



wwPDB EM Validation Summary Report ⓘ

May 7, 2026 – 03:19 PM JST

PDB ID : 8Z5U / pdb_00008z5u
EMDB ID : EMD-39782
Title : Cryo-EM structure of the rod-export apparatus with partial hook within the polar flagellar motor
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2024-04-18
Resolution : 3.04 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

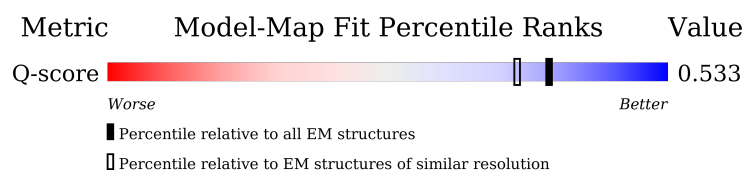
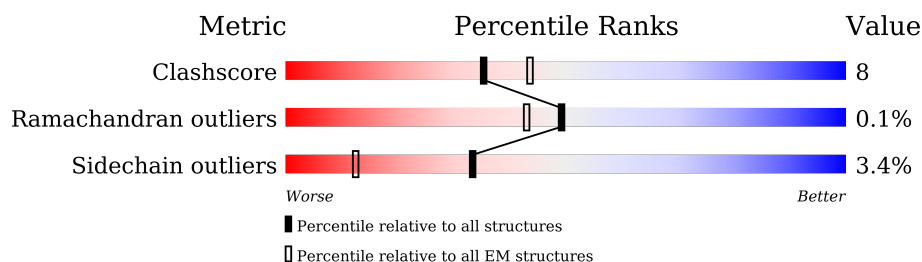
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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	13952 (2.54 - 3.54)

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	D	437	
1	E	437	
1	F	437	
1	G	437	

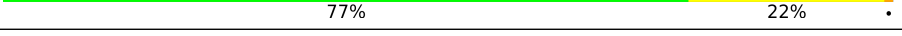
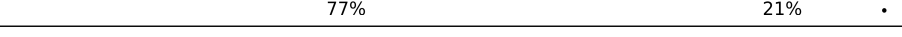
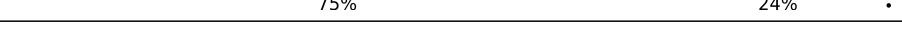
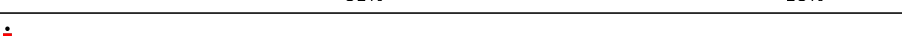
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Mol	Chain	Length	Quality of chain
1	H	437	
1	I	437	
1	J	437	
1	K	437	
1	L	437	
1	M	437	
1	N	437	
1	O	437	
2	0	199	
2	9	199	
3	1	289	
3	2	289	
3	3	289	
3	y	289	
3	z	289	
4	4	89	
4	5	89	
4	6	89	
4	7	89	
5	8	260	
6	A	262	
6	AP	262	
6	AQ	262	
6	AR	262	
6	AS	262	

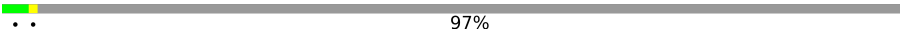
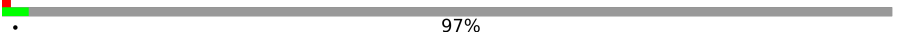
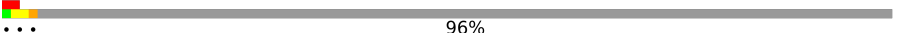
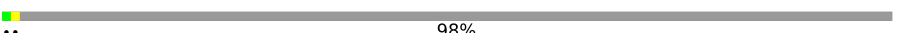
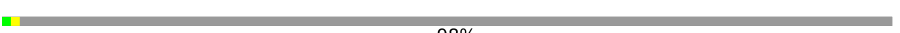
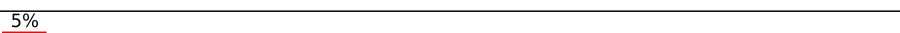
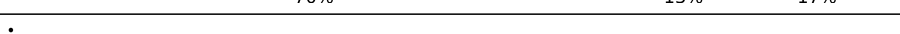
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Mol	Chain	Length	Quality of chain
6	AT	262	 77% 16% 5%
6	AU	262	 74% 20% 5%
6	AV	262	 77% 16% 5%
6	AW	262	 82% 17% .
6	AX	262	 79% 19% .
6	AY	262	 81% 18% .
6	AZ	262	 78% 21% .
6	Aa	262	 79% 20% .
6	B	262	 77% 22% .
6	C	262	 78% 20% .
6	P	262	 77% 21% .
6	Q	262	 82% 16% .
6	R	262	 81% 18% .
6	S	262	 75% 24% .
6	T	262	 69% 29% .
6	U	262	 79% 20% .
6	V	262	 79% 20% .
6	W	262	 74% 25% .
6	X	262	 81% 18% .
6	Y	262	 81% 17% .
6	Z	262	 83% 15% .
6	a	262	 80% 19% .
7	AA	580	 97% ..
7	AB	580	 97% ..
7	AC	580	 97% .

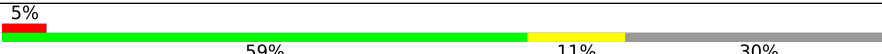
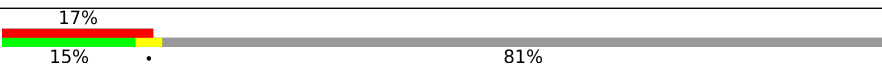
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Mol	Chain	Length	Quality of chain
7	AD	580	 97%
7	AE	580	 97%
7	AF	580	 96%
7	AG	580	 98%
7	AH	580	 98%
7	AI	580	 98%
7	AJ	580	 96%
7	AK	580	 96%
7	AL	580	 5% 94%
7	AM	580	 5% 94%
7	AN	580	 5% 94%
7	AO	580	 5% 94%
8	b	131	 69% 14% 17%
8	c	131	 8% 66% 15% 18%
8	d	131	 5% 70% 13% 17%
8	e	131	 66% 15% 18%
8	f	131	 69% 13% 18%
9	g	137	 5% 79% 16% 5%
9	h	137	 72% 23% 5%
9	i	137	 64% 27% 5%
9	j	137	 81% 13% 5%
9	k	137	 75% 20% 5%
9	l	137	 74% 20% 5%
10	m	249	 77% 22%
10	n	249	 70% 29%

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Mol	Chain	Length	Quality of chain
10	o	249	
10	p	249	
10	q	249	
11	r	103	
11	s	103	
11	t	103	
11	u	103	
11	v	103	
11	w	103	
12	x	376	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 118072 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 protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	E	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	F	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	G	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	H	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	I	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	J	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	K	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	L	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	M	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	N	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	O	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		

- Molecule 2 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	180	Total	C	N	O	S	0	0
			1361	876	231	253	1		
2	9	180	Total	C	N	O	S	0	0
			1361	876	231	253	1		

- Molecule 3 is a protein called Flagellar biosynthetic protein FlhP.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	207	Total	C	N	O	S	0	0
			1599	1055	243	282	19		
3	2	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
3	3	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
3	y	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
3	z	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		

- Molecule 4 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
4	5	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
4	6	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
4	7	89	Total	C	N	O	S	0	0
			722	489	107	117	9		

- Molecule 5 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	242	Total	C	N	O	S	0	0
			1896	1265	295	315	21		

- Molecule 6 is a protein called Flagellar basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	B	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	C	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AP	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AQ	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	AR	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AS	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AT	249	Total	C	N	O	S	0	0
			1866	1156	318	383	9		
6	AU	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AV	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AW	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AX	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AY	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AZ	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Aa	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	P	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Q	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	R	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	S	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	T	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	U	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	V	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	W	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	X	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Y	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Z	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		

- Molecule 7 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AA	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AB	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AC	20	Total	C	N	O	S	0	0
			139	84	24	30	1		
7	AD	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AE	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AF	23	Total	C	N	O	S	0	0
			158	97	27	33	1		
7	AG	11	Total	C	N	O		0	0
			73	46	13	14			
7	AH	11	Total	C	N	O		0	0
			73	46	13	14			
7	AI	11	Total	C	N	O		0	0
			73	46	13	14			
7	AJ	24	Total	C	N	O	S	0	0
			163	100	28	34	1		
7	AK	25	Total	C	N	O	S	0	0
			169	104	29	35	1		
7	AL	32	Total	C	N	O	S	0	0
			220	134	38	46	2		
7	AM	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AN	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AO	32	Total	C	N	O	S	0	0
			220	134	38	46	2		

- Molecule 8 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	109	Total	C	N	O	S	0	0
			845	523	155	166	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	107	Total	C	N	O	S	0	0
			835	518	153	163	1		
8	d	109	Total	C	N	O	S	0	0
			845	523	155	166	1		
8	e	108	Total	C	N	O	S	0	0
			837	519	154	163	1		
8	f	108	Total	C	N	O	S	0	0
			837	519	154	163	1		

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	h	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	i	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	j	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	k	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	l	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

- Molecule 10 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	n	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	o	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	p	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	q	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		

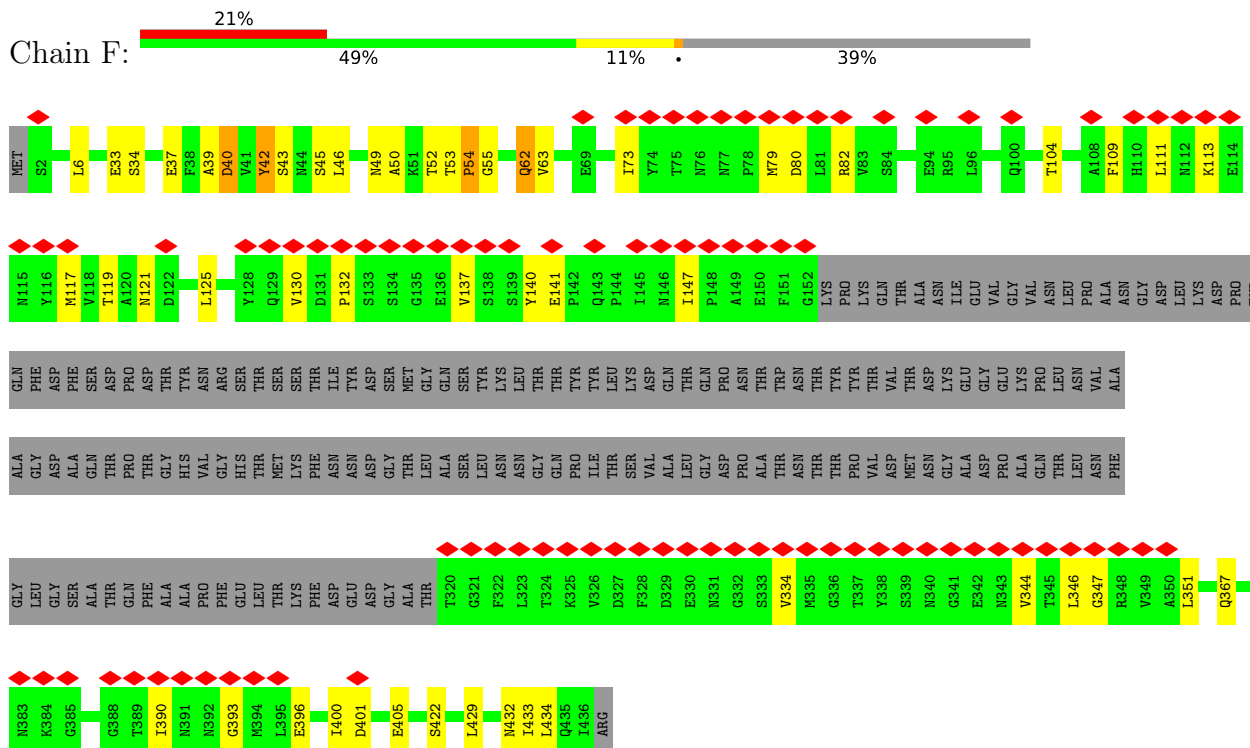
- Molecule 11 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	r	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
11	s	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
11	t	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
11	u	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
11	v	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
11	w	40	Total	C	N	O	S	0	0
			311	194	53	61	3		

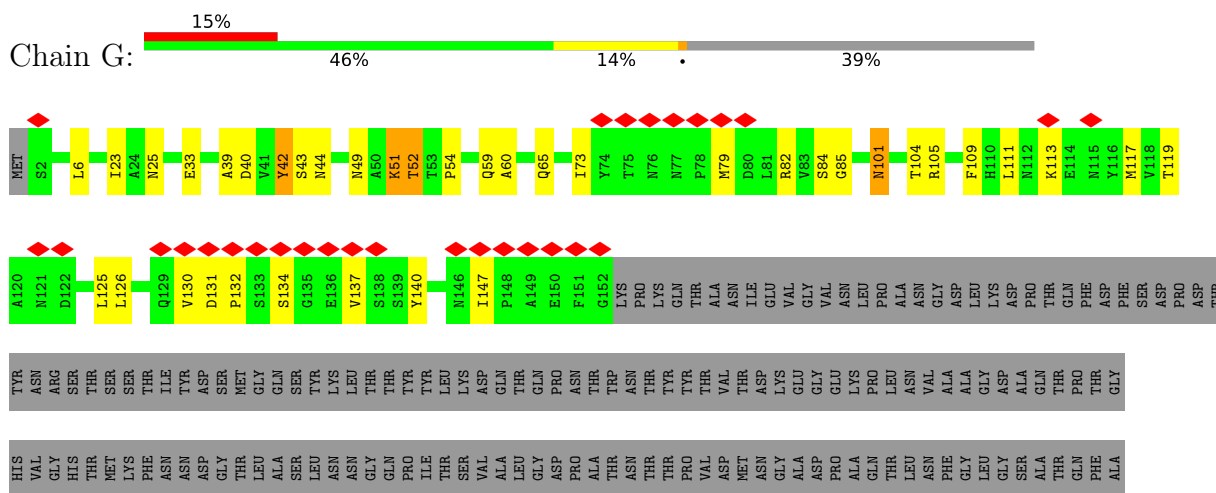
- Molecule 12 is a protein called Flagellar biosynthetic protein FlhB.

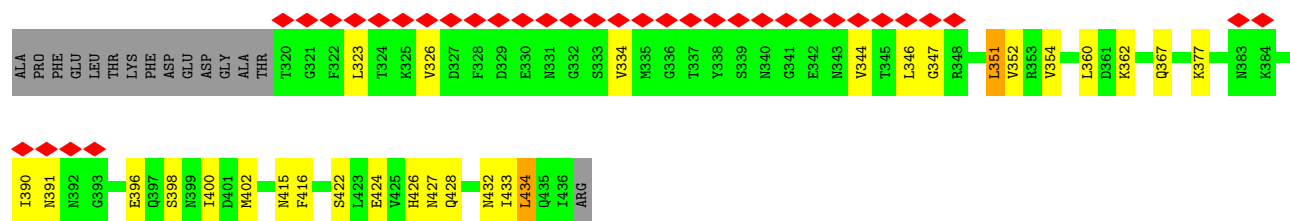
Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	71	Total	C	N	O	S	0	0
			552	370	83	95	4		

- Molecule 1: Flagellar hook protein FlgE

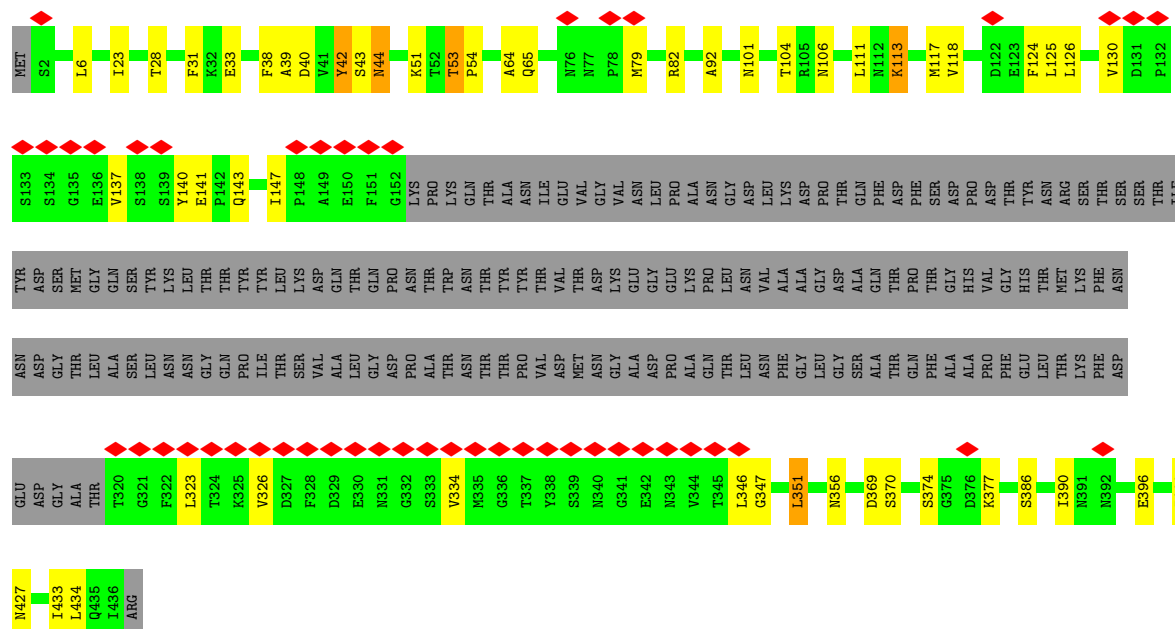


- Molecule 1: Flagellar hook protein FlgE

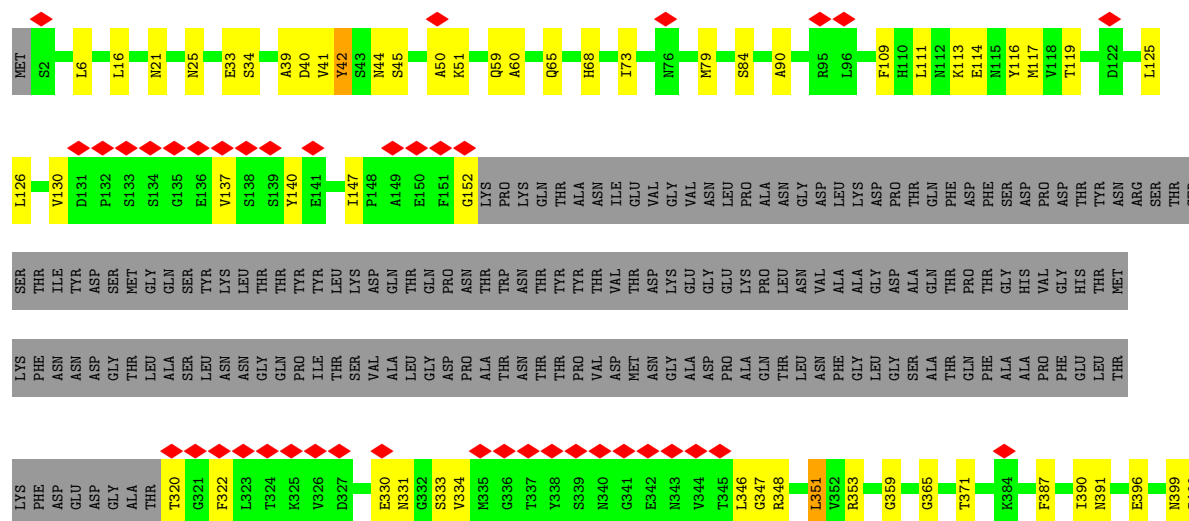




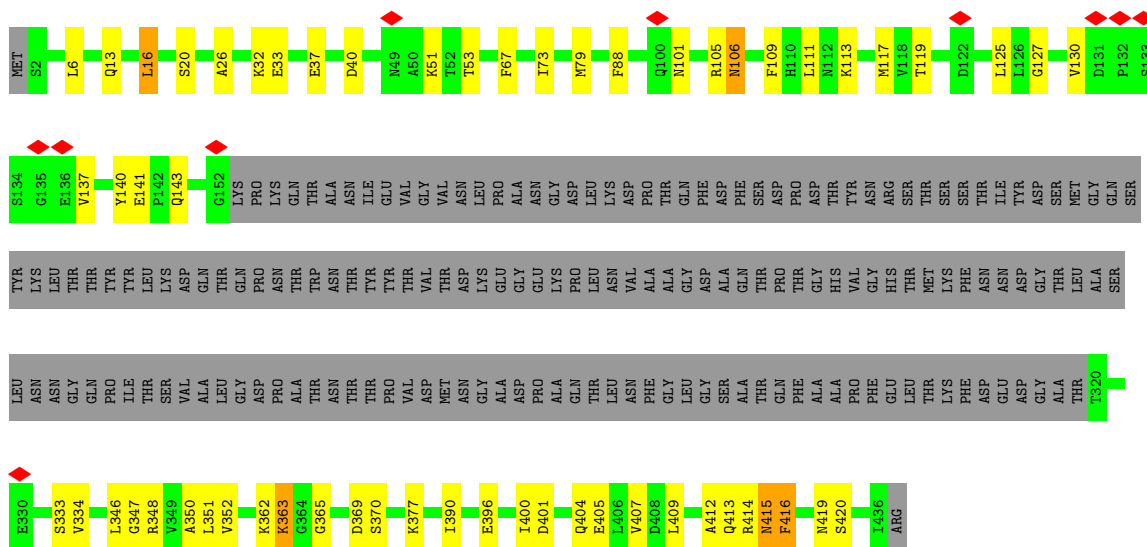
• Molecule 1: Flagellar hook protein FlgE



