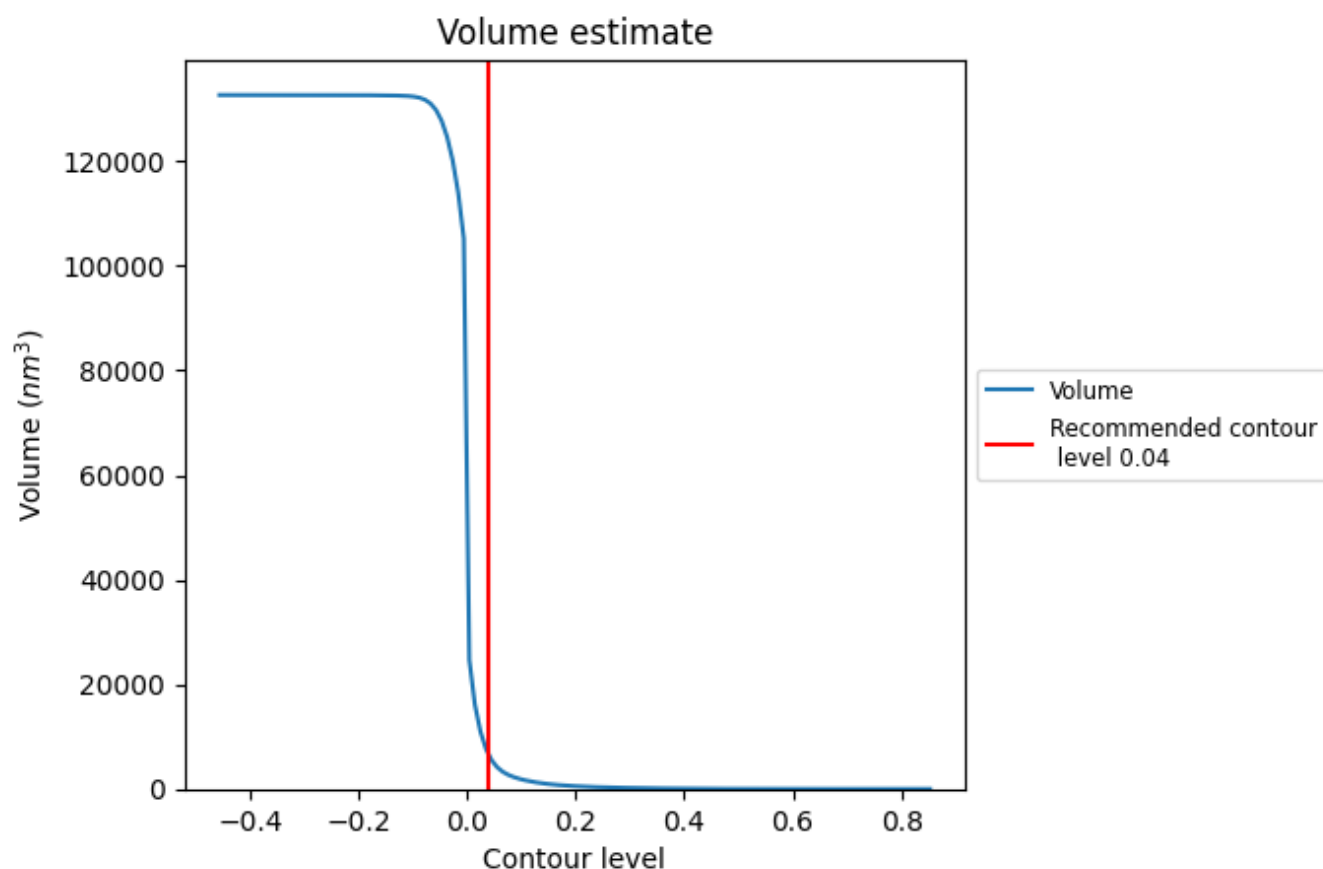
This section contains the results of statistical analysis of the map.

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.