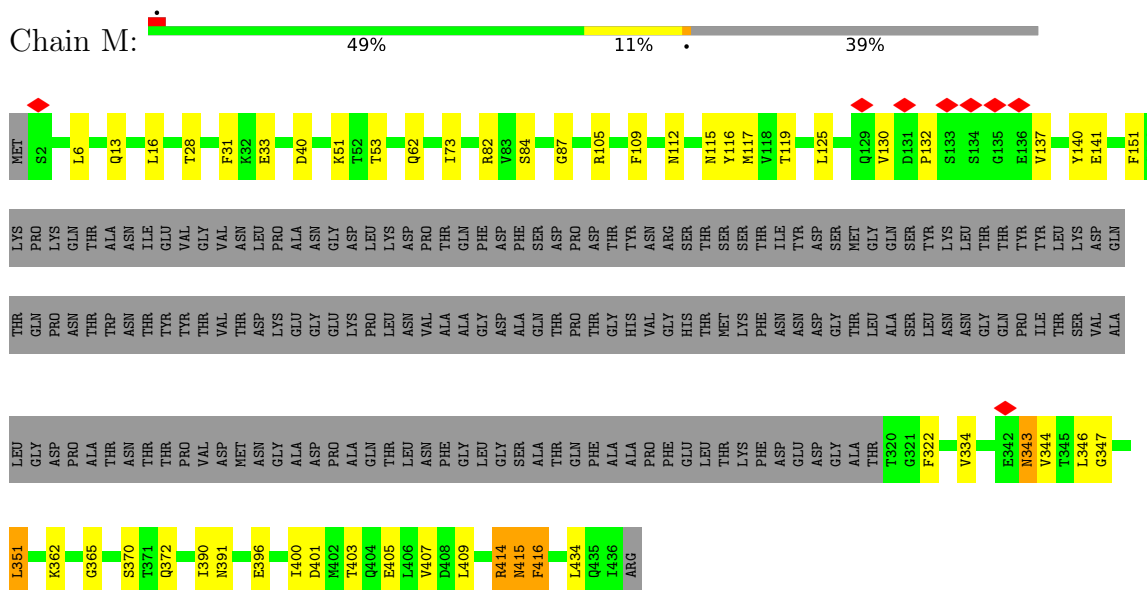
• Molecule 1: Flagellar hook protein FlgE



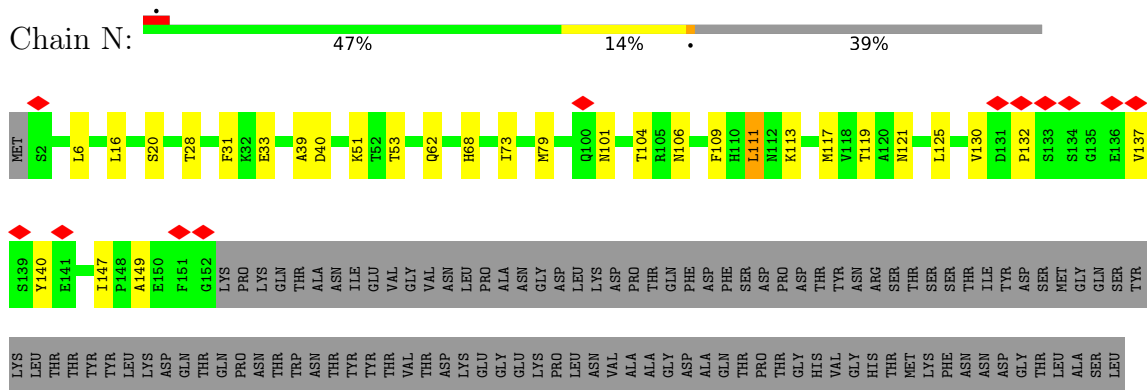


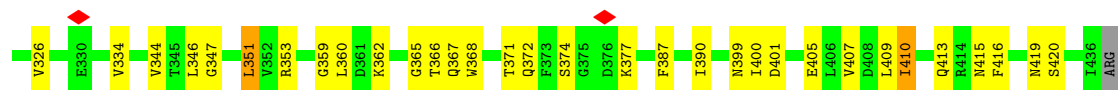


- Molecule 1: Flagellar hook protein FlgE

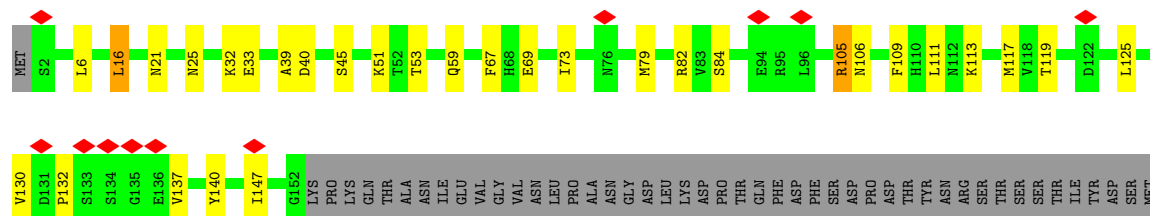


- Molecule 1: Flagellar hook protein FlgE

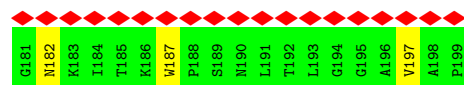
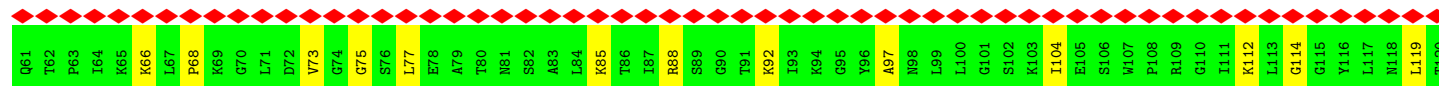




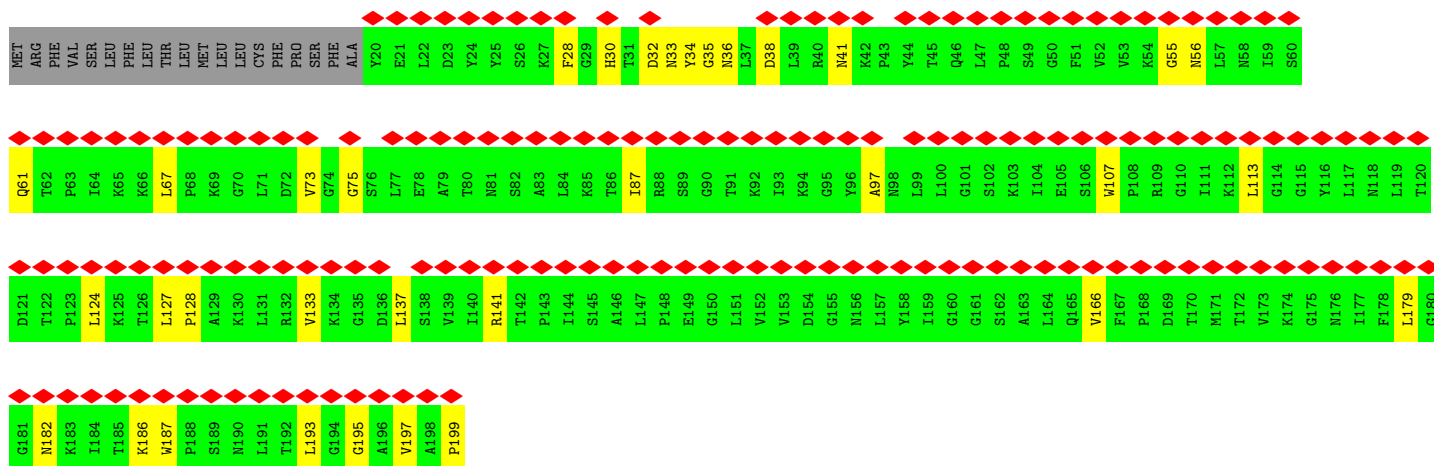
Chain 0:



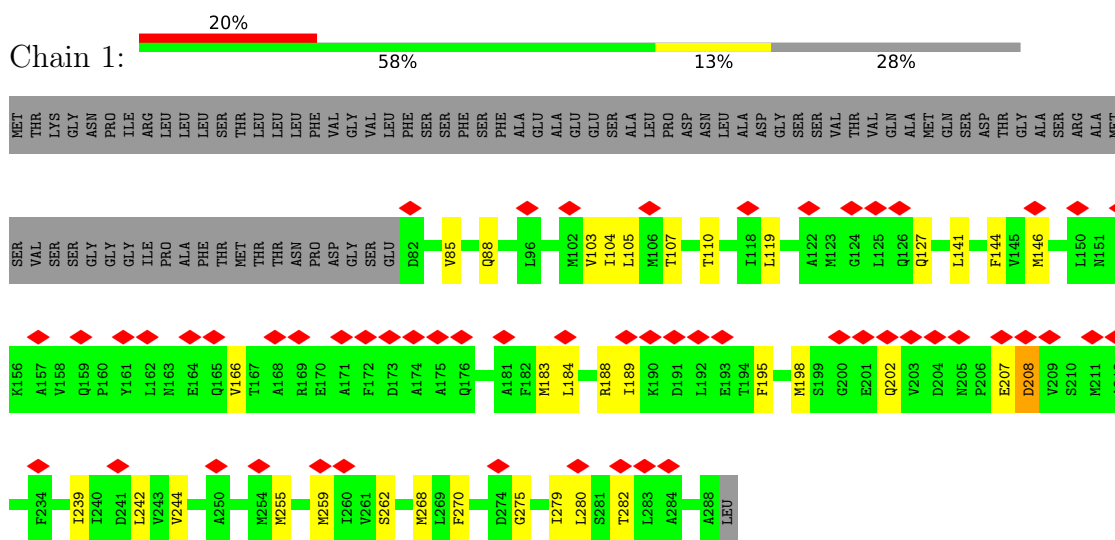
Chain 0: 89% 67% 22% 10%



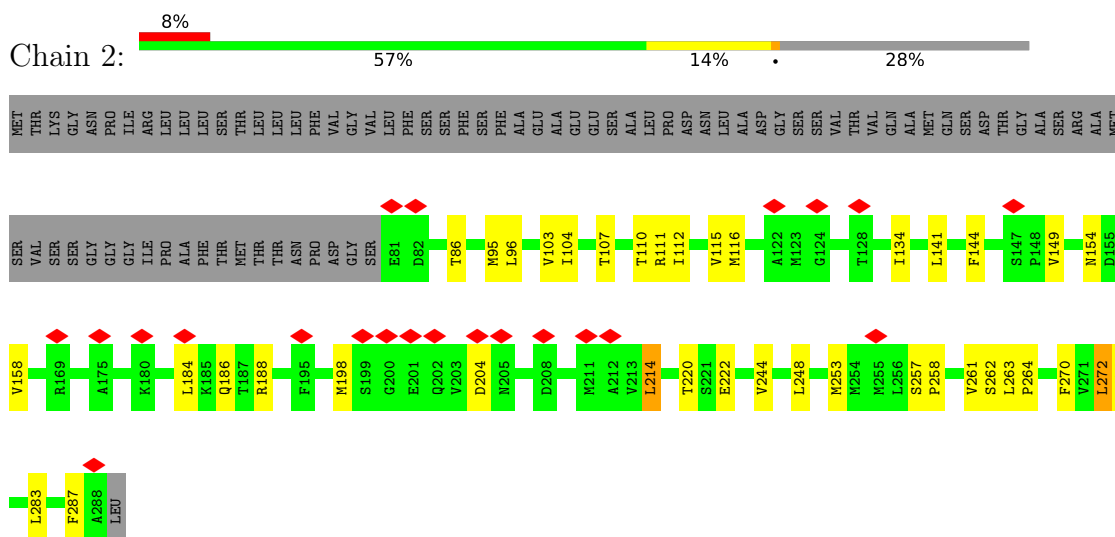
Chain 9: 84% 73% 17% 10%



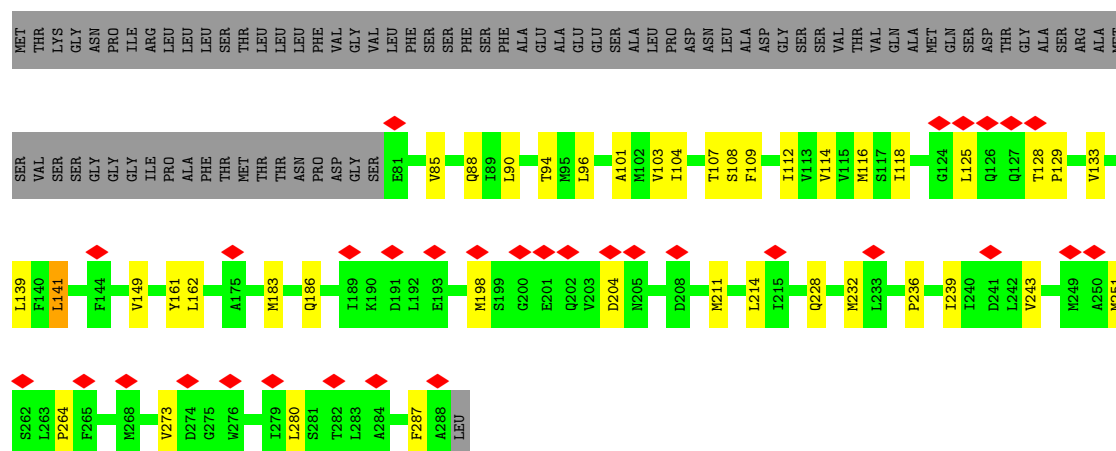
- Molecule 3: Flagellar biosynthetic protein FlhP



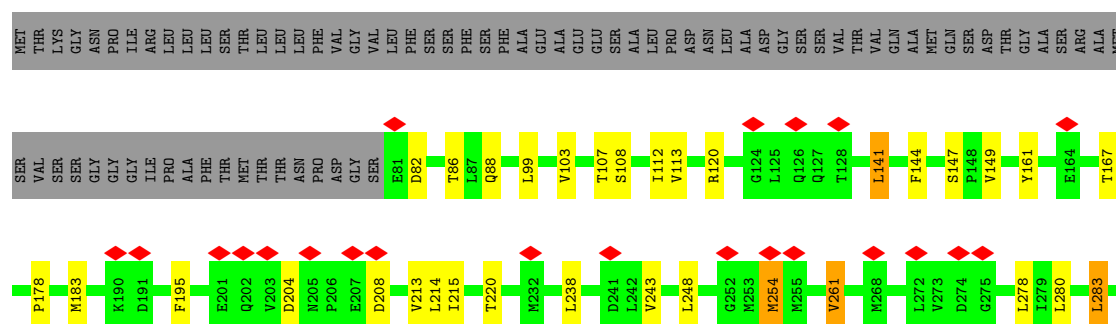
- Molecule 3: Flagellar biosynthetic protein FlhP



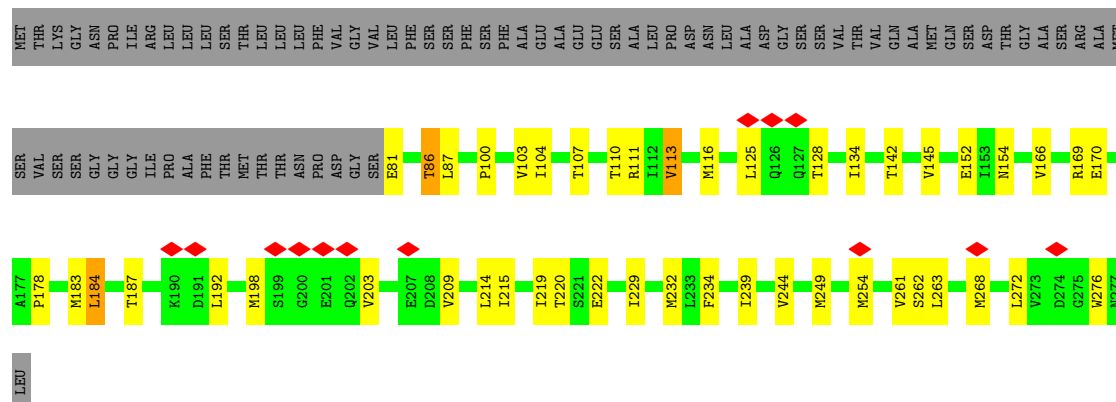
- Molecule 3: Flagellar biosynthetic protein FlpP



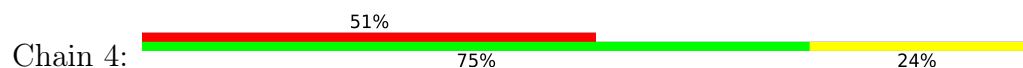
• Molecule 3: Flagellar biosynthetic protein FliP

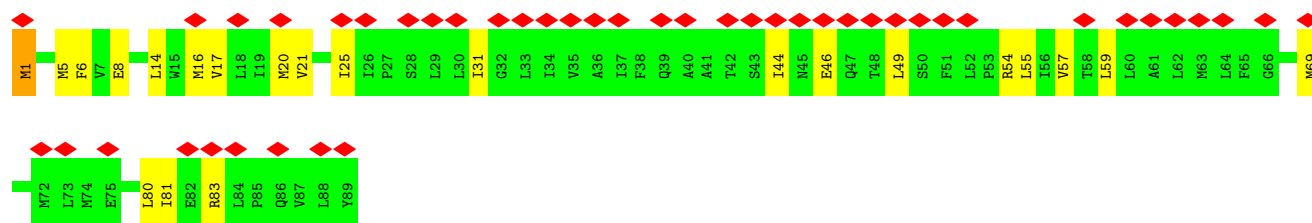


• Molecule 3: Flagellar biosynthetic protein FliP

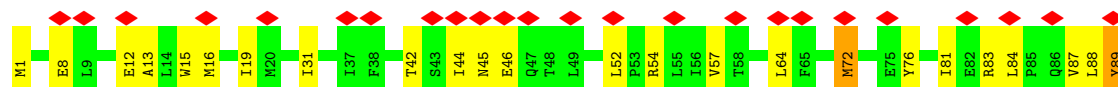
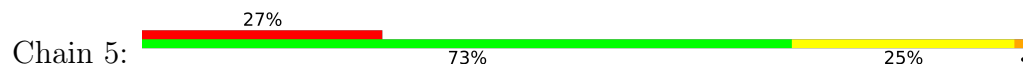


• Molecule 4: Flagellar biosynthetic protein FliQ

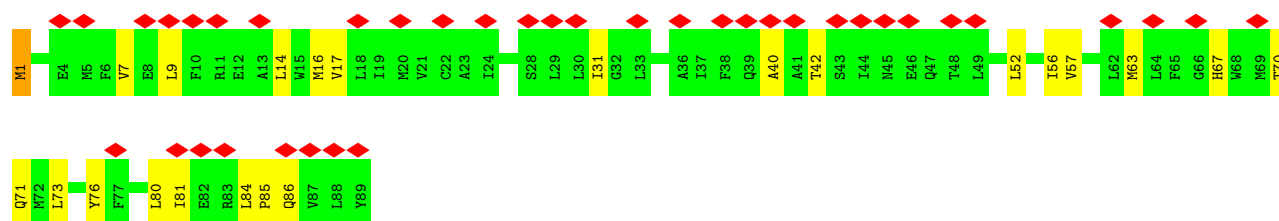
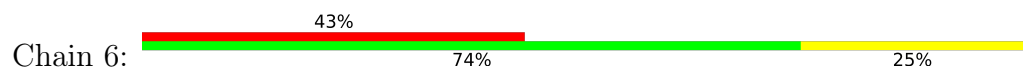




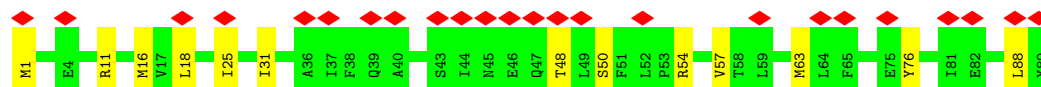
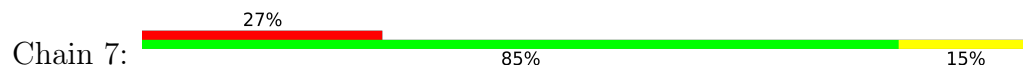
• Molecule 4: Flagellar biosynthetic protein FliQ



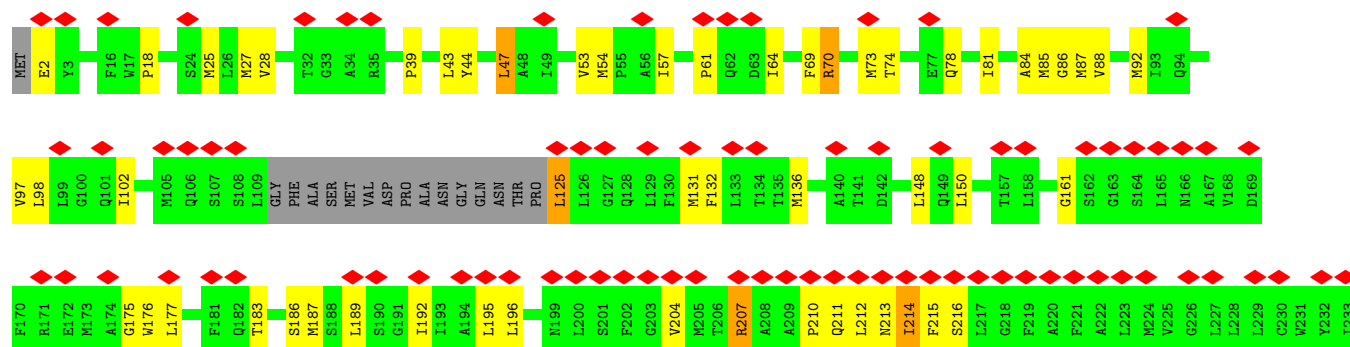
• Molecule 4: Flagellar biosynthetic protein FliQ

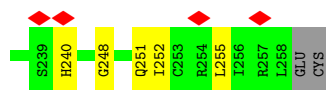


• Molecule 4: Flagellar biosynthetic protein FliQ



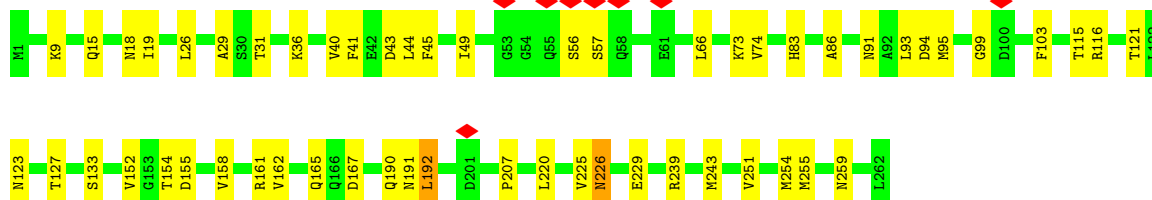
• Molecule 5: Flagellar biosynthetic protein FliR





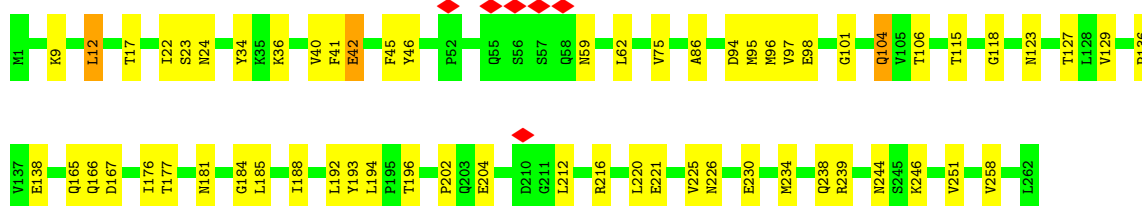
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain A: 79% 20%



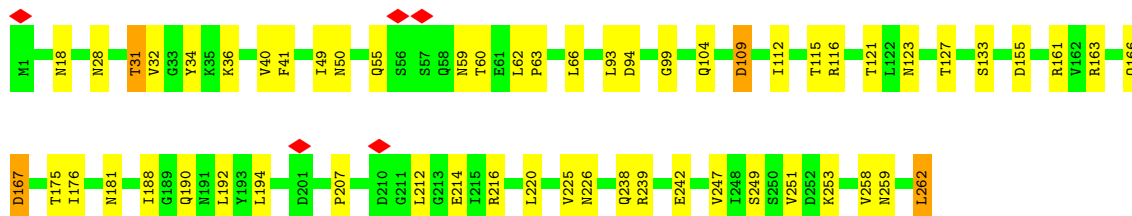
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain B: 77% 22%



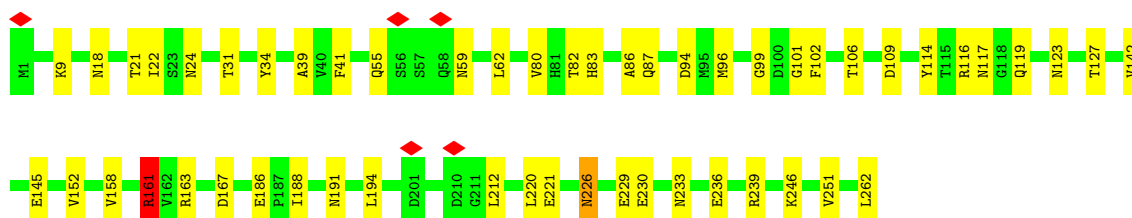
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain C: 78% 20%



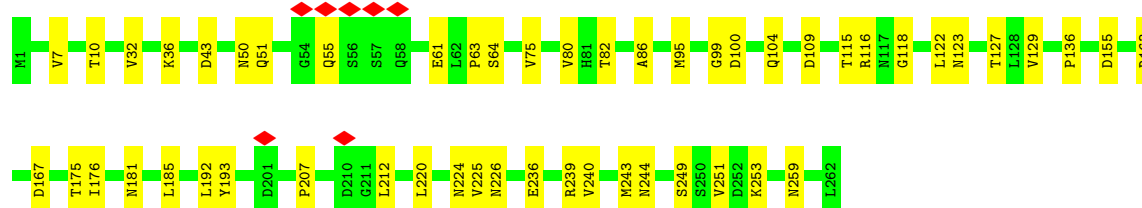
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AP: 80% 19%



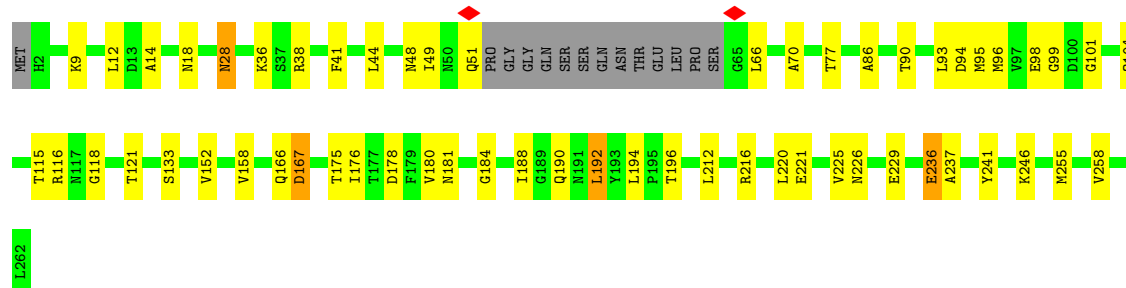
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AQ:  80% 20%



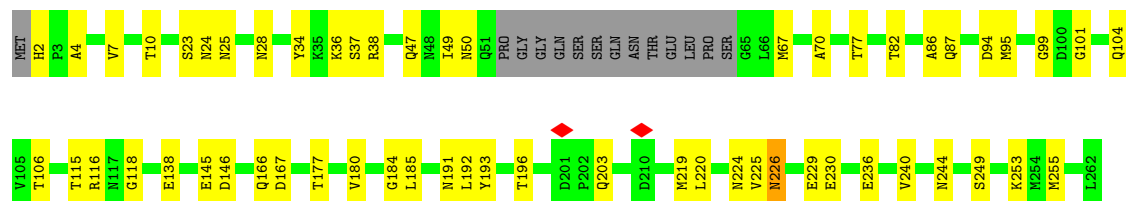
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AR:  73% 21% 5%



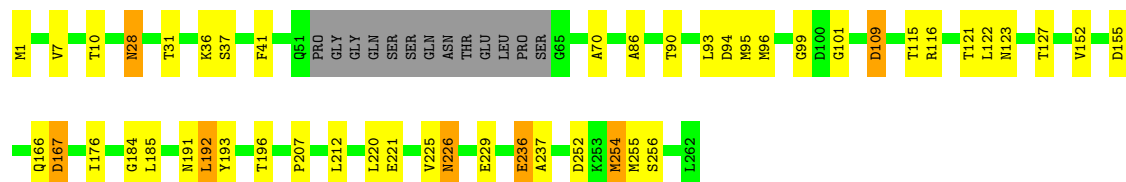
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AS:  73% 21% 5%



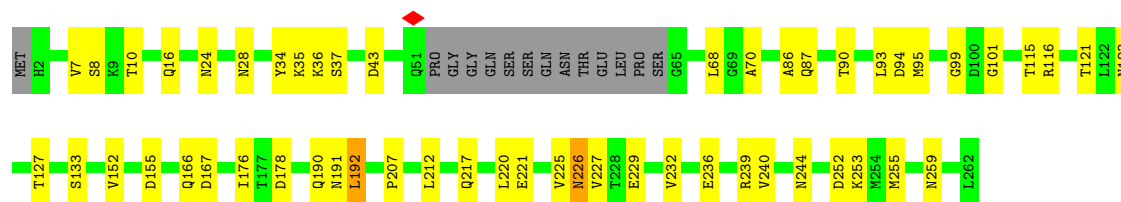
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AT:  77% 16% 5%

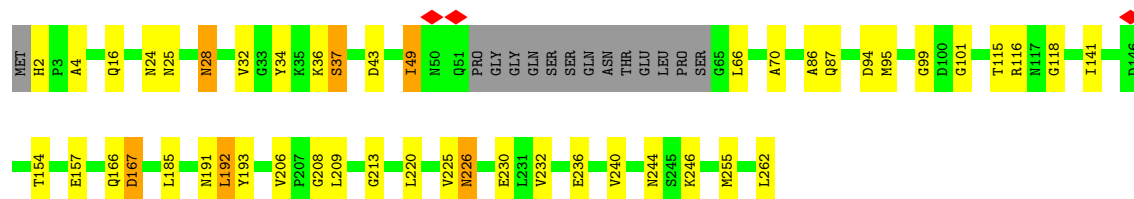
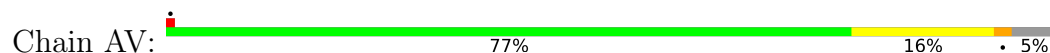


- Molecule 6: Flagellar basal-body rod protein FlgG

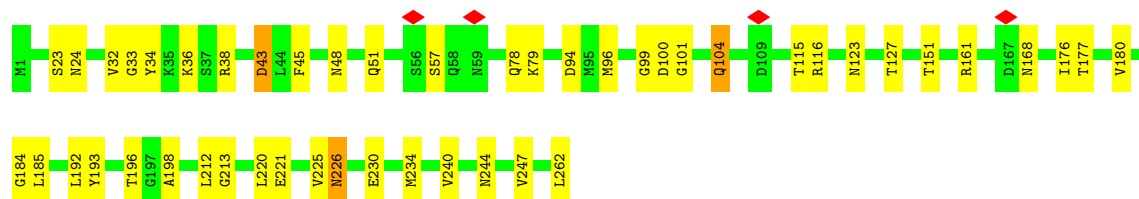
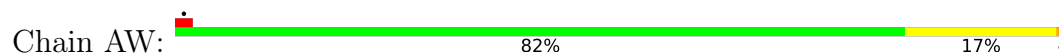
Chain AU:  74% 20% 5%



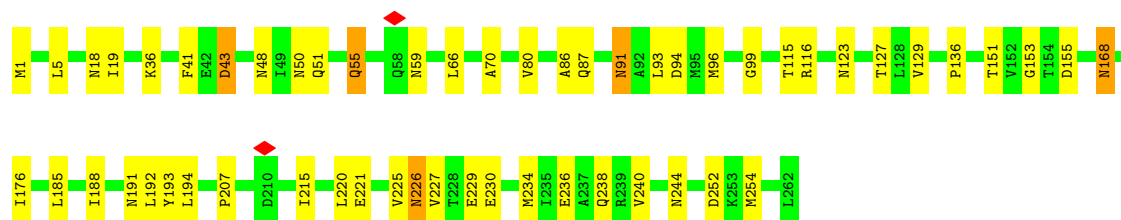
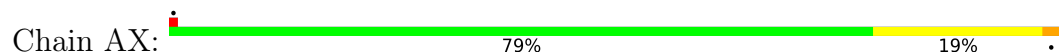
• Molecule 6: Flagellar basal-body rod protein FlgG



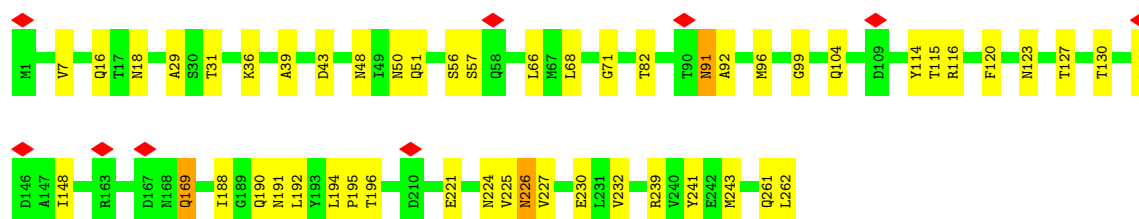
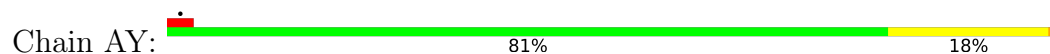
• Molecule 6: Flagellar basal-body rod protein FlgG



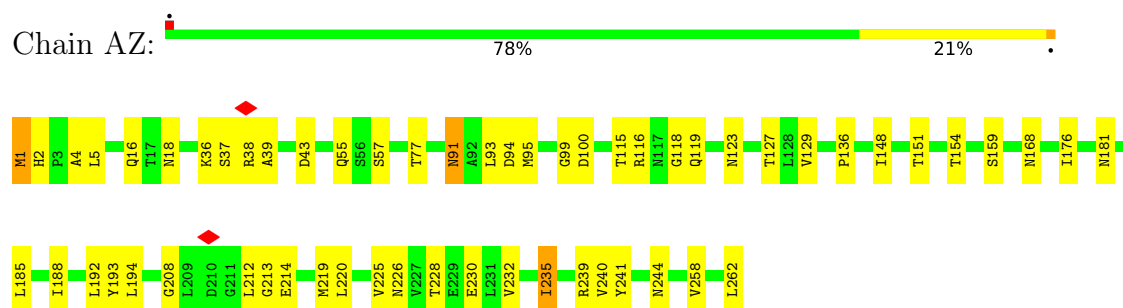
• Molecule 6: Flagellar basal-body rod protein FlgG



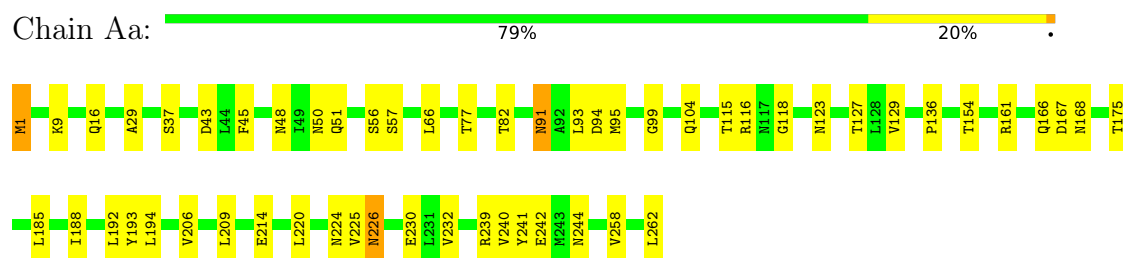
• Molecule 6: Flagellar basal-body rod protein FlgG



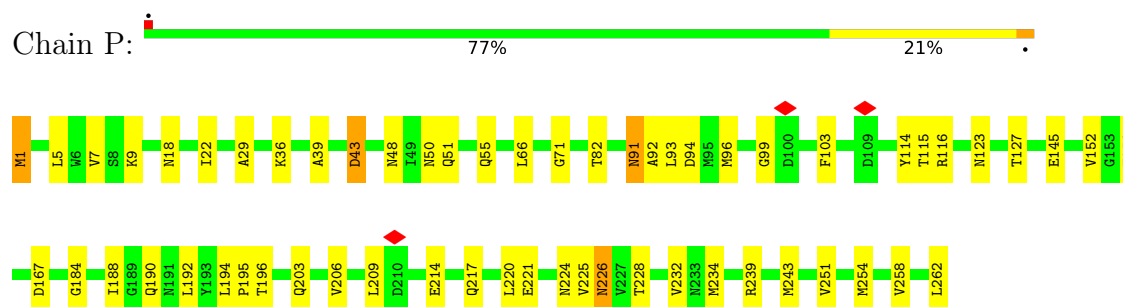
- Molecule 6: Flagellar basal-body rod protein FlgG



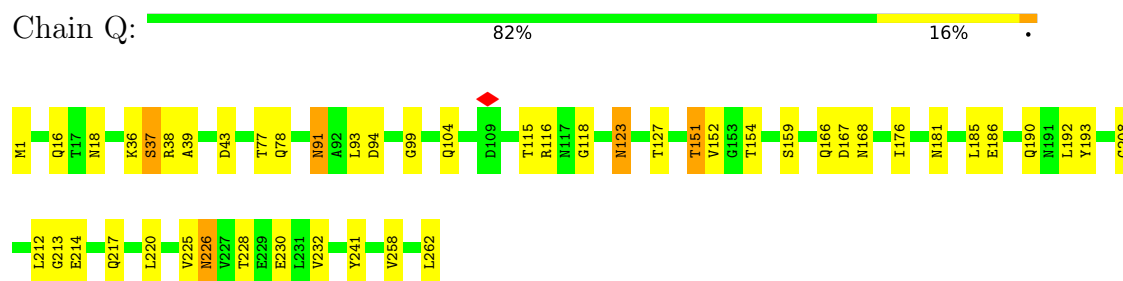
- Molecule 6: Flagellar basal-body rod protein FlgG