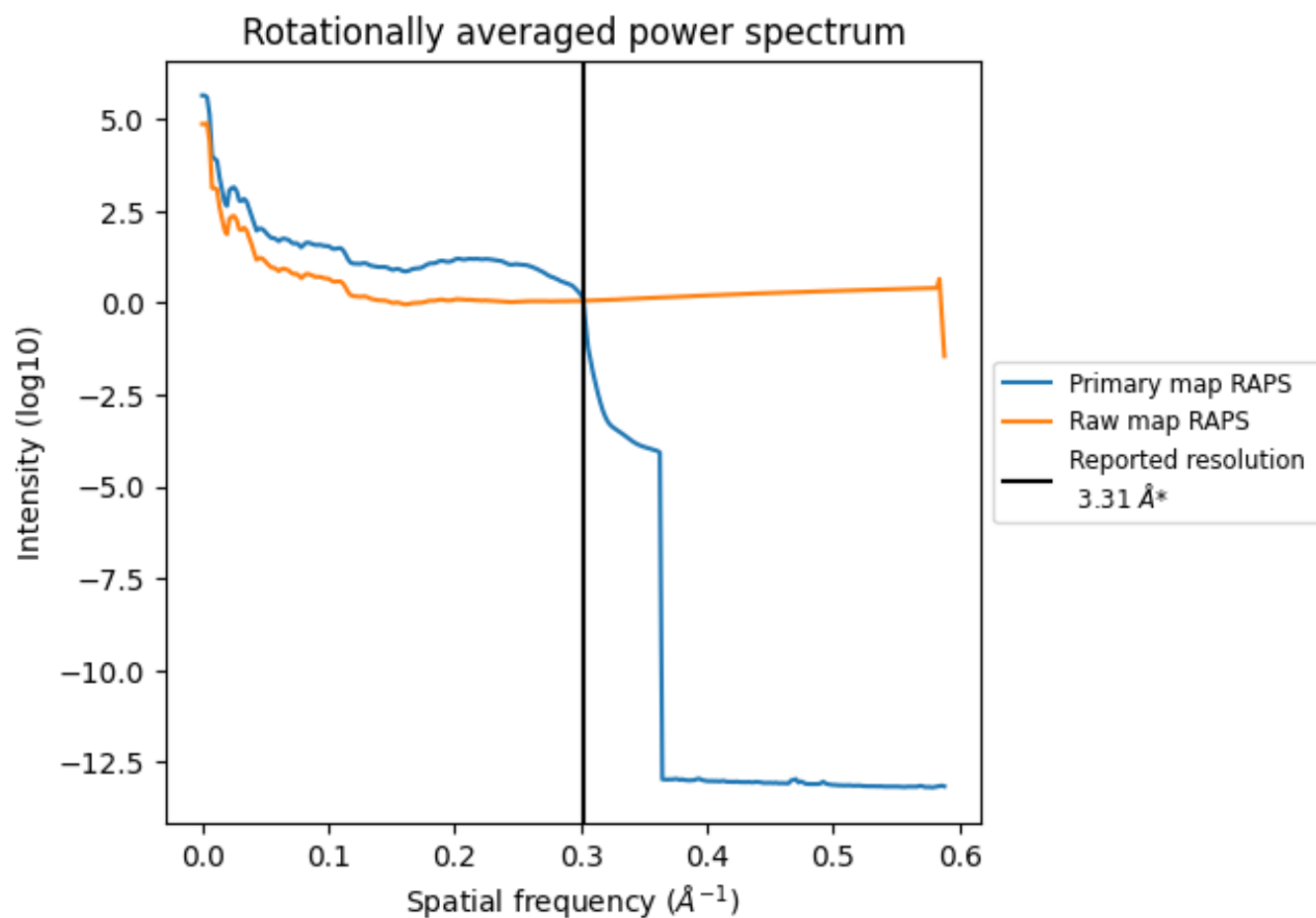
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6548 nm^3 ; this corresponds to an approximate mass of 5915 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 ⓘ

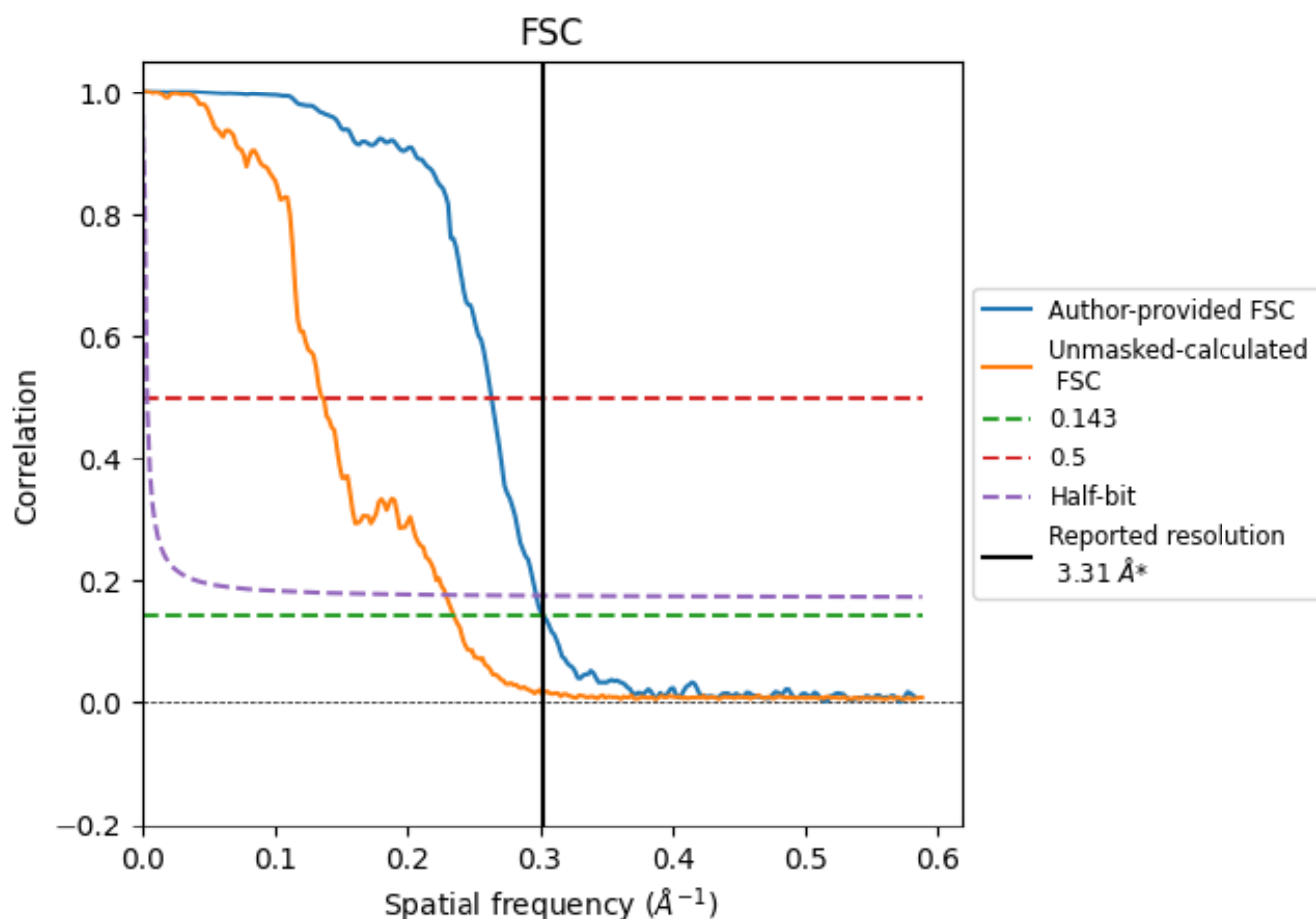


*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.302 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

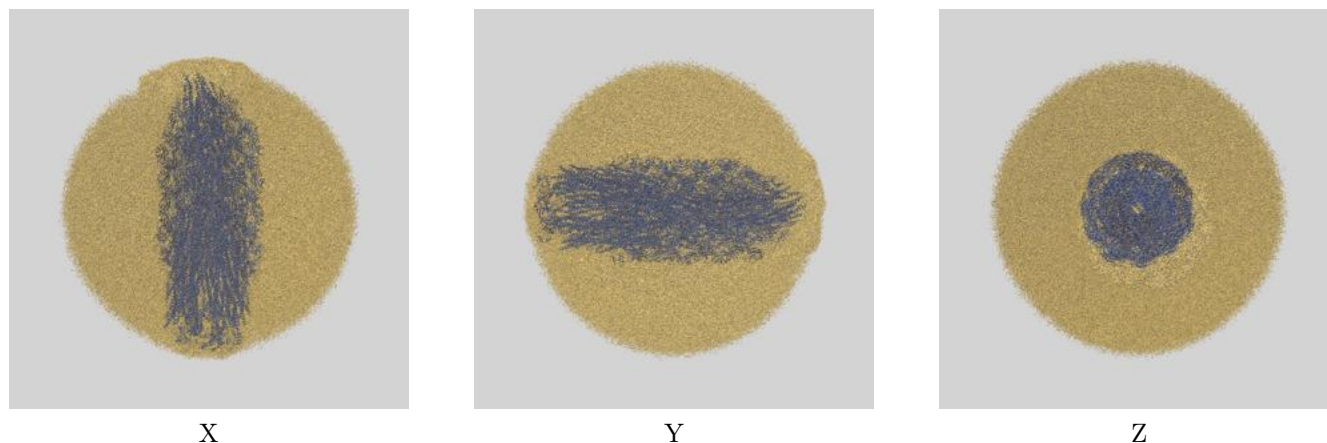
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.79	3.37