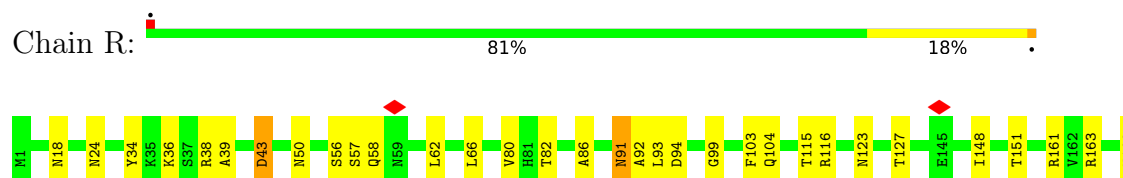
- Molecule 6: Flagellar basal-body rod protein FlgG

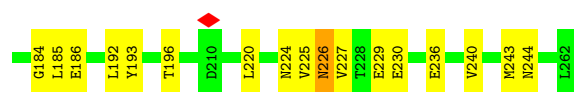


- Molecule 6: Flagellar basal-body rod protein FlgG

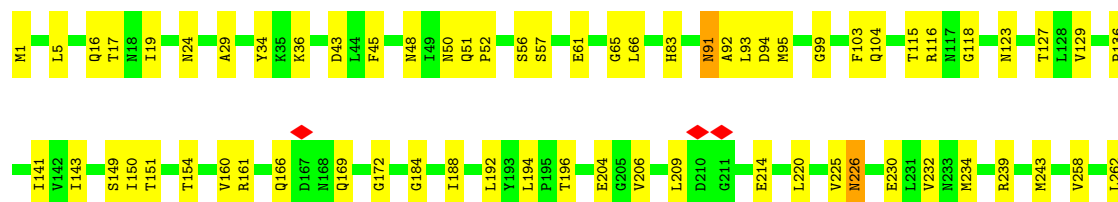
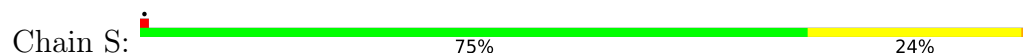


- Molecule 6: Flagellar basal-body rod protein FlgG

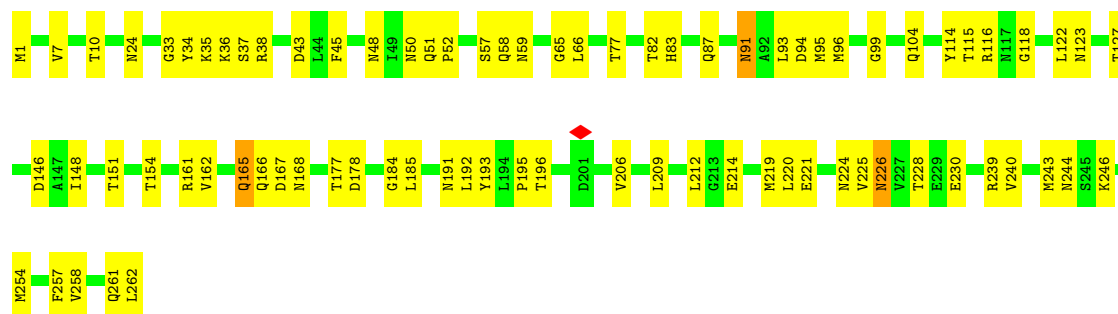




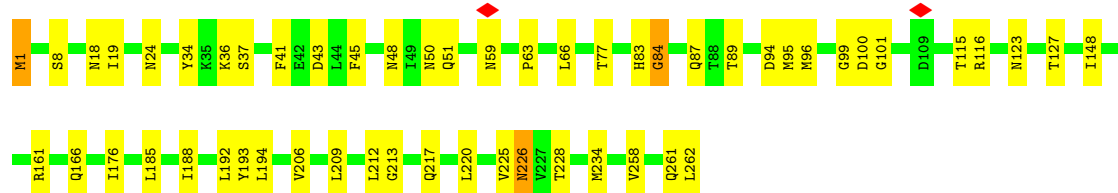
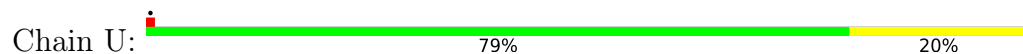
- Molecule 6: Flagellar basal-body rod protein FlgG



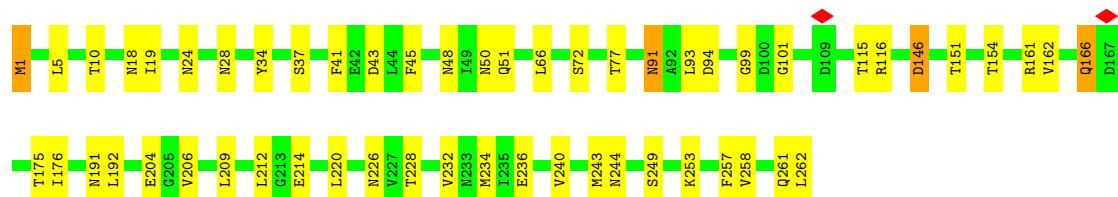
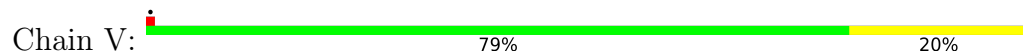
- Molecule 6: Flagellar basal-body rod protein FlgG



- Molecule 6: Flagellar basal-body rod protein FlgG

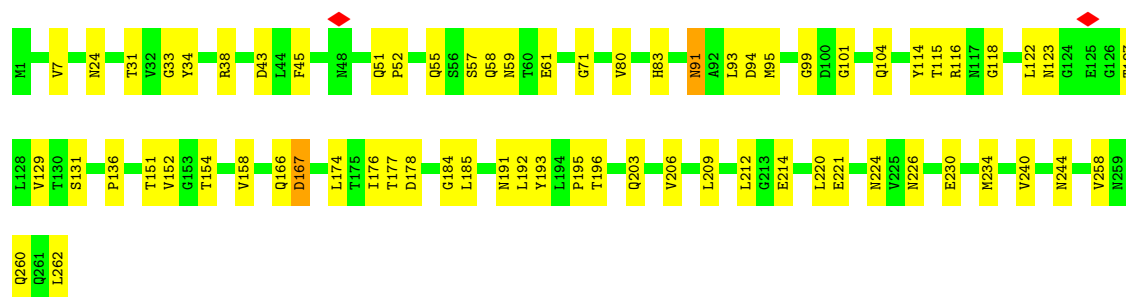


- Molecule 6: Flagellar basal-body rod protein FlgG



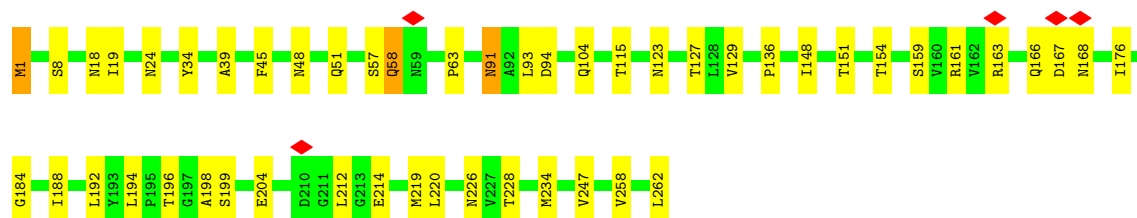
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain W:  74% 25%



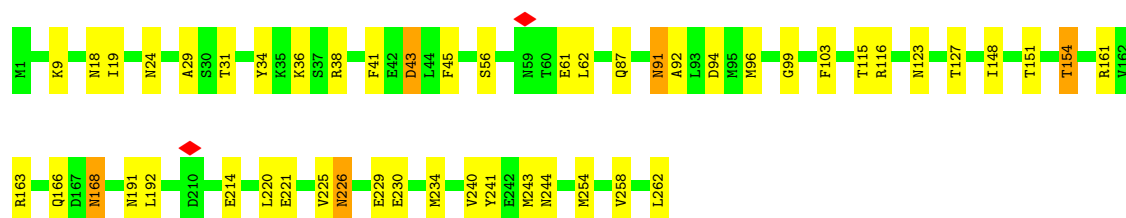
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain X:  81% 18%



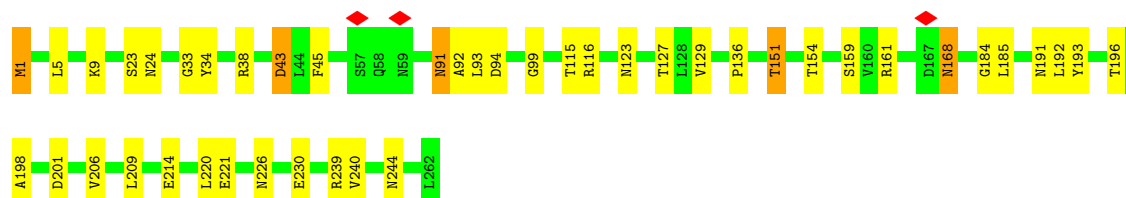
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain Y:  81% 17%



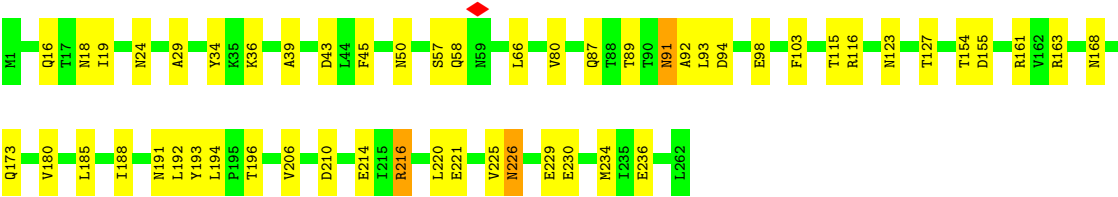
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain Z:  83% 15%

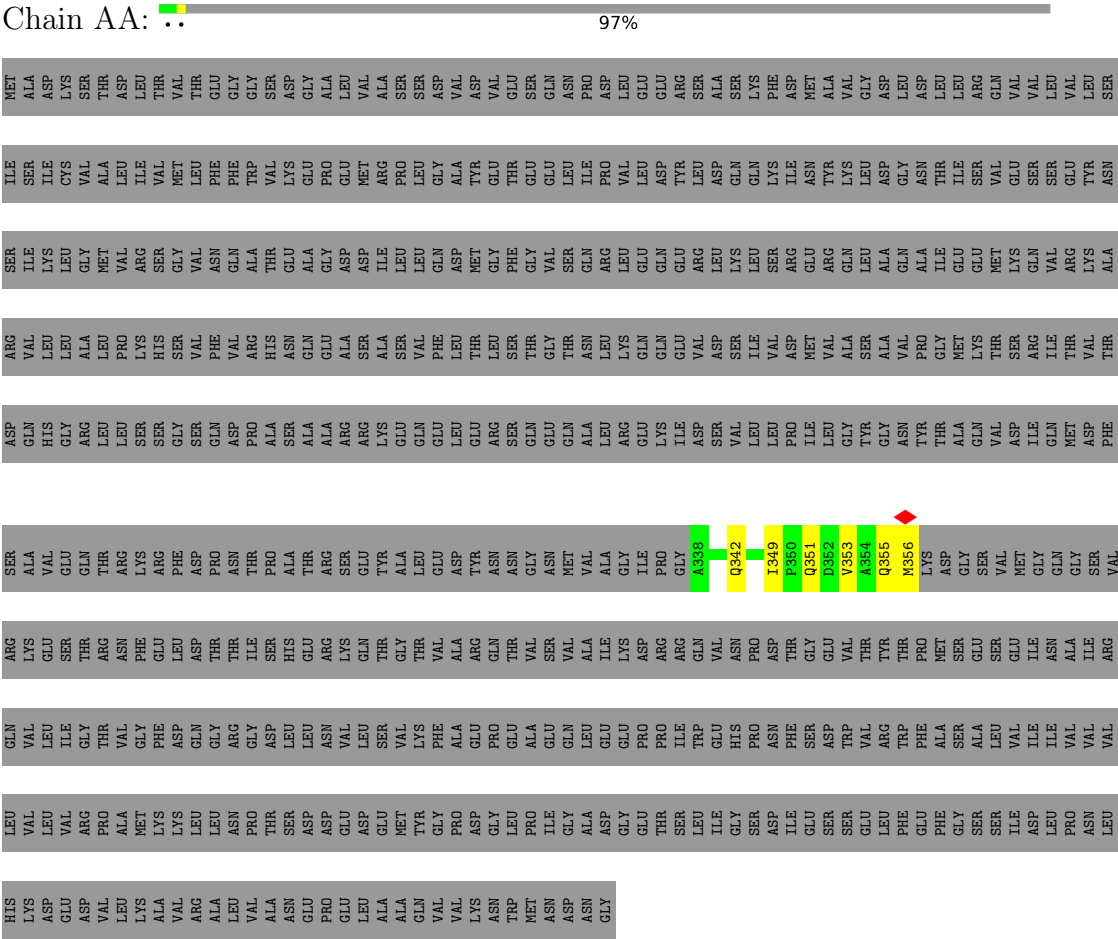


- Molecule 6: Flagellar basal-body rod protein FlgG

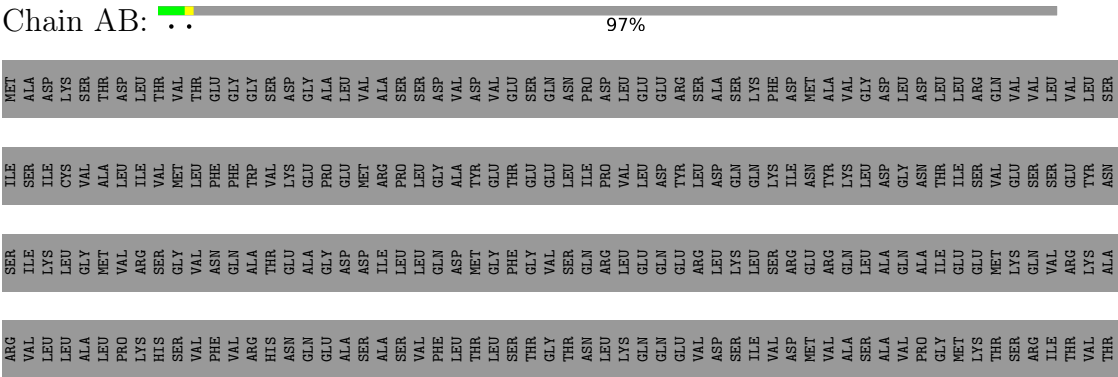
Chain a:  80% 19%



• Molecule 7: Flagellar M-ring protein



• Molecule 7: Flagellar M-ring protein

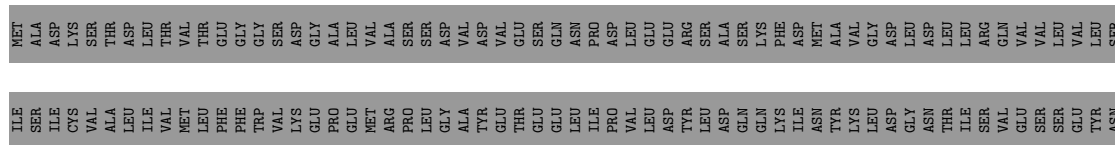








WORLD WIDE
PDB
PROTEIN DATA BANK





Chain AK: 96%



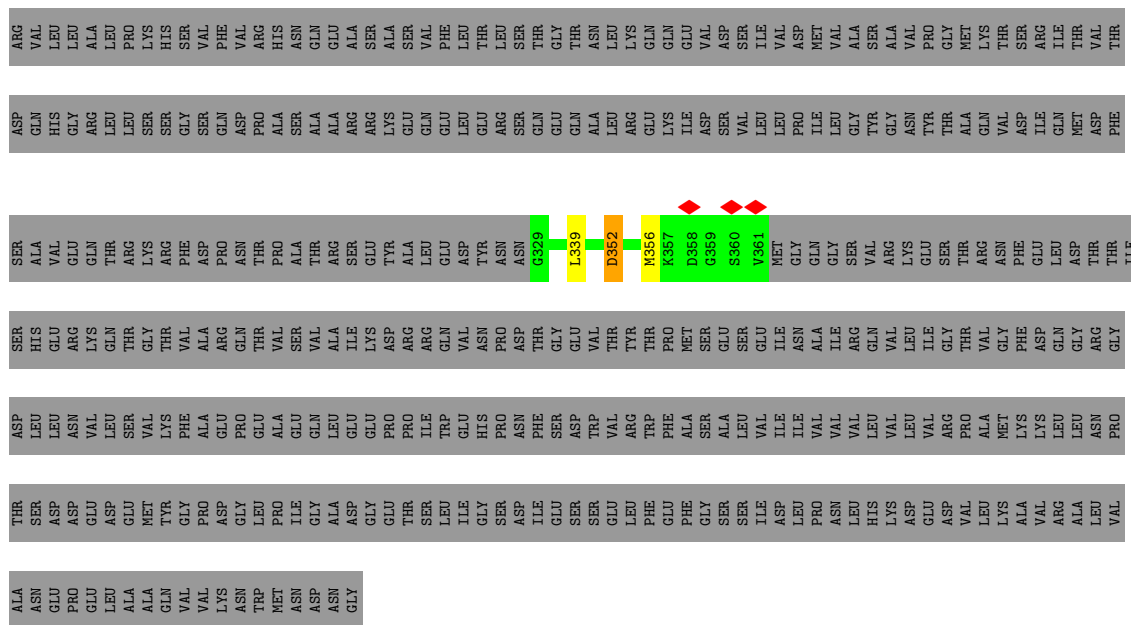
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- Molecule 7: Flagellar M-ring protein

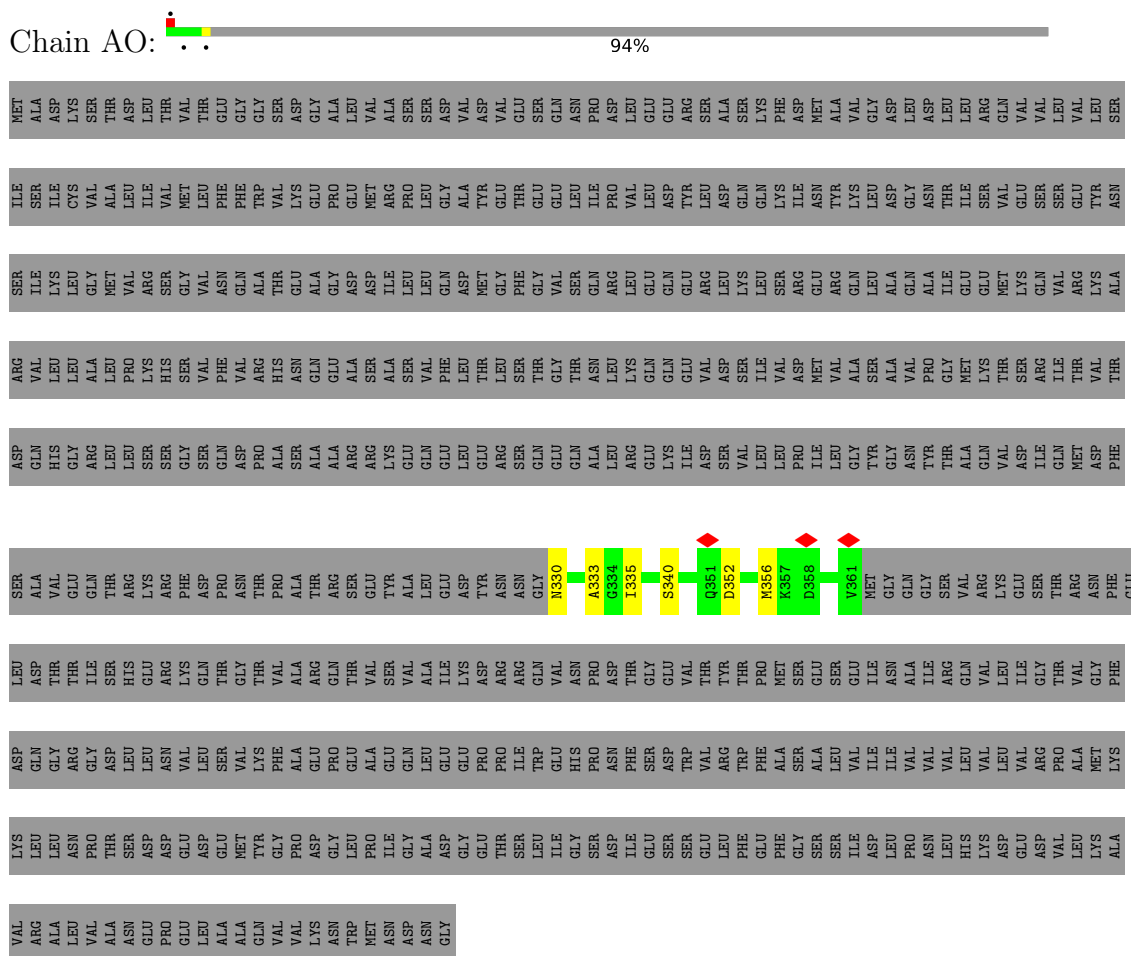
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- Molecule 7: Flagellar M-ring protein

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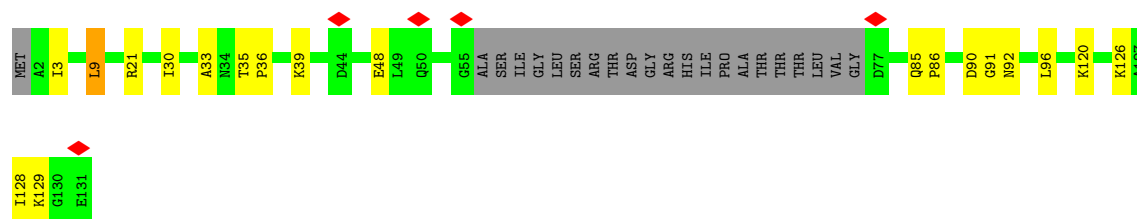


- Molecule 7: Flagellar M-ring protein



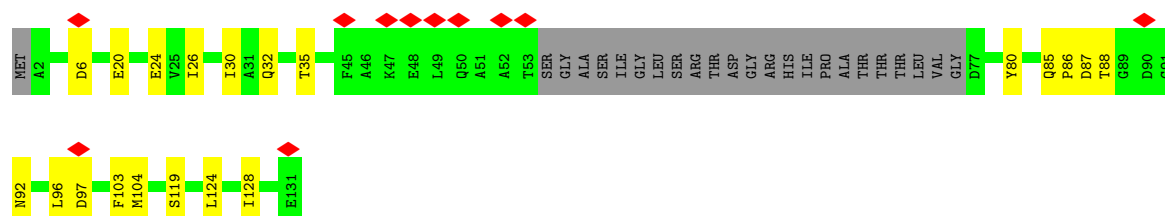
- Molecule 8: Flagellar basal body rod protein FlgB

Chain b: 



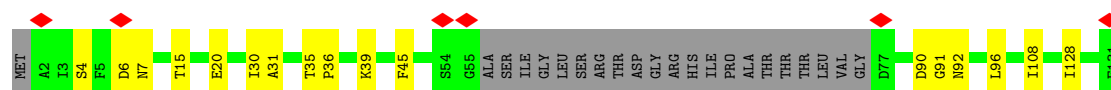
- Molecule 8: Flagellar basal body rod protein FlgB

Chain c: 



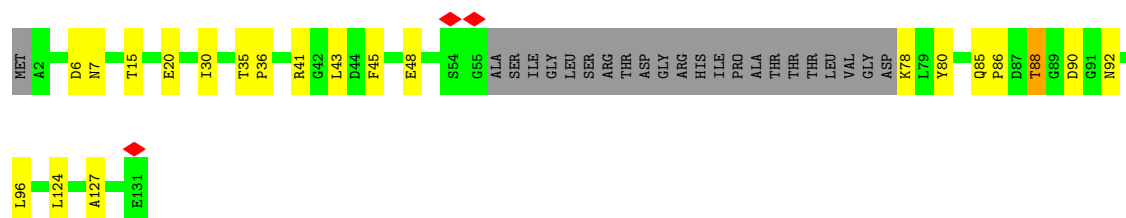
- Molecule 8: Flagellar basal body rod protein FlgB

Chain d: 



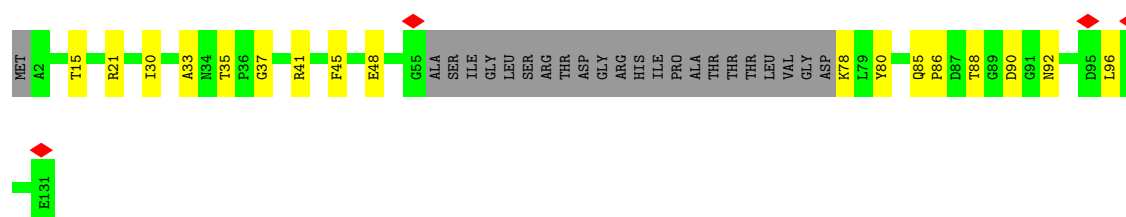
- Molecule 8: Flagellar basal body rod protein FlgB

Chain e: 

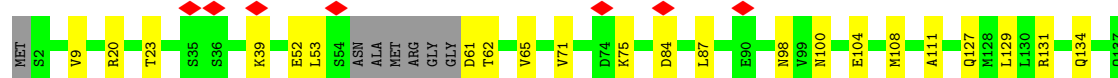
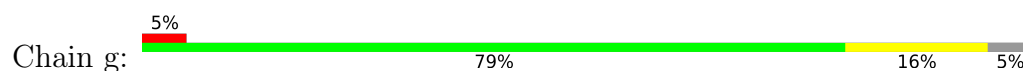


- Molecule 8: Flagellar basal body rod protein FlgB

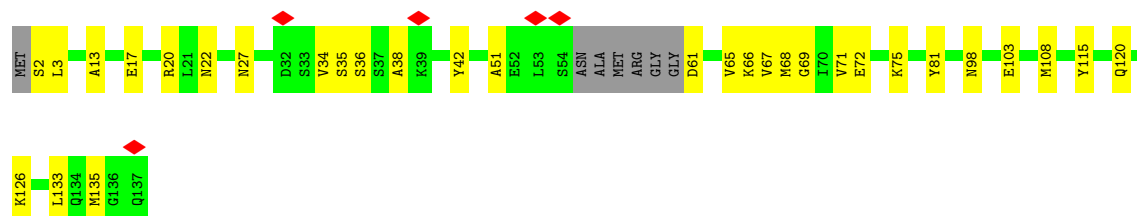
Chain f: 



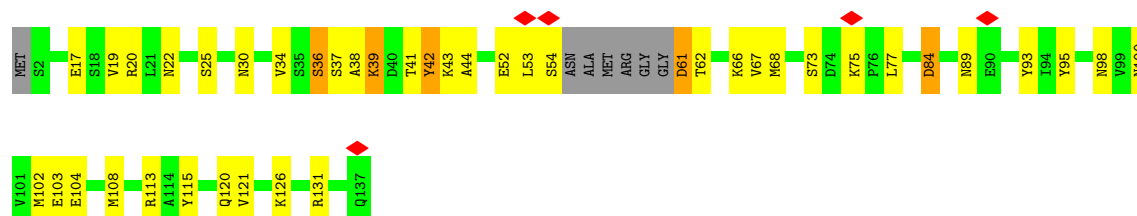
- Molecule 9: Flagellar basal-body rod protein FlgC



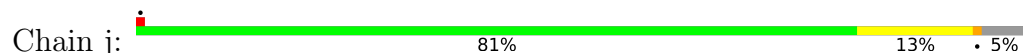
- Molecule 9: Flagellar basal-body rod protein FlgC



- Molecule 9: Flagellar basal-body rod protein FlgC



- Molecule 9: Flagellar basal-body rod protein FlgC

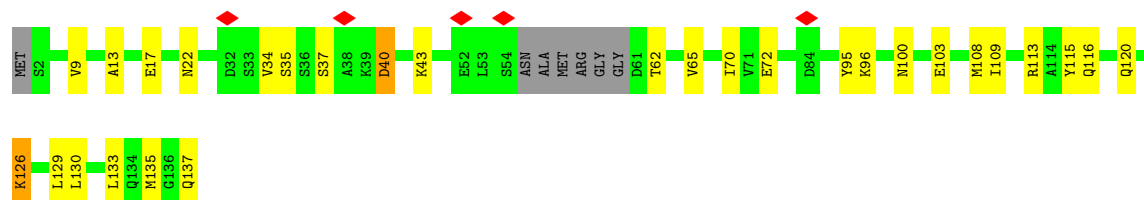


- Molecule 9: Flagellar basal-body rod protein FlgC

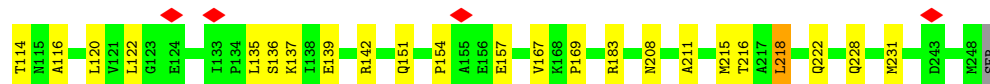
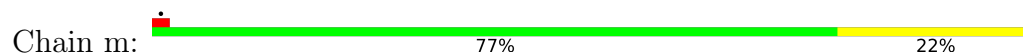


- Molecule 9: Flagellar basal-body rod protein FlgC

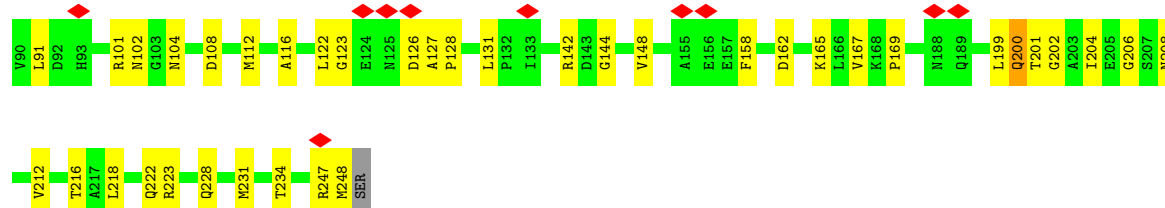
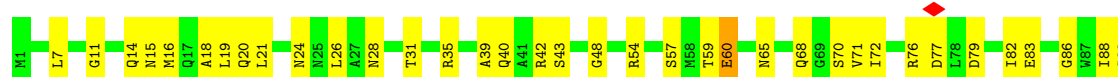




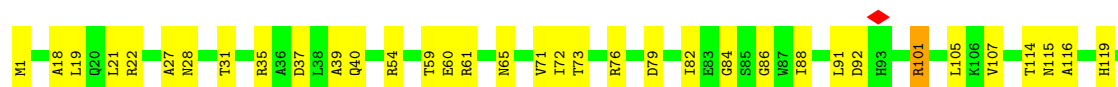
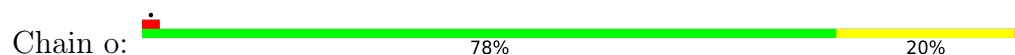
- Molecule 10: Flagellar basal-body rod protein FlgF



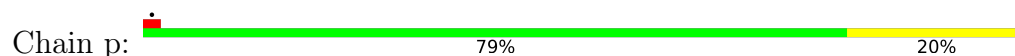
- Molecule 10: Flagellar basal-body rod protein FlgF

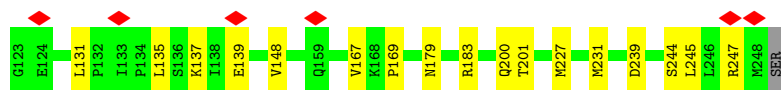


- Molecule 10: Flagellar basal-body rod protein FlgF

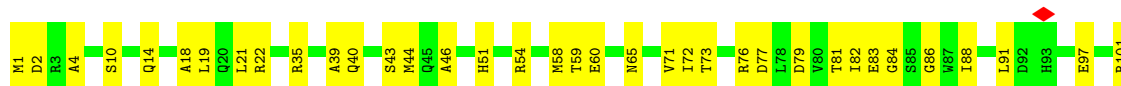
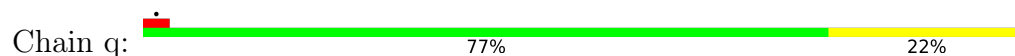


- Molecule 10: Flagellar basal-body rod protein FlgF

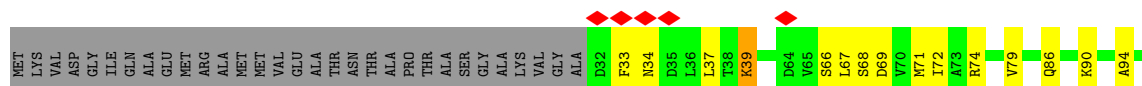




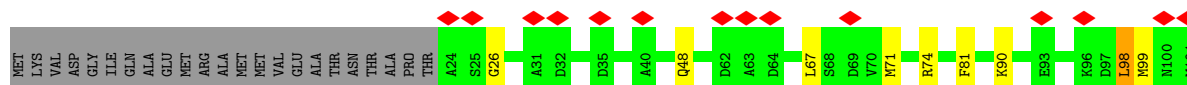
- Molecule 10: Flagellar basal-body rod protein FlgF



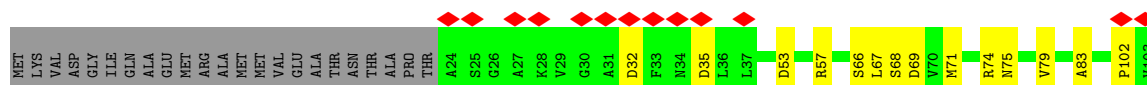
- Molecule 11: Flagellar hook-basal body complex protein FliE



- Molecule 11: Flagellar hook-basal body complex protein FliE

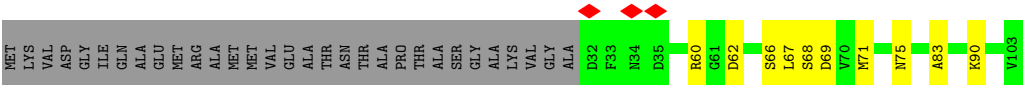


- Molecule 11: Flagellar hook-basal body complex protein FliE

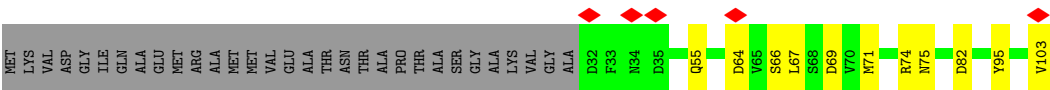


- Molecule 11: Flagellar hook-basal body complex protein FliE

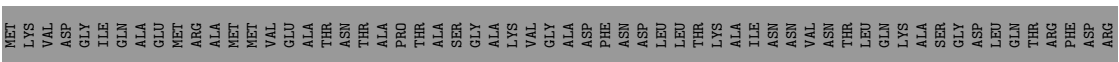




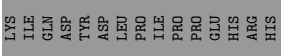
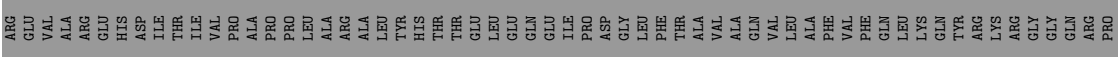
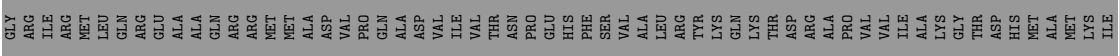
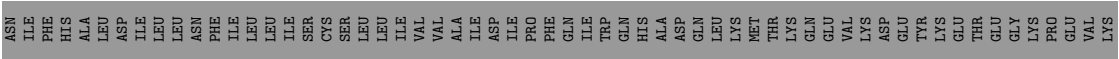
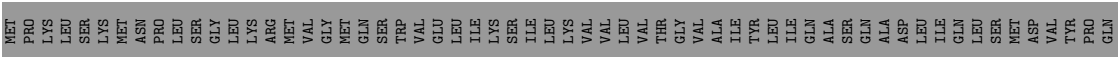
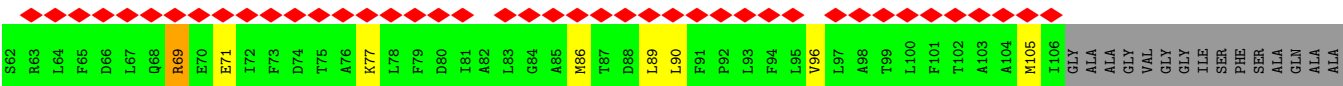
• Molecule 11: Flagellar hook-basal body complex protein FliE



• Molecule 11: Flagellar hook-basal body complex protein FliE



• Molecule 12: Flagellar biosynthetic protein FlhB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.745	Depositor
Minimum map value	-1.973	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	744.0, 744.0, 744.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	D	0.35	0/2092	0.57	4/2833 (0.1%)
1	E	0.31	0/2092	0.52	0/2833
1	F	0.35	0/2092	0.58	4/2833 (0.1%)
1	G	0.39	0/2092	0.61	1/2833 (0.0%)
1	H	0.32	0/2092	0.53	2/2833 (0.1%)
1	I	0.31	0/2092	0.50	2/2833 (0.1%)
1	J	0.32	0/2092	0.55	3/2833 (0.1%)
1	K	0.25	0/2092	0.43	1/2833 (0.0%)
1	L	0.15	0/2092	0.36	2/2833 (0.1%)
1	M	0.20	0/2092	0.42	2/2833 (0.1%)
1	N	0.14	0/2092	0.33	0/2833
1	O	0.10	0/2092	0.25	0/2833
2	0	0.09	0/1389	0.25	0/1884
2	9	0.09	0/1389	0.28	0/1884
3	1	0.13	0/1628	0.29	0/2209
3	2	0.16	0/1637	0.33	0/2221
3	3	0.09	0/1637	0.26	0/2221
3	y	0.10	0/1637	0.27	0/2221
3	z	0.11	0/1637	0.28	0/2221
4	4	0.12	0/739	0.31	0/1005
4	5	0.16	0/739	0.34	0/1005
4	6	0.28	0/739	0.49	0/1005
4	7	0.15	0/739	0.33	0/1005
5	8	0.08	0/1941	0.25	0/2631
6	A	0.16	0/1985	0.33	0/2697
6	AP	0.15	0/1985	0.34	1/2697 (0.0%)
6	AQ	0.09	0/1985	0.24	0/2697
6	AR	0.14	0/1884	0.28	0/2558
6	AS	0.13	0/1884	0.29	0/2558
6	AT	0.12	0/1892	0.25	0/2568
6	AU	0.11	0/1884	0.24	0/2558
6	AV	0.10	0/1884	0.24	0/2558
6	AW	0.10	0/1985	0.25	0/2697
6	AX	0.11	0/1985	0.26	0/2697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	AY	0.10	0/1985	0.25	0/2697
6	AZ	0.10	0/1985	0.23	0/2697
6	Aa	0.10	0/1985	0.25	0/2697
6	B	0.14	0/1985	0.32	0/2697
6	C	0.10	0/1985	0.24	0/2697
6	P	0.11	0/1985	0.25	0/2697
6	Q	0.21	1/1985 (0.1%)	0.28	0/2697
6	R	0.11	0/1985	0.25	0/2697
6	S	0.10	0/1985	0.24	0/2697
6	T	0.11	0/1985	0.24	0/2697
6	U	0.22	0/1985	0.37	3/2697 (0.1%)
6	V	0.10	0/1985	0.25	0/2697
6	W	0.24	1/1985 (0.1%)	0.39	0/2697
6	X	0.11	0/1985	0.25	0/2697
6	Y	0.10	0/1985	0.25	0/2697
6	Z	0.10	0/1985	0.24	0/2697
6	a	0.10	0/1985	0.24	0/2697
7	AA	0.35	0/137	0.45	0/188
7	AB	0.28	0/137	0.43	0/188
7	AC	0.14	0/141	0.31	0/193
7	AD	0.30	0/137	0.46	0/188
7	AE	0.12	0/137	0.28	0/188
7	AF	0.92	0/161	1.23	0/221
7	AG	0.16	0/75	0.32	0/103
7	AH	0.20	0/75	0.42	0/103
7	AI	0.94	0/75	1.34	0/103
7	AJ	0.37	0/166	0.57	0/228
7	AK	0.31	0/172	0.69	0/237
7	AL	0.39	0/223	0.61	0/304
7	AM	0.19	0/227	0.44	0/309
7	AN	0.23	0/227	0.49	0/309
7	AO	0.16	0/223	0.40	0/304
8	b	0.22	0/856	0.36	0/1151
8	c	0.21	0/846	0.30	0/1138
8	d	0.24	0/856	0.31	0/1151
8	e	0.19	0/848	0.31	0/1140
8	f	0.22	0/848	0.35	0/1140
9	g	0.10	0/996	0.26	0/1348
9	h	0.10	0/996	0.26	0/1348
9	i	0.30	0/996	0.46	0/1348
9	j	0.09	0/996	0.24	0/1348
9	k	0.10	0/996	0.28	0/1348
9	l	0.13	0/996	0.30	0/1348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	m	0.10	0/1905	0.26	0/2572
10	n	0.13	0/1905	0.26	0/2572
10	o	0.10	0/1905	0.26	0/2572
10	p	0.17	0/1905	0.36	1/2572 (0.0%)
10	q	0.09	0/1905	0.25	0/2572
11	r	0.31	0/564	0.43	0/759
11	s	0.07	0/609	0.20	0/819
11	t	0.07	0/609	0.17	0/819
11	u	0.07	0/564	0.16	0/759
11	v	0.06	0/564	0.18	0/759
11	w	0.09	0/313	0.19	0/420
12	x	0.07	0/562	0.19	0/760
All	All	0.18	2/119906 (0.0%)	0.34	26/162571 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
1	J	0	2
1	K	0	1
1	M	0	1
3	2	0	1
6	AP	0	2
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	52	PRO	C-O	-5.55	1.17	1.23
6	Q	37	SER	CA-CB	-5.44	1.45	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	LEU	N-CA-C	-8.64	102.51	113.23
1	J	54	PRO	N-CA-CB	-8.45	93.30	102.76
10	p	227	MET	N-CA-C	-8.15	103.46	113.41
6	AP	161	ARG	CB-CA-C	-7.50	97.38	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	54	PRO	N-CA-CB	-6.69	96.22	103.25