Unmasked-calculated*	4.26	7.37	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.31 by more than 10 %

9 Map-model fit [i](#)

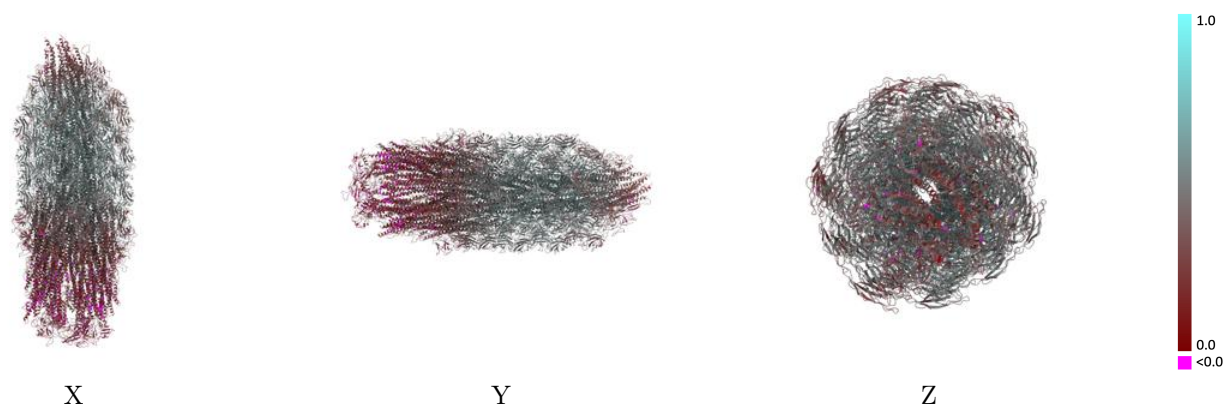
This section contains information regarding the fit between EMDB map EMD-63802 and PDB model 9MCG. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



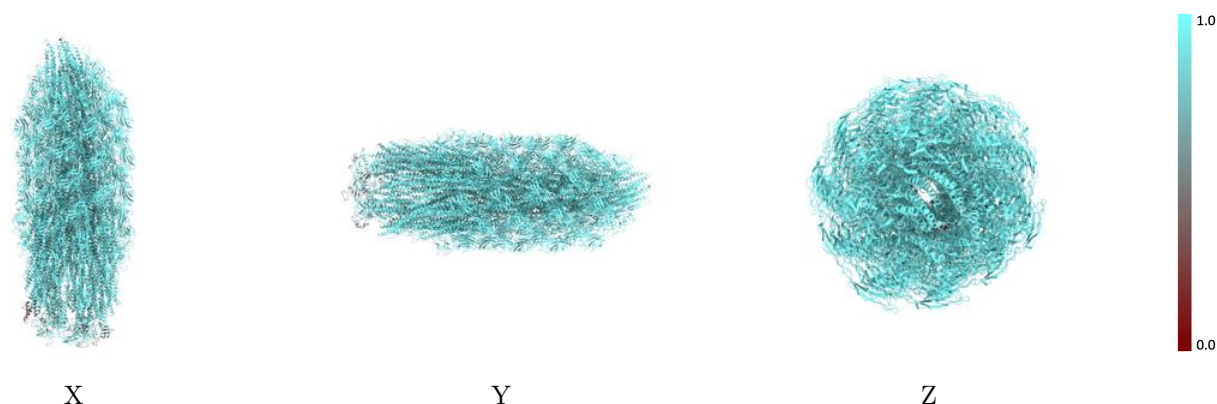
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



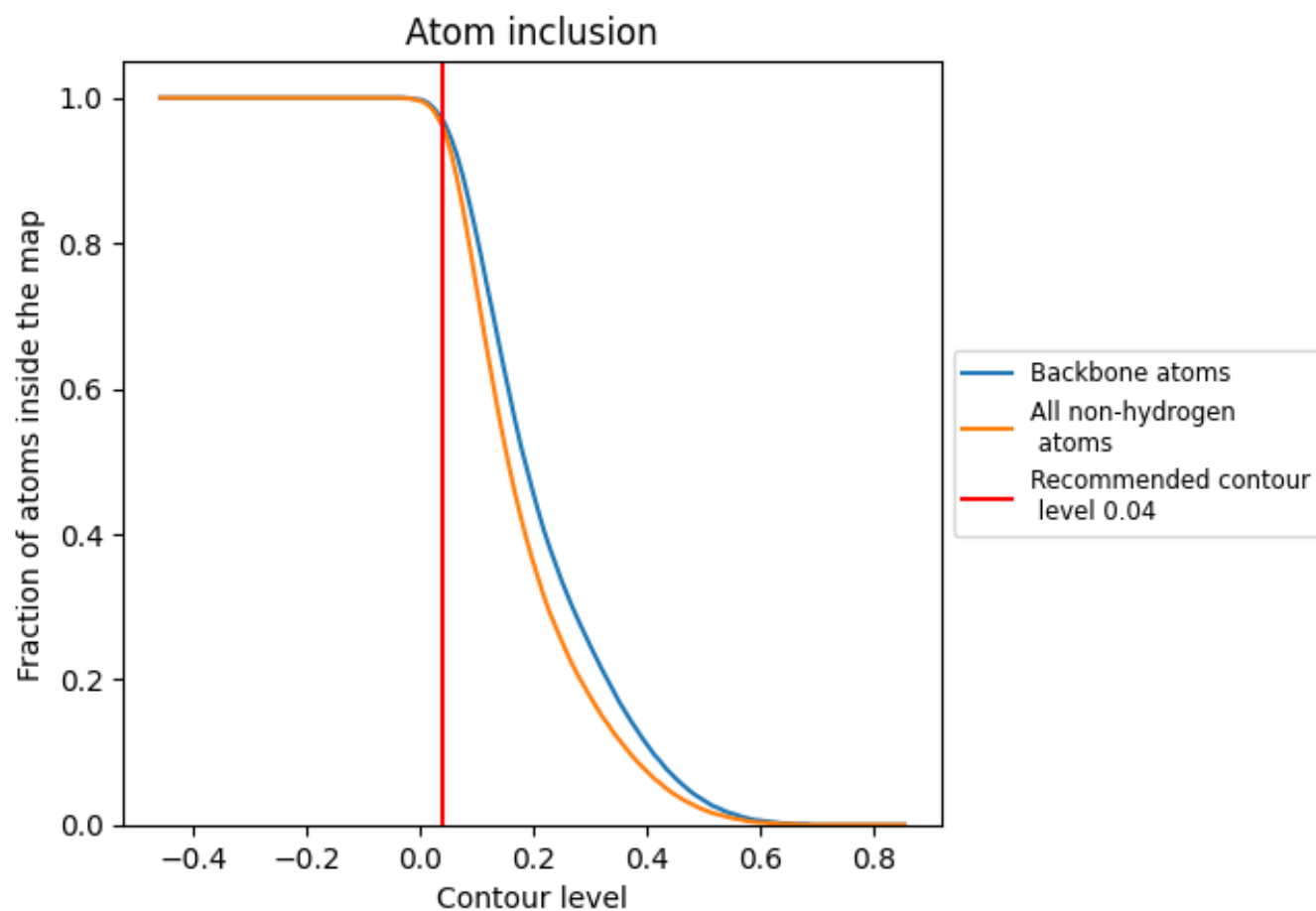
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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	 0.9610	 0.4090