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	414	ARG	Sidechain
1	I	50	ALA	Mainchain
1	J	414	ARG	Sidechain
1	J	50	ALA	Mainchain
1	K	414	ARG	Sidechain

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	D	2057	0	1944	28	0
1	E	2057	0	1944	37	0
1	F	2057	0	1944	39	0
1	G	2057	0	1944	48	0
1	H	2057	0	1944	38	0
1	I	2057	0	1944	44	0
1	J	2057	0	1944	33	0
1	K	2057	0	1944	38	0
1	L	2057	0	1944	39	0
1	M	2057	0	1944	38	0
1	N	2057	0	1944	41	0
1	O	2057	0	1944	31	0
2	0	1361	0	1418	28	0
2	9	1361	0	1418	23	0
3	1	1599	0	1685	23	0
3	2	1608	0	1691	27	0
3	3	1608	0	1691	33	0
3	y	1608	0	1691	24	0
3	z	1608	0	1691	34	0
4	4	722	0	768	16	0
4	5	722	0	768	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	6	722	0	768	15	0
4	7	722	0	768	10	0
5	8	1896	0	1968	44	0
6	A	1956	0	1907	39	0
6	AP	1956	0	1907	39	0
6	AQ	1956	0	1907	30	0
6	AR	1858	0	1813	43	0
6	AS	1858	0	1813	36	0
6	AT	1866	0	1825	33	0
6	AU	1858	0	1813	42	0
6	AV	1858	0	1813	34	0
6	AW	1956	0	1907	36	0
6	AX	1956	0	1907	38	0
6	AY	1956	0	1907	36	0
6	AZ	1956	0	1907	39	0
6	Aa	1956	0	1907	37	0
6	B	1956	0	1907	41	0
6	C	1956	0	1907	38	0
6	P	1956	0	1907	37	0
6	Q	1956	0	1907	35	0
6	R	1956	0	1907	34	0
6	S	1956	0	1907	44	0
6	T	1956	0	1907	50	0
6	U	1956	0	1907	36	0
6	V	1956	0	1907	37	0
6	W	1956	0	1907	39	0
6	X	1956	0	1907	33	0
6	Y	1956	0	1907	36	0
6	Z	1956	0	1907	30	0
6	a	1956	0	1907	37	0
7	AA	135	0	128	4	0
7	AB	135	0	128	2	0
7	AC	139	0	131	0	0
7	AD	135	0	128	2	0
7	AE	135	0	128	2	0
7	AF	158	0	152	16	0
7	AG	73	0	72	4	0
7	AH	73	0	72	4	0
7	AI	73	0	72	8	0
7	AJ	163	0	157	5	0
7	AK	169	0	164	5	0
7	AL	220	0	215	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AM	224	0	218	5	0
7	AN	224	0	218	2	0
7	AO	220	0	215	3	0
8	b	845	0	833	12	0
8	c	835	0	825	18	0
8	d	845	0	833	10	0
8	e	837	0	829	14	0
8	f	837	0	829	11	0
9	g	983	0	958	12	0
9	h	983	0	958	24	0
9	i	983	0	958	37	0
9	j	983	0	958	12	0
9	k	983	0	958	20	0
9	l	983	0	958	25	0
10	m	1879	0	1864	37	0
10	n	1879	0	1864	55	0
10	o	1879	0	1864	36	0
10	p	1879	0	1864	33	0
10	q	1879	0	1864	41	0
11	r	560	0	561	12	0
11	s	605	0	609	9	0
11	t	605	0	609	9	0
11	u	560	0	561	7	0
11	v	560	0	561	10	0
11	w	311	0	320	8	0
12	x	552	0	577	13	0
All	All	118072	0	115897	1850	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 8.

The worst 5 of 1850 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)
9:i:52:GLU:HG3	9:i:52:GLU:O	1.47	1.06
9:i:52:GLU:O	9:i:52:GLU:CG	2.15	0.94
1:H:42:TYR:CD1	1:M:362:LYS:HB2	2.06	0.91
6:AP:161:ARG:NH1	6:a:196:THR:HG22	1.89	0.88
1:H:42:TYR:HE2	1:H:44:ASN:HB2	1.39	0.87

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	D	264/437 (60%)	257 (97%)	7 (3%)	0	100	100
1	E	264/437 (60%)	256 (97%)	8 (3%)	0	100	100
1	F	264/437 (60%)	257 (97%)	7 (3%)	0	100	100
1	G	264/437 (60%)	259 (98%)	3 (1%)	2 (1%)	16	46
1	H	264/437 (60%)	256 (97%)	6 (2%)	2 (1%)	16	46
1	I	264/437 (60%)	256 (97%)	8 (3%)	0	100	100
1	J	264/437 (60%)	256 (97%)	8 (3%)	0	100	100
1	K	264/437 (60%)	258 (98%)	6 (2%)	0	100	100
1	L	264/437 (60%)	260 (98%)	4 (2%)	0	100	100
1	M	264/437 (60%)	257 (97%)	7 (3%)	0	100	100
1	N	264/437 (60%)	259 (98%)	5 (2%)	0	100	100
1	O	264/437 (60%)	259 (98%)	5 (2%)	0	100	100
2	0	178/199 (89%)	173 (97%)	5 (3%)	0	100	100
2	9	178/199 (89%)	174 (98%)	4 (2%)	0	100	100
3	1	205/289 (71%)	202 (98%)	3 (2%)	0	100	100
3	2	206/289 (71%)	203 (98%)	3 (2%)	0	100	100
3	3	206/289 (71%)	204 (99%)	2 (1%)	0	100	100
3	y	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
3	z	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
4	4	87/89 (98%)	87 (100%)	0	0	100	100
4	5	87/89 (98%)	86 (99%)	0	1 (1%)	11	39
4	6	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
4	7	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
5	8	238/260 (92%)	232 (98%)	6 (2%)	0	100	100
6	A	260/262 (99%)	251 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AP	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
6	AQ	260/262 (99%)	248 (95%)	11 (4%)	1 (0%)	30	61
6	AR	244/262 (93%)	240 (98%)	3 (1%)	1 (0%)	30	61
6	AS	244/262 (93%)	235 (96%)	9 (4%)	0	100	100
6	AT	245/262 (94%)	239 (98%)	5 (2%)	1 (0%)	30	61
6	AU	244/262 (93%)	240 (98%)	4 (2%)	0	100	100
6	AV	244/262 (93%)	242 (99%)	1 (0%)	1 (0%)	30	61
6	AW	260/262 (99%)	254 (98%)	5 (2%)	1 (0%)	30	61
6	AX	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
6	AY	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
6	AZ	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
6	Aa	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
6	B	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
6	C	260/262 (99%)	252 (97%)	7 (3%)	1 (0%)	30	61
6	P	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
6	Q	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
6	R	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
6	S	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	T	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	U	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
6	V	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
6	W	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
6	X	260/262 (99%)	250 (96%)	9 (4%)	1 (0%)	30	61
6	Y	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	Z	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	a	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
7	AA	17/580 (3%)	17 (100%)	0	0	100	100
7	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
7	AC	18/580 (3%)	18 (100%)	0	0	100	100
7	AD	17/580 (3%)	17 (100%)	0	0	100	100
7	AE	17/580 (3%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	9
7	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
7	AH	9/580 (2%)	9 (100%)	0	0	100	100
7	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
7	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100
7	AK	23/580 (4%)	23 (100%)	0	0	100	100
7	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
7	AM	31/580 (5%)	31 (100%)	0	0	100	100
7	AN	31/580 (5%)	31 (100%)	0	0	100	100
7	AO	30/580 (5%)	30 (100%)	0	0	100	100
8	b	105/131 (80%)	104 (99%)	1 (1%)	0	100	100
8	c	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
8	d	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
8	e	104/131 (79%)	104 (100%)	0	0	100	100
8	f	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
9	g	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
9	h	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
9	i	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	46
9	j	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
9	k	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
9	l	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
10	m	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
10	n	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
10	o	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
10	p	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
10	q	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
11	r	70/103 (68%)	70 (100%)	0	0	100	100
11	s	78/103 (76%)	78 (100%)	0	0	100	100
11	t	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
11	u	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
11	v	70/103 (68%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	w	38/103 (37%)	38 (100%)	0	0	100	100
12	x	69/376 (18%)	69 (100%)	0	0	100	100
All	All	15361/27193 (56%)	14986 (98%)	358 (2%)	17 (0%)	49	78

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	52	THR
1	G	54	PRO
1	H	64	ALA
6	X	58	GLN
1	H	65	GLN

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	D	225/366 (62%)	216 (96%)	9 (4%)	28	59
1	E	225/366 (62%)	215 (96%)	10 (4%)	25	56
1	F	225/366 (62%)	213 (95%)	12 (5%)	20	51
1	G	225/366 (62%)	213 (95%)	12 (5%)	20	51
1	H	225/366 (62%)	217 (96%)	8 (4%)	31	62
1	I	225/366 (62%)	214 (95%)	11 (5%)	22	53
1	J	225/366 (62%)	211 (94%)	14 (6%)	16	45
1	K	225/366 (62%)	213 (95%)	12 (5%)	20	51
1	L	225/366 (62%)	211 (94%)	14 (6%)	16	45
1	M	225/366 (62%)	214 (95%)	11 (5%)	22	53
1	N	225/366 (62%)	212 (94%)	13 (6%)	18	48
1	O	225/366 (62%)	211 (94%)	14 (6%)	16	45
2	0	149/167 (89%)	145 (97%)	4 (3%)	39	68
2	9	149/167 (89%)	148 (99%)	1 (1%)	76	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1	181/247 (73%)	175 (97%)	6 (3%)	33	64
3	2	182/247 (74%)	176 (97%)	6 (3%)	33	64
3	3	182/247 (74%)	177 (97%)	5 (3%)	39	68
3	y	182/247 (74%)	175 (96%)	7 (4%)	29	60
3	z	182/247 (74%)	175 (96%)	7 (4%)	29	60
4	4	80/80 (100%)	77 (96%)	3 (4%)	29	60
4	5	80/80 (100%)	76 (95%)	4 (5%)	22	53
4	6	80/80 (100%)	75 (94%)	5 (6%)	16	45
4	7	80/80 (100%)	79 (99%)	1 (1%)	61	79
5	8	204/218 (94%)	194 (95%)	10 (5%)	22	53
6	A	218/218 (100%)	214 (98%)	4 (2%)	51	74
6	AP	218/218 (100%)	214 (98%)	4 (2%)	51	74
6	AQ	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	AR	206/218 (94%)	200 (97%)	6 (3%)	37	67
6	AS	206/218 (94%)	200 (97%)	6 (3%)	37	67
6	AT	207/218 (95%)	200 (97%)	7 (3%)	32	63
6	AU	206/218 (94%)	202 (98%)	4 (2%)	50	73
6	AV	206/218 (94%)	199 (97%)	7 (3%)	32	63
6	AW	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	AX	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	AY	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	AZ	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	Aa	218/218 (100%)	215 (99%)	3 (1%)	59	78
6	B	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	C	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	P	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	Q	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	R	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	S	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	T	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	U	218/218 (100%)	212 (97%)	6 (3%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	V	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	W	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	X	218/218 (100%)	215 (99%)	3 (1%)	59	78
6	Y	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	Z	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	a	218/218 (100%)	211 (97%)	7 (3%)	34	64
7	AA	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AB	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AC	15/500 (3%)	15 (100%)	0	100	100
7	AD	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AE	15/500 (3%)	15 (100%)	0	100	100
7	AF	17/500 (3%)	13 (76%)	4 (24%)	1	4
7	AG	8/500 (2%)	8 (100%)	0	100	100
7	AH	8/500 (2%)	7 (88%)	1 (12%)	4	18
7	AI	8/500 (2%)	8 (100%)	0	100	100
7	AJ	17/500 (3%)	16 (94%)	1 (6%)	18	47
7	AK	18/500 (4%)	15 (83%)	3 (17%)	2	10
7	AL	24/500 (5%)	23 (96%)	1 (4%)	26	58
7	AM	24/500 (5%)	24 (100%)	0	100	100
7	AN	24/500 (5%)	22 (92%)	2 (8%)	10	34
7	AO	24/500 (5%)	23 (96%)	1 (4%)	26	58
8	b	89/106 (84%)	88 (99%)	1 (1%)	65	80
8	c	88/106 (83%)	86 (98%)	2 (2%)	44	70
8	d	89/106 (84%)	86 (97%)	3 (3%)	32	63
8	e	88/106 (83%)	85 (97%)	3 (3%)	32	63
8	f	88/106 (83%)	88 (100%)	0	100	100
9	g	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	h	111/115 (96%)	107 (96%)	4 (4%)	31	62
9	i	111/115 (96%)	103 (93%)	8 (7%)	13	40
9	j	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	k	111/115 (96%)	105 (95%)	6 (5%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	l	111/115 (96%)	106 (96%)	5 (4%)	24	56
10	m	204/205 (100%)	199 (98%)	5 (2%)	42	69
10	n	204/205 (100%)	198 (97%)	6 (3%)	37	67
10	o	204/205 (100%)	198 (97%)	6 (3%)	37	67
10	p	204/205 (100%)	202 (99%)	2 (1%)	68	81
10	q	204/205 (100%)	200 (98%)	4 (2%)	48	73
11	r	63/84 (75%)	59 (94%)	4 (6%)	16	45
11	s	66/84 (79%)	64 (97%)	2 (3%)	36	66
11	t	66/84 (79%)	63 (96%)	3 (4%)	24	56
11	u	63/84 (75%)	62 (98%)	1 (2%)	55	76
11	v	63/84 (75%)	63 (100%)	0	100	100
11	w	36/84 (43%)	35 (97%)	1 (3%)	38	67
12	x	58/317 (18%)	55 (95%)	3 (5%)	21	51
All	All	13048/22951 (57%)	12603 (97%)	445 (3%)	33	63

5 of 445 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	AR	180	VAL
3	z	192	LEU
6	P	91	ASN
3	z	86	THR
10	n	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 620 such sidechains are listed below:

Mol	Chain	Res	Type
6	V	217	GLN
9	i	118	ASN
6	W	169	GLN
6	V	203	GLN
6	Z	58	GLN

5.3.3 RNA ⓘ

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.

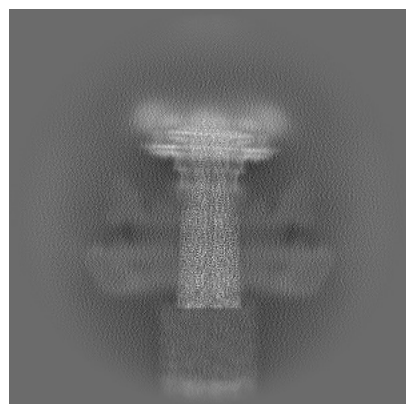
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39782. These allow visual inspection of the internal detail of the map and identification of artifacts.

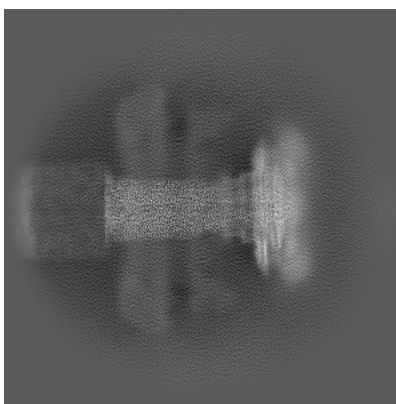
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

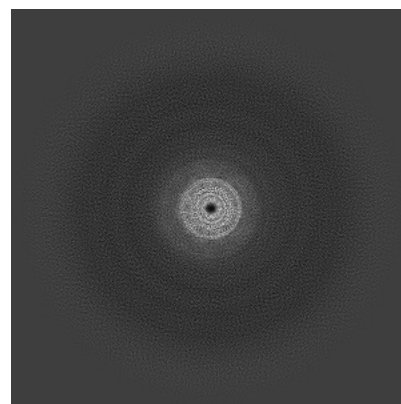
6.1.1 Primary map



X

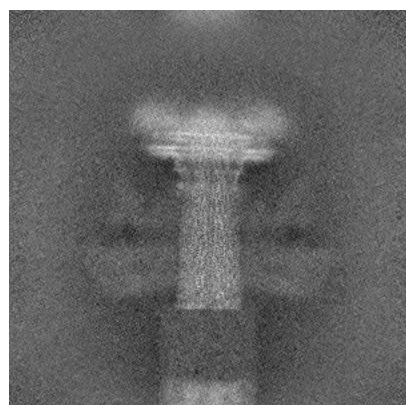


Y

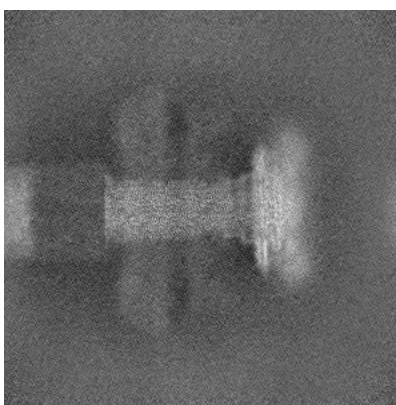


Z

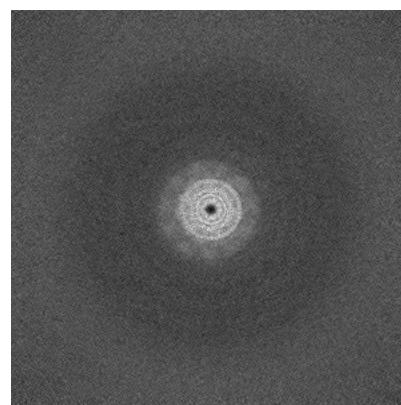
6.1.2 Raw map



X



Y

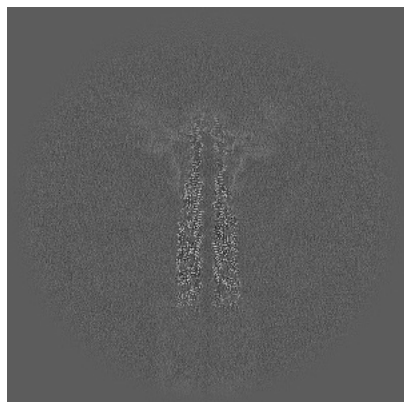


Z

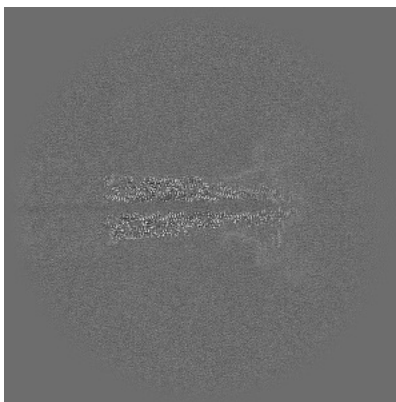
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