AA	 0.7970	 0.2160
AB	 0.8240	 0.2340
AC	 0.7570	 0.2210
AD	 0.7860	 0.2150
AE	 0.8160	 0.2240
BA	 0.9550	 0.2950
BB	 0.9660	 0.2760
BC	 0.9710	 0.3030
BD	 0.9550	 0.2710
BE	 0.9790	 0.3030
BF	 0.9200	 0.2590
BG	 0.8630	 0.2500
BH	 0.9690	 0.3040
BI	 0.9660	 0.3090
BJ	 0.9000	 0.2480
BK	 0.9700	 0.2710
BL	 0.6470	 0.2070
CA	 0.9580	 0.3770
CB	 0.9730	 0.3870
CC	 0.9790	 0.3800
CD	 0.9730	 0.3480
CE	 0.9760	 0.3980
CF	 0.9750	 0.3570
CG	 0.9590	 0.3360
CH	 0.9790	 0.4160
CI	 0.9800	 0.4010
CJ	 0.9740	 0.3480
CK	 0.9600	 0.3440
DA	 0.9580	 0.4210
DB	 0.9850	 0.4810
DC	 0.9870	 0.4750
DD	 0.9900	 0.5140
DE	 0.9850	 0.4820
DF	 0.9900	 0.5030



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Chain	Atom inclusion	Q-score
DG	 0.9860	 0.4640
DH	 0.9940	 0.5150
DI	 0.9740	 0.4480
DJ	 0.9920	 0.4960
DK	 0.9760	 0.4370
EA	 0.9900	 0.5080
EB	 0.9940	 0.5270
EC	 0.9960	 0.5350
ED	 0.9910	 0.5380
EE	 0.9920	 0.5310
EF	 0.9930	 0.5310
EG	 0.9940	 0.5250
EH	 0.9940	 0.5190
EI	 0.9910	 0.5230
EJ	 0.9940	 0.5260
EK	 0.9910	 0.5180
FA	 0.9920	 0.5320
FB	 0.9890	 0.5100
FC	 0.9930	 0.5260
FD	 0.9840	 0.4730
FE	 0.9920	 0.5150
FF	 0.9840	 0.4550
FG	 0.9940	 0.5120
FH	 0.9880	 0.4710
FI	 0.9930	 0.4970
FJ	 0.9900	 0.4750
FK	 0.9940	 0.5300
GA	 0.9850	 0.4950
GB	 0.9750	 0.4120
GC	 0.9760	 0.4370
GD	 0.9530	 0.3380
GE	 0.9700	 0.3870
GF	 0.9580	 0.3190
GG	 0.9810	 0.4040
GH	 0.9790	 0.3370
GI	 0.9860	 0.4060
GJ	 0.9790	 0.3630
GK	 0.9850	 0.4470