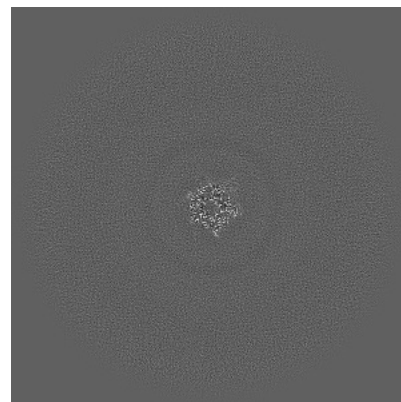
6.2.1 Primary map



X Index: 310



Y Index: 310

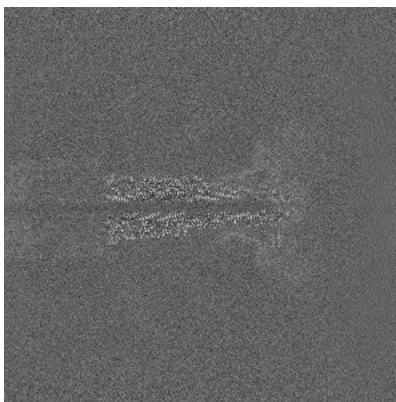


Z Index: 310

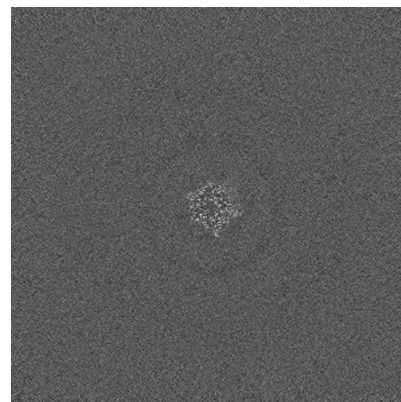
6.2.2 Raw map



X Index: 310



Y Index: 310

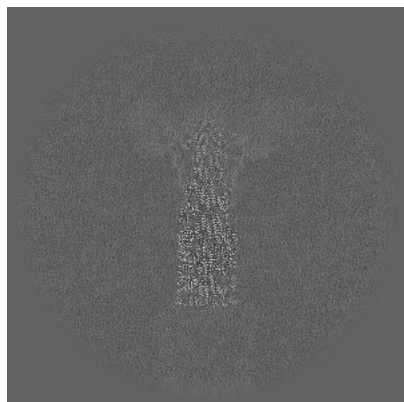


Z Index: 310

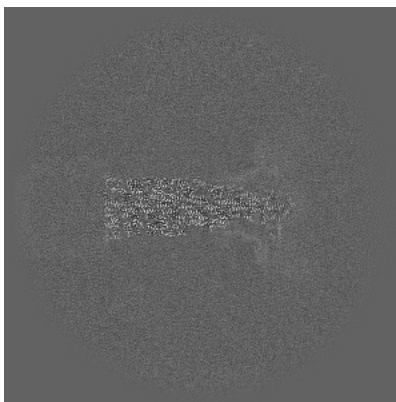
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

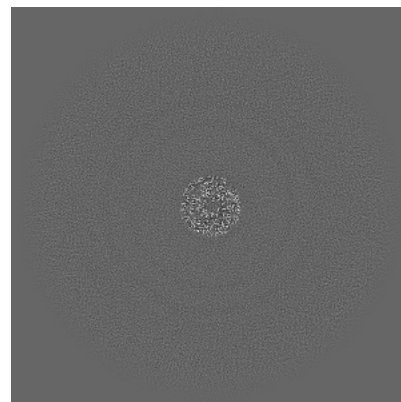
6.3.1 Primary map



X Index: 323

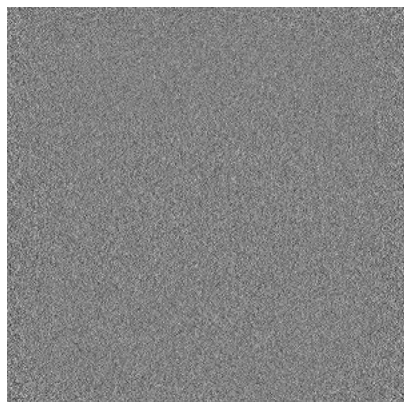


Y Index: 296

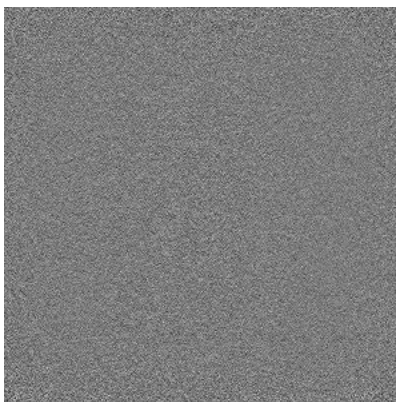


Z Index: 255

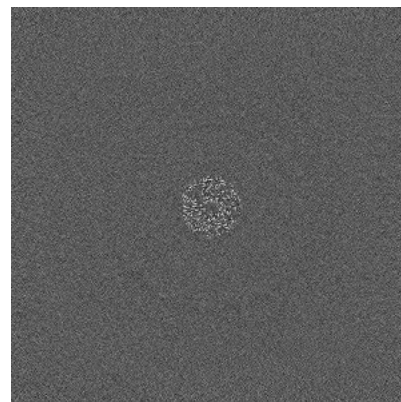
6.3.2 Raw map



X Index: 0



Y Index: 0

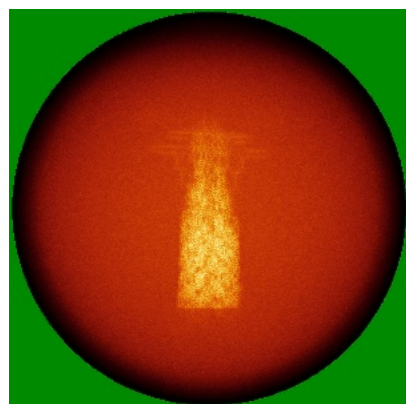


Z Index: 253

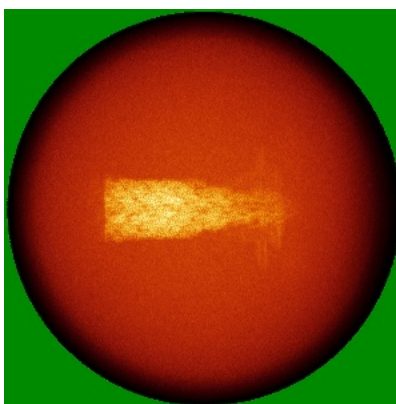
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

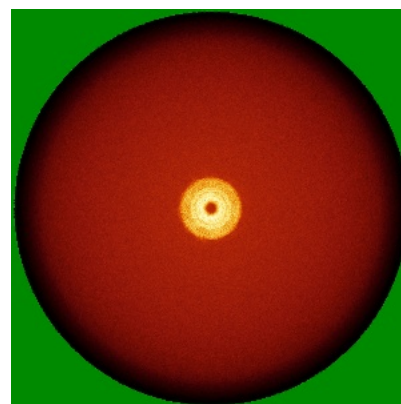
6.4.1 Primary map



X

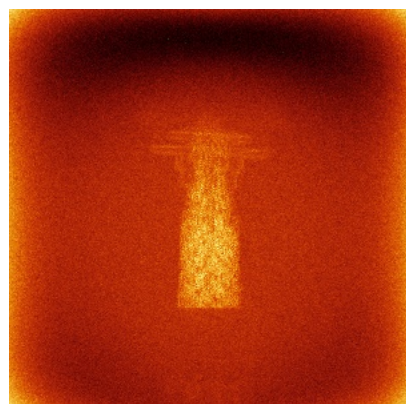


Y

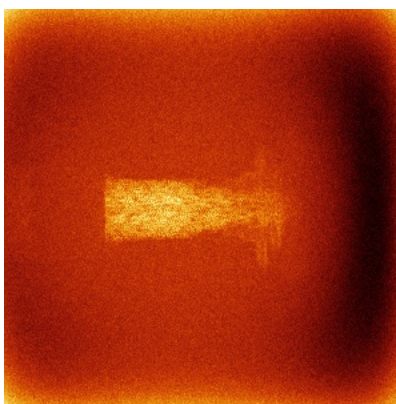


Z

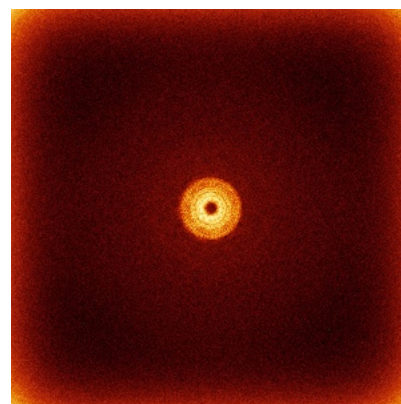
6.4.2 Raw map



X



Y

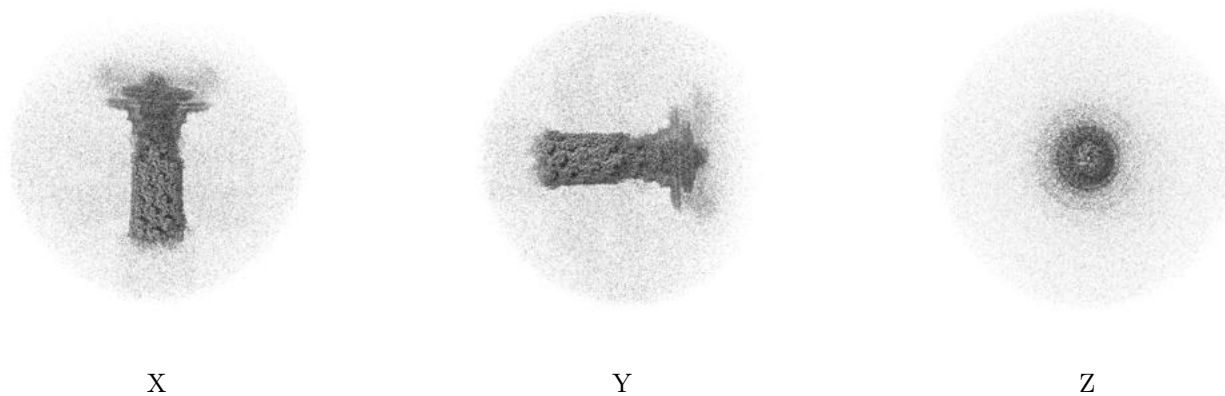


Z

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

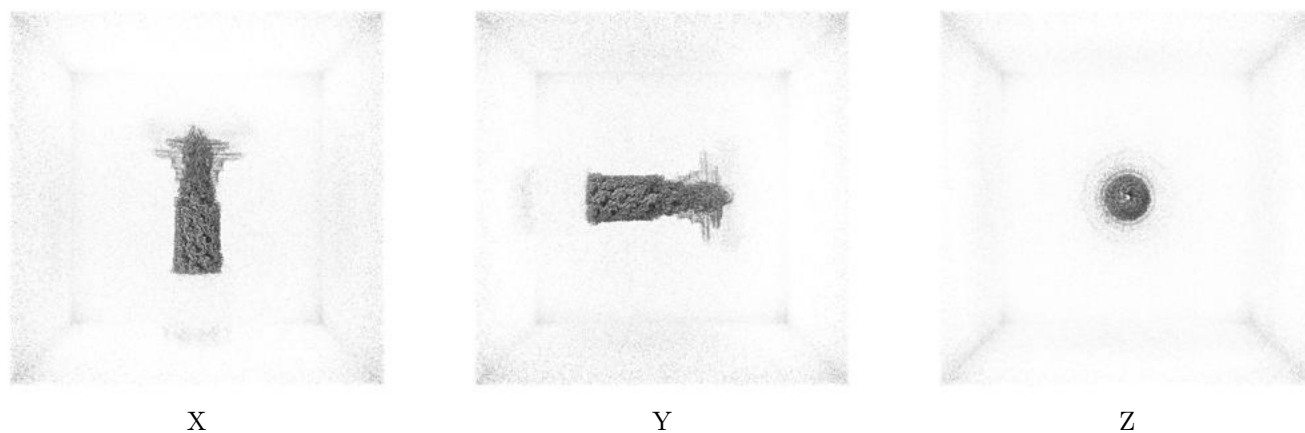
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

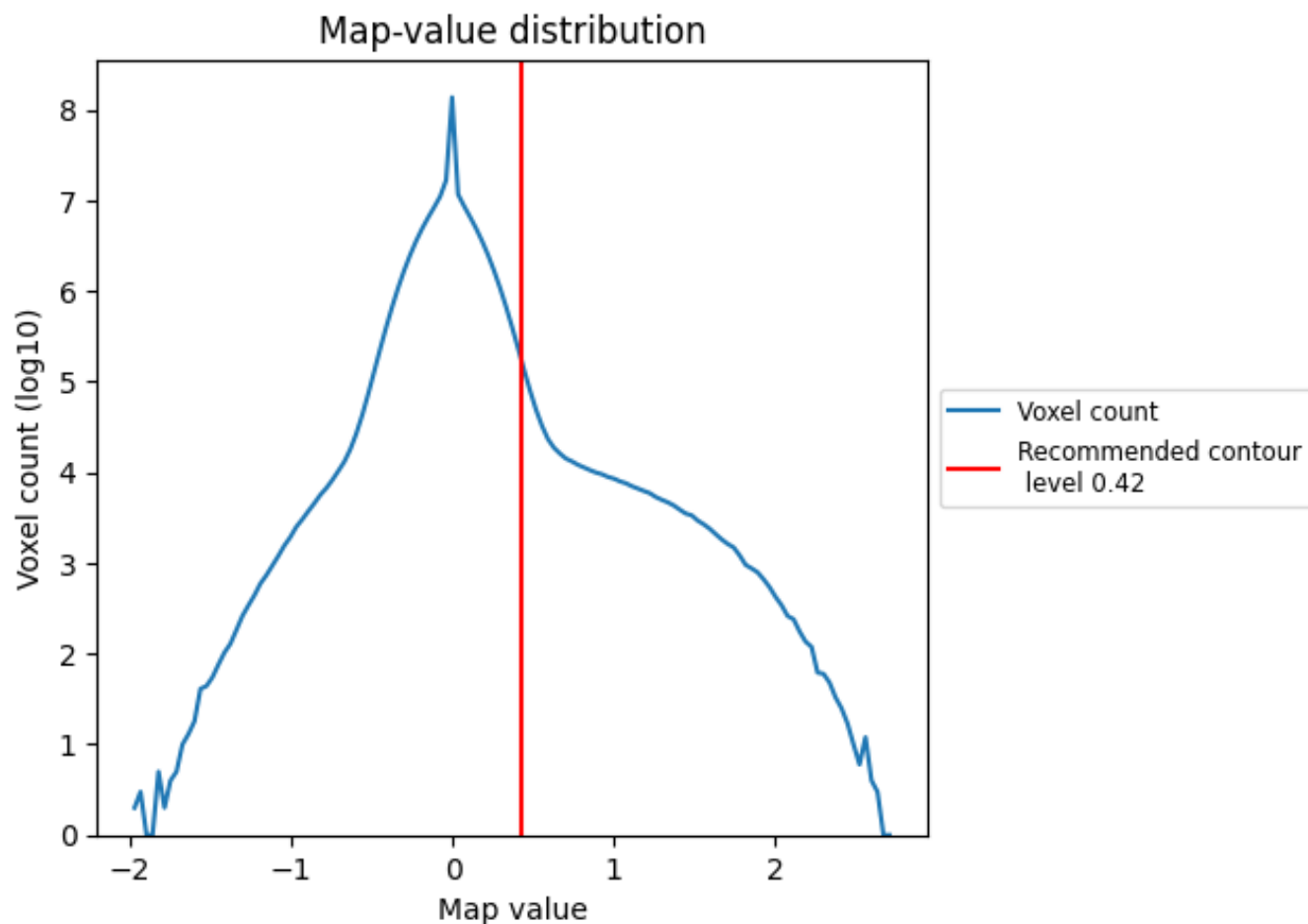
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

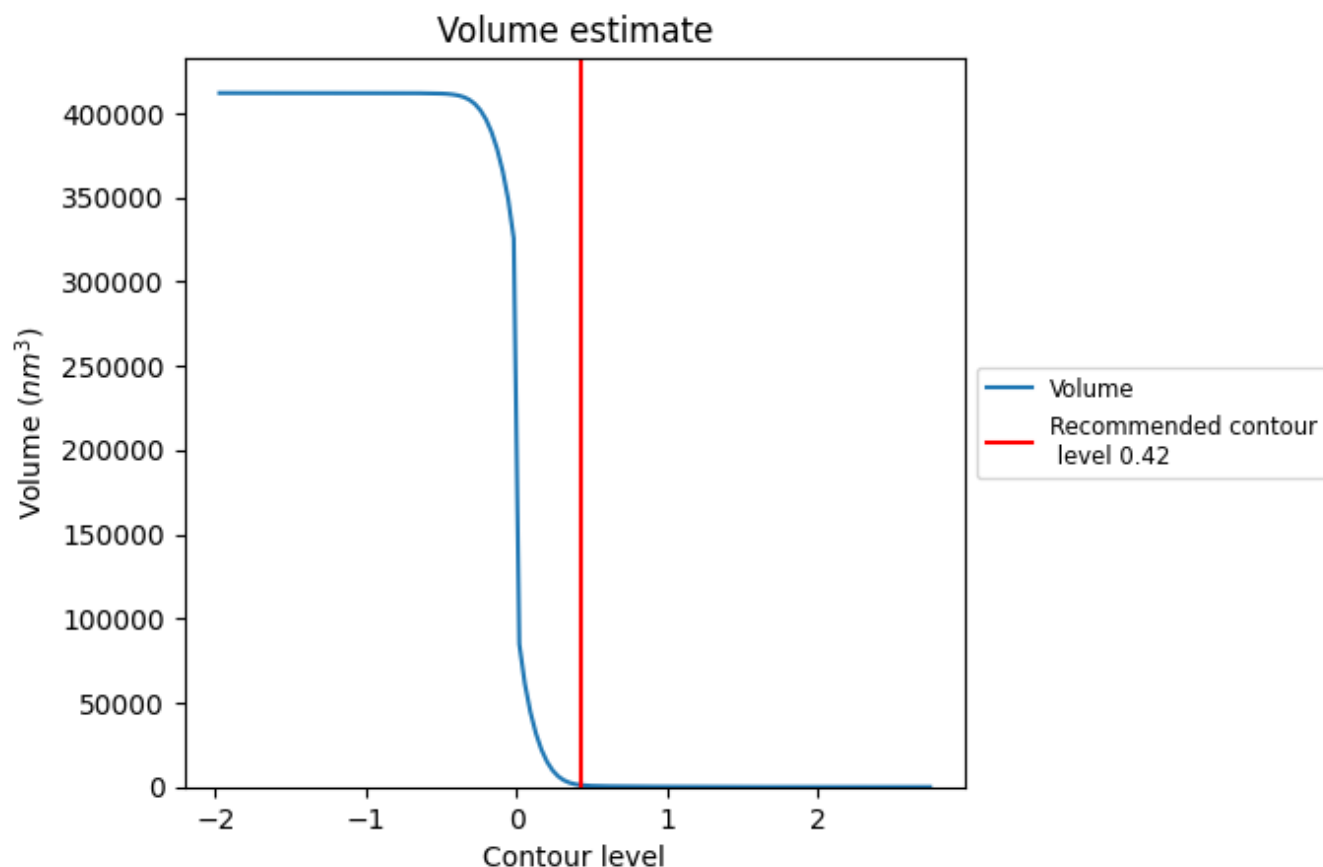
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

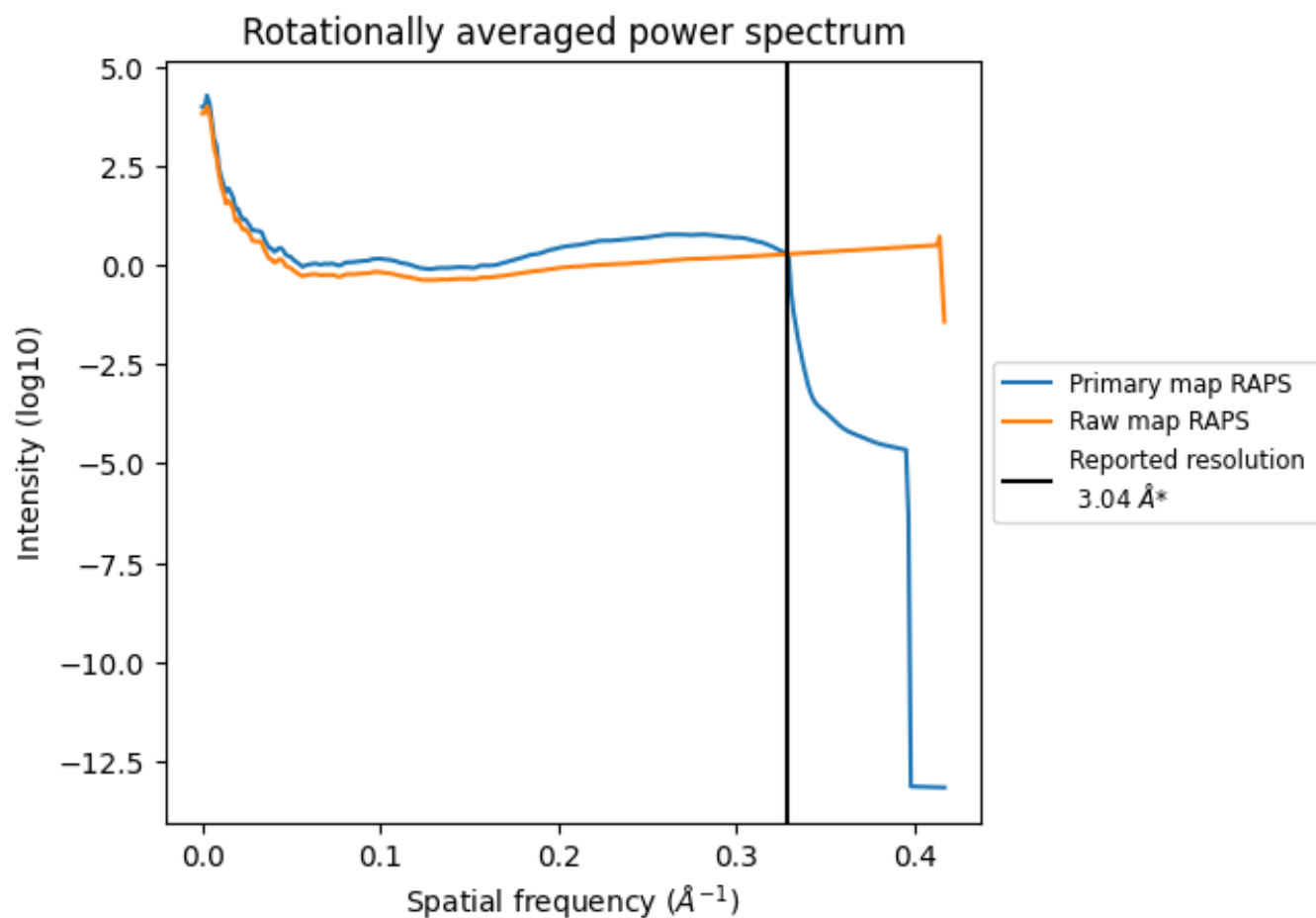
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1170 nm³; this corresponds to an approximate mass of 1057 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 ⓘ

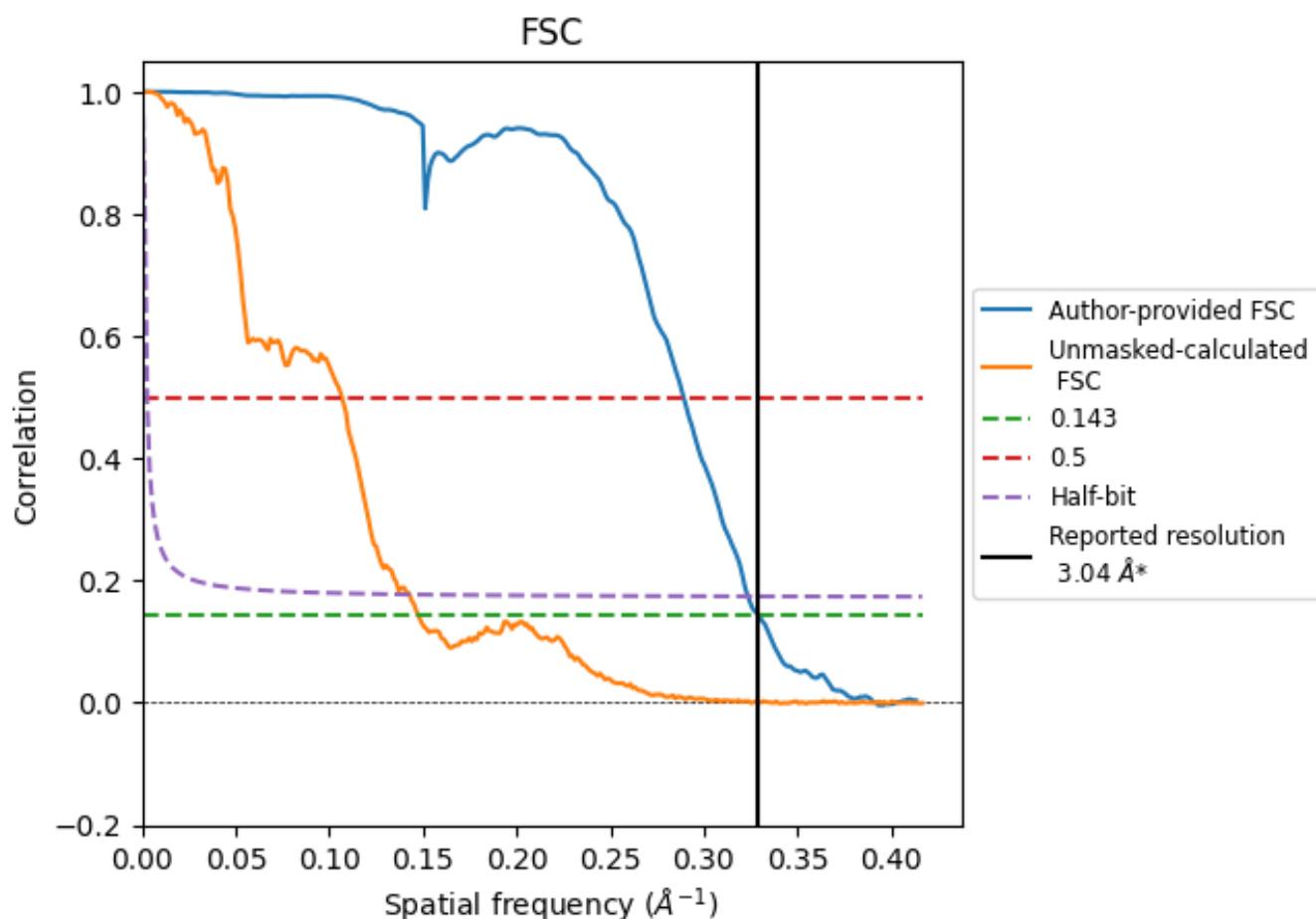


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

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 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

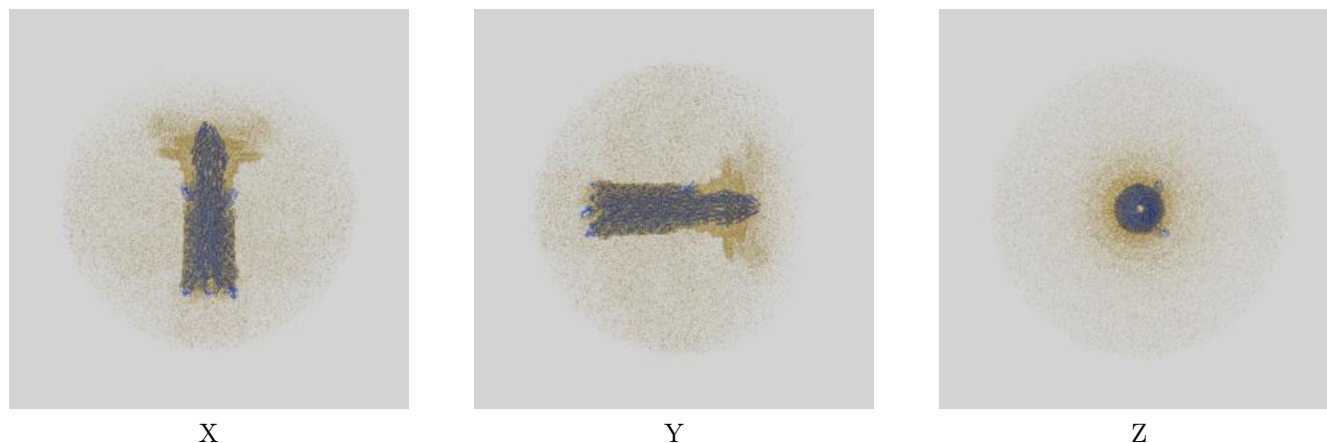
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.46	3.09
Unmasked-calculated*	6.78	9.37	7.01

*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 6.78 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

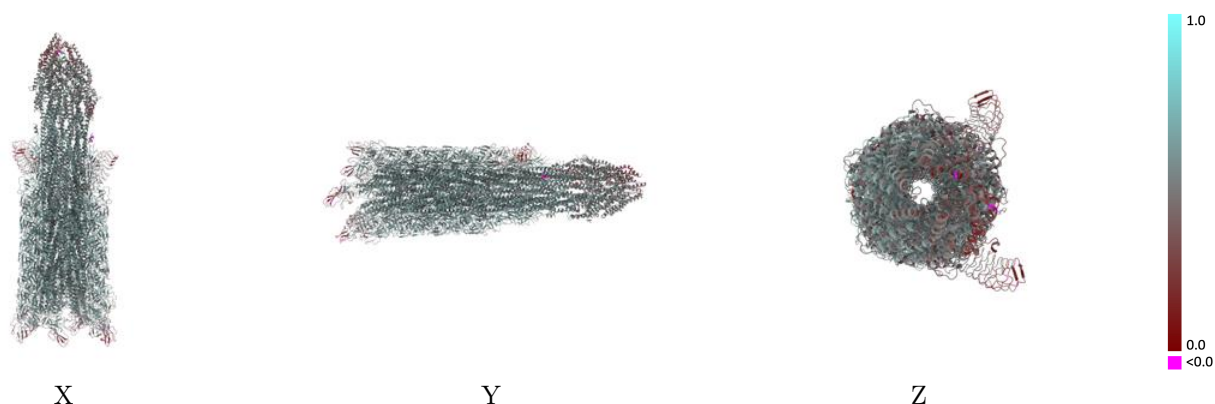
This section contains information regarding the fit between EMDB map EMD-39782 and PDB model 8Z5U. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



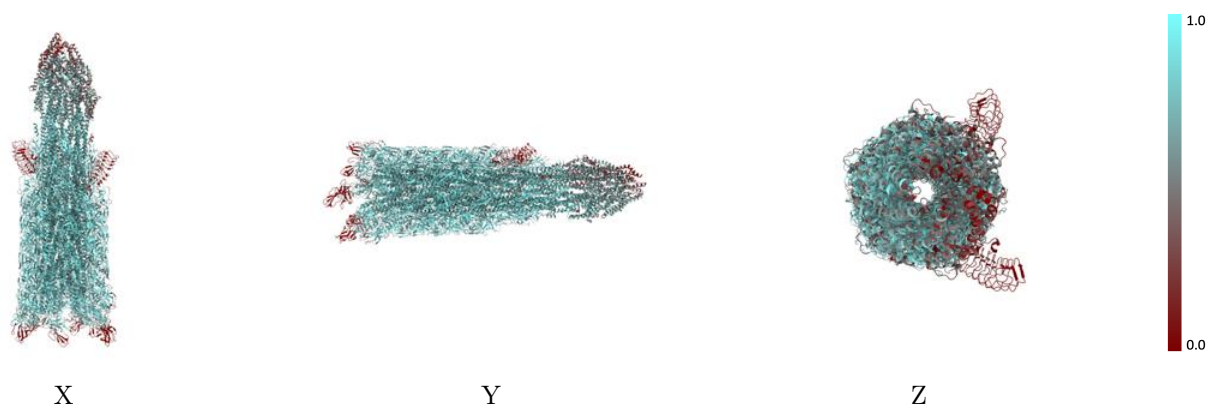
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



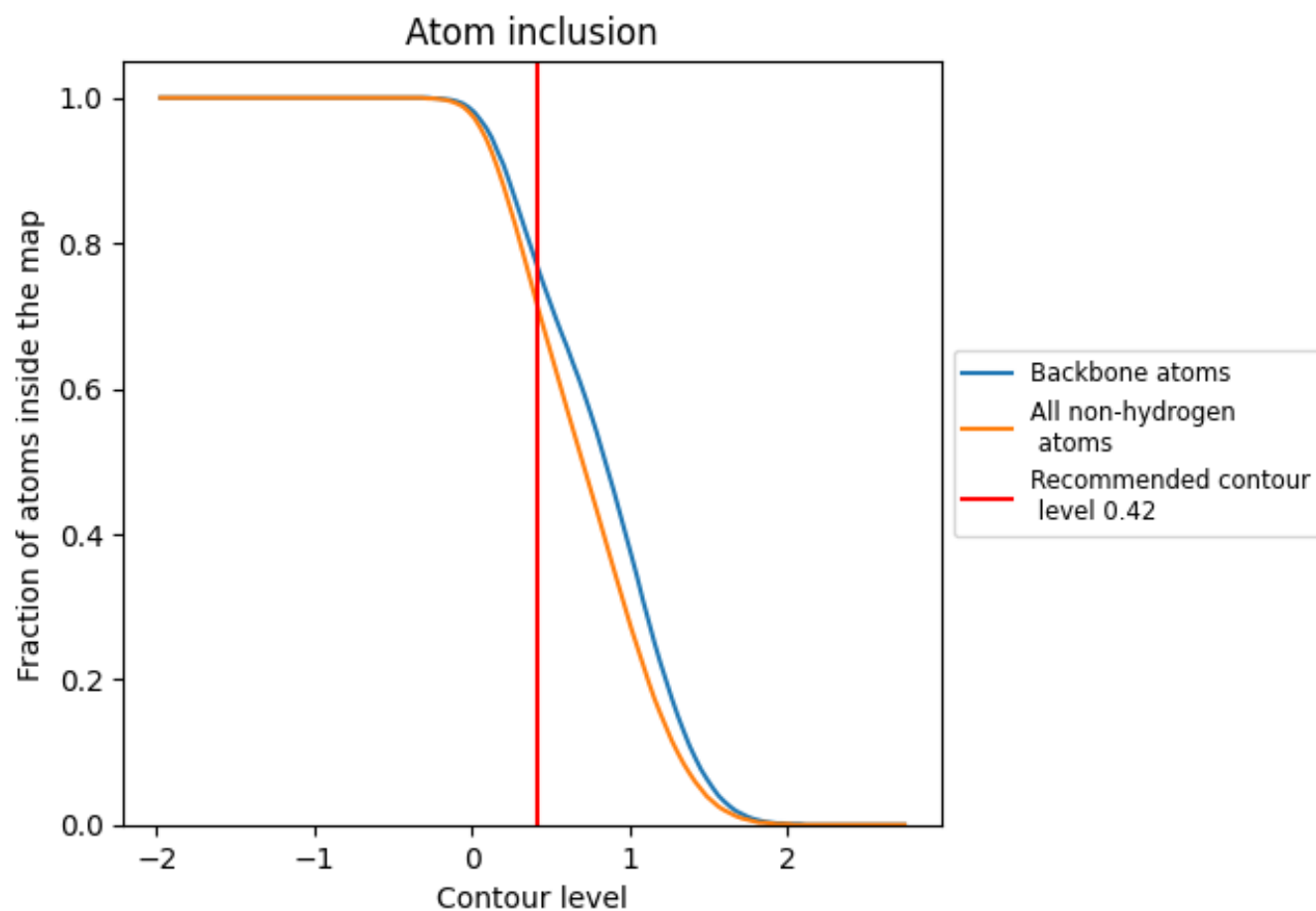
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.5330
0	 0.0790	 0.3420
1	 0.5180	 0.4720
2	 0.6340	 0.5060
3	 0.5580	 0.4790
4	 0.4360	 0.4260
5	 0.5180	 0.4410
6	 0.4560	 0.4420
7	 0.5320	 0.4750
8	 0.4870	 0.4550
9	 0.1120	 0.3640
A	 0.7890	 0.5650
AA	 0.6890	 0.5130
AB	 0.7190	 0.5490
AC	 0.6980	 0.5370
AD	 0.7630	 0.5690
AE	 0.6000	 0.5200
AF	 0.3800	 0.4110
AG	 0.7260	 0.5260
AH	 0.7810	 0.5510
AI	 0.6300	 0.4960
AJ	 0.2940	 0.3850
AK	 0.6800	 0.5320
AL	 0.6450	 0.4940
AM	 0.7100	 0.5130
AN	 0.7190	 0.5280
AO	 0.7360	 0.5420
AP	 0.7920	 0.5630
AQ	 0.7710	 0.5530
AR	 0.8010	 0.5660
AS	 0.8160	 0.5580
AT	 0.8140	 0.5770
AU	 0.8130	 0.5760
AV	 0.8050	 0.5640
AW	 0.8070	 0.5630



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Chain	Atom inclusion	Q-score
AX	 0.8030	 0.5690
AY	 0.7490	 0.5490
AZ	 0.7880	 0.5610
Aa	 0.8040	 0.5720
B	 0.7900	 0.5720
C	 0.8060	 0.5760
D	 0.3880	 0.4380
E	 0.4520	 0.4520
F	 0.5360	 0.4880
G	 0.6060	 0.5080
H	 0.6390	 0.5000
I	 0.6600	 0.5000
J	 0.7110	 0.5230
K	 0.7270	 0.5320
L	 0.7560	 0.5430
M	 0.7650	 0.5460
N	 0.7370	 0.5190
O	 0.7520	 0.5470
P	 0.7930	 0.5560
Q	 0.7920	 0.5550
R	 0.8210	 0.5860
S	 0.7900	 0.5560
T	 0.8010	 0.5650
U	 0.8190	 0.5770
V	 0.8100	 0.5760
W	 0.7940	 0.5580
X	 0.7860	 0.5510
Y	 0.8050	 0.5630
Z	 0.8050	 0.5720
a	 0.8110	 0.5660
b	 0.7510	 0.5550
c	 0.7250	 0.5180
d	 0.7800	 0.5620
e	 0.7850	 0.5630
f	 0.7970	 0.5680
g	 0.7560	 0.5330
h	 0.7910	 0.5530
i	 0.7410	 0.5310
j	 0.8040	 0.5650
k	 0.7940	 0.5670
l	 0.7830	 0.5580
m	 0.8010	 0.5660

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Chain	Atom inclusion	Q-score
n	 0.7290	 0.5340
o	 0.7780	 0.5600
p	 0.7900	 0.5640
q	 0.7450	 0.5390
r	 0.7170	 0.5410
s	 0.6110	 0.4990
t	 0.6560	 0.5060
u	 0.7150	 0.5370
v	 0.6860	 0.5340
w	 0.6830	 0.5240
x	 0.1910	 0.2950
y	 0.6510	 0.5070
z	 0.6720	 0.5190